ICSBEP Guide to the Expression of Uncertainties

Editor

V. F. Dean

Subcontractor to Idaho National Laboratory

Independent Reviewer

Larry G. Blackwood (retired)

Idaho National Laboratory

ACKNOWLEDGMENT

We are most grateful to Fritz H. Fröhner**,** Kernforschungszentrum Karlsruhe**,** Institut für Neutronenphysik und Reaktortechnik, for his preliminary review of this document and for his helpful comments and answers to questions.

This guide was prepared by an ICSBEP subgroup led by G. Poullot, D. Doutriaux, and J. Anno of IRSN, France. The subgroup membership includes the following individuals:

J. Anno	IRSN (retired), France
J. B. Briggs	INL, USA
R. Bartholomay	Westinghouse Safety Management Solutions, USA
V. F. Dean, editor	Subcontractor to INL, USA
D. Doutriaux	IRSN (retired), France
K. Elam	ORNL, USA
C. Hopper	ORNL, USA
R. Jeraj	J. Stefan Institute, Slovenia
Y. Kravchenko	RRC Kurchatov Institute, Russian Federation
V. Lyutov	VNIITF, Russian Federation
R. D. McKnight	ANL, USA
Y. Miyoshi	JAERI, Japan
R. D. Mosteller	LANL, USA
A. Nouri	OECD Nuclear Energy Agency, France
G. Poullot	IRSN (retired), France
R. W. Schaefer	ANL (retired), USA
N. Smith	AEAT, United Kingdom
Z. Szatmary	Technical University of Budapest, Hungary
F. Trumble	Westinghouse Safety Management Solutions, USA
A. Tsiboulia	IPPE, Russian Federation
O. Zurron	ENUSA, Spain

The contribution of French participants had strong technical support from Benoit Queffelec, Director of the Société Industrielle d'Etudes et Réalisations, Enghien (France). He is a consultant on statistics applied to industrial and fabrication processes.

FOREWORD

The methods used by the International Criticality Safety Benchmark Evaluation Project (ICSBEP) to treat uncertainties encountered in experimental data and in the derivation of benchmark models have evolved significantly since the project was initiated in 1992. At an ICSBEP Meeting in Portland, Maine (1999), the Working Group expressed the need for a guide to the treatment of uncertainties in order to assist the work of both evaluator and reader.

Because of this historic background, when using an evaluation reported in the "International Handbook of Evaluated Criticality Safety Benchmark Experiments," the reader will often encounter, especially in evaluations written before 2001,

- mixing of uncertainties in physical parameters that are standard deviations coming from a large number of measurements with those given as tolerances, or bounds,
- lack of information about the sources of given uncertainty values, including level of confidence and degrees of freedom corresponding to reported uncertainties,
- inconsistencies in the coverage factor (corresponding to 1, 2 or 3 σ) between the different uncertainties,
- after the uncertainties in physical parameters are propagated to obtain an equivalent reactivity uncertainty of k_{eff}, this total experimental uncertainty is given without mentioning the level of confidence.

The mean and standard deviation are now recommended as optimal estimates for a parameter and its uncertainty. If these are used for the benchmark model and to calculate the uncertainty in k_{eff}, then, when the probability distribution of k_{eff} is Gaussian (a reasonable assumption in many cases), the level of confidence of the k_{eff} uncertainty range will be approximately 68%.

This guide, written to develop a consistency among evaluators in the uncertainty treatment (Sections 2, 3.1, and 3.5 of the ICSBEP evaluation), is based on two main references, which are the respective U.S. and European standards. The standards are very similar and have the same origin, namely, the International Standard Organization (ISO) Guide to the Expression of Uncertainty in Measurement, published in 1995. These two main references are

- Reference 1 – "American National Standard for Expressing Uncertainty - U.S. Guide to the Expression of Uncertainty in Measurement," ANSI/NCSL Z540-2-1997 (Copyright © 1997 by National Conference of Standards Laboratories, All rights reserved.). and

- Reference 2 – "Guide pour l'expression de l'incertitude de mesure." European Pre-standard NF ENV 13005 Août 1999.

TABLE OF CONTENTS

TABLE OF CONTENTS (cont'd)

TABLE OF CONTENTS (cont'd)

APPENDICES

TABLE OF CONTENTS (cont'd)

1.0 GENERAL CONSIDERATIONS IN THE DETERMINATION OF UNCERTAINTIES

1.1 Benefits of determining best estimates of uncertainties

Every criticality experiment has numerous associated uncertainties. How close the assembly was to critical, k_{eff}=1.0000, is perhaps the most obvious uncertainty for a critical benchmark, but usually is among the least significant. An important uncertainty is in the exact contents of the assembly, the masses and compositions of constituents. Similarly, the geometry (dimensions and relative positions such as tank diameter or array pitch) is never known perfectly. While absolute truth, in this case the *exact* configuration, is unknowable, the attainable goals are an estimate of it (the benchmark model) and an estimate of how well the configuration and its neutronic state are known.

But why should the evaluator make a substantial effort to identify and quantify all the uncertainties? There is no disputing the principle that estimates of physical quantities (here the input quantities that define the benchmark model) are of little use if there is no knowledge of how reliable the estimates are. The real question is, why is it important to carry out a rigorous uncertainty analysis? Why is a rough estimate of the total uncertainty not good enough?

An immediate benefit of a rigorous analysis accrues in qualifying codes and cross sections used in criticality assessments. If the benchmark models used in the validation analysis have realistic uncertainties, then the resulting calculation bias and its associated uncertainty will better reflect the accuracy of the criticality calculations.

A longer-term benefit is improvement of the state of the art of criticality safety. Criticality safety benchmarks can be used for this purpose only if their total uncertainties are well known. Realistic uncertainties from a diverse set of experiments provide the data needed to uncover weaknesses in neutron cross section data and calculational methods. Once these weaknesses have been characterized, it should be possible to reduce or eliminate them. This process holds the promise of more accurate criticality safety calculations in the future. This is important despite the fact that a large safety margin usually is added.[a] Firm knowledge of the uncertainty provides a foundation for setting appropriate safety margins. As the state of the art improves, smaller safety margins can be justified.

Best-estimate parameter values and uncertainties are needed to attain these goals. The evaluator should resist any tendency to either overestimate or underestimate uncertainty. It is a misconception that making large uncertainty estimates is always a conservative approach for criticality safety. **If the total uncertainty is unrealistically large, some existing biases may be hidden in the uncertainty margins when comparing calculational results and benchmark values.** In that case the computer code/nuclear data might be considered as validated in the domain of the benchmarks, while actually a bias may exist. On the other hand, **if the total uncertainty is unrealistically low, calculation results may appear erratic or indicate a bias where none exists. This may lead, incorrectly, to modifications of cross sections or lack of**

[a] Safety margins are added for many reasons, not only as a result of qualification.

confidence in codes or experiments, when the real deficiency was neglected uncertainty. Therefore the uncertainty reported in the benchmark evaluation must be as realistic and accurate as possible. This requires the evaluator to be rigorous, complete, and objective.

1.2 The uncertainty analysis

1.2.1 Evaluation of experimental data

The evaluator typically must perform an uncertainty analysis for the experiment that goes beyond that reported by the experimenters. Experimenters often have not performed as thorough an uncertainty analysis as required for the benchmarks. In the case of decades-old measurements, the experimenters did not have calculational tools as powerful as those available today with which to estimate uncertainty components. Effects of small experimental uncertainties that may have been recognized as negligible in validation of calculational methods available at that time might be larger than current methods' uncertainties. That is, the experimenters may not have perceived a need for the rigorous uncertainty determination expected by today's code users. Small effects that may have seemed negligible at the time of the experiments are recognized today as worth considering as sources of uncertainty. Accordingly, the evaluator needs to make a critical assessment of the uncertainties described by the experimenters and try to remedy any weaknesses.

It is often in the context of filling gaps in the experimenter's uncertainty analysis that the most difficult challenges arise for the evaluator. In this situation there is usually a lack of information in the reported experimental data. For example, no uncertainty is reported, or an uncertainty is reported without indicating its level of confidence, its source, or how it was measured. Faced with a lack of information the evaluator might be inclined to assign a large uncertainty, e.g. by assuming arbitrarily that the "questionable" uncertainty corresponds to one standard deviation (1σ). As discussed above, this inclination should be resisted. Instead, the evaluator should base the uncertainty estimate on an understanding of the physical phenomena causing the parameter to vary about its nominal value. If the phenomena involved are not within the scope of the evaluator's expertise, it is prudent to consult experts and/or the pertinent literature. Methods and habits at the time of the experiment may also be considered.

1.2.2 Additional uncertainty from creating the benchmark model

Even if the experimenters provide a thorough uncertainty analysis for the experimental configuration, the evaluator must extend it to the benchmark model. It is always necessary to transform, or simplify, the as-built experimental configuration into a practical benchmark model. At a minimum, the extent to which the surrounding environment is included in the model must be limited. Typically, additional simplifications are made. Each simplification introduces a bias in k_{eff} compared to the experiment, with an associated uncertainty. When calculations are used to determine the bias, as is usually the case, the evaluator should consider cross section data and the limitations of calculation methods as potential contributors to the uncertainty in the bias, as well as limitations of his knowledge of the details that are modeled and then omitted or simplified.

The transformation-related biases and uncertainties must be combined with the k_{eff} and Δk_{eff}, respectively, of the as-built experiment to obtain the benchmark-model k_{eff} [a] and uncertainty.

The evaluator should strive for a reasonable balance between making the benchmark model amenable to calculation and keeping the total k_{eff} uncertainty of the model as small as practical. Obviously, simplifications that make the benchmark model easier to use tend to make it more attractive to criticality safety analysts. However, each simplification introduces an additional uncertainty contribution. The use of benchmark models to validate a criticality safety analysis or to identify weaknesses in cross section data and calculational methods is more effective if the uncertainties are small. The only stage in the evaluation process where the evaluator legitimately can influence the magnitude of the total uncertainty is in deciding what simplifications to make to create the benchmark model.

1.2.3 An objective, rigorous, graded approach

Since performing a rigorous uncertainty analysis requires a lot of work, there is motivation to perform the task efficiently. The most efficient strategy for the uncertainty analysis is a graded approach, in which the effort expended in quantifying an uncertainty component is roughly proportional to the contribution of the component to the total uncertainty. **Little effort is warranted if a simple estimate shows that the uncertainty in the parameter makes a small contribution to the total uncertainty in k_{eff}. Conversely, a large contributor warrants careful consideration.** If a potentially large contributor is one for which there is a lack of readily available information (a "questionable" uncertainty), then it must be further investigated through, for example, extra measurements or analysis, checking in logbooks and other reference documents, or interviews.

To put into perspective what constitutes a small contributor, consider that a single component that is 10% as large as the total uncertainty makes a ½% contribution to the total when the components are added in quadrature (i.e., square root of sum of squares of components).[b] Thus, a small number of components of this size or less have little effect on the total. When the evaluator cannot anticipate the relative magnitudes of the various uncertainty components, an iterative strategy may be appropriate. In that approach, simple, scoping estimates would be made for all parameters in the first iteration and, in subsequent iterations, the important contributors would be estimated more carefully.

[a] The **benchmark-model k_{eff}** is the best estimate of the value of k_{eff} that would be observed for an isolated experiment having exactly the geometry and materials described in the benchmark model. Therefore, it is also the result expected from a calculation of the benchmark model.

[b] For example, an uncertainty of 0.003 added in quadrature to an uncertainty of 0.03 gives $\sqrt{(0.03)^2 + (0.003)^2}$ = 0.03015, which is an increase of only 0.00015/0.03 = 0.005 = 0.5%.

1.3 Level of confidence

Although the true value of k_{eff} of the configuration described by the benchmark model is not known, the evaluator estimates its value, based on all relevant experimental data and knowledge. The evaluator's estimate is called the "benchmark-model k_{eff}." The evaluator also estimates the overall uncertainty in order to indicate how k_{eff} would vary as values of the parameters vary within their uncertainty ranges. Of course, the value of each parameter in the model is the evaluator's best estimate of its true value. Similarly, the probability distributions of the parameters used to calculate the k_{eff} uncertainty are best estimates based on all available data and knowledge.

In order for the overall uncertainty in the benchmark-model k_{eff} to be useful, it is necessary that its approximate level of confidence be stated. The preferred uncertainty for the benchmark-model k_{eff} is an estimate of its standard deviation, σ.

As mentioned previously, experiment documentation may give uncertainty without specifying its source or how many standard deviations it represents. As part of the evaluation, the evaluator describes whatever is known about the sources of reported uncertainty values so that standard uncertainties (estimates of standard deviations) can be determined. Then the effects of the standard uncertainties are calculated and combined to obtain the overall uncertainty of k_{eff} of the benchmark model.

For a parameter whose probability distribution is normal, or Gaussian, one standard deviation ($\pm\sigma$) represents a 68% confidence level; i.e., the probability that the true value of the parameter is within $\pm\sigma$ of its mean value is 68%. Because k_{eff} depends on many physical parameters, the assumption of a normal probability distribution for k_{eff} of the benchmark-model configuration is usually reasonable (§G.2 of Reference 1). If the uncertainty of k_{eff} is not dominated by the contribution from any single non-normal parameter distribution, and if k_{eff} is approximately linear within the uncertainty ranges of the independent parameters, the standard deviation of k_{eff}, obtained from standard deviations of the independent parameters affecting it, will represent an approximate 68% level of confidence.

1.4 The guide

While this guide describes the important principles and suggests procedures, it is not a "cookbook". This point is well stated in §3.4.8 of Reference 1.[a]

> Although this guide provides a framework for assessing uncertainty, it cannot substitute for critical thinking, intellectual honesty, and professional skill. The evaluation of uncertainty is neither a routine task nor a purely mathematical one; it depends on detailed knowledge of the nature of the measurand and of the measurement. The quality and utility of the uncertainty quoted for the result of a measurement therefore ultimately depend on the understanding, critical analysis, and integrity of those who contribute to the assignment of its value.

[a] ANSI/NCSL Z540-2-1997

The importance of using sound technical judgment cannot be overemphasized. It is the primary asset in performing the uncertainty analysis.

This guide presents a recommended methodology, more or less already used by the scientific community, in a form that each ICSBEP evaluator can implement. Its purpose is to provide guidelines on the treatment of uncertainties in the evaluation of critical experiments by ICSBEP participants.

The remaining sections of this document contain more specific guidance. In particular, see Appendix C for several illustrative examples.

- Section 2 – Definitions of key terms and statistical quantities.
- Section 3 - An inventory of the usual uncertain parameters on which k_{eff} depends.
- Section 4 - Approaches for calculating the Δk effect of the uncertainty in a parameter.
- Section 5 - Systematic effects and their uncertainties.
- Section 6 - Method of obtaining the combined k_{eff} uncertainty.
- Section 7 - References.
- Appendices – A glossary and specific methods.

2.0 METROLOGY AND ASSOCIATED STATISTICS[a]

"Experience shows that practically all measured values differ from the true ones, not only because of uncontrollable experimental errors and limited counting statistics but also because auxiliary quantities employed in the process of data reduction, such as geometric dimensions, sample composition, backgrounds, and reference data, are not known with perfect precision. The true values can therefore never be known exactly, and around a reported experimental value there is always a certain range of similar, more or less plausible values that could also be true. Thus all inferences, predictions, engineering, or other applications of measured data can at best be based on weighted averages over all those possible true values, with weights indicating how plausible each value is. These weights and averages are, of course, what we call probabilities and expectation values. Persons possessing different knowledge about some quantity assign different probabilities and adjust them whenever they get new information. Obviously probabilities encode incomplete and uncertain information. It follows that they cannot be considered as measurable physical properties. They are subjective in the sense that they depend on a person's knowledge, but that does not mean they are arbitrary. They must obey the rules of logic that demand, for instance, that rational persons with the same knowledge assign the same probabilities.

"Clearly the full information gained from a typical measurement of some physical quantity x consists not in a single numerical value but in a whole probability distribution, i.e., a set of discrete probabilities p_j if the possible values x_j form a discrete set, or of infinitesimal probabilities $p(x)\,dx$ of the true value lying between x and $x + dx$ if they form a continuum with probability density function p(x). Most users of a measured datum are, however, not interested in the detailed distribution of possible values. What they want is one recommended value and error bars that indicate the accuracy. Decision theory tells us that if the distribution is to be summarized by just two numbers, it is best to give its mean $\langle x \rangle$ and its variance var x = $\left\langle (x - \langle x \rangle)^2 \right\rangle$, and to state the experimental result as $\langle x \rangle \pm \Delta x$, where $\Delta x \equiv \sqrt{\text{var}\, x}$ is the standard deviation (root-mean-square error). This "estimate under quadratic loss" minimizes the mean square error and thus, for any reasonably smooth loss function, the penalty expected for not using the true value.

"Arguing backwards one can interpret data given in the form $\langle x \rangle \pm \Delta x$ as abbreviating a whole distribution of possible x values, with explicitly specified mean and standard deviation (or first and second moment). Except for Gaussians this information is not sufficient for reconstruction of an unknown original distribution, but the maximum-entropy principle (the modern generalization of the principle of insufficient reason) tells us to use a Gaussian with the given specifications for all further inference, since any other type of distribution would imply additional information that we do not have. This is a remarkable extension of the domain where Gaussians can be employed, far beyond the familiar justification of many small independent errors acting together, and valid

[a] The four introductory paragraphs to this section were provided by Fritz H. Fröhner, Kernforschungszentrum Karlsruhe. For more detail about terms used in these four paragraphs, see References 5 and 6.

also for correlated and common errors. If only bounds (tolerances) are given, so that all one knows is $a < x < b$, the maximum-entropy distribution is rectangular, with mean $\langle x \rangle = (b + a)/2$ and standard deviation $\Delta x = \sqrt{\text{var}\, x} = (b - a)/(2\sqrt{3})$.

"If a measured quantity y is a function of several auxiliary (e.g., data reduction) parameters x_j, one finds the "sandwich rule" for mean square errors,

$$\text{var } y \cong \sum_{j,k} \frac{\partial y}{\partial x_j} \text{cov}(x_j, x_k) \frac{\partial y}{\partial x_k},$$

if the usual linear approximation of error propagation, $\delta y \cong \Sigma_j (\partial y/\partial x_j)\delta x_j$, is used for $y - \langle y \rangle$. The partial derivatives (sensitivities) are, of course, to be taken at the mean values $\langle x_j \rangle$, and $\text{cov}(x_j, x_k) \equiv \left\langle \left(x_j - \langle x_j \rangle\right)\left(x_k - \langle x_k \rangle\right) \right\rangle$ is the jk element of the covariance matrix. In terms of standard deviations σ_j and correlation coefficients ρ_{jk} one has $\text{cov}(x_j, x_k) = \sigma_j \rho_{jk} \sigma_k$ with $\rho_{jj} = 1$ and $\text{cov}(x_j, x_j) = \text{var}\, x_j$. In the simplest case where the unknown error is just a sum of uncorrelated component errors, $\delta y = \Sigma_j \delta x_j$, one has

$$\text{var } y = \sum_j \text{var } x_j .$$

This means the (root-mean-square) component errors have to be added in quadrature, regardless of their nature: Against widely held belief it is perfectly correct to add "statistical" (e.g., counting, type A) and "systematic" (e.g., calibration, common) root-mean-square errors in quadrature to get the total error."

In this section, the following concepts, widely published in the international scientific literature and further discussed in the references, are reviewed: Type A uncertainty (random, based on a finite number of measurements proper for statistical analysis), Type B uncertainty (scientific judgment based on all available information, since there is no possibility to carry out measurements for statistical analysis), standard uncertainty, and combined standard uncertainty. A glossary of other terms extensively used in metrology and in statistics is given in Appendix A.

For the purpose of benchmark-experiment evaluation, the parameters of interest are particular values of quantities that define the physical setup (dimensions, material compositions, masses, temperature, etc.) at the time of the experiment. Their uncertainties come from best estimates of the probability distributions of the true parameter values. Best estimates of characteristics of the parameter probability distributions (called "posteriors" in References 5 and 6) are obtained from combining the available experimental data with whatever prior knowledge exists.

Sections 2.1 and 2.2 deal with the basic uncertainty that arises when measurements are made of one parameter, such as the mass of fuel in a particular fuel rod. The formulas in Section 2.1 include the assumption that the n measured values are taken from an infinite population; i.e., the repeated measurements of the same parameter could, theoretically, be continued indefinitely to obtain an infinite population. There is another Type A uncertainty due to estimating the mean parameter value of a finite population by measuring only part of the population. An example is using the average fuel mass of n measured fuel rods to estimate the mean fuel mass of the N fuel rods used in an experiment. This additional Type A uncertainty is discussed in Section C.12.

2.1 Type A evaluation of standard uncertainty (§4.2 of Reference 1; References 5 and 6)[a]

Type A evaluation (of uncertainty)
method of evaluation of uncertainty by the **statistical analysis** of a series of observations.

Type A estimate of variance
The experimental variance of the observation (n independent repeated measurements), which characterizes the variability or dispersion of the observed values (§4.2.2 of Reference 1), is given by

$s^2 = \frac{1}{n-1}\sum_{i=1}^{n}\left(x_i - \bar{x}\right)^2$ in which $\bar{x}$ is the arithmetic mean or average of the n observations.

It is often used to estimate the variance σ^2 of the probability distribution of the parameter x.

However, whenever a Gaussian distribution of the parameter can be assumed, the best estimate of the variance under quadratic loss (i.e., minimizing the expected error) is

[a] [In this section, two different formulas for Type A uncertainty are given, differing by a factor of $\sqrt{(n-1)/(n-3)}$. The first, smaller one is included because it is the traditional one and is the one given in Reference 1. For small n, Reference 1 also recommends considering the Student t distribution. (See §4.2.3, note 1.) The second, larger one, which is based on the assumption of a Gaussian probability distribution for the parameter whose uncertainty is being estimated, effectively includes the correction for small n. Its derivation from the basic product rule of probability theory is explained in parts 1.6 and A.3 of Reference 6. The explanation includes reference to the Student t distribution. Note that the difference between the two is negligible for large n. For small n, the second formula is recommended. – *editor*]

$$\left\langle \sigma^2 \right\rangle = \frac{1}{n-3}\sum_{i=1}^{n}\left(x_i - \bar{x}\right)^2 .$$ (See eqn. 38 of Reference 6.)

experimental standard deviation
positive square root of the experimental variance

experimental standard deviation of the mean
positive square root of the experimental variance of the mean. It is equal to s/√n (§4.2.3 of Reference 1) or $s\sqrt{(n-1)/n(n-3)}$, the best estimate under quadratic loss for a Gaussian (eqn. 34 of Reference 6). It estimates the uncertainty of a measurement result $\bar{x}$ = the sample mean, which is the expectation of the parameter x, based on the n observations.

least-squares fitting
If a quantity is obtained by least-squares fitting, its empirical standard deviation is also considered as a Type A estimate of uncertainty (§4.2.5, §G3.3, and §H.3.2 of Reference 1).

Type A standard uncertainty
This is the uncertainty of parameter x, which has been repeatedly measured (n observations), whose true value is unknown but which is estimated by $\bar{x} = \frac{1}{n}\sum_{i=1}^{n} x_i$. The Type A standard uncertainty u of the value of parameter x is an estimate of $\sigma(\bar{x})$, the square root of the variance of $\bar{x}$. It is

$u = \sqrt{\frac{1}{n(n-1)}\sum_{i=1}^{n}\left(x_i - \bar{x}\right)^2}$ (see §4.2.3 of Reference 1), or

$u = \sqrt{\frac{1}{n(n-3)}\sum_{i=1}^{n}\left(x_i - \bar{x}\right)^2}$ (best estimate under quadratic loss for an assumed normal, or Gaussian, distribution of the parameter; see References 5 and 6).

2.2 Type B evaluation of standard uncertainty (§4.3 of Reference 1)

Type B evaluation (of uncertainty)
evaluation of uncertainty by a method or consideration other than the statistical analysis of a series of observations. Scientific judgment, based on all the available information on the possible variability of the measurand, and other relevant knowledge are used.

Type B standard uncertainty
The Type B standard uncertainty is a best estimate of the standard deviation of the measurand, based on whatever relevant information is available about the probability distribution of the value of the measurand.

- If the estimate of a measurand is taken from a manufacturer's source (e.g., specification, calibration certificate), and its quoted uncertainty is stated to be a particular multiple of a standard deviation, the standard deviation is simply the total quoted value divided by the particular multiplier. This multiplier is called the coverage factor (defined in Section 2.4).

- If there is no specific knowledge about the possible values of a variable given as $x \pm \Delta x$, where $\pm \Delta x$ seems to refer to the bounds (upper and lower limits) of the quantity (e.g., tolerance), then one may assume that the distribution is equally probable everywhere within the interval. The corresponding standard uncertainty is then $\Delta x/\sqrt{3}$.[a] If only the bounds of the interval are given with no specific information about the values of the parameter p within the interval, one may assume that the distribution is uniform within the interval[b] and the parameter's expected value is the midpoint of the interval. Again, the standard uncertainty corresponding to the standard deviation equals the half interval divided by $\sqrt{3}$, or the total interval divided by $\sqrt{12}$. (See §4.3.7 of Reference 1.)

- Sometimes, the tolerances are asymmetric and the parameter value is given as x_i $(-\Delta x_-,+\Delta x_+)$ or $[x_i+0, x_i+\Delta x]$. Reference 1 (§4.3.8 and §G.5.3) suggests that, in the absence of additional information, the standard uncertainty may be estimated as $(\Delta x_+ + \Delta x_-)/(2\sqrt{3})$, without using the mid point of the interval as the best value of the parameter, if this uncertainty is not a large contributor to the total uncertainty. An alternate method is the following: If a best value x_i is given within the interval [a, b], one can assume that x_i is the estimate under quadratic loss, i.e., the average $\langle x \rangle$. The maximum-entropy distribution is then an exponential distribution between a and b with this average, and the standard deviation is well approximated by

$$\Delta x \cong \frac{h}{\sqrt{3}}\left[1-\left(\frac{\langle x\rangle - x_{mid}}{h}\right)^2\right], \qquad -1 < \frac{\langle x\rangle - x_{mid}}{h} < +1$$

  where $x_{mid} \equiv (b + a)/2$ is the midpoint and $h \equiv (b - a)/2$ is the half width of the interval. Note that if the recommended value is the midpoint, $\langle x \rangle = x_{mid}$, the maximum-entropy distribution becomes uniform, with the correct standard deviation $h/\sqrt{3}$. If the recommended value tends toward one of the bounds, the exponential distribution becomes a sharp spike and the standard deviation goes to zero.

- If the probability distribution of a quantity is known empirically or theoretically or in a combined way, the standard uncertainty is estimated on the basis of this distribution.[c]

- If the uncertainty is not given, then judgment may be used to assign an uncertainty based on typical values (e.g., reported, measured uncertainties on the same parameter, perhaps from

---

[a] See Appendix G for the derivation of this standard uncertainty.

[b] The compelling rationale for this assumption is the principle of insufficient reason (James Bernoulli, 1713) or its modern generalization, the principle of maximum entropy (Jaynes, 1957). (personal communication, F. Fröhner, July, 2002)

[c] If p(x) is the probability distribution of parameter x and μ is the mean value of x, then the standard uncertainty (standard deviation) is $\sigma = \sqrt{\int_{\text{all x}} (x-\mu)^2 p(x)dx}$. (See Appendix G.)

the same laboratory, at approximately the same time period as the experiments being evaluated), reasoning based on a knowledge of the manufacturing process, etc.

