



Methods for Quantifying Uncertainty in Fast Reactor Analyses

Global Nuclear Energy Partnership

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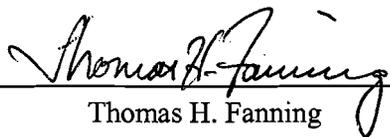


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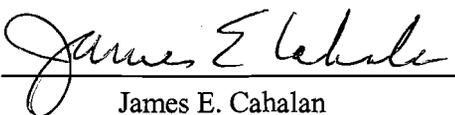
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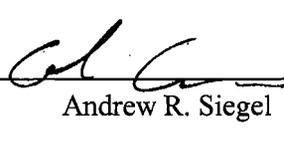
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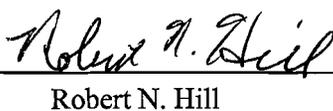
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ABSTRACT

Liquid-metal-cooled fast reactors in the form of sodium-cooled fast reactors have been successfully built and tested in the U.S. and throughout the world. However, no fast reactor has operated in the U.S. for nearly fourteen years. More importantly, the U.S. has not constructed a fast reactor in nearly 30 years. In addition to reestablishing the necessary industrial infrastructure, the development, testing, and licensing of a new, advanced fast reactor concept will likely require a significant base technology program that will rely more heavily on modeling and simulation than has been done in the past. The ability to quantify uncertainty in modeling and simulations will be an important part of any experimental program and can provide added confidence that established design limits and safety margins are appropriate.

In addition, there is an increasing demand from the nuclear industry for best-estimate analysis methods to provide confidence bounds along with their results. The ability to quantify uncertainty will be an important component of modeling that is used to support design, testing, and experimental programs.

Three avenues of UQ investigation are proposed. Two relatively new approaches are described which can be directly coupled to simulation codes currently being developed under the Advanced Simulation and Modeling program within the Reactor Campaign. A third approach, based on robust Monte Carlo methods, can be used in conjunction with existing reactor analysis codes as a means of verification and validation of the more detailed approaches.

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REACTOR CAMPAIGN METHODS FOR QUANTIFYING UNCERTAINTY IN FAST REACTOR ANALYSES

1. Introduction

The creation of the U.S. Department of Energy's Global Nuclear Energy Partnership (GNEP) has led to renewed interest in liquid-metal-cooled fast reactors for the purposes of closing the nuclear fuel cycle and making more efficient use of future repository capacity. Liquid-metal-cooled fast reactors in the form of sodium-cooled fast reactors have been successfully built and tested in the U.S. and throughout the world.[1] However, no fast reactor has operated in the U.S. for nearly fourteen years. More importantly, the U.S. has not constructed a fast reactor in nearly 30 years. In addition to reestablishing the necessary industrial infrastructure, the development, testing, and licensing of a new, advanced fast reactor concept will likely require a significant base technology program that relies more heavily on modeling and simulation than has been done in the past. The ability to quantify uncertainty in modeling and simulations will be an important part of any experimental program and can provide added confidence that established design limits and safety margins are appropriate.

In the late 1960s, the then U.S. Atomic Energy Commission gave development of a liquid-metal-cooled fast reactor (LMR) a high priority, and the development of the Fast Flux Test Facility (FFTF) became a cornerstone of that program. To provide adequate support for the FFTF and for the expected LMRs to follow, a major base technology program was established which provided a continuous stream of experimental information and design correlations. This experimental data would either confirm design choices or prove the need for design modifications. At the time, the "tremendous amount of data and experience pertaining to thermal design" of LMRs was recognized as providing the technical foundation for the future commercial development of LMRs.[2]

Presently, there is limited infrastructure for the development of advanced LMR concepts. Although significant technical data from the earlier LMR programs still exists, much of the experience and expertise related to that data cannot be recovered. The ability of advanced modeling and simulation methods to quantify uncertainties can be used to corroborate past experimental data and to redevelop the experience and expertise that has been lost. Furthermore, simulation methods that quantify uncertainties and propagate them to anticipated outcomes will play a crucial role in developing new testing and experimental programs that will be needed to support the goals and objectives of GNEP while limiting testing that may be unnecessary, redundant, or ineffective. Combined, advanced simulation methods and experimental testing will provide greater confidence that the established design and safety margins are appropriate. Neither can accomplish that alone.

