Proceedings of the ASME 2010 3rd Joint US-European Fluids Engineering Summer Meeting and 8th International Conference on Nanochannels, Microchannels, and Minichannels
FEDSM-ICNMM2010
August 1-5, 2010, Montreal, Canada

FEDSM-ICNMM2010-31270

RESPONSE SURFACE MODELING OF A LARGE BREAK LOSS OF COOLANT ACCIDENT WITH COMPARISONS TO ORDER STATISTICS APPROACHES

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ABSTRACT

NUREG/CR-5249 "Quantifying Reactor Safety Margins Application of Code Scaling, Applicability, and Uncertainty Evaluation Methodology to a Large Break, Loss-of-Coolant Accident" provides the general methodologies to be used in the development of realistic loss of coolant safety analyses. The objective of this paper is to start with NUREG/CR-5249 and develop a modified methodology. The modified approach will include a response surface, model adequacy checks, and development of the 95/95% confidence peak clad temperature cumulative distributions function. The response surface model will then be used to develop simulated results and conclusions about the order statistics best estimate approach. All work is conducted using a verified safety analysis input deck and RELAP as the thermal hydraulic best estimate analysis code.

The objective of the order statistics comparison is to investigate the number of cases in which the maximum PCT, in a simulated order statistics approach, falls below the 95th percentile value of the distribution and to assess the standard deviation in the maximum peak clad temperature of order statistics sets.

Although order statistics may be a more economic approach to satisfying regulatory requirements, response surface models have several benefits that can complement the use of order statistics. The primary benefit is the insight gained into which parameters are most important in determining the peak clad temperature. This is of particular value to the licensee in convincing the regulator that its analysis is robust. The disadvantage is the number of runs required to develop the models. If we examine the main effects, the most significant input parameter is pipe break size. In support of a proposed modification to 10CFR50.46, the U.S. Nuclear Regulatory Commission undertook an expert elicitation to assess the change in frequency of pipe break accidents as a function of break size. The result of that elicitation was a probability density function that decreases approximately as (pipe diameter)$^{-1.5}$ in the region of large pipe diameters. Because break diameter is shown to be such a large contributor to PCT by the response surface, it is evident that calculated PCT could be substantially reduced if credit were given for this form of the uncertainty distribution rather than for the flat distribution used in the analysis (and industry).

INTRODUCTION

Loss of Coolant Accidents (LOCAs) are design basis accidents which must be analyzed to obtain an operating license for nuclear power plants. Reanalysis is also required whenever a major change is made to the plant, such as a new fuel design. The objective of this paper is to use statistical techniques to develop a response surface model. A response surface model is an empirical model, typically a polynomial, which is used to approximate an unknown function given a range of inputs. The fit of the response surface model will be assessed. Once the adequacy of the fit is determined, the model will be used to analyze the applicability of the order statistics approach to LOCA analyses. The order statistics approach is a non parametric best estimate approach currently used by Westinghouse and AREVA. Finally, future modeling techniques will be recommended.

BACKGROUND

10 CFR 50 "Domestic Licensing of Production and Utilization Facilities" [1] provides the framework for which nuclear power plants are regulated by the United States government. Section 50.46 "Acceptance Criteria for Emergency Core Cooling Systems for Light-Water Nuclear Power Reactors," provides the specific regulatory guidelines for a loss of coolant accident, a design basis accident. Appendix K "ECCS Evaluation Modules," of 10 CFR 50, provides the required features of a loss of coolant evaluation model as well as the required documentation. At the time of the development of these sections of 10 CFR 50, computing power and research on loss of coolant accidents were limited. As a result, the methodologies developed and analyses were treated conservatively. The requirements and guidelines were subsequently modified to allow for a realistic or best estimate analysis with consideration of uncertainties. The

treatment of uncertainties is performed in a manner such that the results have a high degree of confidence that the acceptance criteria set forth in Section 50.46 are not violated. Currently, two major pressurized water reactor vendors in the United States, Westinghouse and AREVA, apply both the conservative (commonly referred to as Appendix K calculations) and best estimate or realistic methodologies. The percent difference in PCT between the realistic methodology and Appendix K methodology can be on the order of 45% difference. The conservative Appendix K calculations, in many cases, are the limiting accident analysis, meaning that the LOCA analysis can dictate fuel designs, cycle time and operating power, ultimately having an impact on profitability of the plant.

