Appendix S

COMBINED UNCERTAINTY – THE MISSING LINK

Summary

\( K_{\text{eff}} \) as applied in criticality safety is often not very well understood by specialists. It is a property of a system with fissionable material, of a fissionable material or of component of that system, not an observation or estimation of real neutron transport. \( K_{\text{eff}} \) of a system depends on many specifications, parameters and variables. Uncertainties in those as well as in approximations need to be evaluated in combination, not as individual contributions determined from a base configuration. A significant contributor to the lack of understanding for \( K_{\text{eff}} \) is the assumption that \( K_{\text{eff}} \) can be modelled as a sum or product of independent reactivities. This is not possible in a single system at the same time since any change will influence the neutron flux which is a global variable. However, such an approximation may be appropriate if the uncertainties are very small, not perturbing the converged neutron flux distribution in a system property simulation, but that needs to be justified whenever such an assumption is used. The important message is that the total change or uncertainty in \( K_{\text{eff}} \) caused by multiple variations or uncertainties is not determined by multiple reactivities but by multiple changes to the neutron flux and to system specifications.

Introduction

Evaluation of criticality safety variations and incidents as well as of \( K_{\text{eff}} \) uncertainties requires a good model of neutron physics. The combined uncertainty in \( K_{\text{eff}} \) due to various parameter uncertainties needs to be determined in benchmark, reference value and criticality safety evaluations.

In this appendix, some terms and notations that may be different from definitions in other applications will be used. This is not intentional; the purpose is to describe the physics of the system in simple terms. Neutron removal refers to the fraction and energies of neutrons that are removed from the system or a system region through absorption (capture, fission, etc.). The neutron production properties refer to the probabilities for neutron-atom interactions that produce new neutrons and to other information that determines the result of the neutron removal.

\( K_{\text{eff}} \) at or near criticality is often defined as the ratio between chain-reaction-induced neutrons (excluding spontaneous fission and other fixed neutron sources) divided by removed (lost) neutrons. Not only fission but also other neutron producing reactions such as n-2n are covered. The removed neutrons refer to neutrons that were produced in the previous generation. Each generation corresponds to a converged process, meaning that a new generation only differs from the previous generation in the number of neutrons produced (amplitude), not in their spatial or energy distributions. A better definition for criticality safety is that \( K_{\text{eff}} \) is the inverse of the factor that is needed to keep the amplitude stable.
An incorrect $k_{\text{eff}}$ model

A model that is commonly used to determine the combined $k_{\text{eff}}$ uncertainty leads to the conclusion that individual $k_{\text{eff}}$ uncertainties in the same system can be independent. Such conclusions seem to be based on the relationships between the probabilities for the input parameter uncertainties. Something is missing in such a model; the global uncertainty caused by a local uncertainty in a material property. The global uncertainty is related to the neutron flux and not to a $k_{\text{eff}}$ value.

The combined uncertainty is given in an ICSBEP guide [69] (a factor 2 is missing in [92]).

\begin{equation}
    u_{\text{c}}^2(k_{\text{eff}}) = \sum_{i=1}^{N} (\Delta k_i)^2 + 2 \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} (\Delta k_i)(\Delta k_j)r_{i,j} \tag{1}
\end{equation}

This equation is a form of the general “law of propagation of uncertainties” in [94] and given below in equation (3). In equation (1), $\Delta k_i$ and $\Delta k_j$ correspond to the products of partial derivatives (sensitivity coefficients) and uncertainties as used in [94]. The correlation coefficient $r_{i,j}$ is the ratio between the covariance and the product of the uncertainties. It is always between -1 and +1. Linearity in the sensitivity of $k_{\text{eff}}$ to each input parameter and in particular to correlations is essential.

If one of the partial derivatives is zero, the correlation always becomes zero, independent of the other derivative, correlation coefficient and system changes. Correct application of reactivity equivalence covering the uncertainty range gives such a case if the linearity requirement is complied with also when the uncertainties are combined.

\begin{equation}
    k_{\text{eff}} = \sum_{i=1}^{N} k_i \tag{2}
\end{equation}

\begin{equation}
    k_{\text{eff}} = \prod_{i=1}^{N} k_i \tag{3}
\end{equation}

Besides a requirement for linearity, equation (1) with the terms representing uncertainties also assumes that $k_{\text{eff}}$ is a sum of $k_i$ over $i$, as in equation (2). If the terms had represented relative uncertainties, it is required that $k_{\text{eff}}$ is a product of $k_i$ over $i$, as in equation (3). Both these equations are possible (see below) but not if the terms or factors need to be independent. The $k_i$ values could not be reactivities determined at the same base configuration. Equation (1) is not appropriate for criticality safety evaluation of uncertainties. The missing link is the neutron flux. A combination of individual reactivities is not representative of the total system reactivity caused by multiple changes or uncertainties.