- In some cases, when the uncertainty on a physical parameter is not stated, the evaluator may judge that the number of significant digits used to report the parameter reflects its uncertainty. If so, one of two interpretations may be appropriate. For instance, consider a thickness reported as 0.3175 cm. (i) If precision is represented by the final digit (10^{-4} cm), assume the standard uncertainty to be half of the final digit, i.e., 0.5×10^{-4} cm. (ii) If precision is represented by the final two digits (i.e., the next to the last digit is known and the last digit is a best estimate), assume the standard uncertainty to be half of the last digit that is known, i.e., 0.5×10^{-3} cm.

  However, it is important to note that precision (number of digits) may not represent uncertainty of the reported value. Instead, more decimal places may be reported in order to avoid introducing additional, small, rounding error that can affect the result of subsequent calculations that use the value. Perhaps extra digits are a result of conversion of units, as with the present example: 0.3175 cm ≡ 1/8-inch. In this case, number of significant digits should not be used to estimate uncertainty, as this would cause underestimation of the uncertainty by orders of magnitude.

- The Type B standard uncertainty may be also modified by "evaluator judgment", but this should be justified and documented in the evaluation. Extreme caution is recommended in this particular process.

2.3 "Uncertainty of the uncertainty"

Both Type A and Type B uncertainties can be reliable estimates, but some estimates are more reliable than others. For example, a Type A uncertainty based on only a few measurements is less reliable than one based on many measurements. A Type B uncertainty given in a reference simply as $\pm\Delta x$ is less reliable than one given as a "standard deviation that estimates the random error" or "bounding."

The reliability of an uncertainty estimate can be quantified by the "uncertainty of the uncertainty" (the standard deviation of the uncertainty) or with an estimated number of degrees of freedom. (See §E.4.3 and §G.4.2 of Reference 1.) In general, the larger the number of degrees of freedom (defined in Section A.2), the more reliable is the uncertainty estimate.

Type A standard uncertainties are not necessarily superior to Type B uncertainties. For example, the relative standard deviation of the standard deviation for n observations of a normally distributed random variable is approximately $[2(n-1)]^{-1/2}$. This formula shows that the standard deviation of a statistically estimated standard deviation is not negligible for many practical values of n; e.g., for n=10 observations it is approximately 24 percent.

Sometimes Type B uncertainties that are tolerances are assigned ∞ for the number of degrees of freedom. This may reflect the fact that the possibility of the parameter value being outside

the permissible range is extremely small (§G.4.3 of Reference 1). If, on the other hand, there is some basis for a subjective estimate of the reliability of a Type B uncertainty, the estimate may be used to assign the number of degrees of freedom. This method is discussed in Section 6.4.

2.4 Determining combined standard uncertainty

standard uncertainty, u_x
uncertainty of the result of a measurement of parameter x expressed as one standard deviation. (The number of degrees of freedom may also be specified. Its value may be used in some cases to determine the level of confidence of the combined uncertainty.[a])

combined standard uncertainty, $u_c(z)$ (§5 of Reference 1)
standard uncertainty of the result of a measurement of z derived from the standard uncertainties of the several quantities, or parameters, upon which the measurand (the measured quantity) depends. It is equal to the positive square root of a sum of sample variances and sample covariances of the basic quantities, weighted according to how the measurement result varies with changes in these quantities. (Here sample covariances and sample variances are used as estimates of the true, but unknown, ones.) The weighting factors are often called "sensitivities."

For example, the combined standard uncertainty $u_c(z)$, where z is the estimate of the measurand $Z(X, Y)$[b], and thus the result of the measurement, is obtained by combining the standard uncertainties of the input estimates x and y. It is given by the formula for the combined variance

$$u_c^2(z) = \left[\frac{\partial z}{\partial x}\right]^2 u_x^2 + \left[\frac{\partial z}{\partial y}\right]^2 u_y^2 + 2\,\frac{\partial z}{\partial x}\frac{\partial z}{\partial y} r_{x,y}\, u_x\, u_y \ .$$

The degree of correlation between x and y is characterized by the estimated correlation coefficient r defined by $r = \mathrm{cov}(x, y)/(u_x u_y)$, with $-1 \le r \le +1$. If x and y are perfectly correlated, the correlation coefficient r is either +1 or -1. If x and y are uncorrelated, $r_{x,y}$ is zero and the last term is equal to 0. For n independent pairs of simultaneous observations x_i and y_i, the covariance is $\mathrm{cov}(x, y) = \frac{1}{n-1}\sum_{i=1}^{n}\left(x_i - \bar{x}\right)\left(y_i - \bar{y}\right)$,

where $\bar{x}$ and $\bar{y}$ are the mean values. Furthermore, $\mathrm{cov}(\bar{x}, \bar{y}) = \frac{1}{n(n-1)}\sum_{i=1}^{n}\left(x_i - \bar{x}\right)\left(y_i - \bar{y}\right)$. (See §5.2.3 and §C.3.4 of Reference 1.)[c]

The formula for $u_c^2(z)$ is an application of the general formula (13) of Reference 1 (sometimes called the "law of propagation of uncertainty") developed for N input-quantity estimates. The general formula is

[a] See Section 6.4.
[b] Z is assumed to be a linear function of X and Y, which is often a good approximation for small changes in X and Y.
[c] Examples of parameters whose uncertainties may be correlated are fissile material density and critical mass. (See Section C.3 in Appendix C.)

$$u_c^2(z) = \sum_{i=1}^{N} \left[\frac{\partial z}{\partial x_i} \right]^2 u_i^2 + 2 \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} \frac{\partial z}{\partial x_i} \frac{\partial z}{\partial x_j} r_{i,j} u_i u_j \ .$$

In the case of finding the combined standard uncertainty of k_{eff}, the measurand z is k_{eff}, the u_i's are the standard uncertainties of the physical parameters, and the first derivatives $\partial z/\partial x_i$ are the calculated (or measured) sensitivities of k_{eff} to changes of the parameters.

level of confidence
an estimate of the probability, often expressed as a percent, that the true value of the measurand is within a particular interval, such as within ±u of the expected value of the measurand

coverage factor
numerical factor used as a multiplier of a standard uncertainty in order to obtain an uncertainty with a different level of confidence. For a normal distribution, the coverage factor is typically equal to 1, 1.96, 2, or 3, with a level of confidence of, respectively, 68.27%, 95%, 95.45%, or 99.73%.

For a function that can be approximated by a linear function[a] of many parameters, the coverage factor for a particular level of confidence may be estimated by the Student-t tables (Table G.2 of Reference 1), using the effective number of degrees of freedom of the function. Use of this table assumes that the combined standard uncertainty has been obtained from standard uncertainties (Type A or B estimated standard deviations) of the parameters. This method and the Welch-Satterthwaite formula for calculating the effective number of degrees of freedom (ν_{eff}) are summarized in Appendix G of Reference 1. (See Section 6.0 for further discussion.)

[a] §5.1.5 of Reference 1 says that a first-order approximation "is usually an adequate approximation…for the purposes of an analysis of uncertainty." See Section 4.0 for discussion of possible non-linearity of k_{eff}.

3.0 INVENTORY OF UNCERTAINTIES

Table 1 is a checklist that is useful for making an inventory of all uncertainties.

Uncertainties in data listed in the last column of Table 1 contribute only second-order effects in many cases. This is because their values are the same in both the base case and the perturbed case when used in the calculations of Δk_{eff} for experimental parameter uncertainties. However, they are given so that the effect of their uncertainties on k_{eff} may be considered and evaluated for particular experiments where the effects are possibly significant as first-order effects (for instance, $^{10}B/^{11}B$ in natural boron).

Note that the only possible effects of nuclear cross section data on determining the benchmark model are model-simplification decisions based on calculations, calculated k_{eff} effects of parameter uncertainties, and the magnitude of any calculated corrections to the benchmark-model k_{eff} due to simplifications. Because their values are the same in both the base case and the perturbed case, the effect of nuclear cross sections is, in most cases, small. (The evaluator should be alert to possible exceptions.) The closeness of the calculated k_{eff} value of the experimental configuration to 1.00 is not used to decide the acceptability of a benchmark experiment. Rather, nuclear cross sections are included in the calculational method to be validated with the benchmark model.

Preferably, uncertainties of physical parameters have been given by the experimentalist in the reported experimental data, along with the basis for their values. The effect of these uncertainties on the total uncertainty for k_{eff} must be ascertained. The evaluator considers the nearby environment (for room return effect), the structure containing the experimental device, the fissile solution or the array of fissile rods, neutron absorber materials, etc.

For every volume in the represented configuration, parameters that describe material concentrations and geometry are listed. Then, for each parameter, the evaluator considers if the corresponding uncertainty is of Type A or B.

It is recommended that the description of an uncertainty of Type A include the following information: parameter's mean measured value, reported uncertainty (including coverage factor), number of measurements, and the deduced standard deviation (standard uncertainty). In many cases, the experimentalist will have given, in his report or logbook, exhaustive information such as number of measurements and results, as well as corrections for the finite number of measurements. The evaluator should clearly explain any use of this unpublished data for his evaluation of parameters or uncertainties.

One uncertainty of Type A comes from sampling without replacement from a finite population. (See Section C.12 in Appendix C.) For example, suppose fuel-rod diameter is measured for only n rods from a total population of N rods, and the average is used to represent the mean diameter of the N fuel rods. In this case, the uncertainty of the mean value, which is $1/\sqrt{n}$ times the standard deviation of the n measured values in the case of an infinite population, is multiplied by the factor 1-f, where f = n/N, the fraction of the population that was measured. Note that if the mean value is the measured average of the entire population of N rods used in the experiment

(i.e., n=N), this 'uncertainty of the mean' is zero. However, in addition to the uncertainty of the mean, the uncertainty of the measurements themselves must always be included, as discussed in the first part of Section C.9.

The description of an uncertainty of Type B includes the following information: parameter's mean value, reported uncertainty and whatever is known about its source, the deduced standard uncertainty (best estimate of standard deviation) and how it is obtained (evaluated by scientific judgment based on what particular available information or assumed probability distribution). (See §4.3.7 - 4.3.9 of Reference 1 and Section 2.2.)

For a variable (Type A or B) given as $x \pm \Delta x$, where $x + \Delta x$ and $x - \Delta x$ bound the quantity x, the corresponding standard deviation is $\Delta x/3$, $\Delta x/\sqrt{3}$, etc., according to whether the variable distribution is normal, equally probable everywhere within the interval, or is believed to follow some other distribution. (See Section §4.3.9 of Reference 1.)

Table 1. Identification of possible uncertainties to include in the evaluation of a critical experiment

Origin →		**Result of a fabrication or of a measurement**			**Result of calculations and tables**
Uncertainty Type → **Experiment ↓**		**Geometry**	**Physics and Chemistry**	**Time**	**Universal**
Experimental Device	**Environment: walls, tanks, pedestal, grids, support plates, detectors, etc .** **Measurement systems for the critical approach**	Dimension Sphericity Planeity Curvature Deformation Distance Height Spacing Gap Positioning Pitch Adjustment Centering Eccentricity	Nature Size, shape of particles or layers (resonance shielding, particle effect) Moisture Constitution Density Isotopic percentage Concentration Homogeneity Sampling Radiolysis Hydrolysis Acidity Valence Impurity Temperature	Dates of measurements and analyses Dates of experiments	Nuclear data Cross sections (origin, type, group structure, resonance approximations) Constants (e.g. Avogadro's) Water density Atomic mass Half-life Natural isotopics Truncation, round-off Approximation Simplification Counting statistics Adjustment, fitting Extrapolation
Fissile Material (FM)	**Fissile material** **FM cladding**				
Reflector	**Intentional reflector** **Surroundings external to experiment**				
Moderator					
Poison	**Internal to core and reflector** **External**				

3.1 Uncertainties from physics, chemistry, and isotopics of materials

The uncertainties from materials include the parameters listed in the following table, which may be used by filling in the empty columns, for clarification. This list is not exhaustive; it was prepared for experiments using fissile uranium. A similar table can be developed for configurations with other materials.

The numerical values of the first line are given as an illustration. The illustration is a Type A uncertainty for fuel enrichment.

Parameter Identification[(a)]	Mean measured value	Reported uncertainty in parameter	Type of uncertainty (A or B)	ν Number of degrees of freedom	Number of standard deviations associated with the uncertainty	Standard uncertainty
^{235}U enrichment (wt.%) [(b)]	4.348	0.004	A	4	2	0.002
Fuel density (g/cm^3 fuel rod or g/cm^3 in solution)						
Solid absorber content (g/cm^3)						
Poison content (g/l) in solution						
Absorbing isotope concentration in natural element (eg. ^{10}B in B)						
B equivalent to 1/2 of undetected impurities						
Acidity [H^+] of solution						
Temperature (°C or K)						

(a) Parameter units, assumed here to apply to the second, third, and last columns, should be clearly specified.

(b) Depending on how enrichment is measured and reported, this may be at.%.

Although fuel is sometimes thought of as the most important material, composition uncertainties for moderators, structures, reflectors, etc. may or may not have a larger impact on k_{eff} than do uncertainties in the fuel materials. Consequently, the effects on k_{eff} of all significant materials must be assessed. In most cases, these uncertainties will be Type B. In many instances, their small contribution to the overall uncertainty may allow a rather coarse estimate of their value.

The effect of **impurities** must also be assessed (see, for example, Section C.6). The potential sources of impurity information, in typical order of decreasing reliability for the material actually used in the experiment, are:

1) measured on the components of the experiments,
2) measured for material of the same stock from which the components of the experiment were made,
3) provided by the manufacturer as typical of that material,
4) industry or government specifications for that particular material.

The first three sources come from chemical or physical analyses, while the last source indicates what is required to meet the material standard.

Sometimes impurities might not be reported. Nevertheless, the possibility of their presence and effect should be considered, and if the effect is thought to be important, it should be quantified.

Impurity amounts may be reported in two ways, depending on the possibility to detect them: some have a concentration above the detection limit, are detected and well known; others have a concentration lower than the ability of the device to measure them; they may be detected or not. Therefore, impurity measurement possibilities are the following:

- Impurity concentration is measured. It is reported with an uncertainty.
- Impurity concentration is measured. No uncertainty is reported.
  - If the measurement method is known, an uncertainty typical of the method may be assigned.
  - If the measurement method is not known, because impurity measurements typically have large uncertainty, a large uncertainty is assigned; 25-100% is suggested, depending on the evaluator's judgment of how accurately the measurement was probably done.
- Impurity is detected and reported as <D, where D is 50% of the minimum amount that can with certainty be detected; in this case D ± D may be assigned as the impurity amount.
- Impurity is reported as <D, where D is the minimum amount that can be detected or measured.
  - If D is the minimum amount whose presence can be detected, the evaluator must decide whether to check the effect of D, considered as the complete range of the uncertainty, or not, depending on
    - his expectation of a significant effect and
    - the likelihood that some was present.
  - If D is the minimum amount whose presence can be measured, the evaluator should try to learn
    - if the impurity was detected but could not be measured (in this case, D/2 ± D/2 may be assigned as the impurity amount),
    - if the impurity was sought but was not detected.

The evaluator may choose to assign a larger uncertainty depending on the source of the impurity data. The uncertainty just described applies when components of the experiment were measured (source number 1 in the source list given above). The more removed the measurement is from the experiment, the more uncertainty there may be in the applicability of the measurement to the experiment.

Impurity amounts obtained from materials standards (source number 4) are interpreted differently from those obtained from chemical analyses. Materials standards give maximum permissible amounts of impurities that can adversely affect the properties of the material. In some instances, this is indicated explicitly by specifying "Max." values. In other instances, the symbol "<" is used, and it is implicit that this is the maximum amount allowed.

The best estimate for a specification "<D" in a standard is closer to D than it is to D/2. The reason is that the manufacturer of the material is unlikely to expend resources to reduce the impurity amount much below the allowable maximum. A reasonable assumption for the probability distribution is a right triangular distribution spanning the range of impurity amounts from 0 to D. Implicit here is the assumption that the probability of exceeding the maxiumum allowable impurity amount, D, is negligible. This distribution has a mean impurity amount of 2D/3 and a standard deviation of $D/\sqrt{18}$. Of course, other distributions could be assumed, but it is rare for an impurity to have a large enough impact on k_{eff} that choosing a different distribution would matter significantly.

Impurities are included in the benchmark model, or they are removed with a k_{eff} correction calculated and uncertainty assigned to the correction. An example of treatment in a thermal spectrum is given in Appendix C.6.

3.2 Uncertainties on geometry

The uncertainties on geometry include the parameters listed in the following table, in which the empty columns may be filled as an aid to clarify the uncertainties. As noted for the previous table, this list is not exhaustive. It was established for a fuel-rod array in a tank containing either water or a solution. Different parameters will be listed for other types of configurations.

Parameter Identification	Mean measured value or design value	Reported uncertainty in parameter	Type of uncertainty (A or B)	ν Number of degrees of freedom [(a)]	Number of standard deviations associated with the uncertainty	Standard uncertainty
Fuel Pellet Diameter (cm)						
Clad Outer Diameter (cm)						
Absorber Position (cm)						
Fissile Column Height (cm)	90.	1.	B	∞	$\sqrt{3}$	$1/\sqrt{3}$
Solution Height (cm)						
Solution-Tank Diameter (cm)						

(a) See the discussion in Section 6.4 and in §G.4.2 and §G.4.3 of Reference 1.

In the table, an illustration of Type B uncertainty is given for the fissile column height. In this example, the fissile column height is given as 90 ± 1 cm, where ± 1 cm is stated as a tolerance by the manufacturer. If there is no more knowledge about this quantity, one may assume an equiprobable distribution and that the tolerance bounds the variable, and the standard uncertainty will be taken as $1/\sqrt{3}$. If the manufacturing process is "under statistical control,"[a] or if it may be assumed that the distribution is Gaussian and that the stated tolerance includes >99% of the possible values, the standard uncertainty may be taken as 1/3.

In some cases, a Type A standard uncertainty of the mean is obtained from a well-characterized measurement (i.e., the measurement is one of many very similar, carefully controlled and documented ones of the same random variable). Then the standard uncertainty may be best represented by $s_p/\sqrt{n}$, where s_p is the pooled experimental standard deviation characterizing all the similar measurements, and n is the number of independent observations used to determine the mean of this particular measurement. (See §4.2.4 and §H.3.6 of Reference 1.)

In experiments involving a *fissile solution in a cylindrical tank*, the diameter is an important parameter because its uncertainty can have a large effect. Its uncertainty is either a result of calibration measurements (Type A) or a tolerance (assumed to be Type B, if no other information is given).

3.3 Uncertainties of dates

In the case of experiments carried out with decaying isotopes, all important dates should be reported in order to better determine the isotopes' concentrations when the experiment was performed.

Three dates are important:
1. the date of isotopic analysis,
2. the date of chemical analysis (giving the plutonium and uranium concentrations),
3. the date of the experiment.

In the case of fuel rods, isotopic and chemical analyses are usually performed just before fuel-rod fabrication. Then these two dates are the same for all experiments performed with these rods. This is not generally the case with fuel solutions.

For experiments with plutonium, dates of separation (when ^{241}Am concentration is set to zero), fuel-rod fabrication, experiment, and isotopic analysis are essential to compute the correct ^{241}Pu and ^{241}Am concentrations. Unfortunately, there is sometimes a lack of information for old experiments, and an uncertainty on possible dates must be added.

[a] "Under statistical control" implies that, instead of measuring each individual, one uses sampling theory. It is assumed that measured quantities follow a Gaussian law. Each sample of measurement gives an estimation of the population mean and variance. (See §H.3.6, note 1, of Reference 1.)

3.4 Uncertainties from modeling

The evaluator may simplify the representation of the experiment in the benchmark model in order to make the modeling of the configurations easier and the verification process more efficient.

For instance, the evaluator may choose to always use the same temperature, although it may vary from one experiment to another in a series. In this way, the water density is the same in all model calculations, although in reality it varies. The discrepancy between the real temperature and the temperature of calculation may be taken into account by calculating the Δk_{eff} sensitivity to a temperature change. Then, if the effect is small, the deviation in temperature of the model from experiment may be combined with the uncertainty of the temperature measurement to obtain the temperature uncertainty. If the effect of the temperature difference is significant (but still relatively small), the evaluator includes a k_{eff} correction for the temperature difference between model and experiment, with additional uncertainty (see Section 5.0).

A similar method may be used with plutonium fuel containing ^{241}Am produced by β decay of ^{241}Pu with a half-life of 14.4 years. The evaluator may choose for all models of a series of experiments to contain the same ^{241}Pu and ^{241}Am percentages. Then a calculated correction to k_{eff} may be applied to take into account the gaps between the real values (or likely values, if real values or dates are unknown) and model values of ^{241}Pu and ^{241}Am percentages. If the correction is very small, it may be treated as a Type B uncertainty instead of a correction. If it is larger (but still relatively small), it may be treated as a small correction with additional Type B uncertainty. If the correction would be significant, the best estimates of the actual percentages should be used in the model instead of the correction, with best estimates of their uncertainties included in the total uncertainty.

Using this approach on temperature and ^{241}Pu decay time is acceptable when

- this uncertainty is smaller than the uncertainty of measurement,
- the effect of this uncertainty is much smaller than the combined effect of other uncertainties.

The evaluator, when making model simplifications, and the user, when using a benchmark model, should both be aware that any deviation of the model from reality introduces the possibility of a bias whose magnitude may not be easily or reliably estimated, and which can never be known exactly. This applies whether the deviation was deliberate, by the evaluator creating the benchmark model, or simply due to lack of knowledge about true values.

3.5 General remarks on calculations of uncertainties

When it is relevant, it is recommended to give as much information as possible about the calculations of uncertainties, such as (non-exhaustive list)

- the nuclear cross section library used and its release number (because some nuclear data errors may affect calculated corrections and uncertainties),
- the P_N approximation used for cross section development,

- the order of quadrature in S_N calculations (which might induce truncation errors),
- nuclear data, such as Avogadro's number, decay rate, atomic mass, isotopic composition,
- density of water in calculations of effects of its impurities,
- atmospheric conditions of air (moisture, pressure), when its effect is calculated.

These items correspond more or less to the last column of Table 1. Note that the evaluator is expected to use methods, codes, and data adequate to investigate the reactivity effects of the experiment. Typically, the evaluator uses recent versions of recommended codes and data libraries, assuming that errors have been corrected and methods improved in recent versions.

Note that, in general, uncertainties are small quantities relative to the values of their parameters, due to the experimentalist's work to provide a worthwhile experiment by carefully performing and documenting it. Also, uncertainties are generally assumed to be symmetric around the nominal values of their parameters, both in sign and in magnitude, but this is not necessarily so. Although evaluators are not usually in the position of determining experimental parameter uncertainties, if one does have the opportunity to reduce experimental data, the following is recommended:

> When a quantity and its uncertainty are given in the form $x \pm \Delta x$, the uncertainty (i.e., Δx) should be given with at least two significant digits, while x should have the same number of decimal places as Δx. For example, 6.987±0.035 would be acceptable. But none of the following would be acceptable: 6.99±0.035, 6.987±0.04, or 6.99±0.04.

This way of specification does not distort significantly the weighted averages[a] nor the level of confidence based on the uncertainties. However, the ways described above as unacceptable may lead to unexpected alteration of the level of confidence. (See Appendix F.) It is important to note that this recommendation does not apply to uncertainties that have been provided by the experimentalists. Uncertainties on experimental parameters should be given in the evaluation exactly as specified in the experimental references.

As mentioned in Section 1, the evaluator must report an accurate estimate of the combined standard uncertainty for k_{eff} of the benchmark model of an experiment in order to permit meaningful use of the value. The evaluator must use care to interpret reported uncertainties correctly. For example, it is incorrect to arbitrarily use a Type B uncertainty reported as upper and lower limits as equivalent to the standard deviation, thereby neglecting to divide the half-range value by the appropriate factor of 3, $\sqrt{6}$, or $\sqrt{3}$. Such practice expands unnecessarily the overall standard uncertainty for an experiment, thereby reducing its value as a benchmark. On the other hand, if no uncertainty was reported for a particular parameter, this does not mean that there is no uncertainty. In this case, the evaluator should estimate one and consider its effect on k_{eff}. If the reactivity effect of a "questionable," or poorly known, uncertainty is small relative to the total k_{eff} uncertainty, an in-depth analysis is not needed. If the reactivity effect of this uncertainty is large, a more in-depth analysis is required, because in this case, a coarse approximation will alter the quality and usefulness of the experiment and its benchmark model.

[a] See Reference 6, eqns. 62-67, about combination of data with different accuracies leading to weighted averages.

4.0 CALCULATION OF EFFECTS OF UNCERTAINTIES ON k_{eff}

The aim of this task of the evaluator, which is documented in Section 2 of the ICSBEP evaluation, is to find the effect on k_{eff} due to the variation of each single parameter by one of several available methods.

Suppose that,
the number of uncertain parameters on which k_{eff} depends is N,
the reference value (best estimate) of the i^{th} parameter is x_i,
the standard uncertainty (corresponding to 1σ) of the i^{th} parameter is $\pm u_i$, and
the reactivity effect on k_{eff} of changing x_i by u_i is Δk_i.

(In this and following sections, the subscript "eff" will usually be dropped and k should be understood to mean k_{eff}.)

Almost always, each u_i is small enough to have a first-order effect on k. This means that for $\Delta x_i \leq u_i$, the change in k produced by Δx_i is proportional to the magnitude of Δx_i.

The evaluator may choose a different parameter perturbation, δx_i, to compute the corresponding δk_i. The δx_i is chosen to be large enough to minimize ambiguity arising from roundoff, numerical convergence limits or statistical noise, depending on the method used to compute δk_i. At the same time, it is necessary that δx_i be kept small enough not to violate the linearity (first-order-effect) assumption, so that both u_i and δx_i are proportional to the corresponding changes in k by the same factor. (The evaluator should verify compliance by calculational tests if there is doubt.) Then the desired reactivity effect is $\Delta k_i = u_i \delta k_i / \delta x_i$. The proportionality factor $\delta k_i / \delta x_i$ is the sensitivity of k_{eff} to x_i.

The rare instance where a u_i is not a linear perturbation requires caution and concern. First, it is necessary to determine whether the sensitivity of k to this parameter is too large. If Δk_i due to u_i is not so large as to warrant rejection of the experiment, then it would be prudent to calculate the effects of both $+u_i$ and $-u_i$ perturbations. If the resulting two values of Δk_i have comparable or small magnitudes, it is acceptable to average the magnitudes and carry the result forward into the uncertainty-combining step (see Section 6) as if it were symmetric. If the two values of Δk_i are large and significantly different, they should probably be treated as asymmetric uncertainty.[a] It should be noted, however, that the validity of using a simple coverage factor to go from 1σ to some other confidence level (see Section 6) is in doubt if a u_i is not a linear perturbation.

4.1 One-variable-at-a-time strategy

The easiest way to find the effect of each single parameter on k is to compute each effect individually, changing one parameter at a time. First k_{ref} is obtained using the reference values for all the parameters. Then parameter x_i is perturbed, with all other parameters at their reference

[a] See Section 2.2, **Type B standard uncertainty**, 3rd bullet.

values, and k_i corresponding to the perturbation u_i is calculated. The change in k, $\Delta k_i = k_i - k_{ref}$, is the reactivity effect of u_i. A total of N separate perturbed-k calculations yields all the needed reactivity effects.

The evaluator should preserve other measured quantities during this process. If, for example, the mass of a constituent part has been measured, the density of that part is altered to preserve the mass when a dimension of that part is perturbed.

The differences between the two input files whose k_{eff}'s are subtracted to obtain Δk_i should be obvious or made clear in the description of the uncertainty-effect calculation.

