# NON-PARAMETRIC ORDER STATISTICS: PROVIDING ASSURANCE OF NUCLEAR SAFETY

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#### **ABSTRACT**

Analysis methods relying on non-parametric order statistics have been used in the nuclear industry over the past decade to provide assurance that regulatory criteria will be met in the event of a hypothetical accident. Thermal-hydraulic codes are used as a surrogate for the system being modeled, and the code is exercised within a statistical analysis framework to make predictions of the population of results that would occur in the real system. The code is reasonable representative of the real system, and non-parametric order statistics are used to demonstrate the regulatory expectation that there is high probability that the limits would not be exceeded in the event of an accident.

With a large database of large-break loss-of-coolant accident (LBLOCA) simulation results, it is possible to show the sensitivity of the peak cladding temperature (PCT) prediction to different analysis assumptions. A comparison between the known 95<sup>th</sup> quantile of the population of code predictions and the prediction for that result using various sampling techniques is made, and the conclusions are compared with expectations based on the underlying statistical theory. The effect of an imperfect code is examined to determine the degree to which claims can be made with respect to the regulatory criteria being met in the real system when there is uncertainty or variability in code predictions beyond the definition of initial and boundary conditions. It shown that, even when relying on simulated results, order statistics-based analysis techniques provide a robust solution to the engineering problem of assuring that nuclear safety will be upheld in the event of an accident.

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**KEYWORDS** 

Best-estimate, LOCA, 10 CFR 50.46, statistics

## 1. INTRODUCTION

The goal of best-estimate loss-of-coolant accident (LOCA) analysis is to provide assurance, with "high probability," that core coolable geometry is met in the unlikely event of an accident. This is done demonstrating that criteria that ensure cladding ductility and survivability are not exceeded. [1] US Nuclear Regulatory Commission (NRC) Regulatory Guide 1.157 [2] proposes that 95% probability is sufficient to satisfy this goal. This is a threshold that has generally been accepted by industry and is also typical of engineering practice outside of the nuclear field.

LOCA analyses rely on thermal-hydraulic (T-H) system codes. Under normal operations, a nuclear plant operates predictably and its behavior is well understood. It has been designed to operate in a condition that can be analyzed with precision and accuracy. Under accident scenarios, the system is taken far from

its normal operating point, and the behavior (flow regimes, heat transfer phenomena, localized effects) cannot be predicted with such precision. T-H system codes solve the complex response of the system to a postulated piping break, but rely on empirical closure relationships and use relatively coarse spatial nodalizations. As a result, the codes will inevitably contain some amount of inaccuracy (bias, consciously included to ensure conservatism and compensate for deficiencies) and imprecision (variability due to the reliance on closure relationships rather than fully resolving the T-H response to the smallest scales).

In addition to uncertainty arising from the predictive tools, there is uncertainty related to the accident itself. It is unknown when the break will occur, what the state of the plant will be, or even what the break will be. These scenario uncertainties also must be considered if one wishes to show "high probability" of success.

Given these contributors to uncertainty, the practitioner must apply some form of uncertainty analysis to arrive at a probabilistic statement of success. Many approaches are available, and several have been successfully licensed. Response surface techniques, in which a surrogate model of the system is constructed based on the predictions from the thermal-hydraulic code with changing values for the contributors to uncertainty, are limited by the ever-increasing number of simulations required to resolve the responses to the individual input parameters. These methods also can be very labor-intensive. On the other extreme, full Monte Carlo simulation provides a robust convolution of uncertainty for an unlimited number of input parameters, but requires too many simulations to make performing such an analysis practical with the complex T-H codes used for LOCA analysis (at least historically).

After Guba et al. [3] published a general framework for applying Wilks' [4] statistical theorem to safety analysis applications, best-estimate methods have gravitated toward the use of non-parametric order statistics. The state-of-the-art has been well summarized in [5], and the use of Wilks' theorem has generally been accepted and applied widely.

