Appendix M
NUMERICAL AND STATISTICAL CONSIDERATIONS

This appendix collects a number of issues related to precision, accuracy, convergence, interpolation, extrapolation, etc. that determine the quality of the results.

Precision of reference values

A reasonable target for the numerical and statistical values obtained from deterministic and Monte Carlo codes is a k_{eff} with a precision of 0.001. Better precision is achievable but may not be meaningful at this stage. This k_{eff} target is translated into units of reference values by taking the logarithm of the reference value unit to changes in k_{eff} (Appendix D). This is how the least significant digit before (positive logarithmic value) or after the decimal point (negative logarithmic value) is obtained. The precision in the reference value will thus correspond to between 0.0001 and 0.001 in k_{eff}.

The useful precision in biases and uncertainties depends on the application and whether systematic effects are to be evaluated. As proposed in [69], at least two significant digits are motivated in each standard deviation. However, the recommendation that a measured value should have the same precision is not clear. Systematic effects could motivate much better precision in the standard deviation than in the measured value. A coverage factor larger than one may motivate a higher precision of the standard deviation.

Accuracy of reference values

Unlike the precision, a requested accuracy may be difficult to achieve. It depends on many error sources. The availability and quality of adequate benchmarks (for cross-sections, nuclide densities and other data) is of particular importance. The propagation of uncertainties from various error sources, using results of verification to a total uncertainty related to an overall validation is often very complicated. There are not many benchmarks that cover validation in one step.

Linearity of relations, normality of statistical distributions

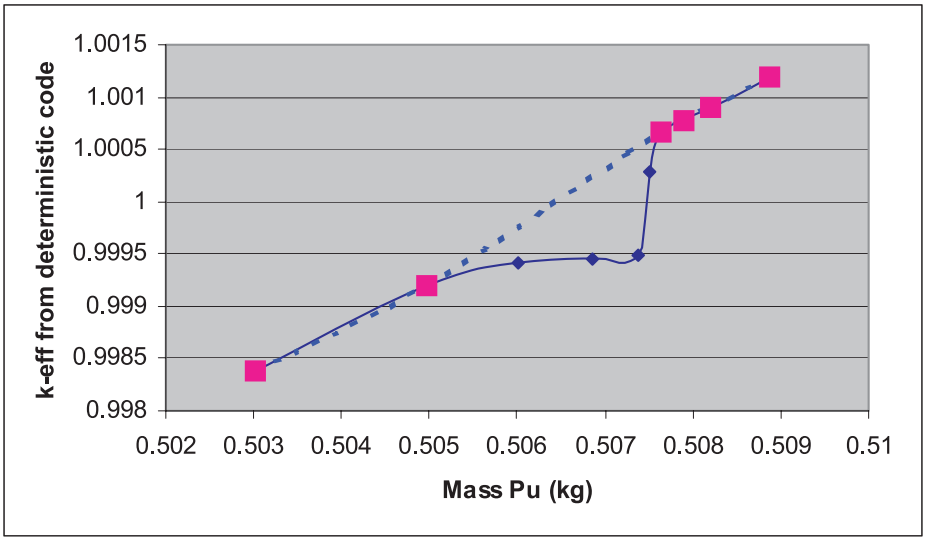
Many equations and other relations are based on approximations that require linearity or normal distribution. The treatment of uncertainties is an example where linear relations are often required. Normal distribution of statistical data is another requirement related to uncertainty treatment that is sometimes taken for granted.

A combination is found where the statistical distribution near the mean is more or less symmetrical while it becomes very asymmetrical further away from the mean. This is one of the reasons why the uncertainty allowance is better represented by a 95% rather than a 66% limit of confidence. In criticality safety, even a 99.9% limit of confidence is required by many authorities.

Numerical convergence

During the evaluation of reference values using SCALE 4 in 2000, it became apparent that there was a problem with convergence, see [29].

Figure M1. Convergence deviation



The line with the diamond markers correspond to actual calculation results with XSDRNPM using the default convergence criterion of 10^{-4}. The dotted line and the squares correspond to the correct values. The calculations and the figure were made to demonstrate a problem to the code developers at ORNL. Their conclusion was that it was a convergence problem. Sure enough, increasing the convergence criterion to 10^{-5} solved the problem. SCALE 5 now has that as a default criterion. ORNL improved such parameters in its SCALE 4.3 contributions to this study.

It is easy to see the potential for serious mistakes if unconverged results are used to determine sensitivities, reactivities, etc.

