

Uncertainty Quantification Approaches for Advanced Reactor Analyses

Nuclear Engineering Division

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Abstract

The original approach to nuclear reactor design or safety analyses was to make very conservative modeling assumptions so as to ensure meeting the required safety margins. Traditional regulation, as established by the U. S. Nuclear Regulatory Commission required conservatisms which have subsequently been shown to be excessive. The commission has therefore moved away from excessively conservative evaluations and has determined best-estimate calculations to be an acceptable alternative to conservative models, provided the best-estimate results are accompanied by an uncertainty evaluation which can demonstrate that, when a set of analysis cases which statistically account for uncertainties of all types are generated, there is a 95% probability that at least 95% of the cases meet the safety margins.

To date, nearly all published work addressing uncertainty evaluations of nuclear power plant calculations has focused on light water reactors and on large-break loss-of-coolant accident (LBLOCA) analyses. However, there is nothing in the uncertainty evaluation methodologies that is limited to a specific type of reactor or to specific types of plant scenarios. These same methodologies can be equally well applied to analyses for high-temperature gas-cooled reactors and to liquid metal reactors, and they can be applied to steady-state calculations, operational transients, or severe accident scenarios.

This report reviews and compares both statistical and deterministic uncertainty evaluation approaches. Recommendations are given for selection of an uncertainty methodology and for considerations to be factored into the process of evaluating uncertainties for advanced reactor best-estimate analyses.

UNCERTAINTY QUANTIFICATION APPROACHES FOR ADVANCED REACTOR ANALYSES

1. Introduction

The original approach to nuclear reactor design or safety analyses was to make very conservative modeling assumptions so as to ensure meeting the required safety margins. Traditional regulation, as established by the U S. Nuclear Regulatory Commission (USNRC) required conservatisms which have subsequently been shown to be excessive. The commission has therefore moved away from excessively conservative evaluations and has determined best-estimate calculations to be an acceptable alternative to conservative models, provided the best-estimate results are accompanied by an uncertainty evaluation which can demonstrate that, when a set of analysis cases which statistically account for uncertainties of all types are generated, there is a 95% probability that at least 95% of the cases meet the safety margins [NRC 2007, NRC 1989]. The use of best-estimate results plus uncertainty analysis for demonstrating safety margins for licensing is also supported by the International Atomic Energy Agency [Sollima 2005].

This change in regulatory requirements makes a shift from conservative to best-estimate modeling tools very attractive. Motivating factors for performing best-estimate calculations with uncertainty quantification include [Petruzzi 2005b]:

- More realistic evaluation of plant safety margins for licensing
- Improvements in emergency response when the response can be based on more realistic evaluations
- Identification of parameters which most impact output uncertainty, thus guiding prioritization of model development and future experiments.

While there is general agreement as to the distinction between conservative and best-estimate models, there is no universally accepted approach to bounding and quantifying the effect of uncertainties on analysis results.

The types of sources of uncertainty which can affect analysis results are almost as diverse as the perspectives of the analysts attempting to account for uncertainties (see, for example, [Aragones 2005], [CSNI 2005], [Fanning 2008], [Petruzzi 2008], [Petruzzi 2005b]). Major categories are:

- Modeling uncertainties, which can include modeling assumptions and simplifications, solution schemes, model options,
- Experimental data uncertainties, including uncertainties in data libraries, instrument errors, material properties measurements,
- Plant data uncertainties, such as uncertainty in instrument response, unavailability of measurements for some plant parameters, manufacturing tolerances on plant components, or variations in reactor operating conditions,

- Representation/simulation uncertainties, including approximations in the representation of the facility geometry, mesh size, imperfect knowledge of initial and boundary conditions,
- Human reliability, such as variation in development of nodalization, different interpretations of the information supplied for the problem to be analyzed, variations in judgment for accepting the steady-state results upon which the transient will be based, differences in interpretation of the results for the transient and subsequent refinement of the solution, plus outright errors.

Many of these types of uncertainties (e.g., experimental data uncertainties, human reliability) are common to all modeling efforts, regardless of the type of physics being modeled, while others are specific to the physical system. In thermal-hydraulic models, for example [D’Auria 2005], uncertainties are introduced by the approximate nature of the conservation equations (not all interactions between phases are included) and by commonly used approximations such as assigning the same velocity to different fields of the same phase (for example, liquid film and liquid droplets), geometry averaging at the cross-section scale (thus ignoring any velocity profile), and geometry averaging at the volume scale (one velocity vector is associated with a hydraulic mesh point for each phase). In addition, empirical correlations are typically used to close the thermal-hydraulic balance equations; these correlations introduce uncertainty due to the scatter and error in the data upon which they are based, due to the fact that most correlations are developed for steady-state, fully developed flow (conditions which do not apply over much of the range of interest of the analysis), and due to the fact that their range of validity often does not encompass all of the problem being analyzed.

To date, nearly all published work addressing uncertainty evaluations of nuclear power plant calculations has focused on light water reactors and on large-break loss-of-coolant accident (LBLOCA) analyses (two exceptions are [Morris 2007] and [Morris 1981], which discuss uncertainty analyses of liquid metal reactor (LMR) transients). However, as demonstrated by the two Morris papers, there is nothing in the uncertainty evaluation methodologies that is limited to a specific type of reactor or to specific types of plant scenarios. These same methodologies can be equally well applied to analyses for high-temperature gas-cooled reactors (HTGR) and to LMR’s, and they can be applied to steady-state calculations, operational transients, or severe accident scenarios.