One such application is within the Westinghouse ASTRUM evaluation method [6], which relies on the WCOBRA/TRAC T-H code. The large break LOCA (LBLOCA) scenario has been analyzed using this methodology for a significant number of operating plants. With this database of results, an illustration of the adequacy of non-parametric order statistics uncertainty methods, and a characterization of the effects of the T-H code performance, is possible.

## 1.1 Non-Parametric Order Statistics: Theory

Guba et al. [3] developed formulations to define upper and lower tolerance limits of a population based on the non-parametric multivariate tolerance limits of Wilks [4]. Eq. 19 of [3] provides the confidence level  $\beta$  that a fraction  $\gamma$  of a population is bounded by the highest rank from a sample is given by

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

where N is the sample size. This well-known equation can be used to derive the minimum sample size N=59 needed to make a 95% probability ( $\gamma$ =0.95), 95% confidence ( $\beta$ ) prediction. The derivation of Eq. 1 arises from the more general form in Eq. 16 of [3]:

$$\beta = 1 - I(\gamma, s - r, N - s + r + 1) = \sum_{j=0}^{s-r-1} {n \choose j} \gamma^j (1 - \gamma)^{N-j}$$
 (2)

where  $\beta$  represents the confidence level that the fraction of the population  $\gamma$  is bounded by the upper and lower tolerance limits set by the samples of rank r (low rank) and s (high rank). I is the incomplete beta function defined by Eq. 17 of [3], and

$$\binom{N}{j} = \frac{N!}{j!(N-j)!} \,. \tag{3}$$

For the special case where only the upper tolerance interval is of interest (r=0), the relation can be expressed as:

$$\beta = 1 - I(\gamma, s, N - s + 1) = \sum_{j=0}^{s-1} {N \choose j} \gamma^j (1 - \gamma)^{N-j}.$$
 (4)

The sample chosen to define the upper tolerance limit can be defined as rank k, where k=1 for the highest rank of the sample, k=2 for the second rank, etc. Then s=N-k+1, and Eq. 4 becomes:

$$\beta = 1 - I(\gamma, N - k + 1, k) = \sum_{j=0}^{N-k} {N \choose j} \gamma^{j} (1 - \gamma)^{N-j}$$
 (5)

[3] also addresses the problem of multiple outcomes. If the number of outcomes of a process (or a prediction in this case) is p, and no correlation between the outcomes is assumed, then it is shown that the confidence level that the fraction  $\gamma$  of the population of the respective outcomes is bounded by upper and lower tolerance limits defined by rank  $r_p$  (low rank) and  $s_p$  (high rank) is:

$$\beta = 1 - I(\gamma, s_p - r_p, N - s_p - r_p + 1). \tag{6}$$

For a one-sided confidence interval where the highest rank is chosen,  $r_p=0$  and  $s_p=N-p+1$ , and

$$\beta = 1 - I(\gamma, N - p + 1, p + 2). \tag{7}$$

Similar to the definition in Eq. 5, if rank k is used to define the upper tolerance limit,  $s_p$ =N-p-k+2, and

$$\beta = 1 - I(\gamma, N - p - k + 2, p + k + 1) = \sum_{j=0}^{N-p-k+1} \binom{N}{j} \gamma^{j} (1 - \gamma)^{N-j}.$$
 (8)

Eq. 8 can be used to determine the sample size N, with predictor rank k, needed to support a 95% confidence level ( $\beta$ =0.95) that the 95<sup>th</sup> quantile ( $\gamma$ =0.95) has been bounded for p outcomes. Table I provides the sample size required to provide a 95/95 predictor for one or two outcomes based on Eq. 8.

The motivation for using lower ranks is described in [5]. Because the tolerance limit is an approximation to the true population, there is inherent conservatism in the typical prediction made using these techniques. Figure 7 of [5] illustrates the theoretical distribution of 95/95 predictions in relation to the true population when making predictions using Eq.5 for a single outcome. With N=59, there is a tendency to strongly over-estimate the 95<sup>th</sup> quantile of the population, a conservatism that diminishes as the size of the sample increases (and the rank used to define the 95/95 predictor decreases). However, when setting a tolerance limit using samples of any size, 95% of the analyses will over-predict the true 95<sup>th</sup> quantile, and 5% of the analyses will under-predict it. This is, in essence, the notion of confidence.