It is assumed that input files for sensitivity studies closely represent the benchmark model, but the base case for sensitivity studies is not required to be the benchmark model. The evaluator considers whether any difference between the model used for sensitivity studies and the benchmark model might significantly affect his calculated result. If so, he improves his method. Any significant difference between models used in sensitivity studies and the benchmark model should be mentioned.

The k values can be computed by an analytical method, a deterministic method, or a Monte Carlo code.

4.1.1 Analytical method

For simple configurations, the use of derivatives of neutronic formulas enables the calculation of Δk versus a parameter change. This method, which has commonly been used for critical height, was used extensively in the past, before high-performance computers and codes were commonplace.

4.1.2 Deterministic method

The use of a code based on a deterministic method is recommended, when practical. Applications where the analytical method can be used are very limited, whereas detailed one- or two-dimensional deterministic calculations, and sometimes even three-dimensional deterministic calculations, can be run economically on modern computers. It is usually much more computationally efficient to calculate a small perturbation deterministically than by Monte Carlo. This is because a very large number of neutron histories is needed in the Monte Carlo calculations to make the statistical fluctuations in k small compared to the reactivity effect. A deterministic method may be used when the configuration geometry can be well enough represented by the code.

A deterministic method solves numerically an approximation to the Boltzman neutron transport equation. The discrete-ordinates transport approximation, commonly referred to as the S_N method, is probably the most widely used method. Alternative approximations include collision probability, simplified spherical harmonics, variational nodal transport, and diffusion theory. The approximation selected by the evaluator depends on the computer codes available and on the tradeoff between computational effort and accuracy. For example, diffusion theory requires the

least computational effort. Diffusion theory is accurate enough when computing the reactivity effect of a fuel enrichment uncertainty for some experiments, but probably is not accurate enough when computing room-return effects.

All the approximations involve iterative solutions. The iterations are terminated when successive iterates agree within convergence criteria. Depending on how slowly the iterative process converges, the actual deviation of the final iterate from a completely converged solution can be as much as an order of magnitude larger than the convergence criterion. Thus, for example, if it is desired to know Δk_i to four decimal places, then the user-specified convergence criterion for k should be no larger than 10^{-5}. The evaluator should also always be aware of the impact of approximations in modeling, such as spatial-mesh and energy-mesh effects. For example, in calculating the effect of a dimension change, it is important not to introduce a large nonuniformity in the spatial mesh, which could cause a significant change in numerical accuracy. If possible, the spatial mesh for the perturbed calculation should be the same as the spatial mesh for the reference calculation, with more mesh points in regions where large changes in flux or fission source occur.

It is helpful if the evaluator reports key modeling parameters used for the k calculations, such as number of energy groups, geometry type, and quadrature order, so that users of the evaluation may conclude that the method was sufficiently accurate.

4.1.3 Monte Carlo method

The Monte Carlo method usually is preferred only when the necessary geometric complexity for the model is beyond the capability of deterministic methods. It can also be a good choice when a large, three-dimensional deterministic calculation is not computationally efficient or when the energy detail of continuous-energy Monte Carlo is important. Monte Carlo calculations are run with a statistical standard deviation s_{MC} for the mean k as low as reasonably achievable with respect to the computation time. The uncertainty in the value of Δk_i obtained from two Monte Carlo calculations is $\sqrt{s_{MC1}^2 + s_{MC2}^2}$, or, if both calculations have the same statistical uncertainty, $\sqrt{2} \times s_{MC}$. Therefore, to obtain a meaningful result for $\delta k_i = k_{\delta xi} - k_{ref}$, it should be much larger than $\sqrt{2} \times s_{MC}$.

To strike a balance with the expense of long-running calculations, the evaluator may be tempted to use large changes of a parameter in order to have a significant reactivity effect larger than $\sqrt{2} \times s_{MC}$. However, an evaluator must be careful in this process. Sometimes too large a parameter change can provide a poor estimate of a small effect, for example in a domain where the variation of k versus this parameter is not linear.

4.1.4 Monte Carlo perturbation method

Statistical uncertainty associated with probabilistic calculations can hide the change between results of two very similar configurations. New algorithms introduced in Monte Carlo codes have been developed that can calculate small changes in k. These algorithms seem to be especially well suited for calculating effects of changes in solutions or material compositions.

4.1.5 Uncertainties of the calculated uncertainties

As discussed in Section 4.1.3, when using Monte Carlo codes to calculate the k_{eff} of the reference configuration and the k_{eff} of the parameter variation, the statistical uncertainty of the calculation by the Monte Carlo code (s_{MC}) must be considered. For the case with no correlations among parameter uncertainties, the variance of the k_{eff} uncertainty caused by the parameter uncertainty is

$$(\Delta k_i)^2 = \frac{u_i^2}{\delta x_i^2}\left[(k_{\delta xi} - k_{ref})^2 \pm \left(s_{MC,\delta xi}^2 + s_{MC,ref}^2\right)\right] \quad (4.1)$$

where $(k_{\delta xi} - k_{ref})$ represents the change in k_{eff} induced by change δx_i on parameter x_i, u_i is the standard uncertainty of parameter x_i, $s_{MC,\delta xi}$ and $s_{MC,ref}$ are the statistical standard deviations of the two calculations of k_{eff}.

Note that $s_{MC,\delta xi}$ and $s_{MC,ref}$ are scaled by the factor $u_i/\delta x_i$ and that they are preceded by ±, indicating that they are uncertainties. Typically, s_{MC} is nominally the same for both Monte Carlo calculations, and in such cases, the notation can be simplified to become

$$(\Delta k_i)^2 = \frac{u_i^2}{\delta x_i^2}\left[(k_{\delta xi} - k_{ref})^2 \pm 2s_{MC}^2\right]$$

From this equation, the contribution to the standard uncertainty of k_{eff} from the standard uncertainty of parameter i is

$$\Delta k_i = \frac{u_i}{\delta x_i}(k_{\delta xi} - k_{ref}) \quad (4.2)$$

and the "uncertainty of the uncertainty" is equal to $\frac{u_i}{\delta x_i}\sqrt{2}s_{MC}$.

Whenever practical, the uncertainty of the uncertainty should be made small (negligible is the ideal) compared to the uncertainty. The most economical way to achieve this is to make δx_i relatively large. This approach is limited by the requirement that δx_i be kept small enough that the assumption of linear dependence of k_{eff} on parameter x_i is valid.

The other way to achieve this is to calculate a relatively large number of neutron histories. Due to ever increasing computer speed and decreasing computer cost, it has become practical to make $s_{MC} \leq 0.0002$ in most cases. In such cases, the uncertainty in the uncertainty is <0.0003, and it is likely that the δx_i yielding δk_i values at least twice that large are within the linear range.

It could be the case that resource constraints require s_{MC} to be much larger than 0.0002 and nonlinear behavior prevents δk_i from being made large compared to $s_{MC}\sqrt{2}$. Under these conditions, a deterministic calculational method would seem preferable to the Monte Carlo method. Alternatively, it might be reasonable to use $s_{MC}\sqrt{2}$ as an estimate of δk_i, especially if the resulting Δk_i is small compared to some other Δk_j. If this alternative is adopted, it should be made clear in the presentation that the uncertainty is obtained in this way and is therefore not representative of the sensitivity of the configuration to parameter i.

Factors other than Monte Carlo statistics contribute to the uncertainty of the uncertainty. Multigroup Monte Carlo calculations have uncertainty due to cross section processing approximations, as do deterministic k_{eff} calculations. Deterministic methods can suffer from incomplete convergence or inadequate refinement of space and angle meshes. As an example, the potential for slow convergence makes it prudent to set the convergence criterion for k_{eff} an order of magnitude smaller than the precision that is being counted on when forming δk_i.

Approximate modeling of the experimental geometry and compositions add uncertainty. If the analysis is approached with these pitfalls in mind, often these errors can be minimized. Also, there is often much error cancellation because the difference between two highly correlated k_{eff} calculations is the quantity of interest.

While factors contributing to uncertainty of the uncertainty give cause for careful analysis, concern with these issues should be tempered by the graded approach advocated in Section 1.2.3. Parameters that make relatively small contributions to $u_c(k_{eff})$ warrant a relatively small portion of the total resources expended on uncertainty analysis. Conversely, the major contributors deserve the most attention.

4.2 Experimental-design methodology

The aim of uncertainty or sensitivity calculations is always to find the reactivity effect of each single parameter on k, i.e., for each parameter x_i the difference $\Delta k_i = (k_{\delta xi} - k_{ref})u_i/\delta x_i$. Experimental design methodology can be used to determine the effect on k of a number of selected input parameters varying together in the k calculation, according to a specified protocol. (See Chapter 15 of Reference 3, and Reference 4.) A least-squares estimation yields a fitted equation:

$\Delta k = a_0 + a_1X_1 + \ldots.. + a_nX_n$ in which

- $a_1X_1,\ldots,a_nX_n$ represent the variations of Δk_{eff} corresponding to changes of "coded" variables $X_1,\ldots,X_n$,
- a_0 is a constant term, which gives a proof of the model linearity, when it is not significantly different from 0,
- a "coded" variable X_i is defined by: $X_i = (x_i - x_{ref}) / (x_{max} - x_{ref})$.

The advantage of having the parameters varying in several simulations is to obtain several simulations for every single parameter and therefore **to reduce the variance of each parameter coefficient a_i** (see §C.3.2 of Reference 1 and Chapter 4 of Reference 4). For instance, performing 4 simulations (equivalent to measurements) of a variable instead of 1 will divide the variance of the mean by 4.

Since several parameters vary at the same time in simulations, experimental design methodology is well suited to derive correlations between parameters, if any.

As in the former section, k is computed either by a discrete-ordinates method or a Monte Carlo method. When using the experimental design methodology, care should be taken if Monte Carlo is used to calculate the parameter sensitivity. As mentioned earlier, the size of the variations should be selected to be large enough to be statistically significant but not so large as to challenge the assumption of linearity. The Monte Carlo perturbation method is an alternative method that may also be applied to small variations of concentrations in several materials at the same time.

Preparing the input data requires more attention from the user. The calculations and results can be written in a matrix format, convenient to compute the coefficients of the least-squares fit of the first-order development of k_{eff}, by a regression analysis. In this way,
$\Delta k_i = a_i X_i$ is determined for each individual parameter. (See Appendix D.)

5.0 ESTIMATIONS OF SYSTEMATIC EFFECTS AND THEIR UNCERTAINTIES

5.1 Systematic error

Systematic effects that result in systematic errors[a] in measured values may come from many sources. Usually the experimentalist has carefully worked to avoid systematic errors in measurement, or has included a description of any suspected systematic effect and his best estimate of the error and its uncertainty in the experimental report. If he has high confidence in his non-zero estimate of systematic error, he may include it as a correction to reported values. However, uncertainty of the value of the correction, whether the correction is zero or non-zero, remains. This uncertainty, the remaining possibility of systematic error, is called "systematic uncertainty."

Whenever a measuring device is used, there is the possibility of systematic error (systematic uncertainty). Systematic error can be reduced by frequent calibration of the device with a standard, but systematic uncertainty can never be eliminated. Imperfections in the standard and slow drift of the device away from its setting at the time of calibration are examples of remaining sources of systematic error after calibration.

Systematic error is defined as the difference between the mean of an infinite number of measurements of the measurand, under repeatability conditions, and the unknown, true value of the measurand (Reference 1, §B.2.22). Therefore, the systematic error is impossible to know and, perhaps more importantly, the magnitude of systematic uncertainty is not indicated by the range of results of repeated measurements.

An example of a source of systematic error is an improperly zeroed measuring instrument. If a systematic effect in the measurement of a parameter is discovered and the value of the error can be estimated with some confidence, the benchmark model includes the correction to the measured parameter. The correction is equal in magnitude and opposite in sign to the estimate of the error.

5.2 Uncertainty of the estimate of systematic error

As is true for the best estimates of parameter values, the best estimate of systematic error has an uncertainty. Its standard uncertainty is typically difficult to estimate. Usually only a rough approximation is possible. In many cases, the best estimate of the systematic error itself is zero, but this does not mean that its uncertainty is zero. Systematic uncertainty should be evaluated carefully, as its presence can contribute significantly to the total uncertainty and can even invalidate the conclusions of the experiment.

The possibility of remaining, uncorrected systematic errors (i.e., systematic uncertainty) should be included in the total uncertainty. Evaluators are encouraged to always estimate the systematic uncertainty, no matter how small. This requires the evaluator to think about what the remaining systematic error might be and to search for something (e.g., calibration data; systematic

[a] A "systematic error" is also sometimes called "common error." It is an error that is common to all measurements of the same type. Thus the error is the same, in sign and magnitude, for each measurement.

component of the accuracy of the measurement method found in the documentation for the measuring equipment; half of the last digit of the specified average value) that can provide a reasonable value. (See Section C.11 in Appendix C for a suggested method of estimating the magnitude of systematic uncertainty.)

Because a systematic error has the same value for all similar pieces of an assembly, the effect of its uncertainty is cumulative and is not divided by the square root of number of pieces. An example of how to include suspected systematic error of mass measurements is included in Section C.9 of Appendix C.

Because a systematic uncertainty in a parameter specified for pieces of an assembly has a larger effect than a random uncertainty of the same magnitude, it is important that the evaluator clearly indicate which uncertainties are systematic and how estimates of their values were obtained.

5.3 Systematic effect of modeling simplifications

Besides searching for all possible systematic effects in the experiment, the evaluator considers systematic effects induced by the modeling simplifications, such as in geometry, chemistry, isotopics, or impurities. To counteract systematic error due to modeling simplifications, the evaluator calculates the reactivity (Δk) of a modeling simplification, and includes it as a correction to the experimental k_{eff} to obtain the benchmark-model k_{eff}.

As an example of modeling simplifications that may have a systematic effect, suppose a proposed benchmark model does not include surroundings. This is often the case because details of the assembly room are not described in the references, or would be complicated to model if they are known. A calculation with an approximate model of the surroundings may indicate that k_{eff} of the proposed model should have a small negative correction. If the main contributor to the room-return correction is known (e.g. steel support plate, concrete walls, etc.), the evaluator may choose to include an approximate model of the object rather than a correction. An advantage of this approach is that such a model may better represent the neutron spectrum of the experiment.

Omitting impurities may be a source of systematic error and may require a correction to the k_{eff} value of the benchmark model compared to the experimentally determined k_{eff}. However, when impurities are well known, the evaluator may prefer to include them in order to better preserve the neutron spectrum of the experiment.

Another source of systematic error in modeling is rounding of parameter values. This is discussed in Appendix F.

5.4 Uncertainty from modeling simplifications

Besides the correction, the evaluator assigns some fraction of the correction as additional uncertainty (an approximate standard deviation), due to lack of knowledge of whatever was omitted or simplified, the approximate nature of its model, and use of a calculational technique to estimate the correction. The standard uncertainty of the correction is included the same way other uncertainties are included: its reactivity effect on k_{eff} is combined with effects of other parameter uncertainties to obtain Δk_{tot}, the combined uncertainty of k_{eff}.

5.5 Systematic effect of modeling similar components as equal

Another way that modeling can create systematic error is by use of a single value (best estimate of the mean value) for many similar components, for example fuel rods. In reality, variations among rods are usually random, with compensating effects. But in the benchmark models, there are no random variations. All rods have the same value of each parameter. The effect of assigning a slightly incorrect value to all rods can be large.[a]

Related to this possibility of systematic measurement error is the fact that using the mean parameter value is not necessarily the best representation of a critical array. This can be understood by considering an example: Suppose a critical configuration is a stack of nominally equal plates whose fuel masses vary about the average. Suppose that when the experiment is built, plates in the center of the array (region of greatest neutronic importance) happen to have more fuel than the rest of the array. If this experiment is modeled with plates that each contain the average fuel mass, the expected calculated k_{eff} will be less than 1.00. Such an experiment would be better represented by a model whose plates have a fuel mass that is greater than average, namely, one equal to the average of fuel masses weighted by the neutronic importance of their position in the array.[b]

This potential problem is mitigated by experimentalists rerunning the experiment several times, with different plates in different positions each time, and by using the average value of the critical parameter (e.g. spacing, number of plates, moderator height) for the benchmark model. If the average result of repeated experiments defines the critical configuration, benchmark users are more confident that using average parameter values in the model of the experiment is appropriate and will not introduce systematic error.

The helpful evaluator will be alert to the possibility that small errors in average parameter values may lead to large systematic effects for certain types of configurations, and will mention this in the evaluation of these configurations.

[a] See the Section C.8 of Appendix C for an example of an ICSBEP evaluation where this occurred.

[b] However, large homogeneous configurations of many fuel elements, because the variation of the neutronic importance over most of the core is typically very small, are well represented by models using average parameter values.

6.0 ESTIMATION OF THE FINAL COMBINED STANDARD UNCERTAINTY

6.1 General formula

In Section 4, expressions were presented for determining, Δk_i, the effect on k_{eff} of u_i, the standard (1σ) uncertainty in an experimental parameter i. Here, the effects of all N experimental parameters are combined. The **total standard uncertainty in k_{eff}, Δk_{tot},** is the square root of the combined variance, which is the quadratic sum of the Δk_i effects of the individual standard uncertainties (i.e., uncertainties that are estimates of 1σ) in the N experimental parameters and any correlations among the uncertainties. The general formula for the combined variance is

$$(\Delta k_{tot})^2 = \sum_{i=1}^{N}\left[\frac{\partial k_{eff}}{\partial x_i}\right]^2 u_i^2 + 2\sum_{i=1}^{N-1}\sum_{j=i+1}^{N}\frac{\partial k_{eff}}{\partial x_i}\frac{\partial k_{eff}}{\partial x_j} r_{i,j} u_i u_j = \sum_{i=1}^{N}(\Delta k_i)^2 + 2\sum_{i=1}^{N-1}\sum_{j=i+1}^{N}(\Delta k_i)(\Delta k_j) r_{i,j}.$$

Each individual Δk_i represents the change in k_{eff} that occurs when the particular physical parameter x_i is changed by an amount equal to u_i, the standard uncertainty of that parameter. As previously discussed in Section 4, to find Δk_i, first the reference value k_{ref} is calculated. This is k for values of all parameters equal or close to their nominal values in the experiment. Then k is calculated for a variation in parameter x_i, with all other parameters held constant. The difference in the two k values, δk_i, divided by the parameter variation in the calculation, δx_i, represents $\frac{\partial k_{eff}}{\partial x_i}$, the sensitivity of k to the parameter x_i. (The sensitivities may, alternatively, be experimentally obtained from the appropriate reactivity measurements.) Multiplying the sensitivity by u_i, the standard uncertainty of parameter x_i, gives the k_{eff} uncertainty due to the standard uncertainty in that particular parameter: $\Delta k_i = \frac{\delta k_i}{\delta x_i} u_i = \frac{\partial k_{eff}}{\partial x_i} u_i$.

6.2 Application cases

As discussed in Section 4.1.5, when using Monte Carlo codes to calculate the k_{eff} of the reference configuration and the k_{eff} of the parameter variation, the statistical uncertainty of the calculation by the Monte Carlo code (s_{MC}) must be considered. Three cases may be considered when Monte Carlo methods are used to calculate uncertainties:

1. $(k_{\delta xi} - k_{ref})^2 > 2s_{MC}^2$
2. $(k_{\delta xi} - k_{ref})^2 \approx 2s_{MC}^2$
3. $(k_{\delta xi} - k_{ref})^2 < 2s_{MC}^2$

For Case 1 it is clear that the equation (6.2) should be applied. Cases 2 and 3 are more problematic. For Case 2, it is recommended that the evaluator either calculate with more neutron

histories, to reduce s_{MC}, or with larger parameter variation. Then the true effect of the uncertainty can be better estimated.

For Case 3, if s_{MC} is reasonably small (0.0002 or less), the uncertainty may be neglected. If s_{MC} is larger, the evaluator may choose to use $\sqrt{2}\ s_{MC}$ as an estimate of Δk_{eff}, if time and resources do not allow more investigation; but in this case it should be clear that the uncertainty is obtained in this way and is therefore not representative of the sensitivity of the configuration to this parameter. If the evaluator has reason to believe that the calculated change in k_{eff} is unrealistically small, then the recommendation for Case 2 applies: either additional neutron histories may be run (either as a continuation of the original case or as a second case with a different random-number seed), or the case may be run with a larger parameter variation.

The evaluator should be aware of the possibility that dropping a large number of separate, apparently insignificant uncertainty effects could lead to underestimation of the total uncertainty.

When giving the final combined standard uncertainty, it is recommended to give an assessment of the significant parameters and point out those that are not significant.

6.3 Value, small or dominant, of individual uncertainty

Because k_{eff} generally may be approximated by a linear function of its variables within their uncertainty ranges, and because k_{eff} generally depends on many parameters with small uncertainties that contribute comparable amounts to the combined uncertainty, k_{eff} will usually have an approximately normal distribution. In other words, the Central Limit Theorem applies (see §G.2 and §5.1.5 of Reference 1). Then, the combined standard uncertainty in k_{eff}, obtained from the standard uncertainties of its variables, will represent an approximate 68% level of confidence.

If, however, the uncertainty in k_{eff} is dominated by one or two parameter uncertainties whose distributions are not normal, or if the effective number of degrees of freedom (see §G.4.1 of Reference 1) of the k_{eff} distribution is small ($\nu_{eff}<10$), then the k_{eff} standard uncertainty will not represent a probability of 68%. In this case, this condition should be described in Section 3.5 of the benchmark evaluation.

If a significant fraction of the k_{eff} standard uncertainty is from a parameter with a non-normal probability distribution, then the level of confidence of u_i of that parameter distribution may be given,[a] as an indication of how much the level of confidence of the combined k_{eff} uncertainty may deviate from 68%. (See §G.1.4, G.1.5, and G.1.6 of Reference 1.)

6.4 Effective degrees of freedom and level of confidence

In most cases, the number of degrees of freedom of k_{eff} will be sufficiently large, and the shape of its distribution will be sufficiently Gaussian, so that its combined standard uncertainty will represent a range within which the true benchmark-model k_{eff} is estimated to lie with an

[a] See Appendix G for a demonstration of how to calculate the level of confidence of the standard uncertainty u_i from a given probability distribution.

approximate 68% level of confidence. Therefore, it is usually not necessary to determine the degrees of freedom for k_{eff} or for each parameter. Only if k_{eff} or its uncertainty is determined by very few parameters and measurements does the number of degrees of freedom become a concern. This can be understood from the following discussion, which is also useful for dealing with the unusual case, as well as to provide a rough estimate of the reliability of uncertainty values.

The effective number of degrees of freedom ν_{eff} of the total, combined uncertainty, Δk_{tot}, may be estimated from the degrees of freedom of the individual parameters using the Welch-Satterthwaite formula (§G.4 of Reference 1):

$$\nu_{eff} = \frac{\left(\Delta k_{tot}\right)^4}{\sum_{i=1}^{N} \frac{\Delta k_i^4}{\nu_i}}$$

where Δk_i is the effect on k_{eff} of changing parameter x_i by u_i. The value of the effective number of degrees of freedom of an uncertainty of a parameter (assuming a Gaussian probability distribution) determines the level of confidence of the uncertainty. The level of confidence is often expressed as percent probability that the true value lies within plus-or-minus the uncertainty of the estimated value of the parameter. Alternatively, the number of degrees of freedom determines the factor by which the uncertainty may be multiplied to give a particular level of confidence.

If the effective number of degrees of freedom of k_{eff} is small, the revised level of confidence of the combined standard uncertainty of k_{eff} may be stated, or the standard uncertainty of k_{eff} may be multiplied by the coverage factor that gives a 68% level of confidence. Both revised level of confidence and appropriate coverage factor may be found in Table G.2 (Student-t distribution) of Reference 1. The coverage factor for the 68% level of confidence is the value of t in the 68% column of Table G.2 in the row corresponding to the effective number of degrees of freedom ν_{eff}.

A method of assigning the number of degrees of freedom to a Type B uncertainty is given in §G.4.2 of Reference 1. This is based on the expression relating the degrees of freedom to the relative uncertainty of u_i: The relative "uncertainty of the uncertainty" is approximately $0.7/\sqrt{\nu_i}$. For example, if a Type B uncertainty is thought to be "reliable to about 35%" (interpreted to mean that the relative uncertainty of the uncertainty is 0.35), then $0.7/\sqrt{\nu_i} = 0.35$, and $\nu_i = (0.7/0.35)^2 = 4$. For Type B uncertainties that are known to be strict tolerances, an estimate for the degrees of freedom is ∞ because the probability that the value is outside the tolerance range is assumed to be extremely small.

For small ν_{eff} it is recommended to state the approximate relative uncertainty of the k_{eff} standard uncertainty, which is large for small degrees of freedom. It is estimated by the expression $0.7/\sqrt{\nu_{eff}}$. (See §E.4.3 and Table E.1 of Reference 1.)

Note that the coverage factor for a 68% level of confidence for number of degrees of freedom between 3 and 10 (Table G.2 of Reference 1) is approximately 1.1. This means that, for ν_{eff}

between 3 and 10, the combined standard uncertainty should be increased by only 10% to give an uncertainty that represents a 68% level of confidence. For $\nu_{eff} \geq 10$, the increase in the combined standard uncertainty to give a 68% confidence level is 5% or less. So the increase in the combined standard uncertainty due to a small effective number of degrees of freedom is not great.[a]

In general, because the uncertainties and probability distributions of input parameters and their number of degrees of freedom are estimates, it is unrealistic to expect that the level of confidence associated with the combined standard uncertainty of k_{eff} is well known. However, following this method will generally give a level of confidence that is within a few percent of 68%. In other words, the probability that k_{eff} of the configuration described by the benchmark model is within the combined standard uncertainty [$\pm\Delta k_{tot}$] of the benchmark-model k_{eff} value is approximately 68%.

[a] Consider this extreme example: Suppose the combined benchmark-model k_{eff} uncertainty is 0.005. Suppose that the dominant parameter uncertainty contributes 90% (i.e., is 0.0045) and has 2 degrees of freedom, and all other uncertainties have degrees of freedom which are very large. According to the Welch-Satterthwaite formula, $\nu_{eff} \approx \frac{0.005^4}{\frac{0.0045^4}{2}} = 3$. Then, using Table G.2 of Reference 1, the coverage factor is 1.2, so that the combined k_{eff} uncertainty should be increased by a factor of 1.2. The revised combined benchmark-model k_{eff} uncertainty for a 68% level of confidence is then 0.006.

7.0 REFERENCES

1. "American National Standard for Expressing Uncertainty - U.S. Guide to the Expression of Uncertainty in Measurement," National Conference of Standards Laboratories, ANSI/NCSL Z540-2-1997.

2. Guide pour l'expression de l'incertitude de mesure - European Prestandard NF ENV 13005 Août 1999.

3. G. Box, W.G. Hunter, J.S. Hunter, "Statistics for Experimenters," John Wiley and Sons (1971).

4. J. Goupy, La méthode des plans d'expérience (translation: "Experimental Design Method") Dunod, Paris, 1996.

5. F. H. Fröhner, "Assigning Uncertainties to Scientific Data," *Nucl. Sci. Eng.* **126** (1997) 1.

6. F. H. Fröhner, "Evaluation and Analysis of Nuclear Resonance Data," JEFF Report 18, OECD Paris (2000).

APPENDIX A: GLOSSARY OF METROLOGY AND ASSOCIATED STATISTICS

A.1 Metrology

In this section, some definitions are given, so that those words are well known when they are used in the main text. These definitions are taken from Appendices B, C, and D of References 1 and 2, except where noted.

metrology
the science of weights and measures or of measurements

measurement
set of operations having the object of determining a value of a quantity, or measurand

measurand
particularly defined quantity subject to measurement

result of a measurement
value attributed to a measurand, obtained by measurement

accuracy of measurement
closeness of the agreement between the result of a measurement and true value of the measurand[a]

conventional true value (of a quantity)
value attributed to a particular quantity and accepted, sometimes by convention

repeatability
closeness of the agreement between the results of successive measurements of the same measurand carried out under the same conditions of measurement

reproducibility
closeness of the agreement between the results of measurements of the measurand carried out under changed conditions of measurement

experimental standard deviation

$$s = \sqrt{\frac{1}{n-1}\sum_{i=1}^{n}(q_i - \bar{q})^2}$$

q_i being the result of the i^{th} measurement and $\bar{q}$ the arithmetic mean of the n considered results. It expresses the closeness of the agreement between a series of n measurements of the same measurand and characterizes the dispersion of the results.