2. Classification of Uncertainty Quantification Methodologies

The term “uncertainty analysis” is not always defined consistently by authors in the field. In particular, there is sometimes confusion as to the distinctions between uncertainty analysis and the related area of sensitivity analysis. Most authors classify uncertainty analysis of a modeling evaluation as the determination of the amount of imprecision present in the predicted output parameters of interest, while sensitivity analysis is the means of identifying the contribution to this imprecision made by the uncertainty in each input parameter to the model [Saltelli 2000, Ionescu-Bujor 2004]. If a sensitivity analysis is performed first and identifies the dependence, or sensitivity, of a given output parameter on the variation in each uncertain input parameter, then these sensitivities, once known, can be combined in an uncertainty analysis to predict the overall uncertainty in the output parameter. By contrast, if an uncertainty analysis is performed first, it may

or may not be possible to estimate the sensitivities of the output parameters to individual input parameters, depending upon how the uncertainty analysis is conducted.

Most methods for performing uncertainty analyses on a physical model involve propagating uncertainties in the model input parameters through the model in order to quantify the resulting uncertainty in the model responses (outputs) which are of interest. These methods fall into one of two categories: statistical or deterministic. There is an additional approach based upon evaluation of output uncertainties; this method is briefly described in Sec. 6.

The majority of techniques which evaluate uncertainties in model output parameter predictions are statistical. These characterize the uncertainties in output parameters by estimating statistical quantities such as the mean value and variance of an output parameter before evaluating the sensitivity of the parameter to variation in each individual input parameter [Cacuci 2004].

By contrast, deterministic methods first evaluate the sensitivity of an output parameter to each input parameter, then use an approach such as the method of moments to linearly combine the sensitivities and characterize the parameter uncertainty by estimating the mean value and variance. Deterministic methods compute local partial derivatives of a particular system response (or output) with respect to each input parameter of interest; these local partial derivatives are the local sensitivities of the response [Ionescu-Bujor 2004].

Statistical and deterministic methods share some common characteristics. Both propagate input uncertainties to determine uncertainties in output parameters of interest. With both approaches, it is necessary to assign a range of uncertainty and a distribution function to each input parameter which is included in the evaluation. Because both rely upon results from propagating input parameter values through the analysis model, both introduce uncertainty from the model limitations, in addition to the uncertainties in the input parameters [CSNI 2007]. This added uncertainty could be separately quantified only by writing several different versions of the code, each with different modeling assumptions, then applying uncertainty analysis to each model version.

There are also significant differences between statistical and deterministic approaches. As a practical matter, statistical methods usually assign uncertainties to only a limited number of input parameters, so that application of a statistical method is preceded by a determination of which input parameters are the most influential on the model responses of interest when uncertainties are considered. By contrast, deterministic methods establish sensitivities for all input parameters; in fact, one application of deterministic methods is to generate sensitivities which can be used to identify those input parameters which are of greatest importance to include in a model uncertainty analysis using a statistical method. The number of uncertain input parameters which is included in an analysis is often limited by the number of parameters for which the range of uncertainty and a distribution function can be established either by experimental data or by expert judgment.

Statistical methods are much easier and cheaper to develop than deterministic methods and are generally easier to use, but they can require many repetitions, or realizations, of the original high-fidelity model or a lower-fidelity surrogate for the model. Since

licensing requires uncertainty bounds to a specified probability and confidence level, the number of runs required to establish an acceptable uncertainty bound on best-estimate calculations is determined by the sample size needed to set the required tolerance limits [CSNI 2007, Wilks 1941, DeVictor 2005], as discussed in more detail below in Sec. 3.1.2.

3. Statistical Methods

As mentioned above, most approaches for quantifying uncertainties in best-estimate model predictions are based on statistical methods. The most commonly used of these are described briefly below.

3.1 Sampling and Propagation of Input Uncertainties

This is the most basic and robust approach to evaluating uncertainties. Several methods, discussed below, use some variation of this approach. The process begins by identifying the dominant uncertain input parameters to be used in the analysis and defining a probability distribution function (PDF) for the uncertainty in each input parameter. Ideally, the function is determined from representative experimental data; however, in practice, such data are often incomplete or unavailable. Frequently, all that is available for an input parameter is an experimentally determined range of uncertainty; in this case, it is common practice to assume a uniform distribution for the PDF [Chojnacki 2005b]. If no experimental data are available, expert judgment must be used to estimate an uncertainty range. This is a fallback position which is problematic for severe accident analyses and licensing evaluations [CSNI 2007]; however, in practice, it is difficult to avoid using expert judgment for at least some of the basis for the PDF's for uncertain input parameters. Information on interdependencies among the input parameters should be used when available, but it is often the case that little or no dependency information is known, and so the input parameters are assumed to be independent [Chojnacki 2005b].

The set of uncertain input parameters is then sampled N times; several types of sampling techniques may be used, as discussed below. Then N runs are made with the model code, each run using a different one of the N sets of input parameters generated by the sampling. These N runs produce a sampling of the output parameters of interest, from which the mean and variance of the distribution of each output quantity may be estimated [DeVictor 2005, Chojnacki 2005a].

3.1.1 Sampling Techniques

There are several techniques commonly used to sample input parameters for uncertainty analyses. These are described below.

Simple random sampling. This is the simplest of the sampling techniques, and probably the most widely used. A sample is generated independently for each uncertain parameter according to the parameter probability distribution. This method is preferred when the uncertainty in the model output parameters is significantly impacted by the uncertainty in a number of the input parameters. Because it is purely random, statistical estimation methods can be applied to estimate the distributions of the output parameters. The main drawback to this technique is that often the number of samples drawn, and therefore the number of runs of the model code, must be quite large in order to give an acceptably

small variance, and this can be quite expensive if the model code is a high-fidelity, CPU-intensive code [Chojnacki 2005a, DeVactor 2005].

Computational costs can be lowered if sampling is done with a variance reduction technique, rather than with simple random sampling. The two most commonly used of these are stratified sampling and Latin Hypercube sampling.