For nuclear safety applications, interest lies only in the upper tolerance limit (e.g., PCT must remain below 2200 °F (1206 °C) but has no minimum limit), but multiple figures of merit (PCT and maximum local oxidation (MLO)) are of interest. For an analysis, 95% confidence means that *both* PCT and MLO are bounded 95% of the time.

Table I. Rank k Required to Achieve 95/95 Predictor

Sample Size N	1 outcome ( <i>p</i> =1)	2 outcomes (p=2)
59	1	-
93	2	1
124	3	2
153	4	3
181	5	4

## 1.2 Non-Parametric Order Statistics: Safety Analysis Context

In the context of non-parametric order statistics methods, "high probability" has, in the US, been interpreted to mean 95% probability with 95% confidence (95/95). Or, it has been accepted that the 95<sup>th</sup> quantile must be predicted or over-predicted at least 95% of the time by the statistical method.

It is important to specify *of what* the 95/95 prediction is being made, as this will inform the analysis method itself and the interpretation of the results. For example, should one wish to demonstrate that 95% of all LOCAs that might occur during the month of January will meet the acceptance criteria, then the uncertainty distributions associated with boundary conditions sensitive to the environment, such as containment temperatures, should reflect conditions possible in January only. If it is desired that 95% of all LOCAs that occur with a particular axial power distribution meet the limits, then it would be inappropriate to treat the axial power distribution as a contributor to uncertainty.

Along these lines, the 95/95 prediction made using a T-H code must be accepted for what it is. It is a statement claiming that the 95<sup>th</sup> quantile of the outcome of interest will be equal to or less than the prediction, with 95% confidence, for the scenario and distributions of uncertainty parameters as defined *and as predicted by the T-H code*. If the T-H code is a perfect model for the real system, then the 95/95 prediction applies directly. However, this is never the case, so the practitioner is compelled to introduce biases (conservatism) to ensure that the T-H code *bounds* reality. This is the essential reason why 95/95 predictions from these analyses must be interpreted subjectively as satisfying the need to show that the real system will behave acceptably with "high probability."

#### 2. ILLUSTRATIONS

A database of analysis results generated using the ASTRUM methodology provides a reasonable test case for illustrating the predictions using non-parametric order statistics theory. Furthermore, the studies shown here illustrate the effect on the predictor conservatism that finite sample sizes, code bias and variability, and the consideration of multiple outcomes will introduce.

Fig. 1 shows the distribution of 2,725 predictions from LBLOCA analyses covering 3- and 4-loop plants. Fig. 1(a) shows the PCT distribution, 1(b) shows the MLO distribution, and 1(e) shows MLO as a function of PCT. The two are highly correlated, with a Pearson correlation coefficient of 0.723 (P-Value = 0.000), and each has a continuous cumulative distribution function. Neither distribution is normal (Figs. 1(c) and 1(d)).

Although the results represent T-H predictions for a wide range of plants, each with its own range of uncertainty distributions assumed in is respective analysis, no two values are numerically identical. This satisfies the assumption implicit in [3] that the outcome of the process is continuous.

For the illustrative studies presented here, the PCT and MLO results shown in Fig. 1 are assumed to represent the true population; they are a surrogate for the "real system." Because the database is large, the 95<sup>th</sup> quantile is known for both PCT and MLO: 1771 °F (966 °C) and 1.96%.