[a] [Reference 1 calls accuracy a "qualitative concept." It might also be called a "quantitative approximation of uncertainty" when it is expressed as a value. – *editor*]

uncertainty (of measurement)
parameter, associated with the result of a measurement, that characterizes the dispersion of the values that could reasonably be attributed to the measurand

error (of measurement)
result of a measurement minus the true value of measurand

relative error
error of measurement divided by true value of the measurand

random error
result of a measurement minus the mean that would result from an infinite number of measurements of the same measurand carried out under repeatability conditions

systematic error
mean that would result from an infinite number of measurements of the measurand carried out under repeatability conditions minus the true value of the measurand
(The error of measurement is the sum of systematic error and random error.)

true value
value of the measurand that would be obtained by a perfect measurement[a]

A.2 Basic statistical terms

Common statistical concepts such as probability distribution, distribution function, expected value, variance, standard deviation, normal distribution, (two-sided) confidence interval, confidence level, degrees of freedom, covariance, and Student-t distribution are defined extensively in Appendix C of Reference 1, entitled: "Basic statistical terms and concepts" or in Appendix C of Reference 2 entitled "Termes et Concepts Statistiques Fondamentaux".

degrees of freedom
number of terms in a sum minus the number of constraints on the terms of the sum.
The number ν of degrees of freedom is equal to n-1 for a single quantity estimated by the arithmetic mean of n independent observations. For a Type B uncertainty that bounds all possible values of the measurand, ν is taken as infinite (∞).

probability
degree of plausibility or rational expectation on a numerical scale ranging from 0 (impossibility) to 1 (certainty), intermediate values indicating intermediate degrees of plausibility[b]

[a] Definitions that include the terms “infinite number of measurements” or “true value” are ideal quantities that generally cannot be known exactly. Their values can only be estimated.
[b] Reference 6, p. 4.

APPENDIX B: SUMMARY OF SOME PRINCIPLES FOR UNCERTAINTY EVALUATION

This section presents a summary of some general principles for calculating uncertainties, as may be understood from the main text of this guide.

1. It is, of course, basic to know if the parameter uncertainty u_i is Type A (statistical type) or Type B (non-statistical type), as described in Section 2. However, once the parameter uncertainty u_i is determined, the effect on k_{eff} is calculated without regard to its type.

2. The estimated probability distribution can be used to derive an estimate of the standard deviation for a Type B uncertainty (see one example in Appendix G).

3. After a preliminary, cursory evaluation of effects of parameter uncertainties on k_{eff}, the evaluator may list all parameters and classify them in order to determine their importance relative to the total uncertainty. Except when possible estimation errors are suspected, it is not necessary to make detailed evaluations for parameters that contribute a small part of the total. Instead, the evaluator may refer to the smallness of the effects or to his specific knowledge of previous evaluations of similar experiments with similar devices, apparatus, or configurations, to explain why he does not more fully investigate the small parameter uncertainties.

4. Uncertainties in k_{eff} of the benchmark model have two main sources: parameter measurements and modeling simplifications.

5. In arrays of fissile units that are nominally the same, parameters may vary slightly from one unit to another in the actual experiment. But in the benchmark model, the fissile units in an array are almost always modeled as identical, with all having the mean measured values of the parameters. Using the mean value for each parameter is a simplification of the benchmark model. It is generally assumed that the net effect on k_{eff} of physical variation among the units in the array is zero, so there is no correction to k_{eff} from using the mean value in the model. However the physical variation in the experiment compared to lack of physical variation in the model contributes to the uncertainty in k_{eff} of the benchmark model.

6. Parameter x may be estimated by an average, $\bar{x}$, of n observations of its value. Its standard uncertainty is the experimental standard deviation (square root of the variance) divided by $\sqrt{n}$. This can be derived by considering the combined uncertainty of the function $\bar{x} = \frac{1}{n}\sum_{i=1}^{n} x_i = \sum_{i=1}^{n} \frac{1}{n} x_i$. The standard uncertainty of each observation, x_i, is $u_i = s$. Therefore, the combined variance of $\bar{x}$ (assuming no correlations among observations) is

$$\left\langle \sigma^2 \right\rangle = \sum_{i=1}^{n} \left(\frac{\partial \bar{x}}{\partial x_i} \right)^2 u_i^2 = \sum_{i=1}^{n} \left(\frac{1}{n} \right)^2 s^2 = n \times \left(\frac{1}{n} \right)^2 s^2 = \frac{s^2}{n}.$$

Taking the square root of this gives $s/\sqrt{n}$, the combined standard uncertainty.

.

7. Error is the difference between measured result and true value of the measurand. The error is unknown. Uncertainty is an estimate of the possible error, based on the expected (but unknown) probability distribution for the parameter. The standard uncertainty is the best estimate of the standard deviation of that probability distribution. Standard uncertainties are estimated from a series of measurements (Type A) or from whatever other data is given (Type B), combined with any relevant prior information.

8. The combined standard uncertainty of a quantity (measurand) that depends on other parameters is the best estimate of its standard deviation, obtained from the standard uncertainties of the independent parameters and sensitivities of the quantity to variations of the parameters. If the parameters and measurements of the parameters are independent, there are no correlation terms.

9. The combined standard uncertainty of k_{eff} is obtained by combining the reactivity effects of the standard uncertainties of the parameters upon which k_{eff} depends. The reactivity effect of each parameter standard uncertainty is the change in k_{eff} from increasing (or decreasing) the parameter value by its standard deviation. If parameter variations are independent (no correlations between them), the k_{eff} combined standard uncertainty is the square root of the sum of the squares of the effects of the individual standard uncertainties of all parameters.

10. The probability distribution of the benchmark-model k_{eff} (as parameters of the configuration vary according to their respective probability distributions) is usually a normal, or Gaussian, distribution. This assumption is justified whenever none of the non-normal parameter distributions dominate the uncertainty in k_{eff}, and whenever k_{eff} may be approximated as a linear function of its parameters (which is usually true, at least for small variations of the parameters). Therefore, the standard deviation of k_{eff} represents an interval with a 68% level of confidence. This means that the estimated probability is 68% that the value of k_{eff} of the configuration described by the benchmark model is within the standard deviation of the benchmark-model k_{eff}.

11. Use of a measuring device introduces two kinds of measurement uncertainty: from possible random error and from possible systematic error. Both uncertainties should be included in the combined standard uncertainty, but the algorithms for calculating their contributions to the combined standard uncertainty are sometimes different.

12. A Type A uncertainty evaluation usually does not provide systematic uncertainty. Therefore, by itself it may be of little value, since measurements with nothing but random uncertainties are the exception rather than the rule in physics.

13. When using the term "systematic uncertainty," its definition should be clear. It might refer to 1) the (unknown) systematic error, 2) the best estimate of the systematic error included as a correction, or 3) the uncertainty in the estimate of the systematic error, whether that estimate is zero or is non-zero and included as a correction. In this guide, it is used only in the last sense. The effect of systematic uncertainty should be combined with other uncertainties to obtain the total combined standard uncertainty of k_{eff}.

14. Often the effect on k_{eff} of the uncertainty in the estimate of systematic error can be most easily determined by considering δ_c, a small correction to each observation. This correction δ_c represents the systematic error. The value of δ_c, the estimate of the systematic error, is zero unless there is a

basis for a non-zero estimate. The uncertainty in δ_c is the uncertainty in the estimate of the systematic error, called the "systematic uncertainty."

15. For correctly evaluating uncertainties of arrays, all of the following numbers are important:
    N – the number of fissile units in the array,
    N_p – the total population of fissile units,
    N_m – the number of fissile units that have been measured,
    n – the number of measurements of the parameter per unit.

16. Generally, physical variation of a measurand is not easily distinguished from random uncertainties of the measuring device.

17. If the mean parameter value is obtained by averaging measurements of each unit in the array, so that the number of measurements (n) is the same as number of units in the array (N), the calculation of the effect of the standard uncertainty of the parameter for an array is much simpler.

18. When calculating $\frac{\partial k_{eff}}{\partial x_i}$, the sensitivity of k_{eff} to a parameter, it is not necessary to change the parameter by its standard uncertainty, u_i, in the calculation. Instead, Δk_{eff} may be calculated by changing x_i to $x_i + \delta x_i$, as long as δx_i and u_i are both small enough that the change in k_{eff} is linear with the change in the parameter. Then the effect of the standard uncertainty is

$$\Delta k_i = \frac{\left| k_{eff}(x_i) - k_{eff}(x_i + \delta x_i) \right|}{\delta x_i} \times u_i .$$

19. Because the effect of systematic error does not diminish with number of elements in an assembly (like the effect of random uncertainty does), it is important to include estimates of systematic uncertainty in the uncertainty analysis. Otherwise the combined k_{eff} uncertainty may be underestimated.

APPENDIX C: EXAMPLES OF UNCERTAINTY EVALUATIONS

This section presents a few examples applying the principles of Appendix B, in particular, examples evaluating Δk_i for arrays of fissile units.

It should be noted that the depth of the discussion of the examples is not meant to imply that all uncertainties should be scrutinized to such detail. In fact, for the example in Section C.1, the differences in the results of different analyses are practically insignificant. (This fact, itself, may be instructive.) Here, the depth of discussion is not related to the particular size of the uncertainty. As mentioned in Appendix B (#3), the larger the uncertainty, the more scrutiny is appropriate.

Also, examples of UO_2 rods are emphasized. This is because effects of uncertainties of array parameters are typically more difficult to evaluate than other uncertainties, for some of the reasons mentioned in the discussion.

C.1 Examples of determining Δk_i, the effect on k_{eff} of the standard uncertainty σ_i of a parameter x_i for a critical array of fuel rods

In a fuel rod array, many parameters are random variables. If the parameter measurement is of statistical type (Type A), the parameter value obtained from the series of n measurements is defined by its mean $\overline{m}$, variance $<\sigma^2>$, and number ν of degrees of freedom (see Section A.2). The standard uncertainty of $\overline{m}$ is then $<\sigma>/\sqrt{n}$, corresponding to the standard deviation of the mean (see §4.2 of Reference 1, pp. 65-68 of Reference 3, and References 5 and 6).

The parameters of an array either characterize the fuel rod itself and are due to the way rods were manufactured:

- fuel linear density,
- inner and outer clad diameter,
- clad thickness,
- fissile column diameter,
- fissile column height,

or they characterize the array, such as the pitch. (Pitch uncertainty is further discussed in Section C.2.5.)

A few parameters of fuel rod arrays may be measured separately and are already assumed to apply to all rods, such as fuel enrichment, stoichiometry (O/U or O/Pu ratio), fuel-pellet density, impurities, and clad density and composition. (Fuel-enrichment uncertainty is discussed in Section C.4.)

Consider an **example**. Suppose that the following is known about the fuel mass in fuel rods of a critical configuration: The configuration comprises 100 fuel rods that are nominally the same. The mass of fuel in 36 rods is measured by a measuring device that has an accuracy of 0.1 grams. Therefore, the measurement consists of 36 values, one observation of each rod. The 36

observations result in a measurement of average mass of fuel (UO_2) in a rod. The result is 580.00±0.21 g (1σ).

The question to be answered is "What is Δk_{mass}, the effect on k_{eff} of u_{mass}, the standard uncertainty in UO_2 mass in the rods of the critical configuration?"

For clarity, it is advisable to first evaluate the standard uncertainty u_i in the particular parameter x_i. (Here, x_i is fuel mass per rod.) Then use u_i to find the uncertainty in k_{eff}, Δk_i, due to the particular value of the parameter uncertainty. Also, the evaluator should be careful to distinguish between N=100, the number of rods in the configuration, and n=36, the number of measurements of the parameter from which the mean parameter value is derived.

There are several acceptable answers, depending on additional data and evaluator judgment.

C.1.1 One acceptable answer

C.1.1.1 Parameter uncertainty

1. The following is known about the measurement:
    a. The value of the fuel mass of 36 of the rods used in the configuration was observed.
    b. The mean value of fuel mass per rod was 580 g.
    c. The standard deviation (s) of the 36 observations was 0.21 g.
    d. The accuracy of the measuring device was 0.1 g.
2. The evaluator must make the following judgments, based on further investigation of data about the measurement and the measuring device and, if necessary, best guesses about the meaning of the available data:
    a. Is the ±0.21-g uncertainty the experimental standard deviation, i.e., is it the square root of the variance of the measurement (36 observations)? Or was the variance divided by √n=6 to give the standard deviation of the mean mass?
    b. Does the 0.1-g accuracy of the measuring device represent a standard deviation, the entire range of possible values, or something else?
    c. What is the shape of the probability distribution curve of measurement uncertainty represented by the 0.1-g accuracy of the device? (normal, flat, etc.)
    d. The evaluator has learned that the word "accuracy" has no generally accepted definition and that it is often used differently in different contexts. He wonders, "Does the stated accuracy include estimates of possible systematic error as well as possible random error?"
    e. If it includes possible systematic error, what is the best estimate of the value of the systematic error? If the best estimate of the systematic error is not zero (for example, if an estimate, including direction, of the expected drift of the device's zero from the time of last calibration is known), then a correction, equal to the best estimate of the drift, to each measured value of fuel mass should be made.
3. Suppose the evaluator decides the following:
    a. Logbook data show that 0.21 g is the experimental standard deviation (square root of the variance) of the 36 observations.

   b. The measuring device has no known systematic error: the device was calibrated immediately before the measurements with a highly accurate standard (contributing negligible additional uncertainty) and the device was checked with the standard after the mass measurements and showed no drift, or change.
   c. The ±0.1-g accuracy is the entire range of the possible random error.
   d. There is no basis for estimating the shape of the probability distribution of the uncertainty.
4. The evaluator revises what is known about uncertainty from the measuring device. He assumes that ±0.1 g represents the entire range of the probability distribution of each observation and that the probability distribution is uniform (flat) over the range. Therefore, the standard uncertainty of each observation is $0.1/\sqrt{3}$ g (derived in Appendix G), and it is assumed symmetric about the observed mass value.
5. #1, above, is revised to the following:
   a. The value of the fuel mass of 36 of the 100 fuel rods used in the configuration was observed.
   b. The mean value of fuel mass per rod was 580 g.
   c. The experimental standard deviation of the 36 observations was 0.21 g.
   d. The standard uncertainty of each observation from the measuring device is $0.1/\sqrt{3}$ g = 0.058 g.
6. Now the evaluator wants to decide whether the 0.21 g is only from physical variation of UO_2 mass among rods, or whether the 0.21 g includes the 0.058-g standard uncertainty of the measuring device. (Reference 1 in §4.3.10 says it is important not to "double-count" uncertainties.)
   a. Suppose he decides that the 0.21 g includes both physical variation among rods and the measurement uncertainty, so that $0.21^2 = u_{mv}^2 + 0.058^2$, where u_{mv} is the mass variation among the rods. Therefore, the standard deviation of physical variation among rods may be estimated as $u_{mv} = \sqrt{0.21^2 - 0.058^2} = 0.202$ g.
   b. Then the two uncertainties in rod mass are 0.202 g, from physical variation among rods, and 0.058 g standard uncertainty of the measurement of each rod.

C.1.1.2 k_{eff} uncertainty (effect of 0.022 g/rod)

Uncertainty from simplification of the benchmark model. The benchmark model uses $x_i = \bar{m}$, the mean fuel mass per rod, for all rods. This is a simplification from the actual experiment, in which there is small physical variation (standard deviation of 0.202 g) of the fuel mass among the rods. Since the best estimate of x_i (mean $\bar{m}$) is used in the model, there is no correction to k_{eff} of the benchmark model. However, this simplification contributes uncertainty to k_{eff} of the benchmark model.

To estimate the k_{eff} effect of this standard uncertainty from physical variation, add 0.202 g of UO_2 to the mass of every rod. Divide the resulting Δk_v by number of rods in the configuration,

N=100, to find the approximate effect from each rod, $\Delta k_j = \frac{\Delta k_v}{100}$.[a] Since the physical variations among rods are assumed independent, add, in quadrature, the Δk_j effect from each rod to get the k_{eff} uncertainty from rod variation. The resulting reactivity effect is

$$\Delta k_{mv} = \sqrt{\sum_{j=1}^{N} (\Delta k_j)^2} = \sqrt{\sum_{j=1}^{100} \left(\frac{\Delta k_v}{100}\right)^2} = \sqrt{100 \times \left(\frac{\Delta k_v}{100}\right)^2} = \frac{\Delta k_v}{\sqrt{100}} = \frac{\Delta k_v}{\sqrt{N}}.$$

This is the k_{eff} uncertainty due to the mass variation among rods in the experiment compared to the simpler benchmark model, which has the same mass $\overline{m}$ in each and every rod.

Measurement uncertainty. There is an uncertainty in mean mass of the rod due to the 0.058-g uncertainty in the observation of each rod from the measuring device. The mean mass per rod is

$$x_i = \overline{m} = \frac{1}{n}\sum_{j=1}^{n} m_j = \sum_{j=1}^{n} \frac{1}{n} m_j .$$

The combined variance of x_i (see the general formula in Section 2.4) is

$$\sum_{j=1}^{n} \left(\frac{\partial x_i}{\partial m_j}\right)^2 u_{mj}^2 = \sum_{j=1}^{n} \left(\frac{1}{n}\right)^2 0.058^2 = n\left(\frac{1}{n}\right)^2 0.058^2 = \frac{0.058^2}{n}.$$

So the standard uncertainty of x_i due to accuracy of the measuring device is $\frac{0.058}{\sqrt{n}}$ g.

To find the effect, Δk_{mm}, of this mass-measurement uncertainty, change x_i by $\frac{0.058}{\sqrt{36}} = 0.0096$ g and calculate Δk_{mm}. Since the evaluator has already calculated Δk_v for changing all rods by δm=0.202 g, he multiplies Δk_v by $\frac{0.0096}{(\delta m)} = \frac{0.0096}{0.202}$. So $\Delta k_{mm} = \Delta k_v \left(\frac{0.0096}{0.202}\right)$.

Combined mass uncertainty, Δk_{mass}. The combined k_{eff} uncertainty due to uncertain fuel mass is the square root of the quadratic sum of the two above calculated uncertainties.

$$\Delta k_{mass} = \sqrt{\Delta k_{mv}^2 + \Delta k_{mm}^2}$$

[a] Actually, the Δk_j's are not the same, as discussed in Section C.2. Rods at the center will contribute more than those near the edges due to greater neutronic importance of central rods. But equal contributions from every rod may be used as an approximation.

$$= \sqrt{\frac{\Delta k_v^2}{100} + \Delta k_v^2 \left(\frac{0.0096}{0.202}\right)^2} = \sqrt{\frac{\Delta k_v^2}{100}\left(\frac{0.202}{0.202}\right)^2 + \frac{\Delta k_v^2}{36}\left(\frac{0.058}{0.202}\right)^2}$$

$$= \frac{\Delta k_v}{0.202}\sqrt{\frac{0.202^2}{100} + \frac{0.058^2}{36}} = \frac{\Delta k_v}{0.202} \times 0.022 .$$

More generally, $$\Delta k_i = \frac{\Delta k_{\delta xi}}{\delta x_i}\sqrt{\frac{u_{iv}^2}{N} + \frac{u_{im}^2}{n}} \qquad \text{(C1)}$$

where

- Δk_i = change in k_{eff} due to standard uncertainty u_i of parameter x_i (In the example, x_i is $\bar{m}$, mean fuel mass in a fuel rod.),
- $\Delta k_{\delta xi}$ = change in k_{eff} if parameter x_i is changed by δx_i,
- δx_i = increment of x_i in the perturbed k_{eff} calculation,
- u_{iv} = the standard uncertainty of x_i representing physical variation of the parameter among units of the array,
- N = number of units in the array,
- u_{im} = the standard uncertainty of x_i due to measurement accuracy,
- n = number of measurements used to determine $x_i = \bar{m}$.

Therefore, in the case of parameter x_i whose value, the average of n measurements, is used for each of N fissile units of a critical configuration, the standard uncertainty used to obtain Δk_i for that parameter is

$$u_i = \sqrt{\frac{u_{iv}^2}{N} + \frac{u_{im}^2}{n}}. \qquad \text{(C2)}$$

The evaluator observes that if all 100 rods of the configuration had been measured to obtain the mean value of UO_2 mass per fuel rod, so that $n \geq N$,[a] then the resulting reactivity effect of the standard uncertainty would have been much simpler to calculate. In this case, the result for Δk_{mass} would have been the same obtained by assuming that the standard uncertainty in mass x_i of each rod was

$$\frac{\sqrt{0.202^2 + 0.058^2}}{\sqrt{N}} = \frac{0.21}{\sqrt{N}} \text{ g} = 0.021 \text{ g}.$$

[a] If n>N, according to Reference 1 (see, for example, §H.1.3.2) the "pooled" experimental standard deviation is divided by the square root of the number relevant to the current case, which is N, number of rods in the critical configuration.

C.1.2 Another acceptable answer

C.1.2.1 Parameter standard uncertainty

Suppose the evaluator makes the same judgments through #5 in Section C.1.1.1. Then he decides that the observed experimental standard deviation 0.21 g does not include the uncertainty of the measuring device. Perhaps he reasons that there are other random influences (e.g. rod variation, air temperature and pressure at times of measurement) besides the measuring device that cause the observed 0.21-g experimental standard deviation, and that the uncertainty of the device contributes additional uncertainty. Or perhaps he has reason to believe that the experimentalists intended the 0.21 g to represent variation among rods and, therefore, the 0.21 g was after correction for the accuracy of the measuring device.

(Including both the observed variation and the stated uncertainty of the measuring device follows the method of examples in Reference 1 (note 2 of §4.3.7 and §H.1.3.2). In §H.1.3.2 the standard deviation of the mean of measurements is combined with the two standard uncertainties of the comparator (measuring device) – one standard uncertainty from possible random error and one from possible systematic error.)

C.1.2.2 k_{eff} uncertainty, Δk_{mass} (effect of 0.0231 g/rod)

The evaluator knows from experience (e.g., Section C.1.1.2) that unless n (number of measurements of the parameter) is equal to N (number of rods in the array), it is necessary to make an estimate of physical variation among the rods and distinguish it from measurement uncertainties in order to obtain the combined k_{eff} uncertainty. Therefore, he uses formula (C2) to find the standard uncertainty u_{xi}. The standard uncertainty representing physical variation among the rods is the observed standard deviation of the Type A measurement, $\sigma_{mv} = 0.21$ g. The standard uncertainty of each mass measurement is $\sigma_{mm} = 0.058$ g. Therefore, the standard uncertainty of the mean mass (fuel mass in each rod) is

$$u_i = \sqrt{\frac{u_{mv}^2}{N} + \frac{u_{mm}^2}{n}} = \sqrt{\frac{0.21^2}{100} + \frac{0.058^2}{36}} = \sqrt{0.00044 + 0.000093} = \sqrt{5.34 \times 10^{-4}} = 0.0231 \text{ g.}$$

The evaluator obtains Δk_{mass} by changing x_i by 0.231 g and dividing the resulting Δk by 10.

C.1.3 A third possible acceptable answer

C.1.3.1 Parameter standard uncertainty

Suppose the evaluator learns, from studying the mass-weighing device's calibration certificate, that the 0.1-g accuracy of the measuring device is the entire range of a possible systematic error (see Section 5.0). Therefore, ±0.1 g bounds the uncertainty of an unknown correction δ_{cor} that should be added to each measurement. (For example, the correction might be the drift of the zero point, or calibration reference point, since the time of calibration.) So each observation of mass should be corrected by a small amount, δ_{cor} grams, which is approximately the same for each

observation, but is unknown. The calibration certificate also states that, based on repeated calibrations of other individual weighing devices of the same kind, the expected value of the error is zero and the distribution of the possible error about its expected value is approximately normal. Because the distribution is normal and not flat, 0.1 g represents approximately 3σ (not $\sqrt{3}\sigma$). The standard uncertainty u_{cor} of δ_{cor} is then $0.1/3 = 0.033$ g (not $0.1/\sqrt{3} = 0.058$ g).

The evaluator understands that the observed Type A experimental standard deviation, 0.21 g, probably includes both physical variation among the 36 measured rods as well as random uncertainty of the measurement procedure, but he does not know how to apportion the two sources of the observed random variation. He decides to ask the experimenter to make some repeated measurements of a single mass sample of approximately 580 g, in order to obtain an estimate of the random uncertainty of the measurement procedure. The result of 20 repeated measurements of the sample gave an experimental standard deviation of 0.08 g. The evaluator takes this value as the experimental standard deviation of the random error of a measurement. The remaining $\sqrt{0.21^2 - 0.08^2} = 0.19$ g is assumed to be due to physical variation among the rods.

The mean value of fuel mass per rod is $x_i = \overline{m} = \frac{1}{N}\sum_{i=1}^{N}(m_i + \delta_{cor}) = \delta_{cor} + \frac{1}{N}\sum_{i=1}^{N} m_i$. So the combined standard uncertainty of x_i due to measurement uncertainties is

$$\sqrt{\left(\frac{\partial x_i}{\partial \delta_{cor}}\right)^2 u_{cor}^2 + \sum_{i=1}^{N}\left(\frac{\partial x_i}{\partial m_i}\right)^2 u_{mi}^2} = \sqrt{0.033^2 + \left(\frac{1}{n}\right)^2 \sum_{i=1}^{n} u_{mi}^2} = \sqrt{0.033^2 + \frac{1}{n^2}\times n \times 0.08^2}\ \text{g.}$$

$$= \sqrt{0.033^2 + \frac{0.08^2}{36}} = 0.036 \text{ grams.}$$ This standard uncertainty must be combined with uncertainty from physical variation, $0.19\ \text{g}/\sqrt{100} = 0.019$ g. Therefore, the combined uncertainty of the mass of fuel in a fuel rod is $\sqrt{0.019^2 + 0.036^2} = 0.041$ g/rod.

C.1.3.2 k_{eff} uncertainty, Δk_{mass} (effect of 0.041 g/rod)

The reactivity effect of the ±0.041-g uncertainty of x_i can be estimated by adding 0.041 grams of fuel mass to every rod to find Δk_{mass}.

Note that this is the largest of the possible Δk_{mass} values considered. This is because the uncertainty of the systematic error, which is estimated as zero and so requires no correction, contributes 0.033-g uncertainty to the mass of each rod.

C.1.4 Other possible acceptable answers

Other acceptable answers are possible, depending on available data and judgment of the evaluator. The evaluator should attempt to discover what is known about the measurements and

uncertainties of the measuring devices. Whatever the answer, it should be justified by including reference to the data, assumptions, and the reasons for the assumptions.

C.2 Estimating more realistically the effect of random variation among units of an array, Δk_{array}

As described in Section C.1, the effect of the uncertainty in a parameter is calculated by varying the parameter in a k_{eff} calculation. To find the effect of the random variation of a parameter among rods or units of an array, the Δk_{eff} effect may be estimated by dividing by $\sqrt{N}$, the number of rods or units in the array. (See Section C.1.1.2.)