Stratified sampling. In this approach [Iman 1982], the probability distribution for each uncertain input parameter is divided into N strata of equal marginal probability, and one sample is drawn from each stratum for each input parameter. This technique results in a more even distribution of sampled values throughout the range of each uncertain parameter and prevents the clustering of sample values which can result if a moderate number of random samples is taken. Stratified sampling thus generally reduces the number of samples required for good statistics.

Latin Hypercube sampling. This technique [Iman 1982, Helton 2005] improves upon stratified sampling, at a slight additional computational cost. First, a stratified sampling is performed, then the samples for each input parameter are permuted using some method of randomization. The first set of sampled input parameters is then made up of the first value for each input parameter in the permuted order, the second set is made up of the second value for each input parameter in the permuted order, etc. This approach assumes that the input variables are uncorrelated. If there is a known correlation among the input variables, the correlation matrix for the parameters, rather than a randomization scheme, can be used to permute the order of the stratified samples [Chojnacki 2005a, Iman 1982]. Generally, Latin Hypercube sampling produces a more accurate estimate of the output PDF than does random sampling, if the same number of samples is drawn when applying each technique.

3.1.2 Number of Samples Required

Because simple random sampling samples the uncertain input variables one at a time and runs the model code once for each sampling, it can require thousands of code runs to generate good statistics. This is a parametric approach, since the number of samples taken is dependent upon the number of input parameters to be sampled. The number of random samples, and therefore code runs, can be substantially reduced if a nonparametric approach is used instead. In this case, all uncertain parameters are sampled simultaneously, and the number of samples is decoupled from the number of uncertain input parameters.

The criterion for setting the number of samples taken when the nonparametric approach is used is to take at least as many samples as will ensure that, when the model code is run for each of these samples and a set of values of the output quantity of interest is generated, this set of values meets the tolerance limit required for that output quantity with a specified confidence level [Muftuoglu 2007, Glaeser 2008, CSNI 2007]. The method for determining the minimum sample size for specified upper and/or lower tolerance limits was developed by Wilks [Wilks 1941] and extended to the multivariate case by Wald [Wald 1943] and Tukey [Tukey 1947]. Somerville [Somerville 1958] generalized Wilks' approach to establish the minimum number of samples required so that the set of response values lying between the r^{th} smallest and the s^{th} largest of all the

response values meets the required tolerance limit. In the case of uncertainty estimates for best-estimate calculations, $r=0$, and Wilks' theorem provides an upper bound on the calculational uncertainty [Cadet-Mercier 2002]. The case of $s=1$, i.e., the Wilks formula at the first order, gives the minimum number N of samples required so that all N response values meet the tolerance limit with the specified confidence level, but this result often produces an upper bound value that is more conservative than desired. The BEMUSE analysis of the LOFT L2-5 test [CSNI 2007] indicated that applying the Wilks formula to the 4th or 5th order usually produced a more satisfactory tolerance, at the price of some additional code runs. Thus, if N runs are performed using N samples of the input parameters and the resulting values of Y , the output parameter of interest, are ordered, with $Y(1)<Y(2)<...<Y(N)$, then, for a tolerance limit of the 95% percentile at a confidence level of 95% [NRC 2007, NRC 1989], the first four orders of Wilks' method give upper bounds as follows:

- $Y(N)$, with $N = 59$: Wilks at the first order ($r = 1$).
- $Y(N-1)$, with $N = 93$: Wilks at the second order ($r = 2$).
- $Y(N-2)$, with $N = 124$: Wilks at the third order ($r = 3$).
- $Y(N-3)$, with $N = 153$: Wilks at the fourth order ($r = 4$), etc.

Thus, taking greater numbers of samples can reduce the maximum value Y that satisfies the USNRC 95/95 criterion [CSNI 2007].

3.1.3 Monte Carlo Method

This is the simplest technique by which to propagate input parameter uncertainties. Parametric random sampling of the input parameters is used, and for each set of input parameters, the full, high-fidelity model is run to produce samples of the output responses of interest. This method has the drawback of often being very expensive to apply, but it is one of the most straightforward and therefore economical to implement, and all statistical evaluation methods may be rigorously used on the resulting sample space [Devictor 2005]. It will also correctly account for any discontinuities and transitions between physical regimes, can incorporate correlations between input parameters, and works well for input parameters with large uncertainty ranges [Gorham 1993].

3.1.4 GRS and IPSN

These approaches also use the full numerical/computational model, but instead of parametric sampling, they apply nonparametric simple random sampling in the form of the Wilks method [Glaeser 2008]. Thus, the number of code runs is much reduced over that required by the Monte Carlo method. Both approaches address the effects of uncertainties in the code models, boundary and initial conditions, and the solution algorithms upon calculation results. The GRS (Gesellschaft für Anlagen- und Reaktorsicherheit) method was developed in Germany and is used with several versions of the ATHLET best-estimate thermal-hydraulics code [Austregesilo 2005, Petruzzi 2007], while the IPSN (Institut de Protection et de Sureté Nucléaire) method is French and is applied to the CATHARE V2.5 best-estimate thermal-hydraulics code [Petruzzi 2007].

3.1.5 ENUSA

The ENUSA method was developed in Spain and is very similar to the GRS and IPSN methods. It propagates input uncertainties by running the full, high-fidelity model and uses nonparametric sampling of the uncertain input parameters, with the number of samples taken determined by the Wilks method. It differs from the GRS and IPSN approaches in that it selects the subset of uncertain input parameters to be sampled by applying the Phenomena Identification and Ranking Table process, a subjective approach which uses expert opinion to rank the dominant phenomena in the transient of interest [Boyack 1990]. This method is distinguished from the USNRC's CSAU method (see Sec. 4) only by 1) the use of a high-fidelity model instead of a response surface (see Sec. 3.1.6) and 2) by using nonparametric sampling [Petruzzi 2007].