NUREG/CR-5249 "Quantifying Reactor Safety Margins Application of Code Scaling, Applicability, and Uncertainty Evaluation Methodology to a Large Break, Loss-of-Coolant Accident" [2] provides the general methodologies to be used in the development of a realistic loss of coolant safety analysis. NUREG/CR-5249 also provides a sample methodology and analysis of a realistic loss of coolant accident.

REVIEW OF CURRENT (ORDER STATISTICS) LBLOCA METHODOLOGY

NUREG/CR-5249 provides the building blocks on which today's RLBLOCA methodologies are based. In practice, the capabilities and assessment and ranging of parameters sections of the CSAU methodology are still followed in the development of current RLBLOCA methodologies. However, the response surface methodology presented in NUREG/CR-5249 is not the preferred methodology in use by the reactor vendors. Both AREVA's and Westinghouse's current methodologies for RLBLOCA are non-parametric, order statistics, based methodologies [3,4].

Order statistics are, as the name implies, an ordering of random variables from independent and identical distributions where each random variable has a probability density and a cumulative distribution function. For example, in LBLOCA the PCT is the primary safety criterion reported. Assume "n" sets of parameters are developed by randomly selecting values from each of the uncertainty distributions. The "n" LOCA cases are then run with the RELAP code resulting in "n" PCTs. These "n" PCT results are then ordered smallest to largest. The smallest PCT value would be the first order statistic, $PCT_{(1)}$, and the largest PCT value would be, $PCT_{(n)}$. Let the smallest order statistic be V and the largest be U while values in between are the K_{th} order statistics (remember the PCT order statistic are random variables). Order statistics can be used to answer the following questions:

- What are the CDF and PDF of V?
- What are the CDF and PDF of K?

Before describing how order statistics are applied, a basic understanding of current RLBLOCA methodologies is required. AREVA and Westinghouse have similar methodologies. Both methodologies follow the steps prescribed by the CSAU methodology (frozen code, nodalization analysis, PIRT, etc.). Rather than using a response surface along with a Monte Carlo sampling to derive the bias and uncertainties associated with code scaling, code limitations and operating condition as recommended in the CSAU methodology, AREVA and Westinghouse use order statistics. In the order statistics approach input parameters are randomly sampled from known and bounding ranges. Then the frozen code, with the sampled input parameters, is run resulting in a PCT. If one were to sample and run the frozen code several thousand times, this would be a direct Monte Carlo analysis resulting in a CDF of the PCTs. In the case of the CSAU methodology, a response surface model would be developed. Because the response surface model can be run very quickly on a computer, the input parameters could be sampled for several hundred thousand cases resulting in a CDF of PCTs that has very little statistical variability. The objective of the order statistics method is not to approximate the CDF of the PCT. The objective is to develop a tolerance level where the result states that you are 95% confident that one of the cases is in the 95th percentile of PCTs for an unknown CDF of PCTs. Thus, when the licensee submits the value of the PCT to the regulator, they are not stating that the value quoted is the 95th percentile value but that they are 95% confident that the 95th percentile value is smaller than the value submitted. Put another way if one samples a set of inputs and determines a PCT and repeats this process at some point, you could ask the question "how confident am I that a PCT in the 95% is included in this set of PCTs?" The question then is how many cases are required using the order statistics method? The answer to this question was presented by Wilks where a simplified summery of Wilks work is presented by Frepoli [3] as:

$$\beta = (1-\gamma)^N \tag{1}$$

Where
β = confidence level input
γ = percentile input
N= number of trials

For β= 1-0.95= 0.05 (95% confidence level) and γ= 1-0.95= 0.05 (95th percentile PCT) then the required number of cases N is 59. 59 cases was the number of cases required in the AREVA methodology. Westinghouse requires 124 samples. The reason for the difference is that there are actually three different criteria (PCT, local oxidation, and core wide oxidation) that must be satisfied in the analysis.

