MOCADATA
Monte Carlo Aided Design and Tolerance Analysis:
General hierarchical Bayesian procedure for calculating the bias and the a posteriori uncertainty of neutron multiplication factors including Usage of TSUNAMI in a hierarchical Bayesian procedure for calculating the bias and the a posteriori uncertainty of k_{eff}

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Abstract

In the paper on hand hierarchical Bayesian Monte Carlo procedures are described which make it possible to consider all the uncertainties associated with criticality safety analysis including burnup credit. These uncertainties are related to the validation of the depletion calculations performed in burnup credit applications, the uncertainties associated with the validation of the criticality calculations, the uncertainties associated with the parameters characterizing the application cases, as well as the uncertainties of the nuclear data with respect to the application cases. A lot of the hierarchical Bayesian procedures described in the paper on hand are incorporated in a system of computer codes which is named as MOCADATA. This code system has been developed by the authors of the paper on hand.

1 Introduction

It is an indispensable part of a criticality safety analysis of a nuclear fuel system performed by using numerical methods for calculating the neutron multiplication factor k_{eff} of the system to determine the confidence that one has in the numerical result obtained for k_{eff}. The determination of this confidence is necessary in order to be able to demonstrate that the probability that the neutron multiplication factor k_{eff} of the system, calculated by means of a specific criticality calculation procedure adequately chosen with respect to the system, exceeds the maximum allowable neutron multiplication factor k_{max}, is not greater than an administratively established margin γ, i. e. meets the following inequality:

$$\pi_S = P\left((k_{eff} + \Delta k_B) > k_{max} \mid S\right) \leq \gamma . \qquad (1)$$

S stands for the nuclear fuel system of interest; π_S is the probability $P\left((k_{eff} + \Delta k_B) > k_{max} \mid S\right)$ that $k_{eff} + \Delta k_B$ is greater than k_{max} given by an adequate administrative margin Δk_m according to

$$k_{max} = 1 - \Delta k_m ; \qquad (2)$$

and Δk_B denotes the bias in k_{eff} characteristic of the employed criticality calculation procedure with respect to the system S.

1.1 Observations on the neutron multiplication factor k_{eff} and its bias Δk_B

The neutron multiplication factor k_{eff} of the system S is a function of

- a set of parameters $\mathbf{x} = (x_1, x_2, \ldots)$ describing the material compositions and geometric arrangement of the materials forming the system and
- a set of nuclear data $\boldsymbol{\xi} = (\xi_1, \xi_2, \ldots)$ (cross sections, fission spectra, neutron-per-fission quantities) related to the isotopic compositions of the system and their impact on the neutron spectrum of the system.

Since characterized by uncertainties due to variations, tolerances or variances and covariances the sets of parameters $x_1, x_2, \ldots$ and $\xi_1, \xi_2, \ldots$ represent sets of random variables and hence random vectors $\mathbf{x}$ and $\boldsymbol{\xi}$, respectively.

Random variables are completely defined by the probability distribution

$$P\big((\mathbf{x},\boldsymbol{\xi}) \in R\big) = \int_R p(\mathbf{x},\boldsymbol{\xi})\, d\mathbf{x}\, d\boldsymbol{\xi}; \tag{3}$$

where R is some region in the $(\mathbf{x},\boldsymbol{\xi})$-space, and

$$p(\mathbf{x},\boldsymbol{\xi}) = p(\mathbf{x}) \cdot p(\boldsymbol{\xi}) \tag{4}$$

is the joint probability density function (pdf) of $\mathbf{x}$ and $\boldsymbol{\xi}$.

As a function of random variables $k_{eff}(\mathbf{x},\boldsymbol{\xi})$ is a random variable completely defined by a probability distribution $F(k_{eff})$. This distribution is determined by the pdf eq. (4). This pdf is however unknown in general. But even if $p(\mathbf{x},\boldsymbol{\xi})$ is assumed to be known the distribution $F(k_{eff})$ remains unknown, in general, because the direct functional relationship $k_{eff} = k_{eff}(\mathbf{x},\boldsymbol{\xi} \mid S)$ with the parameters $\mathbf{x}$ and $\boldsymbol{\xi}$ for a given system S is unknown, in general. So therefore, any numerical result obtained for $k_{eff}(\mathbf{x},\boldsymbol{\xi} \mid S)$ is a random sample on the underlying distribution $F(k_{eff})$.

This statement goes not only for the system S for which the proof of sufficient subcriticality shall be furnished (application case) but also for those experimental or experiment-based systems chosen as benchmarks adequate to estimate the bias Δk_B that is characteristic of the applied criticality calculation procedure with respect to the application case S. The bias Δk_B is usually derived by evaluating the statistic

$$S_B\{(\Delta k_B)_i = B[k_{eff}]_i - (k_{eff})_i,\ i = 1,\ldots,N_B\}, \tag{5}$$

of the deviations $(\Delta k_B)_i$ of the observed results $(k_{eff})_i$ from their respective expected benchmark values $B[k_{eff}]_i$, $i = 1,\ldots,N_B$. N_B denotes the number of evaluated benchmarks. Since the

distributions $F((k_{eff})_i)$ usually remain unknown the distributions $F((\Delta k_B)_i)$ usually remain unknown. Consequently the distribution $F(\Delta k_B)$ remains unknown, in general.

Since $F(k_{eff})$ and $F(\Delta k_B)$ usually remain unknown, the distribution $F(\kappa)$ of the sum $\kappa \equiv k_{eff} + \Delta k_B$ remains unknown. Consequently the probability π_S on the left-hand side of inequality (1) cannot be calculated, in general, since this probability is just given by the distribution $F(\kappa) = F(k_{eff} + \Delta k_B)$,

$$\pi_S = P(\kappa > k_{max} \mid S) = F(\kappa > k_{max} \mid S) = \int_{k_{max}}^{\infty} \frac{dF(\kappa \mid S)}{d\kappa} d\kappa \equiv \int_{k_{max}}^{\infty} f(\kappa \mid S)\, d\kappa \; ; \; \kappa \equiv k_{eff} + \Delta k_B . \tag{6}$$

However, the sum

$$\kappa_j \equiv [k_{eff} + \Delta k_B]_j \equiv (k_{eff})_j + (\Delta k_B)_j . \tag{7}$$

of the two individual numerical results $(k_{eff})_j$ and $(\Delta k_B)_j$ obtained for $k_{eff}(\mathbf{x},\boldsymbol{\xi} \mid S)$ and Δk_B, respectively, is a random sample on the distribution $F(k_{eff} + \Delta k_B \mid S)$, since any numerical result obtained for k_{eff} is a sample on $F(k_{eff} \mid S)$ and any numerical result obtained for Δk_B is a sample on $F(\Delta k_B)$. Therefore, a procedure is required which makes it possible to draw a sufficient number M of different, mutually independent samples κ_j such that the probability $F(\kappa \mid S) = F(k_{eff} + \Delta k_B \mid S)$ can be studied as a random variable. Then it becomes possible to determine the probability $(1-\alpha)$ that the probability π_S given by eq. (6) meets inequality (1):

$$\begin{aligned} 1-\alpha = P(\pi_S \le \gamma) = \int_0^{\gamma} d\pi_S\, p(\pi_S) = P\big(F(\kappa > k_{max} \mid S) \le \gamma\big) = P\left(\int_{k_{max}}^{\infty} \frac{dF(\kappa \mid S)}{d\kappa} d\kappa \le \gamma\right) \\ = P\big(F(\kappa \le k_{max} \mid S) \ge (1-\gamma)\big) = P\left(\int_0^{k_{max}} \frac{dF(\kappa \mid S)}{d\kappa} d\kappa \ge (1-\gamma)\right) \end{aligned} . \tag{8}$$

The probability $(1-\alpha)$ expresses the confidence that one has in the statement that the probability, that $\kappa = k_{eff} + \Delta k_B$ exceeds k_{max}, is not greater than the administrative limit γ.

Note that in case of prescribing definite values for γ and α the last line of expression (8) becomes

$$1-\alpha = P\big(F(\kappa \le k(\gamma,\alpha) \mid S) \ge (1-\gamma)\big) = P\left(\int_0^{k(\gamma,\alpha)} \frac{dF(\kappa \mid S)}{d\kappa} d\kappa \ge (1-\gamma)\right), \tag{9}$$

where the integration limit $k(\gamma,\alpha)$ is the so-called "one-sided $(1-\gamma)/(1-\alpha)$ tolerance limit" of $k_{eff} + \Delta k_B$ (e. g., for $\gamma = \alpha = 0.05$ the one-sided upper 95%/95% tolerance limit).

1.2 Determination of a confidence level (1-α) at unknown probability distribution $F(k_{eff}+\Delta k_B)$

Since the numerical results κ_j defined by eq. (7) do not depend on the subscript j the notation can be chosen such that a set $\{\kappa_j, j = 1,\ldots,M\}$ of M samples can be arranged in an order statistic

$$\kappa_1 \le \kappa_2 \le \ldots \le \kappa_{M-1} \le \kappa_M . \tag{10}$$

According to the previous section the results κ_i are assumed to be mutually independent, which is in fact the usual case. Thus, the probability of occurrence of a result κ_i does not depend on the occurrence of any of the other results $\kappa_j, j \ne i$. So therefore, the probability that $(i-1)$ values are smaller than κ_i, that the value κ_i occurs, and that $(M-i)$ values are greater than κ_i amounts to

$$P(\lambda_1 = i-1, \lambda_2 = 1, \lambda_3 = M-i) = \binom{M}{\lambda_1\ \lambda_2\ \lambda_3} \cdot \prod_{j=1}^{3} P_j^{\lambda_j} ,$$

where

$$\binom{M}{\lambda_1\ \lambda_2\ \lambda_3} = \frac{M!}{\lambda_1!\,\lambda_2!\,\lambda_3!} = \frac{M!}{(i-1)!\,1!\,(M-i)!} = \frac{\Gamma(M+1)}{\Gamma(i)\,\Gamma(M-i+1)}$$

is the number of realizations of grouping M samples into the three groups of size $\lambda_1 = i-1$, $\lambda_2 = 1$, and $\lambda_3 = M-i$, respectively.

The probabilities P_j, $j = 1,2,3$, are related to these groups as follows: The probability P_1 related to the first group $\lambda_1 = i-1$ is the probability that there is one value κ smaller than κ_i, the probability P_2 related to the second group $\lambda_2 = 1$ is the probability that the value κ_i occurs, i. e. that there is one value κ falling into the infinitesimal interval $[\kappa_i, \kappa_i + d\kappa_i]$, and the probability P_3 related to the third group $\lambda_3 = M-i$ is the probability that there is one value κ greater than κ_i. Since the results κ_i are samples on the probability distribution $F(\kappa) \equiv F(k_{eff} + \Delta k_B)$ the probabilities P_j, $j = 1,2,3$, are given by the following expressions:

$P_1 = F(\kappa_i)$,

$P_2 = dF(\kappa_i) = \varphi(\kappa_i)\, d\kappa_i$ with $\varphi(\kappa_i) = dF(\kappa_i)/d\kappa_i$,

$P_3 = 1 - F(\kappa_i)$.

The pdf of κ_i becomes, therefore,

$$f(\kappa_i) = \frac{\Gamma(M+1)}{\Gamma(i)\,\Gamma(M-i+1)} \left[F(\kappa_i)\right]^{i-1} \left[1-F(\kappa_i)\right]^{M-i} \varphi(\kappa_i) . \tag{11}$$

Using the transformation

$$F = F(\kappa_i) = \int_{-\infty}^{\kappa_i} \varphi(\tilde{\kappa}_i)\, d\tilde{\kappa}_i ,$$

the pdf eq. (11) can be transformed into a pdf $h(F)$ with F regarded as a random variable. Because of

$$h(F)\,dF = f(\kappa_i)\,d\kappa_i \text{ and } h(F) = \frac{f(\kappa_i)}{\left|\frac{dF}{d\kappa_i}\right|} = \frac{f(\kappa_i)}{\varphi(\kappa_i)},\ h(F) \text{ becomes}$$

$$h(F) = h(F;a,b) = \frac{\Gamma(a+b)}{\Gamma(a)\,\Gamma(b)}\, F^{a-1}\,[1-F]^{b-1}. \tag{12}$$

with

$$a \equiv i \text{ and } b \equiv M - i + 1. \tag{13}$$

Since being a probability, F is only defined on the interval $[0,1]$. Therefore, according to eq. (12), the probability F taken as a random variable, follows a Beta-distribution, cf. Ref. [1]. This is a remarkable result because it has been stated above that F remains unknown, in general, apart from the fact that F is a probability and hence defined on the interval $[0,1]$, i.e. $F \in [0,1]$.

The integration problem eq. (8) can now be solved, in fact. As follows from eq. (8), the probability $P\big(F < (1-\gamma)\big)$ that F is less than $(1-\gamma)$ is just α. So therefore, using eq. (12), α becomes

$$\alpha = P\big(F < (1-\gamma)\big) = \int_0^{1-\gamma} dF\ h(F) = \frac{B_{(1-\gamma)}(a,b)}{B(a,b)} \equiv I_{(1-\gamma)}(a,b), \tag{14}$$

where $B_{(1-\gamma)}(a,b)$ denotes the incomplete Beta function [2] and

$$B(a,b) = \frac{\Gamma(a)\ \Gamma(b)}{\Gamma(a+b)} \tag{15}$$

is the complete Beta function [2]. Applying the relationship between the incomplete Beta function and the binomial expansion $I_{(1-\gamma)}(a,b)$ (cf. Ref. [2]), eq. (14) becomes, using definition eq. (13),

$$\alpha = I_{(1-\gamma)}(i, M-i+1) = \sum_{m=i}^{M} \binom{M}{m} (1-\gamma)^m\, \gamma^{M-m}. \tag{16}$$

This equation provides for each member κ_i of the order statistic eq. (10) a probability $\alpha_i = \alpha(\kappa_i;\gamma)$ as a function of γ. So therefore, for a specified probability γ the confidence level $(1-\alpha_i)$ can be calculated for the greatest κ_i value which just meets the inequality $\kappa_i \le k_{max}$; and it can be checked then whether $(1-\alpha_i)$ is sufficiently large or not. (Note, usually specific figures are administratively prescribed for γ and α.)

For $i = M$ eq. (16) becomes

$$\alpha = (1-\gamma)^M . \tag{17}$$

So therefore, if α shall not exceed a certain value α_0 and γ shall not exceed the administrative margin γ_0, then the minimum required number M of samples κ_j, eq. (7), amounts to

$$\min(M) = \frac{\log(\alpha_0)}{\log(1-\gamma_0)} . \tag{18}$$

After having clarified that the confidence $(1-\alpha)$, defined by eq. (8), can be determined even if the probability distribution $F(\kappa \mid S) = F(k_{eff} + \Delta k_B \mid S)$ is unknown, it is time now to develop the procedure required to draw a sufficient number of samples $\kappa_j = [k_{eff} + \Delta k_B]_j$ on $F(\kappa \mid S)$.

1.3 Reflections on the information needed and the information flow required

As stated in section 1.1, the probability distribution $F(\kappa \mid S)$ is determined by

- the probability density functions of the material and design data $\mathbf{x}_S$ and $\mathbf{x}_B$ of the system S of interest and the benchmarks (B), respectively, selected for estimating the bias Δk_B as well as
- the probability density function of the nuclear data ξ related to the system S.

Since these probability density functions are unknown, in general, the sampling procedure sought-after must have the capability to gain information on these probability density functions from empirical data or quantities derived from empirical information or nuclear reaction models. About the flow of required information on $\mathbf{x}_S$, $\mathbf{x}_B$ and ξ the following reflections can be made:

- The task in criticality safety analysis usually is to demonstrate that a given nuclear fuel system S meets inequality (8) at the administrative limit γ with a sufficiently large confidence level $(1-\alpha)$.
- For this purpose criticality calculations are performed using a specific criticality calculation code with a specific nuclear data library.
- Possible biased errors in the applied nuclear data as well as algorithmic und numerical weaknesses of the employed criticality calculation code may result in a non-zero bias Δk_B in the calculated k_{eff} values. This bias Δk_B is characteristic of the employed nuclear data library and the used criticality calculation code with respect to the system S of interest.
- In order to be able to determine the bias Δk_B that applies to the system S under the given nuclear data library and the given calculation code, it is necessary to analyze benchmark configurations which are similar to the application case S with respect to neutron physics properties and hence representative for the system S. The representativeness of a benchmark B with respect to S can be measured by the correlation between the neutron multiplication factors k_B of the benchmark and k_S of the system

$$\mathrm{corr}\left(k_B, k_S\right) \propto \boldsymbol{\Lambda}\,\mathbf{cov}(\xi)\,\boldsymbol{\Lambda}^T, \tag{19}$$

as obtained in first-order perturbation theory [3]. $\mathbf{cov}(\xi)$ in eq. (19) denotes the covariance matrix of the nuclear data, and $\boldsymbol{\Lambda}$ is the vector of the sensitivities

$$\Lambda_{cv} = \frac{\xi_v}{k_c}\frac{\partial k_c}{\partial \xi_v}, \quad c = \left\{\begin{matrix} B \\ S \end{matrix}\right\}, \tag{20}$$

of k_B and k_S, respectively, to the nuclear data ξ.

- Since the bias Δk_B of interest is that one which is characteristic of the combined use of the given nuclear data library and the given criticality calculation code with respect to the system S, there is no need for considering the uncertainties in the nuclear data ξ when calculating the set $S_B\{(\Delta k_B)_i\,,\ i = 1,...,N_B\}$ of bias values eq. (5) for the set of the representative benchmarks selected. The bias Δk_B is in fact related, at given neutron energy E, to the use of fixed values $\xi_v(E)$ from the employed nuclear data library by the applied calculation code when calculating the neutron multiplication factor k_S of the system of interest.

- The uncertainties in the material and design data $\mathbf{x}_B$ of the benchmarks have to be taken into account, since they lead to uncertainties of the $(\Delta k_B)_i$ values observed for the benchmarks $i = 1,...,N_B$.

- Since the correlation coefficients eq. (19), $\mathrm{corr}\left((k_B)_i, k_S\right)$, are less than 1, i. e., since the benchmark configurations $i = 1,...,N_B$ are similar but not equal to the system S with respect to neutron physics properties, a model is required which is capable to derive the bias Δk_B related to the system S from the results $(\Delta k_B)_i$ obtained for the benchmarks $i = 1,...,N_B$, taking into account the uncertainties in $(\Delta k_B)_i$ due to the uncertainties in the data $\mathbf{x}_B$. For this purpose a set $\mathbf{z}$ of explanatory variables is required which characterizes the benchmarks $i = 1,...,N_B$ as well as the system S: $\mathbf{z} = \mathbf{z}_i$, $i = 1,...,N_B$, and $\mathbf{z} = \mathbf{z}_S$, respectively. The required model therefore consists in a trending analysis $\Delta k_B = \Delta k_B(\mathbf{z})$ concluding from the points $\mathbf{z}_i$ in the $\mathbf{z}$-space to the point $\mathbf{z}_S$ in this space.

- The procedure used to estimate the neutron multiplication factor k_S of the system S must include consideration of the uncertainties in the material and design data $\mathbf{x}_S$ of the system.

- In addition, the procedure used for estimating k_S must include consideration of the uncertainties in the nuclear data ξ. It is in fact the application case S for which the impact of the uncertainties in ξ on the neutron multiplication factor is of interest.

Part of the elements of the system's material and design vector $\mathbf{x}_S$ characterizes the nuclear fuel in the system S. Application of burnup credit to the system S significantly increases the number of elements of $\mathbf{x}_S$ describing the fuel characteristics and introduces additional uncertainties related to the estimation and validation of the fuel composition as a function of initial enrichment

and burnup. Therefore, to get a full picture of the flow of required information on the parameters $\mathbf{x}_S$, $\mathbf{x}_B$ and ξ, a complete overview of the sources and the hierarchy of uncertainties is needed. This overview is given in the next section.

2 Sources and hierarchy of uncertainties

A burnup credit criticality safety analysis consists in implementation of two key steps:

- Depletion analysis: Estimation and validation of the isotopic composition of the fuel
- Criticality analysis: Estimation and validation of the neutron multiplication factors for evaluating the loading criterion (e. g., the loading curve indicating the minimum burnup required for fuel with a specific initial enrichment to be loaded in the system S of interest)

Accordingly, the uncertainties in k_{eff} arising for the depletion analysis can be distinguished from the uncertainties arising from the criticality analysis.

2.1 Depletion analysis

The upper part of Figure 1 summarizes the sources and the hierarchy of uncertainties arising out the depletion analysis:

- The estimation of the fuel's isotopic composition as a function of initial enrichment and burnup is performed by means of depletion calculations. Due to possible biased errors in the nuclear data applied to the depletion calculations and due to algorithmic and numerical weaknesses in the employed depletion calculation code, the calculated isotopic number densities may be biased.
- To validate the depletion calculations and to eliminate the biases in the isotopic number densities, comparisons between predicted, i. e. calculated, and measured isotopic concentrations are made. The measured isotopic concentrations are obtained from chemical assays of samples from irradiated fuel. Accordingly, the comparison of calculated to measured concentrations inevitably introduces
  - all the uncertainties in the measured concentrations arising from the applied assay methods and
  - all the uncertainties in the parameters (such as irradiation history and burnup of the fuel samples) required to perform the calculations.

  The uncertainties in the parameters needed for performing the calculations lead to uncertainties in the calculated concentrations.
- Isotopic Correction Factors (ICFs) are derived from the statistics of comparisons between measured and calculated isotopic concentrations. Due to the uncertainties in these concentra-

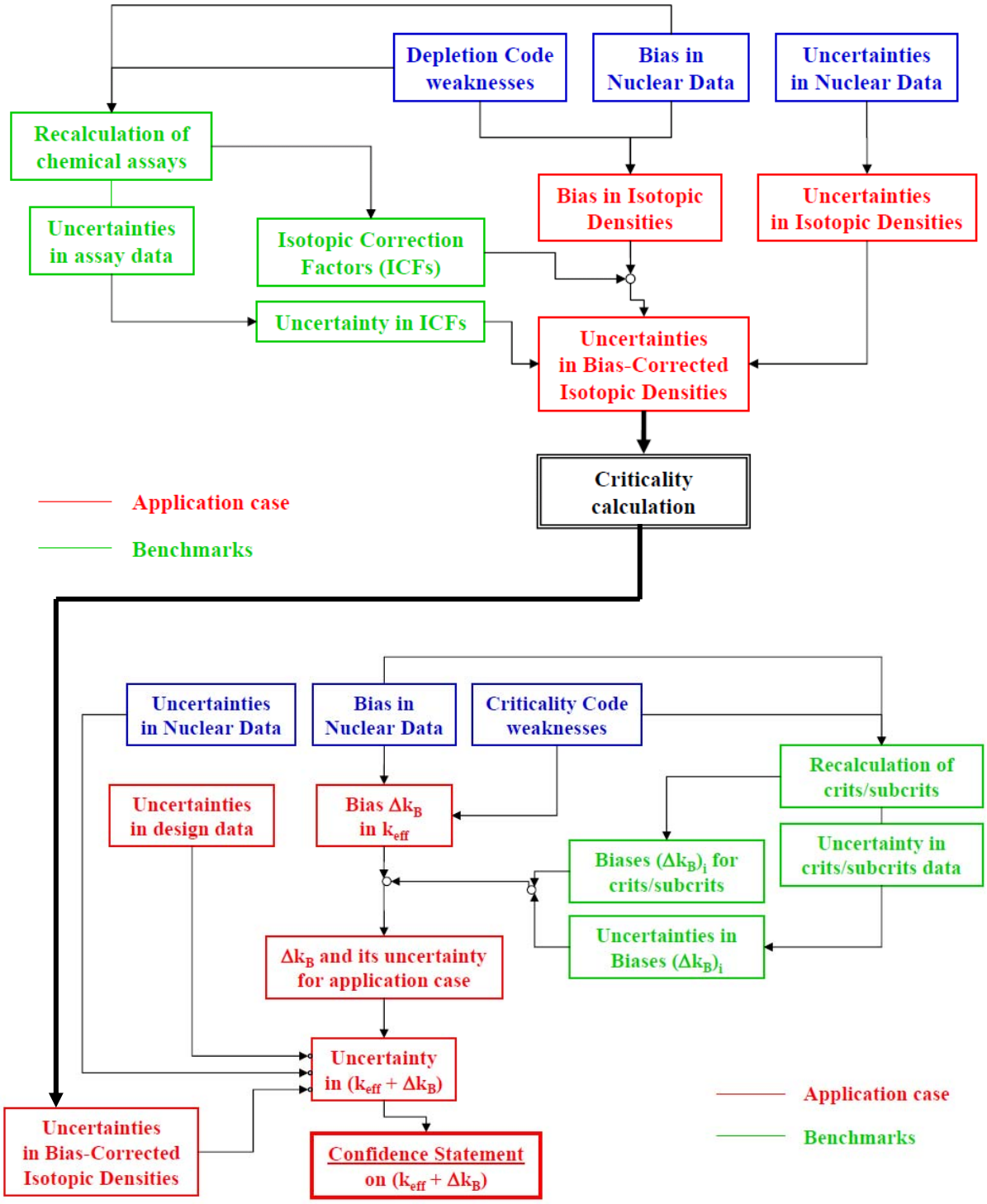

***Figure 1**: Hierarchy of uncertainties in burnup credit criticality safety analysis*

tions the ICFs have uncertainties that have to be considered when the ICFs are applied to the isotopic number densities calculated for the application case, i. e. for the fuel to be loaded in the system S:

$$[N_i^{(S)}]_{corr.} = (ICF)_i \cdot N_i^{(S)}, \qquad (21)$$

$N_i^{(S)}$:= number density of the i-th isotope calculated for the application case S, and $[N_i^{(S)}]_{corr.}$:= "bias-corrected" number density of this isotope.

- There is no need to consider the uncertainties in the nuclear data in the evaluation of the ICFs because the isotopic biases to be corrected by applying the ICFs are those which are characteristic of the combined use of the given nuclear data library and the given depletion calculation code with respect to the neutron spectrum of the application case.
- However, the uncertainties in the nuclear data have to be considered, in principle, in the calculation of the isotopic number densities $N_i^{(S)}$ of the application case.
- With respect to the calculation of these number densities $N_i^{(S)}$, uncertainties in the irradiation history have to be taken into account only in so far as they have to be covered by a bounding irradiation history required in the analysis of the application case [4].

2.2 Criticality analysis

As appears from Figure 1, the bias-corrected number densities and their uncertainties are input to the criticality analysis. All the other uncertainties related to the determination of the k_{eff} value of the system S of interest (application case) and the bias Δk_B of the employed criticality code with respect to S are summarized in the lower part of Figure 1. These uncertainties were already discussed in detail in section 1.3.

3 Hierarchical Bayesian Monte Carlo procedures

The flow of the information on the random vectors $\mathbf{x}_S$, $\mathbf{x}_B$ and ξ required for solving eq. (8) has to follow the hierarchy of uncertainties presented in Figure 1. The uncertainties in the parameters related to some level in that hierarchy determine the uncertainties of the parameters of the following level. Figure 2 gives an example related to the validation of the depletion calculations:

The uncertainties in the measured and the calculated isotopic concentrations determine the uncertainties of the ICFs; the uncertainties of the ICFs impact the uncertainties of the isotopic concentrations of the application case S; and these uncertainties contribute to the uncertainty of $k_{eff} = k_{eff}(S)$. So, in generalized terms, as illustrated in Figure 3, to gain information on the uncertainty $\mathbf{x} = \mathbf{x}(\mathbf{a}, \mathbf{b})$ depending on the parameters $\mathbf{a}$ and $\mathbf{b}$ of the preceding hierarchical level information about the parameters $\mathbf{\Theta_a}$ and $\mathbf{\Theta_b}$ is required characterizing the probability density

distributions $p(\mathbf{a}\,|\,\boldsymbol{\Theta}_{\mathbf{a}})$ and $p(\mathbf{b}\,|\,\boldsymbol{\Theta}_{\mathbf{b}})$ which determine the expectation values and the variances and covariances of the components of $\mathbf{a}$ and $\mathbf{b}$, respectively, according to the expressions given in the following equations:

- Expectation $E[\eta_i]$ of η_i: $E[\eta_i] = \int_{\Omega_\eta} \eta_i \, p(\boldsymbol{\eta}\,|\,\boldsymbol{\Theta}_{\boldsymbol{\eta}})\, d\boldsymbol{\eta}, \; \forall i,$ (22)

  where η_i stands either for the i-th component of $\mathbf{a}$ or the i-th component of $\mathbf{b}$, so that $\boldsymbol{\eta}$ stands either for $\mathbf{a}$ or $\mathbf{b}$.