The derivation of $\Delta k_{array} = \Delta k_{eff}/\sqrt{N}$ included using $\Delta k_{eff}/N$ for the average effect of each rod. However, this approximation is not realistic, because it is known that rods near the center of the array have a greater neutronic importance than rods near the periphery. Because the effects from each rod are added in quadrature (i.e., square root of sum of squares), this uneven weighting must be taken into account if the effect of random variation is desired.

C.2.1 The correcting factor κ_{corr}

For all such parameters, a more realistic Δk_{eff} effect of the random parameter variations in the configuration may be obtained by dividing Δk, obtained from changing all rods by the experimental standard deviation of the parameter, by the square root of the number N of rods multiplied by a correcting factor:

$$\Delta k_{array} = \frac{\Delta k}{\sqrt{\kappa_{corr} N}} \ .$$

The factor κ_{corr} is a correcting factor introduced to take into account the unequal importance of fuel rods in the reactor core. The order of magnitude of κ_{corr} lies roughly between 0.5 and 1.[a]

Since it is difficult to find the value of κ_{corr}, an alternative method divides the array of N rods into l concentric zones of N_j rods (j = 1,...l), using for the standard uncertainty the expression

$$\Delta k_{array} = \sqrt{\sum_{j=1}^{l} \frac{\Delta k_j^2}{N_j}} \quad \text{with} \quad N = \sum_{j=1}^{l} N_j \ .$$

Each Δk_j is calculated with only the N_j rods in zone j changed.

It is interesting to notice that, **if κ_{corr} equals 1 or if l equals 1, then Δk_{array} is probably slightly underestimated. Nevertheless it still may be considered a good approximation**, as shown in recent calculations, comparing the formula to calculations using zones. For small pitch (e.g. 1.1 cm, 1.3 cm) the difference is larger, but still not significant. Of course, as N gets larger, the effect

[a] For large N, a better estimate for the interval is 0.8 to 1. Since n is often very large and we divide by $\sqrt{N}$, then the uncertainty is small, so that the effect of κ_{corr} differing slightly from 1 is very small for large N.

of slightly different correction terms κ_{corr} becomes smaller, as mentioned above. On the other hand, if $\kappa_{corr} \cdot N$ equals 1, then Δk_{array} is overestimated.

If l =N and all N_j are equal to 1, then the correct value is calculated. However, this requires N+1 calculations of k_{eff} that differ from each other by the characteristics of only one rod. Therefore, the Δk_{eff}'s are very small.

If u_i is too small to yield a reliable Δk_{eff}, a larger variation δx_i of the parameter is used to compute Δk_{eff}. The real change in k_{eff} will be

$$\Delta k = \frac{\Delta k_{eff}}{\delta x_i} \times u_i .$$

Of course, this formula is only reliable for small variations, when the effect is linear.

This treatment of uncertainty is explained in the following paragraphs by using one selected parameter (the outer clad diameter) and a progressive approach.

C.2.2 Progressive approach

Array Type 1 : array with N identical rods

The k_{eff} change due to a variation of fuel-rod diameter can be evaluated as illustrated in Steps 1 and 2, below.

Step 1: Two arrays, each with n identical fuel rods

One way to obtain Δk_{array} is to consider two arrays, each of them with identical rods. A reference calculation is performed for the first array, having rods with the mean diameter $\bar{d}$. Another calculation is performed for the second array, having rods with diameter $\bar{d} + u_d$, where u_d is the standard deviation of the diameter distribution of the fuel rods for the experiment.

For *Step 1*, the Δk obtained by subtraction is equal to Δk_1.

$$\Delta k_1 = k_{eff}(\bar{d}) - k_{eff}(\bar{d} + u_d) \qquad (1)$$

Step 2: k_{eff} variation due to one single rod in an array of N identical rods

Assuming that the k_{eff} variation due to each rod is independent of the grid position, the variation of k_{eff} of an array of rods with diameter $\bar{d}$ due to one single rod of diameter $\bar{d} + u_d$, is given by

$$\Delta k_{rod} = \frac{\Delta k_1}{N} \qquad (2)$$

However, as discussed above, this is not perfectly true. Actually, each rod contributes according to its neutronic importance, which is proportional to the adjoint of the flux distribution. The rods in the middle of the array contribute most to k_{eff}. In fact, the contributions from rods near the center of the array are greater than $\Delta k_1/N$. (Note that, in the case of undermoderated arrays, peripheral rods located next to a water reflector will have higher worth than peripheral rods of an optimally moderated or overmoderated array.)

Array Type 2 : array with no identical rods

Suppose that each position of the grid holds one rod or another, diameters being different. The position that each single rod takes is random, i.e., each position contains a random variable.

The array variance is obtained by adding the variances of each rod:

$$\Delta k^2_{array} = \Delta k^2_{rod1} + \Delta k^2_{rod2} + \Delta k^2_{rod3} + ... + \Delta k^2_{rodN}$$

In addition, the variance of each position in this array is considered as identical to the one calculated in *Step 2*, above.

Therefore,

$$\Delta k^2_{array} = N\Delta k^2_{rod} = N\left(\frac{\Delta k_1}{N}\right)^2 = \frac{(\Delta k_1)^2}{N},$$

and the standard deviation of the array due to the parameter is

$$\Delta k_{array,diam} = \frac{\Delta k_1}{\sqrt{N}} \qquad (3)$$

(This formula gives also the standard deviation of the mean value of k_{eff} for N arrays containing identical rods, where each array has rods identical to one of the rods in the original array.)

C.2.3 Finding a more realistic Δk_{array}

1. Formula (1) overestimates the uncertainty worth, because it assumes that all rods are identical and have the same parameter change, which is not at all the real situation. Rods have independent variations, so that there are compensating effects. Formula (3) underestimates the uncertainty worth because unequal neutronic importance is not accounted for.

2. The k_{eff} change due to each rod is not independent of the grid position, because the central rods are the most important in terms of reactivity worth and their contribution to a k_{eff} change is greater than $\Delta k_{eff}/N$.

   Therefore, several Δk_{rod}'s are bigger than $\Delta k_{eff}/N$. In general, when uncertainties are combined by taking the square root of the sum of their squared values, the bigger ones will dominate. Therefore, $\Delta k_{array,\ diam}$ should be larger than $\Delta k_{eff}/\sqrt{N}$.

3. For this reason, it is recommended to consider several concentric zones (e.g. 3 zones) and to calculate for each zone the value $\Delta k_{eff}/N_i$ as explained hereafter:

   - calculation 1: all rods of the whole configuration with diameter $\bar{d}$,
   - calculation 2: rods of zone 1 with diameter $\bar{d}+u_d$,

     rods of zones 2 and 3 with diameter $\bar{d}$,
   - calculation 3: rods of zone 2 with diameter $\bar{d}+u_d$,

     rods of zones 1 and 3 with diameter $\bar{d}$,
   - calculation 4: rods of zone 3 with diameter $\bar{d}+u_d$,

     rods of zones 1 and 2 with diameter $\bar{d}$,

   The standard k_{eff} uncertainty for the array is

$$\Delta k_{array} = \sqrt{\sum_{j=1}^{3}\sum_{i=1}^{N_j}\left(\frac{\Delta k_j}{N_j}\right)^2} = \sqrt{\sum_{j=1}^{3} N_j\left(\frac{\Delta k_j}{N_j}\right)^2} = \sqrt{\sum_{j=1}^{3}\frac{(\Delta k_j)^2}{N_j}}$$

$$\Delta k_{array} = \sqrt{\frac{(\Delta k_1)^2}{N_1}+\frac{(\Delta k_2)^2}{N_2}+\frac{(\Delta k_3)^2}{N_3}} \qquad (4)$$

   where each Δk_j is the difference between results from calculation 1 and the calculation where rods of zone *j* have diameter $\bar{d}+u_d$, and each N_j is the number of rods in zone *j*.

4. Another way to evaluate the uncertainty worth is to use the correction factor κ_{corr} in the formula

$$\Delta k_{array} = \frac{\Delta k}{\sqrt{\kappa_{corr} N}}. \qquad (5)$$

   Here Δk is equal to Δk_1 in *Step 1* in Section C.2.2. It is obtained by subtracting the result of calculation 1 from the result of a calculation where all rods have diameter $\bar{d}+u_d$, and $N = \sum_{j=1}^{3} N_j$. In this case, the correction factor κ_{corr} is obtained by equating formulae (4) and (5).

C.2.4 Example: Uncertainty in fuel-rod diameter

As mentioned in the introduction of this appendix, two cases can be considered, according to the fact that the uncertainty of the parameter (here the rod diameter) is Type B (not of statistical type) or is Type A (statistical type).

The rod diameter values have been measured (using a micrometer, for instance) on a sample of n fuel rods: this allows a Type A evaluation of uncertainty. It was observed that in many cases, the parameter distribution is nearly centered in the middle of the tolerance range, is much narrower than the tolerance range, and shows almost the shape of a normal distribution.

As a numerical application, let us consider the U(4.738%)O_2 Zircaloy-clad fuel rods used for the PWR experiments in Valduc:

- diameter design value : 9.50 ± 0.06 mm
- value from 300 measurements : 9.4924 ± 0.0044 (1σ) mm

The observed distribution shows almost the shape of a normal distribution.

The minimum and maximum values are

- diameter design value : 9.44 , 9.56 mm
- value from 300 measurements : 9.479 , 9.506 (3σ) mm

The experimental standard deviation of the mean is the experimental standard deviation divided by √n, or 0.0044/√300 = 0.000254 mm.[a]

By application of §4.2 in Reference 1, the standard uncertainty $u_{\bar{d}}$ is this experimental standard deviation of the mean, 0.000254 mm, for configurations containing ≥ 300 rods.

The mean value $\bar{d}$ is used for each and every rod in the benchmark model. The standard uncertainty of $\bar{d}$ is used to compute the uncertainty on k_{eff} by using the formula

$$\Delta k_{\bar{d}} = \frac{\left\{\left|k_{eff}\left(\bar{d}\right) - k_{eff}\left(\bar{d} + u_d\right)\right| + \left|k_{eff}\left(\bar{d}\right) - k_{eff}\left(\bar{d} - u_d\right)\right|\right\}}{2}$$

in which the values of k_{eff} are obtained by special Monte Carlo or S_N calculations.

[a] However, this does not include possible systematic error (systematic uncertainty) of the diameter measurement. See Section C.11.

This differs from the uncertainty calculated in the previous section in the following ways:

Previous section (Section C.2.3)	This section (Section C.2.4)
Uncertainty due to physical variation among rods, as opposed to their all being the same. (This is an uncertainty due to model simplification.)	Uncertainty of the mean value, used for all rods in the model. (The true mean value is not known. This uncertainty is an estimate of the possible error in the mean value.)
Values of N and N_i in the formulae refer to number of rods in the critical configuration.	Value of n in the formulae refers to number of rods for which the parameter was measured.
This method accounts for the fact that not all rods have the same neutronic importance.	It is not necessary to account for unequal importance because, to calculate the effect of this uncertainty, all rods are changed by the amount of the uncertainty.
This uncertainty represents the effect of actual physical variation, not measurement uncertainty.	This uncertainty represents the effect of our not knowing the true mean value.

C.2.5 Uncertainty in spacing of fissile units

Consider the case of an array of N equally spaced fissile rods or units. Pitch uncertainty (from either variation in rod positions or measurement uncertainty) depends upon the grid for the rods or units and their placement in the grid. In the case of rods, random variation of pitch is due to the gap between the rod and the grid hole and also to the location of the hole itself in the grid. In rare cases, it may be affected by slight bowing of the fuel rods.

Uncertainty in pitch may include both random uncertainty and systematic uncertainty. If the standard deviation of the distance between fissile units has been determined and Δk is calculated for an increase in the distance between all units by that amount, the effect from each unit may be roughly estimated as $\frac{\Delta k}{N}$. (This is only a rough estimate partly because the value of pitch at the center of an assembly has a larger effect than the value of pitch near the edges due to the greater neutronic importance at the center of an assembly.) Then the total effect on k_{eff} of the random variation among unit positions is the total of the effects from each, combined, as usual, as the square root of the sum of their squared values:

$$\sqrt{\sum_{i}^{N}\left(\frac{\Delta k}{N}\right)^2} = \sqrt{N\frac{(\Delta k)^2}{N^2}} = \frac{\Delta k}{\sqrt{N}}.$$

Another example of random spacing uncertainty is that due to holes in a grid plate being larger than the fuel rods in them. Rods are free to move in any direction within these holes. Therefore, assuming a normal distribution of rod positions within the hole, the effect of changing the pitch

by Δr (difference in radii of hole and rod) divided by $3\sqrt{N}$ gives an estimate of the effect of this random-spacing standard uncertainty.

This random spacing uncertainty from rods not being centered in their holes should not be confused with the uncertainty in the mean pitch value, which applies to the entire array. The uncertainty in mean pitch comes from possible imprecision in manufacture of the grid, so that hole centers might be, for example, actually spaced 1.2001 cm apart (mean value), rather than 1.2000 cm apart, as specified for fabrication of the grid (and as specified in the benchmark model). The standard deviation or tolerance in pitch is specified by the grid manufacturer, and/or is measured by the experimentalists. If the uncertainty (standard deviation or tolerance in hole spacing) is specified by the manufacturer, he should clearly differentiate between uncertainty in the mean spacing, or pitch, which applies to the whole array, and random spacing uncertainty. If pitch has been measured by the experimentalists, the standard uncertainty in mean pitch is equal to the experimental standard deviation of the pitch measurements divided by the square root of the number of measurements. The Δk_{eff} effect is calculated for a change to the entire array by the standard uncertainty of mean pitch. It should not be divided by $\sqrt{N}$.

C.3 Uncertainty in fuel-rod linear density (including example of perfect correlation)

Usually, the following quantities are given for the fuel rod:

- the pellet diameter $D \pm \Delta D$,
- the pellet density $\rho \pm \Delta\rho$,
- the fissile column mass $M \pm \Delta M$,
- the fissile column height $L \pm \Delta L$.

The linear density M_L, or fuel mass per unit length, is equal to the ratio M/L.

From the point of view of neutronics, the main parameter is the linear density. In the determination of effects on k_{eff} of uncertainties due to diameter and density, we should be cautious not to include the effect of any uncertainty twice. To avoid this, the density-uncertainty effect should be obtained by keeping constant the pellet diameter, and the diameter-uncertainty effect should be obtained by keeping constant the linear density.

Two densities may be known: the pellet density and the fissile column density deduced from the linear density, the latter one being the best one to use.

The uncertainty on the fissile column *fuel density* ρ (g/cm^3) is calculated by using the following formula: $\rho = \dfrac{4M_L}{\pi D^2}$

in which: M_L = fuel mass per unit length of fissile rod (g/cm)
D = pellet diameter (cm)

The general formula for the combined variance (see Section 2.4) of ρ gives

$$u_c^2 = \left[\frac{\partial \rho}{\partial M_L}\right]^2 u_{M_L}^2 + \left[\frac{\partial \rho}{\partial D}\right]^2 u_D^2 + 2\frac{\partial \rho}{\partial M_L}\frac{\partial \rho}{\partial D} u_{M_L} u_D$$

assuming that M_L and D are perfectly correlated with correlation coefficient r=1. Perfect correlation with r=1 means that whenever a measurement of M_L exceeds the mean of M_L, then a measurement of D correspondingly exceeds the mean value of D; and similarly, whenever a measurement of M_L is less than the mean of M_L, then a measurement of D for that rod is correspondingly less than the mean value of D. This is reasonable, but the correlation is not necessarily true. Other influences may affect M_L, such as material density of the particular pellets, flatness of the pellets' upper and lower surfaces, and chips in the edges of some pellets. Ideally, the covariance would be measured, using simultaneous measurements of D and M_L. (See the formulas for covariance in Section 2.4.)

Guidance from Reference 1 (§F.1.2.1) says that the covariance of two measured quantities may be taken as zero or treated as insignificant in the following three cases:

1. if the two random variables representing the physical parameters are uncorrelated because they were measured independently of each other;
2. if either can be treated as a constant, or
3. if there is insufficient information to evaluate their covariance.[a]

Using the formula for ρ in terms of M_L and D,

$\frac{\partial \rho}{\partial M_L} = \frac{4}{\pi D^2}$ and $\frac{\partial \rho}{\partial D} = -\frac{8M_L}{\pi D^3}$. These values can be used in the formula for the combined uncertainty of ρ (with or without the correlation term, as appropriate) to find the standard uncertainty in fuel density.

C.4 Combining enrichment uncertainties of two batches (including example of perfect correlation)

If fuel pellets come from two or more batches, each with its own measured enrichment value and standard uncertainty, then the overall value of the enrichment and its standard uncertainty (combined from the uncertainties observed for each batch) are weighted by the estimated fraction of pellets from each batch. If the fraction from each batch is unknown, then the uncertainty of the fraction is also included in the combined uncertainty of the parameter.

[a] It should be pointed out that if there is an unknown covariance, omitting it will lead to an overestimated or underestimated uncertainty. An argument can be made that a covariance cannot be simply ignored just because there is insufficient data to estimate it. The effect of possible correlations on the uncertainty can be checked. In cases where the covariance is unknown but expected to be positive, it is sometimes recommended that perfect correlation be assumed (so that the covariance is at its maximum value) to estimate its maximum effect on the uncertainty. Or some kind of Type B estimate of covariance might be appropriate. (personal communication, Larry Blackwood, August, 2002)

For example, suppose fuel rods in a critical configuration each contain fuel from one of two batches. Consider the enrichment and its uncertainty. Suppose the enrichment of the first batch is given as 2.36 ± 0.03 wt.% ^{235}U and the enrichment of the second batch is 2.34 ± 0.02 wt.% ^{235}U, with uncertainties reported as standard deviations. Suppose 40±2% of the rods contain fuel from the first batch, and 60±2% of the rods contain fuel from the second batch, where the ±2% is also an estimated standard deviation. The average enrichment is

$$e = f_1 \times e_1 + f_2 \times e_2 = 0.4\times 2.36 + 0.6\times 2.34 = 2.348 \text{ wt.\% } ^{235}\text{U}.$$

A first estimate for the combined uncertainty in enrichment, σ_e, is

$$\sqrt{\left(\frac{\partial e}{\partial e_1}\right)^2 u_{e1}^2 + \left(\frac{\partial e}{\partial e_2}\right)^2 u_{e2}^2 + \left(\frac{\partial e}{\partial f_1}\right)^2 u_{f1}^2 + \left(\frac{\partial e}{\partial f_2}\right)^2 u_{f2}^2}$$

$$= \sqrt{(f_1 \times u_{e1})^2 + (f_2 \times u_{e2})^2 + (e_1 \times u_{f1})^2 + (e_2 \times u_{f2})^2}$$

$$= \sqrt{(0.4\times 0.03)^2 + (0.6\times 0.02)^2 + (2.36\times 0.02)^2 + (2.34\times 0.02)^2} = \sqrt{0.0047}$$

$$= 0.0686 \text{ wt.\% of } ^{235}\text{U}.$$

However, correlations must be considered. The two measured enrichments are assumed to be uncorrelated (e.g., the two batches were made at different times and at different factories). Enrichments are obviously not correlated with their fraction in the core. But there is a correlation between f_1 and f_2. Because the sum of f_1 and f_2 is always the same, the correlation coefficient between them, $r(f_1,f_2)$, is –1. According to the equation in Section 2.4, the correlation term is

$$2\times\left(\frac{\partial e}{\partial f_1}\right)\left(\frac{\partial e}{\partial f_2}\right) u_{f1} u_{f2}\, r(f_1, f_2) = 2 e_1 e_2 u_{f1} u_{f2} (-1) = -2 \cdot 2.36 \cdot 2.34 \cdot 0.02 \cdot 0.02 = -0.0044.$$

If this correlation term is included under the square-root sign, the result for the combined uncertainty in enrichment is $\sqrt{0.0047 - 0.0044} = 0.017$ wt.% ^{235}U. So the enrichment and its standard uncertainty are 2.348 ± 0.017 wt.% ^{235}U.

If the fractions f_1 and f_2 are known exactly (if rods from each enrichment batch were identified, and 4 rods of every 10 that were inserted in the core were from the first batch and 6 were from the second), then u_{f1} and u_{f2} are each zero. Then, the combined uncertainty in enrichment u_e is $\sqrt{\left(\frac{\partial e}{\partial e_1}\right)^2 u_{e1}^2 + \left(\frac{\partial e}{\partial e_2}\right)^2 u_{e2}^2} = 0.017$ wt.% ^{235}U. This result has the same value as the result when batch fractions were only known to ±2%. The two results are so similar because of the negative correlation, as can be seen by comparing the correlation term with the two terms that include the fraction uncertainties.

In general, if there are several batches with standard uncertainties u_{ei} and if fractions f_i of each enrichment are known, the standard enrichment uncertainty is $= \sqrt{\sum_i (f_i \times u_{ei})^2}$.

C.5 Correlation between mass and density uncertainties

Mass and density are an example of two input parameters that depend on a common independent parameter, mass. Suppose that both mass and density with their standard uncertainties are given in the experimental data. The evaluator's task is to find the effect on k_{eff} from their uncertainties.

The general case is described in §F.1.2.3 of Reference 1. Each of two parameters, x_1 and x_2, is a function of several independent variables (q_1, q_2, q_3, etc.). The combined uncertainty of each parameter x_i can be calculated from

$$u_i = \sum_j \left(\frac{\partial x_i}{\partial q_j} \right)^2 u_{qj}^2 .$$

But what if the two parameters have one (or more) independent variables in common? Suppose that both x_1 and x_2 depend on q_2. The covariance between x_1 and x_2 due to their common independent variable q_2 is given by

$$\mathrm{cov}(x_1,x_2) = \frac{\partial x_1}{\partial q_2} \frac{\partial x_2}{\partial q_2} u_{q2}^2 .$$

Therefore, using the first formula in Section 2.4 (from equation 13 in §5.2.2 of Reference 1), the combined uncertainty of k_{eff} due to both x_1 and x_2 is equal to

$$\Delta k_{x1,\,x2} = \sqrt{\left(\frac{\partial k_{eff}}{\partial x_1} \right)^2 u_{x1}^2 + \left(\frac{\partial k_{eff}}{\partial x_2} \right)^2 u_{x2}^2 + 2 \left(\frac{\partial k_{eff}}{\partial x_1} \right) \left(\frac{\partial k_{eff}}{\partial x_2} \right) \frac{\partial x_1}{\partial q_2} \frac{\partial x_2}{\partial q_2} u_{q2}^2} .$$

If x_1 is mass and x_2 is density, both parameters are a function of the independent variable mass, m. The functions are

$$x_1 = m \quad \text{and} \quad x_2 = \rho = m/v,$$

where v is the volume, another independent variable. Assume, for this example, that v is known and has negligible uncertainty. Then the standard uncertainty in k_{eff} due to mass and density is

$$\Delta k_{mass,\,dens} = \sqrt{\left(\frac{\partial k_{eff}}{\partial m} \right)^2 u_m^2 + \left(\frac{\partial k_{eff}}{\partial \rho} \right)^2 u_\rho^2 + 2 \left(\frac{\partial k_{eff}}{\partial m} \right) \left(\frac{\partial k_{eff}}{\partial \rho} \right) \frac{\partial m}{\partial m} \frac{\partial \rho}{\partial m} u_m^2}$$

$$= \sqrt{\left(\frac{\partial k_{eff}}{\partial m} \right)^2 u_m^2 + \left(\frac{\partial k_{eff}}{\partial \rho} \right)^2 u_\rho^2 + 2 \left(\frac{\partial k_{eff}}{\partial m} \right) \left(\frac{\partial k_{eff}}{\partial \rho} \right) 1 \cdot \frac{1}{v} u_m^2} .$$

However, complications arise because volume and dimensions contribute additional uncertainty, and density is not a linear function of volume.

To avoid the complications of including correlations, it is recommended (§5.2.4 of Reference 1), to calculate the combined k_{eff} uncertainty from parameters that are not correlated, if possible. For example, in the present case, it would be preferable to calculate Δk_{eff} using uncertainties in mass and dimensions, rather than using density uncertainty.

However, mass uncertainty may be represented by change in density if volume is kept constant. Similarly, dimension uncertainty may be represented by change in density if mass is held constant and if each dimension (whose measurement is uncorrelated with measurement of other dimensions) is varied separately.

C.6 Uncertainty from impurities

This section provides guidance on determining the effect on reactivity due to a Type B uncertainty, impurities. In some cases, the measured value of an impurity may be so small or is so poorly known that the presence of the parameter itself (the impurity) may be considered an uncertainty.

However, in one case, even small amounts of impurities may have very large effect. This is the case of impurities in fissile material. If the impurity mass is included in the reported fuel mass (or solution density, in the case of fissile solution), the effect of impurities may be large due to their replacing fuel (or solution). In this case, two effects are calculated separately: 1) subtracting fuel mass equal to the best estimate of the total mass of impurities, 2) adding best estimates of the impurities. Often, the first effect is the larger one. It is easy to include in the benchmark model by simply reducing the fissile material by the total mass of impurities. The smaller effect, the impurities themselves, may be included in one of three ways, discussed in more detail in Section C.6.2:

- Include best estimates of impurities in the benchmark model.
- Omit impurities and, instead, include the calculated effect of best estimates of impurities as a small correction to the benchmark-model k_{eff}.
- Omit impurities and add additional uncertainty. (This option is usually chosen when identities and amounts of impurities are poorly known.)

C.6.1 Type B uncertainty

The Type B parameter uncertainty may be given as $x_0 \pm \Delta x$, where Δx represents the tolerance, assumed to bound the possible values of the parameter. The standard uncertainty is $\Delta x/\sqrt{3}$ or $\Delta x/3$ according to whether the parameter distribution is expected to be flat or normal.

Sometimes, a tolerance is given as $[x_0+\Delta x_1, x_0-\Delta x_2]$. The best estimate of the value of parameter x may be x_0 or it may be chosen by using an estimated probability distribution. If a uniform probability distribution seems reasonable, the parameter value is then $x_i = x_0 + \frac{\Delta x_1 - \Delta x_2}{2}$, varying between $x_0+\Delta x_1$ and $x_0-\Delta x_2$.

If the parameter, given as $x_0 \pm \Delta x$, is expected to follow a Gaussian distribution within the bounds of the tolerance (perhaps indicated by previous measurements on the same type of parameter), the standard uncertainty is $\Delta x/3$. In order to find the corresponding change in k_{eff}, two calculations are run, taking a parameter value successively equal to $x_0 + \Delta x/3$ and $x_0 - \Delta x/3$. The contribution to the k_{eff} uncertainty is then

$$\Delta k_i = \{|k_{ref} - k_{x0+\Delta x/3}| + |k_{x0-\Delta x/3} - k_{ref}|\} / 2 = |k_{x0+\Delta x/3} - k_{x0-\Delta x/3}| / 2.$$

Note that, as mentioned previously, whether the uncertainty is Type A or Type B is not relevant to the calculation of the effect of the uncertainty on k_{eff}. Type A or B only refers to two methods of determining the standard uncertainty (which is always defined as the best estimate of the standard deviation) of a measured parameter.

C.6.2 Impurities

The effect of impurities must be assessed. There are three possible results of measurements of impurities: 1) those whose concentrations can be measured (with an uncertainty), 2) those that can be detected but the amounts are not known because they are so small, and 3) those that are not detected.