3.1.6 Surrogate models

For complex models, using the full-fidelity model to propagate each set of sampled uncertain input parameters can be prohibitively expensive. It is therefore sometimes necessary to replace the full complex model with a surrogate model. The surrogate model represents the same physical situation as the full model but is derived with simplifying assumptions, resulting in a model which runs much more quickly than the original code, at the price of reduced accuracy and range of applicability. Each set of sampled input parameters is then propagated through the surrogate model, and the resulting responses are used to estimate the uncertainty distribution for the output of interest.

There are several possibilities for surrogate models:

Simplified modeling. The detailed code model may simply be replaced by a model which makes simplifying assumptions about the problem to be analyzed. This approach was used by Morris [Morris 2007] in a study of uncertainty in best-estimate analyses of three unprotected fast reactor accident scenarios. Instead of using the SAS4A/SASSYS high-fidelity severe accident code [Cahalan 1994], Morris substituted the MATWS program [Cahalan 2002], which coupled the SAS4A/SASSYS point-kinetics model with a simplified modeling of the reactor thermal-hydraulics. This substitution allowed him to use the Monte Carlo approach to estimating uncertainty and make thousands of code runs to propagate the input uncertainties while still keeping the required computing time to a reasonable amount.

Response surfaces. The response surface approach generates a simplified model using a three-step approach [Morris 1981]:

- 1) The input parameters are evaluated to determine those which have the greatest influence on the model response(s) of interest, and from these a set is chosen to use as the uncertain input parameters.
- 2) The responses of the full-fidelity model are evaluated over a range of samples of the input parameter space.
- 3) These responses are used to generate a linear parametric expression which adequately approximates the model responses over the range of interest of the uncertain input variables. This expression constitutes the response surface.

The response surface thus represents the full-fidelity model as an interpolation of a few solutions to the complex model generated by sampling the uncertainty in a few dominant input parameters. This approach assumes that the code responses behave smoothly over the range of interest. It also requires having a means to make a judicious selection of the dominant uncertain input parameters [Morris 2008]. If the complex model is sufficiently well-behaved, use of a response surface can produce accurate results while being much less expensive to run repeatedly with a set of sampled input parameters than would be the case with the full-fidelity model.

Stochastic Finite Element Methods (SFEM). These methods effectively create a higher order response surface surrogate model using finite elements as the approximation functions for the parametric expression which approximates the full model responses. They are more accurate than linear models and more computationally efficient than running the high-fidelity model, but the number of basis functions required expands rapidly as the dimension of the system of interest increases. They are most efficiently used if a sensitivity analysis is performed first to serve as a basis for selecting the subset of uncertain input parameters to be sampled and used to generate the higher-order response model [Roderick 2008, Fanning 2008].

Neural networks. This method has been proposed by Martinez [Martinez 2005]. A learning set of surrogate models is built by sampling the full model using either simple random sampling or Latin Hypercube sampling.

3.1.7 Dempster-Shafer

Dempster-Shafer uncertainty methodology is an extension of the classical Monte Carlo approach that provides one way of addressing lack of knowledge about the true distribution of an uncertain output parameter. This theory provides a means for assigning probability distribution functions to some uncertain input parameters about which sufficient information is available and possibility functions to other parameters when the information available can be associated only with a fuzzy number. The combined use of PDF's and fuzzy numbers produces a plausibility distribution which gives accurate knowledge about the lower and upper probabilities of the uncertain parameter. The uncertainty assigned to the parameter of interest is represented by the lower and upper probabilities, and the difference between these probabilities is a measure of the lack of knowledge modeled by the fuzzy numbers [Chojnacki 2005b].

3.2 Variance-Based Methods

These methods use variance ratios to assess the importance of an input parameter in contributing to the uncertainty of a model output parameter. An example of these is the Fourier Amplitude Sensitivity Test, which is based on using a Fourier series to approximate the full model. These methods have the advantage that they do not assume a linear relationship between the model input parameters and the model responses. However, they are computationally expensive, requiring many thousands of realizations if the problem involves more than a few input parameters. Knowledge of the inverse cumulative distribution function for the PDF of each uncertain input parameter is also required [Lu 2001, Cacuci 2004].

3.3 First-Order and Second-Order Reliability Methods (FORM and SORM)

These methods focus specifically on estimating a probability of failure. They make use of optimization algorithms which identify the most likely point of failure within the space of uncertain parameters, then approximate the probability of failure by fitting a first-order (linear) or second-order (quadratic) surface at that point. They can be much faster than sampling-based methods for determining the particular mode of failure of the system under consideration. With respect to severe accident and licensing analyses, these methods are primarily suited to structural mechanics evaluations. Structural mechanics analyses are interested in failure probabilities, not just uncertainties, so behavior in the tail of a distribution function is of the greatest interest. The FORM/SORM methods are therefore appropriate [DeVictor 2005, Cacuci 2004].

4. The CSAU Method: The Methodology Approved for Licensing of Operating Reactors

CSAU, or the Code Scaling, Applicability, and Uncertainty evaluation method, is a complete specification of steps to prepare for and execute an uncertainty evaluation. Because CSAU, which employs a statistical uncertainty analysis approach, covers not only the actual uncertainty evaluation but also steps leading to performing both the scenario calculations and the uncertainty assessment, it is discussed separately from the other statistical methods. Fourteen steps, which are grouped into three elements, are specified by the CSAU method. It was developed by the USNRC for evaluating uncertainty in best-estimate code calculations performed for design and safety analyses of light water reactors [Boyack 1990, Lellouche 1990], but there is really nothing in the method specific to a particular category of reactor; in fact, the approach could be applied to calculations for systems other than nuclear reactors. The method should require little modification to make it applicable to HTGR and LMR best-estimate calculations. Although a common application of this method is determination of the uncertainties in LBLOCA analyses, the approach can be applied to any steady-state or transient analyses for which sufficient experimental data are available.