- Covariance $\mathrm{cov}(\eta_i, \eta_j)$ of the components η_i and η_j of $\boldsymbol{\eta}$:

$$\mathrm{cov}(\eta_i, \eta_j) = E\left[(\eta_i - E[\eta_i])\cdot(\eta_j - E[\eta_j])\right] = \int_{\Omega_\eta} (\eta_i - E[\eta_i])\cdot(\eta_j - E[\eta_j])\, p(\boldsymbol{\eta}\,|\,\boldsymbol{\Theta}_{\boldsymbol{\eta}})\, d\boldsymbol{\eta}, \; \forall i \wedge j, \quad (23)$$

$\Omega_{\boldsymbol{\eta}}$ in equations (22) and (23) denotes the definition region of $\boldsymbol{\eta}$.

For $i = j$ eq. (23) gives the variances $\sigma^2(\eta_i)$ of $\boldsymbol{\eta}$,

$$\sigma^2(\eta_i) \equiv \mathrm{cov}(\eta_i, \eta_i) = \int_{\Omega_\eta} (\eta_i - E[\eta_i])^2 \; p(\boldsymbol{\eta}\,|\,\boldsymbol{\Theta}_{\boldsymbol{\eta}})\, d\boldsymbol{\eta}, \; \forall i. \quad (24)$$

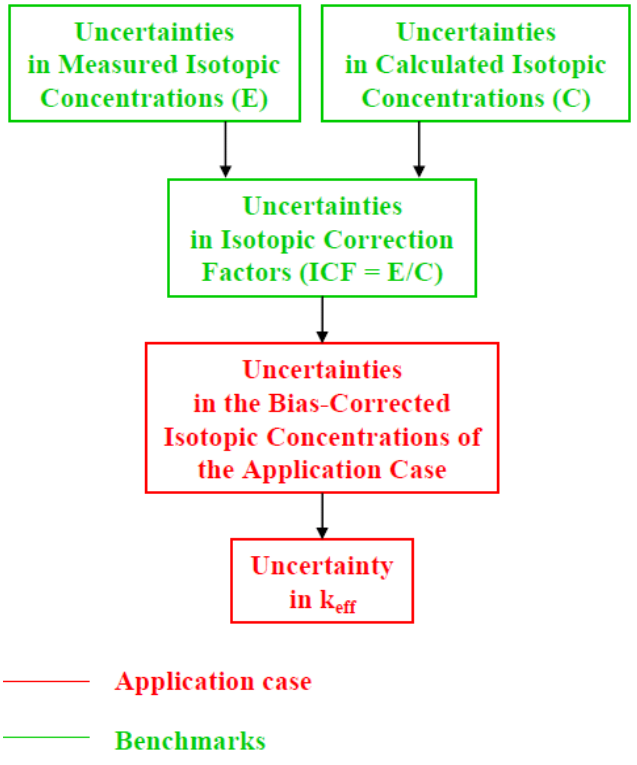

***Figure 2**: Example for the dependency of the uncertainties of the parameters of a given level on the uncertainties of the parameters of the preceding level in the hierarchy of uncertainties*

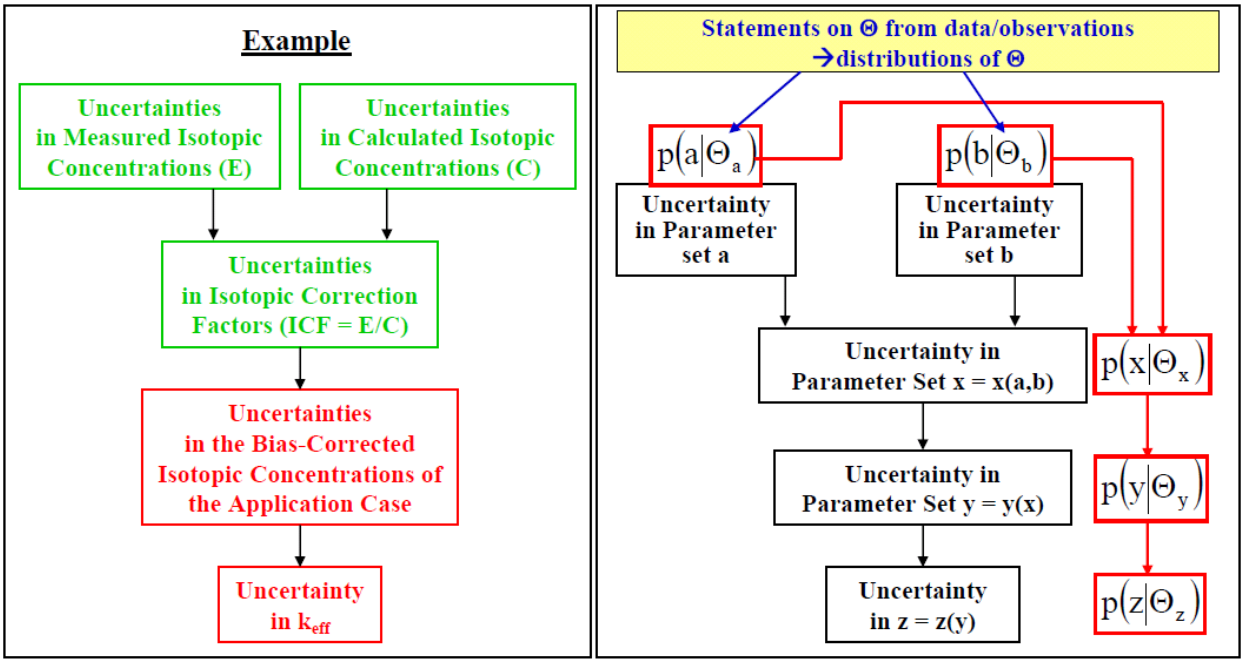

***Figure 3**: Illustration of the information flow required for the estimation of the uncertainties in the parameters of the different levels in the hierarchy of uncertainties*

The correlation $\mathrm{corr}(\eta_i, \eta_j)$ (also named as "correlation coefficient") of the components η_i and η_j of $\boldsymbol{\eta}$ is defined by the expression given in eq. (25),

$$\mathrm{corr}(\eta_i, \eta_j) = \frac{\mathrm{cov}(\eta_i, \eta_j)}{\sqrt{\sigma^2(\eta_i)\ \sigma^2(\eta_j)}},\ \forall i \wedge j. \tag{25}$$

If the variables η_i are mutually independent, the covariance and the correlation vanish for $i \neq j$. (The converse statement is not necessarily true.) The random variables are mutually independent if and only if their joint pdf is completely factorizable as

$$p(\boldsymbol{\eta}\,|\,\boldsymbol{\Theta}) \equiv p(\eta_1,\ldots,\eta_m\,|\,\boldsymbol{\Theta}_1,\ldots,\boldsymbol{\Theta}_m) = \prod_{i=1}^{m} p_i(\eta_i\,|\,\boldsymbol{\Theta}_i)\,.$$

with $\boldsymbol{\Theta} = (\Theta_1,\ldots,\Theta_n) = (\boldsymbol{\Theta}_1,\ldots,\boldsymbol{\Theta}_m)$, $\boldsymbol{\Theta}_i = (\Theta_{1,i},\ldots,\Theta_{n_i,i})$, $i = 1,\ldots,n$, $n = \sum_{i=1}^{m} n_i$.

In matrix notation the expectation values (means), eq. (22), of the components are summarized in the expectation (mean) vector

$$\mathbf{E}[\boldsymbol{\eta}] = \left(E[\eta_1],\ldots,E[\eta_m]\right)^T, \tag{26}$$

and the variances, eq. (24), and covariances, eq. (23), are summarized in the covariance matrix

$$\mathbf{cov}(\boldsymbol{\eta}) \equiv \mathbf{V}(\boldsymbol{\eta}) = \begin{pmatrix} \sigma^2(\eta_1) & \mathrm{cov}(\eta_1,\eta_2) & \cdots & \mathrm{cov}(\eta_1,\eta_m) \\ \mathrm{cov}(\eta_2,\eta_1) & \sigma^2(\eta_2) & \cdots & \mathrm{cov}(\eta_2,\eta_m) \\ \vdots & \vdots & \ddots & \vdots \\ \mathrm{cov}(\eta_m,\eta_1) & \mathrm{cov}(\eta_m,\eta_2) & \cdots & \sigma^2(\eta_m) \end{pmatrix}. \tag{27}$$

Since $\mathrm{cov}(\eta_i,\eta_j) = \mathrm{cov}(\eta_j,\eta_i)$ by definition (cf. eq. (23)), the matrix $\mathbf{cov}(\boldsymbol{\eta})$ is symmetric, i. e., $\mathbf{V}(\boldsymbol{\eta}) = \mathbf{V}^T(\boldsymbol{\eta})$.

Let us assume that the parameters $\boldsymbol{\Theta}_\mathbf{a}$ and $\boldsymbol{\Theta}_\mathbf{b}$, and hence the pdfs $p(\mathbf{a}\,|\,\boldsymbol{\Theta}_\mathbf{a})$ and $p(\mathbf{b}\,|\,\boldsymbol{\Theta}_\mathbf{b})$, are known (e. g., for a multivariate Gaussian density $p(\boldsymbol{\eta}\,|\,\boldsymbol{\Theta}_\boldsymbol{\eta})$ the parameter set $\boldsymbol{\Theta}_\boldsymbol{\eta}$ is given by equations (26) and (27), i. e. $\boldsymbol{\Theta}_\boldsymbol{\eta} = \big(\mathbf{E}[\boldsymbol{\eta}], \mathbf{cov}(\boldsymbol{\eta})\big)$). Then Monte Carlo (MC) samples $\mathbf{a}_{MC}$ and $\mathbf{b}_{MC}$ on $\mathbf{a}$ and $\mathbf{b}$, respectively, can be drawn from the respective pdfs. If all the functional relationships $\mathbf{x} = \mathbf{x}(\mathbf{a},\mathbf{b})$, $\mathbf{y} = \mathbf{y}(\mathbf{x})$ and $\mathbf{z} = \mathbf{z}(\mathbf{y})$ mentioned in Figure 3 can be solved analytically then insertion of the draws $\mathbf{a}_{MC}$ and $\mathbf{b}_{MC}$ in $\mathbf{z} = \mathbf{z}\big(\mathbf{y}\big(\mathbf{x}(\mathbf{a},\mathbf{b})\big)\big)$ yields a set of MC samples $\{\mathbf{z}_{MC}\}$ and hence an empirical distribution of $\mathbf{z}$. From this distribution information on the parameters $\boldsymbol{\Theta}_\mathbf{z}$ of the pdf $p(\mathbf{z}\,|\,\boldsymbol{\Theta}_\mathbf{z})$ can be derived which may be useful for evaluation or further application. If each of the relationships $\mathbf{x} = \mathbf{x}(\mathbf{a},\mathbf{b})$, $\mathbf{y} = \mathbf{y}(\mathbf{x})$ and $\mathbf{z} = \mathbf{z}(\mathbf{y})$ can only be solved numerically, the following can be stated: Use of the draws $\mathbf{a}_{MC}$ and $\mathbf{b}_{MC}$ in the numerical procedure applied to solve $\mathbf{x} = \mathbf{x}(\mathbf{a},\mathbf{b})$ provides a set of MC samples $\{\mathbf{x}_{MC}^{(num)}\}$ and hence an empirical distribution of $\mathbf{x}$. From this distribution information on the parameters $\boldsymbol{\Theta}_\mathbf{x}$ of the pdf $p(\mathbf{x}\,|\,\boldsymbol{\Theta}_\mathbf{x})$ can be derived which can be used to draw MC samples $\mathbf{x}_{MC}^{(p)}$ on $p(\mathbf{x}\,|\,\boldsymbol{\Theta}_\mathbf{x})$. These samples are inserted in the numerical procedure employed for solving $\mathbf{y} = \mathbf{y}(\mathbf{x})$. The set of MC samples $\{\mathbf{y}_{MC}^{(num)}\}$ thus obtained provides information on the parameters $\boldsymbol{\Theta}_\mathbf{y}$ of the pdf $p(\mathbf{y}\,|\,\boldsymbol{\Theta}_\mathbf{y})$, which can be used to draw MC samples $\mathbf{y}_{MC}^{(p)}$ on $p(\mathbf{y}\,|\,\boldsymbol{\Theta}_\mathbf{y})$. These samples are now used in the numerical procedure applied to solve $\mathbf{z} = \mathbf{z}(\mathbf{y})$; a set $\{\mathbf{z}_{MC}^{(num)}\}$ of MC samples is thus obtained which provides information about the parameters $\boldsymbol{\Theta}_\mathbf{z}$ of $p(\mathbf{z}\,|\,\boldsymbol{\Theta}_\mathbf{z})$.

The upper part of Figure 4 illustrates the just outlined MC procedure for two consecutive levels of a hierarchy of uncertainties: MC samples $\mathbf{x}_{MC}^{(p)}$ are drawn form the definition region of $\mathbf{x}$. These MC samples are used in the analytical or numerical procedure to be employed for solving $\mathbf{y} = \mathbf{y}(\mathbf{x})$. An empirical distribution of $\mathbf{y}$ is thus obtained which can be used for further evaluations.

However, to be able to perform MC sampling on the definition region of $\mathbf{x}$, the pdf $p(\mathbf{x}\,|\,\boldsymbol{\Theta})$ and hence the parameter set $\boldsymbol{\Theta} \equiv \boldsymbol{\Theta}_\mathbf{x}$ has to be known. However, such pdfs are usually unknown. In particular, as already stated in section 1.1, the pdfs of those parameters are usually unknown which refer to top levels of the hierarchy of uncertainties presented in Figure 1. Therefore, it is necessary to gain knowledge about the parameters $\boldsymbol{\Theta}$ from empirical data.

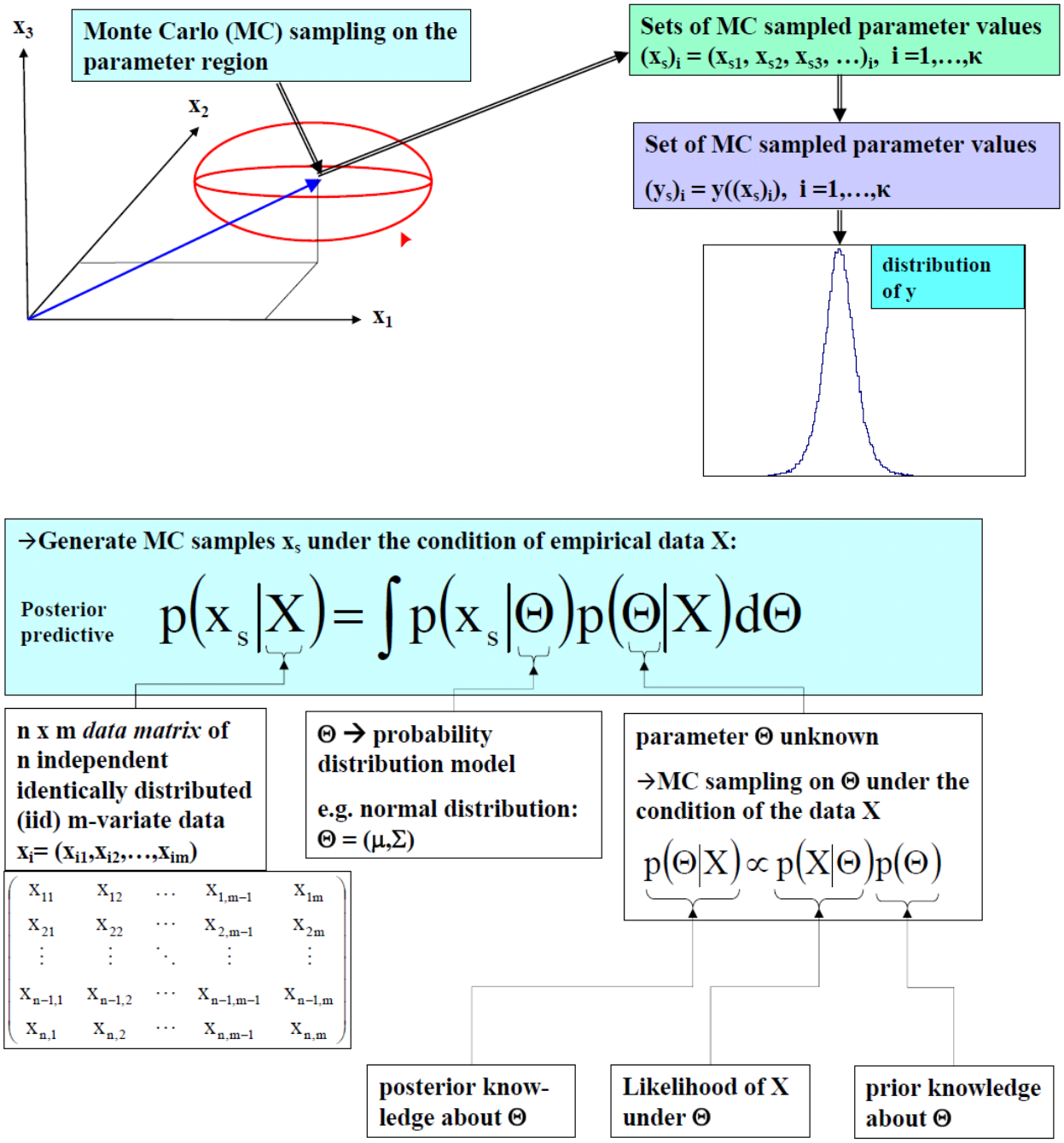

***Figure 4**: Illustration of the concept of Bayesian Monte Carlo procedures*

Let us assume that the data matrix $\mathbf{X}$ represents n independent identically distributed observations of the parameters $\mathbf{x} = (x_1, \ldots, x_m)^T$ of interest drawn to gain information on the unknown parameters $\boldsymbol{\Theta} = (\Theta_1, \ldots, \Theta_r)^T$:

$$\mathbf{X}^T = \begin{pmatrix} x_{11} & x_{12} & \cdots & x_{1m} \\ x_{21} & x_{22} & \cdots & x_{2m} \\ \vdots & \vdots & \ddots & \vdots \\ x_{n1} & x_{n2} & \cdots & x_{nm} \end{pmatrix}. \tag{28}$$

According to Bayes' theorem [1] the posterior knowledge about $\boldsymbol{\Theta}$, i. e., the knowledge gained from the empirical data $\mathbf{X}$ is represented by the posterior pdf $p(\boldsymbol{\Theta} \mid \mathbf{X})$ according to eq. (29),

$$p(\boldsymbol{\Theta} \mid \mathbf{X}) = \frac{p(\mathbf{X} \mid \boldsymbol{\Theta})\, p(\boldsymbol{\Theta})}{\int\limits_{\Omega(\boldsymbol{\Theta})} d\boldsymbol{\Theta}\, p(\mathbf{X} \mid \boldsymbol{\Theta})\, p(\boldsymbol{\Theta})} \propto p(\mathbf{X} \mid \boldsymbol{\Theta})\, p(\boldsymbol{\Theta}), \tag{29}$$

where $\Omega(\boldsymbol{\Theta})$ denotes definition region of $\boldsymbol{\Theta}$.

As indicated in Figure 4, $p(\boldsymbol{\Theta})$ is the prior pdf representing the knowledge about $\boldsymbol{\Theta}$, if there is some, prior to the information contained in $\mathbf{X}$. If there is no prior knowledge available, a so-called "non-informative" prior is chosen for $p(\boldsymbol{\Theta})$, cf. References [5] through [7]. $p(\mathbf{X} \mid \boldsymbol{\Theta})$ represents the Likelihood function of the observations $\mathbf{X}$ under $\boldsymbol{\Theta}$. $p(\mathbf{X} \mid \boldsymbol{\Theta})$ is not a pdf, but a function of $\boldsymbol{\Theta}$ only, determining the amount of information $\mathbf{I}_{\mathbf{X}}(\boldsymbol{\Theta})$ of $\mathbf{X}$ about $\boldsymbol{\Theta}$, [1],

$$\left[\mathbf{I}_{\mathbf{X}}(\boldsymbol{\Theta})\right]_{ij} = E_{\mathbf{X}}\left[\frac{\partial \ln p(\mathbf{X} \mid \boldsymbol{\Theta})}{\partial \Theta_i} \cdot \frac{\partial \ln p(\mathbf{X} \mid \boldsymbol{\Theta})}{\partial \Theta_j}\right], \; i.j = 1, \ldots, m. \tag{30}$$

Despite this information the parameters $\boldsymbol{\Theta}$ remain random parameters in general, whatever the size n of the samples (observations) $\mathbf{x}_i = (x_{i1}, \ldots, x_{im})^T$ might be. In fact, it is not possible, in general, to obtain a set of certain values $\boldsymbol{\Theta}_0$ from a finite sample of any size n. This fundamental uncertainty due to the finite number n is expressed by the fact that the posterior pdf $p(\boldsymbol{\Theta} \mid \mathbf{X})$ is a pdf which is, in general, different from a delta distribution $\delta(\boldsymbol{\Theta} - \boldsymbol{\Theta}_0)$. Thus, for any region R falling into the definition region $\Omega(\boldsymbol{\Theta})$, i. e. $R \subseteq \Omega(\boldsymbol{\Theta})$, the probability

$$P(\boldsymbol{\Theta} \in R \mid \mathbf{X}) = \int\limits_R d\boldsymbol{\Theta}\, p(\boldsymbol{\Theta} \mid \mathbf{X}) \tag{31}$$

remains less than 1 (and is equal to 1 for $R = \Omega(\boldsymbol{\Theta})$). $\boldsymbol{\Theta}$ under $\mathbf{X}$ is completely defined by the probability given in eq. (31).

So therefore, to be able to perform MC sampling on the definition region of $\mathbf{x}$, first MC samples $\boldsymbol{\Theta}_{MC}$ from the posterior pdf $p(\boldsymbol{\Theta} \mid \mathbf{X})$ have to be drawn. The samples can then be used in the pdf model $p(\mathbf{x} \mid \boldsymbol{\Theta})$ so that MC samples $\mathbf{x}_{MC}$ under the condition of the empirical data $\mathbf{X}$ are drawn according to the so-called "posterior predictive pdf"

$$p(\mathbf{x}_{MC} \mid \mathbf{X}) = \int_{\Omega(\mathbf{\Theta})} d\mathbf{\Theta}\, p(\mathbf{x}_{MC} \mid \mathbf{\Theta})\, p(\mathbf{\Theta} \mid \mathbf{X}) . \tag{32}$$

Note that a probability distribution model $p(\mathbf{x} \mid \mathbf{\Theta})$ is needed for evaluating the empirical data according to eq. (29). This brings in a further fundamental uncertainty due to the selection of probability distribution models. However, this uncertainty can be reduced, if not actually surmounted, by performing sensitivity studies on the use of different distribution models.

As appears from the Bayes' theorem eq. (29), the use of Bayesian MC procedures requires the definition of a prior pdf $p(\mathbf{\Theta})$. Accomplishment of this requirement involves the probability-theoretical problem of the Bayesian methodology, see Appendix to this paper.

For those who are not so familiar with Bayesian MC procedures the principle of such procedures is illustrated by means of a simple example shown in Figure 5: Let us assume that we want to draw MC samples x_{MC} on the one-dimensional parameter x according to eq. (32), where $\mathbf{X}$ reduces now to the vector of observations x_i, $i = 1,\ldots,n$: $\mathbf{x}_{obs} = (x_1,\ldots,x_n)^T$. Whatever the pdf $p(\mathbf{x} \mid \mathbf{\Theta})$ of the random variable x might be, the sample mean of the observations x_i is given by

$$\bar{x} = \frac{1}{n}\sum_{i=1}^{n} x_i \tag{33}$$

and the corresponding sample variance is given by

$$\hat{\sigma}^2 = \frac{1}{n-1}\sum_{i=1}^{n} (x_i - \bar{x})^2 . \tag{34}$$

Let us assume that we can justify that $\mathbf{x}_{obs}$ represents n observations on a Normal distribution with unknown expectation (mean) μ and unknown variance σ^2,

$$p(x \mid \mathbf{\Theta}) = p(x \mid \mu, \sigma^2) \equiv N(\mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2} \right). \tag{35}$$

With equations (33) and (34) the Likelihood in eq. (29) thus becomes

$$\begin{aligned} p(\mathbf{x}_{obs} \mid \mathbf{\Theta}) = p(\mathbf{x}_{obs} \mid \mu, \sigma^2) &= \frac{1}{\left(\sqrt{2\pi\sigma^2}\right)^n} \exp\left(-\frac{1}{2\sigma^2}\sum_{i=1}^{n} (x_i - \mu)^2 \right) \\ &= \frac{1}{\left(2\pi\sigma^2\right)^{n/2}} \exp\left(-\frac{1}{2}\frac{(\bar{x}-\mu)^2}{\sigma^2/n} \right) \exp\left(-\frac{1}{2\sigma^2}\sum_{i=1}^{n} (x_i - \bar{x})^2 \right) \\ &= \frac{1}{\left(2\pi\sigma^2\right)^{n/2}} \exp\left(-\frac{1}{2}\frac{(\mu-\bar{x})^2}{\sigma^2/n} \right) \exp\left(-\frac{1}{2}(n-1)\frac{\hat{\sigma}^2}{\sigma^2} \right). \end{aligned} \tag{36}$$

Let us assume that no prior knowledge about $\mathbf{\Theta} = (\mu, \sigma^2)$ is available. Accordingly, the commonly proposed non-informative prior density

$$p(\mu,\sigma^2) \propto \sigma^{-2} \tag{37}$$

is chosen (cf. eq. (A-39) in the Appendix to this paper).

Multiplying the Likelihood eq. (36) with this prior density results, according to eq. (29), in the posterior density

$$p(\mu,\sigma^2 \mid \mathbf{x}_{obs}) \propto p\left(\mu \mid \mathbf{x}_{obs},\sigma^2\right) \cdot p(\sigma^2 \mid \mathbf{x}_{obs}), \tag{38}$$

where $p(\mu \mid \mathbf{x}_{obs},\sigma^2)$ is the Normal pdf

$$p(\mu \mid \mathbf{x}_{obs},\sigma^2) = N\left(\bar{x},\frac{\sigma^2}{n}\right) = \sqrt{\frac{n}{2\pi\sigma^2}}\ \exp\left(-\frac{1}{2}\frac{(\bar{x}-\mu)^2}{\sigma^2/n}\right) \tag{39}$$

and $p(\sigma^2 \mid \mathbf{x}_{obs})$ is the Inverse-Wishart pdf (cf. equations (A-12) and (A-40) in the Appendix)

$$\begin{aligned} p(\sigma^2 \mid \mathbf{x}_{obs}) &= \text{Inv}-\text{Wishart}\left((n-1)^{-1}\hat{\sigma}^{-2};\, n-1;\, m=1\right) \\ &= \left[2^{\frac{n-1}{2}} \cdot \Gamma\left(\frac{n-1}{2}\right)\right]^{-1} \left((n-1)\hat{\sigma}^2\right)^{(n-1)/2} \left(\sigma^2\right)^{-(n-1+2)/2}\ \exp\left(-(n-1)\frac{\hat{\sigma}^2}{\sigma^2}\right) \\ &= \text{Inv}-\chi^2(\sigma^2 \mid (n-1),\hat{\sigma}^2) \end{aligned} \tag{40}$$

with $(n-1)$ degrees of freedom and scale factor $(n-1)\,\hat{\sigma}^2$. As indicated in eq. (40), in the one-dimensional case $(m=1)$ the Inverse-Wishart distribution is identical with the scaled Inverse-χ^2-distribution with $(n-1)$ degrees of freedom and scale factor $\hat{\sigma}^2$ [6].