In the following section, a brief background on the role of uncertainty in establishing design limits and safety margins is provided along with a short discussion of existing methods for the treatment of uncertainty. Of particular importance is the evaluation of design basis margins by the quantification and use of hot channel factors. In addition, past methods for statistical quantification during transient analyses are briefly discussed. Subsequent sections present methods that may be applied to advanced simulation methods for the purpose of quantifying uncertainty, as well as implementation options for their use.

2. Background

There is increasing demand from the nuclear industry and regulatory agencies for best-estimate analysis methods to provide confidence bounds along with their results. In response to this, the Organization for

Economic Cooperation and Development/Nuclear Energy Agency (OECD/NEA) formed an expert group on “Uncertainty Analysis in Modeling” and held a workshop in April 2006. A second workshop is planned for April 2008.[3] A goal of these workshops is to develop a benchmark program to define uncertainty and modeling tasks for design, operation, and safety analysis of light-water reactors (LWRs). Although the focus is on LWRs, it is expected that demand for confidence bounds in best-estimate analyses will also exist for LMRs.

Uncertainty plays a key role in two different aspects of evaluating safety margins: setting design limits and assessing operating conditions. First, experimental or analytical determination of design limits for materials or components is often carried out under well-controlled conditions. Irregular geometries, compositions, or operating histories in a real system introduce uncertainty in the actual operating conditions experienced by the materials. In addition, experimental uncertainty must also be considered. Together, the actual failure limits for a material or component may be lower than that measured under nominal laboratory conditions.

Second, analytical or quantitative measurements of the current state of the reactor introduce several different forms of uncertainty. Furthermore, reactor operations may allow for overpower conditions. Together, actual operating conditions may be closer to the failure limits than predicted by nominal conditions alone.

The role of uncertainty in these two aspects of design margin evaluation is illustrated in Figure 1, where the margin to fuel melting is qualitatively considered. Uncertainties contribute to reducing the estimate of the power-to-melt design limit by accounting for a non-ideal geometry (maximum cold gap) and experimental uncertainties. Uncertainties also contribute to increasing the estimate of peak linear power by accounting for control and instrumentation uncertainties and potential overpower conditions. As a result, the minimum margin to fuel melting is considerably smaller than that predicted by nominal conditions alone.