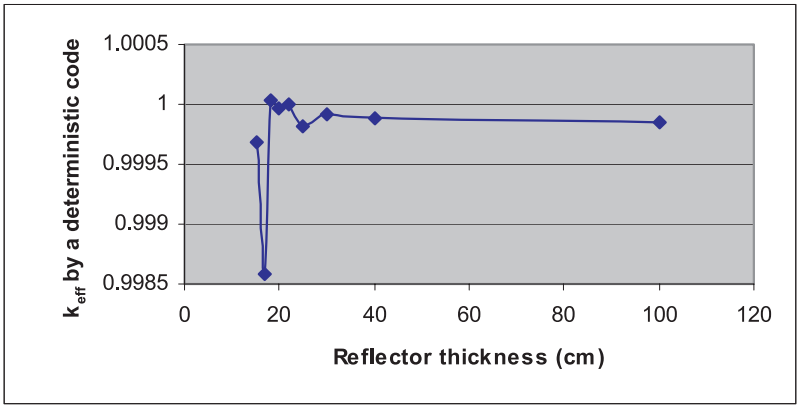
Geometry mesh

Modern computer codes are built into packages that simplify the work for the user in different ways. One way is to determine default parameters that are adequate for typical user problems. The mesh distribution for deterministic codes is important for the accuracy of the result but also for the calculation time. A balance between these objectives is determined by the code developers. It is the user's responsibility to make sure that the automatically generated mesh is sufficient for the problem being solved.

In SCALE 4, the mesh distributions in the fissile material centre and in the reflector are calculated by default. The user can change them by a size factor (SZF) in the calculation sequence CSAS1X or by running the XSDRNPM code separately, with full control of all input. The difference between an external reflector and a moderator between heterogeneously distributed fissile "lumps" is clear to the user. It may not be so easy when a default mesh strategy is implemented in the calculation system.

During evaluations of graphite and other reflectors, a peculiar consequence of inadequate default mesh distributions was discovered, see Figure M2. Increasing the reflector thickness, it was found that k_{eff} went through a sequence of variations, with an optimum at some thickness. The figure was generated for water but the behaviour was more dramatic for graphite. From a physics point of view there is nothing to explain the behaviour; there is only a water reflector and nothing else outside this water.

Figure M2. Optimum reflection



The default mesh was sufficient for a lattice of fuel rods or similar problems. For a thick reflector, it was not sufficient. Similar conclusions can be made for several of the systems covered by the study reported here. In particular for thin (neutronically) slabs such as solid $U(100)O_2$ and all plutonium isotope distributions in PuO_2, the mesh distribution had to be tightened to get good results. This was demonstrated by comparison of XSDRNPM and KENOVa calculations with the same cross-section libraries.

Angular quadrature

During the comparison of XSDRNPM and KENOVa calculations using the same cross-section libraries, it was found that the default angular quadrature of 8 in SCALE is not sufficient for fast systems. It was particularly important to increase the quadrature for volumes, less important for cylinder diameters and least for slabs. The example inputs for ICSBEP Handbook benchmarks give examples of an angular quadrature of 64. This was found to be necessary also for fast spheres in the current study. For cylinder and slabs the quadrature used for fast systems was 32.

Source convergence and initial transients in Monte Carlo calculations

The systems involved in the reference value calculations are simple and no difficulty is expected concerning source convergence. The benchmarks used to validate the reference values are not very complicated either. However, to reduce the uncertainty due to source convergence and initial transients (insufficient number of initial neutrons skipped), the total number of generations were often increased compared with sample inputs and the number of skipped neutrons were also increased. Similar statistics were also applied to the calculation of reference values with the Monte Carlo codes KENOVA (SCALE 5) and MCNP5.

Error sources, uncertainties, systematic and random effects

Various error and uncertainty terms have been described in Appendix B. In general they seem to comply with the recommendations in the U.S. standard [94] and in the ICSBEP Handbook [68].

Examples of these terms can be taken from the validation of reference values in this study. The average deviation between calculation results and benchmarks is a combined bias of many error sources. The remaining statistical uncertainty, obtained from making the average determination, is often assumed to be normally (Gaussian) distributed. The uncertainty gives a random effect for a single application but a systematic effect for a group of applications. The safety and economic effects of the uncertainty, as applied to many systems or operations, are systematic.

Combination of uncertainties

This issue seems to be controversial but has direct support in the U.S. standard [94] and in an ICSBEP Guide [69]. Before the discussion on combined uncertainties, an example follows.

Consider the neutron absorption rate A in a plate. Two equations are used to demonstrate the determination of the combined (total) uncertainty. The first equation is a simple sum of the absorptions A_1, A_2 and A_3 in the present nuclides 1, 2 and 3.

$$A = A_1 + A_2 + A_3 \qquad (1)$$

The other equation is related to the three input parameters neutron flux Φ in the plate, to the total absorption cross section Σa of the plate material and to the thickness T of the plate. The constant c is used to obtain the following relation:

$$A = c * \Phi * \Sigma_a * T \qquad (2)$$

How do the uncertainties in the individual input parameters influence the total uncertainty in A?

The following equation is taken from the ICSBEP Guide [69]:

$$u_c^{\,2}(k_{eff}) = \sum_{i=1}^{N} (\Delta k_i)^2 + 2\sum_{i=1}^{N-1} \sum_{j=i+1}^{N} (\Delta k_i)(\Delta k_j) r_{i,j} \qquad (3)$$

The input parameters are indicated by “i” and “j”. The equation is used to combine uncertainties in k_{eff} to a combined uncertainty. Standards, guides and handbooks often refer to this equation or the same principle. A necessary requirement is that all relations (sensitivities) are linear, also when the uncertainties are combined. If all uncertainties are independent, the second summation term vanishes. Can Δk values in the same system at the same time be independent? Is the equation (3) representative for the uncertainty in k_{eff}, in particular when the system is significantly sub- or supercritical?