Eq. (39) says that the unknown mean μ follows a Normal distribution with expectation $\bar{x}$ and variance σ^2/n, which is unknown since σ^2 is unknown. However, eq. (40) tells that the unknown σ^2 follows a scaled Inverse-χ^2-distribution with $(n-1)$ degrees of freedom and scale factor $\hat{\sigma}^2$, which is the known sample variance eq. (34). So therefore, as illustrated in Figure 5, to get an MC sample x_{MC} the following steps have to be taken successively:

- Drawing of a MC sample σ^2_{MC} from the pdf eq. (40)
- Inserting of σ^2_{MC} into the pdf eq. (39) and then drawing of a MC sample μ_{MC} from the pdf $p\left(\mu \mid \bar{x},\frac{\sigma^2_{MC}}{n}\right)$.
- Inserting of μ_{MC} and σ^2_{MC} into the pdf eq. (35) and then drawing of a sample x_{MC} from the pdf $p(x \mid \mu_{MC},\sigma^2_{MC})$.

To get the next sample x_{MC} one has to return to the first step and to repeat the procedure.

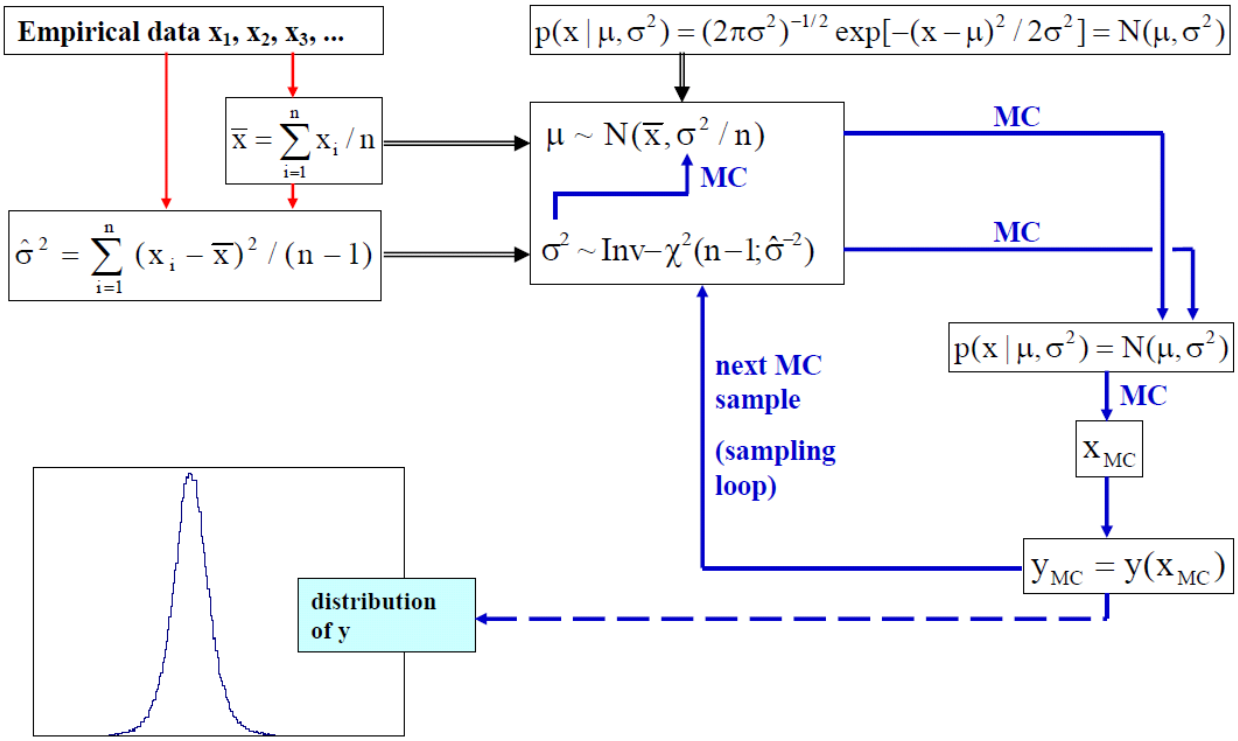

***Figure 5**: Example for a Bayesian Monte Carlo procedure*

As illustrated in Figure 5, the obtained samples x_{MC} can be used to solve (analytically or numerically, as the case may be) the relation $y = y(x)$ so that one gets an empirical distribution of samples $y_{MC} = y(x_{MC})$ which bares information about the pdf of y.

In the following sections the Bayesian Monte Carlo procedure summarized in eq. (32) will be applied to the analysis of uncertainties involved in burnup credit criticality safety analysis. The description of the application of the Bayesian Monte Carlo procedure follows the hierarchy of uncertainties shown in Figure 1. Since the paper on hand was written for a burnup credit workshop, the attention is mainly focused on the depletion validation issues in the following.

4 Validation of depletion calculation

As well-known, validation of a depletion calculation for a burnup credit (BUC) criticality safety analysis consists in implementation of two key steps:

- Evaluation of chemical assay data from samples from irradiated fuel
- Evaluation of the ICFs (isotopic correction factors) for the isotopes to be used in a BUC criticality safety analysis

4.1 Evaluation of assay data

The evaluation of the assay data includes the following steps:

- Evaluation of the measurement results obtained from the laboratories which performed the assays of the fuel samples
- Evaluation of the burnup of the fuel samples
- Evaluation of the calculated isotopic concentrations and of the resulting ICFs

The notation which is used for indices in the following sections is as follows:

- J := number of an analyzed fuel sample, $J = 1,..., N_{FS}$;
- L = L(J) := number of the laboratory which participated in the analysis of the J-th fuel sample, $L(J) = 1,\ldots, N_{lab}(J)$; i. e., the J-th sample is divided in $N_{lab}(J)$ subsamples which are independently analyzed by $N_{lab}(J)$ laboratories;
- I = I(L(J)) := number of an isotope considered in the analysis of the J-th fuel sample by the L(J)-th laboratory, $I(L(J)) = 1,\ldots, N_{isot}(L(J))$; note that the number $N_{isot}(L(J))$ can differ from laboratory to laboratory at given J.

4.1.1 Evaluation of the measured isotopic concentrations

The L-th laboratory that has participated in the analysis of the J-th assay delivers a set of measured isotopic concentrations (experimental results)

$$\mathbf{E}_{JL}(\mathbf{p}) = \left(E_{IJL}(\mathbf{p}),\ldots, E_{IJL}(\mathbf{p}),\ldots\right)^T,\ I = 1,\ldots, N_{isot}(L(J)). \tag{41}$$

The vector $\mathbf{p}$ in eq. (41) denotes the set of experimental parameters on which the estimation of the isotopic concentrations E_{IJL} has been based. Kind and number of these parameters depend on the applied experimental analysis methods and devices and may therefore vary with L and J.

Let us assume that the laboratory has repeated the measurement of the isotopic concentrations N times and that the results $E_{IJL}(\mathbf{p})$ in eq. (41) represent the sample means

$$E_{IJL}(\mathbf{p}) = \frac{1}{N}\sum_{n=1}^{N}\left(E_{IJL}(\mathbf{p})\right)_n \tag{42}$$

of the single results $\left(E_{IJL}(\mathbf{p})\right)_n$. The covariance of the sample means, eq. (41), becomes therefore

$$\operatorname{cov}(E_{IJL}(\mathbf{p}), E_{\tilde{I}JL}(\mathbf{p})) = \frac{1}{N^2}\sum_{n,\tilde{n}=1}^{N}\operatorname{cov}\left((E_{IJL}(\mathbf{p}))_n, (E_{\tilde{I}JL}(\mathbf{p}))_{\tilde{n}}\right),\ I, \tilde{I} = 1,\ldots, N_{isot}(L(J)). \tag{43}$$

Assuming that each of the functions $(E_{IJL}(\mathbf{p}))_n$ can be expanded about the sample means $\hat{\mathbf{p}}_n = (\hat{p}_{1n}, \hat{p}_{2n},\ldots, \hat{p}_{\rho n})^T$ in a Taylor series

$$\left(E_{IJL}(\mathbf{p})\right)_n = \sum_{\lambda_1=0}^{\infty} \cdots \sum_{\lambda_\rho=0}^{\infty} \frac{(p_1 - \hat{p}_{1n})^{\lambda_1} \cdots (p_\rho - \hat{p}_{\rho n})^{\lambda_\rho}}{\lambda_1! \ldots \lambda_\rho!} \left[\frac{\partial^{\lambda_1 + \ldots + \lambda_\rho} (E_{IJL}(\mathbf{p}))_n}{\partial p_1^{\lambda_1} \ldots \partial p_\rho^{\lambda_\rho}} \right]_{\mathbf{p}=\hat{\mathbf{p}}_n} \tag{44}$$

and assuming that terms of order $m = \sum_{i=1}^{\rho} \lambda_i > 1$ can be ignored, eq. (43) becomes

$$\operatorname{cov}(E_{IJL}, E_{\tilde{I}JL}) \approx \frac{1}{N^2} \sum_{n,\tilde{n}=1}^{N} \left[\sum_{\nu,\mu=1}^{\rho} \left(\frac{\partial (E_{IJL})_n}{\partial p_\nu} \right)_{\hat{p}_{\nu n}} \left(\frac{\partial (E_{\tilde{I}JL})_{\tilde{n}}}{\partial p_\mu} \right)_{\hat{p}_{\mu\tilde{n}}} \operatorname{cov}(p_{\nu n}, p_{\mu\tilde{n}}) \right]. \tag{45}$$

The N measurements are usually performed in such a way that they are mutually independent. Thus $\operatorname{cov}(p_{\nu n}, p_{\mu\tilde{n}})$ in eq. (45) becomes $\operatorname{cov}(p_{\nu n}, p_{\mu\tilde{n}}) = \operatorname{cov}(p_{\nu n}, p_{\mu\tilde{n}}) \delta_{n,\tilde{n}}$ and hence

$$\operatorname{cov}(E_{IJL}, E_{\tilde{I}JL}) \approx \frac{1}{N^2} \sum_{n=1}^{N} \left[\sum_{\nu,\mu=1}^{\rho} \left(\frac{\partial (E_{IJL})_n}{\partial p_\nu} \right)_{\hat{p}_{\nu n}} \left(\frac{\partial (E_{\tilde{I}JL})_n}{\partial p_\mu} \right)_{\hat{p}_{\mu n}} \operatorname{cov}(p_{\nu n}, p_{\mu n}) \right]. \tag{46}$$

For the case that the parameters p_ν are mutually independent eq. (46) reduces to

$$\operatorname{cov}(E_{IJL}, E_{\tilde{I}JL}) \approx \frac{1}{N^2} \sum_{n=1}^{N} \left[\sum_{\nu=1}^{\rho} \left(\frac{\partial (E_{IJL})_n}{\partial p_\nu} \right)_{\hat{p}_{\nu n}} \left(\frac{\partial (E_{\tilde{I}JL})_n}{\partial p_\nu} \right)_{\hat{p}_{\nu n}} \sigma^2(p_{\nu n}) \right]. \tag{47}$$

The expressions eq. (46) or, as the case may be, eq. (47) are the elements $(S_{JL})_{I\tilde{I}}$ of the covariance matrix $\mathbf{S}_{JL}$ of the vector $\mathbf{E}_{JL}(\mathbf{p})$ of observations eq. (41).

So therefore, for the determination of the uncertainties of the bias-corrected number densities eq. (21) it is a crucial step (cf. Figure 1) to determine the elements of the covariance matrix $\mathbf{S}_{JL}$ very carefully, i. e.,

- to take all the contributions to the covariances eq. (46) or eq. (47) and hence to the correlations of the results $\mathbf{E}_{IJL}$ and $\mathbf{E}_{\tilde{I}JL}$ into account (e. g., the contribution due to the uncertainty of the assay mass used in a measurement) and
- to check whether terms of order $m = (\lambda_1 + \ldots + \lambda_\rho) > 1$ of the Taylor series expansion eq. (44) can really be ignored or not. If not, the Taylor series expansion with the required order m has to be inserted into the definitions of the expectation and the covariance (cf. equations (22) and (23), for instance) to get the expressions for the mean values E_{IJL} and the covariances $\operatorname{cov}(E_{IJL}, E_{\tilde{I}JL})$ which have to be applied in case of $m > 1$.

The number N of measurements usually amounts to 1, $N = 1$. If a fuel sample is divided in subsamples it is in fact preferable to give the subsamples to different laboratories, because it has been observed many a time that results from different laboratories are incompatible, i. e., that a statistical compatibility test [1] of these results leads to the outcome that the hypothesis under test that these results have one and the same expectation is rejected. Very often no explanation of the

observed incompatibilities can be given; and so these incompatibilities have to be considered in the validation of depletion calculations because, even if it is obvious that an observed incompatibility is due to the results from one particular laboratory, statistics cannot tell whether the results from this laboratory are wrong and the results from the remaining laboratories are right, or vice versa. So therefore, giving subsamples to different laboratories makes it possible to include the consideration of errors which may be hidden in the applied radiochemical analysis procedures. It is to be expected, in fact, that the results obtained by the different laboratories from the respective subsamples are compatible. Inexplicable incompatibility of these results can hence be understood as an indication of underestimation of the uncertainties of at least some of the individual sets of results $\mathbf{E}_{\mathrm{JL}}(\mathbf{p})$, eq. (41). This underestimation can be rectified by evaluating the results from all the laboratories by means of on and the same probability distribution model. The use of one and the same probability distribution model expresses the expectation that the results from the different laboratories shall be compatible.

But before a joint probability distribution model can be obtained the evaluation of the results eq. (41) and eq. (46) or eq. (47) from the individual laboratories has to be completed. Since N in eq. (42) and eq. (46) or eq. (47) usually amounts to 1, there is usually not enough information available to gain knowledge about the parameters $\boldsymbol{\Theta}$ of the pdf underlying the outcomes of eq. (41). One is therefore committed to go the usual way, i. e., to assume that the vector eq. (41) with N = 1 in eq. (42) represents a sample on a multivariate Normal distribution. In fact, Normality is assumed because it is simple to use and, to some extent, empirically supported. With respect to the results from only one laboratory there are suggestions from the mathematical and experimental side that the assumption of Normality is at least a good approximation to the actual pdf [1].

Since no further information about the parameters $\boldsymbol{\Theta}$, i. e., about the expectation vector and the covariance matrix of the assumed Normal distribution model is available in case of N = 1, one is forced to take the sample eq. (41) and the sample covariance matrix $\mathbf{S}_{\mathrm{JL}}$ with the elements eq. (46) or, as the case may be, eq. (47) for the expectation vector and the covariance matrix, respectively. By means of the pdf-model $\mathrm{N}(\mathbf{E}_{\mathrm{JL}}, \mathbf{S}_{\mathrm{JL}})$ thus assumed Monte Carlo (MC) samples $\mathbf{E}_{\mathrm{JL}}^{\mathrm{MC}}$ can be drawn, the variation of which represents the uncertainty of the results eq. (41) which has turned out to be revealable with respect to the analysis methods used by the L(J)-th laboratory.

By the way, if the matrix $\mathbf{S}_{\mathrm{JL}}$ were the actual ("true") covariance matrix then the MC samples $\mathbf{E}_{\mathrm{JL}}^{\mathrm{MC}}$ drawn from $\mathrm{N}(\mathbf{E}_{\mathrm{JL}}, \mathbf{S}_{\mathrm{JL}})$ would be samples on the actual ("true") expectation vector $\mathbf{E}[\mathbf{E}_{\mathrm{JL}}]$ of $\mathrm{N}(\mathbf{E}_{\mathrm{JL}}, \mathbf{S}_{\mathrm{JL}})$ because of the symmetry of the covariance form of $\mathrm{N}(\mathbf{E}[\mathbf{E}_{\mathrm{JL}}], \mathbf{S}_{\mathrm{JL}})$.

The MC samples $\mathbf{E}_{\mathrm{JL}}^{\mathrm{MC}}$ are used in the next steps to be taken to obtain the required ICFs.

4.1.2 Evaluation of the burnup

The next step to be taken is the evaluation of the burnup of the fuel sample to be able to determine the sample's isotopic concentration from depletion calculations performed by means of the depletion calculation code of interest for the sample's irradiation history.

The following cases have to be distinguished:

(a) Each laboratory L = L(J) that participates in the analysis of the J-th fuel sample has estimated the burnup value from measured isotopic concentrations $E_{\nu JL}$ of burnup indicators (as Nd-148, for example).

(b) The burnup value of the J-th fuel sample has been calculated only, i. e., none of the laboratories has estimated the burnup from any measurement results.

(c) Only part of the laboratories accomplished the estimation of the sample's burnup according to (a).

4.1.2.1 Case (a)

In case (a) the results $E_{\nu JL}$ are part of the set of outcomes presented by the vector $\mathbf{E}_{JL}(\mathbf{p})$, eq. (41). For each burnup indicator a MC sample $E_{\nu JL}^{MC}$ is thus included in the MC sample vector $\mathbf{E}_{JL}^{MC}$ drawn from the model $N(\mathbf{E}_{JL}, \mathbf{S}_{JL})$ as described in section 4.1.1. So therefore, insertion of the MC sample value $E_{\nu JL}^{MC}$ into the relation

$$B = g_\nu(c_\nu) \tag{48}$$

of the Burnup B to the isotopic concentration c_ν of the ν-th burnup indicator provides a MC sample $B_{\nu JL}^{MC}$ for the burnup:

$$B_{\nu JL}^{MC} = g_\nu(E_{\nu JL}^{MC}),\ \nu = 1,\ldots,\beta(L)\,. \tag{49}$$

$\beta(L)$ in eq. (49) denotes the number of burnup indicators considered by the L-th laboratory.

It is to be expected that the actual burnup of the fuel sample can be assumed to be sufficiently well-defined. Otherwise it would be highly unlikely that the sample is appropriate for being applied to depletion calculation validation. Therefore, the set of outcomes $\left\{B_{\nu JL}^{MC},\ \nu = 1,\ldots,\beta(L)\right\}$ can be taken for a sample of size $\beta(L)$ on the underlying burnup pdf. Because of being relations for burnup indicators, the relations eq. (48) can be assumed to be linear functions of the form

$$B = g_\nu(c_\nu) = a_\nu \cdot c_\nu \tag{50}$$

with a factor a_ν which

- depends on parameters such as the irradiated fuel mass, the energy released per fission, as well as the fission yield of the ν-th burnup indicator, its atomic mass and, in case that this indicator is not stable, its radioactive decay constant, but which

- does not depend on c_ν.

It follows therefore that B given by eq. (50) is a Normal variable (cf. section 4.2.2 in Ref. [1]). In section 4.1.1 it has been assumed that the variables $c_\nu \equiv E_{\nu JL}$ are Normal variables. So therefore, the set of MC samples $\left\{B_{\nu JL}^{MC},\ \nu = 1,\ldots,\beta(L)\right\}$ resulting from eq. (50) according to eq. (49) can be taken for a sample of size $\beta(L)$ on the Normal pdf $p(B_J \mid E[B_J], V[B_J]) = N(E[B_J], V[B_J])$ of the burnup B_J of the J-th fuel sample.

The expectation $E[B_J]$ and the variance $V[B_J] = \sigma^2(B_J) = \sigma_J^2$ remain unknown.

If the size $\beta(L)$ amounts to 1, $\beta(L) = 1$, there is nothing more to be done, i. e., one stays with

$$B_{JL}^{MC} \equiv B_{1JL}^{MC} \text{ for } \beta(L) = 1 \tag{51}$$

as MC sample on the burnup.

But in case of $\beta(L) > 1$ the Bayesian MC procedure for one-dimensional random variables described in section 3 can be employed (cf. equations (33) through (40) and Figure 5):

- The sample mean

$$\overline{B}_{JL} = \frac{1}{\beta(L)} \sum_{\nu=1}^{\beta(L)} B_{\nu JL}^{MC},\ \beta(L) > 1, \tag{52}$$

  and the sample variance

$$\hat{\sigma}_{JL}^2 = \frac{1}{\beta(L)-1} \sum_{\nu=1}^{\beta(L)} (B_{\nu JL}^{MC} - \overline{B}_{JL})^2,\ \beta(L) > 1, \tag{53}$$

  are evaluated (cf. eq. (33) and (34)).

- A MC sample $(\sigma_{JL}^2)^{MC}$ on the variance $V[B_J]$ is drawn from the scaled inverse-χ^2-distribution $\text{Inv}-\chi^2(\beta(L)-1;\hat{\sigma}_{JL}^2)$ (cf. eq. (40) and Figure 5).

- Insertion of $(\sigma_{JL}^2)^{MC}$ into the pdf $N(\overline{B}_{JL}, V[B_J]/\beta(L))$ (cf. eq. (39)) and draw of a MC sample $E[B_{JL}]^{MC}$ on the expectation $E[B_{JL}]$ from the resulting pdf $N(\overline{B}_{JL}, (\sigma_{JL}^2)^{MC}/\beta(L))$ (cf. Figure 5).

- Insertion of $E[B_{JL}]^{MC}$ and $(\sigma_{JL}^2)^{MC}$ into the pdf $N(E[B_J], V[B_J])$ (cf. eq. (35) and Figure 5) and draw of a MC sample

  $$B_{JL}^{MC} \text{ from } N(E[B_{JL}]^{MC}, (\sigma_{JL}^2)^{MC}) \text{ for } \beta(L) > 1. \tag{54}$$

One may raise criticism of the taken route of evaluating the results $E_{\nu JL}$, $\nu = 1,\ldots,\beta(L)$, from the different laboratories $L = L(J) = 1,\ldots,N_{lab}(J)$ separately. In principle one can put in fact the results $E_{\nu JL}$ from the different laboratories for each of the burnup indicators ν together because

the expectation $E[B_J]$ is, as already stated above, to be expected to be applicable to all the burnup values $B_{\nu JL}$ resulting from $B_{\nu JL} = g_\nu(E_{\nu JL})$ according to the relations eq. (48). However, if one put the results $E_{\nu JL}$ from the different laboratories together the question immediately arises why one does not proceed in the same way with all the results $\mathbf{E}_{JL}(\mathbf{p})$, eq. (41), from the different laboratories. The answer to this question is that evaluating the results $\mathbf{E}_{JL}(\mathbf{p})$ from the different laboratories separately is more powerful than averaging these results, because evaluating the outcomes $\mathbf{E}_{JL}(\mathbf{p})$ separately ensures that the maximum possible amount of experimental information can be made available for the estimation of the ICFs of those nuclides which are actually used in an actual burnup credit application case, cf. section 4.2.

Case (a) was defined as the case that each laboratory has estimated the burnup value from the results $E_{\nu JL}$ obtained for the burnup indicators $\nu = 1,\ldots,\beta(L)$. So, the question naturally arises why the drawing of burnup MC samples $B_{\nu JL}^{MC}$ is based, according to eq. (49), on the drawing of MC samples $E_{\nu JL}^{MC}$ from the distribution model $N(\mathbf{E}_{JL}, \mathbf{S}_{JL})$ of the complete set $\mathbf{E}_{JL}$ of measured isotopic concentrations instead of being based on a distribution model of the burnup already estimated by the L-th laboratory. Let us assume that this laboratory has delivered the estimated burnup in form of the total average

$$\hat{B}_{JL} = \frac{1}{\beta(L)} \sum_{\nu=1}^{\beta(L)} B_{\nu JL} = \frac{1}{\beta(L)} \sum_{\nu=1}^{\beta(L)} g_\nu(E_{\nu JL}) = \frac{1}{\beta(L)} \sum_{\nu=1}^{\beta(L)} a_\nu \cdot E_{\nu JL} \,. \tag{55}$$

So therefore, the variance of this estimate is

$$V[\hat{B}_{JL}] = \frac{1}{\beta(L)^2} \sum_{\nu,\mu=1}^{\beta(L)} \mathrm{cov}\left(B_{\nu JL}, B_{\mu JL}\right) = \frac{1}{\beta(L)^2} \sum_{\nu,\mu=1}^{\beta(L)} a_\nu \, a_\mu \, \mathrm{cov}\left(E_{\nu JL}, E_{\mu JL}\right). \tag{56}$$

Even if one makes the pretty idealized assumption that all the covariances $\mathrm{cov}\left(E_{\nu JL}, E_{\mu JL}\right)$ are really considered the following statement has to be recognized: If the burnup MC samples are drawn from a Normal distribution model with the estimate eq. (55) as expectation and with the estimate eq. (56) as variance then, in contrast to the procedure described above, only the part $(\mathbf{S}_{\beta\beta})_{JL}$ of the empirical covariance matrix $\mathbf{S}_{JL}$ is involved,

$$\mathbf{S}_{JL} = \begin{pmatrix} (\mathbf{S}_{\alpha\alpha})_{JL} & (\mathbf{S}_{\alpha\beta})_{JL} \\ (\mathbf{S}_{\alpha\beta})_{JL}^{T} & (\mathbf{S}_{\beta\beta})_{JL} \end{pmatrix}, \tag{57}$$

- $(\mathbf{S}_{\beta\beta})_{JL}$ is the covariance matrix with the elements $\mathrm{cov}\left(E_{\nu JL}, E_{\mu JL}\right)$ of the burnup indicators, $\nu, \mu = 1,\ldots,\beta(L)$
- $(\mathbf{S}_{\alpha\alpha})_{JL}$ is the covariance matrix related to the remaining isotopes called “nbi-isotopes” (i.e., “non-burnup-indicator-isotopes”) in the following, $\alpha = N_{isot}(L(J)) - \beta(L)$, and
- $(\mathbf{S}_{\alpha\beta})_{JL}$ contains covariances between these nbi-isotopes and the burnup indicators.

The actual (i. e. "true", but unknown) concentrations of all the isotopes are functions of the fuel sample's burnup at given irradiation history. All experimental results $\mathbf{E}_{JL}(\mathbf{p})$, eq. (41), contain therefore empirical information about the burnup of the fuel sample. Consequently, if only the partial matrix $(\mathbf{S}_{\beta\beta})_{JL}$ is involved all the information is lost which is transmitted by means of the partial covariance matrix $(\mathbf{S}_{\alpha\beta})_{JL}$ from the nbi-isotopes to the burnup indicators. Since the number β of burnup indicators is usually significantly smaller than the number α of nbi-isotopes the loss of information can be heavy, the heavier the higher the correlations between nbi-isotopes and burnup indicators are. So therefore, drawing MC samples $\mathbf{E}_{JL}^{MC}$ for all the isotopes from the distribution model $N(\mathbf{E}_{JL},\mathbf{S}_{JL})$ and then using the MC samples $E_{\nu JL}^{MC}$ for the burnup indicators included in $\mathbf{E}_{JL}^{MC}$ for obtaining MC samples B_{JL}^{MC} on the burnup according to eq. (51) or eq. (54) is a much more powerful procedure since it makes use of all the available experimental information.

4.1.2.2 Case (b)

Case (b) may be regarded as a case that results in misbegotten outcomes since the available burnup information is not blessed by any experimental information from the chemical analysis of the fuel sample of interest. However, since no further information is available one is committed to go the usual way, i. e., to assume that the burnup B_J of the J-th fuel sample follows a probability distribution $p(B_J|\boldsymbol{\Theta})$. Neither the type nor the parameters $\boldsymbol{\Theta}$ of $p(B_J|\boldsymbol{\Theta})$ can be really fixed here, since they depend on the procedure used for calculating the burnup of the fuel sample. However, what can be done here is to suggest to evaluate the whole amount of validation data, which has been compiled for the applied burnup calculation procedure, as indicated in Figure 6:

- Plot the frequency of occurrence $H(B_P - B_M)$ of the observed deviations $\Delta B = B_P - B_M$ of the predicted (calculated) burnup B_P from the measured burnup B_M against $\Delta B = B_P - B_M$.
- Derive an empirical pdf $h(\Delta B|\hat{\boldsymbol{\Theta}}_{\Delta B})$ ($\hat{\boldsymbol{\Theta}}_{\Delta B}$ denotes the resulting estimate of the "true" distribution parameters $\boldsymbol{\Theta}_{\Delta B}$) by using one of the methods described in Ref. [1], sections 11.2 through 11.4.

The empirical pdf $h(\Delta B|\hat{\boldsymbol{\Theta}}_{\Delta B})$ is usually expected to be a Normal pdf. In fact, there are suggestions from the mathematical as well as from the empirical side that the assumption of Normality for $h(\Delta B|\hat{\boldsymbol{\Theta}}_{\Delta B})$ is at least a good approximation to the actual pdf $h(\Delta B|\boldsymbol{\Theta}_{\Delta B})$.