A realistic $k_{\text{eff}}$ model

A way of describing $k_{\text{eff}}$ is as a function $F(S)$ where $S$ or rather $S(V,E)$ is a variable standing for system or material (equivalent when the material positions are specified) properties covering all volume positions ($V$) and all neutron energies ($E$). The dependences on $V$ and $E$ will not be specified for each variable and parameter but they must be considered. $S$ contains all parameters required to determine the $k_{\text{eff}}$ related physics of the system. $S$ is a global variable. If it is divided into components (volume and/or energy region), each component is dependent on other components. This is easy to realise, e.g. by exchanging the locations of fissile material with reflector material components.
The function $F(S)$ can be written as $R_r(S)\Sigma_p$, where $R_r(S)$ stands for the neutron removal distribution. This distribution consists of neutrons removed from a converged chain-reaction-induced neutron source (fission, n-2n, etc.) generation that is normalised to one neutron. Leaked neutrons are included as captured neutrons in an outer, non-fissionable region. $\Sigma_p$ contains all sub-parameters needed to determine the number and properties of produced neutrons from information on each neutron removal, but not to determine the interaction relations between different regions. This distinction makes $S$ very different to $\Sigma$. The neutron production is determined by $R_r(S)\Sigma_p$.

The equation is first written as a function $F$, then as a vector product which is then described by the sum of products and finally translated into a sum of $k_{eff}$ contributions. The large $\Sigma$ is a summation symbol, not to be confused with the parameter $\Sigma$. The dimension $N$ of both vectors (1xN and Nx1) is determined by the number of regions. The vector product gives the normalised sum of produced neutrons in each region. This is equivalent to a numerical $k_{eff}$ contribution from this region (not to be confused with a reactivity value of the region). The corresponding equations using integrals are not needed here. A region may be related both to volume and to energy properties of the material (making $N$ equal to the product of volume and energy regions).

A local change in a material specification not only changes the $k_{eff}$ contribution from the associated regions but also all other $k_{eff}$ contributions. This is already obvious from a physics point of view and the equation (4) shows the connections. The missing link is that every $R_{r,i}$ is correlated, not only to every $\Sigma_{p,j}$, but to other $R_{r,j}$.

The combined variance of $k_{eff}$ due to combined uncertainties in $R_r$ and $\Sigma_p$ and where $\nu(R_r, \Sigma_p)$ is the covariance can be expressed [94] as

$$u_e^2(k) = \left( \frac{\partial F}{\partial \Sigma_p} \right)^2 u^2(\Sigma_p) + \left( \frac{\partial F}{\partial R_r} \right)^2 u^2(R_r) + 2 \frac{\partial F}{\partial \Sigma_p} \frac{\partial F}{\partial R_r} \nu(R_r, \Sigma_p)$$

This is a first order Taylor series expansion of the variance, assuming linearity in the relations. The linearity of the sensitivity coefficients (the partial derivatives) need to be preserved not only for the single variance terms but also for the correlated term which should mirror the physics effect of the combination. Linearity when only one parameter at a time is changed is not sufficient. Correlations between only two uncertainties at a time are not sufficient when there are more uncertainties. The linearity compliance may be realistic for measurements but not for many criticality safety evaluations.

A more practical solution is found if the system is divided into the $N$ regions mentioned above. An uncertainty in $S_i$ in the system region $i$ may lead to an uncertainty in $\Sigma_{p,i}$ and in $\Sigma_{p,j}$ in other regions $j$ (zero in a non-fissionable region and in many other cases) but always leads to uncertainties in $R_{r,j}$ in every region $j$. The uncertainties in $R_{r,j}$ and $\Sigma_{p,j}$ are always correlated (the covariance is not zero) if the $\Sigma_{p,j}$ uncertainty is not zero. Uncertainties in $R_{r,i}$ and $R_{r,j}$ are always correlated.

$R_{r,j}$ for each region $j$ is a function of the global system parameter $S$. $\Sigma_{p,i}$ is a function of the local system parameter $S_i$. Uncertainties in $S_i$ in the same or in different regions are correlated through $R_r$.

Since the function $F$ can be given as the product $R_r(S)\Sigma_p$, the variance equation above can be simplified by referring to relative uncertainties. The partial derivatives are easy to calculate ($\Sigma_p$ and
\[ R_r(S) \text{ respectively) and after division by } R_r(S)\Sigma_p \text{ (to create relative uncertainties) and introducing the coefficient } r \text{ to indicate correlation between the uncertainties, the equation can be transformed to} \]

\[
\left( \frac{u_c(k)}{k} \right)^2 = \left( \frac{u^2(\Sigma_p)}{\Sigma_p} \right)^2 + \left( \frac{u^2(R_r)}{R_r} \right)^2 + 2r \frac{u(\Sigma_p) u(R_r)}{\Sigma_p R_r} \tag{6} \]

An uncertainty in a material parameter \( X_j \) in a system is equivalent to uncertainties in the system variable \( S \) (always in \( R_r(S) \) and sometimes in \( \Sigma_p \)). The parameter \( X_j \) can be divided into the \( N \) regions referred to above. Each regional parameter is referred to as \( X_{j,i} \).