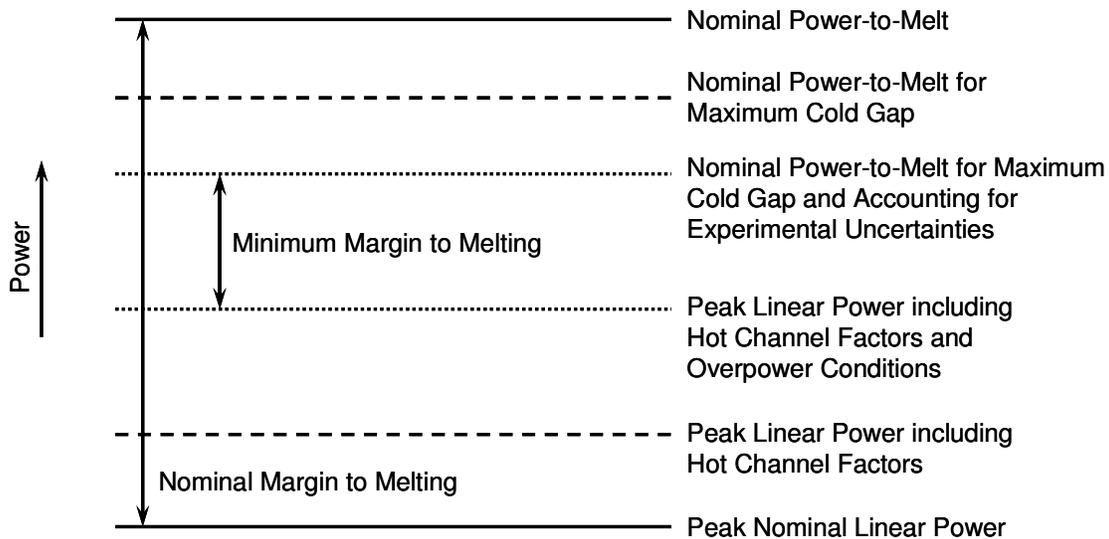


Figure 1: Accounting for Uncertainty when Assessing Design Margins

2.1 Design Limits and Uncertainty

Thermal, hydraulic, mechanical, and nuclear design requirements are established for LMRs for a variety of event classifications with different severity levels. These classifications range from normal operation (including steady-state and operational transients) to emergency or faulted conditions that are extremely unlikely to occur. To satisfy design requirements, design limits are established that consider material properties and all potential environmental conditions. Design limits must also allow adequate margins to account for all design, fabrication, and operational uncertainties. The specification of design limits and the treatment of uncertainties depend on the type of event classification being considered. While one approach may be to select the most pessimistic assumptions and define extremely conservative limits, this approach is impractical and will impose a significant economic burden and unacceptable limits on plant operations.

Instead of extremely conservative limits, reasonably-conservative design limits are defined. Historically, this has been done through extensive in-pile and out-of-pile experimental programs for materials and components that attempt to confirm design limits for steady-state and transient operations under a wide variety of thermal, hydraulic, mechanical, and nuclear loading conditions and histories. The defined design limits must account for uncertainty which ultimately influences allowable plant operating conditions.

While advanced simulation methods will never make given materials stronger or components last longer, two important contributions can be made. First, being able to better resolve the various loads expected to be imposed on a material or component may result in better-targeted experimental conditions and procedures. As a result, identified failure modes and behaviors are representative of actual conditions and not overly conservative. Second, being able to account for and quantify the effects of experimental and modeling uncertainties will result in more confidence that established failure limits are appropriate.

2.2 Steady-State Analyses and Hot Channel Factors

Plant operating conditions are set to ensure that design limits are not exceeded. The impact of modeling and experimental uncertainties, instrumentation and control inaccuracies, manufacturing tolerances, material properties uncertainties, and other variations in reactor operating conditions must be accounted for when confirming reactor conformance with established limits. For normal, steady-state operations and operational transients, a method of hot-channel analyses similar to that employed for light-water reactors is used.[2,4] One significant difference between hot channel analyses for LMRs compared to LWRs is that LMRs may have multiple hot channels as a result of assembly ducting and flow orificing. Therefore, multiple potential hot channels need to be analyzed rather than just the nominal maximum-temperature channel.

Hot channel factors are defined by a combination of factors that account for statistical and non-statistical contributions. Some of the non-statistical factors, such as inlet and intra-assembly flow maldistributions, mixing uncertainties, and cladding circumferential temperatures variations can be better quantified through direct, higher-order numerical simulations. Even so, the impact of manufacturing tolerances and material properties uncertainties will contribute to uncertainty in these evaluations. Other non-statistical factors, including power level measurement uncertainties and control system tolerances, are not likely to benefit from improved simulation methods.

Statistical contributions to hot channel factors include numerous components. Examples include uncertainties in nuclear data, fissile fuel distribution, material properties, and flow areas. In conventional hot-channel analyses, it is assumed that these components are independent of each other. However this is not always the case. For example, variations in fissile fuel distribution will affect material (fuel)

properties and local power distributions. The assumption of parameter independence is made to simplify the statistical analyses.

A number of methods have been proposed for combining the effects of the numerous components that make up hot channel factors. Commonly, a semistatistical method is employed where non-statistical contributions are combined by a direct, cumulative method, and statistical contributions are combined by treating the uncertainties as statistically independent variables.[4] The cumulative method assumes that all uncertainties have the most unfavorable values. The statistical method assumes variances are independent and can be added linearly.

As previously described, many non-statistical contributions may be better quantified through direct, higher-order numerical simulations. This avoids the pessimistic assumptions used in the cumulative method and can result in a more realistic assessment of the contribution. For the statistical contributions, incorporating uncertainty quantification methods directly into the numerical simulation will allow for coupled effects to be modeled and the assumption of independence can be relaxed.