Criticality safety specialists often answer: “Yes, if the input parameters are independent, then the uncertainties are also independent”. “Yes, this equation can be applied to evaluation of the uncertainty in k_{eff} “.

Now, to consider the input parameters, let's look at a more general source for combination of uncertainties, the U.S. standard [94]:

$$u_c{}^2(y) = \sum_{i=1}^{N}\left(\frac{\partial f}{\partial x_i}\right)^2 u^2(x_i) + 2\sum_{i=1}^{N-1}\sum_{j=i+1}^{N}\frac{\partial f}{\partial x_i}\frac{\partial f}{\partial x_j}v(x_i, x_j) \quad (4)$$

Here $y = f(x_1, x_2 \ldots x_N)$. The equation (4), often referred to as the law of propagation of uncertainty, contains input uncertainties $u^2(x_i)$ and input covariances $v(x_i, x_j)$. An important factor now is the partial derivative $\partial f/\partial x_i$. It is sometimes referred to as a sensitivity coefficient. Does that make it a constant? Certainly not, as will be seen by the continuation of the example started in the beginning of this section. The equation is based on a first order Taylor expansion of the function y. This is probably not sufficient for many criticality safety evaluations with crude approximations and associated uncertainties.

Going from equation (4) to (3) means that the neutron flux has to be considered as a parameter within the range "i" of parameters. This will not be easy to do. The flux uncertainty is a function of every other parameter uncertainty. The sensitivity of k_{eff} to a flux uncertainty (a probability distribution) is a very complex problem to solve. The covariances between the flux and other uncertainties will not be zero.

If equation (1) includes only independent uncertainties, each partial derivative becomes one and the equation becomes a summary of the variances (square of standard deviations).

$$u_c{}^2(A)_{total} = \sum_{i=1}^{N} u^2(A_i) \quad (5)$$

Are the uncertainties independent? The three terms in equation (1) are essentially based on equation (2) for each nuclide.

If the input parameters in equation (2) are independent, the partial derivatives becomes $c*\Sigma_a*T$, $c*\Phi*T$ and $c*\Phi*\Sigma a$ respectively. The independence of the input parameters makes **their** correlation term vanish. However, the uncertainty terms are correlated to the input parameters through the partial derivatives (all but one term) or the input parameter uncertainty (the remaining term). The terms in the sum are correlated through their common dependence on each input parameter.

$$u_c{}^2(A)_{total} = \left(c\sum_a T\right)^2 u^2(A_1) + \left(c\Phi T\right)^2 u^2(A_2) + \left(c\sum_a \Phi\right)^2 u^2(A_3) \quad (6)$$

There is a simpler way of writing this relationship using relative uncertainties. It applies to functions that depend on products of parameters (covers division since it is a product of the inverse parameter). It is easy to derive by dividing the equation with the square of the function (A or $c*\Phi*\Sigma_a*T$).

$$\frac{u_c{}^2(A)_{total}}{A^2} = \frac{u^2(A_1)}{A_1^2} + \frac{u^2(A_2)}{A_2^2} + \frac{u^2(A_3)}{A_3^2} \quad (7)$$

The ratios are relative variances. The relationship still requires independence between the input parameters. It must not be more complicated than a product of two ore more parameters.

Of the three input parameters Φ, Σ_a and T, there is one that is influenced by the others. It is of course the neutron flux Φ. Even if the beam from some neutron source will not be influenced by the other two input parameters, Σ_a and T, the neutron flux in the plate will be. Self-shielding related to resonance absorption is familiar to criticality safety specialists. The neutron energy spectrum will be depleted by strong absorption in the plate. Each absorber nuclide will change the spectrum for the other nuclides. Moderation and reflection will do the same. This is dependence.

In a critical system, the situation is much more complex. The relationship of k_{eff} to the transport equation is not a simple product of independent parameters. Unlike the neutron beam in the previous paragraph, the neutron source is very strongly dependent on the changes in the system. A reduction of the plate thickness or removal of strong neutron absorbers from the plate may actually increase the neutron absorption in the plate. The reason would be that the removal of the absorber nuclides causes the fundamental mode to change to give a very strong neutron flux in the plate (an increase of the neutron flux by ten orders of magnitude and more is possible).

The answers to the two questions are thus “No, the Δk values can’t be independent” and “No, equation (3) is not a reasonable representation of the k_{eff} uncertainty”. The neutron flux correlation is a missing link. Rather than rewriting this section to propose a solution, a separate Appendix S is added.

Interpolation

The different contributors have approached the issue of moderation optimisation differently. Similarly, the issue of interpolation to obtain critical values from values near criticality has been treated differently. An important issue is how close the calculation points are. Significant interpolation errors have been observed.

In the EMS contribution from 2001, an effort had been made to determine a reasonable precision of the requested values. This is the same logarithmic method as used in this report, Appendix D. Optimisation and interpolation were made to allow such precision. A comparison with other contributions shows that they sometimes are not as precise. Large spacing between parameter values without adequate curve-fitting leads to quite large errors in a few cases.