The three elements of the CSAU method, and the steps they cover, are as follows [Boyack 1990]:

- 1) Requirements and code capabilities. This element encompasses the first six steps of the CSAU method, namely
 - i. Specify a scenario and thus determine the parameters to be evaluated.
 - ii. Select the nuclear power plant for which calculations are to be performed.
 - iii. Identify and rank the physical processes involved. In this step, the dominant phenomena which drive the scenario are identified by expert judgment, then ranked and summarized in a Phenomena Identification and Ranking Table (PIRT). From these rankings, the actual relevant model input parameters to which uncertainties must be assigned are determined.
 - iv. Select a frozen version of an analysis code.

- v. Provide code documentation.
 - vi. Determine the applicability of the code to the scenario by comparing the modeling requirements established in steps (i) through (iii) against the information on the code capabilities assembled in steps (iv) and (v).
- 2) Assessment and Ranging of Parameters. The next four steps in the process are grouped into this element and are
- vii. Establish an assessment matrix. In this step, test data are assembled from both separate effects tests and integral tests to be used to evaluate if the code can accurately model the phenomena determined in step (iii) and to address any code shortcomings identified in step (vi).
 - viii. Generate the nodalization of the plant that will be used by the analysis code.
 - ix. Determine code and experiment accuracy by using the code selected in step (iv) with the nodalization established in step (viii) to simulate the experiments from which the data assembled in step (vii) were collected. Any biases which must be included to compensate for deficiencies in the code models will be determined in this step also.
 - x. Determine effects of scale, i.e., verify that the best-estimate code can scale up phenomena measured in test facilities to the same phenomena in the full-size plant.
- 3) Sensitivity and Uncertainty Analyses. In this element, the actual uncertainty and sensitivity analyses are performed through the final four steps:
- xi. Determine the effect of the reactor input parameters and state. This step quantifies how uncertainty in the reactor state and operating conditions at the start of the transient affect the simulation.
 - xii. Perform nuclear power plant sensitivity calculations, to determine the effect of variability in individual parameters on the dominant safety parameters.
 - xiii. Combine biases and uncertainties established in earlier steps into an assessment of total uncertainty, justifying the particular method used to perform the combination. This step combines the uncertainties of each of the processes identified in step (iii) to estimate the total uncertainty in the calculated parameters.
 - xiv. Determine total uncertainty. Use the output of step (xiii) to make a statement of total uncertainty for the code.

The USNRC requires that an uncertainty evaluation of a best-estimate calculation of any output parameter identify a bounding value of that parameter that covers 95% or more of the domain of that parameter with a 95% confidence level. In other words, there is a 95% probability that at least 95% of the values within the uncertainty range of the output parameter fall at or below the bounding value identified through the uncertainty analysis. This 95/95 criterion is considered sufficiently conservative by the USNRC for LBLOCA analyses for light water reactors [Martin 2005, Muftuoglu 2007, Boyack 1990]. This is

the criterion which must be met by the overall uncertainty determined using the CSAU method.

As described above, the original implementation of the CSAU approach determined the set of uncertain input parameters to be considered by applying the PIRT process, then used simple random sampling to sample the uncertain input parameters and propagated these uncertainties through a surrogate model in the form of a response surface [Boyack 1990]. However, these are not fundamental limitations of the method. For example, AREVA has applied the fourteen steps of the CSAU approach to several LBLOCA analyses for pressurized water reactors, using the S-RELAP5 code; however, instead of using response surfaces and simple random sampling, AREVA substituted the GRS method, which made use of the full-fidelity model and nonparametric sampling (see Sec. 3.1.4). This modification to the original CSAU methodology has been approved by the USNRC for licensing of fuel reloads [Martin 2005].

The CSAU approach has been demonstrated by Westinghouse [Young 1998], as well as by AREVA [Martin 2005]. It has been applied to updates of the Final Safety Analysis Reports of about twenty U. S. light water reactors by Westinghouse [Glaeser 2002, IAEA 2003], to the AP600 LBLOCA analysis [Glaeser 2002], and to boiling water reactor licensing in Japan [IAEA 2003].

5. Deterministic Methods

Deterministic methods are used to find the local sensitivity of a particular output parameter to variations in the input parameters to the analysis model. The methods assume that the sensitivity of the output parameter depends linearly on the variation in each input parameter. Once the local sensitivities have been found, the mean value and variance of the output parameter can be determined from application of the Propagation of Errors method to express the value of the output parameter as a linear function of the sensitivities and the uncertainties in the input parameters.

There are two deterministic methods which have been applied to large-scale, complex systems: the Forward Sensitivity Analysis Procedure and the Adjoint Sensitivity Analysis Procedure, sometimes called differential sensitivity theory. These two methods will be briefly described.