The impurity that is detected but is below the detection limit, DL, may be considered to have an average value of DL/2, with bounding values 0 and DL.[a] Therefore, if impurities are omitted in the benchmark model, the effect of the impurity can be divided in two parts: one half (DL/2) is considered as a correction to k_{eff}, whereas the other half (DL/2) is considered as an uncertainty that bounds the value. Since there is no more knowledge on the distribution, one may assume that the distribution is equally probable within the interval, and therefore the corresponding standard uncertainty will be $DL/(2\sqrt{3})$.

Consider fuel rods in water. Concentrations C_i (μg/g UO_2 or PuO_2) are given for all impurities in the fuel. In a thermal spectrum, it is possible to determine for each element concentration an equivalent boron concentration C_{Bi} (μg/g UO_2 or PuO_2) giving the same reaction rate of absorption. For an element i, we have: $N_i \sigma_{ai} = N_{Bi} \sigma_{aB}$, or

$$\frac{C_i \sigma_{ai}}{A_i} = \frac{C_{Bi} \sigma_{aB}}{A_B}$$

Therefore, $C_{Bi} = C_i \frac{\sigma_{ai}}{\sigma_{aB}} \frac{A_B}{A_i}$

with:

N_i	concentration (atom/barn-cm) of impurity,
σ_{ai}	thermal absorption cross section of impurity,
C_i	concentration (μg/g UO_2 or mixed oxide) of impurity,
A_i	atomic mass of impurity,
N_{Bi}	concentration (atom/barn-cm) of boron equivalent to the impurity,

[a] However, this depends on the analytical laboratory's definition of detection limit. For example, it might be half of the amount that can be detected with certainty.

σ_{aB} thermal absorption cross section of boron,
C_{Bi} equivalent boron concentration (μg/g UO_2 or mixed oxide) of impurity,
A_B atomic mass of boron.

The equivalence coefficient c_i is defined as $c_i = \frac{C_{Bi}}{C_i} = \frac{\sigma_{ai}}{\sigma_{aB}} \frac{A_B}{A_i}$ for each element.

The following table gives equivalence coefficients c_i for impurities found in fuel pellets.

Table C.1. Equivalence coefficients ($c_i = C_{Bi} / C_i$) of impurities in a thermal spectrum

Element	Atomic mass	σ_{ai}	$c_i \times 10^4$	Element	Atomic mass	σ_{ai}	$c_i \times 10^4$
B	10.811	760.0	10,000	In	114.82	197.0	244.06
Ag	107.868	63.0	83.08	Li	6.941	71.0	1455.09
Al	26.981	0.23	1.21	Mg	24.305	0.063	0.37
C	12.011	0.0035	0.04	Mn	54.938	13.3	34.44
Ca	40.078	0.43	1.53	Mo	95.94	2.5	3.71
Cd	112.411	2520	3188.92	N	14.00674	1.9	19.30
Co	58.9332	37.19	89.77	Ni	58.893	4.5	10.87
Cr	51.9961	3.1	8.48	Pb	207.2	0.171	0.12
Cl	35.453	33.6	134.82	Si	28.0855	0.17	0.86
Cr	51.996	3.1	8.48	Sm	150.36	5600	5297.95
Cu	63.546	3.8	8.51	Sn	118.71	0.61	0.73
Dy	162.5	930.0	814.11	Ta	180.9479	20.0	15.72
Eu	151.96	4600.0	4306.07	Th	232.038	7.4	4.54
F	18.9984	0.0095	0.07	Ti	47.88	6.1	18.12
Fe	55.847	2.56	6.52	V	50.9415	5.0	13.96
Gd	157.25	48800	44144.99	W	183.85	18.0	13.93
Hf	178.49	106.0	84.48	Zn	65.39	1.1	2.39

By adding the equivalent boron concentrations of each impurity, all impurities can be treated as boron giving the same absorption rate in the thermal system. The summary natural-boron equivalent of impurities is then

$$C_B = \sum_i C_i \times c_i = \sum_i C_{Bi} .$$

This can be used to calculate the k_{eff} correction and uncertainty due to impurities that are omitted from the benchmark model.

C.7 Uncertainty in geometry: the diameter of a cylindrical tank

The diameter of the cylindrical tank containing the fuel lattice or solution is known, either by the nominal value and its tolerance, or by calibration measurements.

In the first case, (a Type B uncertainty) if only the tolerance [$-t_-$, $+t_+$] is given and there is no specific knowledge about the diameter within the tolerance range, the diameter distribution may be assumed to be equally probable in the interval, and the diameter expected value corresponds to the midpoint of the interval. Therefore, the change in k_{eff} is obtained by taking a standard uncertainty equal to
$(t_- + t_+) / 2\sqrt{3}$.

In the second case, the diameter could be better known through calibration measurements: calibrated volumes of water are poured into the tank and the corresponding water height is measured. From the reported set of both values, the tank internal diameter is deduced and is valid in the range of corresponding heights. A sample of "N" diameter values is available. From this sample, it is possible to know the distribution law and its properties (mean, standard deviation). The standard deviation is used as the value of standard uncertainty.

C.8 Example of small measurement errors having a large systematic effect

An example of small measurement errors in array parameter values causing large effects occurred during an ICSBEP evaluation. The experiments were thin, steel-clad, highly enriched UO_2-Al fuel rods at two close pitches, performed at RRC Kurchatov Institute in 1997.[a] The combined total k_{eff} uncertainty was ~0.5%, a typical value. Calculated k_{eff} results were ~1.00, as expected, except for configurations at the larger pitch, which had calculated k_{eff} values that were 1.5% high.[b] Fortunately, components of the experiment were still available so that parameter measurements could be checked. The experimentalists discovered that the problem was the steel clad. The nominal thickness was 0.1 cm. More accurate, clad-volume measurements (measuring volume changes from displacement of water) gave an average thickness of 0.119 cm. The clad density, reported as 8.0 ± 0.2 g/cm^3, was measured and found to be 7.86 ± 0.07 g/ cm^3. The new clad dimensions and density, when used for all fuel rods, gave good calculated results for both pitch values (within 0.3% of the expected k_{eff} values). The combined effects of the uncertainties of clad OD, thickness, and density had not predicted the possibility of the high k_{eff} values, even though the uncertainties bracketed the revised parameter values. This is because the uncertainty effects had been combined as if they were random among the rods (dividing by $\sqrt{N}$), rather than systematic.

[a] HEU-COMP-THERM-011, -012, -013, and –014.
[b] As discussed at the ICSBEP meeting in Dijon, France, May, 1998.

C.9 Combining random, systematic, round-off, and sampling uncertainties of a parameter measured for a collection of pieces

The following equations can be used for estimating the uncertainty of a parameter for a collection of pieces of material based on measurements and uncertainties of some or all of the individual pieces. For our purposes, the collection usually refers to a critical assembly. Cases 1 and 2 apply when measured values for all pieces of the collection are known. An example of such an application is the estimation of uranium mass uncertainty for the Big Ten critical assembly (IEU-MET-FAST-007). Big Ten is a uranium metal cylinder made up of many pieces of different enrichments, sizes, and shapes. Another example is the mass uncertainty for the Zeus assembly (HEU-MET-INTER-006). Cases 3-5 apply to pieces that may not all have been measured but are nominally the same, such as assemblies of fuel rods or cans of fissile solution.

The cases described here concern the uncertainty in total mass of the collection. However, the equations may be applied to the uncertainty of other parameters besides mass for collections of items that have been measured individually.

These equations apply when there are no correlations among the measurement uncertainties considered, which is often a reasonable assumption. (If there are correlations among the uncertainties, then additional terms would be required in the calculation. See Section 2.4).

C.9.1 Background and definitions

There are four types of uncertainty terms to consider when calculating the uncertainty in the mean mass or total mass of an assembly:

u_{ph} = 1σ uncertainty due to physical variation in the mass or density from piece to piece
u_r = 1σ random mass-measurement uncertainty
u_s = 1σ systematic mass-measurement uncertainty
r_r = round-off resolution

The first uncertainty term u_{ph} due to physical variation[a] is also sometimes called the "sampling uncertainty." It is a characteristic of collections of individual pieces. This term is non-zero only when the set of pieces that were measured is not the same as the set of pieces used in the assembly (see Cases 3-5 here). It is discussed further in Section C.12. The other three terms all derive from the individual measurements that were made.

The standard uncertainty of a single measured mass value of a particular piece x_i is

$$u_{xi} = \sqrt{u_{ri}^2 + u_{si}^2 + \frac{r_{ri}^2}{12}} \qquad (1)$$

The three uncertainty components u_{ri}, u_{si}, and r_{ri} are defined below.

[a] Note that possible effect of physical variation on k_{eff} from unequal importance of relative positions in the assembly when the mean mass or density is used in the model is not considered here. This is discussed in Section C.2.

The sources of u_{ri} are random variations in the measuring device and procedure. The value u_{ri} may be estimated by the standard deviation of results of several weighings of one typical piece (Type A) or by some other method (Type B), such as by the specified accuracy of the measuring device.

The value u_{si} is the uncertainty of the systematic error. A systematic error occurs when a series of measured values are incorrect by approximately the same amount. An example of systematic error is incorrectly zeroing the measuring device. Unlike random uncertainty, repeated measurements of the parameter cannot reduce or reveal the systematic uncertainty. However measurements that show trends over time (called "drift") or with scale of the measuring device can reveal the existence of systematic error that changes with time or with scale. Estimations of systematic uncertainty can be based on such trends. Another way to estimate systematic uncertainty is by using results of occasional calibrations of the measuring device with a standard unit.

If the magnitude of a systematic error becomes known, it is added as a correction to the parameter value. But uncertainty of the exact value of the correction remains; this possible systematic error is called the systematic uncertainty.

The third kind of uncertainty, r_{ri}, corresponds to the smallest readable unit marked on the scale of the measuring device or to numerical round-off, whichever is larger. If, for example, measurements are made to the nearest gram, then r_{ri} is 1 gram, and it is assumed that the true value can be anywhere within ±0.5 g of the stated value and has a uniform probability distribution. Therefore, the standard uncertainty for each piece is $r_{ri}/(2\sqrt{3}) = r_{ri}/\sqrt{(12)}$. For example, if r_{ri} is 1 gram, this standard uncertainty is 0.29 grams.

C.9.2 Particular Cases

In the following sections, equations for calculating the uncertainty of the total assembly mass are discussed for particular situations regarding the selection of pieces used and measured that may occur in an experiment. Each equation combines the u_{xi} of the individually measured pieces plus estimates of the u_{ph} term when appropriate. Note that in cases where the measurement uncertainties u_{ri}, u_{si}, and r_i are assumed to be the same for all pieces measured, the subscript i is dropped.

In all cases, the total mass of the assembly is equal to the mean of the measured masses times N, the number of pieces used in the assembly. Whenever the total is obtained by multiplying a mean mass by the number of pieces N, then by standard uncertainty propagation, the uncertainty in total mass is

$$u_T = \sqrt{N^2 u_{\bar{x}}^2}$$
$$= \sqrt{N^2 \left(u_{ph\bar{x}}^2 + u_{r\bar{x}}^2 + u_{s\bar{x}}^2 + r_{r\bar{x}}^2 \right)}$$

where the terms in parentheses are (in the order in which they appear) the uncertainties in the mean mass due to

- piece-to-piece physical variation,
- possible random measurement errors,
- possible systematic errors, and
- round-off

in the n measured mass values.

First, consider each of the 4 types of uncertainty of the mean.

$u_{ph\bar{x}}$ This uncertainty of the mean value due to physical variation is also called the sampling uncertainty. It is also sometimes called "the uncertainty of the mean," referring to cases when the set of measured pieces is different from the set of pieces in the collection. If the set of all pieces of the collection is identical to the set of pieces measured and used to determine the mean or sum of the collection, this uncertainty due to physical variation is zero. It is further discussed in Section C.12.

$u_{r\bar{x}}$ This random measurement uncertainty of the mean is due to random variations in the measuring device and procedure. Assuming the measurements are independent, the square of this uncertainty is $u_{r\bar{x}}^2 = \sum_{i=1}^{n}\left(\frac{\partial \bar{x}}{\partial x_i}\right)^2 u_{ri}^2 = \sum_{i=1}^{n}\left(\frac{1}{n}\right)^2 u_{ri}^2 = n \times \left(\frac{1}{n}\right)^2 u_r^2 = \frac{u_r^2}{n}$ whenever the random measurement uncertainties of each x_i are the same. So $u_{r\bar{x}} = \frac{u_r}{\sqrt{n}}$.

$u_{s\bar{x}}$ The systematic uncertainty is the uncertainty of the systematic error, which is an error that is the same (both in magnitude and in sign) for each measured piece. A non-zero estimate of the systematic error can be added as a correction to the parameter value, but usually the systematic error is estimated as zero. Because the systematic uncertainty is the same in magnitude and sign for each piece (although whether the sign is + or – is not known), the systematic uncertainties add algebraically rather than quadratically. Therefore the systematic uncertainty of the mean value is $u_{s\bar{x}} = \sum_{i=1}^{n}\left(\frac{\partial \bar{x}}{\partial x_i}\right) u_{si} = n \times \frac{1}{n} u_s = u_s$.

$r_{r\bar{x}}$ The roundoff error is assumed to be random for each of the n measured pieces. Therefore the roundoff uncertainties of the n measured pieces are combined quadratically to obtain the roundoff uncertainty of the mean. (It is assumed that the mean value itself is not rounded.[a]) The value r_{ri} is the larger of the smallest readable unit of the scale of the measuring device and the last decimal place of the rounded value. The probability distribution of the true value of the mass of each of

[a] If the mean value is rounded, then the sum, $N \times \bar{x}$, includes an error equal to N times the value of the dropped or added increment.

the n measured pieces is assumed to be uniform within the interval ±0.5 r_{ri}. When r_{ri} is the same for each of the n measured pieces, the squared roundoff uncertainty of the mean value is

$$r_{\bar{x}}^2 = \sum_{i=1}^{n}\left(\frac{\partial \bar{x}}{\partial x_i}\right)^2 \frac{r_{ri}^2}{12} = \sum_{i=1}^{n}\left(\frac{1}{n}\right)^2 \frac{r_r^2}{12} = n \times \left(\frac{1}{n}\right)^2 \frac{r_r^2}{12} = \frac{r_r^2}{12n} \quad \text{and} \quad r_{\bar{x}} = \frac{r_r}{12\sqrt{n}} .$$

Further consideration of the individual uncertainties gives the equations for the following cases. In Cases 1 and 2, the set of pieces measured is the same as the set of pieces used in the assembly. For these cases, the u_{ph} term for the uncertainty due to the physical variation in mass from piece to piece does not appear in the equations because, of course, its effect on the uncertainty in the mean or total mass for the assembly goes to zero when the mean or total mass is calculated from the measured masses values of all pieces of the assembly. (This uncertainty is discussed in Section C.12.) The formulas in Cases 3-5 are used when all pieces are nominally the same and have the same measurement uncertainties, but the set of pieces measured is not identical to the set used in the assembly. More explanation of these equations is given at the end of this section.

Case 1. All N pieces in the assembly are measured and have the same measurement uncertainties.

For Case 1, the mass of the assembly is calculated as

$$T = \sum_{i=1}^{N} x_i = N\bar{x} \tag{2}$$

where T is the total mass, $\bar{x} = \frac{1}{N}\sum_{i=1}^{N} x_i$, and x_i is the measured mass of the i^{th} piece in the assembly.

Since the uncertainties are the same for all of the N pieces measured, the standard uncertainty of T is

$$u_T = \sqrt{N u_r^2 + N^2 u_s^2 + \frac{N r_r^2}{12}} \tag{3}$$

where u_r, u_s, and r_r are the common values for all N pieces.

Because the measured mass of every piece being used has been included in the sum, there is no uncertainty in the total mass or in the mean mass due to random physical variation in mass from piece to piece, i.e., $u_{ph} = 0$.

Case 2. All N pieces are measured and their uncertainties are different.

This case might occur when pieces are of different sizes. The formula for total mass is the same as for Case 1 except that each individual piece is treated explicitly. The uncertainty is

$$u_T = \sqrt{\sum_{i=1}^{N} u_{ri}^2 + \left(\sum_{i=1}^{N} u_{si}\right)^2 + \frac{\sum_{i=1}^{N} r_{ri}^2}{12}} \quad (4)$$

where u_{ri}, u_{si}, and r_{ri} are the uncertainty values for the i^{th} piece in the assembly.

Case 3. Only n of the N nominally equivalent pieces in the assembly are measured and they have the same measurement uncertainties.

For Case 3, it is assumed that the n pieces measured have been randomly selected from the N pieces used in the assembly, so that statistical properties of mean and variance estimates apply (e.g. the equations in Section C.12).

When only a subset n of the N pieces in the assembly have been measured, the total mass is estimated as

$$T = N\bar{x} \quad (5)$$

where $\bar{x}$ is the mean mass of the n measured pieces

$$\bar{x} = \frac{1}{n}\sum_{i=1}^{n} x_i \ . \quad (6)$$

The uncertainty in T in this case is

$$u_T = \sqrt{N^2\left[\left(\frac{N-n}{N}\right)\left(\frac{1}{n}\right)\left(s_n{}^2 - u_r^2\right) + \frac{u_r^2}{n} + u_s^2 + \frac{r_r^2}{12n}\right]} \quad (7)$$

where $s_n{}^2$ is the variance of the sample, Equation 6 in Section C.12.

$$s_n{}^2 = \frac{\sum_{i=1}^{n}(x_i - \bar{x})^2}{n-1}. \quad (8)$$

The terms in brackets are the uncertainties of the mean $\bar{x}$. The first term, which is the u_{ph} term due to physical variation among pieces, includes the "finite population correction" $\frac{N-n}{N}$, which is discussed further in Section C.12.

Case 4. The N pieces are selected from a larger population of N' nominally equivalent pieces. All N' pieces have been measured, but it is unknown which N were selected. All measured pieces have the same measurement uncertainties.

In this case it is assumed that values for the mean and standard deviation of the N' pieces are all that is known and available for use in the uncertainty calculations for the subset of N pieces. The formula for the total mass is still the same as Equation 5 except that now the mean $\bar{x}$ is based on measurements of N' items.

Equation 7 becomes

$$u_T = \sqrt{N^2\left[\left(\frac{N'-N}{N'}\right)\left(\frac{1}{N}\right)\left(s^2 - u_r^2\right) + \frac{u_r^2}{N'} + u_s^2 + \frac{r_r^2}{12N'}\right]} \tag{9}$$

where now the estimate of s^2 is calculated as

$$s^2 = \frac{\sum_{i=1}^{N'}(x_i - \bar{x})^2}{N'-1}. \tag{10}$$

Case 5. The N pieces are selected from a larger population of N' nominally equivalent pieces of which n pieces have been measured. The number of pieces common to N and n is k, but the number k may not be known. All measured pieces have the same measurement uncertainties.

The expression for the uncertainty in total mass is[a]

$$u_T = \sqrt{N^2\left[\left(\frac{N+n-2k}{N}\right)\left(\frac{1}{n}\right)\left(s^2 - u_r^2\right) + \frac{u_r^2}{n} + u_s^2 + \frac{r_r^2}{12n}\right]} \tag{11}$$

If k is not known, then,

if $N + n \leq N'$, $k = 0$;

if $N + n > N'$, $k = N + n - N'$.

As for the previous cases, s^2 is the experimental standard deviation of the measured sample,

$$s^2 = \frac{\sum_{i=1}^{n}(x_j - \bar{x})^2}{n-1}. \tag{12}$$

More Explanation for Equations 7, 9, and 11.

[a] See derivation of the factor (N+n-2k)/(Nn) at the end of Section C.12.

The last three terms in the square brackets in Equation 7 (i.e., those involving u_r, u_s, and r_r) are the propagated random, systematic, and round-off uncertainties for the mean value used in calculating T.

The first term in the sum in the square brackets, $\left(\frac{N-n}{N}\right)\left(\frac{s_n^2 - u_r^2}{n}\right)$, is the variance in the mean due to piece-to-piece variation. Thus it is an estimate of u_{ph}^2. The observed variance is a result of both piece-to-piece variation and random errors in the measurement from various random influences. The estimated squared standard deviation of these random errors, u_r, is therefore subtracted from the observed variance of the measured pieces to obtain the piece-to-piece variation. The value $s_n^2 - u_r^2$ is divided by n to estimate the variance of the mean value due to physical variation. The factor (N-n)/N is the finite population correction (see Section C.12). Note that when the mean is the average of all N pieces used in the assembly, as in Cases 1 and 2, then n=N and N-n is zero and this u_{ph} term becomes zero.

When multiplied by N^2, the estimate of u_{ph} used in Equation 7 is consistent with Equation 12 in Section C.12, except for the subtraction of the random measurement error term u_r^2. The subtraction of the random measurement error term is not necessary in Section C.12 because there it is assumed that each x_i is know exactly (or, the measurement uncertainty is so small that it is insignificant). Only when there is no appreciable measurement error does Equation 12 in Section C.12 provide an unbiased estimate of u_{ph}. When the x_i are measured with errors, s_n^2 contains both the piece-to-piece variability (u_{ph}) and the random measurement error (u_r). So the random measurement error component must be subtracted out to get a result solely involving piece-to-piece variation.

Note that s_n^2 is not used directly as a simple estimate of $u_{ph}^2 + u_r^2$ because the finite population correction (N-n)/N applies only to true piece-to-piece variation component of s_n^2, not to the measurement error. However, when N is much larger than n, overestimating the finite-population correction slightly as 1 and using only s_n^2/n for the first two terms is simpler and acceptible, as long as this uncertainty is not one that significantly affects the overall uncertainty of k_{eff} of the experiment.

It should be noted that in many cases, the actual data needed to calculate s_n^2 will not be available, rather s_n^2 will be obtained from experiment reports or other sources, as will u_r^2 and u_s^2. Often the value of n, number of measurements, is not known. In this case, the evaluator may choose to estimate n as a low reasonable value (e.g., 1 to 4) and s^2/n may replace the u_{ph} and u_r terms with likely small impact on the reliability of the uncertainty estimate.

The differences between Equations 7, 9, and 11 are based on recognizing how many observations contributed to the calculation of the mean mass value used in the calculation of $T = N\bar{x}$. But the numbers in the first term in the brackets in Equations 7, 9, and 11 are further adjusted based on how many of the actually measured pieces are retained in the sample selected for use in the experiment, because the uncertainty is increased when not all the measured pieces are used in the assembly. For example, if all the pieces are measured and also used in the assembly, then the variation between pieces has no effect on the uncertainty in the total. However, if all the pieces

are measured and only a randomly selected subset is used in the assembly, then some uncertainty due to piece-to-piece variability is introduced even though every piece has been measured.

C.10 Plutonium valency

Chemists have known for a long time that in plutonium nitrate solution, the Pu valency state might not always be IV, which gives $Pu(NO_3)_4$. The valence of plutonium depends on many conditions, including temperature, PH and acidity, particularly. Plutonium with valency III, forming $Pu(NO_3)_3$, which is generally a more reactive solution composition from a criticality viewpoint, may coexist with Pu IV.[a] Moreover, other phenomena, such as radiolysis and polymerization, may contribute to the formation of this and other valency states.[b]

A proposed method to determine the effect of the possible valency state III is to take as its possible fraction the same fraction as the NO_3^- relative uncertainty, and then to calculate, by proportionality, the effect by changing all Pu IV to Pu III in the Pu nitrate solution. That is, for the Pu III calculation, assume that the molecular form of plutonium nitrate is $Pu(NO_3)_3$ and derive the remaining solution components, as usual, from the experimental data of the chemical analysis. The difference in k_{eff} results multiplied by the NO_3^- relative-uncertainty fraction may be used as an estimate of the effect of Pu valency uncertainty. (See, for example, Section C.6 in PU-SOL-THERM-028.) Until now, this type of calculation shows that the uncertainty effect is low.

C.11 An estimate of systematic uncertainty

A rough estimate of the order of magnitude of systematic uncertainty can be the scale interval of the measuring device.

However, another basis of estimate of a value for systematic uncertainty comes from the following considerations: Whenever a part used in an experimental assembly is made, the manufacturer works hard to ensure that the piece is within specifications. How closely the part matches specifications will be carefully checked during its manufacture as well as during its certification or approval by the quality assurance department of the company or factory. Both machinists and certifying personnel strive to reduce error in the part. If it is assumed that reducing random and systematic error are approximately equally difficult and that the difficulties grow approximately as E^{-2}, where "E" is the magnitude of the error, then it is easier and more economical for the manufacturers of the part (and also for manufacturers of measuring instruments) to approximately equally reduce both random and systematic error. Therefore, in the absence of additional information, a reasonable estimate is that half of the accuracy provided by the manufacturer of the part (or measuring device) comes from possible systematic error and half comes from possible random error. Since these two types of uncertainty are combined

---

[a] O.J. Wick, ANS - Plutonium Handbook.A Guide to the Technology, Vol 1, 1980, pp 403 – 439; M. Benedict, T. Pigford, H. Levi, *Nuclear Chemical Engineering*, MacGraw Hill, 1981.

[b] H. K. Clark, *Subcritical Limits for Plutonium Systems*, Nuclear Science & Engineering, **79**, p 65, 1981; H.C. Paxton and N.L. Pruvost, Critical Dimensions of Systems Containing ^{235}U, ^{239}Pu, and ^{233}U, LA 10860 - rev 1986.

quadratically to obtain the total uncertainty, an estimate for systematic uncertainty is the stated accuracy divided by √2. The same value is taken as an estimate for the random uncertainty.

If many similar parts are used in the assembly, the effect of the random component of the uncertainty will be reduced (often by 1/√N, where N is the number of parts in the assembly), but the effect of the systematic component of the uncertainty of the part will not be so reduced. This also applies to the effect of systematic uncertainty in the measurements for all parts measured by the same device.

C.12 Sampling uncertainty: Variance of the mean when sampling without replacement from a finite population

Basic uncertainty analysis assumes an infinite population of endlessly repeated measurements of the parameter value. In practice we often deal with parameters (such as the mean, sum, standard deviations, etc. of mass, enrichment, dimensions, etc.) of finite populations of equivalent items, such as N fuel elements in a critical configuration. When N is a large number of items carefully manufactured according to strict specifications (several hundred fuel elements is typical), it seems impractical to measure all N. Using measurements of only n of the N fuel elements to estimate parameters for the entire population is an example of *sampling without replacement*.[a] There is additional uncertainty from assuming that measurements of only part of the population apply to the entire population.

This additional uncertainty from measuring only a sample rather than measuring the entire population is called the *sampling uncertainty*. It is due to physical variation among members of the population. If the manufacturing process was indeed tightly controlled and the measurements are accurate, this additional *sampling uncertainty* will be small.

In the following discussion of sampling uncertainty, the random, systematic, and round-off uncertainties of the individual measurements are ignored, or are considered as so small that they are completely inconsequential. However, the random, systematic, and round-off uncertainties are usually not negligible and should be included, as described in Section C.9.

In the following discussion about using measured values of a sample to estimate population values (and vice versa), simple random sampling is assumed. This means that each item of the population has an equal chance of being chosen for the sample.

Let a population have a finite number N of elements with some quantity or characteristic X. Let $x_1, x_2, \ldots, x_N$ be characteristic values of elements of this population with equal statistical weight.