2.3 Transient Analyses and Statistical Quantification

Transient analyses present additional complications not present in steady-state analyses. In steady-state analysis, individual components, including core assemblies, can be modeled independently with appropriate (and possibly uncertain) boundary conditions. Transient events, on the other hand, can involve whole-plant dynamics with complex and coupled feedback mechanisms with non-linear behaviors. This significantly expands the parameter space of interest and makes incorporation of uncertainty quantification methods directly into numerical simulation methods impractical.

For example, in the SAS4A/SASSYS-1 LMR analysis code system,[5] there are hundreds of internal parameters that characterize correlations for items such as decay heat as well as coolant, cladding, and fuel properties. In addition, there are well over 1,000 user-supplied input parameters that may be used to define a problem, many of which represent vector quantities. It is impractical to identify in advance which of these parameters should be treated internally by uncertainty quantification methods, and it is virtually impossible to incorporate them all. Furthermore, many methods for incorporating and propagating uncertainty assume that uncertainties behave in a linear fashion even if the system is nonlinear. Instead, statistical quantification using sampling methods have been proposed and demonstrated.

Vaurio, et al., demonstrated the feasibility of using a statistical sensitivity analysis procedure to rank the input data for large computer codes in order of sensitivity importance.[6,7] This ranking identifies the importance of a large number of input variables to the uncertainty of selected output quantities. The method also identifies input parameters that contribute to non-linear threshold effects. Such information can be used to direct modeling that uses statistical sampling techniques. Morris, et al., compared the effectiveness of a response surface methodology with differential sensitivity theory (DST).[8] This comparison led to the conclusion that the development and implementation costs for DST were likely to be significant in comparison to the development of forward solutions. Both Vaurio and Morris[9] developed techniques for statistically sampling input parameters of large codes to propagate and measure the impact of uncertainty on selected output parameters. Vaurio developed the PROSA code[10,11] to evaluate probabilistic response surfaces to obtain probability distributions for consequences of reactor transients. Morris used the statistical analysis capabilities of the commercial GoldSim probabilistic simulation tool[12] to perform direct sampling of a model (rather than a response surface) and evaluate probability distributions for the consequences. Neither of these methods required modifications to the underlying solution methods or algorithms and are amenable to computer codes with very large sets of input parameters. In addition, the impacts of uncertainty are not assumed to be linear.

3. Methods for Quantifying Uncertainty and Variability

A number of methods are available that can be incorporated into simulations for the purpose of quantifying and propagating uncertainty. As described above, transient analyses present complications in terms of the size of the parameter space and in the complex and coupled nature of non-linear feedback mechanisms with the potential for threshold effects. As described above, existing methods for statistical quantification using sampling techniques can be applied to transient analyses. In the subsections that follow, the primary focus is on methods that can be applied to the practical evaluation of design limits and margins during steady-state operations.

3.1 Reduced Basis Models

A significant challenge in uncertainty quantification is to be able to compute expected system responses over large-dimensional parameter spaces. For complex systems, the simulation cost is generally too high to permit solution evaluation for the very large number of cases required to confidently identify all critical points, particularly for systems governed by partial differential equations (PDEs) where each individual simulation requires the use of high-performance computing. One approach to reducing the interrogation cost is to build a response surface, which characterizes the behavior of a few output values of interest as a function of a few input parameters.

Typically, response surfaces are constructed as interpolants of the outputs over the distribution of input parameters, where the interpolation nodes are specific solution points – each consisting of the solution to the governing PDE for a given set of input parameters. In an offline stage, one solves a large system of dimension N (> 1 million, typically) characterizing the discretized PDE at a number of points M ($\ll N$) in parameter space. In a subsequent “online” stage, one can interrogate the solution rapidly (at cost scaling with M , rather than N) either at points of direct interest to the designer or within a Monte Carlo context to characterize the probability of reaching critical regimes in the output space. Straightforward interpolation, however, has several drawbacks. First, stability typically dictates that subsequent queries be restricted to the convex hull of the selected nodes, lest the interpolant become an extrapolant. Second, interpolation does not provide rigorous error bounds with the estimate.