5.1 Forward Sensitivity Analysis Procedure

This method begins with a system of linear equations,

$$\mathbf{Ax} = \mathbf{b}, \quad (1)$$

where the components of the $n \times n$ matrix \mathbf{A} and the vector \mathbf{b} are parameters with associated uncertainties. The responses, or output quantities, of this system are scalar quantities of the form

$$R = \mathbf{cx}, \quad (2)$$

where the components of \mathbf{c} are also parameters with associated uncertainties. The sensitivity of a response R , δR , to variation in any of the uncertain parameters can be determined by perturbing Eq. (1) around the best-estimate, or nominal, system of equations and substituting the solution into the perturbation of Eq. (2) around the best-estimate

response R^0 . However, this approach requires inverting a new matrix, $\mathbf{A}^0 + \delta\mathbf{A}$, for each variation of a parameter. A less burdensome approach is to solve the Forward Sensitivity System,

$$\mathbf{A}^0(\delta\mathbf{x}) = \delta\mathbf{b} - (\delta\mathbf{A})\mathbf{x}^0 \quad (3)$$

for $\delta\mathbf{x}$ and calculate the sensitivity of R to the perturbed parameter as

$$\delta R = \mathbf{c}^0(\delta\mathbf{x}) + (\delta\mathbf{c})\mathbf{x}^0. \quad (4)$$

This approach requires inversion (or iterative solution) only of the same matrix \mathbf{A}^0 which must be inverted to generate the best-estimate solution anyway. However, to determine the local sensitivity of each input parameter, solution of the differentiated system, Eq. (3), must be repeated each time an input parameter is perturbed. Thus, the Forward Sensitivity Analysis Procedure is a feasible approach only if the number of system responses of interest exceeds the number of uncertain input parameters, which is rarely the case in practice. Also, since Eq. (3) is linear, the method is accurate only for small perturbations of the input parameters. For further details on the Forward Sensitivity Analysis Procedure, see [Cacuci 2005, Ionescu-Bujor 2004, Ionescu-Bujor 2005].

5.2 Adjoint Sensitivity Analysis Procedure

The Adjoint Sensitivity Analysis Procedure (ASAP) is an alternative to the Forward Sensitivity Analysis Procedure and avoids having to repeatedly invert matrix \mathbf{A}^0 in Eq. (3) above. The method is derived by forming the inner product of Eq. (3) with an n-component vector $\boldsymbol{\psi}$, giving

$$\langle \boldsymbol{\psi}, \mathbf{A}^0(\delta\mathbf{x}) \rangle = \langle \boldsymbol{\psi}, \delta\mathbf{b} - (\delta\mathbf{A})\mathbf{x}^0 \rangle. \quad (5)$$

Transposing the left side of Eq. (5) gives

$$\langle \boldsymbol{\psi}, \mathbf{A}^0(\delta\mathbf{x}) \rangle = \langle \delta\mathbf{x}, (\mathbf{A}^0)^+ \boldsymbol{\psi} \rangle. \quad (6)$$

Since $\boldsymbol{\psi}$ is arbitrary, it can be set by identifying the right-hand side of Eq. (6) with the first term on the right side of Eq. (4), giving

$$(\mathbf{A}^0)^+ \boldsymbol{\psi} = \mathbf{c}^0. \quad (7)$$

Combining Eqs. (3) through (7) then gives

$$\langle \boldsymbol{\psi}, \delta\mathbf{b} - (\delta\mathbf{A})\mathbf{x}^0 \rangle = \langle \delta\mathbf{x}, (\mathbf{A}^0)^+ \boldsymbol{\psi} \rangle = \mathbf{c}^0(\delta\mathbf{x}) = \delta R - (\delta\mathbf{c})\mathbf{x}^0,$$

which can be rearranged to give

$$\delta R = (\delta\mathbf{c})\mathbf{x}^0 + \langle \boldsymbol{\psi}, \delta\mathbf{b} - (\delta\mathbf{A})\mathbf{x}^0 \rangle. \quad (8)$$

The vector $\boldsymbol{\psi}$ is the adjoint function which solves the adjoint sensitivity system, Eq. (7). Since Eq. (7) is independent of the input parameter uncertainties ($\delta\mathbf{A}$) and $\delta\mathbf{b}$ and is linear in $\boldsymbol{\psi}$, the adjoint function can be found by solving Eq. (7) just once. The local sensitivity of the system response, δR , to all system input parameters can then be found by solving Eq. (8), which is a much less costly calculation than inverting \mathbf{A}^0 or repeatedly solving Eqs. (1) and (2) for multiple samples of the uncertain input parameters. The adjoint equations must be solved backwards in time, starting from the solution to the original system of equations [Cacuci 2004, Ounsy 1994, Ionescu-Bujor 2000]. The sensi-

tivities thus determined can then be used to perform an uncertainty analysis of the system.

The ASAP has been implemented and tested in the light water reactor analysis codes RELAP5/MOD3.2 [Cacuci 2000], CATHARE [Ounsy 1994], and ATHLET [Glaeser 2002], all of which couple point kinetics and thermal-hydraulics. It has also been applied to a simple model of loss of decay heat in a gas-cooled fast reactor [Morris 1981]. While these implementations demonstrated that the ASAP can be used for sensitivity and uncertainty analyses, they also brought out some drawbacks to the method:

- 1) Since the adjoint is a function of the model response R , a new adjoint must be developed for each model response parameter for which uncertainty is to be characterized.
- 2) Development of an adjoint set of equations to be added to an existing code is usually difficult, expensive, and time-consuming [Glaeser 2002, Cacuci 2005]. Even when the forward equations and adjoint equations are developed and coded simultaneously, the addition of the adjoint equations adds extensively to the development effort [Morris 1981].
- 3) The adjoint produces a linear approximation to the output parameter probability distribution function; for thermal-hydraulic problems, the true distribution may be significantly non-linear [Morris 2008].
- 4) If the range of responses of interest expands after the main code development effort, a large amount of additional development effort must be expended to develop additional adjoint functions. Also, if the forward model is evolving, the associated adjoint models must be redeveloped to account for the evolution of the forward model.

The conclusion is that, while the ASAP has some attractive features, the drawbacks of this approach are significant and the method requires further development.