Parameters of the population are the following:

population mean is $$X_{\text{mean},N} = \frac{1}{N}\sum_{i=1}^{N} x_i \qquad (1)$$

[a] W. Cochran, *Sampling Techniques*, Wiley, New York, copyright 1953, Chapter 2.

population sum is $$X_{sum,N} = \sum_{i=1}^{N} x_i \quad (2)$$

variance of the population is $$S_N^2 = \frac{1}{N-1}\sum_{i=1}^{N}(x_i - X_{mean,N})^2 \quad (3)$$

Let n elements from this population be measured by sampling without replacement. (This name indicates that the measured element cannot be replaced to be measured a second time. In this case, sample draws are not independent: the first element is drawn from N elements, the second is drawn from N – 1 elements, and so on.) Values of the sample are the following:

sample mean is $$x_{mean,n} = \frac{1}{n}\sum_{i=1}^{n} x_i \quad (4)$$

sample sum is $$x_{sum,n} = \sum_{i=1}^{n} x_i \quad (5)$$

variance of the sample is $$s_n^2 = \frac{1}{n-1}\sum_{i=1}^{n}(x_i - x_{mean,n})^2 . \quad (6)$$

Using the measured values of the sample, one can estimate *unbiased* values of the mean, the sum, and the variance of the population. The sampling method to estimate a population value "is *unbiased* if the average value of the estimate, taken over all possible samples of given size *n*, is exactly equal to the true population value." [a] Estimates (denoted below by ^) of parameters of the population are the following:

unbiased estimate of the mean of the population, $$\hat{X}_{mean,N} = x_{mean,n} = \frac{1}{n}\sum_{i=1}^{n} x_i \quad (7)$$

unbiased estimate of the sum of the population, $$\hat{X}_{sum,N} = N x_{mean,n} = N \times \frac{1}{n}\sum_{i=1}^{n} x_i \quad (8)$$

unbiased estimate of the variance of the population,[b] $$\hat{S}_N^2 = s_n^2 = \frac{1}{n-1}\sum_{i=1}^{n}(x_i - x_{mean,n})^2 \quad (9)$$

Note that the estimate of the variance of the population is simply (6), the variance of the sample.

The uncertainty of using the sample mean $x_{mean,n}$ as an estimate of the population mean derives from the fact that the number of possible samples of size n drawn from a population of N is $\frac{N!}{n!(N-n)!}$. This creates a collection of $\frac{N!}{n!(N-n)!}$ possible sample mean values that can occur. These different sample mean values form their own population, so the uncertainty of a sample mean value is the square root of the variance of this population of sample mean values. The variance of the mean, defined as the expected value ("expectation") of the squared difference

[a] Ibid., Sec 2.3, p. 14.
[b] Ibid., Theorem 2.4, p. 18.

between the mean of the sample and the mean of the population, obtained by averaging over all possible samples of size n, is equal to [a]

$$S^2_{mean,N,n} \equiv E\left[\left(x_{mean,n} - X_{mean,N}\right)^2\right] = \left(\frac{N-n}{N}\right)\frac{S_N{}^2}{n} \tag{10}$$

where $S_N{}^2$ is defined by (3).

Using (9) for the estimate of $S_N{}^2$, an unbiased estimate of the variance of (7), the mean of the population obtained from the sample mean, is [b]

$$\hat{S}^2_{mean,N,n} = \left(\frac{N-n}{N}\right)\frac{s_n{}^2}{n}. \tag{11}$$

Similarly, the unbiased estimate of $S^2_{sum,N,n}$, the variance of (8), the sum of the population obtained from the sample mean, is [c]

$$\hat{S}^2_{sum,N,n} = N^2\left(\frac{N-n}{N}\right)\frac{s_n{}^2}{n}. \tag{12}$$

Taking the square root of these variance estimates gives the additional uncertainty due to measuring only a sample of the population to obtain estimates of the population's mean or sum. This result is used in Case 3 of Section C.9, where the uncertainty of the sum of pieces is derived.

The factor $\left(\frac{N-n}{N}\right)$ is called the *finite population correction*. Note that the factor is close to 1 whenever N is very large compared to n, giving for equation (11)

$$\hat{S}^2_{mean,N,n} \approx \frac{s_n{}^2}{n} \tag{13}$$

This is the formula for the variance in the mean when sampling with replacement (in which case the sample draws are independent) from an infinite population. This is also the formula for variance of the measured value of a parameter obtained as the mean of n repeated measurements of it (which is a type of sampling with replacement from an infinite population).

Of course, when all members of the population are measured (n = N), the sample mean and sum become identical, respectively, to the the population mean and sum. Then the variances of the mean and of the sum are 0, as are their estimates (11) and (12), because they include the factor (N - n). In this special case, there is, of course, no additional uncertainty from using the sample mean as an estimate of the population mean.

[a] Ibid., Theorem 2.2, p. 15.
[b] Ibid., eqn. 2.18, p. 19.
[c] Ibid., eqn. 2.19, p. 19.

Because the upper limit of $\left(\frac{N-n}{N}\right)$ is 1, the effect of not using this correction factor and using, instead, only $\frac{s_n^2}{n}$ or $\frac{S_N^2}{n}$ is to overestimate the additional uncertainty from measuring only a fraction of the nominally equivalent items, or from using only a fraction of the measured items.

Because of the symmetry of $x_{mean,n}$ and $X_{mean,N}$ in (10), this variance of the mean also applies when the mean of a large population N', obtained from measurements of all its members, is used to estimate the mean of an assembly of fewer items N that are randomly drawn from the population. This is Case 4 of Section C.9. The uncertainty is due to not knowing which members of the entire population were used in the assembly. In this case, the result (10) is used directly as the variance of the mean value for the N items used in the assembly. The unbiased estimate of the variance of the sum of the N items is then

$$\hat{s}^2_{sum,N,N'} = N^2\left(\frac{N'-N}{N'}\right)\frac{S_{N'}^2}{N} \tag{14}$$

For some experiments, a double sampling without replacement occurs. This is Case 5 of Section C.9. In the first step, a sample of n elements is drawn from the population of size N for the purpose of measurement. After the measurements, the n elements are returned to the population. Then, another sample of size m to be used in the experiment is drawn from the population N. If m < n, the N items may be totally, partially, or not at all from the set of n items measured. If m > n, some or all elements used in the experiment are elements that were not measured. Using the mean of measured elements as the mean of the assembly introduces additional uncertainty because these two sets are different. Derivation of the additional uncertainty is given below.

Derivation[a] of the additional uncertainty of the mean for Case 5 of Section C.9

If the mean of sample n from a population N of nominally identical pieces is used to estimate the mean of m pieces for an assembly chosen randomly from the same population N, using the methods of Cochran,[b] the variance of the mean may be defined as $E\left[\left(\bar{x}_n - \bar{x}_m\right)^2\right]$,

where E is the expectation,

$\bar{x}_n = \frac{1}{n}\sum_{i=1}^{n} x_i$ = mean of the measured sample, and

$\bar{x}_m = \frac{1}{m}\sum_{i=1}^{m} x_i$ = mean of pieces in the assembly.

The mean is of some measured parameter, such as mass.

[a] Derived by V. F. Dean, October 2007.

[b] Cochran, William G., *Sampling Techniques*, Modern Asia Edition, John Wiley & Sons, Inc., New York, 1966 (sixth printing).

To find $E\left[\left(\bar{x}_n - \bar{x}_m\right)^2\right]$ first add and subtract $\bar{Y} = \frac{1}{N}\sum_{i=1}^{N} x_i$, the mean of the whole population N. Get

$$E\left[\left(\bar{x}_n - \bar{x}_m\right)^2\right] = E\left[\left\{\left(\bar{x}_n - \bar{Y}\right) - \left(\bar{x}_m - \bar{Y}\right)\right\}^2\right]$$

$$= E\left[\left(\bar{x}_n - \bar{Y}\right)^2 - 2\left(\bar{x}_n - \bar{Y}\right)\left(\bar{x}_m - \bar{Y}\right) + \left(\bar{x}_m - \bar{Y}\right)^2\right]$$

$$E\left[\left(\bar{x}_n - \bar{x}_m\right)^2\right] = E\left[\left(\bar{x}_n - \bar{Y}\right)^2\right] - 2E\left[\left(\bar{x}_n - \bar{Y}\right)\left(\bar{x}_m - \bar{Y}\right)\right] + E\left[\left(\bar{x}_m - \bar{Y}\right)^2\right] \qquad (15)$$

The variance of the N values x_i of the population is $S^2 \equiv \frac{\sum_{i=1}^{N}\left(x_i - \bar{Y}\right)^2}{N-1}$. [a]

The variance of the mean of the population, when $\bar{\bar{x}}_n$ (the mean of n pieces sampled randomly from the population) is used to estimate $\bar{Y}$ (the mean of the population of N items), is defined as $E\left[\left(\bar{x}_n - \bar{Y}\right)^2\right]$.

Theorem 2.2 of Cochran proves that $E\left[\left(\bar{x}_n - \bar{Y}\right)^2\right] = \frac{S^2}{n}\frac{(N-n)}{N}$.

Theorem 2.4 of Cochran shows that an unbiased estimate of S^2 is the variance of the sample,

$s_n^{\,2} \equiv \frac{\sum_{i=1}^{n}\left(x_i - \bar{x}_n\right)^2}{n-1}$, where $\bar{x}_n \equiv \frac{1}{n}\sum_{i=1}^{n} x_i$.

So the first and third expectations in the last expression of Equation (15) are

$$E\left[\left(\bar{x}_n - \bar{Y}\right)^2\right] = \frac{N-n}{nN}s^2 \qquad \text{and} \qquad E\left[\left(\bar{x}_m - \bar{Y}\right)^2\right] = \frac{N-m}{mN}s^2.$$

The middle expectation of Equation (15) is $-2E\left[\left(\bar{x}_n - \bar{Y}\right)\left(\bar{x}_m - \bar{Y}\right)\right]$. We need to derive the value of this expectation in order to find the variance of the mean of the m pieces, randomly drawn from population N and used in an assembly, when estimated by the mean of n pieces of another sample of n pieces randomly drawn from the same population.

By the definition of the means, $\bar{\bar{x}}_n$ and $\bar{\bar{x}}_m$, this middle term equals

$$-2E\left[\frac{1}{n}\left(\sum_{i=1}^{n}\left(x_i - \bar{Y}\right)\right) \times \frac{1}{m}\left(\sum_{i=1}^{m}\left(x_i - \bar{Y}\right)\right)\right] = \frac{-2}{mn}E\left[\left(\sum_{i=1}^{n}\left(x_i - \bar{Y}\right)\right) \cdot \left(\sum_{i=1}^{m}\left(x_i - \bar{Y}\right)\right)\right].$$

So now the task is to fine the average value (expectation) of $\left(\sum_{i=1}^{n}\left(x_i - \bar{Y}\right)\right) \cdot \left(\sum_{i=1}^{m}\left(x_i - \bar{Y}\right)\right)$ over all possible samples from N of sizes m and n.

[a] *Ibid.*, Equation 2.7.

Note that, when considering all possible samples, some, all, or none of the pieces of sample n can be the same pieces as those of sample m. This is because the n measured pieces are replaced in population N before randomly choosing the m pieces to be used in the assembly, or vice versa. Suppose that the number of same, or common, pieces in the two samples is k. Then $k \le m$ and $k \le n$. That is, k is equal to or less than the smaller of m and n. Also, of course, $m \le N$ and $n \le N$. Therefore,

$$\left(\sum_{i=1}^{n}\left(x_i-\bar{Y}\right)\right)\cdot\left(\sum_{i=1}^{m}\left(x_i-\bar{Y}\right)\right)=\left[\left(x_1-\bar{Y}\right)+\left(x_2-\bar{Y}\right)+\ldots+\left(x_k-\bar{Y}\right)+\left(x_{k+1}-\bar{Y}\right)+\ldots+\left(x_n-\bar{Y}\right)\right]\times$$
$$\left[\left(x_1-\bar{Y}\right)+\left(x_2-\bar{Y}\right)+\ldots+\left(x_k-\bar{Y}\right)+\left(x'_{k+1}-\bar{Y}\right)+\ldots+\left(x'_{m}-\bar{Y}\right)\right]$$

The primes remind us that $x_a \neq x'_a$ because only the k pieces are the same. Also, abbreviate $\left(x_i - \bar{Y}\right)$ as X_i. So we have

$$\left[X_1+X_2+\ldots+X_k+X_{k+1}+\ldots+X_n\right]\cdot\left[X_1+X_2+\ldots+X_k+X'_{k+1}+\ldots+X'_{m}\right].$$

Doing the multiplication of terms gives

$$\left(\sum_{i=1}^{n}\left(x_i-\bar{Y}\right)\right)\cdot\left(\sum_{i=1}^{m}\left(x_i-\bar{Y}\right)\right)=\sum_{i=1}^{k}X_i^2+\sum_{i=1}^{k}X_i\cdot\sum_{\substack{j=1\\ j\neq i}}^{k}X_j+\sum_{i=1}^{k}X_i\cdot\sum_{j=k+1}^{m}X'_j+\sum_{i=k+1}^{n}X_i\cdot\sum_{j=1}^{k}X_j+\sum_{i=k+1}^{n}X_i\cdot\sum_{j=k+1}^{m}X'_j$$

Now we need to find the expectations of these 5 terms, which together make up the middle expectation of Equation (15). To do this, we average each of these sums over all possible samples of sizes n and m from N, so that we can get the result in terms of the population variance. Then we can estimate the population variance by s_n^2, the variance of the measured sample n, as mentioned previously.

To do this we use the number-ratio proof [a] of Theorem 2.1 and Equations 2.10 and 2.11 of Cochran.[b]

From Equation 2.10, by considering the ratio of number of terms on each side of the equation, the first of the 5 expectations is

$$E\left[\sum_{i=1}^{k}X_i^2\right]=\frac{k}{N}\sum_{i=1}^{N}X_i^2$$

From Equation 2.11, the same considerations give a value for the second of the 5 expectations:

$$E\left[\sum_{i=1}^{k}X_i\cdot\sum_{\substack{j=1,\\ j\neq i}}^{k}X_j\right]=2E\left[\sum_{i=1}^{k}X_i\cdot\sum_{j=i+1}^{k}X_j\right]=\frac{2k\left(k-1\right)}{N\left(N-1\right)}\sum_{i=1}^{N}X_i\cdot\sum_{j=i+1}^{N}X_j.$$

[a] The number-ratio proof is the following: "Since every unit appears in the same number of samples [when averaging over all possible samples], it is clear that [the sums over the samples in left-hand side] must be some multiple of [the sums over the population in the right-hand side]. The multiplier must be [t_s, number of terms in the left-hand side divided by T_N, number of terms in the right-hand side], since the expression on the left has [t_s] terms and the expression on the right has [T_N] terms." (See Cochran, p. 15; it is true because all pieces of the sample have approximately the same value.)

[b] *Ibid.*, pp. 14-16.

Note that for this term, because the two sums $\sum_{i=1}^{k} X_i$ and $\sum_{\substack{j=1,\\ j\neq i}}^{k} X_j$ have the same k pieces in each, there are two individual terms equal to $X_i \cdot X_j$ with $i \neq j$; for example, there is a $X_3 \cdot X_4$ term as well as a $X_4 \cdot X_3$ term. As Cochran notes, the product $\sum_{i=1}^{k} X_i \cdot \sum_{j=i+1}^{k} X_j$ has k(k-1)/2 terms, while the product $\sum_{i=1}^{N} X_i \cdot \sum_{j=i+1}^{N} X_j$ has N(N-1)/2 terms. So the ratio of the numbers of near-equal terms on each side is $\frac{k(k-1)}{N(N-1)}$.

For the third expectation term, $\sum_{i=1}^{k} X_i \cdot \sum_{j=k+1}^{m} X'_j$ with k(m – k) separate terms and again using the number-ratio proof of Theorem 2.1, it must be that

$$E\left[\sum_{i=1}^{k} X_i \cdot \sum_{j=k+1}^{m} X'_j\right] = \frac{2k(m-k)}{N(N-1)} \sum_{i=1}^{N} X_i \cdot \sum_{j=i+1}^{N} X_j .$$

The 2 is here because the right hand side has N(N-1)/2 terms, so the ratio of number of terms in the left-hand side to the number of near-equivalent terms in the right-hand side is $\frac{2k(m-k)}{N(N-1)}$.

Similarly,

$$E\left[\sum_{i=k+1}^{n} X_i \cdot \sum_{j=1}^{k} X_j\right] = \frac{2k(n-k)}{N(N-1)} \sum_{i=1}^{N} X_i \cdot \sum_{j=i+1}^{N} X_j$$

and

$$E\left[\sum_{i=k+1}^{n} X_i \cdot \sum_{j=k+1}^{m} X'_j\right] = \frac{2(n-k)(m-k)}{N(N-1)} \sum_{i=1}^{N} X_i \cdot \sum_{j=i+1}^{N} X_j .$$

Using the equalities established above, we obtain for the middle expectation of the right-hand side of Equation (15) the following:

$$\begin{aligned}
&\frac{-2}{mn} E\left[\left(\sum_{i=1}^{n}\left(x_i - \bar{Y}\right)\right) \cdot \left(\sum_{i=1}^{m}\left(x_i - \bar{Y}\right)\right)\right] \\
&\quad = \frac{-2}{mn}\left\{\frac{k}{N}\left[\sum_{i=1}^{N}\left(x_i - \bar{Y}\right)^2\right]\right. \\
&\qquad \left. +2\left[\frac{k(k-1)}{N(N-1)} + \frac{k(m-k)}{N(N-1)} + \frac{k(n-k)}{N(N-1)} + \frac{(n-k)(m-k)}{N(N-1)}\right] \times \left[\sum_{i=1}^{N}(x_i - \bar{Y})\right] \times \left[\sum_{j=i+1}^{N}(x_j - \bar{Y})\right]\right\} \\
&\quad = \frac{-2}{mnN}\left\{k\left[\sum_{i=1}^{N}\left(x_i - \bar{Y}\right)^2\right]\right. \\
&\qquad \left. + 2\frac{k(k-1+m-k+n-k)+(n-k)(m-k)}{N-1} \times \left[\sum_{i=1}^{N}\left(x_i - \bar{Y}\right)\right] \times \left[\sum_{j=i+1}^{N}\left(x_j - \bar{Y}\right)\right]\right\}
\end{aligned}$$

$$= \frac{-2}{mnN}\left\{ k\left[\sum_{i=1}^{N} \left(x_i - \bar{Y} \right)^2 \right] + 2\frac{mk + nk - k^2 - k + nm - nk - km + k^2}{N-1} \times \left[\sum_{i=1}^{N} \left(x_i - \bar{Y} \right) \right] \times \left[\sum_{j=i+1}^{N} \left(x_j - \bar{Y} \right) \right] \right\}$$

$$= \frac{-2}{mnN}\left\{ k\left[\sum_{i=1}^{N} \left(x_i - \bar{Y} \right)^2 \right] + 2\frac{nm - k}{N-1} \times \left[\sum_{i=1}^{N} \left(x_i - \bar{Y} \right) \right] \times \left[\sum_{j=i+1}^{N} \left(x_j - \bar{Y} \right) \right] \right\}$$

$$= \frac{-2k}{mnN}\left\{ \left[\sum_{i=1}^{N} \left(x_i - \bar{Y} \right)^2 \right] + 2\frac{nm - k}{k\left(N-1\right)} \times \left[\sum_{i=1}^{N} \left(x_i - \bar{Y} \right) \right] \times \left[\sum_{j=i+1}^{N} \left(x_j - \bar{Y} \right) \right] \right\}.$$

Now, as Cochran does in his proof of Theorem 2.2, "complete the square on the cross-product term." The middle expectation of Equation (15) becomes

$$\frac{-2}{mn} E\left[\left(\sum_{i=1}^{n} \left(x_i - \bar{Y} \right) \right) \cdot \left(\sum_{i=1}^{m} \left(x_i - \bar{Y} \right) \right) \right] = \frac{-2k}{mnN}\left\{ \left[1 - \frac{nm - k}{k(N-1)} \right] \left[\sum_{i=1}^{N} \left(x_i - \bar{Y} \right)^2 \right] + \frac{nm - k}{k(N-1)} \left[\sum_{i=1}^{N} \left(x_i - \bar{Y} \right) \right]^2 \right\}$$

Because $\sum_{i=1}^{N} \left(x_i - \bar{Y} \right) = 0$, by the definition of $\bar{Y}$, the last term on the right-hand side is zero.

So $$\frac{-2}{mn} E\left[\left(\sum_{i=1}^{n} \left(x_i - \bar{Y} \right) \right) \cdot \left(\sum_{i=1}^{m} \left(x_i - \bar{Y} \right) \right) \right] = \frac{-2k}{mnN} \left[1 - \frac{nm - k}{k(N-1)} \right] \left[\sum_{i=1}^{N} \left(x_i - \bar{Y} \right)^2 \right].$$

Simplifying further and using the definition of S^2, the variance of the population N, it equals

$$\frac{-2k}{mnN} \left[\frac{kN - k - nm + k}{k(N-1)} \right] \left[\sum_{i=1}^{N} \left(x_i - \bar{Y} \right)^2 \right] = \frac{-2}{mnN} \left[\frac{kN - nm}{(N-1)} \right] \left[\sum_{i=1}^{N} \left(x_i - \bar{Y} \right)^2 \right] = \frac{-2\left(kN - nm\right)}{mnN} S^2.$$

This is the value of the middle term in the right-hand side in the original expression, Equation (15), which is repeated here:

$$E\left[\left(\bar{x}_n - \bar{x}_m \right)^2 \right] = E\left[\left(\bar{x}_n - \bar{Y} \right)^2 \right] - 2E\left[\left(\bar{x}_n - \bar{Y} \right)\left(\bar{x}_m - \bar{Y} \right) \right] + E\left[\left(\bar{x}_m - \bar{Y} \right)^2 \right] \qquad (15)$$

Therefore, using the values obtained for these 3 expectations in terms of the sample variance s_n^2, which estimates the population variance S^2, this becomes

$$E\left[\left(\bar{x}_n - \bar{x}_m \right)^2 \right] = \left\{ \left[\frac{N - n}{nN} \right] + 2\left[\frac{mn - kN}{mnN} \right] + \left[\frac{N - m}{mN} \right] \right\} \cdot s_n^2.$$

Simplifying further, $$E\left[\left(\bar{x}_n - \bar{x}_m \right)^2 \right] = \frac{1}{mnN}\left[mN - mn + 2mn - 2kN + nN - mn \right] \cdot s_n^2 = \frac{N(m + n - 2k)}{mnN} \cdot s_n^2$$

or $$E\left[\left(\bar{x}_n - \bar{x}_m \right)^2 \right] = \frac{m + n - 2k}{mn} \cdot s_n^2,$$

where k is the number of pieces common to random samples m and n. If k is the smaller of m and n (which is the largest possible value for k, and implies either that all measured pieces are in the assembly or that the whole assembly comprises measured pieces), this can be written as

$$E\left[\left(\bar{x}_n - \bar{x}_m\right)^2\right] = \frac{|m - n|}{mn} \cdot s_n^2 = \left(\frac{1}{min(m,n)} - \frac{1}{max(m,n)}\right) \cdot s_n^2 .$$

Note, however, that the additional uncertainty will be proportional to the square root of $\frac{m + n - 2k}{mn}$, which increases as k decreases.

Usually, we do not know how many pieces are common to both samples. Therefore, we must assume the worst case, which is the smallest possible value of k.

For k = 0, indicating that there are no pieces common to samples n and m, the variance of the mean becomes

$$E\left[\left(\bar{x}_n - \bar{x}_m\right)^2\right] = \frac{m + n}{mn} \cdot s_n^2 = \left(\frac{1}{n} + \frac{1}{m}\right) \cdot s_n^2 .$$

However, if m + n > N, it is impossible that samples m and n have no common pieces. In this case, the smallest possible k is m + n – N. For this case, the expectation of the variance of the mean becomes

$$E\left[\left(\bar{x}_n - \bar{x}_m\right)^2\right] = \frac{m + n - 2(m + n - N)}{mn} \cdot s_n^2 = \frac{2N - m - n}{mn} \cdot s_n^2 = \left(\frac{2N}{mn} - \frac{1}{n} - \frac{1}{m}\right) \cdot s_n^2 .$$

In summary, if the mean of m pieces used in an assembly is estimated by using the mean of a sample of n pieces of a larger population N, from which both assembly pieces and measured pieces were randomly taken, the variance of the mean is $E\left[\left(\bar{x}_n - \bar{x}_m\right)^2\right] = \frac{m + n - 2k}{mn} \cdot s_n^2$, where k is the number of pieces common to the assembly and measured sample, and s_n^2 is the variance of the measured sample n. If k is not known, the smallest possible k is assumed:

k = 0, if m + n ≤ N, or
k = m + n – N, if m + n > N.

APPENDIX D: EXAMPLE OF EXPERIMENTAL-DESIGN METHODOLOGY

LEU-COMP-THERM-052: Uranium Dioxide (4.738%-Enriched) Fuel-Rod Arrays Moderated and Reflected by Gadolinium Nitrate Solution

Critical experiments with 4.738%-enriched uranium dioxide rod arrays in a large water-filled tank were carried out in testing equipment called Apparatus B in the experimental criticality facility at the "Service de Recherches et d'Etudes en Criticité" in Valduc (C.E.A. France) in 1978. Experiments were subcritical approaches extrapolated to critical, with the multiplication factor reached being very close to 1.000 (~0.99).

The six configurations of the experimental program were:

- either one hexagonal assembly of 1261 fuel rods (21 rods per side of the hexagon)
- or one pseudo-cylindrical assembly of 1285 fuel rods (10 rods added on each side of the hexagon and 6 rods removed at each corner)

Configurations were performed at three triangular pitches (1.35, 1.72 and 2.26 cm). The array was moderated and reflected by a gadolinium nitrate solution. The gadolinium concentration was such that the solution critical height (between 87.5 and 89.6 cm) obtained by an extrapolation method covered most of the fissile column (90 cm).

For this example, only Case 1 of LEU-COMP-THERM-052 will be treated, because of reference values varying from one case to the other. This example of the experimental design method should be considered from a "mathematical" point of view. "Physical" aspects are treated in LEU-COMP-THERM-052.

In the original evaluation, many uncertainties are of Type B. Later evaluations should include most recent statistical measurements giving therefore more uncertainties of Type A.

D.1 Inventory of uncertainties

D.1.1 Uncertainties on materials

The uncertainties on materials should include at least the parameters listed in the following table (non-exhaustive list), in which the columns are filled, for clarification.

Parameter Identification (unit of measurement)	Mean measured value	Reported uncertainty in parameter[(a)]	Type of uncertainty (A or B)	ν Number of degrees of freedom [(b)]	Number of standard deviations associated with the uncertainty	Standard uncertainty
^{235}U Enrichment (wt.%)	4.738	0.004	A	∞ [(c)]	2	0.002
Fuel Density (g/cm^3 fuel rod)	10.38	0.04	B	∞	3	0.04/3
Temperature (°C)	22.0	1	B	∞	none	1/√3
Gadolinium Content (g/l) in solution	0.6	3 %	A	unknown	2	3 % / 2

(a) The uncertainty is usually reported with the same unit as quoted in the first column. In a few cases, relative uncertainties are given, in %.
(b) The number ν of degrees of freedom is equal to n-1 for a single quantity estimated by the arithmetic mean of n independent observations.
(c) Actually, the number of measurements is unknown, but data indicates that many measurements were made; therefore, for practical purposes, it is assumed to be infinite. (Value confirmed by 5 points of measurement.)

The uncertainty in temperature will have an effect on water density and nuclear temperatures of isotopes.

D.1.2 Uncertainties in geometry

The uncertainties in geometry should include at least the parameters listed in the following table (non-exhaustive list), in which the columns are filled, for clarification.