Given that order statistics analyses and best estimate approaches are fairly new to the regulator, the reporting requirements are sometimes satisfied by the licensee by submitting results similar in format to parametric Appendix K analyses. For example, the regulator often requires that the peak case (case with the highest PCT) and the associated inputs with the peak case must be submitted. Historically parametric calculations determine the limiting input condition for each input and each input is reported. However, this is not appropriate for order statistics based analyses as each input parameter is randomly sampled from a predetermined and bounding range (typically a uniform distribution). Thus no conclusions should be drawn from one case alone. In general, the only conclusion that can be drawn from an order statistics analysis is that one is 95% confident that the largest PCT obtained in a set of 59 cases is greater than the 95th percentile value.

METHODOLOGY

The methodology used to develop the response surface is a derivative of the CSAU methodology and current realistic LOCA methodologies.

A response surface model is an empirical model developed to approximate an unknown function. In our case, the function being approximated is PCT as calculated by the RELAP computer code. There are 14 input parameters that are treated as having uncertainty distributions. A response surface model is typically a linear or polynomial function. Equation 2 represents a second order polynomial with cross term effects. Response surfaces are typically developed based on results from experiments in a lab or a manufacturing process. Since it is impractical to run physical LOCA experiments over a variety of conditions in an operating reactor, the response surface developed is a meta-model. A meta-model is a model developed from a computer simulation, where the computer simulation is designed to represent a physical process. In our case the meta-model is a model of a LOCA event run using RELAP. The motivation for developing the model is to be able to run a large number of cases quickly.

$$PCT = \beta_0 + \sum_{j=1}^{k} \beta_j x_j + \sum_{j=1}^{k} \beta_{jj} x_j^2 + \sum_{i}^{j-1} \sum_{j=2}^{n} \beta_{ij} x_i x_j + \varepsilon \qquad (2)$$

The first step in the development of the response surface model is to select input parameters that will be included in the response surface model. The goal is to select parameters that have the largest impact on PCT. Table 1 presents the 14 parameters that were selected based on engineering judgment and considerations related to ease of execution. After a response surface model is developed it can be examined to determine which parameters have the largest significant impact on PCT. If parameters are shown to have a very small impact they should be removed from the model and the model should be developed again. This iterative screening process was not possible due to the logistics of running a large set of cases multiple times. For this reason the 14 parameters selected (see Table 1) are all included in the response surface models.

Once the input parameters are selected a design matrix must be developed. The design matrix (X) is used to solve for the coefficients (βs) in the regression model. The coefficients are obtained using classic linear regression techniques. The linear regression is preformed using the built-in functions *regress* and *regstats* in Matlab (Matlab R2006b).

The biggest challenge in obtaining a response surface that represents the unknown function (PCT) accurately, in the region of interest, is in the choice of the design input matrix. In typical response surface applications a small set of parameters is varied. With a limited number of parameters factorial designs are commonly used. With 14 parameters, a full factorial design would require 16,384 cases. Partial factorial designs and various other designs are also frequently used when the performance of a full factorial design is impractical. However, a latin hypercube design, also called a space filling design, was selected to develop the input matrix. The concept of the latin hypercube design is to evenly cover the range of each input parameter and evenly fill the operating space. The latin hypercube design is developed using the Matlab function *lhsdesign*. Finally, the number of cases to be run in RELAP is dictated by the response surface model that is to be fit: linear, second order, second order with cross effects, etc. Solving for the regression coefficients requires the design matrix be over defined (more cases than regression coefficients). In the cases of the second order polynomial fit with cross effects 150 total cases were run. In addition to the 150 cases a set of 24 additional cases were run to test the model accuracy.