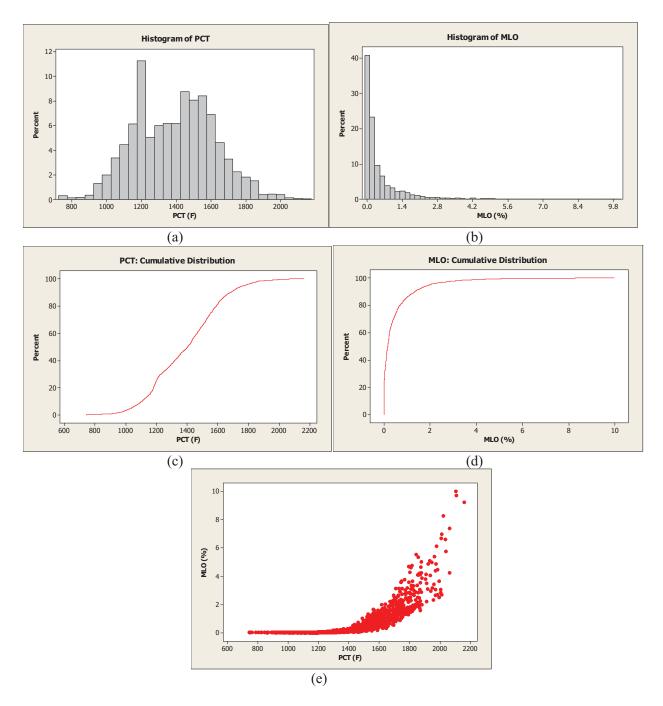


Figure 1. PCT and MLO distributions for the database. (e) Implies correlation.

## 2.1. Study 1: Illustration of Method Adequacy, Effect of Sample Size

A set of ten thousand (10,000) PCT 'analyses' are performed, each by randomly sampling from the population of results and using rank statistics to determine a 95/95 predictor. In the first set, a random sample of 59 results (N=59) is taken for each of the 10,000 analyses, and the highest rank case is chosen as the 95/95 predictor. Fig. 2 shows the distribution of analysis results along with the distribution from analyses of sample size N=124 (rank 3 is 95/95 predictor) and N=181 (rank 5).

In comparison with the true value for the 95<sup>th</sup> quantile of 1771 °F (966 °C), the mean predictions are 1921 °F (1049 °C), 1859 °F (1050 °C), and 1839 °F (1004 °C) for N=59, 124, and 181 respectively, corresponding to average levels of conservatism of approximately 150 °F (83 °C), 90 °F (50 °C), and 70 °F (39 °C). The measured standard deviation of the prediction populations – the width of the distribution shown in Fig. 2 - is an indicator of the stability of the predictor, and decreases as the sample size increases: 101 °F (56 °C) for N=59, 62 °F (34 °C) for N=124, and 46 °F (26 °C) for N=181. As expected, 5% of the predictions under-estimate the true 95<sup>th</sup> quantile regardless of the sample size used in the analyses. However, as the sample size used in the analysis increases, the severity of the under-prediction decreases as a result of the reduced standard deviation of the prediction population.

While an increase in sample size tends to move the 95/95 predictor closer to the true 95<sup>th</sup>, a reduction in the predictor is not guaranteed (Fig. 3). For most of the 10,000 analyses, the change in the predictor in going from N=59 to N=124 or N=181 samples is less than zero. For over 10% of the analyses, however, the predictor increases. For those analyses, the N=59 prediction was toward the bottom end of the range of predictors.

These observations are inherent in the statistical method itself, and reflect the disadvantage associated with using relatively small samples compared with, e.g., full Monte Carlo analysis. With limited knowledge of the true distribution around the 95<sup>th</sup> quantile of the population, bounding (conservative) tolerance limits are constructed.

The safety regulator, interested in ensuring large margins between safety analysis predictions and physical limits, prefers larger sample sizes to reduce the variation in the 95/95 predictor and to minimize the severity of the under-prediction that could occur 5% of the time. The plant operator, interested in avoiding large over-predictions that could unduly restrict plant operation, also prefers larger sample sizes. Both perspectives are well served when a large sample size is used and a stable predictor results.