6. Method of Extrapolation of Output Uncertainties

As mentioned in Sec. 2, one uncertainty analysis method (the Uncertainty Method based upon Accuracy Extrapolation “embedded” into the code with the Capability of Internal Assessment of Uncertainty, or UMAE-CIAU [Petruzzi 2007, Petruzzi 2008, Petruzzi 2005b]) extrapolates output uncertainties by comparing best-estimate results against relevant experimental data from small-scale single-effects test facilities, integral test facilities, and, if available, the power plant. This approach requires an extensive set of data which covers the full range of interest and is considered both representative of the problem being analyzed and reliable, and so the method is appropriate primarily to steady-state scenarios and operational transients and is not readily applicable to severe accident analysis. It also cannot be used to determine the sensitivity of a model response to the uncertainty in a particular input parameter. However, the method has the advantage that it does not require determination of either uncertainty ranges or distribution functions for uncertain input parameters, nor does it require selection of a set of uncertain parameters to be considered. Thus, the need for application of engineering judgment is largely circumvented and is limited to the judgment required in selecting the experiments and data against which to compare model responses.

7. Comparisons of Uncertainty Methodologies

A summary of the strengths and weaknesses of the various methodologies discussed in Secs. 3-6 is given below in Table 1. As can be seen by examining the table, all methods have both strengths and weaknesses, and no one method stands out as the consensus choice for uncertainty evaluations. The selection of an uncertainty evaluation method for a particular best-estimate analysis must take into account several factors:

- The tradeoff between the expense of using the full high-fidelity model equations compared with the loss of accuracy incurred when a surrogate model, such as response surfaces, is used. For modeling of a sufficiently complex system, the high-fidelity model may simply take too long, using the available computer hardware, to run multiple times for a statistical uncertainty evaluation, but the system must also be evaluated to determine if it is sufficiently well-behaved in the range of interest so that it can be represented by a surrogate model. It should also be remembered that the use of high-fidelity models becomes increasingly attractive as faster computers with larger memory and improved reliability become available. Given the rate at which computer hardware has improved for a number of years, it is prudent to consider whether the time and effort required for development and implementation of a sufficiently accurate surrogate for a particular model may not be better spent in addressing considerations which will not benefit from hardware improvements, such as methods for determining uncertainty distributions for input parameters and for identifying dominant uncertain input parameters.
- The level of difficulty in implementing an uncertainty evaluation method and the flexibility of the method once implemented. The success of the GRS and similar implementations of the simple Monte Carlo approach, coupled with the Wilks method (see Secs. 3.1.4 and 4), demonstrates the benefits of an approach that is simple to implement and flexible to use. By contrast, adjoint procedures for sensitivity analysis have been under development for about thirty years and have yet to gain much acceptance; as discussed in Sec. 5.2, the ASAP is both expensive to develop, even if developed in parallel with the original model, and it is inflexible in that a new adjoint must be developed for each model response of interest or if the original model is changed.
- The expense of applying an uncertainty evaluation method once it is in place. If the original high-fidelity model is not likely to change for a long period of time and the model responses of interest are not expected to change, an evaluation method, such as ASAP, that is more difficult to implement but inexpensive to run once it is developed may be the best choice.
- Deterministic approach or statistical approach. The deterministic methods provide insight into which uncertain input parameters most influence the model responses of interest. However, these methods add another layer of complexity in that the uncertainty analysis can be performed only once a sensitivity analysis is

Table 1. Comparison of Strengths and Weaknesses of Uncertainty Analysis Methods

Method	Easy to implement	Number of code runs	Cost per run	Selection of uncertain input parameters	Flexible to add new model responses?	Flexible to model changes?	Accuracy
Statistical							
Monte Carlo	Yes	Parametric - may be large	Full model - may be high	Data, experts	Yes	Yes	Accuracy of input uncertainties
GRS/IPSN	Yes	Nonparametric (Wilks)	Full model - may be high	Data, experts	Yes	Yes	Accuracy of input uncertainties
ENUSA	Yes	Nonparametric (Wilks)	Full model - may be high	PIRT	Yes	Yes	Accuracy of input uncertainties
Simplified modeling	Additional model devel.	Can use nonparametric	Low	Data, experts	Redevelopment of simplified model		< full model
Response surfaces	Resp. surface development	Can use nonparametric	Low	Data, experts	Redevelopment of response surface		< full model, no discontinuities
SFEM	Additional model devel.	Can use nonparametric	Low for small no. of inputs	Data, experts	Redevelopment of approximation model		< full model
Dempster-Shafer	Yes	Parametric - may be large	Full model - may be high	Data, experts	Yes	Yes	Accuracy of input uncertainties
FAST	Fourier series expansion	Increases rapidly with no. of input parameters	May be high	Data, experts	Yes	Yes	Accuracy of input uncertainties
Original CSAU	Resp. surface development	Parametric - may be large	Low	PIRT	Redevelopment of response surface		Less than the full model
AREVA CSAU	Yes	Nonparametric (Wilks)	Full model - may be high	PIRT	Yes	Yes	Accuracy of input uncertainties
Deterministic							
FSAP	Yes	One per input parameter variation for each response	Full model - may be high	Data, experts	Yes	Yes	Assumes small input uncertainties, no discontinuities
ASAP	Adjoint development	One per input parameter for each response	Adjoint model < full model	None required	New adjoint must be developed.		Assumes small input uncertainties, no discontinuities
UMAE-CIAU	Yes	One	Full model - may be high	None required	Possible extensive additional experimental data	Yes	Dependent on quality of experimental data

completed, and the analyst must then decide on a suitable method for combining the sensitivities in order to execute the uncertainty analysis.

- Suitability of linear approximation. Methods such as response surface and ASAP represent the model response distribution linearly; consideration needs to be given to the physics of the system to determine if it is appropriate to approximate the distribution as a linear function.