If this true, then

$$\hat{\boldsymbol{\Theta}}_{\Delta B} = \left(\delta B, s^2(\Delta B)\right), \tag{58}$$

where δB is the expectation value of the empirical distribution $h(\Delta B|\hat{\boldsymbol{\Theta}}_{\Delta B})$ (cf. Figure 6) and $s^2(\Delta B)$ denotes the variance of this distribution. The distribution of the burnup B_J of the J-th fuel sample can then be approximated by the Normal pdf $N\left(B_J^{(c)} - \delta B, s^2(\Delta B)\right)$ with expectation

$B_J^{(c)} - \delta B$, where $B_J^{(c)}$ is the burnup calculated for the J-th fuel sample. Therefore, by means of $N\left(B_J^{(c)} - \delta B, s^2(\Delta B)\right)$ MC samples B_J^{MC} on the burnup B_J can be drawn:

$$B_J^{MC} \text{ from } N\left(B_J^{(c)} - \delta B, s^2(\Delta B)\right). \tag{59}$$

If the assumption of Normality for $h(\Delta B \mid \hat{\boldsymbol{\Theta}}_{\Delta B})$ is rejected by a method chosen from Ref. [1], sections 11.2 through 11.4, for fitting $N \cdot h(\Delta B \mid \hat{\boldsymbol{\Theta}}_{\Delta B})$ to the distribution $H(B_P - B_M)$ of the N observed deviations $\Delta B = B_P - B_M$, then one has to stay with a "real life distribution" for $h(\Delta B \mid \hat{\boldsymbol{\Theta}}_{\Delta B})$. The Johnson families of empirical distributions are particularly appropriate for this purpose [1]. The MC samples B_J^{MC} can then be obtained by drawing MC samples ΔB^{MC} from $h(\Delta B \mid \hat{\boldsymbol{\Theta}}_{\Delta B})$ and subtracting these samples from $B_J^{(c)}$:

$$B_J^{MC} = B_J^{(c)} - \Delta B^{MC} \text{ with } \Delta B^{MC} \text{ from } h(\Delta B \mid \hat{\boldsymbol{\Theta}}_{\Delta B}). \tag{60}$$

It is obvious that eq. (59) is a special case of eq. (60).

In contrast to the MC samples eq. (51) or eq. (54), a MC sample B_J^{MC} obtained from eq. (59) or eq. (60) has to be applied to all the laboratories $L = L(J)$ which participated in the analysis of the J-th fuel sample.

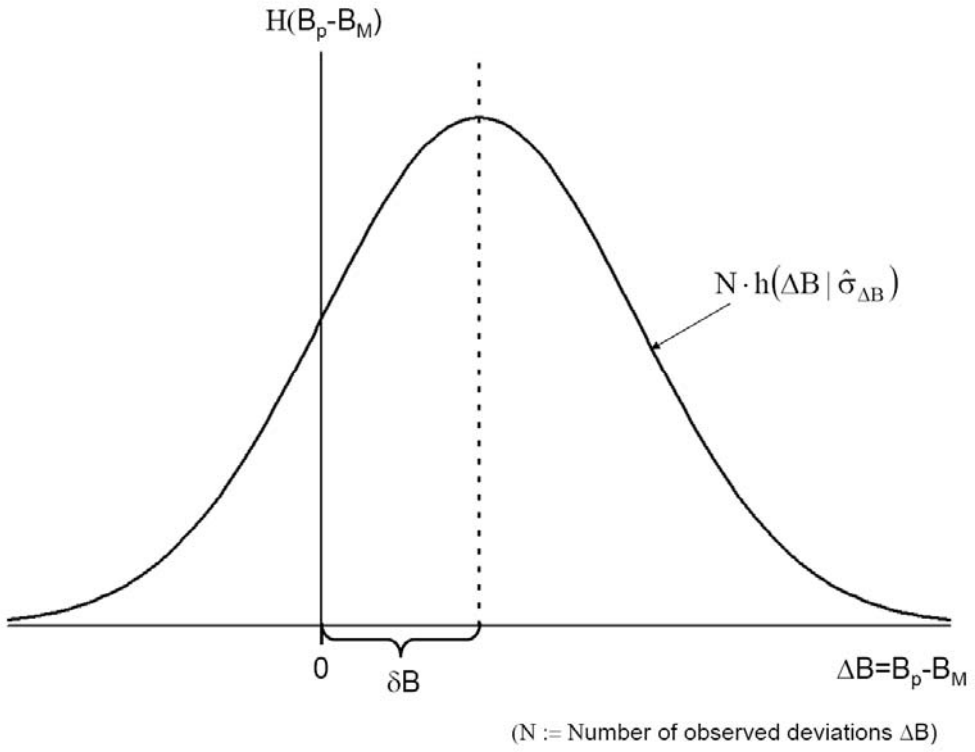

***Figure 6**: Illustration of the evaluation of the statistics of validation data compiled for a burnup calculation procedure*

4.1.2.3 Case (c)

It is obvious that in case (c) for those laboratories which accomplished the estimation of the fuel sample's burnup according to case (a) laboratory-specific MC samples B_{JL}^{MC} are drawn according to eq. (51) or eq. (54). For all other laboratories one has to proceed according to case (b) and hence according to eq. (59) or eq. (60).

In this conjunction the question naturally arises if it is possible to combine MC sample values B_J^{MC} based on calculated burnup values $B_J^{(c)}$ with MC sample values $B_{\nu JL}^{MC}$ based on measured burnup indicator concentrations. The answer is "yes" if and only if the following conditions are met:

- The set of validation data, which has been applied to the validation of the burnup calculation procedure used for the determination of $B_J^{(c)}$, must not include any information resulting from the analysis of the J-th fuel sample, i. e., from the fuel sample of interest.
- The assumption of Normality for $h(\Delta B \mid \hat{\boldsymbol{\Theta}}_{\Delta B})$ must not be rejected by the method chosen from [1], sections 11.2 through 11.4, for obtaining $h(\Delta B \mid \hat{\boldsymbol{\Theta}}_{\Delta B})$. In other words, B_J^{MC} shall be drawn according to eq. (59).

If these conditions are met, then and only then $B_J^{MC(c)} \equiv B_J^{MC}$ can be added to equations (52) and (53), which then become

$$\overline{B}_{JL} = \frac{1}{\beta(L)+1}\left(B_J^{MC(c)} + \sum_{\nu=1}^{\beta(L)} B_{\nu JL}^{MC} \right) \tag{61}$$

and, respectively,

$$\hat{\sigma}_{JL}^2 = \frac{1}{\beta(L)}\left\{ \left(B_J^{MC(c)} - \overline{B}_{JL} \right)^2 + \sum_{\nu=1}^{\beta(L)} \left(B_{\nu JL}^{MC} - \overline{B}_{JL} \right)^2 \right\}, \tag{62}$$

where we have written $B_J^{MC(c)}$ instead of B_J^{MC} to make clear that this MC sample is based on the calculated burnup $B_J^{(c)}$ and originates from eq. (59).

So, when instead of equations (52) and (53) equations (61) and (62) are used in the above-described Bayesian MC procedure for generating MC samples B_{JL}^{MC}, then $\beta(L)$ has obviously to be replaced by $\beta(L)+1$.

4.1.3 Evaluation of the calculated isotopic concentrations

The calculation of the isotopic concentrations of an irradiated fuel sample by means of the depletion calculation code of interest is usually performed as follows: The fuel sample's irradiation history is described (modeled) and the fuel is then depleted according to this history up to a fixed burnup value specified for the sample. Then the radioactive decay is followed as long as required,

i.e., till the date of chemical analysis is reached. So, one set of calculated isotopic concentrations is thus obtained referring to just one burnup value. However, to be able to consider the uncertainty in the fuel sample's burnup one needs the calculated isotopic concentrations $\mathbf{c} = \left(c_1,\ldots,c_I,\ldots,c_{N_{isot}}\right)^T$ as a function of the burnup, $\mathbf{c} = \mathbf{c}(B)$, for a certain burnup range the width of which depends on the uncertainty of the burnup.

The burnup value up to which the fuel is depleted in a depletion calculation performed under a specific irradiation history is given by eq. (63),

$$B = \sum_{\lambda=1}^{L_{fin}} \int_{t_{BOC(\lambda)}}^{t_{EOC(\lambda)}} P_S(t)\, dt\,, \tag{63}$$

where $P_S(t)$ denotes the specific power history (as a function of time t), λ numbers the irradiation cycles, $\lambda = 1,\ldots,L_{fin}$, L_{fin} is the last irradiation cycle, $t_{BOC(\lambda)}$ is the time of the begin of the λ-th irradiation cycle, and $t_{EOC(\lambda)}$ is the time of the end of this cycle. Due to the downtime periods Δt_D between the irradiation cycles, $t_{BOC(\lambda)}$ is given by eq. (64),

$$t_{BOC(\lambda)} = \begin{cases} 0 & , \quad \lambda = 1 \\ t_{EOC(\lambda-1)} + \Delta t_{D(\lambda-1)} & , \quad 1 < \lambda \le L_{fin} \end{cases}, \tag{64}$$

where $\Delta t_{D(\lambda-1)}$ is the downtime period after cycle no. $\lambda - 1$ for $\lambda > 1$.

The irradiation history specified for a fuel sample is, by definition, related to the time periods $\left(t_{EOC(\lambda)} - t_{BOC(\lambda)}\right)$ and $\Delta t_{D(\lambda)}$, but the lengths of these time periods are fixed independently from the fuel sample's irradiation history. So, therefore, the only chance to determine the calculated isotopic concentrations $\mathbf{c} = (c_1,\ldots,c_{N_{isot}})^T$ as a function of burnup, $\mathbf{c} = \mathbf{c}(B)$, for a specified burnup range by means of the depletion code of interest is to vary the specific power $P_S(t)$ such that the burnup varies over the full burnup range specified. A change of the specific power does not only result in a change of the fission rate but impacts also other depletion parameters such as, in particular, the fuel temperature and hence the moderator density (PWR) or void history (BWR). It is therefore recommended to study the amount of such impacts and to take, if required, account of these impacts by changing the depletion parameters concerned.

So, it turns out that the determination of the calculated isotopic concentration as a function of burnup makes it necessary to vary the irradiation history of the fuel sample of interest. This obviously brings in some arbitrariness since the number of variations of the specific power $P_S(t)$ leading to one and the same change of the burnup is infinite. Since there is no other chance to consider the uncertainty of the fuel sample's burnup, this arbitrariness reflects a fundamental uncertainty which is characteristic of the validation of depletion calculations. The impact of this uncertainty on the calculated isotopic concentrations can be analyzed in sensitivity studies using different variations of $P_S(t)$ which all results in one and the same burnup change. It is obvious

that the outcomes of such studies depend on the height of the fuel sample's burnup and the width of the burnup range over which the burnup is to be varied.

Since the variation of the irradiation history is due to the necessity of varying the burnup over a specified range and is not due to any uncertainty in the recorded irradiation history is seems to be reasonable to vary the specific power stepwise by multiplying all the recorded specific power values $P_S(t)$ of all the irradiation periods $\left(t_{EOC(\lambda)} - t_{BOC(\lambda)}\right)$, $\lambda = 1,\ldots,L_{fin}$, by one and the same factor f_μ (less or greater than 1, as the case may be) and repeat for each of these variations, i.e. for each of the factors f_μ applied, $\mu = 1,\ldots,n$, the depletion calculation and the following of the radioactive decay. Thus, sets if isotopic concentration $\mathbf{c}_\mu = \mathbf{c}(B_\mu)$ are obtained referring to different burnup values B_μ, $\mu = 1,\ldots,n$, obtained according to the factors f_μ applied to the specific power $P_S(t)$. For a sufficiently large number n of sets $\mathbf{c}_\mu = \mathbf{c}(B_\mu)$ the isotopic concentrations c_I, $I = 1,\ldots,N_{isot}$, can be determined as functions of the burnup by applying adequate interpolation procedures (e.g., spline interpolation) or fitting procedures (e.g., linear least squares using a polynomial model) to the sets $\mathbf{c}_\mu = \mathbf{c}(B_\mu)$, $\mu = 1,\ldots,n$. Thus the functional relation $\mathbf{c} = \mathbf{c}(B) = (c_1(B),\ldots,c_{N_{isot}}(B))^T$ sought after is obtained.

This procedure has to be applied to all the analyzed fuel samples $J = 1,\ldots,N_{FS}$, so that one gets the calculated isotopic concentrations

$$\mathbf{c}_J = \mathbf{c}_J(B) = \left(c_{1J},\ldots,c_{IJ},\ldots,c_{M_{isot}(J),J}\right)^T, \text{ with } M_{isot} = \underset{L(J)=1,..,N_{LAB}(J)}{\text{Max}}\left\{N_{isot}(L(J))\right\}. \qquad (65).$$

The question naturally arises if uncertainties in the fuel sample's irradiation history have still to be included in the procedure just described. It goes without saying that in cases of doubt this question can only be answered by means of sensitivity studies. However, apart from the question if the uncertainties in the fuel sample's irradiation history are really known, it seems to be quite unlikely to be confronted with doubtful cases, because it seems to be reasonable to assume that the impacts on the calculated isotopic concentrations due to uncertainties in the fuel sample's irradiation history are covered by far by the impacts arising from the variation of the irradiation history due to the variation of the fuel sample's burnup. This can be concluded from a simple example: Experience shows that the square root of the sample variance s_{JL}^2 of burnup values $B_{\nu JL}$ estimated by some laboratory L from the results $E_{\nu JL}$ for some burnup indicators $\nu = 1,\ldots,\beta(L)$, usually amounts to about $1\,\text{MWd/kg}$. Assuming a normal pdf model $N(\hat{B}_{JL}, s_{JL}^2)$ using the sample mean eq. (55) as the expectation and the sample variance s_{JL}^2 as the variance, the interval $[\hat{B}_{JL} - 3s_{JL}, \hat{B}_{JL} + 3s_{JL}]$ contains 99.7% of the cumulative distribution of $N(\hat{B}_{JL}, s_{JL}^2)$:

$$\int_{\hat{B}_{JL}-3s_{JL}}^{\hat{B}_{JL}+3s_{JL}} dB\, N(\hat{B}_{JL}, s_{JL}^2) = 0.997.$$

Let us assume a constant specific power P_S of 30 kW / kg for all the irradiation periods and a total time of 1500 effective full power days (resulting from 3 irradiation cycles with 500 effective full power days each). So, the burnup of the fuel at the end of its operation time amounts to 45 MWd / kg U. A variation of the burnup by $\pm 3 s_{JL} = \pm 3\,\mathrm{MWd/kg\,U}$, i.e. on the interval $[42\,\mathrm{MWd/kg}\ ,\ 48\,\mathrm{MWd/kg}]$ results in a variation of the specific power by

$$\pm \Delta P_S = \frac{\pm 3\ \mathrm{MWd/kg}}{1500\,\mathrm{d}} = \pm 2 \frac{\mathrm{kW}}{\mathrm{kg}}.$$

Due to the normal pdf model $N(\hat{B}_{JL}, s^2_{JL})$ used for the burnup, the specific power is thus assumed to be normal distributed with $P_S = 30\,\mathrm{kW/kg}$ as expectation value and $\sigma^2 = (\Delta P_S / 3)^2 = (0.667)^2\,(\mathrm{kW/kg})^2 = 0.444\,(\mathrm{kW/kg})^2$ as variance. The standard deviation $\sigma = 0.667\,\mathrm{kW/kg}$ covers the uncertainty of the values $P_S(t)$ of the specific power history recorded together with the values of the other irradiation history parameters (such as fuel and moderator temperature etc).

Now, having described the procedures for evaluating the measured isotopic concentrations and the burnup values of the fuel samples as well as the procedures for determining the calculated isotopic concentrations as functions of burnup, we are prepared to the estimate the Isotopic Correction Factors (ICFs) as set forth in the next section

4.1.4 Monte Carlo sampling on isotopic correction factors (ICFs)

The upper part of Figure 7 summarizes what has been hitherto described:

- $\mathbf{E}_{JL}$ represents the set of measured isotopic concentrations observed for the J-th fuel sample in the L(J)-th laboratory (cf. eq. (41)), and $\mathbf{S}_{JL}$ is the empirical covariance matrix of the components E_{IJL} of $\mathbf{E}_{JL}$ (cf. eq. (46) or eq. (47)), $I = 1,\ldots, N_{isot}(L(J))$.
- Assuming a normal distribution model $N(\mathbf{E}_{JL}, \mathbf{S}_{JL})$ using $\mathbf{E}_{JL}$ as expectation and $\mathbf{S}_{JL}$ as covariance matrix, Monte Carlo (MC) samples $\mathbf{E}^{MC}_{JL}$ on the random vector $\mathbf{E}_J$ are drawn.
- The values of the components $\mathbf{E}^{MC}_{\nu JL}$ of $\mathbf{E}^{MC}_{JL}$ related to the burnup indicators $\nu = 1,\ldots,\beta(L)$ are inserted into the respective well-known functional relations of the burnup to the burnup indicator isotopic concentrations c_ν (case (a), cf. equations (48) and (50)). Thus, a MC sample B^{MC}_{JL} on the random variable B_J is obtained, either from eq. (51) in case of $\beta(L) = 1$, or from eq. (54) in case of $\beta(L) > 1$ using a Bayesian MC procedure for evaluating the $B^{MC}_{\nu JL}$ values obtained for the individual burnup indicators $\nu = 1,\ldots,\beta(L)$ according to eq. (50).
- If the burnup value of the fuel sample is not based on any measurement, but calculated only (case (b)), a MC sample B^{MC}_J on the random variable B_J is drawn by evaluating all the vali-

dation results compiled for the applied burnup calculation procedure (cf. eq. (59) or eq. (60) and Figure 6).

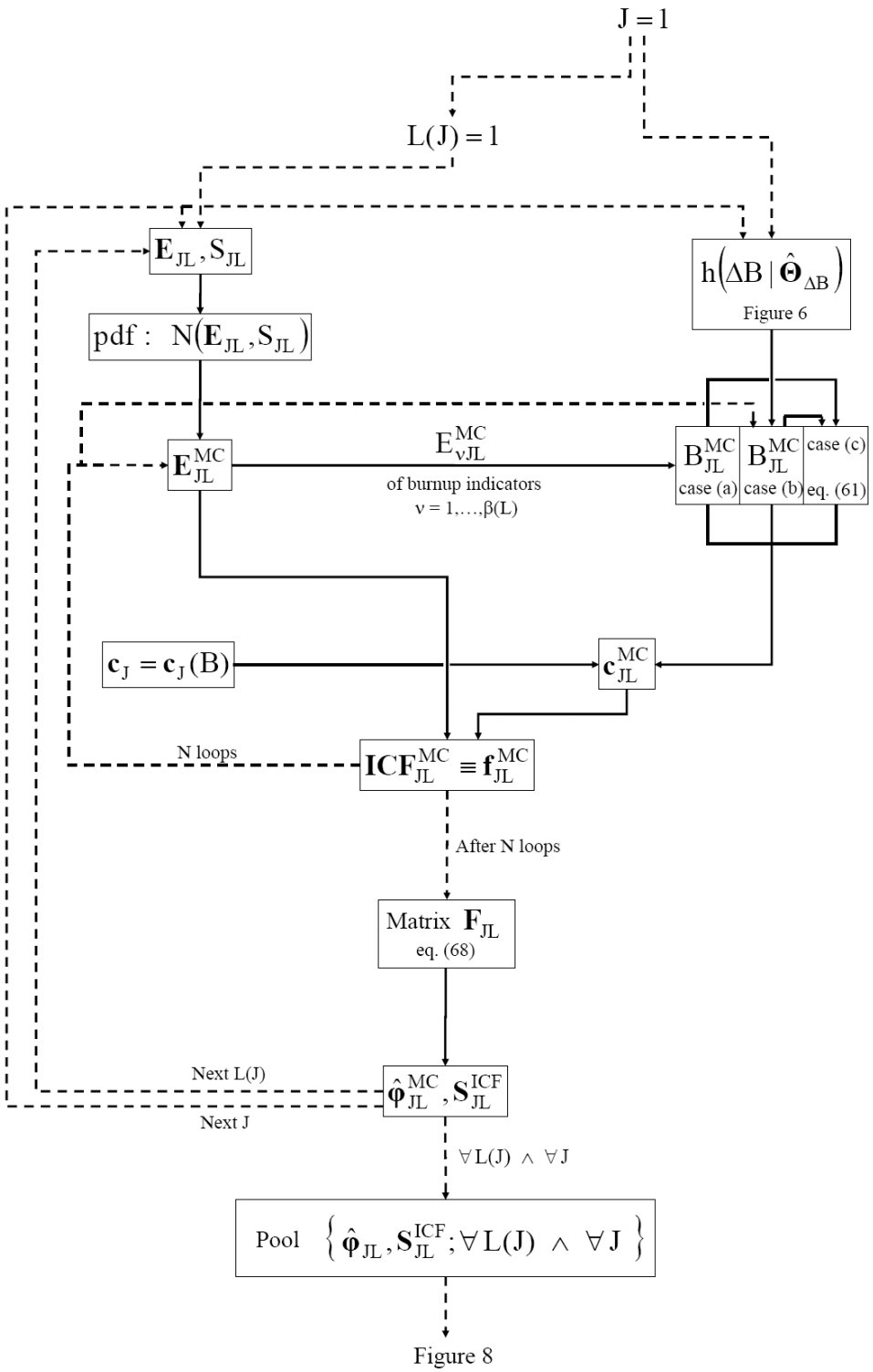

***Figure 7**: Flow chart of the procedure of generating an ICF working pool*

- If only part of the laboratories $L = 1,\ldots,N_{lab}(J)$ performed measurements on burnup indicator isotopic concentrations (case (c)), a MC sample B_J^{MC} is drawn according to the case (b) procedure for all those laboratories which did not accomplish a burnup indicator isotopic concentration measurement. For all the other laboratories laboratory specific MC samples B_{JL}^{MC} are drawn according to the case (a) procedure. Under certain conditions described in section 4.1.2.3 the MC sample B_J^{MC} drawn according to the case (b) procedure can be added to equations (52) and (53) of the case (a) procedure (cf. equations (61) and (62)).

In any case a burnup MC sample value is available. As indicated in Figure 7, this value is now inserted into the relations eq. (45), $\mathbf{c}_J = \mathbf{c}_J(B)$, of the isotopic concentrations $\mathbf{c}_J$, calculated for the J-th fuel sample, to the burnup. Thus a MC sample

$$\mathbf{c}_{JL}^{MC} = \left(c_{1JL},\ldots,c_{M_{isot}(J),J,L}\right)^T, \tag{66}$$

is obtained. With this MC sample and with the MC sample $\mathbf{E}_{JL}^{MC}$ derived by means of the empirical distribution $N(\mathbf{E}_{JL},\mathbf{S}_{JL})$ a MC sample of the ICFs is obtained for the fuel sample J analyzed in the laboratory L:

$$\mathbf{ICF}_{JL}^{MC} \equiv \mathbf{f}_{JL}^{MC} = \left(\frac{E_{1JL}^{MC}}{C_{1JL}^{MC}},\ldots,\frac{E_{I_{max}JL}^{MC}}{C_{I_{max}JL}^{MC}}\right)^T, \tag{67}$$

with $I_{max} \equiv N_{isot}(L(J))$.

As indicated in Figure 7, the whole procedure described, starting with the drawing of the MC sample $\mathbf{E}_{JL}^{MC}$, is now repeated a good lot of times to get a sufficiently large number of MC samples $\mathbf{ICF}_{JL}^{MC} \equiv \mathbf{f}_{JL}^{MC}$.

After N loops the result $\mathbf{f}_{JL}^{MC-n}$, $n = 1,\ldots,N$, form a matrix

$$\mathbf{F}_{JL}^{MC} = \begin{pmatrix} \left[\mathbf{f}_{JL}^{MC\_1}\right]^T \\ \vdots \\ \left[\mathbf{f}_{JL}^{MC\_N}\right]^T \end{pmatrix} \tag{68}$$

containing MC samples $\left\{f_{IJL}^{MC-n},\ n = 1,\ldots,N\right\}$ of size N for each of the isotopes $I = 1,\ldots,N_{isot}$. So, this matrix contains all that information about the ICFs and the uncertainty of the ICFs which results from the measurement outcomes obtained for the J-th fuel sample in the L(J)-th laboratory. As appears from Figure 1, both the information about the ICFs and the information about the uncertainty of the ICFs are contributions to the flow of information following the hierarchy of uncertainties. To make the information contained in the matrix eq. (68) available for the Bayesian MC hierarchical procedure to be used, as explained in section 3, for translating the uncertainties of the ICFs into uncertainties of the bias-corrected isotopic number densities of a burnup credit application case, the sample mean vector

$$\hat{\boldsymbol{\varphi}}_{JL} = \left(\hat{\varphi}_{1JL},\ldots,\hat{\varphi}_{IJL},\ldots\right)^{T} \tag{69}$$

with the components

$$\hat{\varphi}_{IJL} = \frac{1}{N}\sum_{n=1}^{N} \ln\left(\frac{f_{IJL}^{MC\_n}}{a_I}\right) = \frac{1}{N}\sum_{n=1}^{N} \ln\left(f_{IJL}^{MC\_n}\right) - \ln a_I\,, \quad I = 1,\ldots,N_{Isot}(L(J)) \tag{70}$$

and the related sample covariance matrix

$$\mathbf{S}_{JL}^{ICF} = \frac{1}{N-1}\sum_{n=1}^{N}\left(\boldsymbol{\varphi}_{JL}^{MC\_n} - \hat{\boldsymbol{\varphi}}_{JL}\right)\left(\boldsymbol{\varphi}_{JL}^{MC\_n} - \hat{\boldsymbol{\varphi}}_{JL}\right)^{T}, \tag{72}$$

with

$$\boldsymbol{\varphi}_{JL}^{MC\_n} = \begin{pmatrix} \ln\left(\dfrac{f_{1JL}^{MC\_n}}{a_1}\right) \\ \vdots \\ \ln\left(\dfrac{f_{IJL}^{MC\_n}}{a_I}\right) \\ \vdots \end{pmatrix} = \begin{pmatrix} \ln\left(f_{1JL}^{MC\_n}\right) - \ln\left(a_1\right) \\ \vdots \\ \ln\left(f_{IJL}^{MC\_n}\right) - \ln\left(a_I\right) \\ \vdots \end{pmatrix} \tag{73}$$

are derived from the MC sample values contained in the matrix eq. (68).

Because of

$$\Delta\varphi_{IJL}^{MC\_n} \equiv \varphi_{IJL}^{MC\_n} - \hat{\varphi}_{IJL} = \ln\left(f_{IJL}^{MC\_n}\right) - \frac{1}{N}\sum_{n=1}^{N}\ln\left(f_{IJL}^{MC\_n}\right),\ I = 1,\ldots,N_{Isot}(L(J))\,, \tag{74}$$

the elements of the sample covariance matrix eq. (72) do not depend on the quantities a_I introduced by equations (70) and (73); and the sample covariance matrix can be therefore written as

$$\mathbf{S}_{JL}^{ICF} = \frac{1}{N-1}\sum_{n=1}^{N}\boldsymbol{\Delta\varphi}_{JL}^{MC\_n}\left(\boldsymbol{\Delta\varphi}_{JL}^{MC\_n}\right)^{T} \tag{75}$$

with vector $\boldsymbol{\Delta\varphi}_{JL}^{MC\_n}$ the elements of which are given by eq. (74).

The quantities (fixed numbers) a_I, $I = 1,\ldots,N_{Isot}$, are introduced to represent the experience already available for the applied depletion calculation procedure with respect to the ICFs. Experience shows that for a good lot of isotopes observed ICF values are distributed around 1, so that $a_I = 1$ is an adequate choice to represent the experience already available for these isotopes. Only for a few isotopes ICFs have been observed for some depletion procedures which significantly differ from 1 (Gd-155 is a prominent example for that). In such cases it is recommendable to choose a_I according to the available experience.