Reduced-basis (RB) methods [13,14,15] offer an alternative means of constructing response surfaces that provide rigorous error bounds in the output. Such bounds yield a confidence measure at any point in the parameter space, even outside the convex hull. Moreover, the size of the bound gap indicates increased uncertainty and can be used to identify regions of critical behavior (i.e., local “cliff” phenomena). In addition, availability of inexpensive error bounds permits the development of an efficient bootstrapping procedure in developing the M -dimensional sample set. Given an initial set of nodes, one interrogates the response surface on a fine mesh. The next interpolation node is then selected as the fine-mesh point where uncertainty is maximal. This procedure, repeated recursively, generally gives rapid reduction (i.e., exponential with M) in the bound-gap. Moreover, critical regions are automatically identified by resultant high concentrations of nodal points in the input parameter space.

The essential idea behind the RB approach is to use the full (order- N) solutions to the PDE as basis vectors to generate approximate solutions at other points in parameter space. The convergence tends to be quite rapid because the parametric response surface is generally smooth. Moreover, rigorous lower- and upper-bound error estimates can be developed from coercivity and boundedness of the governing differential operators. A significant computational savings can be realized if the operator is affine in the parameter, which allows the nonlinear operator to be expressed as a low-dimensional expansion in which the solution and parameter dependence are separable. If the output functional is also affine in the parameter, then one rapidly compute the output bounds in complexity scaling only with M and having no N dependence.

Rigorous RB methods have undergone significant development in the past decade. Patera and co-workers have developed RB methods for elliptic and parabolic problems that are characteristic of the steady and unsteady Navier-Stokes equations, respectively [16,17]. To date, the methods have been applied to relatively small problems tractable on workstations, but we are currently extending these to three-dimensional Navier-Stokes problems solved on large parallel clusters. In addition, the methods are constrained to relatively low Reynolds numbers and thus unsuitable for application to direct numerical simulation (DNS) or large-eddy simulations (LES) of turbulence. We anticipate, however, that the methods will be applicable to characterizing the response surfaces of Reynolds-averaged Navier-Stokes (RANS) models of turbulent flows, for which eddy-viscosity provides the coercivity needed to establish the bound estimates.[18] The validity of the constituent RANS solutions will be established through detailed comparisons with high-fidelity LES models at selected parameter points. Such comparisons have already been performed for the particular case of a 7-pin subassembly with wire-wrap[19] and investigations of larger subassemblies are currently underway.

3.2 Higher-Order Methods

Prior investigations have shown that, while linear perturbation models (as are the ones resulting from sensitivity analysis) are very important tools for uncertainty quantification, they are also not sufficient for tackling complex nonlinear systems,[20] including in the context of core disruptive accidents analysis.[8] On the other hand, sampling methods by themselves are having an extremely difficult time in creating a complete uncertainty picture for systems with a very large number of parameters.[20] Recent investigations have shown that spectral stochastic finite element methods (SFEM, see References 21 and 22) can fill the gap between sensitivity methods and sampling methods, by creating higher order approximation models of complex systems (effectively, higher order global sensitivity methods, or higher order response surface methods) that take advantage of the smoothness existent in the system, while needing a sampling-like approach (co-location, [23]) to determine their parameters. A significant challenge is that such methods suffer a rapid increase in the required number of basis functions with the dimension of the system. Initial investigation into the approximation properties of such methods for nonlinear problems has been carried out in Reference 24.

To alleviate these shortcomings and thus realize the full potential of such methods, second-order adjoint sensitivity analysis can guide the selection of significant directions in the parameter space that result in major variation of the merit functions under consideration. The eigenvectors corresponding to the largest eigenvalues of the Hessian of a merit function are excellent prospects to significantly reduce uncertainty if higher order terms involving them are considered in the SFEM expansion. These eigenvectors can be identified using a matrix free approach. The most significant eigenvectors of the Hessian of the merit function with respect to the uncertain parameters can be used to guide the higher order uncertainty quantification approach based on SFEM. The matrix free aspect is important, since otherwise one would have to store matrices that are generally dense and whose sizes may be products of the state space with the parameter space, and may therefore be beyond the storage possibilities of the most advanced computers. Once the dominant eigenvectors of the Hessian are so determined, an SFEM polynomial basis is generated that has higher degrees in the directions of these eigenvectors, after which a co-location procedure is carried out to determine the coefficients of the SFEM approximation that best explains the variation in the merit function. We expect that such methods will rapidly explain the smooth variation with respect to the uncertain parameters and, for best efficiency, can be used in a hybrid fashion with RB models.