x_1	Assembly Burnup
x_2	Peaking Factor, Fq
x_3	Axial Sku (bottom,top)
x_4	Radial Peaking Factor A
x_5	Radial Peaking Factors B
x_6	One-Sided Break Size
x_7	Decay Heat Coefficient
x_8	Pressurizer Critical Flow Coefficient
x_9	Film Boiling Heat Transfer Coefficient
x_{10}	Biasi CHF
x_{11}	Initial Stored Energy
x_{12}	Condensation Interphase HTC
x_{13}	Accumulator Pressure
x_{14}	Accumulator Volume

Table 1:
Input Parameters

ANALYSIS APPROACH

Once the response surface model is developed the models are checked for fit and accuracy. A limiting PCT is determined from the CDF derived from the response surface model. Finally, sets of 59 and 124 cases are run and comparisons are made to the order statistics approach.

Since RELAP is a deterministic code (the same results will be repeated given the same inputs, no random error) the only error associated with deterministic models is a bias term. For this reason many classic statistic tests, for example F-tests and t-tests, are not applicable [5]. Simpson [6] recommends model adequacy be based on R-squared tests, residuals and validation though additional data points. Because R-squared values always improve with additional parameters, R-squared adjusted values will be reported [5]. Residual plots for the base set of runs, plus residual plots including a set of 24 additional cases that were not used in the development of the response surface, are used to determine the adequacy of fit.

A limiting PCT is determined based on CDFs that are generated from multiple runs of the response surface model. Inputs to the response surface models are generated using Monte Carlo sampling. The model is then run resulting in one PCT. This sampling process is repeated 1,000 times and the results are ordered. This results in an ordered array of 1,000 PCTs. The plot of ordered PCTs produces an approximation to the CDF of the response surface model. The development of the CDF process is repeated again 1,000 times and

1,000 CDFs are plotted on the same graph. The 95th percentile value for each of the CDFs is then plotted in a histogram and a set of 1,000 of the 95th percentile PCTs is plotted. The result is an approximation of the PDF (histogram) and CDF of the 95th percentile PCTs. The limiting PCT is reported as the 95th percentile point from the 95th percentile CDF. The result provides 95 percent confidence that the 95th percentile PCT is less than or equal to the value quoted. Thus 1,000,000 simulated LOCA cases total are run with the response surface model.

To test the ability of order statistics to reliably bound the 95th percentile PCT, 1,000 sets of 59 cases and 124 cases are run. Two results are derived from these sets of cases. First the standard deviation of the peak PCT is reported. Second, a CDF is developed from the response surface by running 100,000 trials. This CDF is assumed to approximate the actual CDF. To verify the validity of the order statistics approach one can compare the number of times the peak case from the sets of 1,000 runs of 59 and 124 cases falls below the 95th percentile PCT of the approximated CDF. The peak PCT value in the sets of 59 and 124 would be expected to be greater than the 95th percentile value predicted by the approximated CDF 952 out of the 1,000 sets of runs for the 59 cases and 998 out of 1,000 sets for the 124 case runs.

RESULTS OF THE SECOND ORDER RESPONSE SURFACE MODEL

The linear regression coefficients of the response surface model provides insight into what parameters are the most significant in the resulting PCT. A linear model, which is not presented here, indicated that break size was, by a large margin, the most statistically important input parameter to PCT during a large break LOCA. Similar results were seen in the coefficients of the second order model. In addition to break size, power peaking factor, axial skew, and decay heat coefficient were shown to be some of the most statistically important inputs when calculating PCT.

The response surface model must be checked for adequacy of fit to both the input data and a set of points that were not used in the development of the response surface. The model has an R squared adjusted value of 0.94, indicating that the quadratic model matched the design matrix point fairly well. Figure 1 is a plot of the residuals from the linear regression modeling. The quadratic models residuals are approximately +/- 150 °F. From Figure 2 the residuals based on cases which were not part of the design matrix are larger than those shown in Figure 1, +/- approximately 225 °F. This is not unexpected but is an indication that the response surface does not capture the complete behavior of the RELAP5 analysis. In a regulatory application, a characteristic value for the residual would be added to the 95/95 PCT for conservatism. In practice, these residuals and the fit of the models would have to be improved. To do this an iterative screening and modeling process could be done. The residuals of the cases that were not part of the screening might indicate that more data points are needed.