As explained in section 3, a probability distribution model $p\left(\mathbf{f}_{JL} \mid \boldsymbol{\Theta}\right)$ is needed for evaluating the empirical data eq. (68) according to Bayes' theorem eq. (29). The ratios

$$R_{IJL} = \frac{f_{IJL}}{a_I}, \quad I = 1,\ldots,N_{Isot}(L(J)) \tag{76}$$

represent the values of the observed variables f_{IJL} as random proportions of numbers resulting from previous observations. It is therefore appropriate to choose a multivariate log-Normal distribution for the distribution model $p(\mathbf{R}_{JL} \mid \boldsymbol{\Theta})$ of the random vector

$$\mathbf{R}_{JL} = \left(\frac{f_{1JL}}{a_1},\ldots,\frac{f_{IJL}}{a_I},\ldots \right)^T, \tag{77}$$

cf. References [12] and [13]. For this reason the logarithmical values $\ln\left(f_{IJL}^{MC-n}\right)$ of the data contained in the matrix eq. (68) are used in equations (69) through (75).

The definition region of the log-Normal distributed variables R_{IJL} is $R_{IJL} \in (0,\infty)$, $I = 1,\ldots,N_{Isot}(L(J))$. In fact, it is evident that an ICF number must be greater than zero, but a minimum possible value cannot be specified; and, likewise, it is obvious that an ICF cannot become infinite, but a maximum possible value cannot be specified. So, the choice of a log-Normal distribution model $p(\mathbf{R}_{JL} \mid \boldsymbol{\Theta})$ is also appropriate with respect to the definition region of the random vector $\mathbf{f}_{JL}$ determining the definition region of the random vector $\mathbf{R}_{JL}$, eq. (77).

Now, as indicated in Figure 7, all the procedures hitherto described are repeated till the measurement results from all the laboratories $L(J) = 1,\ldots,N_{lab}(J)$ for each of the fuel samples $J = 1,\ldots,N_{FS}$ are evaluated. Thus one gets a set of sample mean vectors eq. (69) and related covariance matrices eq. (75):

$$\left\{ \hat{\boldsymbol{\varphi}}_{JL}\ ,\ \mathbf{S}_{JL}^{ICF}\ ;\ L(J) = 1,\ldots,N_{lab}(J),\ J = 1,\ldots,N_{FS} \right\} \tag{78}$$

This set serves as a pool for generating ICFs for burnup credit (BUC) application cases.

4.2 Evaluation of the isotopic correction factors for burnup credit applications

It is well-known that the sets of isotopes considered in radiochemical analyses differ from the set of isotopes which can principally be used in BUC applications [14]. The sets of isotopes studied in radiochemical analyses usually include a good lot of isotopes which cannot be used in BUC applications, but which deliver necessary information about the fuel samples analyzed (as for instance obtained from burnup indicators as Cs-137, Ce-144) or information needed for different applications (e.g., source term validation for shielding calculations). So, the set of BUC isotopes considered in a radiochemical analysis is usually only a subset of the total set of isotopes studied in this analysis. It is observed that this subset often differs from analysis to analysis and sometimes also from laboratory to laboratory; and it is therefore found that many sets of analyzed isotopes do not contain all the isotopes which can principally be used in BUC criticality safety analysis.

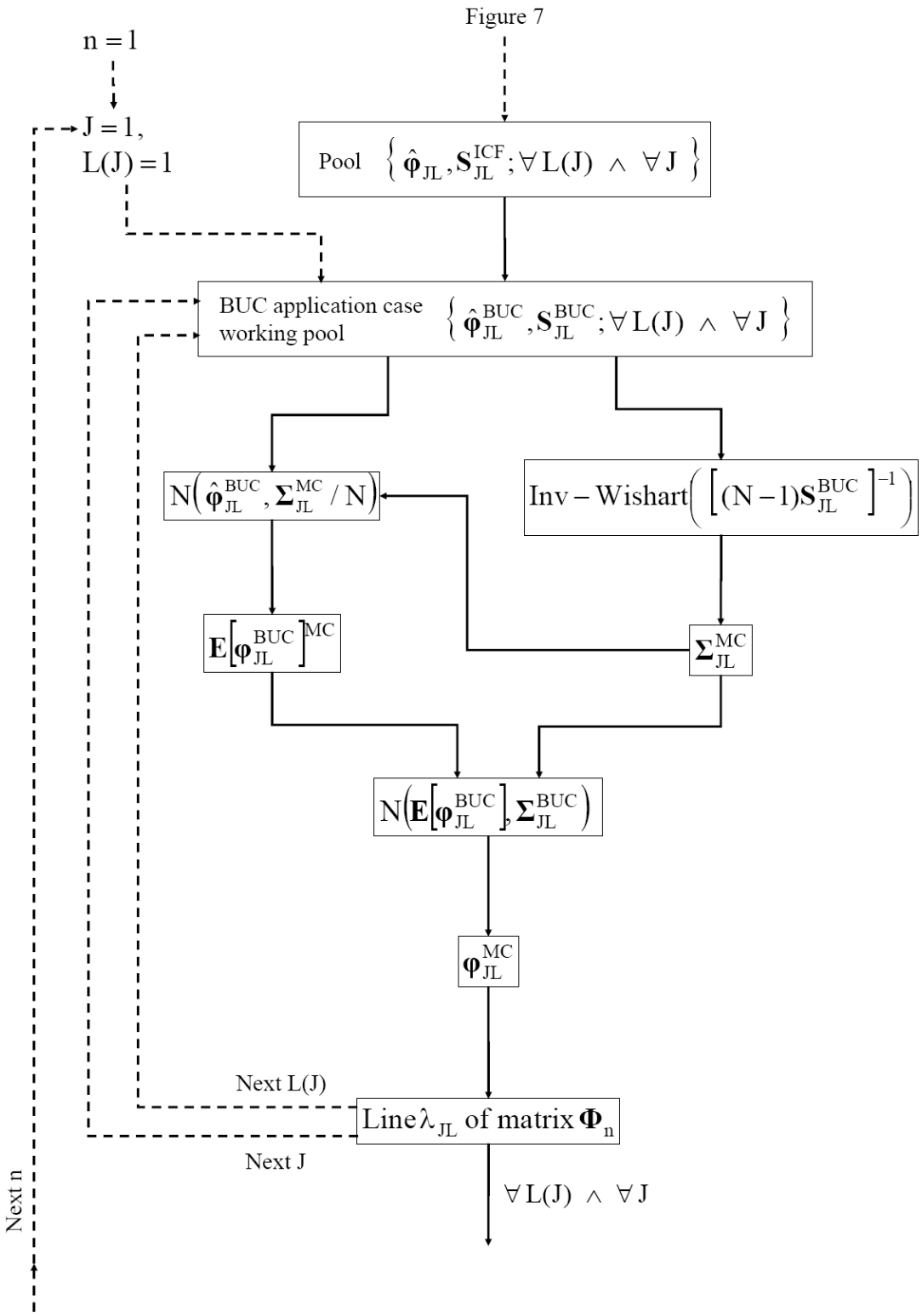

Figure 8: *Flow chart of the procedure for evaluating the ICFs for BUC applications*
(Figure continued on next page)

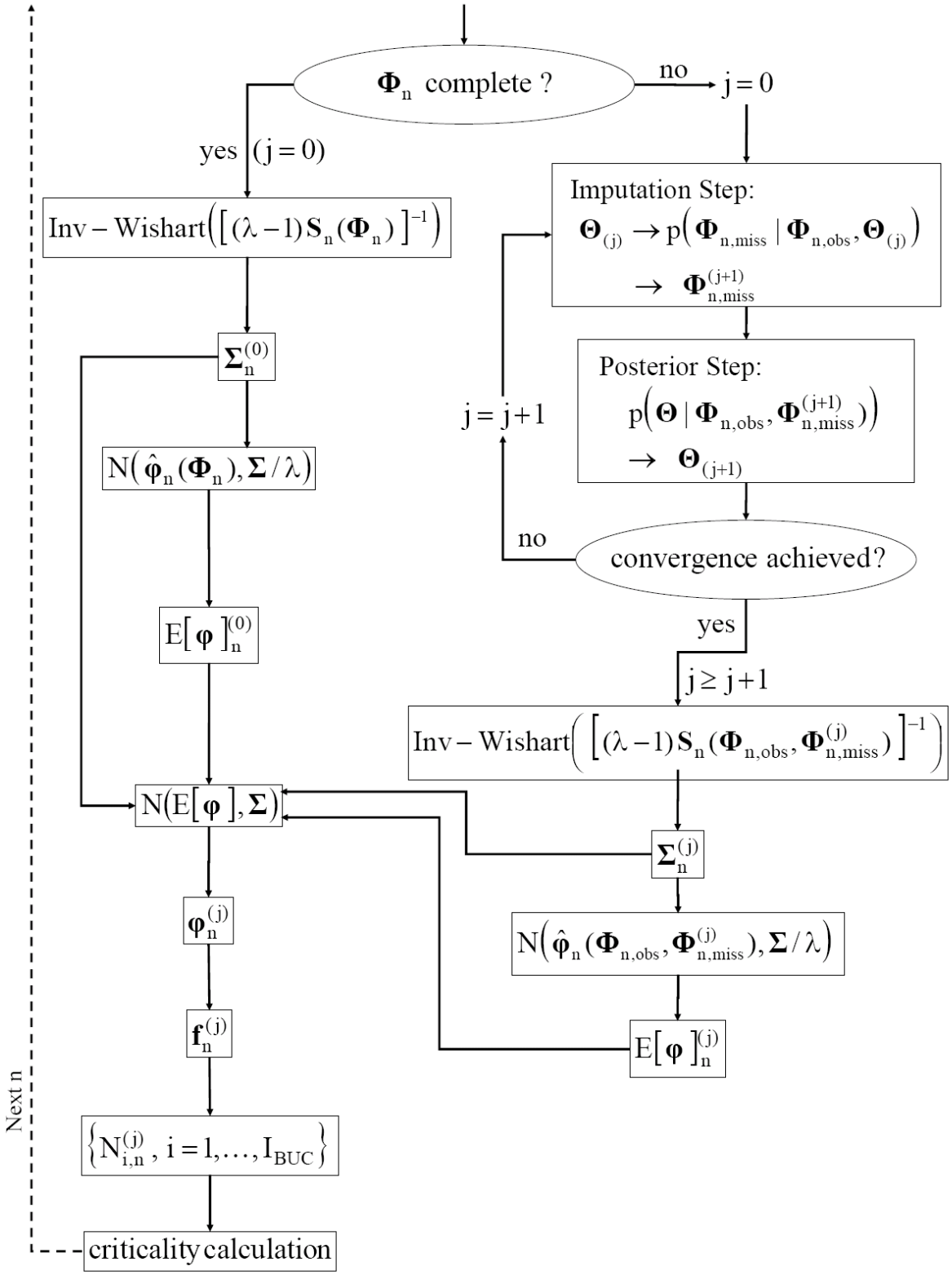

Figure 8 (continuation)

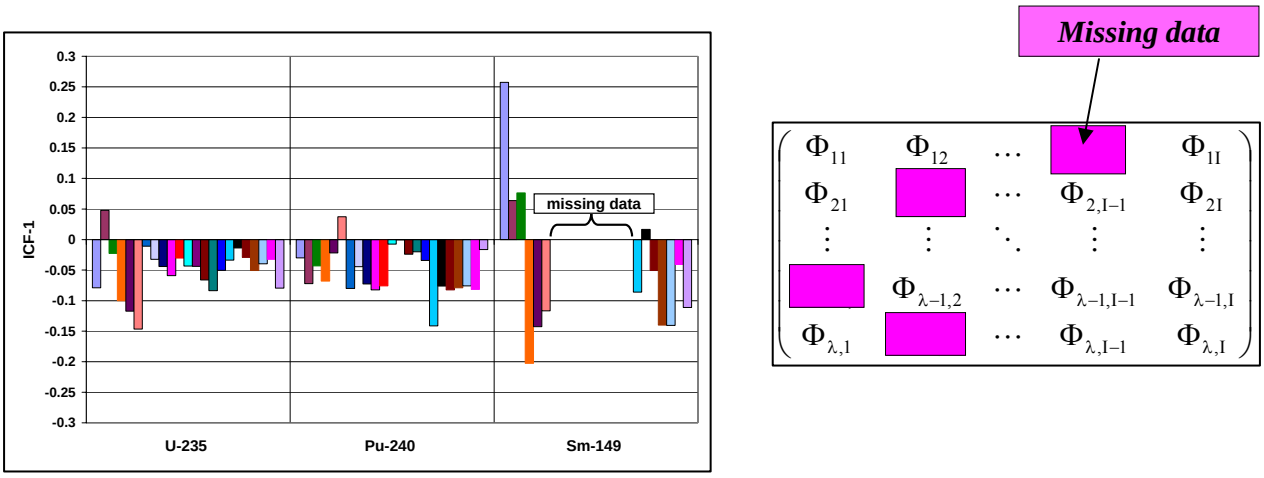

Figure 9: *Example for missing data [15]*

Which isotopes are really used in an actual BUC application case depends on the BUC level applied to this case (e.g., "actinide-only" level or "actinide plus fission product" level with different numbers of BUC fission products, cf. Ref. [14]). So, for an actual BUC application case first, as indicated in Figure 8, a "BUC-application-case-specific working pool"

$$\left\{\hat{\boldsymbol{\varphi}}_{JL}^{BUC}\,,\,\mathbf{S}_{JL}^{BUC}\,;\,L(J)=1,\ldots,N_{lab}(J),\,J=1,\ldots,N_{FS}\right\} \tag{79}$$

has to be extracted from the pool eq. (78), i.e. a working pool which includes all the information contained in eq. (78) about the ICFs of the isotopes used in the actual BUC application case.

Then, a BUC ICF data matrix $\boldsymbol{\Phi}$ has to be derived from the working pool eq. (79) in such a way that $\boldsymbol{\Phi}$ is capable to play a role of the matrix eq. (28) so that MC samples on the ICFs of the actually used BUC isotopes can be drawn according to eq. (32).

The number of columns of the matrix $\boldsymbol{\Phi}$ is given by the number of BUC isotopes actually used, and the number of rows of $\boldsymbol{\Phi}$ is given by the sum

$$\lambda=\sum_{J=1}^{N_{FS}}N_{lab}(J)\,. \tag{80}$$

Since it is observed, as stated above, that many sets of isotopes studied in radiochemical analyses do not contain all the isotopes principally applicable in BUC criticality safety analysis, it may happen that some of the actually used BUC isotopes do not appear in some of the data $\hat{\boldsymbol{\varphi}}_{JL}^{BUC}$ and $\mathbf{S}_{JL}^{BUC}$ of the working pool eq. (79). It may therefore happen that some elements of the matrix $\boldsymbol{\Phi}$ are missing, i.e. remain unknown, as exemplified in Figure 9. So therefore, the procedure of drawing MC samples on the ICFs of the actually used BUC isotopes according to eq. (32) must include a solution of the case that the matrix $\boldsymbol{\Phi}$ is incomplete. cf. References [13] and [15]. Then and only then, when a solution of this case is included, it is possible to use all the information

contained in the working pool eq. (79) about the ICFs of the isotopes used, even if some of these isotopes do not appear in some of the data sets $\hat{\boldsymbol{\varphi}}_{JL}^{BUC}$ and $\mathbf{S}_{JL}^{BUC}$, [16], [17].

4.2.1 Generation of working pools for BUC applications

The extraction of a BUC-application-case-specific working pool eq. (79) from the pool eq. (78) is carried out by projecting each random vector $\boldsymbol{\varphi}_{JL}$ related to $\hat{\boldsymbol{\varphi}}_{JL}$ and $\mathbf{S}_{JL}^{ICF}$ into the lower space spanned by the random vector $\boldsymbol{\varphi}_{JL}^{BUC}$.

The random vectors $\boldsymbol{\varphi}_{JL}$ are defined by

$$\boldsymbol{\varphi}_{JL} \equiv \ln \mathbf{R}_{JL} = \left(\ln \frac{f_{1JL}}{a_1}, \ldots, \ln \frac{f_{IJL}}{a_I}, \ldots \right)^T, \; L = L(J) = 1, \ldots, N_{lab}(J), \; J = 1, \ldots, N_{FS}, \tag{81}$$

cf. equations (69), (70), (76) and (77). Since $\mathbf{R}_{JL}$ obeys, by definition (cf. Section 4.1.4), a multivariate log-Normal distribution model, $\boldsymbol{\varphi}_{JL}$ follows a multivariate normal distribution [12]. $\hat{\boldsymbol{\varphi}}_{JL}^{BUC}$ in eq. (79) is thus obtained by deleting all the elements of $\hat{\boldsymbol{\varphi}}_{JL}$, eq. (69), which do not belong to the BUC isotopes to be used; and the covariance matrix $\mathbf{S}_{JL}^{BUC}$ is obtained by retaining only those rows and columns of $\mathbf{S}_{JL}^{ICF}$ which belong to these BUC isotopes [1]. So, according to equations (69) through (73) one gets for $\hat{\boldsymbol{\varphi}}_{JL}^{BUC}$ and $\mathbf{S}_{JL}^{BUC}$:

$$\hat{\boldsymbol{\varphi}}_{JL}^{BUC} = \frac{1}{N} \sum_{n=1}^{N} \left(\boldsymbol{\varphi}_{JL}^{BUC} \right)^{MC\_n}, \tag{82}$$

with

$$\left(\boldsymbol{\varphi}_{JL}^{BUC} \right)^{MC\_n} = \begin{pmatrix} \varphi_{1JL}^{MC\_n} \\ \vdots \\ \varphi_{N_{BUC}JL}^{MC\_n} \end{pmatrix} = \begin{pmatrix} \ln \left(\dfrac{f_{1JL}^{MC\_n}}{a_1} \right) \\ \vdots \\ \ln \left(\dfrac{f_{N_{BUC}JL}^{MC\_n}}{a_{N_{BUC}}} \right) \end{pmatrix} \tag{83}$$

where $N_{BUC} = N_{BUC}(L(J))$ is the number of BUC isotopes contained in the set of isotopes studied by the $L(J)$-th laboratory in the analysis of the J-th fuel sample;

$$\mathbf{S}_{JL}^{BUC} = \frac{1}{N-1} \sum_{n=1}^{N} \left(\left(\boldsymbol{\varphi}_{JL}^{BUC} \right)^{MC\_n} - \hat{\boldsymbol{\varphi}}_{JL}^{BUC} \right) \left(\left(\boldsymbol{\varphi}_{JL}^{BUC} \right)^{MC\_n} - \hat{\boldsymbol{\varphi}}_{JL}^{BUC} \right)^T. \tag{84}$$

It should be kept in mind that the working pool eq. (79) thus obtained depends on the isotopes really used in the BUC application case of interest. Accordingly, different BUC application cases usually result in different working pools eq. (79), whereas the pool eq. (78) does not depend on

any application case, but is the basis for all BUC-application-specific working pools eq. (79) that may be of interest.

4.2.2 Evaluation of a working pool of a BUC application

As stated in the preceding section, the random vector $\boldsymbol{\varphi}_{\mathrm{JL}}$, eq. (81), follows a multivariate Normal distribution. Any projection into a lower space gives a marginal distribution which is again Normal [1]. So therefore, the random vector $\boldsymbol{\varphi}_{\mathrm{JL}}^{\mathrm{BUC}}$ follows, by construction, a Normal distribution with unknown expectation $\mathbf{E}[\boldsymbol{\varphi}_{\mathrm{JL}}^{\mathrm{BUC}}]$ and unknown covariance matrix $\boldsymbol{\Sigma}_{\mathrm{JL}}^{\mathrm{BUC}}$,

$$\begin{aligned} p\left(\boldsymbol{\varphi}_{\mathrm{JL}}^{\mathrm{BUC}} \middle| \mathbf{E}[\boldsymbol{\varphi}_{\mathrm{JL}}^{\mathrm{BUC}}], \boldsymbol{\Sigma}_{\mathrm{JL}}^{\mathrm{BUC}}\right) &= N\left(\mathbf{E}[\boldsymbol{\varphi}_{\mathrm{JL}}^{\mathrm{BUC}}], \boldsymbol{\Sigma}_{\mathrm{JL}}^{\mathrm{BUC}}\right) \\ &\propto \left|\boldsymbol{\Sigma}_{\mathrm{JL}}^{\mathrm{BUC}}\right|^{-1/2} \cdot \exp\left\{-\frac{1}{2}\left(\boldsymbol{\varphi}_{\mathrm{JL}}^{\mathrm{BUC}} - \mathbf{E}[\boldsymbol{\varphi}_{\mathrm{JL}}^{\mathrm{BUC}}]\right)^{\mathrm{T}}\left(\boldsymbol{\Sigma}_{\mathrm{JL}}^{\mathrm{BUC}}\right)^{-1}\left(\boldsymbol{\varphi}_{\mathrm{JL}}^{\mathrm{BUC}} - \mathbf{E}[\boldsymbol{\varphi}_{\mathrm{JL}}^{\mathrm{BUC}}]\right)\right\} \end{aligned} \tag{85}$$

The N vectors $\left(\boldsymbol{\varphi}_{\mathrm{JL}}^{\mathrm{BUC}}\right)^{\mathrm{MC\_n}}$, $\mathrm{n} = 1,\ldots,\mathrm{N}$, eq. (83), each of which results, by construction, from an independent MC draw $\mathbf{f}_{\mathrm{JL}}^{\mathrm{MC\_n}}$, represent thus a set of independent observations from the Normal distribution of $\boldsymbol{\varphi}_{\mathrm{JL}}^{\mathrm{BUC}}$. Therefore, assuming that all prior knowledge has been used to fix the numbers $\mathbf{a}_{\mathrm{I}}$ in eq. (70) and hence eq. (83) so that no other prior knowledge is available, it follows, as appears from the Appendix to this paper, that

- the covariance matrix $\boldsymbol{\Sigma}_{\mathrm{JL}}^{\mathrm{BUC}}$ follows an Inverse-Wishart distribution

$$\begin{aligned} &p\left(\boldsymbol{\Sigma}_{\mathrm{JL}}^{\mathrm{BUC}} \middle| \left\{\left(\boldsymbol{\varphi}_{\mathrm{JL}}^{\mathrm{BUC}}\right)^{\mathrm{MC\_n}}, \mathrm{n} = 1,\ldots,\mathrm{N}\right\}\right) \\ &\qquad \propto \mathrm{Inv-Wishart}\left(\left[(\mathrm{N}-1)\,\mathbf{S}_{\mathrm{JL}}^{\mathrm{BUC}}\right]^{-1}; \mathrm{N}-1; \mathrm{N}_{\mathrm{BUC}}(\mathrm{L(J)})\right) \end{aligned} \tag{86}$$

  with (N-1) degrees of freedom and $\mathrm{N}_{\mathrm{BUC}} \times \mathrm{N}_{\mathrm{BUC}}$ scale matrix $(\mathrm{N}-1)\mathbf{S}_{\mathrm{JL}}^{\mathrm{BUC}}$, $\mathbf{S}_{\mathrm{JL}}^{\mathrm{BUC}}$ given by eq. (84), and that

- the expectation vector $\mathbf{E}[\boldsymbol{\varphi}_{\mathrm{JL}}^{\mathrm{BUC}}]$ follows a Normal distribution

$$p\left(\mathbf{E}[\boldsymbol{\varphi}_{\mathrm{JL}}^{\mathrm{BUC}}] \middle| \left\{\left(\boldsymbol{\varphi}_{\mathrm{JL}}^{\mathrm{BUC}}\right)^{\mathrm{MC\_n}}, \mathrm{n} = 1,\ldots,\mathrm{N}\right\}\right) \propto N\left(\hat{\boldsymbol{\varphi}}_{\mathrm{JL}}^{\mathrm{BUC}}, \frac{\boldsymbol{\Sigma}_{\mathrm{JL}}^{\mathrm{BUC}}}{\mathrm{N}}\right) \tag{87}$$

  with expectation vector $\hat{\boldsymbol{\varphi}}_{\mathrm{JL}}^{\mathrm{BUC}}$ given by eq. (83), and covariance matrix $\boldsymbol{\Sigma}_{\mathrm{JL}}^{\mathrm{BUC}}/\mathrm{N}$.

So therefore, the following steps can be taken successively

- Drawing of a MC sample $\boldsymbol{\Sigma}_{\mathrm{JL}}^{\mathrm{MC}}$ from the Inverse-Wishart pdf eq. (86)

- Insertion of $\mathbf{\Sigma}_{JL}^{MC}$ into the normal pdf eq. (87) and then drawing of a MC sample $\mathbf{E}[\boldsymbol{\varphi}_{JL}^{BUC}]^{MC}$ from the resulting pdf $N\left(\hat{\boldsymbol{\varphi}}_{JL}^{BUC};\mathbf{\Sigma}_{JL}^{MC}/N\right)$
- Insertion of $\mathbf{E}[\boldsymbol{\varphi}_{JL}^{BUC}]^{MC}$ and $\mathbf{\Sigma}_{JL}^{MC}$ into the Normal pdf eq. (85) and then drawing of a MC sample $\boldsymbol{\varphi}_{JL}^{MC}$ from the resulting pdf $N\left(\mathbf{E}[\boldsymbol{\varphi}_{JL}^{BUC}]^{MC};\mathbf{\Sigma}_{JL}^{MC}\right)$.

As indicated in Figure 8, the MC sample $\boldsymbol{\varphi}_{JL}^{MC}$ provides the line number

$$\lambda_{JL}=\sum_{j=1}^{J}\left\{\sum_{\ell=1}^{L(J)}\left[(j-1)+\ell\right]\right\} \tag{88}$$

of the BUC ICF data matrix $\mathbf{\Phi}_n$.

To get the next line of this matrix, one has to perform the MC sample procedure just described for the next $L(J)$ value. And, as indicated in Figure 8, on has to proceed in this way till one is through with all $L(J)=1,\ldots,N_{lab}(J)$ and $J=1,\ldots,N_{FS}$. The matrix $\mathbf{\Phi}_n$ thus obtained represents an ICF Monte Carlo sample from all the available data. As already stated, this matrix may be incomplete.

By construction, the line vectors

$$\boldsymbol{\varphi}_{n\ell}=\left(\varphi_{n\ell 1},\ldots,\varphi_{n\ell I_{BUC}}\right),\ \ell=1,\ldots,\lambda, \tag{89}$$

of the matrix $\mathbf{\Phi}_n$ are mutually independent. I_{BUC} in expression (89) denotes the number of BUC isotopes used in the BUC application case of interest; and λ is the total number of lines of $\mathbf{\Phi}_n$, cf. eq. (80).

In addition, even though some components $\varphi_{n\ell i}$ of some line vectors $\boldsymbol{\varphi}_{n\ell}$ may be missing, each line vector is, by construction, a sample $\boldsymbol{\varphi}_{n\ell}$ from a related Normal distribution

$$p\left(\boldsymbol{\varphi}_\ell\,\middle|\,\mathbf{E}[\boldsymbol{\varphi}_\ell],\mathbf{\Sigma}_\ell\right)=N\left(\mathbf{E}[\boldsymbol{\varphi}_\ell],\mathbf{\Sigma}_\ell\right)\propto\left|\mathbf{\Sigma}_\ell\right|^{-1/2}\cdot\exp\left\{-\frac{1}{2}\left(\boldsymbol{\varphi}_\ell-\mathbf{E}[\boldsymbol{\varphi}_\ell]\right)^T\,\mathbf{\Sigma}_\ell^{-1}\left(\boldsymbol{\varphi}_\ell-\mathbf{E}[\boldsymbol{\varphi}_\ell]\right)\right\}, \tag{90}$$
$$\ell=1,\ldots,\lambda,$$

with expectation $\mathbf{E}[\boldsymbol{\varphi}_\ell]$ and covariance matrix $\mathbf{\Sigma}_\ell$.

As explained in section 4.1.1, the results $\mathbf{E}_{JL}$, eq. (41), obtained by the different laboratories $L(J)=1,\ldots,N_{lab}(J)$ for one and the same fuel sample J are expected to be compatible, i.e., have one and the same expectation $\mathbf{E}[\mathbf{E}_{JL}]$, cf. Ref. [1]. Consequently, those line vectors $\boldsymbol{\varphi}_{n\ell}$, which are related to one and the same fuel sample J, shall have one and the same expectation, i.e., shall be compatible.