Parameter Identification (unit of measurement)	Mean measured value or design value	Reported uncertainty in parameter[(a)]	Type of uncertainty (A or B)	ν Number of degrees of freedom[(b)]	Number of standard deviations associated with the uncertainty	Standard uncertainty
Fuel Pellet Radius (cm)	0.395	0.002	B	∞	1	0.002
Clad Outer Radius (cm)	0.470	0.0025	B	∞	none	0.0025/√3
Fuel-Rod Position (cm)		0.06	B	1260	1	0.06/√1261
Solution Height (cm)	89.6	0.2	B[(c)]	∞	3	0.2/3
Fissile column height (cm)	89.6	1	B	∞	3	1/3

(a) The uncertainty is usually reported with the same unit as quoted in the first column. In a few cases, relative uncertainties are given, in %.
(b) $\nu \rightarrow \infty$. See the discussion in Section 6.4 and in Sections G.4.2 and G.4.3 of Reference 1.
(c) The parameter is taken as Type B, because it is the result of an average measurement by 5 counters for each experiment.

The fissile column height design value 90.0 is given as 90 ± 1 cm, where ± 1 cm is given as a tolerance by the manufacturer. However, it is taken as 89.6, to give the possibility of running uncertainty calculations with positive or negative increments (because revising the model to heights greater than 90 cm is difficult). Note that it is not necessary that the reference case exactly match the benchmark model; it is sufficient for parameters to only be close to the benchmark-model specifications.

D.2 Estimation of uncertainties

When experimental design is used as the method of determination of uncertainties, it is convenient to treat the parameters in groups such that within each group all parameters may be easily varied at the same time.

D.2.1 Estimation of uncertainties in a first group of parameters by experimental-design methodology

The first group of parameters x_i , which will vary at the same time includes

x_1 = ^{235}U Enrichment (wt.%)

x_2 = Fuel Density (g/cm^3 fuel rod)

x_3 = Fuel Pellet Radius (cm)

x_4 = Clad Outer Radius (cm)

The parameters' variations in calculations will be, respectively, 0.01, 0.04, 0.001, 0.001. Nine simulations with simultaneous changes in parameters are run. The 9th calculation corresponds to the reference configuration.

calculation n°	x_1	x_2	x_3	x_4	k_{eff}	delta k_{eff} x 10^5
1	4.728	10.34	0.394	0.469	0.998	-169
2	4.748	10.34	0.394	0.471	0.9983	-139
3	4.728	10.42	0.394	0.471	0.99855	-114
4	4.748	10.42	0.394	0.469	1.00054	85
5	4.728	10.34	0.396	0.471	0.9991	-59
6	4.748	10.34	0.396	0.469	1.00111	142
7	4.728	10.42	0.396	0.469	1.00135	166
8	4.748	10.42	0.396	0.471	1.00162	193
9	4.738	10.38	0.395	0.470	0.99969	0

By linear regression from these calculations, we obtain a first order development for the k_{eff} variation:

$$\Delta k_{eff} \times 10^5 = 13.125 + 57.125\frac{(x_1 - 4.738)}{0.01} + 69.375\frac{(x_2 - 10.38)}{0.04} + 97.375\frac{(x_3 - 0.395)}{0.001} - 42.875\frac{(x_4 - 0.470)}{0.001}$$

The first term, 13.125 pcm, is a residual term, which should be as low as possible, its value being small when it is compared with the total variation due to the four parameter changes.
For each parameter change, it is possible to compute the effect on k_{eff}.
For instance, Δk_{eff} [^{235}U Enrichment (wt.%)] = 57.125 (0.002/0.01) 10^{-5} = 11×10^{-5}

Parameter	Parameter Variation in Calculation	Δk_{eff} x 10^5	Parameter Experimental Standard Deviation	Δk_{eff} x 10^5
x_1	0.01	57	0.002	11
x_2	0.04	69	0.01333	23
x_3	0.001	97	0.001	97
x_4	0.001	-43	0.00072	-31

D.2.2 Estimation of uncertainties on a second group of parameters by experimental-design

The second group of parameters x_i, which will vary at the same time includes
x_1 = Solution Height (cm)
x_2 = Fissile Column H eight (cm)

The parameter variations in calculations will be the same: 0.4 cm. Five simulations with simultaneous changes in parameters are run, and the 5th calculation corresponds to the reference configuration.

calculation n°	x_1	x_2	k_{eff}	delta k_{eff} x 10^5
1	89.2	89.2	0.99937	-32
2	90	89.2	0.99984	15
3	89.2	90	0.99953	-16
4	90	90	0.99985	16
5	89.6	89.6	0.99969	0

By linear regression from these calculations, we obtain a first order development for the k_{eff} variation:

$$\Delta k_{eff}\times10^5 = -4.25 + 19.75\frac{(x_1-89.6)}{0.4} + 4.25\frac{(x_2-89.6)}{0.4} - 3.75\frac{(x_1-89.6)}{0.4}\times\frac{(x_2-89.6)}{0.4}$$

The first term, -4.25 pcm, is a residual term, which should be as low as possible, its value being small when it is compared with the total variation due to the two parameter changes.

The cross-term ($x_1\times x_2$) is introduced in order to take into account the correlation between parameters x_1 and x_2. In Section D.2.1, when using the fitted polynomial expression to rebuild

the delta k_{eff} values, the agreement between the calculated values and the rebuilt values was excellent (within 1×10^{-5}), so that it was inferred that there was no correlation between parameters.

For each parameter change, it is possible to compute the effect on k_{eff}.

Parameter	Parameter Variation in Calculation	Δk_{eff} x 10^5	Parameter Experimental Standard Deviation	Δk_{eff} x 10^5
x_1	0.04	20	0.06667	3
x_2	0.04	4	0.33333	4
$x_1 \times x_2$	0.04x0.04	4	0.02222	-0.5

The last interaction term is not taken into account, since it is too small.

D.2.3 Estimation of uncertainties on a last group of parameters by direct calculations

The third group of parameters x_i is investigated independently, by direct calculations, as usual:
x_1 = Temperature (°C)
x_2 = Fuel-Rod Position (cm)
x_3 = Gadolinium Content (g/l) in solution

Parameter	Parameter Variation in Calculation	Δk_{eff} x 10^5	Parameter Experimental Standard Deviation	Δk_{eff} x 10^5
x_1	3	24	$1/\sqrt{3}$	5
x_2	0.06	174	$0.06/\sqrt{1261}$	5
x_3	-4.5 %	597	3 %/2	199

D.2.4 Estimation of the combined uncertainty

All values of uncertainties (1σ) corresponding to the parameters changes are reported in the following table, which corresponds to Table 8 of LEU-COMP-THERM-052.

Case	Pitch (cm)	Parameter Identification (unit of measurement)	Parameter Variation in Calculation	Calculated Effect, $\Delta k_{eff} \times 10^5$	Parameter Reported Uncertainty	Parameter Experimental Standard Deviation	Δk Effect of Standard Uncertainty $\times 10^5$
1	1.35	^{235}U Enrichment (wt.%)	0.010[(a)]	57	0.004	0.004/2	11
		Fuel Density (g/cm^3)	0.04	69	0.04	0.04/3	23
		Fuel Radius (cm)	0.002	97	0.002	0.002	97
		Clad Outer Radius (cm)	0.002	-43	0.0025[(b)]	0.0025 /√3	31
		Temperature (°C)	3	24	1[(c)]	1[(c)] /√3	5
		Fuel-Rod Position (cm)	0.06	174	0.06 [(d)]	0.06/√1261	5
		Gadolinium Content (g/l)	-4.5 %	597	3 %	3 %/2	199
		Solution Height (cm)	0.4	20	0.2	0.2 /3	3
		Fissile column height (cm)	0.4	4	1	1 /3	4
		Quadrature sum					**225**

(a) When changing the ^{235}U enrichment, the ^{238}U concentration was changed correspondingly to maintain constant mass of uranium.
(b) Assumed uncertainty taken as half uncertainty of clad thickness.
(c) Measurement uncertainty is ± 1 °C; measured temperature is 22 °C, except Case 4 where it is 23 °C. Both solution density and cross sections were changed by amounts corresponding to 3 degrees to calculate this effect.
(d) Maximum displacement allowed by diametral gap between grid hole and fuel pin clad is ± 0.03 cm. Uncertainty on fuel pin center-hole position is ± 0.05 cm. The total uncertainty on fuel-rod positioning was given by the quadratic sum $\sqrt{0.03^2 + 0.05^2}$ and the k_{eff} variation was divided by $\sqrt{N}$, where N is the number of fuel rods.

The gadolinium content is the parameter that contributes most to the experimental uncertainty. It is very easy to find its contribution by one-variable-at-a-time strategy. Using the experimental design method would certainly improve the variance of the result. However, the choice of a parameter family for gadolinium concentration is not obvious, and there could be a masking effect between this major contributor and other minor contributors to uncertainty.

APPENDIX E: UNCERTAINTIES CALCULATED FOR LEU-COMP-THERM-040

Four 4.738-wt.%-Enriched Uranium Dioxide Rod Assemblies Contained in Borated Stainless Steel or Boral Square Canisters, Water Moderated and Reflected by Lead or Steel

The following table gives a comparison of calculations performed by three methods:

- two independent Monte Carlo calculations ($\sigma = 33 \times 10^{-5}$), in which the parameter change was the experimental standard deviation multiplied by 5, and the results were divided by the same factor 5;
- 19 Monte Carlo calculations to find by experimental-design methodology five parameter uncertainties: the four listed in the table, and the temperature showing no effect;
- two independent calculations ($\sigma = 33 \times 10^{-5}$) using a perturbation model in the Monte Carlo code; in fact, the standard deviation associated with the result in this case is 1×10^{-5}.

In the three types of Monte Carlo calculations, the associated standard deviations are, respectively,

- $10^{-5}\sqrt{2\times33^2\,\frac{1}{25}} = 9\times10^{-5}$
- $10^{-5}\sqrt{\frac{33^2}{19}\,\frac{1}{25}} = 2\times10^{-5}$
- 1×10^{-5}

Using the experimental design methodology reduces the value of the standard deviation by a factor of $\sqrt{19}$, in this case.

Case	Valduc Reference No.	Parameter Identification (unit of measurement)	Parameter Nominal Value	Experimental Standard Deviation Used for Parameter	$\Delta k_{eff} \times 10^5$ from 2 independent calculations	$\Delta k_{eff} \times 10^5$ from experimental design	$\Delta k_{eff} \times 10^5$ from perturbation model
1	1983	^{235}U Enrichment (wt.%) Fuel Density (g/cm^3) Fuel Radius (cm) Clad Outer Radius (cm)	4.738 10.38 0.395 0.47	0.004 0.04 0.002 0.002	45 68 98 39	38 70 92 34	50 72 87 49

APPENDIX F: ROUNDING EXPERIMENTAL DATA[a]

F.1 Recommended practice

The standard deviation and the measured value of the measurand are equally important when we use interval estimates, i.e., confidence intervals. In spite of this, the standard deviation is frequently specified only with one digit – saying that "the digits within the experimental uncertainty are not interesting anyhow." This is accompanied by rounding the value of the measurand also in the same way. For example, the criticized practice consists of specifying

60 ± 5 instead of 58.72 ± 4.63,

or

59 ± 2 instead of 58.72 ± 1.52.

This kind of easygoing approach can have serious consequences for those who try to use experimental data. Below, are arguments in favor of the following simple practice:

(1) **Give the standard deviation with at least two digits.**
(2) **The decimal place of the last digit of the measurand should be the same as that of the standard deviation.**

For example, data like

58.72 ± 4.63 or 58.7 ± 4.6

can be recommended, but data like 59 ± 5 should be avoided. The first argument will be trivial while the second one will be based on some mathematical analysis.

F.2 Trivial arguments

Let us consider the following simple example, which might appear extreme but is instructive. Assume that we have two measured values of the same measurand: $x_1 = 1.02$ and $x_2 = 3.14$ whose standard deviations are

$s_1 = 1.49$ and $s_2 = 1.51$,

respectively.[b] It is simple to see that there is no significant difference between the measured values. Thus, their weighted average can be used for estimating their common true value: 2.06 ± 1.06. Let us now round the standard deviations to one digit:

$s'_1 = 1$ and $s'_2 = 2$.

Before rounding, the weights were practically equal:

$$w_1 = 1/s_1^2 = 0.4504 \quad \text{and} \quad w_2 = 1/s_2^2 = 0.4444,$$

[a] Contributed by Zoltán Szatmáry, Technical University of Budapest, Hungary.
[b] This is an artificial case presented in order to amplify the effects of rounding. In the usual cases, the problems are less awkward but their effects are rarely negligible.

while, after rounding, their ratio became 4 to 1. The weighted average based on the latter is: 1.44 ± 1.12. The deviation of the two averages is

$$2.06 - 1.44 = 0.62$$

which is of the same order of magnitude as the standard deviations. *It was completely superfluous to introduce such an error by rounding.* According to the approach criticized above, one need not pay attention to errors that are comparable to the standard deviations. Few things are less true than this because the incorrect rounding can change the interval estimates dramatically.

In the case of a Gaussian distribution, the quantile is $\gamma_G = 1.96$ for a confidence level of 95%. We shall take $\gamma_G \approx 2$ in the following. For $s_1 = 1.49$, the half length of the confidence interval (i.e., the experimental uncertainty) is 3 while it is roughly 2 if s_1 is rounded to $s'_1 = 1$. With the better standard deviation (i.e., s_1), the uncertainty of 2 means that the quantile was arbitrarily reduced to

$$\gamma = \gamma_G \cdot 2/3 = 1.33,$$

which corresponds to a confidence probability of 82%. The statistical tests based on the rounded values became thus biased; that is, we think that we work with 95% but the actual confidence level is only 82%. This is an important difference.

We conclude that excessive rounding can make statistical analyses misleading. It may happen that good theories will be rejected just because we neglected to specify one digit more. Of course, the opposite can also happen. Incorrect theories might be confirmed for the same reason.

F.3 Probabilistic arguments

Let us now study, quantitatively, what is the minimum number of digits to be specified. Let ξ be the difference between the experimental value of the measurand and its true value, and let σ be its standard deviation. The interval estimates (i.e., the confidence intervals) are based on the γ quantile defined by the equation

$$\mathrm{P}\{|\xi| < \gamma\sigma\} = 1 - \varepsilon \qquad (1)$$

where $(1 - \varepsilon)$ is the confidence level (99%, 95%, etc.). When the measured value is rounded, a particular value, r, of a uniformly distributed random variable is added to ξ.[a] This means that the quantile γ ought to be calculated from the equation

$$\mathrm{P}\{|\xi + r| < \gamma\sigma\} = 1 - \varepsilon\,. \qquad (2)$$

Introduce the following notation:

$$\Phi(x) = \mathrm{P}\{\xi < x\}$$

leading to

$$\mathrm{P}\{|\xi| < x\} = \Phi(x) - \Phi(-x)\,.$$

Similarly, denote

[a] This model of the rounding is borrowed from the theory of quantizing random processes. It is only an approximation.

$$F(\gamma) = \mathrm{P}\{\xi + r < \gamma\sigma\}$$

leading to

$$\mathrm{P}\{|\xi + r| < \gamma\sigma\} = F(\gamma) - F(-\gamma).$$

If the range of r is Θ, we may write:

$$F(\gamma) = \int_{-\Theta/2}^{\Theta/2} \mathrm{P}\{\xi + r < \gamma\sigma | r\} \frac{\mathrm{d}r}{\Theta} = \int_{-\Theta/2}^{\Theta/2} \Phi(\gamma\sigma - r) \frac{\mathrm{d}r}{\Theta} = \int_{\gamma\sigma-\Theta/2}^{\gamma\sigma+\Theta/2} \Phi(r) \frac{\mathrm{d}r}{\Theta}.$$

Assume, as an example, that ξ is a Gaussian random variable. Then

$$\Phi(x) = \frac{1}{2} + \frac{1}{2}\mathrm{erf}\left(\frac{x}{\sigma\sqrt{2}}\right),$$

where

$$\mathrm{erf}(z) = \frac{2}{\sqrt{\pi}} \int_0^z e^{-t^2} \mathrm{d}t.$$

The integral can be simply calculated leading to

$$1 - \varepsilon = \mathrm{P}\{|\xi + r| < \gamma\sigma\} =$$

$$= \frac{\gamma\sigma + \Theta/2}{\Theta} \mathrm{erf}\left(\frac{\gamma\sigma + \Theta/2}{\sigma\sqrt{2}}\right) + \frac{2\sigma}{\Theta\sqrt{2\pi}} \exp\left[-\frac{(\gamma\sigma + \Theta/2)^2}{2\sigma^2}\right] -$$

$$- \frac{\gamma\sigma - \Theta/2}{\Theta} \mathrm{erf}\left(\frac{\gamma\sigma - \Theta/2}{\sigma\sqrt{2}}\right) - \frac{2\sigma}{\Theta\sqrt{2\pi}} \exp\left[-\frac{(\gamma\sigma - \Theta/2)^2}{2\sigma^2}\right]. \qquad (3)$$

It can be seen that this depends only on the ratio Θ/σ (of course, in addition to γ). Equation 3 can now be applied in two ways:

1. Equation 3 can be solved for γ for any given value of ε and Θ/σ. This quantile allows constructing correct confidence intervals that take into account the fact that the measurand was rounded. This γ quantile will be greater than the γ_G quantile belonging to the Gaussian distribution. Thus, the correct confidence interval is broader than the Gaussian one. We can put this also in the following form: *the experimental uncertainty increases when the measurand is rounded*. We usually never take this into account: we use the Gaussian quantile γ_G, which is correct if and only if there is no rounding. Therefore, it is advisable to choose such a rounding range θ for which the difference between γ and γ_G is negligible. Figure F.1 shows the percentage difference between quantiles γ and γ_G as a function of Θ/σ. It can be seen that the difference is negligible when Θ/σ is less than 0.1.
2. When we neglect the consequences of rounding, we use the Gaussian quantile γ_G for constructing the confidence interval. Due to rounding, this corresponds in fact to another confidence level:

$$\mathrm{P}\{|\xi + r| < \gamma_G\sigma\} = 1 - \varepsilon' \qquad (4)$$

where the left hand side is given by Equation 3. Figure F.1 presents the difference between ε and ε', too. It can be seen that the difference is negligible again when Θ/σ is less than 0.1.

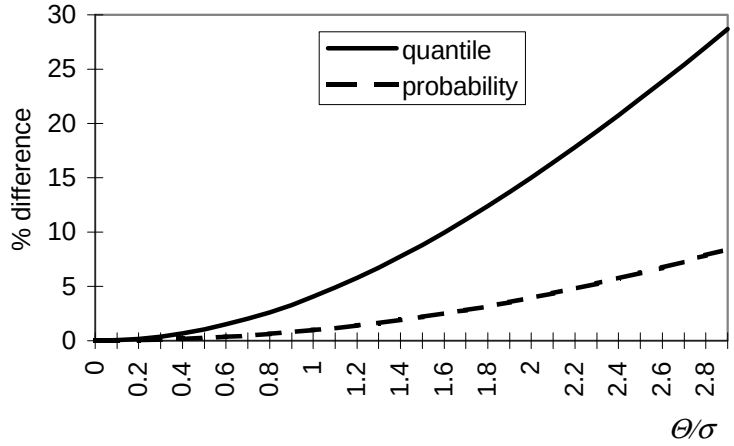

Figure F.1. Percentage difference between quantiles γ and γ_G as well as $(1-\varepsilon)$ and the $(1-\varepsilon')$ given by Equation 4 for various values of Θ/σ. ($\varepsilon = 0.05$.)

Our final conclusion is that the rounding range θ may not be more than one tenth of the standard deviation σ. Rounding to the first digit would correspond to $\theta \approx \sigma$. In plain words: *the measurand may be rounded only up to the second digit of s*. This was our recommendation formulated above. We make this clear by means of our former example where $s = 4.63$. Our conclusion was that θ should be less than $\sigma/10 \approx 0.5$. The simplest way of realizing such a rounding is to round the measurand to its 0.1 digit: we write 58.7 instead of 58.72. It follows from our analysis that we are surely on the safe side since this rounding will not distort confidence intervals.

F.4 Rounding the standard deviation

Let us now turn to the rounding of the standard deviation. One intuitively feels that s should be rounded in the same way as the measurand itself, i.e., we write $s = 4.6$ instead of $s = 4.63$ if the measured value 58.72 was rounded to 58.7. In order to make the reasoning less heuristic, let us model the rounding of s (measured value that estimates σ) in the same way as we did with the measurand. We have then instead of Equation 2:

$$\mathrm{P}\{|\xi| < \gamma(\sigma + r)\} = 1 - \varepsilon\,. \qquad (5)$$

We assume for simplicity that the measurand is not rounded.[a] It is not necessary to repeat the derivations made above because it can simply be seen that Equation 3 is applicable if θ is replaced by $\gamma\theta$ in it. This means that the curves shown in Figure F.1 are now plotted as functions of $\gamma\theta/\sigma$. Consequently, this latter quantity should be less than 0.1, which sets a more severe requirement on the rounding range θ than in case of the measurand.

Let us consider some numerical examples. For a confidence level of 95%, the Gaussian quantile is $\gamma_G = 1.96$. When Equation 5 is solved for $\varepsilon = 0.05$, the resulting γ quantile will be more.

[a] We return to this point later.

Therefore, $\gamma \approx 2$ is a sound underestimation. We have concluded above that $\gamma\theta/\sigma < 0.1$. It follows from this that θ should be less than $\sigma/(10\gamma)$. In the former example, this sets the following condition: $\theta < 0.25$ meaning that σ should be rounded to the 0.1 digit as we stated heuristically.

If we let σ go through an order of magnitude, the upper limit for θ changes also an order of magnitude. For example, for $10 < \sigma < 100$, we get from the above considerations that $0.5 < \theta_{max} < 5$. This means that σ should be rounded to the last digit before the decimal point. For the order of magnitude considered, this requires keeping two valuable digits. Of course, this conclusion is general, it does not depend on the order of magnitude (i.e., $10 < \sigma < 100$) chosen as a numerical example.

It is noted finally that rounding is delicate when $\sigma \approx 10$ because the upper limit of θ is 0.5 for $\gamma = 2$. If we want to keep our results applicable for higher values of the quantile, too, a two-digit rounding may be poor accuracy. For example, for a confidence level of 99.73%, the Gaussian quantile is $\gamma_G = 3$ (the "3σ uncertainty" as it is frequently called), which leads to and upper limit of $\theta_{max} = 0.33$ requiring rounding to the 0.1 digit. Therefore, we prefer, for example, rounding $\sigma = 10.452$ to 10.5 rather than to 10. Due to statistical uncertainties of estimating the standard deviation, a value like $\sigma = 9.752$ could have occurred with the same probability. It is naturally rounded to 9.8, i.e., to the same digit. This approach assures that the last digit is the same for $10 < \sigma$ as for $\sigma > 10$ when $\sigma \approx 10$. If, on the contrary, $\sigma = 10.452$ is rounded to 10 (as to "two valuable digits") while $\sigma = 9.752$ is rounded to 9.8 (again as to "two valuable digits"), this causes an abrupt change in the rounded last digit when σ goes through 10. Such an approach is not only inconsistent but it is also a nasty treatment of the experimental data.

It is a natural question when this exceptional three-digit rounding of σ can be recommended. In our practice, this is the interval $10 < \sigma < 20$ (according to the former numerical example). The reason is that $0.5 < \theta_{max} < 1$ for this range of σ.

We ought to analyze the general case when both the measurand and the standard deviation are rounded. This would require the study of the following equation:

$$P\left\{\left|\xi + r_1\right| < \gamma\left(\sigma + r_2\right)\right\} = 1 - \varepsilon \qquad (6)$$

where r_1 and r_2 are statistically independent random variables uniformly distributed in the range $(-\theta/2, \theta/2)$.[a] We do not go into the details of this because of mathematical complications. It is trivial that the resulting γ values would be more than those presented in Figure F.1, which leads to increasing the severity of the condition set for θ. It is not necessary to perform the rather complicate analysis of Equation 6 because there is a simple way of making plausible that our final conclusion remains valid.

[a] According to our recommendations, the rounded digit is the same for the measurand as for the standard deviation. That is why the range (θ) is the same for r_1 and r_2.

The variance of r_1 is $\theta^2/12$. The total variance of $(\xi + r_1)$ is thus $\sigma^2 + \theta^2/12$. Since θ is less than $\sigma/10$, the latter can not be more than

$$\sigma^2 + \frac{(\sigma/10)^2}{12} = 1.00083\sigma^2$$

which may be taken equal to σ^2 in a very good approximation. Therefore, our reasoning concerning the rounding of σ remains applicable.

APPENDIX G: DERIVATION OF THE STANDARD UNCERTAINTY AND LEVEL OF CONFIDENCE FOR A UNIFORM DISTRIBUTION

The main purpose of this appendix is to show how level of confidence and standard deviation can be derived from any given probability distribution, using a uniform (flat) distribution as an example.

For an assumed uniform probability distribution of possible values of a parameter x between bounds μ-a and μ+a (the mean value of x is μ), the standard deviation σ is a/√3. This can be derived by considering the following:

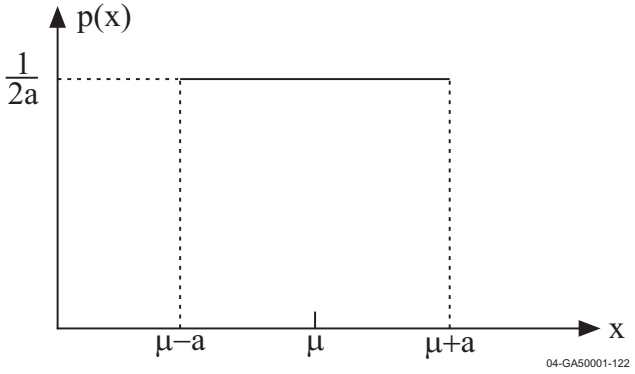

Figure G.1. Probability Density Function p(x) for Variable x, Assumed to Be Uniformly Distributed between μ-a and μ+a.

In order for the total probability over the interval to be 1, the constant value of the uniform probability density is 1/2a from μ-a to μ+a and is zero elsewhere. The variance is therefore

$$\sigma^2(x) = \int_{\text{all } x} (x-\mu)^2 p(x)dx = \int_{\mu-a}^{\mu+a} (x-\mu)^2 \left(\frac{1}{2a}\right)dx .$$

To perform the integration, change variables: Let y = x - μ ; dy = dx. Then

$$\sigma^2(x) = \frac{1}{2a}\int_{-a}^{a} y^2 dy = \frac{1}{2a}\frac{y^3}{3}\bigg|_{-a}^{a} = \frac{1}{2a}\left[\frac{a^3}{3} - \frac{(-a)^3}{3}\right] = \frac{1}{2a}\left(\frac{2a^3}{3}\right) = \frac{a^2}{3} \quad \Rightarrow \quad \sigma(x) = \frac{a}{\sqrt{3}} .$$

Note that the level of confidence that the variable is between μ-σ and μ+σ is not the same for a uniform probability distribution as for a normal probability distribution. For a normal distribution the level of confidence that the variable is between μ-σ and μ+σ is 0.683. However, for a uniform distribution, the level of confidence is (making the substitution $y = x - \mu$)

$$\int_{\mu-\sigma}^{\mu+\sigma} p(x)dx = \int_{-\sigma}^{+\sigma} \frac{1}{2a} dy = \frac{1}{2a} y\Big|_{-a/\sqrt{3}}^{a/\sqrt{3}} = \frac{1}{2a}\left(\frac{a}{\sqrt{3}} - \frac{-a}{\sqrt{3}}\right) = \frac{2a}{2a\sqrt{3}} = \frac{1}{\sqrt{3}} = 0.577 .$$