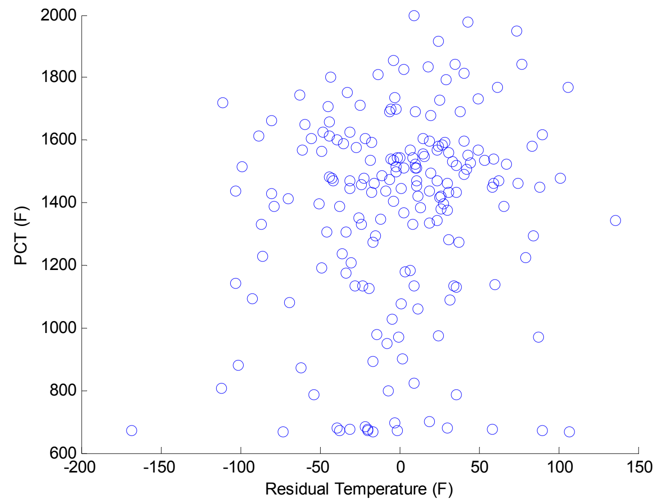

Figure 1:
Residual vs. PCT Scatter Plot, Experimental Cases

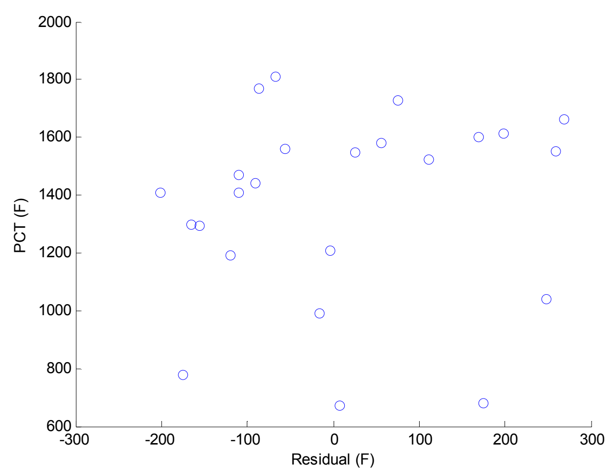

Figure 2:
Residual vs. PCT Scatter Plot, Sample Cases

Figure 3 is a plot of the 1,000 sets of CDFs developed by running the response surface model (each CDF line contains 1,000 PCT points). A histogram approximating the PDF of the 95th percentile PCT is then developed and the accompanying CDF is plotted in Figure 5. The mean 95th percentile PCT was found to be 1820 ^{o}F. The 95th percentile PCT of the CDF of the 95th percentile PCTs is found to be 1846 ^{o}F.