Given these considerations, the best choice for many evaluations would be propagating input uncertainties using the full model and nonparametric sampling, since this approach is straightforward to implement and run, gives good accuracy, and, for many scenario analyses, can be run in a reasonable amount of time, due to the use of order statistics (Wilks method). If running times are excessive for the scenario of interest, either due to number of realizations required or time to run one realization of the full model, then the option of using a surrogate model should be considered. If the dimension of the system of interest is not too large, the SFEM probably will provide the most accurate results of the various types of surrogate models, since it is nonlinear.

8. Considerations in Performing Uncertainty Evaluations

Most of the uncertainty analysis methods discussed above can be applied to transient analyses without regard to whether the system being analyzed involves a particular area of physics. In fact, most of the methods have been used to evaluate uncertainties in best-estimate modeling of light water reactor LBLOCA's, which couples reactor physics and thermal-hydraulics. An exception to this are the FORM/SORM methods, which are most suitable to problems in which a probability of failure is of interest and which therefore, for reactor plant analyses, are primarily of interest in structural mechanics analyses, as discussed in Sec. 3.3. Specific physics comes into play primarily in terms of the type of uncertain input parameters that are selected for the analysis and the type of information available for establishing the uncertain input parameter probability distribution functions and ranges. It is also true that modeling uncertainties are generally smaller for reactor physics analyses than for thermal-hydraulic or fuel behavior analyses, both of which are highly non-linear and strongly influenced by material properties modeling, which is often limited to empirical correlations valid over a limited range of conditions.

There are several important considerations to address for methods other than the UMAE-CIAU approach:

- The means of selecting the dominant uncertain input parameters; in other words, determining which input parameters sufficiently influence the uncertainty in the model responses of interest so that uncertainty in these parameters needs to be included in the uncertainty analysis. A sensitivity analysis can provide quantitative input to this process. Many times, this determination is done simply by the analyst's judgment or by expert elicitation. Also, in current practice, an input parameter is often selected simply because information is available concerning the range of uncertainty of the parameter.
- The means of estimating the range of values and probability density function for each uncertain input parameter. There are three options: perform a literature review to find ranges and distributions derived either from experimental data or

code analyses; fit available experimental data, either from separate effects tests or integral tests; or use expert elicitation if no data or validated calculational results are available [CSNI 2007].

- The choice of how to transfer raw measured data into input parameter ranges and distributions. If sufficient data are available, classical statistics can be applied. If the amount of data available is small, the Bayesian procedure is suitable for performing the best inference possible from the limited data [Glaeser 2002].
- Accounting for interdependencies of input parameter uncertainties. Currently, most uncertainty analyses ignore these interdependencies. While in many practical cases, most input parameters are independent [Devictor 2005], if it is the case that significant interdependencies exist, neglecting them can lead to underestimation of calculational uncertainties. These can be addressed to some extent by fuzzy modeling [Chojnacki 2005b] or by developing a correlation coefficient matrix, if sufficient information on interdependencies is available [Devictor 2005].

9. Conclusions and Recommendations

The uncertainty methodologies reviewed above have primarily been applied to uncertainty evaluation of light water reactor best-estimate calculations. This includes the several variations of the CSAU method which have been approved by the USNRC for licensing analyses. These methods now need to be evaluated and, if necessary, adjusted for application to best-estimate calculations for high-temperature gas-cooled reactors and liquid metal reactors. They also need to be optimally integrated into the development of advanced simulation codes. These goals lead to several observations:

- Initially, ranges and distributions for advanced reactor uncertain input parameters will probably have to be based much more on engineering judgment than is currently the case for comparable parameters in light water reactor analyses, due to a much more limited set of available experimental and operating data. Plans for advanced reactor experimental programs need to include generating data for uncertainty evaluations, as well as for code validation.
- Work is needed to improve the techniques used for identifying the dominant uncertain input parameters to be included in an uncertainty evaluation.
- Step 7 of the CSAU method compares the high-fidelity model code against a range of single effects and integral tests, to assess how well the code is able to predict the dominant physical processes of the transient of interest [Young 1998]. The USNRC will probably require more extensive data from both types of tests than are currently available for HTGR's and LMR's in order to execute this step satisfactorily. This will require expanded experimental programs to generate the necessary validation data.
- Currently, application of the CSAU usually involves making extensive use of the USNRC Reg. Guide 1.157 [NRC 1989], which lists all processes known to affect light water reactor LBLOCA's [Young 1998]. The information in this document guides the analyst in selecting the uncertain input parameters and the output re-

sponses for an uncertainty evaluation of a best-estimate LBLOCA analysis for a particular system. This implies that the USNRC would need to develop a comparable guide for the dominant HTGR and LMR accident scenarios.

- Light water reactor analysis experience has shown that different qualified versions of the same code can predict output temperatures that differ by more than 150K; thus, direct specific code version qualification is needed for uncertainty evaluation [Petruzzi 2008]. Comparable qualifications of advanced simulation codes for HTGR and LMR analyses would be needed for output responses appropriate to these types of reactors.
- Uncertainty assessment needs to be addressed in advanced simulation code documentation. Code manuals should discuss uncertainty assessments and describe preferred methods for making uncertainty evaluations.
- Internal assessment of uncertainty within the analysis is the most desirable approach [Glaeser 2002, Prošek 2003] but is not always feasible. Internal assessment is an integral feature of the UMAE/CIAU method and could probably be implemented in mature codes for the ASAP method. However, incorporating methods that sample and propagate input uncertainties as an optional internal feature of an analysis code would be somewhat challenging and would result in much longer running times.

After considering the advantages and drawbacks of the various approaches to uncertainty evaluation, the recommendation is to use sampling and propagation of input uncertainties, in conjunction with application of the Wilks formula to determine the number of samples required. When possible, this should be done with the full, high-fidelity model, as in the GRS approach, such as AREVA has done with the S-RELAP5 code. If this implementation is simply too expensive, a surrogate model should be substituted for the full model.

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