3.3 Monte Carlo Methods

Monte Carlo (MC) simulations are the classic approach to uncertainty quantification because they accommodate high-dimensional parameter spaces and can treat virtually any nonlinear system using a

black-box approach. The feasibility of such approaches has been demonstrated for uncertainty quantification in unprotected loss-of-heat sink, loss-of-flow, and transient overpower accidents. In the particular case outlined by Morris,[9] the commercial stochastic simulation code GoldSim (developed originally for geological repository modeling) was coupled to simplified point-kinetics and thermal-hydraulics models extracted from the SAS4A/SYSSYS-1 computer code and used to rapidly simulate 10,000 realizations in order to characterize the uncertainty of transient responses within the first hour of a given triggering event. While the large number of realizations used in this demonstration is impractical for high-resolution approaches (e.g., using LES- or RANS-based thermal-hydraulics analysis) it is feasible to consider using MC to simultaneously drive hundreds or thousands of realizations in parallel of existing or future neutronic, thermal-hydraulic, and safety analysis codes. Such a direct approach has the advantage of robustness both with respect to MC sampling and with respect to the significant expert knowledge and validation embedded in the methods and algorithms of best-estimates codes. This approach also avoids the very high costs associated with developing both forward and adjoint solutions for the complex, coupled, non-linear problems being investigated. Furthermore, for the methods that can be practically implemented, MC methods provide a means for validating the newer proposed approaches.

4. Implementation Options for Quantifying Uncertainty

The reduced-basis technology has undergone significant development in the past decade and the group of Patera at MIT has developed Matlab-based drivers that can couple to large-scale PDE codes. We envision, initially, using these codes to drive Nek5000 simulations for convection-diffusion with prescribed hydrodynamic flow fields (computed independently by Nek5000) to study thermal sensitivity with respect to pin and cladding conductivities, velocity distributions, etc. Simulations for three-dimensional unsteady Navier-Stokes computations at moderate Reynolds numbers are also likely tractable within the FY08-10 time frame, at which point geometric sensitivities could also be incorporated. The theory for RANS-based simulations remains to be developed and would require close collaboration with Patera and his collaborators at Paris VI.

A natural starting point for the application of the SFEM method would be on simplified, steady-state thermal-hydraulics models that capture the essential transfer phenomena with comparable parameter dependencies. The objective would be to quantify the uncertainty in thermal-hydraulics state variables with respect to the physical parameters such as thermal diffusion in the fuel or density of the coolant as well as fluctuations in the velocity field (the latter requiring a far larger dimensional space). Error estimation of the resulting approximation would be carried out by sampling methods. The increased accuracy of the higher-order model would be expected to result in the need of a relatively small number of samples for validation.

Monte Carlo methods will play two roles in uncertainty quantification. In the first, it can be applied to problems and models that are not amenable to direct incorporation of uncertainty-quantification methods. These would include problems, such as whole-plant transient dynamics modeling, which involve complex coupling of non-linear feedback mechanisms. In the second, Monte Carlo methods can be applied to existing or new best-estimate codes for the purposes of verification and validation of the advanced methods described above.

5. Summary

Although significant technical data from the earlier LMR programs still exists, the limited infrastructure available for the development of an advanced LMR concept as proposed by GNEP suggests that advanced modeling and simulation methods will play a significant role. With an increasing demand from the nuclear industry for best-estimate analysis methods to provide confidence bounds along with their results,

the ability to quantify uncertainty will be an important component of modeling that is used to support design, testing, and experimental programs.

Three avenues of UQ investigation have been proposed. Two relatively new approaches are described which could be directly coupled to simulation codes currently being developed under the Advanced Simulation and Modeling program within the Reactor Campaign. A third approach, based on robust Monte Carlo methods, can be used in conjunction with existing reactor analysis codes as a means of verification and validation of the more detailed approaches.

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