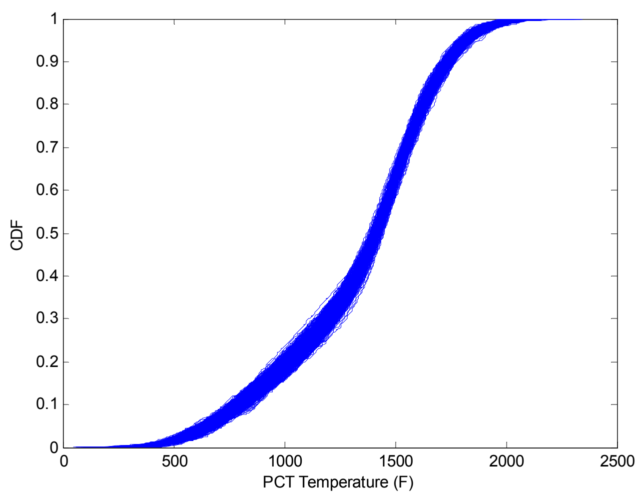

Figure 3:
CDF for 1,000 Trials

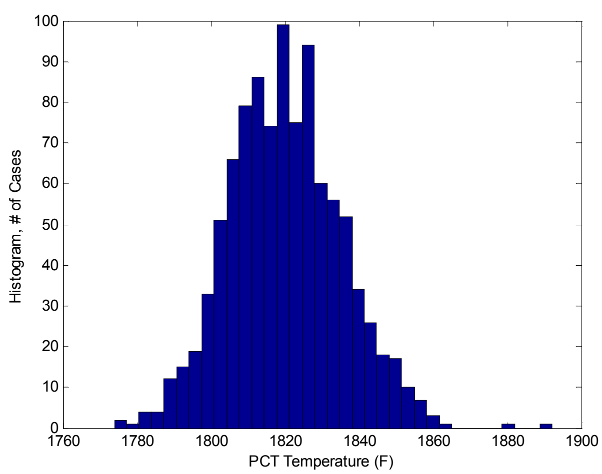

Figure 4:
PDF for 95th Percentile PCT Values

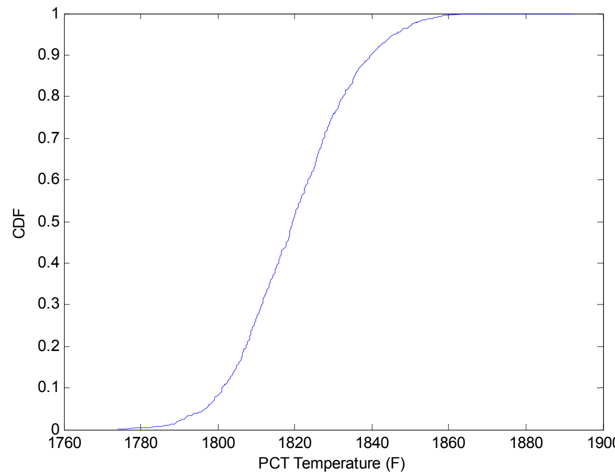

Figure 5:
CDF for 95th Percentile PCT Values

RESULTS OF THE ORDER STATISTICS COMPARISON

Although the response surface developed for PCT is not a precise representation of the RELAP5 analysis of PCT, it has the complexity and characteristics of the RELAP5 analysis. Thus, it provides a suitable surrogate for demonstrating that order statistics predicts the 95th percentile PCT with the required confidence and for indicating how large the deviation might be for those cases in which by chance the licensee's calculated maximum PCT actually does not fall within the 95% confidence interval. The objective of the order statistics comparison is to compare the number of cases in which the maximum PCT in a set of runs falls below the 95th percentile value of the distribution and to assess the standard deviation in the maximum PCT for 1,000 sets of 59 and 124 cases. An accurate CDF is developed by running 100,000 trials. The results can be seen in Figure 5. The 95th percentile PCT from this CDF is 1821 ^{o}F. To verify that the confidence level is met, this 95% value is compared to the peak point in each set of 59 and 124 cases. If the peak PCT in a set is below 1821 ^{o}F, it is considered a failure. 1,000 sets of 59 cases were run. Using the Wilks formula, one would expect 48 sets to fail. The CDFs for 1,000 sets of 59 cases are shown in Figure 6. The number of sets in which the maximum PCT was found to be less than 1821 ^{o}F is 37, which is in reasonable agreement with the 48 cases expected. Similarly for 1,000 sets of 124 cases, the Wilks formula indicates that 2 sets would be expected to have a maximum PCT less than 1821 ^{o}F. The CDFs are shown in Figure 7. The number of sets in which the maximum PCT was found to be less than 1821 ^{o}F is 4, which is in reasonable agreement with the 2 cases expected.

For the regulator, a natural question is "Suppose by chance the licensee's analysis falls outside the 95% confidence level (i.e. the maximum PCT from the set is less than the 95th percentile of the true CDF), how large might the error be?" One standard deviation is approximately 90 ^{o}F. Of the 1,000 trials with 59 cases, the lowest value of maximum PCT obtained was 1735 ^{o}F, which represents a deviation from the true 95th percentile value of approximately 86 ^{o}F.

Similarly, for the 124 cases, the lowest value of maximum PCT obtained was 1796 ^{o}F, which represents a deviation from the true 95th percentile value of 25 ^{o}F.