In addition, to the knowledge of the authors of this paper, it has never been observed up to now that ICFs show a significant dependence on the burnup of the fuel samples analyzed. This means that a compatibility test of the ICFs obtained for the different burnup values leads to the result that the hypotheses that these ICFs have one and the same expectation cannot be rejected on the basis of the available ICF data and the significance level α chosen for the test [1]. Since such a compatibility test is, by definition, a goodness-of-fit test (cf. Ref. [1], section 11.5.2), a significance level of $\alpha = 0.1\%$ is usually chosen. In other words, with a statistical certainty of $(1-\alpha) = 99.9\%$ it cannot be rejected that ICFs obtained for different burnups are compatible.[1] Consequently, it cannot be rejected on the basis of $\alpha = 0.1\%$ that all the line vectors $\boldsymbol{\varphi}_{n\ell}$, eq. (89), $\ell = 1,\ldots,\lambda$, are compatible.

As explained, compatibility of all the line vectors $\boldsymbol{\varphi}_{n\ell}$, $\ell = 1,\ldots,\lambda$, means that all these vectors have one and the same expectation $\mathbf{E}[\boldsymbol{\varphi}_{n\ell}] = \mathbf{E}[\boldsymbol{\varphi}_{\ell}] = \mathbf{E}[\boldsymbol{\varphi}]$ for all $\ell = 1,\ldots,\lambda$; but observation of compatibility of line vectors does not imply, in general, any statement about the covariances

$$\mathrm{cov}(\boldsymbol{\varphi}_{n\ell}) = \mathbf{E}\left[(\boldsymbol{\varphi}_{n\ell} - \mathbf{E}[\boldsymbol{\varphi}])(\boldsymbol{\varphi}_{n\ell} - \mathbf{E}[\boldsymbol{\varphi}])^{T}\right] = \boldsymbol{\Sigma}_{\ell},\ \ell = 1,\ldots,\lambda, \tag{91}$$

of the line vectors apart from the fact that $\mathbf{E}[\boldsymbol{\varphi}_{n\ell}]$ is replaced with $\mathbf{E}[\boldsymbol{\varphi}]$ in expression (91).

However, as told in section 4.1.1, compatibility of the results $\mathbf{E}_{JL}$, eq. (41), obtained by different laboratories $L(J) = 1,\ldots,N_{lab}(J)$ for one and the same fuel sample J, is missed very often. Usually no explanation of the observed incompatibilities can be given. Since results can safely be discarded only on physical arguments, the observed incompatibilities can only be understood as an indication of underestimation of the uncertainties of at least some of the individual sets of results $\mathbf{E}_{JL}$, eq. (41). For rectifying this underestimation one and the same probability distribution model is assumed, as already explained in section 4.1.1, for all the results $\mathbf{E}_{JL}$, $L(J) = 1,\ldots,N_{lab}(J)$, obtained for one and the same fuel sample J. Consequently, for all the line vectors $\boldsymbol{\varphi}_{n\ell}$ which result from one and the same fuel sample the same covariance matrix $\boldsymbol{\Sigma}_J$ is taken in eq. (90), i.e., $\boldsymbol{\Sigma}_{\ell} = \boldsymbol{\Sigma}_J$.

The question naturally arises as for what $\boldsymbol{\Sigma}_J$ stands. For all the line vectors $\boldsymbol{\varphi}_{n\ell}$ which result from a given fuel sample J the covariance matrix $\boldsymbol{\Sigma}_J$ is related to the precision that can be expected for each of these line vectors under the condition that it is considered that these line vectors must be compatible.

The degree of precision is expressed by the information content eq. (30), cf. Ref. [1]. If $\boldsymbol{\Sigma}_{\ell} = \boldsymbol{\Sigma}_J$ were known, eq. (30) would deliver for a line vector $\boldsymbol{\varphi}_{n\ell}$ due to eq. (90)

[1] In section 9 we will outline what can be done when it might have been observed one day that some ICFs show a significant dependence on the burnup.

$$\mathbf{I}_{\ell} = \mathrm{E}\left[\left(\frac{\partial \ln \mathrm{N}(\mathbf{E}[\boldsymbol{\varphi}_{\ell}], \boldsymbol{\Sigma}_{\ell})}{\partial \boldsymbol{\varphi}_{\mathrm{n}\ell}}\right)\left(\frac{\partial \ln \mathrm{N}(\mathbf{E}[\boldsymbol{\varphi}_{\ell}], \boldsymbol{\Sigma}_{\ell})}{\partial \boldsymbol{\varphi}_{\mathrm{n}\ell}}\right)^{\mathrm{T}}\right] = \boldsymbol{\Sigma}_{\ell}^{-1} . \tag{92}$$

Even though it might be that certain fuel samples require certain radiochemical analysis methods, precision is not determined by the analyzed fuel samples $\mathrm{J} = 1,\ldots,\mathrm{N}_{\mathrm{FS}}$ but by the analysis methods used by the laboratories. Therefore, even if we are dealing with a set of fuel samples each of which was only analyzed once, i.e., even if we are dealing with the case $\mathrm{N}_{\mathrm{lab}}(\mathrm{J}) = 1$ for all $\mathrm{J} = 1,\ldots,\mathrm{N}_{\mathrm{FS}}$, it is necessary to use one and the same covariance matrix $\boldsymbol{\Sigma}$ for all the analyzed fuel samples, i.e., $\boldsymbol{\Sigma}_{\mathrm{J}} = \boldsymbol{\Sigma}$, since experience shows that if each and every of these fuel samples were given to all the available laboratories incompatibility of the results would be observed for these samples, at least in many cases, even then if the laboratories apply the same or very similar analysis methods.

So, it turns out that the line vectors $\boldsymbol{\varphi}_{\mathrm{n}\ell}$, $\ell = 1,\ldots,\lambda$, eq. (89), of the matrix $\boldsymbol{\Phi}_{\mathrm{n}}$, which are, by construction, mutually independent, have to be taken as a random sample of size λ from a Normal distribution

$$\mathrm{p}\left(\boldsymbol{\varphi} \mid \mathbf{E}[\boldsymbol{\varphi}], \boldsymbol{\Sigma}\right) = \mathrm{N}\left(\mathbf{E}[\boldsymbol{\varphi}], \boldsymbol{\Sigma}\right) \propto \left|\boldsymbol{\Sigma}\right|^{-1/2} \cdot \exp\left\{-\frac{1}{2}\left(\boldsymbol{\varphi} - \mathbf{E}[\boldsymbol{\varphi}]\right)^{\mathrm{T}} \boldsymbol{\Sigma}^{-1}\left(\boldsymbol{\varphi} - \mathbf{E}[\boldsymbol{\varphi}]\right)\right\} \tag{93}$$

with unknown expectation $\mathbf{E}[\boldsymbol{\varphi}]$ and unknown covariance matrix $\boldsymbol{\Sigma}$.

Therefore, if all line vectors $\boldsymbol{\varphi}_{\mathrm{n}\ell}$ and hence the matrix $\boldsymbol{\Phi}_{\mathrm{n}}$ were complete, all the elements $\varphi_{\mathrm{n}\ell\mathrm{i}}$ ($\mathrm{i} = 1,\ldots,\mathrm{I}_{\mathrm{BUC}}$; $\ell = 1,\ldots,\lambda$) would be completely defined by the probability density function (pdf) $\mathrm{p}\left(\boldsymbol{\Phi}_{\mathrm{n}} \mid \boldsymbol{\Theta}\right) = \mathrm{p}\left(\boldsymbol{\Phi}_{\mathrm{n}} \mid \mathbf{E}[\boldsymbol{\varphi}], \boldsymbol{\Sigma}\right)$ which is named as "complete-data pdf" in the following.

However, as already stated, the matrix $\boldsymbol{\Phi}_{\mathrm{n}}$ may be incomplete, i.e., some elements $\varphi_{\mathrm{n}\ell\mathrm{i}}$ may be missing. This is the case, in particular, if the "actinide-plus-fission-product" BUC level is applied [14]. An incomplete matrix can be split into two parts, one part denoted by $\boldsymbol{\Phi}_{\mathrm{n,obs}}$ contains the observed (i.e., the non-missing) data, the other part denoted by $\boldsymbol{\Phi}_{\mathrm{n,miss}}$ characterizes the missing data. So, the complete-data pdf $\mathrm{p}\left(\boldsymbol{\Phi}_{\mathrm{n}} \mid \boldsymbol{\Theta}\right)$ is the joint pdf $\mathrm{p}\left(\boldsymbol{\Phi}_{\mathrm{n,obs}}, \boldsymbol{\Phi}_{\mathrm{n,miss}} \mid \boldsymbol{\Theta}\right)$ of $\boldsymbol{\Phi}_{\mathrm{n,obs}}$ and $\boldsymbol{\Phi}_{\mathrm{n,miss}}$, which can be rewritten as product of the conditional pdf $\mathrm{p}\left(\boldsymbol{\Phi}_{\mathrm{n,miss}} \mid \boldsymbol{\Phi}_{\mathrm{n,obs}}, \boldsymbol{\Theta}\right)$ and the marginal pdf $\mathrm{p}\left(\boldsymbol{\Phi}_{\mathrm{n,obs}} \mid \boldsymbol{\Theta}\right)$, cf. Ref. [1],

$$\mathrm{p}\left(\boldsymbol{\Phi}_{\mathrm{n}} \mid \boldsymbol{\Theta}\right) = \mathrm{p}\left(\boldsymbol{\Phi}_{\mathrm{n,obs}}, \boldsymbol{\Phi}_{\mathrm{n,miss}} \mid \boldsymbol{\Theta}\right) = \mathrm{p}\left(\boldsymbol{\Phi}_{\mathrm{n,miss}} \mid \boldsymbol{\Phi}_{\mathrm{n,obs}}, \boldsymbol{\Theta}\right) \mathrm{p}\left(\boldsymbol{\Phi}_{\mathrm{n,obs}} \mid \boldsymbol{\Theta}\right). \tag{94}$$

The marginal pdf is the projection

$$\mathrm{p}\left(\boldsymbol{\Phi}_{\mathrm{n,obs}} \mid \boldsymbol{\Theta}\right) = \int \mathrm{p}\left(\boldsymbol{\Phi}_{\mathrm{n}} \mid \boldsymbol{\Theta}\right) \mathrm{d}\boldsymbol{\Phi}_{\mathrm{n,miss}} . \tag{95}$$

of the complete-data pdf; and the conditional pdf $\mathrm{p}\left(\boldsymbol{\Phi}_{\mathrm{n,miss}} \mid \boldsymbol{\Phi}_{\mathrm{n,obs}}, \boldsymbol{\Theta}\right)$ is the section

$$p\left(\boldsymbol{\Phi}_{n,miss} \mid \boldsymbol{\Phi}_{n,obs}, \boldsymbol{\Theta}\right) = \frac{p\left(\boldsymbol{\Phi}_{n,obs}, \boldsymbol{\Phi}_{n,miss} \mid \boldsymbol{\Theta}\right)}{\int p\left(\boldsymbol{\Phi}_{n,obs}, \boldsymbol{\Phi}_{n,miss} \mid \boldsymbol{\Theta}\right) d\boldsymbol{\Phi}_{n,miss}} \tag{96}$$

through the complete-data pdf at given data $\boldsymbol{\Phi}_{n,obs}$. Using eq. (95) in eq. (96) one gets eq. (94).

The conditional pdf $p\left(\boldsymbol{\Phi}_{n,miss} \mid \boldsymbol{\Phi}_{n,obs}, \boldsymbol{\Theta}\right)$ is, by definition, a predictive distribution of the missing data $\boldsymbol{\Phi}_{n,miss}$ under the condition of the observed data $\boldsymbol{\Phi}_{n,obs}$ and given model parameters $\boldsymbol{\Theta} = \left(\mathbf{E}[\boldsymbol{\varphi}], \boldsymbol{\Sigma}\right)$. The problem is that the parameters $\boldsymbol{\Theta}$ are unknown. However, given a guess $\boldsymbol{\Theta}_{(0)}$ on $\boldsymbol{\Theta}$, one can obtain by means of Monte Carlo techniques a first guess $\boldsymbol{\Phi}^{(1)}_{n,mis}$ on the missing data $\boldsymbol{\Phi}_{n,miss}$. With this guess one has a guess $p\left(\boldsymbol{\Phi}_{n,obs}, \boldsymbol{\Phi}^{(1)}_{n,miss} \mid \boldsymbol{\Theta}\right)$ on the complete-data pdf. Using this guess as likelihood in Bayes' theorem eq. (29), a guess $p\left(\boldsymbol{\Theta} \mid \boldsymbol{\Phi}_{n,obs}, \boldsymbol{\Phi}^{(1)}_{n,miss}\right)$ on the "complete-data posterior pdf" $p\left(\boldsymbol{\Theta} \mid \boldsymbol{\Phi}_{n}\right)$ can be obtained. From this guess of $p\left(\boldsymbol{\Theta} \mid \boldsymbol{\Phi}_{n}\right)$ a new guess $\boldsymbol{\Theta}_{(1)}$ on $\boldsymbol{\Theta}$ can be drawn by means of MC techniques, and the whole procedure just described is repeated with $\boldsymbol{\Theta}_{(1)}$ as new starting parameter so that one gets first a new guess $\boldsymbol{\Phi}^{(2)}_{n,mis}$ on the missing data, and then a new guess $\boldsymbol{\Theta}_{(2)}$ on the parameter set $\boldsymbol{\Theta}$. The procedure is then repeated again and again, till convergence is achieved, cf. References [16] through [18]. The whole procedure is known as "data augmentation procedure". The first step, consisting in application of a guess $\boldsymbol{\Theta}_{(j)}$ for achieving a new guess $\boldsymbol{\Phi}^{(j+1)}_{n,mis}$ is named as "imputation step", the second step consisting in applying $\boldsymbol{\Phi}^{(j+1)}_{n,mis}$ for obtaining a complete-data posterior pdf and then a new guess $\boldsymbol{\Theta}_{(j+1)}$ is called "posterior step" [16]:

- Imputation step:

$$\boldsymbol{\Theta}_{(j)} \rightarrow p(\boldsymbol{\Phi}_{n,miss} \mid \boldsymbol{\Phi}_{n,obs}, \boldsymbol{\Theta}_{(j)}) \rightarrow \boldsymbol{\Phi}^{(j+1)}_{n,miss} \rightarrow \text{complete data pdf } p(\boldsymbol{\Phi}^{(j+1)}_{n,miss}, \boldsymbol{\Phi}_{n,obs} \mid \boldsymbol{\Theta}) \tag{97}$$

- Posterior step:

$$p(\boldsymbol{\Phi}^{(j+1)}_{n,miss}, \boldsymbol{\Phi}_{n,obs} \mid \boldsymbol{\Theta}) \xrightarrow{\text{Bayes' theorem}} \text{complete data posterior pdf } p(\boldsymbol{\Theta} \mid \boldsymbol{\Phi}_{n,obs}, \boldsymbol{\Phi}^{(j+1)}_{n,miss}) \rightarrow \boldsymbol{\Theta}_{(j+1)} \tag{98}$$

The starting parameter set $\boldsymbol{\Theta}_{(0)}$ can be generated by using the so-called "Expectation-Maximization (EM) algorithm" [16], [18]. The data augmentation procedure is performed by means of Markov chain MC techniques [18]. When convergence is achieved after j_C iteration steps then all the MC draws $\boldsymbol{\Theta}_{(j)}$ with $j > j_C$ can be used to draw respective MC samples $\boldsymbol{\varphi}_{MC}$ on $\boldsymbol{\varphi}$ from the pdf eq. (93) according to eq. (32).

Since the line vectors $\boldsymbol{\varphi}_{n\ell}$ of the matrix $\boldsymbol{\Phi}_n$ are independent samples from the Normal distribution eq. (93), it follows, as appears from the Appendix to this paper, that the complete data posterior pdf $p\left(\boldsymbol{\Theta} \mid \boldsymbol{\Phi}_{n}\right) = p\left(\mathbf{E}[\boldsymbol{\varphi}], \boldsymbol{\Sigma} \mid \boldsymbol{\Phi}_{n}\right)$ is given, assuming that no prior knowledge about $\boldsymbol{\Theta} = \left(\mathbf{E}[\boldsymbol{\varphi}], \boldsymbol{\Sigma}\right)$ is available, by the product

$$p(\boldsymbol{\Theta} \mid \boldsymbol{\Phi}_n) = p(\boldsymbol{\Sigma} \mid \boldsymbol{\Phi}_n) \cdot p(\mathbf{E}[\boldsymbol{\varphi}] \mid \boldsymbol{\Sigma}, \boldsymbol{\Phi}_n), \tag{99}$$

where

- $p(\boldsymbol{\Sigma} \mid \boldsymbol{\Phi}_n)$, denoting the pdf of the covariance matrix $\boldsymbol{\Sigma}$ under the complete data matrix $\boldsymbol{\Phi}_n$, is given by the Inverse-Wishart distribution

  $$p(\boldsymbol{\Sigma} \mid \boldsymbol{\Phi}_n) \propto \text{Inv} - \text{Wishart}\left((\lambda - 1)^{-1} \mathbf{S}_n^{-1}; \lambda - 1; I_{BUC}\right), \tag{100}$$

  with $(\lambda - 1)$ degrees of freedom and $I_{BUC} \times I_{BUC}$ scale matrix $(\lambda - 1)\,\mathbf{S}_n$ following from the sample covariance matrix

  $$\mathbf{S}_n = \frac{1}{\lambda - 1} \sum_{\ell=1}^{\lambda} (\boldsymbol{\varphi}_{n\ell} - \hat{\boldsymbol{\varphi}}_n)(\boldsymbol{\varphi}_{n\ell} - \hat{\boldsymbol{\varphi}}_n)^T, \tag{101}$$

  with the sample average

  $$\hat{\boldsymbol{\varphi}}_n = \frac{1}{\lambda} \sum_{\ell=1}^{\lambda} \boldsymbol{\varphi}_{n\ell}, \tag{102}$$

  having the components

  $$\hat{\varphi}_{ni} = \frac{1}{\lambda} \sum_{\ell=1}^{\lambda} \varphi_{n\ell i}, \; i = 1, \ldots, I_{BUC}, \tag{103}$$

  and

- $p(\mathbf{E}[\boldsymbol{\varphi}] \mid \boldsymbol{\Sigma}, \boldsymbol{\Phi}_n)$, denoting the pdf of the expectation $\mathbf{E}[\boldsymbol{\varphi}]$ under the complete data matrix $\boldsymbol{\Phi}_n$ and the given covariance matrix $\boldsymbol{\Sigma}$, is given by the Normal distribution

  $$p(\mathbf{E}[\boldsymbol{\varphi}] \mid \boldsymbol{\Sigma}, \boldsymbol{\Phi}_n) \propto N(\hat{\boldsymbol{\varphi}}_n, \boldsymbol{\Sigma} / \lambda), \tag{104}$$

  with expectation $\hat{\boldsymbol{\varphi}}_n$ given by eq. (102) and covariance matrix $\boldsymbol{\Sigma} / \lambda$.

The posterior step eq. (98) of the data augmentation procedure becomes therefore:

- Given a guess $\boldsymbol{\Phi}_{n,mis}^{(j)}$ first a MC sample $\boldsymbol{\Sigma}_n^{(j)}$ is drawn from the Inverse-Wishart distribution eq. (100), using the scale matrix $(\lambda - 1)\,\mathbf{S}_n^{(j)}$ resulting from the sample covariance matrix $\mathbf{S}_n^{(j)} = \mathbf{S}_n\left(\boldsymbol{\Phi}_n^{(j)}\right)$ obtained with the augmented data matrix $\boldsymbol{\Phi}_n^{(j)} = \left(\boldsymbol{\Phi}_{n,obs}, \boldsymbol{\Phi}_{n,miss}^{(j)}\right)$ according to eq. (101).
- Then, using the MC sample $\boldsymbol{\Sigma}_n^{(j)}$ and the sample mean $\hat{\boldsymbol{\varphi}}_n^{(j)} = \hat{\boldsymbol{\varphi}}\left(\boldsymbol{\Phi}_n^{(j)}\right)$ obtained with the augmented data matrix $\boldsymbol{\Phi}_n^{(j)} = \left(\boldsymbol{\Phi}_{n,obs}, \boldsymbol{\Phi}_{n,miss}^{(j)}\right)$ according to eq. (102) a MC sample $\mathbf{E}[\boldsymbol{\varphi}]_n^{(j)}$ is drawn from the Normal distribution eq. (104).

The resulting parameter MC sample $\boldsymbol{\Theta}_{(j)} = \left(\mathbf{E}[\boldsymbol{\varphi}]_n^{(j)}, \boldsymbol{\Sigma}_n^{(j)}\right)$ can either be used to start the next imputation step eq. (97) or, if $j = j_C$ or greater, i.e., if convergence is achieved, to draw a MC

sample $\boldsymbol{\varphi}_n^{(j)}$ from the Normal distribution eq. (93). For numerical details and requirements of performing the data augmentation procedure see References [13] and [18].

When $j > j_C$ is reached and a MC sample $\boldsymbol{\varphi}_n^{(j)}$ is drawn, then a MC sample $\mathbf{f}_n^{(j)}$ of the ICFs is obtained by inverting the transformation introduced with eq. (70), i.e.

$$\mathbf{ICF}_n^{(j)} \equiv \mathbf{f}_n^{(j)} = \left(\left(f_n^{(j)}\right)_1, \ldots, \left(f_n^{(j)}\right)_{I_{BUC}} \right)^T \tag{105}$$

with

$$\left(f_n^{(j)}\right)_1 = a_i \exp\left\{ \left(\varphi_n^{(j)}\right)_i \right\}, \; i = 1, \ldots, N_{BUC}, \tag{106}$$

$\left(\varphi_n^{(j)}\right)_i$ the i-th component of $\boldsymbol{\varphi}_n^{(j)}$.

It is obvious that in case of a complete-data matrix $\boldsymbol{\Phi}_n$ a MC ICF sample set $\mathbf{f}_n^{(0)}$ ($j = 0$), eq. (105), is directly obtained by drawing $\boldsymbol{\Sigma}_n^{(0)}$ from the pdf eq. (100), then $\mathbf{E}[\boldsymbol{\varphi}]_n^{(0)}$ from the pdf eq. (104), then $\boldsymbol{\varphi}_n^{(0)}$ from the pdf eq. (93), and then using the re-transformation eq. (106).

The MC ICF sample set $\mathbf{f}_n^{(j)}$ ($j = 0$ or $j > j_C$, depending on the data matrix $\boldsymbol{\Phi}_n$) is applied, according to eq. (21), to the isotopic number densities calculated for the BUC application case of interest. As indicated in Figures 1 and 8, with the set of bias-corrected isotopic number densities $N_{i,n}^{(j)}$, $i = 1, \ldots, I_{BUC}$, thus obtained a criticality calculation according to section 7 is performed. The resulting neutron multiplication factor $\left(k_{eff}\right)_n$ is one term of the sum eq. (7),

$$\kappa_n = \left(k_{eff}\right)_n + \left(\Delta k_B\right)_n . \tag{107}$$

Now, to get a sufficiently large number n of samples $\left(k_{eff}\right)_n$ such that the uncertainty in the bias-corrected isotopic number densities, which results from the uncertainties in the depletion validation procedure, is sufficiently considered by the resulting distribution of the sample values $\left(k_{eff}\right)_n$ one returns, as indicated in Figure 8, to the first step of the evaluation of the BUC application case working pool eq. (79), i.e., one goes back to the drawing of MC samples from the distributions eq. (86), eq. (87) and then eq. (85) to get the next data matrix $\boldsymbol{\Phi}_n$.

5 Uncertainties in the depletion calculations performed for a burnup credit application case

As indicated in Figure 1, in addition to uncertainties due to manufacturing tolerances in the fuel and core design parameters, uncertainties in the nuclear data ξ result in uncertainties in the isotopic number densities $N_i^{(s)}$, $i = 1, \ldots, I_{BUC}$, calculated for BUC application to a spent fuel system S of interest. Therefore, the bias correction of the number densities $N_i^{(s)}$ according to eq. (21) have to consider not only the uncertainties in the ICFs according to section 4.2.2 but also, in principle, the uncertainties in the number densities $N_i^{(s)}$.

However, as stated in Ref. [19], section 5, the wide variety of fuel irradiation histories to be considered in a BUC application case makes it necessary to look for a bounding history given by those fuel operating conditions which result in the highest spent fuel reactivity in the spent fuel system S of interest. But, as stated in Ref. [20], it is observed that instead of searching for a bounding irradiation history very often a considerably conservative irradiation history is simply chosen (for the difference between the terms "bounding" and "conservative" see Ref. [4]). The choice of such conservative irradiation histories result in number densities $N_i^{(s)}$, $i = 1,\ldots,I_{BUC}$, the use of which in criticality calculations result in neutron multiplication factors which cover by far all reactivity impacts due to the manufacturing tolerances in the fuel and core design parameters and due to the uncertainties in the nuclear data $\boldsymbol{\xi}$.

In BUC application cases it makes sense in fact to define the operating conditions, i.e., the depletion parameters, in such a way that reactivity effects due to variations in fuel and core design parameters are covered. However, studies on the reactivity impacts due to the uncertainties in the nuclear data $\boldsymbol{\xi}$ are of fundamental interest in BUC criticality safety analysis. In the framework of hierarchical Bayesian procedures here presented such a study can be performed by drawing MC samples $\left(N_i^{(s)}\right)_{MC}$ from a distribution $p\left(\mathbf{N}^{(s)} \mid \boldsymbol{\Theta}\right)$ of the BUC-application-case-specific number densities $\mathbf{N}^{(s)} = \left(\mathbf{N}_1^{(s)},\ldots,\mathbf{N}_{I_{BUC}}^{(s)}\right)^T$. This requires to draw MC samples on the nuclear data $\boldsymbol{\xi}$ to represent the variation of these data due to their variances and covariances. We will discuss procedures required for drawing MC samples on $\boldsymbol{\xi}$ in sections 8.1 and 8.2.

Once MC samples $\left(\mathbf{N}^{(s)}\right)_{MC}$ are available, the set of bias-corrected isotopic number densities $N_i^{(j)}$, $i = 1,\ldots,I_{BUC}$, to be used in a subsequent criticality calculation (cf. Figure 1) is generated by multiplying the values $\left(\mathbf{N}^{(s)}\right)_{MC\_n}$ of the n-th MC sample on $\mathbf{N}^{(s)}$ with the respective values $\left(\mathbf{f}_n^{(j)}\right)_i$ of the n-th MC sample on the ICFs.

6 Validation of criticality calculation

As already described in section 1.1 validation of a criticality calculation is achieved by estimating the bias Δk_B which is characteristic of the applied criticality calculation procedure with respect to the application case S. In the framework of the hierarchical Bayesian MC procedures here described this means that to the n-th k_{eff} value $\left(k_{eff}\right)_n$ obtained with the n-th set $\left(\mathbf{N}^{(s)}\right)_{MC\_n} = \left(\left(N_1^{(s)}\right)_{MC\_n},\ldots,\left(N_{I_{BUC}}^{(s)}\right)_{MC\_n}\right)^T$ of isotopic number densities the n-th sample $\left(\Delta k_B\right)_n$ drawn on the bias Δk_B has to be added, cf. eq. (7) or eq. (107).