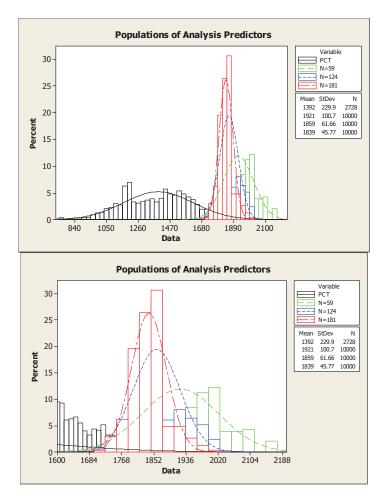


Figure 2. Distribution of 95/95 Predictors (°F) using N=59, N=124, and N=181. True 95<sup>th</sup> quantile is 1771 °F (966 °C).

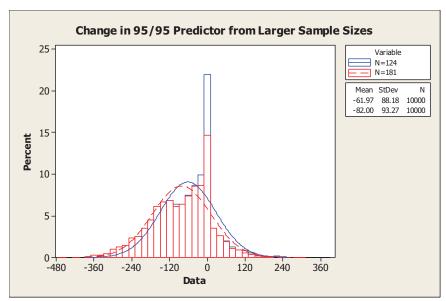


Figure 3. Distribution of 95/95 Predictor Change (°F) in Comparison to Result with N=59.

## 2.2. Study 2: Effect of Code Imprecision (Variability)

Section 2.1 discusses conservatisms introduced in the statistical method due to limited sample sizes, assuming that a sample can be taken directly from the population. In safety analysis, however, samples are generated using T-H codes that are surrogates for the real system, and the 95/95 predictor from the analysis is of the population of code predictions, not the population of results for the real system.

T-H codes suffer from some amount of imprecision, or variability, due to the coarseness of the mesh used to solve the discretized equations. Logical switches in correlations, such as those related to flow and heat transfer regimes, can be smoothed and damped with numerical ramps, but ultimately remain. Phenomenological effects, such as the predicted occurrence of rod burst, can alter the solution path in a discrete manner. As a result, the PCT predictions should be viewed as having some resolution.

This imprecision can be represented as a deviation in the prediction for a given LOCA scenario relative to the result that would occur in the real system. Here, it is represented by introducing a normally distributed error upon sampling from the population of known results.

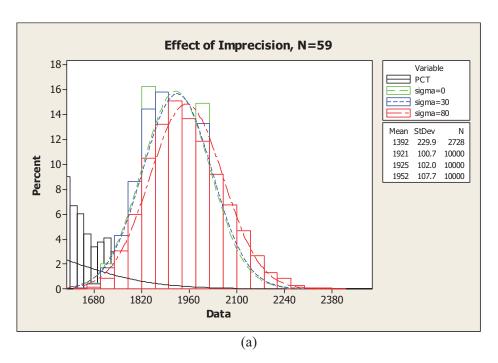
Fig. 4(a) illustrates the effect on the results with N=59. If the code is assumed to predict the true result in each simulation only within a standard deviation ( $\sigma$ ) of 30 °F (17 °C), the mean 95/95 predictor tends to increase, with a mean increase of 4 °F (2 °C). With  $\sigma$ =80°F (44 °C), the mean predictor increases from 1921 °F (1049 °C) to 1952 °F (1067 °C), a change of 31 °F (17 °C). Furthermore, the population of predictors varies more widely. A standard deviation in the predictor of 101 °F (56 °C) with no imprecision increases to 108 °F (60 °C) with  $\sigma$ =80°F (44 °C). Similar trends occur for N=181 (Fig. 4(b)); there is an increase in the mean 95/95 predictor of 26 °F (14 °C) with  $\sigma$ =80°F (44 °C), and an increase in the predictor standard deviation from 46 °F (26 °C) to 49 °F (27 °C).