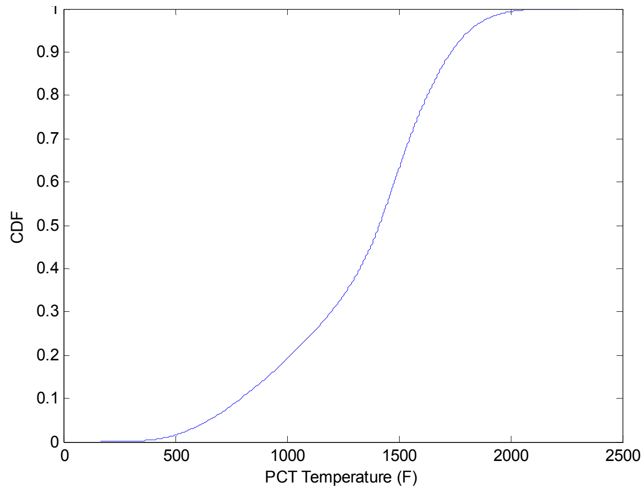

Figure 5:
CDF for 100,000 Trials

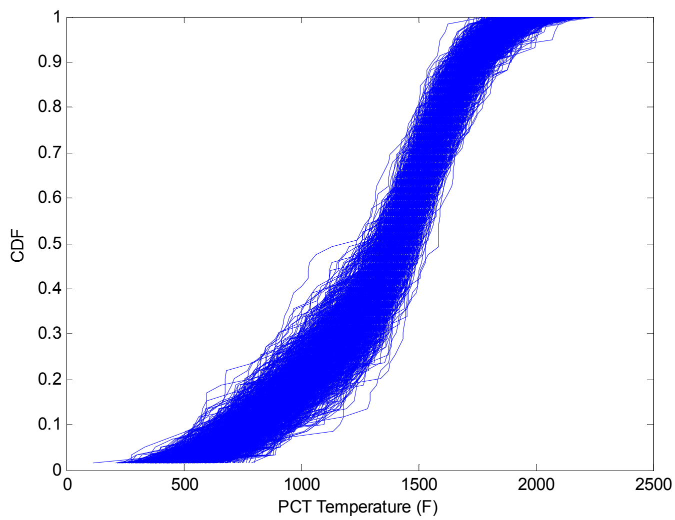

Figure 6:
CDF for 1,000 Trials of 59 Cases

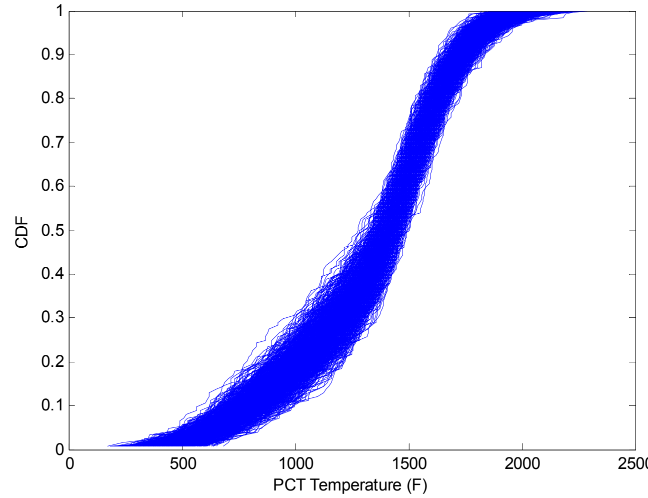

Figure 7:
CDF for 1,000 Trials of 124 Cases

CONCLUSION

Because the response surface is not a perfect fit to the RELAP5 PCT results, it would be necessary to include a bias term in the maximum PCT. Given a 95th percentile PCT of 1821 ^{o}F and adding a bias based on the residuals of approximately 225 ^{o}F will result in a PCT of 2046 ^{o}F. Attempts should be made to reduce this bias by improving the fit of the response surface to the RELAP5 results. A required step to improve the model fit would be an iterative process eliminating parameters that are not statistically important. Alternate modeling techniques could be used in an attempt to improve model accuracy. Simpson [6] recommends neural networks as a possible modeling technique.