The procedure to generate MC samples $\left(\Delta k_B\right)_n$ on Δk_B by means of Bayesian MC procedures has been already described in detail in Ref. [8]. The description is not repeated here, only the main steps are summarized:

- Since the experimental or experiment-based systems chosen as benchmarks (B) adequate to estimate the bias Δk_B, which is characteristic of the applied criticality calculation code with respect to the application case S (cf. section 1.3), may have made use of the same equipments such as the same fuel rods and absorber plates (cf. Ref. [21]), the material design data of all the selected benchmarks are compiled in one material and design data vector $\mathbf{x}_B$. This vector is, so to speak, the joint material and design data vector of all the chosen benchmarks, i.e., some components of $\mathbf{x}_B$ can be related to different benchmarks, others are related to only one benchmark.
- Due to the uncertainties in the material and design data $\mathbf{x}_B$ (cf. Ref. [8]), MC samples $\mathbf{x}_B^{MC}$ on the joint vector $\mathbf{x}_B$ are drawn.
- For each MC sample $\left(\mathbf{x}_B^{MC}\right)_j$ the k_{eff} values of all the benchmarks are calculated. With these k_{eff} values a set of bias samples $(\Delta k_{Bi})_j$, $i = 1,\ldots,N_B$, $j = 1,\ldots,N$, is obtained; N_B is the number of chosen benchmarks, N denotes the number of MC samples drawn on $\mathbf{x}_B$.
- After having reached a sufficiently large number N, the bias samples are averaged thus yielding the sample mean vector

$$\overline{\boldsymbol{\Delta k}}_B = \left(\overline{\Delta k}_{B1},\ldots,\overline{\Delta k}_{BN_B}\right)^T \tag{108}$$

with

$$\overline{\Delta k}_{Bi} = \frac{1}{N}\sum_{j=1}^{N}(\Delta k_{Bi})_j\ ,\ i = 1,\ldots,N_B, \tag{109}$$

and the sample covariance matrix

$$\mathbf{S}_B = \frac{1}{N-1}\sum_{j=1}^{N}\left((\boldsymbol{\Delta k}_B)_j - \overline{\boldsymbol{\Delta k}}_B\right)\left((\boldsymbol{\Delta k}_B)_j - \overline{\boldsymbol{\Delta k}}_B\right)^T\ , \tag{110}$$

with

$$(\boldsymbol{\Delta k}_B)_j = \left((\Delta k_{B1})_j,\ldots,(\Delta k_{BN_B})_j\right)^T,\ j = 1,\ldots,N. \tag{111}$$

- Since the k_{eff} values from which the bias samples $(\Delta k_{Bi})_j$ are derived are usually obtained by means of a MC criticality calculation code, the vectors eq. (111), $j = 1,\ldots,N$, can be taken, due to the Central Limit Theorem of statistics [1], as samples on a normal distribution with expectation $\mathbf{E}[\boldsymbol{\Delta k}_B]$ and covariance matrix $\boldsymbol{\Sigma}_B$. So, as follows from the Appendix, eq. (A-41) and eq. (A-42), assuming that no prior information about $\boldsymbol{\Theta}_B = \left(\mathbf{E}[\boldsymbol{\Delta k}_B], \boldsymbol{\Sigma}_B\right)$ is available, a MC sample $\boldsymbol{\Sigma}_B^{MC}$ can be drawn from the Inverse-Wishart distribution with scale matrix $(N-1)\mathbf{S}_B$, and a MC sample $\mathbf{E}[\boldsymbol{\Delta k}_B]^{MC}$ can be drawn from a normal distribution, the expectation and the covariance matrix of which are the sample mean eq. (109) and the matrix $\boldsymbol{\Sigma}_B^{MC}/N$, respectively.

- Defining explanatory variables $\mathbf{z}_i$, $i = 1,\ldots,N_B$ and $\mathbf{z}_S$ characterizing adequately the chosen benchmarks and the application case S, the MC sample $\boldsymbol{\Theta}_B = \left(\mathbf{E}[\Delta\mathbf{k}_B]^{MC}, \boldsymbol{\Sigma}_B^{MC}\right)$ can be used to perform a Bayesian regression analysis (cf. [6], [8], [16]) which yields a MC sample $\Delta\mathbf{k}_B^{MC} = \Delta\mathbf{k}_B^{MC}(\mathbf{z}_S)$ for the bias to be applied to the application case S. This sample is one of the values $(\Delta k_B)_n$ to be inserted in eq. (107). Drawing of the next sample $\boldsymbol{\Theta}_B = \left(\mathbf{E}[\Delta\mathbf{k}_B]^{MC}, \boldsymbol{\Sigma}_B^{MC}\right)$ leads to the next MC sample $\Delta\mathbf{k}_B^{MC}(\mathbf{z}_S)$, and so forth. In this way one gets the set of MC sample values $(\Delta k_B)_n$ needed for the samples κ_n, eq. (107)

The required explanatory variables $\mathbf{z}_i$, $i = 1,\ldots,N_B$, and $\mathbf{z}_S$ are usually case-dependent [15]. To avoid overfitting, the dimension of $\mathbf{z}_i$ and $\mathbf{z}_S$ shall be reduced to the minimum dimension required for achieving an accepted regression model, i.e., a model which complies with the samples $\boldsymbol{\Theta}_B = \left(\mathbf{E}[\Delta\mathbf{k}_B]^{MC}, \boldsymbol{\Sigma}_B^{MC}\right)$. The minimum required dimension of the explanatory variables can be checked by means of statistical tests [1]. It is often observed that the minimum required dimension amounts to one with $\mathbf{z}_i = 1$, $\forall i$, and $\mathbf{z}_S = 1$, which means that there is no need for any explanatory variable since the simplest regression model given by the weighted means procedure (cf. Ref. [8] and section 11.5.2 in Ref. [1]) fits to the samples $\boldsymbol{\Theta}_B$.

As already stated in section 1.3, consideration of the uncertainties in the nuclear data ξ is not required for the estimation of the bias Δk_B, i.e., for the validation of the criticality calculations. As indicated in Figure 1, these uncertainties have to be taken into account when the neutron multiplication factor k_{eff} of the application case is estimated.

7 Uncertainties in the criticality calculations performed for an application case

In addition to the uncertainty due to the uncertainties in the validation of the depletion calculation, the uncertainties in the material and design data $\mathbf{x}_S$ of the application case S and the uncertainties in the involved nuclear data ξ have to be taken into account in the evaluation of the neutron multiplication factor k_{eff} of the application case. In the framework of the hierarchical Bayesian MC procedures here described this means that in the input to the calculation (yielding the sample value $(k_{eff})_n$ in eq. (107) the isotopic number density MC sample $N_{i,n}^{(j)}$, $i = 1,\ldots,I_{BUC}$ (cf. section 5) is used together with the MC sample $(\mathbf{x}_S^{MC})_n$ on the material and design data $\mathbf{x}_S$ and the MC sample ξ_n^{MC} on the involved nuclear data ξ. As already mentioned in section 1.1, the joint pdf $p(\mathbf{x}_S, \xi)$ of $\mathbf{x}_S$ and ξ factorizes as

$$p(\mathbf{x}_S, \xi) = p(\mathbf{x}_S) \cdot p(\xi) . \tag{112}$$

Therefore, the MC samples $(\mathbf{x}_S^{MC})_n$ and ξ_n^{MC} can be drawn independently from $p(\mathbf{x}_S)$ and $p(\xi)$, respectively.

The procedure of generating MC samples $(\mathbf{x}_S^{MC})_n$ has been already described in detail in Ref. [8]. The description is not repeated here. In the following the attention is focused on the drawing of MC samples $\boldsymbol{\xi}_n^{MC}$.

8 Evaluation of nuclear data uncertainties

8.1 The ideal method

The ideal method of evaluating uncertainties in the nuclear data $\boldsymbol{\xi}$ is, in principle, completely analogous to the method of evaluating the uncertainties in the validation of depletion calculations. On the analogy to the matrix $\boldsymbol{\Phi}$, generated as described in section 4.2.2, one needs a neutron-energy-dependent matrix $\mathbf{M}(E_n)$ (E_n := neutron energy) which contains all the available observations $\xi_\ell(E_n)$ of the involved nuclear data, empirical observations (e.g., measured data), empirically based observations (resulting from evaluations of integral measurements for instance), and data derived by means of theories of nuclear reactions and models of the nuclei (e.g., data related to the experimentally non-resolvable resonance region). Choosing an adequate distribution $p(\boldsymbol{\xi}(E_n)\,|\,\boldsymbol{\Theta}(E_n))$ and a prior pdf $p(\boldsymbol{\Theta}(E_n))$ representing adequately the prior knowledge about the distribution parameters $\boldsymbol{\Theta}(E_n)$ one gets by means of Bayes' theorem eq. (29) the posterior pdf

$$p(\boldsymbol{\Theta}(E_n)\,|\,\mathbf{M}(E_n)) \propto p(\mathbf{M}(E_n)\,|\,\boldsymbol{\Theta}(E_n))\cdot p(\boldsymbol{\Theta}(E_n)) \quad , \tag{113}$$

from which MC samples $\boldsymbol{\Theta}(E_n)^{MC}$ can be drawn which can be used to draw, according to eq. (32), MC samples $\boldsymbol{\xi}(E_n)^{MC}$ from the distribution $p(\boldsymbol{\xi}(E_n)\,|\,\boldsymbol{\Theta}(E_n))$.

In case of missing data, i.e., in case that $\mathbf{M}(E_n)$ is incomplete, the data augmentation procedure described in section 4.2.2 (see equations (94) through (98)) can be used to estimate the posterior pdf $p(\boldsymbol{\Theta}(E_n)\,|\,\mathbf{M}(E_n))$ provided that the missing-data-mechanism is ignorable, i.e., that the missingness does not depend on the missing data (for details see Ref. [16]).

Once a MC sample $\boldsymbol{\xi}(E_n)^{MC}$ is obtained, a continuous cross-section library L_{XS}^{MC} can be generated from $\boldsymbol{\xi}(E_n)^{MC}$ by means of a basis-data evaluation code. This library is used in the calculation of one of the sample values $(k_{eff})_n$ in eq. (107).

The procedure is repeated by drawing the next sample $\boldsymbol{\xi}(E_n)^{MC}$, from which the next library L_{XS}^{MC} is generated which is used for the calculation of the value $(k_{eff})_{n+1}$, and so forth.

8.2 The one-data-set case

Due to the lack of a sufficient amount of nuclear basis data it is hardly to believe that the ideal method described in the preceding section can ever be realized. So, one has to be content with the fact that at least one set of estimates $\hat{\boldsymbol{\xi}}(E_n)$ of the mean of the nuclear basis data is available

together with the estimate $\hat{\mathbf{V}}(E_n)$ of the corresponding covariance matrix of the nuclear basis data. Since more information will scarcely be available one is committed to go the usual way, i.e., to assume that the expectations $\mathbf{E}[\hat{\xi}(E_n)]$ and $\mathbf{E}[\hat{\mathbf{V}}(E_n)]$ are the expectation vector $\mathbf{E}[\xi(E_n)]$ and the covariance matrix $\mathbf{V}(E_n)$ of the Normal distribution $N\left(\mathbf{E}[\xi(E_n), \mathbf{V}(E_n)\right)$. MC samples $\hat{\xi}(E_n)^{MC}$ are therefore drawn from a Normal distribution using the estimates $\hat{\xi}(E_n)$ and $\hat{\mathbf{V}}(E_n)$ as expectation vector and covariance matrix, respectively. The resulting samples $\hat{\xi}(E_n)^{MC}$ are then used for generating the cross section libraries L_{XS}^{MC}.

8.3 Usage of the SCALE module TSUNAMI

We are just installing the one-data-set procedure described in the preceding section. As long as the installation of that procedure has not been finished, we use the module TSUNAMI of the SCALE system [22] for estimating the contribution of the uncertainties of the nuclear data to the neutron multiplication factor k_{eff}.

Application of TSUNAMI to the system S of interest (application case) provides the neutron multiplication factor k_S of the system and, according to equations (19) and (20), the ratio

$$R_{ND} = \frac{\sigma_{ND}}{k_S} \propto \left\{ \sum_{\nu,\mu} \Lambda_{s\nu} \frac{\mathrm{cov}\left(\xi_\nu, \xi_\mu\right)}{\xi_\nu \, \xi_\mu} \Lambda_{s\mu} \right\}^{1/2} \quad \text{with } \Lambda_{sj} = \frac{1}{k_S} \left(\frac{\partial k_S}{\partial \xi_j} \xi_j \right). \tag{114}$$

This ratio is the relative deviation of the system's neutron multiplication factor k_S due to the uncertainties in the nuclear data (ND) ξ, cf. Ref. [22]. Since TSUNAMI uses MC techniques [22], the sample mean $\bar{k}_S$ of the calculated neutron multiplication factor k_S can be assumed to follow a Normal distribution because of the Central Limit Theorem of statistics [1]. It is assumed, therefore, that the estimate

$$\hat{\sigma}_{ND} = R_{ND} \cdot \bar{k}_S \tag{115}$$

follows a normal distribution $N\left(E[\sigma_{ND}], V[\sigma_{ND}]\right)$ with expectation $E[\sigma_{ND}]$ and variance $\tau^2 \equiv V[\sigma_{ND}]$. So, running TSUNAMI m times for the application case S using different starting random numbers one gets a set of results $\left(\hat{\sigma}_{ND}\right)_j$, $j = 1, \ldots, m$, with sample mean

$$\bar{\sigma}_{ND} = \frac{1}{m} \sum_{j=1}^{m} \left(\hat{\sigma}_{ND}\right)_j \tag{116}$$

and sample variance

$$\hat{\tau}^2 = \frac{1}{m-1} \sum_{j=1}^{m} \left(\left(\hat{\sigma}_{ND}\right)_j - \bar{\sigma}_{ND} \right)^2 \quad . \tag{117}$$

Due to the normality assumption it follows

- that $\mathrm{E}[\sigma_{\mathrm{ND}}]$ follows a Normal distribution $\mathrm{N}\left(\overline{\sigma}_{\mathrm{ND}}, \tau^2/\mathrm{m}\right)$ with expectation $\overline{\sigma}_{\mathrm{ND}}$ and variance τ^2/m, cf. eq. (39), and
- that τ^2 follows an Inverse-χ^2 distribution $\mathrm{Inv}-\chi^2\left(\tau^2 \mid (\mathrm{m}-1), \hat{\tau}^2\right)$ with $\mathrm{m}-1$ degrees of freedom and scale feactor $\hat{\tau}^2$, cf. eq. (40).

So the following steps have to be taken

- Drawing of a MC sample τ^2_{MC} from the distribution $\mathrm{Inv}-\chi^2\left(\tau^2 \mid (\mathrm{m}-1), \hat{\tau}^2\right)$
- Insertion of τ^2_{MC} into $\mathrm{N}\left(\overline{\sigma}_{\mathrm{ND}}, \tau^2/\mathrm{m}\right)$ and drawing of a MC sample $\mathrm{E}[\sigma_{\mathrm{ND}}]_{\mathrm{MC}}$ from the resulting distribution
- Insertion of $\mathrm{E}[\sigma_{\mathrm{ND}}]_{\mathrm{MC}}$ and $\tau^2_{\mathrm{MC}} \equiv \mathrm{V}[\sigma_{\mathrm{ND}}]_{\mathrm{MC}}$ into the distribution $\mathrm{N}\left(\mathrm{E}[\sigma_{\mathrm{ND}}], \mathrm{V}[\sigma_{\mathrm{ND}}]\right)$ and drawing of a MC sample $\sigma^{\mathrm{MC}}_{\mathrm{ND}}$ from the resulting distribution
- This MC sample $\sigma^{\mathrm{MC}}_{\mathrm{ND}}$ is inserted into the distribution

$$\mathrm{p}\left(\Delta \mathrm{k}_{\mathrm{ND}} \mid \mathrm{E}[\Delta \mathrm{k}_{\mathrm{ND}}], \sigma^2_{\mathrm{ND}}\right) = \mathrm{N}\left(0, \sigma^2_{\mathrm{ND}}\right) = \frac{1}{\sqrt{2\pi}\sigma_{\mathrm{ND}}} \exp\left(-\frac{1}{2}\frac{\Delta \mathrm{k}^2_{\mathrm{ND}}}{\sigma^2_{\mathrm{ND}}}\right) \tag{118}$$

  and a MC sample $\Delta \mathrm{k}^{\mathrm{MC}}_{\mathrm{ND}}$ on the deviation from the expectation $\mathrm{E}\left[\Delta \mathrm{k}_{\mathrm{ND}}\right] = 0$ is drawn.

Expression (118) results from reflections on the meaning of the ratio eq. (114): It is obvious that $\sigma_{\mathrm{ND}} = \mathrm{R}_{\mathrm{ND}} \cdot \mathrm{k}_{\mathrm{S}}$ is related to a distribution $\mathrm{p}\left(\Delta \mathrm{k}_{\mathrm{ND}} \mid 0, \sigma^2_{\mathrm{ND}}\right)$ of the variable $\Delta \mathrm{k}_{\mathrm{ND}} = \mathrm{k}_{\mathrm{S}} - \mathrm{E}[\mathrm{k}_{\mathrm{S}}]$ with expectation $\mathrm{E}[\Delta \mathrm{k}_{\mathrm{ND}}] = 0$ (by definition) and variance

$$\mathrm{V}[\Delta \mathrm{k}_{\mathrm{ND}}] = \mathrm{E}\left[\left(\Delta \mathrm{k}_{\mathrm{ND}} - \mathrm{E}[\Delta \mathrm{k}_{\mathrm{ND}}]\right)^2\right] = \mathrm{E}\left[\left(\mathrm{k}_{\mathrm{S}} - \mathrm{E}[\Delta \mathrm{k}_{\mathrm{S}}]\right)^2\right] = \sigma^2_{\mathrm{ND}}.$$

In fact, as follows from eq. (114),

$$\sigma^2_{\mathrm{ND}} = \mathrm{k}^2_{\mathrm{S}} \cdot \mathrm{R}^2_{\mathrm{ND}} = \sum_{\nu,\mu} \frac{\partial \mathrm{k}_{\mathrm{S}}}{\partial \xi_\nu} \mathrm{cov}\left(\xi_\nu, \xi_\mu\right) \frac{\partial \mathrm{k}_{\mathrm{S}}}{\partial \xi_\mu} = \mathbf{z}\,\mathrm{cov}(\boldsymbol{\xi})\,\mathbf{z}^{\mathrm{T}} \text{ with } \mathbf{z} = \left(\frac{\partial \mathrm{k}_{\mathrm{S}}}{\partial \xi_1}, \ldots, \frac{\partial \mathrm{k}_{\mathrm{S}}}{\partial \xi_{\mathrm{j}}}, \ldots\right). \tag{119}$$

Expression (119) is just the variance of $\mathrm{k}_{\mathrm{S}}(\boldsymbol{\xi})$ in the first-order perturbation evaluation

$$\mathrm{k}_{\mathrm{S}}(\boldsymbol{\xi}) \approx \mathrm{k}_{\mathrm{S}}\left(\mathrm{E}[\boldsymbol{\xi}]\right) + \mathbf{z}\,\mathrm{d}\boldsymbol{\xi}. \tag{120}$$

with

$$\mathrm{E}\left[\mathrm{k}_{\mathrm{S}}(\boldsymbol{\xi})\right] \approx \mathrm{k}_{\mathrm{S}}\left(\mathrm{E}[\boldsymbol{\xi}]\right). \tag{121}$$

So, assuming $\mathrm{k}_{\mathrm{S}}(\boldsymbol{\xi})$ to be Normal distributed it follows that $\Delta \mathrm{k}_{\mathrm{ND}} = \mathrm{k}_{\mathrm{S}} - \mathrm{E}[\mathrm{k}_{\mathrm{S}}]$ is Normal distributed with expectation $\mathrm{E}\left[\Delta \mathrm{k}_{\mathrm{ND}}\right] = 0$ and variance σ^2_{ND}.

Now, the n-th MC sample $\left(\Delta k_{ND}^{MC}\right)_n$ obtained by means of the above described procedure, i.e, resulting from the successive draws of $\left(\tau_{MC}^2\right)_n$, $E[\sigma_{ND}^{MC}]_n$ and $\left(\sigma_{ND}^{MC}\right)_n$ is added to the right-hand side of eq. (107) to include the uncertainty in the calculated neutron multiplication factors due to the uncertainty in the nuclear data.

9 Conclusions

As summarized in Figure 10, the procedure of including all the uncertainties relevant to BUC criticality safety analysis is now complete. The presented MOCADATA procedure has been developed to make it possible by means of using hierarchical Bayesian MC procedures to consider

- all uncertainties in
  - the depletion calculations performed for the application case,
  - the chemical assay data evaluated for validating the depletion calculations,
  - the critical experiments evaluated for estimating the bias of the criticality calculation code applied,
  - the application case;
- all uncertainties due to
  - empirical data required for performing statistical analysis,
  - the finite number of the data, and
  - the possible incompleteness of the data;
- the fundamental variability due to the selection of probability distribution models required for evaluating empirical data.

Criticism may be raised on the fact that the determination of ICF MC sampled $\mathbf{f}_n^{(j)}$ has been based on the observation that ICFs do not show any significant dependence on the burnup (cf. section 4.2.2). Well, as long as this observation is valid it is justified to take this observation as a basis. And this observation remains valid as long as compatibility tests [1] demonstrate that there is no significant dependence on the burnup.

Let us nevertheless assume that it will be observed one day that some ICFs show a significant dependence on the burnup. In that case it is possible to proceed analogously to section 6, i.e., to evaluate the line vectors eq. (89) by means of a Bayesian MC regression analysis using the burnup as explanatory variable. As appears from Ref. [16], this regression analysis can be performed with missing data, i.e., as described in section 4.2.2, with some missing elements $\varphi_{n\ell i}$ of some line vectors $\boldsymbol{\varphi}_{n\ell}$, eq. (89), of the matrix $\boldsymbol{\Phi}_n$.

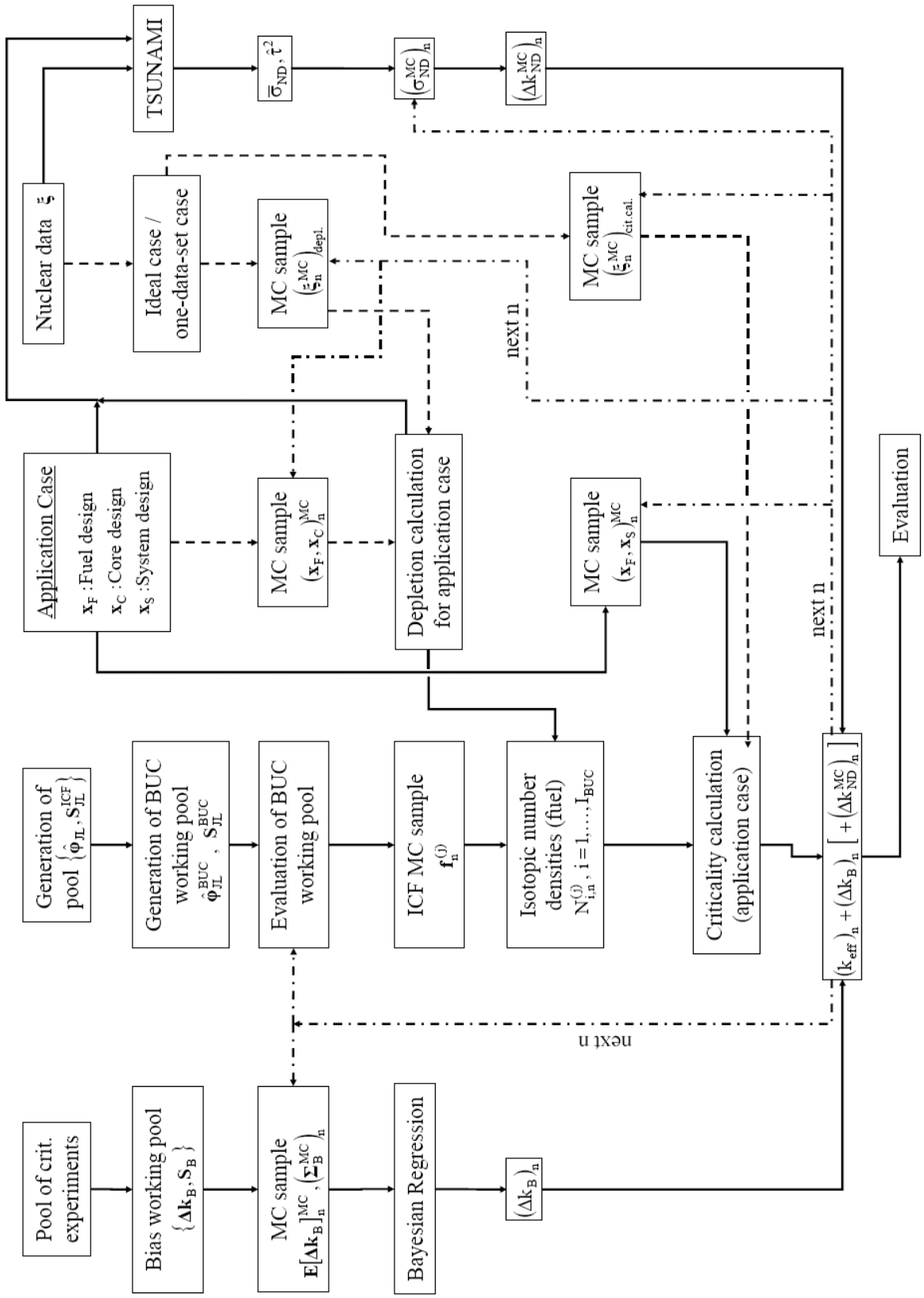

Figure 10: *Summary of the hierarchical Bayesian procedures presented in the paper on hand*

So, whether the ICFs depend on the fuel's burnup or not, in any case one gets, provided that one has a sufficient amount of data [13], MC samples

$$\kappa_n = \left(k_{eff}\right)_n + \left(\Delta k_B\right)_n \left[+\left(\Delta k_{ND}^{MC}\right)_n\right],\ n = 1,\ldots,M. \tag{122}$$

If a sufficiently large number M of samples is reached, the M samples can be evaluated by means of the methods described in sections 1.1 and 1.2

In addition, the distribution of the obtained results κ_n can be fitted by means of a free-of-binning fit procedure [1] using, for instance, a Johnson empirical distribution model [1]. Once such a distribution model is fitted to the data eq. (122) by means of the Maximum Likelihood method [1] yielding the distribution model $f_{fit}\left(\kappa \mid \boldsymbol{\Theta}\right)$ it becomes possible to draw MC samples on the covariance matrix $\mathbf{cov}\left(\boldsymbol{\Theta}\right)$ of the parameters $\boldsymbol{\Theta}$ estimated by $\hat{\boldsymbol{\Theta}}$, to draw then MC samples on the expectation $\mathbf{E}[\boldsymbol{\Theta}]$ of the parameters $\boldsymbol{\Theta}$, and to draw finally MC samples $\boldsymbol{\Theta}^{MC}$ on $\boldsymbol{\Theta}$. These MC samples can be inserted into the applied distribution model so that one gets fit distributions $f\left(\kappa \mid \boldsymbol{\Theta}^{MC}\right)$. If these MC fit distributions correspond to the data, which can be tested by means of a Smirnov-Cramer-von Mises test [1], then MC samples π_S^{MC} on the probability eq. (6) can be calculated:

$$\pi_S^{MC} = P\left(\kappa > k_{max} \mid S\right)^{MC} = \int_{k_{max}}^{\infty} d\kappa\, f\left(\kappa \mid \boldsymbol{\Theta}^{MC}\right). \tag{123}$$

Let us assume that we have drawn N samples π_S^{MC}. Arranging these N samples in an order statistic

$$\left(\pi_S^{MC}\right)_1 \le \ldots \le \left(\pi_S^{MC}\right)_N, \tag{124}$$

the confidence level $(1-\alpha_j)$ can be calculated by means of eq. (16) for the greatest $\left(\pi_S^{MC}\right)_j$ which just meets the inequality $\left(\pi_S^{MC}\right)_j \le \gamma$ and hence eq. (8) for a prescribed margin γ. It can then be checked if the result $(1-\alpha_j)$ complies with the value prescribed for α. Note that for values usually prescribed for α and γ (usually $\alpha = \gamma = 0.05$ is chosen) it is sufficient to evaluate the results κ_n, eq. (122), directly by the methods described in sections 1.1 and 1.2. However, for values of γ significantly smaller than the values usually chosen it is necessary, because of the condition given by eq. (18), to generate MC samples on the probability π_S according to eq. (123).

Appendix

Application of a Bayesian MC procedure requires the definition of a prior pdf $p(\boldsymbol{\Theta})$, cf. eq. (29) in section 3. Accomplishment of this requirement involves the probability-theoretical problem of the Bayesian methodology. As summarized in Ref. [8], there are mainly three approaches for choosing a prior density:

- Concept of conjugate priors using the concept of conjugate distributions: For a given Likelihood function $p(\mathbf{X}\,|\,\boldsymbol{\Theta})$ one is looking for a prior pdf $p(\boldsymbol{\Theta})$ which belongs to the same distribution family as the posterior pdf $p(\boldsymbol{\Theta}\,|\,\mathbf{X})$. This family must be of such a diversity that all information, experiences and subjective suppositions can be described [6].
- Empirical Bayes methods: The methods are decision-theory-based using a decision rule as estimator for $\boldsymbol{\Theta}$ which minimizes the risk with respect to the prior pdf [1], [9], [10].
- Concept of objective priors: The determination of such priors is based on frequentist or logical probability.