If the parameters \( X_{j,i} \) for each region \( i \) are combined into the regional parameter \( S_i \), the equations can be simplified, without losing any information. The correlations between different \( X_j \) parameters need to be observed when the region variables \( S_i \) and associated uncertainties and covariances are determined.

\[
S_i = \sum_{j=1}^{M} X_{j,i} \tag{7} \]

Each change in a system influences the global parameter \( S \) and thus \( R_r(S) \). The uncertainty \( u_c(\Sigma_p) \) due to uncertainties in \( S_i \) in each region \( i \) of the system can be determined as

\[
u^2(\Sigma_p) = \sum_{i=1}^{N} \left( \frac{\partial \Sigma_p}{\partial S_i} \right)^2 \left( u^2(S_i) + 2 \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} \frac{\partial \Sigma_p}{\partial S_i} \frac{\partial \Sigma_p}{\partial S_j} \nu(S_i, S_j) \right) \tag{8} \]

\( \Sigma_p,i \) represents the neutron production related information for each region \( i \), while \( S_i \) represents the total system information for region \( i \). An example of correlated uncertainties is the uncertainties in temperatures of different volume regions. Another example of correlation is the neutron flux.

The variance \( u^2(R_r) \) due to uncertainties in \( S_i \) in each region \( i \) of the system is determined as

\[
u^2(R_r) = \sum_{i=1}^{N} \left( \frac{\partial R_r}{\partial S_i} \right)^2 \left( u^2(S_i) + 2 \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} \frac{\partial R_r}{\partial S_i} \frac{\partial R_r}{\partial S_j} \nu(S_i, S_j) \right) \tag{9} \]

It is repeated that \( S \) does not only represent the material structure and geometry but all system properties, including neutron physics. In general, the “sensitivity coefficients” (partial derivatives) for the neutron removals are more significant than for the material neutron production properties of the materials, making the correlations in equation (9) stronger than in equation (8).

The conclusion is that if there is an uncertainty in the system, whether it is an uncertainty in the material properties or in the configuration of the materials, the system response to other uncertainties will become different. The effect of a combination of uncertainties cannot be determined from the individual uncertainties, the correlations must be considered.
Reality checks

It is easy to find cases where non-linearity applies. Essentially all relations between $k_{\text{eff}}$ and an input parameter are non-linear. Only for small uncertainties, the linearity applies. A linear relation could be valid for a parameter that is designed for that purpose. In the case of combined and significant uncertainties, it would be difficult to maintain the linearity.

An example of combined uncertainties is taken from the reactivity worth of control rods in a nuclear reactor at zero power level. Assume that all uncertainties in $k_{\text{eff}}$ due to the control rod axial position are identical, follow a linear relationship with $k_{\text{eff}}$ and that the events causing the uncertainties are independent. The combined effect of two simultaneous uncertainties is requested. The system is assumed to be maintained just critical using a global parameter (boron concentration or water level).

Some people would now say that there is no correlation between the uncertainties. The combined effect of any two uncertainties are said to be identical, independent of the horizontal locations of the control rods in the reactor. It makes no difference whether they are adjacent or in opposite “corners”.

In reality, a partial insertion of a control rod would reduce the effect of an adjacent cluster since the neutron flux would be depressed in this part of the reactor. The opposite would be true for a partial removal of the control rod. The correlation effects are relatively strong in both cases. On the other hand, a partial insertion or removal of one control rod may not significantly change the effect of a control rod in the opposite “corner” of the reactor. The correlation effect is relatively weak.

It is very likely that the case of a combined uncertainty of two adjacent control rods will violate the linearity requirement of the sensitivity coefficients.

A proper physics model leading to a close simulation is needed to evaluate critical experiments. It may be even more important when simplified benchmarks are designed.

Examples of the various variables and parameters are useful to test and understand the model. The thickness of a steel plate in water between fissile materials is a parameter $X_1$. The thicknesses of the water regions on either side of the plate can be represented by the additional parameters $X_2$ and $X_3$. The total thickness of the three regions is a fourth parameter $X_4$. The dimensions are correlated. The uncertainties are correlated. Correlations to uncertainties in other dimensions (e.g. the fissile material) are not significant. The local neutron flux is changed by a change in water moderation. The global neutron flux is changed since the changed moderation changes the fission distribution. The absorption fractions in the steel and in the water are changed.

The variable $S_1$ may represent the steel plate and the first energy group. All the uncertainties in $X_1$-$X_4$ contribute to the uncertainty in $S_1$ through the uncertainty in the neutron flux. There is no neutron production in the region 1 so the parameter $\Sigma_{p,1}$ remains zero. However, the uncertainty in the global neutron removal distribution $R_r(S)$ is influenced, including $R_{r,1}$. 