Although order statistics may be a more economic approach to satisfying regulatory requirements, response surface models have several benefits that can complement the use of order statistics. The primary benefit is the insight gained into which parameters are most important in determining the peak clad temperature. This is of particular value to the licensee in convincing the regulator that its analysis is robust. The disadvantage is the number of runs required to develop the models.

If we examine the main effects in the response surface, the main effect is pipe break size. In support of a proposed modification to 10CFR50.46, the U.S. Nuclear Regulatory Commission undertook an expert elicitation to assess the change in frequency of pipe break accidents as a function of break size. The result of that elicitation [7] was a probability density function that decreases approximately as (pipe diameter)$^{-1.5}$ in the region of large pipe diameters. Because break diameter is shown to be such a large contributor to PCT by the response surface, it is evident that the calculated PCT could be substantially reduced if credit were given for this form of the uncertainty distribution rather than for the flat distribution used in the analysis (and industry). The second largest term is radial peaking factor. The power level in the highest power fuel pin is directly proportional to this term. Not surprisingly, the cross terms for these two variables are typically large.

Based on 1,000 sets of simulated order statistics analyses with 59 case and 124 case approaches (using the response surface model developed), it was demonstrated that the order statistics approach can be used to estimate 95th percentile PCT with a predictable high degree of confidence. In addition, these analyses showed that, in the event the analyst happened to select a set of inputs that were outside the confidence range (i.e. produced a maximum PCT that was less than the true 95th percentile), the resulting under-estimate of maximum PCT is likely to be small.

NOMENCLATURE

CFR	Code of Federal Regulation
NRC	Nuclear Regulatory Commission
LOCA	Loss of Coolant Accident
LBLOCA	Large Break Loss of Coolant Accident
ECCS	Emergency Core Cooling System
PCT	Peak Clad Temperature
MSE	Mean Squared Error
CDF	Cumulative Distribution Function
PDF	Probability Density Function
SER	Safety Evaluation Report
RLBLOCA	Realistic Large Break Loss of Coolant Accident
β	Confidence level
γ	Percentile
N	Number of cases required
$\beta_0, \ldots, \beta_{14}$	Response surface coefficients
$X_1, \ldots, X_{14}$	Reponses surface input parameters
PCT	Peak clad temperature from the response surface

REFERENCES

1. Code of Federal Regulation. 10 Energy Parts 0 to 50. The Office of the Federal Register National Archives and Records Administration.

2. Boyack, B. et al. NUREG/CR-5249. Quantifying Reactor Safety Margins Application of Code Scaling, Applicability, and Uncertainty Evaluation Methodology to Large-Break, Loss-of-Coolant Accident. Prepared for the Division of Systems Research Office of Nuclear Regulatory Research U.S. Nuclear Regulatory Commission. December 1989.

3. Frepoli, C. "An Overview of Westinghouse Realistic Large Break LOCA Evaluation Model." Science and Technology of Nuclear Installations Volume 2008, Article ID 498737, 15 pages.

4. Landry, R. "Safety Evaluation on Framatome ANP Topical Report EMF-2103(P), Revision 0, "Realistic Large Break Loss-of-Coolant Accident Methodology for Pressurized Water Reactors" (TAC No. MB7554) April 9, 2003.

5. Myers, R. H. and Montgomery, D. C. Response Surface Methodology Process and Product Optimization Using Design Experiments. Second Edition. John Wiley and Sons Inc, 2002.

6. Simpson, T. W., et al. "On The Use of Statistics in Design and the Implications for Deterministic Computer Experiments." 1997 ASME Design Engineering Technical Conference. Sacramento, CA September 14-17, 1997.

7. U.S. NRC, "Framework for Development of a Risk-Informed, Performance-Based Alternative to 10CFR Part 50, Working Draft Report (Does not represent a staff position)" NUREG-1860, July 2006.