The imprecision tends to disperse the population of 95/95 predictors, and shift them to higher values, but the effect on each individual analysis will vary. Fig. 5 shows the distribution of change (increase) in the 10,000 95/95 predictors when the code is assumed to include imprecision with  $\sigma$ = 80°F (44 °C). As in Fig.4, the mean increases are 31 °F (17 °C) and 26 °F (14 °C), respectively, for N=59 and N=181. However, the variation in the change is large, such that some of the 'analyses' would result in lower 95/95 predictors as a result of the imprecision. Nonetheless, the effect of code imprecision is to increase the achieved confidence level in the predictor in comparison with the true 95<sup>th</sup> quantile of the real system (see Table II). With larger sample sizes, the effect is more noticeable since the code imprecision is larger in comparison with the variation associated with the predictor itself (Fig. 2).

Imprecision, or variability, in the T-H code appears as a contributor to the conservatism associated with defining tolerance intervals with non-parametric order statistics. The sample of T-H predictions is dispersed relative to the population of results that would occur in the real system, increasing the chance that the predictor is not a good representative of the true 95<sup>th</sup> quantile. As a result, more than 95% confidence is achieved, as compared with exactly 95% if the T-H code reflected the real system with perfect precision.

Table II. Confidence Level Achieved in the Presence of Code Imprecision

Sample Size N	$\sigma = 0  ^{\circ}F$ $(0  ^{\circ}C)$	$\sigma = 30 \text{ °F}$ $(17 \text{ °C})$	$\sigma = 80 \text{ °F}$ $(44 \text{ °C})$
59	94.9%	94.9%	96.9%
124	94.9%	94.8%	97.4%
181	94.8%	94.6%	97.8%



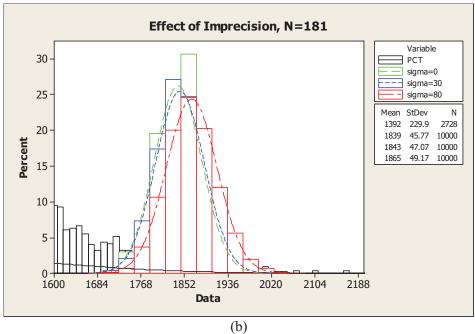


Figure 4. Distribution of 95/95 Predictors (°F) using (a) N=59 and (b) N=181 with standard deviation in each sampled result of 30 °F (17 °C) and 80 °F (44 °C).

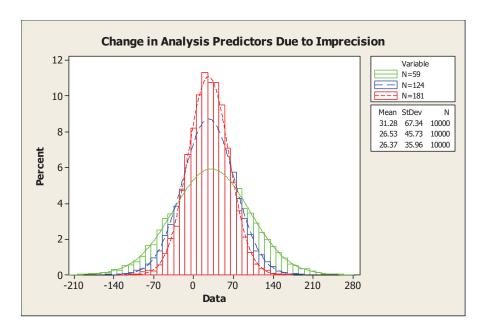


Figure 5. Change (Increase) in 95/95 Predictor (°F) Resulting from Imprecision with  $\sigma$ =80 °F (44 °C) for N=59 and N=181.

#### 2.3. Study 3: Effect of Code Inaccuracy (Bias)

In general, biases are introduced to the codes to compensate for shortcomings, less than complete understanding of the physical phenomena, or inadequate knowledge of the experimental database to which the codes are benchmarked. While some are intentionally introduced, others arise from deficiencies. The codes tend to predict conservative results even when the initial and boundary conditions are known exactly, as endorsed by Regulatory Guide 1.157.

These biases have a predictable effect on 95/95 predictions. Fig. 6(a) shows the population of predictors with N=59 samples in each of 10,000 of the analyses. Additionally, analyses are performed in which each sampled result is assumed to include a code imprecision (variability) of  $\sigma$ =30 °F (17 °C) and a code inaccuracy (bias) of 30 °F (17 °C), as well as a set with  $\sigma$ =30 °F (17 °C) and a bias of 80 °F (44 °C). Similarly, Fig. 6(b) shows the results for N=181. Compared with Figs. 4(a) and 4(b), the effect of the bias is to shift the population of predictors to higher PCT by the amount of the bias, with no effect on the standard deviation of the predictor population. In contrast with Fig.4, the effect of the bias is constant for all samples, and therefore categorically increases the predictor of every analysis.