The first and the second approach give rise to controversy due to scientific-theory-based doubts whereas the latter approach is beyond controversy. The concept of objective priors has however the disadvantage that in many cases coming along in real life no prior is known. The attention is therefore focused not only on this concept in the following, but also on the first concept.

The justification of the concept of conjugate priors is the same as the justification of the apparently arbitrary definition of the information matrix given in eq. (30) of section 3: It reasonably works (with respect to the information matrix see [1], section 5). The concept of conjugate prior pdfs offers computational advantages in many cases. In addition such priors have the property of being interpretable as additional data [6]. The question arises of how the total lack of knowledge, i.e. lack of prior information, is represented in the framework of this concept.

Priors representing lack of knowledge have been derived by H. Jeffreys [5], and these priors, named as "objective priors" by Jeffreys, are now known as "Jeffreys' priors" therefore. These priors are based on the principle that so-called "non-informative" priors, which represent the lack of knowledge, should be invariant under reparameterization [1], [6], [7].

The attention is focused in the following on the Normal distribution model since this model is the most used one in the paper on hand. The multivariate Normal pdf of an m-dimensional random vector $\mathbf{x} = (x_1, \ldots, x_m)^T$ is given by eq. (A-1), [1],

$$p(\mathbf{x}\,|\,\boldsymbol{\Theta}) = p(\mathbf{x}\,|\,\boldsymbol{\mu}, \boldsymbol{\Sigma}) = \frac{1}{(2\pi)^{m/2}\,|\,\boldsymbol{\Sigma}\,|^{1/2}} \cdot \exp\left\{-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^T\,\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})\right\},\ \boldsymbol{\Theta} = (\boldsymbol{\mu}, \boldsymbol{\Sigma}), \tag{A-1}$$

with expectation vector

$$\mathbf{E}[\mathbf{x}] = \boldsymbol{\mu} = (\mu_1, \ldots, \mu_m)^T = (E[x_1], \ldots, E[x_m])^T \tag{A-2}$$

and covariance matrix

$$\mathbf{cov}(\mathbf{x}) = \boldsymbol{\Sigma} = \mathrm{E}\left[(\mathbf{x}-\boldsymbol{\mu})(\mathbf{x}-\boldsymbol{\mu})^{\mathrm{T}}\right]. \tag{A-3}$$

$|\boldsymbol{\Sigma}|$ in eq. (A-1) denotes the determinant of $\boldsymbol{\Sigma}$.

Let $\mathbf{X}$ be the matrix which represents a sample of n mutually independent observation $\mathbf{x}_1,\ldots,\mathbf{x}_n$ from the distribution eq. (A-1),

$$\mathbf{X} = \begin{pmatrix} \mathbf{x}_1^{\mathrm{T}} \\ \vdots \\ \mathbf{x}_n^{\mathrm{T}} \end{pmatrix} = \begin{pmatrix} x_{11} & \ldots & x_{1m} \\ \vdots & & \vdots \\ x_{n1} & \ldots & x_{nm} \end{pmatrix}. \tag{A-4}$$

The Likelihood $p(\mathbf{X}\,|\,\boldsymbol{\Theta}) = p(\mathbf{X}\,|\,\boldsymbol{\mu},\boldsymbol{\Sigma})$ for this sample is

$$p(\mathbf{X}\,|\,\boldsymbol{\mu},\boldsymbol{\Sigma}) \propto |\boldsymbol{\Sigma}|^{-n/2} \cdot \exp\left\{-\frac{1}{2}\sum_{i=1}^{n}(\mathbf{x}_i-\boldsymbol{\mu})^{\mathrm{T}}\,\boldsymbol{\Sigma}^{-1}(\mathbf{x}_i-\boldsymbol{\mu})\right\}. \tag{A-5}$$

By straightforward application of the multiplication rules for vectors and matrices the Likelihood eq. (A-5) becomes

$$p(\mathbf{X}\,|\,\boldsymbol{\mu},\boldsymbol{\Sigma}) \propto |\boldsymbol{\Sigma}|^{-n/2} \cdot \exp\left\{-\frac{1}{2}\mathrm{Tr}\left(\boldsymbol{\Sigma}^{-1}\mathbf{S}_0\right)\right\},\ \mathrm{Tr} := \mathrm{trace}, \tag{A-6}$$

with the $m \times m$ matrix

$$\mathbf{S}_0 = \sum_{i=1}^{n}(\mathbf{x}_i-\boldsymbol{\mu})(\mathbf{x}_i-\boldsymbol{\mu})^{\mathrm{T}}. \tag{A-7}$$

Since, by definition, $\mathbf{E}[\mathbf{x}_i] = \boldsymbol{\mu}$, $\forall i$, and $\mathbf{cov}(\mathbf{x}_i) = \boldsymbol{\Sigma}$, $\forall i$, the expectation of eq. (A-7) is, because of eq. (A-3):

$$\mathbf{S}_0 = n\,\boldsymbol{\Sigma}. \tag{A-8}$$

The right-hand side of eq. (A-6) is proportional to the Wishart pdf with $\nu = n$ degrees of freedom and $m \times m$ scale matrix $\boldsymbol{\Psi}$ [11]

$$p(\mathbf{W}) \equiv \mathrm{Wishart}(\boldsymbol{\Psi};\nu,m) \equiv \mathrm{W}(\boldsymbol{\Psi};\nu,m) = C \cdot |\boldsymbol{\Psi}|^{-\nu/2} \cdot |\mathbf{W}|^{(\nu-m-1)/2} \cdot \exp\left\{-\frac{1}{2}\mathrm{Tr}\left(\boldsymbol{\Psi}^{-1}\mathbf{W}\right)\right\}. \tag{A-9}$$

with the normalization factor [6], [7]

$$C = \left[2^{\nu m/2} \cdot \pi^{m(m-1)/4} \cdot \prod_{j=1}^{m}\Gamma\left(\frac{n+1-j}{2}\right)\right]^{-1}. \tag{A-10}$$

and with the expectation

$$\mathbf{E}[\mathbf{W}] = \nu\,\boldsymbol{\Psi}. \tag{A-11}$$

So, as apparent from a comparison of eq. (A-6) with eq. (A-9) as well as eq. (A-8) with eq. (A-11), $\mathbf{W} = \mathbf{S}_0$ and $\mathbf{\Psi} = \mathbf{\Sigma}$, $\nu = n$.

The natural choice for meeting the concept of conjugate priors is to look for all the pdfs which have the same functional form as the Likelihood, since then it is accomplished that the prior belongs to the same distribution family as the posterior pdf.

So therefore, the Wishart pdf is the conjugate prior distribution for the inverse covariance matrix in a multivariate normal distribution model.

If a matrix follows a Wishart distribution eq. (A-9), then the inverse of the matrix follows an Inverse-Wishart distribution

$$p(\mathbf{\Psi}) \equiv \text{Inv}-\text{Wishart}\left(\mathbf{W}^{-1};\nu,m\right) = C\cdot\left|\mathbf{W}\right|^{\nu/2}\cdot\left|\mathbf{\Psi}\right|^{-(\nu+m+1)/2}\cdot\exp\left\{-\frac{1}{2}\text{Tr}\left(\mathbf{W}\,\mathbf{\Psi}^{-1}\right)\right\}. \tag{A-12}$$

with ν degrees of freedom, $m\times m$ scale matrix $\mathbf{W}$, and factor C given by eq. (A-10) [7].

(The notation $\mathbf{W}^{-1}$ in $\text{Inv}-\text{Wishart}\left(\mathbf{W}^{-1};\nu,m\right)$ may be regarded as confusing, but it is just the notation used in Ref. [6].)

The expectation of (A-12) is (for $\nu > m+1$) [6]

$$\mathbf{E}[\mathbf{\Psi}] = (\nu-m-1)^{-1}\,\mathbf{W}. \tag{A-13}$$

Neither the expectation $\boldsymbol{\mu}$ nor the covariance matrix $\mathbf{\Sigma}$ are usually known in real life. However, as described in section 3, the matrix eq. (A-4) contains information about the parameters $\mathbf{\Theta} = (\boldsymbol{\mu}, \mathbf{\Sigma})$. This information can be used to calculate numerical values, named as "estimates", for the parameters. These estimates are related to the particular set of evaluated observations. To obtain estimates for the parameters one has to choose a method for proceeding from the observations to the estimates, i.e., one has to choose a function of the observations which is named as "estimator". An estimator must have some desirable properties which determine its "goodness" with respect to its task. These properties, such as consistence, unbiasedness and efficiency (i.e., information content, cf. eq. (30) in section 3), are discussed in the theory of estimators, see Ref. [1] for instance.

It is well known that the sample mean vector

$$\bar{\mathbf{x}} = \frac{1}{n}\sum_{i=1}^{n}\bar{\mathbf{x}}_i \tag{A-14}$$

with the components

$$\bar{\mathbf{x}}_j = \frac{1}{n}\sum_{i=1}^{n}\mathbf{x}_{ij}\,,\ j = 1,\ldots,m\,, \tag{A-15}$$

and the sample covariance matrix

$$\mathbf{S} = \frac{1}{n-1}\sum_{i=1}^{n} (\mathbf{x}_i - \bar{\mathbf{x}})\,(\mathbf{x}_i - \bar{\mathbf{x}})^T \tag{A-16}$$

with the elements

$$S_{kj} = \frac{1}{n-1}\sum_{i=1}^{n} (x_{ik} - \bar{x}_k)\,(x_{ij} - \bar{x}_j),\ k, j = 1, \ldots, m, \tag{A-17}$$

are unbiased estimators of $\boldsymbol{\mu}$ and $\boldsymbol{\Sigma}$, i.e.

$$\mathbf{E}[\bar{\mathbf{x}}] = \boldsymbol{\mu} \tag{A-18}$$

and

$$\mathbf{E}[\mathbf{S}] = \boldsymbol{\Sigma}, \tag{A-19}$$

respectively. Therefore $\bar{\mathbf{x}}$ and $\mathbf{S}$ are sometimes written as $\hat{\boldsymbol{\mu}}$ and $\hat{\boldsymbol{\Sigma}}$, respectively.

Equations (A-18) and (A-19) can be easily shown by using the fact that the expectation operator $\mathbf{E}[]$ is a linear operator, i.e. $\mathbf{E}[a\,\mathbf{x} + b\,\mathbf{y}] = a\,\mathbf{E}[\mathbf{x}] + b\,\mathbf{E}[\mathbf{y}]$.

The sum $Q(\mathbf{X}, \boldsymbol{\mu})$ of quadratic forms $q_i(\mathbf{x}_i, \boldsymbol{\mu}) = (\mathbf{x}_i - \boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1} (\mathbf{x}_i - \boldsymbol{\mu})$ in the exponential function on the right-hand side of eq. (A5) can be rewritten as follows

$$Q(\mathbf{X}, \boldsymbol{\mu}) = \sum_{i=1}^{n} q_i(\mathbf{x}_i, \boldsymbol{\mu}) = \sum_{i=1}^{n} \left[(\mathbf{x}_i - \bar{\mathbf{x}}) + (\bar{\mathbf{x}} - \boldsymbol{\mu})\right]^T \boldsymbol{\Sigma}^{-1} \left[(\mathbf{x}_i - \bar{\mathbf{x}}) + (\bar{\mathbf{x}} - \boldsymbol{\mu})\right].$$

This expression becomes since, due to eq. (A-14), only real quadratic forms survive:

$$Q(\mathbf{X}, \boldsymbol{\mu}) = \sum_{i=1}^{n} (\mathbf{x}_i - \bar{\mathbf{x}})^T \boldsymbol{\Sigma}^{-1} (\mathbf{x}_i - \bar{\mathbf{x}}) + \sum_{i=1}^{n} (\bar{\mathbf{x}} - \boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1} (\bar{\mathbf{x}} - \boldsymbol{\mu}). \tag{A-20}$$

By straightforward application of the multiplication rules for vectors and matrices to the first term of the right-hand side of eq. (A-20) one gets

$$Q(\mathbf{X}, \boldsymbol{\mu}) = \mathrm{Tr}\left(\boldsymbol{\Sigma}^{-1}(n-1)\mathbf{S}\right) + (\bar{\mathbf{x}} - \boldsymbol{\mu})^T \left(\boldsymbol{\Sigma}/n\right)^{-1} (\bar{\mathbf{x}} - \boldsymbol{\mu}), \tag{A-21}$$

where $\mathbf{S}$ is the sample covariance matrix eq. (A-16).

The Likelihood eq. (A-5) thus becomes

$$p(\mathbf{X} \mid \boldsymbol{\mu}, \boldsymbol{\Sigma}) \propto \left|\frac{\boldsymbol{\Sigma}}{n}\right|^{-1/2} \exp\left(-\frac{1}{2}(\bar{\mathbf{x}} - \boldsymbol{\mu})^T \left(\frac{\boldsymbol{\Sigma}}{n}\right)^{-1} (\bar{\mathbf{x}} - \boldsymbol{\mu})\right) \cdot |\boldsymbol{\Sigma}|^{-\frac{n-1}{2}} \exp\left(-\frac{1}{2}\mathrm{Tr}\left(\boldsymbol{\Sigma}^{-1}(n-1)\mathbf{S}\right)\right). \tag{A-22}$$

So, the Likelihood has the functional form of

- a normal distribution of the sample mean $\bar{\mathbf{x}}$ with expectation $\boldsymbol{\mu}$ (cf. eq. (A-18)) and covariance matrix $\boldsymbol{\Sigma}/n$

multiplied with

- a Wishart distribution of the inverse covariance matrix with $n-1$ degrees of freedom.

As conjugate prior $p(\boldsymbol{\Theta})$ for $\boldsymbol{\Theta}=(\boldsymbol{\mu},\boldsymbol{\Sigma})$ is therefore chosen

$$p(\boldsymbol{\mu},\boldsymbol{\Sigma}) \propto \left|\frac{\boldsymbol{\Sigma}}{n_0}\right|^{-1/2} \exp\left(-\frac{1}{2}(\hat{\boldsymbol{\mu}}_0-\boldsymbol{\mu})^T\left(\frac{\boldsymbol{\Sigma}}{n_0}\right)^{-1}(\hat{\boldsymbol{\mu}}_0-\boldsymbol{\mu})\right)\cdot|\boldsymbol{\Sigma}|^{-\frac{\nu_0+m+1}{2}}\exp\left(-\frac{1}{2}\mathrm{Tr}\left(\boldsymbol{\Sigma}^{-1}\nu_0\boldsymbol{\Psi}_0\right)\right) \tag{A-23}$$

with hyperparameters $\hat{\boldsymbol{\mu}}_0$, n_0, ν_0 and $\boldsymbol{\Psi}_0$ chosen to meet the requirements of diversity described at the beginning of this Appendix.

These parameters can be interpreted as parameters which are related to a prior sample of n_0 mutually independent observations $\mathbf{x}_{01},\ldots,\mathbf{x}_{0n_0}$ from the distribution eq. (A-1). Accordingly, $\hat{\boldsymbol{\mu}}_0$ is interpreted as sample mean

$$\hat{\boldsymbol{\mu}}_0 = \frac{1}{n_0}\sum_{i=1}^{n_0}\mathbf{x}_{0i} \tag{A-24}$$

with covariance matrix

$$\mathbf{cov}(\hat{\boldsymbol{\mu}}_0) = \boldsymbol{\Sigma}/n_0\,. \tag{A-25}$$

Analogously to eq. (A-16) the matrix $\boldsymbol{\Psi}_0$ in eq. (23) can be interpreted as sample covariance matrix

$$\boldsymbol{\Psi}_0 = \frac{1}{\nu_0}\sum_{i=1}^{\nu_0+1}(\mathbf{x}_{0i}-\hat{\boldsymbol{\mu}}_0)(\mathbf{x}_{0i}-\hat{\boldsymbol{\mu}}_0)^T \tag{A-26}$$

with

$$\nu_0 = n_0 - 1\,. \tag{A-27}$$

The set of prior observations $\mathbf{x}_{01},\ldots,\mathbf{x}_{0n_0}$ and the set of the present observations $\mathbf{x}_1,\ldots,\mathbf{x}_n$ can be considered as one sample with the total sample mean

$$\hat{\boldsymbol{\mu}}_N = \frac{1}{n_0+n}\left(\sum_{i=1}^{n_0}\mathbf{x}_{0i}+\sum_{i=1}^{n}\mathbf{x}_i\right) = \frac{1}{n_0+n}\left(n_0\,\hat{\boldsymbol{\mu}}_0 + n\,\bar{\mathbf{x}}\right) \tag{A-28}$$

and the total sample covariance matrix

$$\boldsymbol{\Psi}_N = \frac{1}{n_0+n-1}\sum_{i=1}^{n_0+n}\left(\mathbf{y}_i-\hat{\boldsymbol{\mu}}_N\right)\left(\mathbf{y}_i-\hat{\boldsymbol{\mu}}_N\right)^T, \tag{A-29}$$

with

$$\mathbf{y}_i = \begin{cases}\mathbf{x}_{0i} & \text{for} \quad i=1,\ldots,n_0\\ \mathbf{x}_{i-n_0} & \text{for} \quad i=n_0+1,\ldots,n_0+n\end{cases}. \tag{A-30}$$

With this definition, the sample mean eq. (A-28) and the definition eq. (A-31),

$$N = n_0 + n\,, \tag{A-31}$$

the sample covariance matrix eq. (A-29) becomes

$$(N-1)\,\boldsymbol{\Psi}_N = \sum_{i=1}^{n_0} \left(\mathbf{x}_{0i} - \hat{\boldsymbol{\mu}}_0\right)\left(\mathbf{x}_{0i} - \hat{\boldsymbol{\mu}}_0\right)^T + \frac{n^2}{N^2}\sum_{i=1}^{n_0} \left(\hat{\boldsymbol{\mu}}_0 - \bar{\mathbf{x}}\right)\left(\hat{\boldsymbol{\mu}}_0 - \bar{\mathbf{x}}\right)^T + \\ + \sum_{i=1}^{n} \left(\mathbf{x}_i - \bar{\mathbf{x}}\right)\left(\mathbf{x}_i - \bar{\mathbf{x}}\right)^T + \frac{n_0^2}{N^2}\sum_{i=1}^{n} \left(\hat{\boldsymbol{\mu}}_0 - \bar{\mathbf{x}}\right)\left(\hat{\boldsymbol{\mu}}_0 - \bar{\mathbf{x}}\right)^T .$$

As follows from equations (A-16), (A-26) and (A-27), this expression becomes

$$(N-1)\,\boldsymbol{\Psi}_N = \nu_0 \boldsymbol{\Psi}_0 + (n-1)\,\mathbf{S} + \frac{n_0\, n}{N}\left(\hat{\boldsymbol{\mu}}_0 - \bar{\mathbf{x}}\right)\left(\hat{\boldsymbol{\mu}}_0 - \bar{\mathbf{x}}\right)^T . \tag{A-32}$$

Multiplying the Likelihood eq. (A-22) with the prior pdf (A-23) results in the posterior density

$$p\left(\boldsymbol{\mu}, \boldsymbol{\Sigma} \mid \mathbf{X}\right) \propto \left|\frac{\boldsymbol{\Sigma}}{N}\right|^{-1/2} \cdot \exp\left\{-\frac{1}{2} Q(\bar{\mathbf{x}}, \boldsymbol{\mu}_0, \boldsymbol{\mu})\right\} \cdot \left|\boldsymbol{\Sigma}\right|^{-\frac{n+\nu_0+m+1}{2}} \cdot \exp\left\{-\frac{1}{2}\left(\boldsymbol{\Sigma}^{-1}(n-1)\mathbf{S} + \boldsymbol{\Sigma}^{-1}\nu_0 \boldsymbol{\Psi}_0\right)\right\} \tag{A-33}$$

with the quadratic form

$$Q(\bar{\mathbf{x}}, \hat{\boldsymbol{\mu}}_0, \boldsymbol{\mu}) = (\bar{\mathbf{x}} - \boldsymbol{\mu})^T \left(\boldsymbol{\Sigma}/n\right)^{-1} (\bar{\mathbf{x}} - \boldsymbol{\mu}) + (\hat{\boldsymbol{\mu}}_0 - \boldsymbol{\mu})^T \left(\boldsymbol{\Sigma}/n_0\right)^{-1} (\hat{\boldsymbol{\mu}}_0 - \boldsymbol{\mu}) . \tag{A-34}$$

Insertion of the total sample mean eq. (A-28) in eq. (A-34) and straightforward application of the multiplication rules for vectors and matrices leads to the expression (A-35) for eq. (A-34),

$$Q(\bar{\mathbf{x}}, \hat{\boldsymbol{\mu}}_0, \boldsymbol{\mu}) = (\hat{\boldsymbol{\mu}}_N - \boldsymbol{\mu})^T \left(\frac{\boldsymbol{\Sigma}}{n_0 + n}\right)^{-1} (\hat{\boldsymbol{\mu}}_N - \boldsymbol{\mu}) + \frac{n_0\, n}{n_0 + n} \mathrm{Tr}\left\{\boldsymbol{\Sigma}^{-1}\left(\hat{\boldsymbol{\mu}}_0 - \bar{\mathbf{x}}\right)\left(\hat{\boldsymbol{\mu}}_0 - \bar{\mathbf{x}}\right)^T\right\}. \tag{A-35}$$

So therefore, using equations (A-27), (A-31) and

$$\nu_N = \nu_0 + n = n_0 - 1 + n = N - 1 \tag{A-36}$$

the posterior pdf eq. (A-33) becomes

$$p\left(\boldsymbol{\mu}, \boldsymbol{\Sigma} \mid \mathbf{X}\right) \propto \left|\frac{\boldsymbol{\Sigma}}{N}\right|^{-1/2} \cdot \exp\left\{-\frac{1}{2}(\hat{\boldsymbol{\mu}}_N - \boldsymbol{\mu})^T \left(\frac{\boldsymbol{\Sigma}}{N}\right)^{-1} (\hat{\boldsymbol{\mu}}_N - \boldsymbol{\mu})\right\} \cdot \\ \cdot \left|\boldsymbol{\Sigma}\right|^{-\frac{\nu_N+m+1}{2}} \cdot \exp\left\{-\frac{1}{2}\mathrm{Tr}\left(\boldsymbol{\Sigma}^{-1}\left(\nu_0 \boldsymbol{\Psi}_0 + (n-1)\,\mathbf{S}\right) + \frac{n_0\, n}{N}\boldsymbol{\Sigma}^{-1}\left(\hat{\boldsymbol{\mu}}_0 - \bar{\mathbf{x}}\right)\left(\hat{\boldsymbol{\mu}}_0 - \bar{\mathbf{x}}\right)^T\right)\right\}$$

and hence with equations (A-32) and (A-36):

$$p\left(\boldsymbol{\mu}, \boldsymbol{\Sigma} \mid \mathbf{X}\right) \propto \left|\frac{\boldsymbol{\Sigma}}{N}\right|^{-1/2} \cdot \exp\left\{-\frac{1}{2}(\hat{\boldsymbol{\mu}}_N - \boldsymbol{\mu})^T \left(\frac{\boldsymbol{\Sigma}}{N}\right)^{-1} (\hat{\boldsymbol{\mu}}_N - \boldsymbol{\mu})\right\} \cdot \\ \cdot \left|\boldsymbol{\Sigma}\right|^{-\frac{\nu_N+m+1}{2}} \cdot \exp\left\{-\frac{1}{2}\mathrm{Tr}\left(\boldsymbol{\Sigma}^{-1}\nu_N \boldsymbol{\Psi}_N\right)\right\} \tag{A-37}$$

As follows from a comparison of this expression with eq. (A-23), the posterior pdf eq. (A-37) is of the same family as the prior pdf eq. (A-23). So the prior pdf eq. (A-23) meets the concept of conjugate priors described at the beginning of this appendix.

Eq. (A-23) can be rewritten as follows

$$p(\boldsymbol{\mu},\boldsymbol{\Sigma}) \propto \exp\left\{-\frac{n_0}{2}(\hat{\boldsymbol{\mu}}_0-\boldsymbol{\mu})^T(\boldsymbol{\Sigma})^{-1}(\hat{\boldsymbol{\mu}}_0-\boldsymbol{\mu})\right\}\cdot|\boldsymbol{\Sigma}|^{-\frac{\nu_0+m+2}{2}}\cdot\exp\left\{-\frac{1}{2}\mathrm{Tr}\left(\boldsymbol{\Sigma}^{-1}\nu_0\boldsymbol{\Psi}_0\right)\right\}. \tag{A-38}$$

In compliance with the interpretation of the hyperparameters $\hat{\boldsymbol{\mu}}_0$, n_0, ν_0 and $\boldsymbol{\Psi}_0$ as parameters which are related to a prior sample $\mathbf{x}_{01},\ldots,\mathbf{x}_{0n_0}$ the lack of any prior knowledge is regarded as the limit of the conjugate prior eq. (A-38) as $n_0 \to 0$, $\nu_0 \to n_0 - 1 \to -1$ and $\boldsymbol{\Psi}_0 \to 0$,

$$p(\boldsymbol{\mu},\boldsymbol{\Sigma}) \propto |\boldsymbol{\Sigma}|^{-\frac{m+1}{2}}. \tag{A-39}$$

This limit is just the multivariate Jeffreys prior density commonly proposed as non-informative prior density [6]. With this prior the posterior pdf eq. (A-37) becomes

$$\begin{aligned} p(\boldsymbol{\mu},\boldsymbol{\Sigma}\,|\,\mathbf{X}) \propto \left|\frac{\boldsymbol{\Sigma}}{n}\right|^{-1/2}\cdot\exp\left\{-\frac{1}{2}(\bar{\mathbf{x}}-\boldsymbol{\mu})^T\left(\frac{\boldsymbol{\Sigma}}{N}\right)^{-1}(\bar{\mathbf{x}}-\boldsymbol{\mu})\right\}\cdot \\ \cdot|\boldsymbol{\Sigma}|^{-\frac{(n-1)+m+1}{2}}\cdot\exp\left\{-\frac{1}{2}\mathrm{Tr}\left(\boldsymbol{\Sigma}^{-1}(n-1)\,\mathbf{S}\right)\right\} \end{aligned}. \tag{A-40}$$

This expression shows that the covariance matrix $\boldsymbol{\Sigma}$ follows an Inverse-Wishart distribution

$$p(\boldsymbol{\Sigma}\,|\,\mathbf{X}) \propto \mathrm{Inv-Wishart}\left((n-1)^{-1}\mathbf{S}^{-1};\, n-1;\, m\right) \tag{A-41}$$

with $n-1$ degrees of freedom and $m \times m$ scale matrix $(n-1)\,\mathbf{S}$ (cf. eq. (A-12)), and that the expectation vector $\boldsymbol{\mu}$ follows a normal distribution

$$p(\boldsymbol{\mu}\,|\,\boldsymbol{\Sigma},\mathbf{X}) \propto N(\bar{\mathbf{x}},\boldsymbol{\Sigma}/n) \tag{A-42}$$

with expectation $\bar{\mathbf{x}}$ and covariance matrix $\boldsymbol{\Sigma}/n$.

So therefore, by means of Monte Carlo (MC) techniques a sample $\boldsymbol{\Sigma}_{MC}$ on $\boldsymbol{\Sigma}$ can be drawn from the pdf eq. (A-41). Inserting this sample $\boldsymbol{\Sigma}_{MC}$ into the pdf eq. (A-42), a sample $\boldsymbol{\mu}_{MC}$ on $\boldsymbol{\mu}$ can be drawn from $N(\bar{\mathbf{x}},\boldsymbol{\Sigma}_{MC}/n)$. And finally, using the samples $\boldsymbol{\mu}_{MC}$ and $\boldsymbol{\Sigma}_{MC}$ in the pdf eq. (A-1), a sample $\mathbf{x}_{MC}$ on the random vector $\mathbf{x}$ can be drawn.

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