Again, Table III shows that more than 95% confidence is achieved due to the bias in the T-H code in its representation of the real system. A constant bias tends to increase the confidence level more for analysis with large sample sizes, since the variation among predictors is smaller (Fig.2), so a larger fraction of the analyses that under-predict the true 95<sup>th</sup> quantile will over-predict it due to the bias. This result may seem trivial, but is important. When benchmarking T-H codes to experimental results, any systematic biases should be expected to directly translate to analysis conservatism, and the effect increases (rather than diminishes) as the sample size increases.

Table III. Confidence Level Achieved in the Presence of Code Imprecision and Bias

Sample Size N	$\sigma = 0 \circ F (0 \circ C)$ bias = 0°F (0 °C)	$\sigma = 30 \text{ °F } (17 \text{ °C})$ bias = 30 °F (17 °C)	σ = 30 °F (17 °C) bias = 80 °F (44 °C)
59	94.9%	97.8%	99.7%
124	94.9%	98.5%	99.9%
181	94.8%	99.0%	99.9%

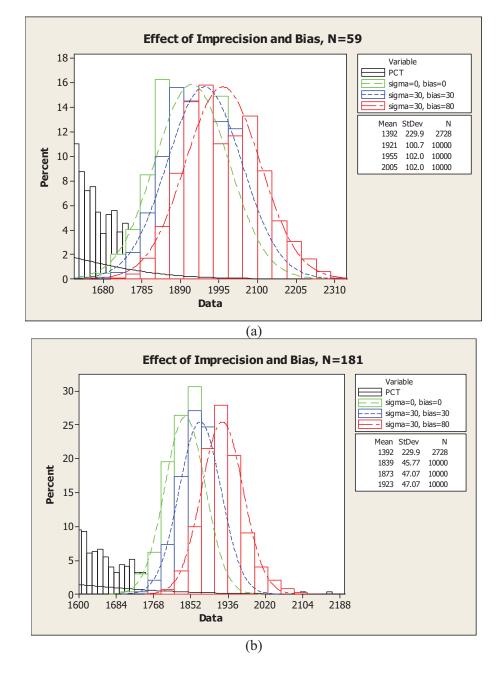


Figure 6. Distribution of 95/95 Predictors using (a) N=59 and (b) N=181 with standard deviation in each sampled result of 30 °F (17 °C), and a bias in each sampled result of either 30 °F (17 °C) or 80 °F (44 °C).

## 2.4. Study 4: Multiple Outcomes

Table I prescribes the rank statistics to make a 95/95 statement jointly about two outcomes. The populations of PCT and MLO allow for an illustration of this process. In this study, 10,000 'analyses' are performed, where pairs of PCT and MLO are taken at random from their populations (e.g., the 350<sup>th</sup> value of PCT and the corresponding 350<sup>th</sup> value of MLO) to populate a sample for each 'analysis.' For sample size N=124, the rank 2 result for both PCT and MLO is taken as the 95/95 predictor. For N=181, rank 4 is used. The confidence level is calculated as the fraction of analyses in which the predictor for both PCT and MLO bounds their respective known 95<sup>th</sup> quantile value. Additionally, rank 1 results from analyses with N=59 are examined to illustrate the effect of multiple outcomes on the confidence level. Table IV shows the results.

With N=59, the sample size is insufficient to jointly make a 95/95 predictor. While PCT and MLO are individually bounded with 95% confidence, they are jointly only bounded with 92% confidence.

When appropriate ranks are used, the confidence level exceeds 95% for the individual outcomes and the joint result. This is the result of the high degree of correlation between the outcomes (Fig. 1(e)).

The confidence level will always exceed the desired confidence level when there is correlation between the outcomes, but the magnitude by which it exceeds the desired level will be a function of the degree of correlation, the population distribution itself, and the sample size used. Table IV implies that the increased confidence is less with N=181 than with N=124. This is because the variation among analysis predictions is larger with N=124; Fig. 7 shows that the individual predictor population tends to both increase and disperse ( $\sigma$  increases) when a higher rank is chosen to accommodate the joint probability statement. The effect is lessened as the sample size increases, since more information is known about the upper portion of the population, and the change in the predictor due to a single rank in the sample is smaller.

Table IV. Confidence Level Achieved in the 95/95 Predictions for PCT and MLO

Sample Size N	PCT Only	MLO Only	PCT and MLO
59 (rank 1)*	94.9%	95.5%	92.3%
124 (rank 2)	98.8%	99.0%	98.1%
181 (rank 4)	97.9%	96.1%	96.9%

<sup>\*</sup>Rank 1 is inadequate to form 95/95 statements with N=59 (Table I)

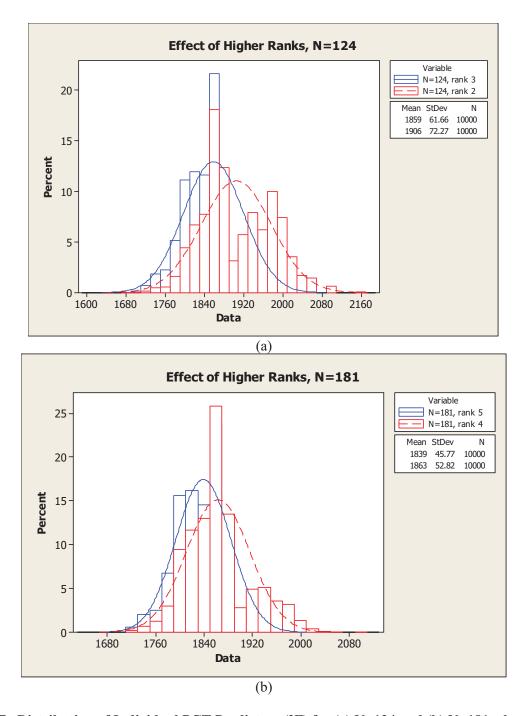


Figure 7. Distribution of Individual PCT Predictors (°F) for (a) N=124 and (b) N=181 when using a rank appropriate for a single-outcome 95/95 statement and a higher rank appropriate for a two-outcome 95/95 statement. True 95<sup>th</sup> quantile is 1771 °F (966 °C).

#### 3. CONCLUSIONS

A population of thermal-hydraulic calculation results has been used as a basis for assessing the adequacy of non-parametric order statistics for providing assurance of meeting nuclear safety limits. The following conclusions have been reached:

- Sample size: The desired confidence level can be achieved with multiple combinations of sample sizes and lower ranks. However, the use of larger sample sizes leads to predictions that tend to be closer to the true 95<sup>th</sup> quantile result. This is desirable for both practitioners and regulators.
- Code imprecision (variability): The inability of a T-H code to exactly model the response of a real system leads to some variability in predictions. This variability tends to disperse the population of predictors, and ultimately increases the confidence level of the prediction at the expense of added conservatism. This effect, in terms of the increase in confidence level, increases with larger sample sizes, since the variability associated with the T-H code increases relative to the predictor variability associated with the statistical method itself.
- Code inaccuracy (bias): When models are skewed toward conservatism to compensate for unmodeled phenomena or lack of knowledge in the physical processes, the analysis predictions categorically increase, again resulting in higher confidence levels at the expense of conservatism. For reasons similar to the effect of code imprecision, this effect increases with larger sample sizes.
- Multiple outcomes: If multiple outcomes are well correlated, the confidence level in the joint 95/95 predictors will exceed the desired level.

T-H codes are imperfect representations of the real system. However, provided that the analysis scenario is defined properly, uncertainty distributions are well defined, and only conservative biases are present in the T-H code, at least 95% confidence in the outcome of the real system will be achieved when using 95/95 predictions based on simulated results.

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