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Confirmation of Wilks' Method with TRACE Modeling of BWR Spray Cooling

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Abstract - *Wilks' formula has been popularly used to quantify the minimum amount of computational work required to meaningfully assess a model's uncertainty, due to its nonparametric statistical nature that does not require knowledge of the distribution of the qualifying parameters of interest, nor does it limit the amount of considered input uncertain parameters in the simulation model. This approach is favorable due to considerable computational expense of typical nuclear safety simulations, providing a quantifiable number of code executions that can statistically verify a desired level of safety. In this work, the U.S. NRC TRACE thermal-hydraulics code was chosen to simulate the separate-effect spray cooling tests for licensing BWR SVEA-64 fuel performed by ASEA-ATOM. Using this validated model, sets of 1000 directly-sampled TRACE models were perturbed over 31 sensitive parameters through forward uncertainty quantification using uniform and normal probability distributions for the input parameters to assess the applicability of Wilks' method in a realistic nuclear safety analysis scenario. The obtained results compare various Wilks-defined 'sample sizes' according to one-sided confidence intervals for the 1st, 2nd and 3rd-order statistics, along with the two-sided confidence interval for the 1st-order statistics. The comparison quantifies that Wilks' method is valid at the 95%/95% tolerance/confidence level as determined by the U.S. NRC for reactor safety licensing modeling.*

I. INTRODUCTION

The widespread adoption of the Best Estimate Plus Uncertainty (BEPU) methodology has encouraged the nuclear industry to pursue more realistic safety limits and accurate prediction of accident phenomena rather than the use of overly-conservative models. Advantageously, an accurate model may reveal worst-case scenarios that would result from rare triggering events not easily observable by experiment. However, there is a considerable computational expense associated with these ever-increasing high-fidelity multi-physics models. In response, Wilks' formula has been popularly used to quantify the minimum amount of computational work required to meaningfully assess a model's uncertainty by specifying acceptable tolerance limits on the model output parameter space. This method possesses certain nonparametric statistical properties that it does not require knowledge of the distribution of the output parameters of interest, nor does it limit the amount of input uncertain parameters in the simulation model [1].

In this work, the U.S. NRC thermal-hydraulics code TRACE version 5.0 Patch 4 was chosen to simulate the separate-effect spray cooling tests for SVEA-64 fuel performed by ASEA-ATOM [2]. This experiment was used to evaluate and eventually license designs for emergency spray cooling injection over SVEA-type fuel assemblies in Sweden. BWR emergency core cooling system (ECCS) designs commonly incorporate a Low-Pressure Core Spray (LPCS) system that introduces coolant through spray nozzles directed to the top of the core, located in the upper plenum region. This design is effective for LOCA response, particularly during the initial refill and reflood stages of accident response where the goal is limiting the peak cladding temperature rise in the core.

The computational model was evaluated by performing forward uncertainty quantification (UQ) using the simplest stochastic method for sensitivity analysis: direct Monte Carlo sampling. The Dakota toolbox from Sandia National Lab was chosen as the analysis tool and code driver for its well-established coupling with TRACE. In prior work, the computational model was evaluated to determine an appropriate set of sensitive parameters [3]. In the following work, an appropriately-large set of sampled model outputs is collected to provide a reference set from which Wilks' method is applied and compared.

II. METHODOLOGY

The simplest approach to stochastic sensitivity and uncertainty analysis of a model is through direct Monte Carlo sampling of uncertain parameters. Although the convergence of Monte Carlo methods is relatively slow, this issue is negligible if the only goal is to establish a tolerance limit on the range of a model's output as considered sufficient from a regulatory standpoint. Wilks' method provides a statement of the sampling parameters required for sufficient statistics. The following section provides a brief overview of the various definitions of Wilks' method as applied to uncertainty quantification of a model, as well as a description of the specific thermal-hydraulic computational model used in this analysis.

1. Wilks' Method Applied to Uncertainty Quantification

Wilks' theorem [4] provides a means of establishing tolerance limits of a sample with a certain level of confidence while disregarding the distribution of the sample through non-parametric statistics. This method allows a code uncertainty quantification study to determine whether a computational model will fulfill some acceptance criteria for any number of input uncertain parameters, each defined by any type of distribution. This approach is favorable due to considerable computational expense of typical nuclear safety simulations, providing a quantifiable number of code executions that can statistically verify a desired level of safety. The basis of Wilks' theorem makes a relatively simple statement based on ordered statistics. For a given number of code runs n that results in a scalar quantity of interest y_i, the total set of output quantities can be put in order of increasing value (y_1, y_2, y_3... y_n) such that a probability distribution $f(y)$ and cumulative distribution $P(y)$ of the output could be determined. Suppose that from all possible model outputs, a tolerance limit α is specified for which the most extreme quantity (y_n) must lie beyond this value, with the intention that a conservative model will reliably represent the most extreme case within the n set of outputs. This limit can be further qualified with a confidence level β to indicate the stability or reliability of the first-ordered statistic from the n set of outputs. The attractiveness of this method lies in the fact that with random sampling of any number of inputs, regardless of their distribution, a set number of code runs can be determined such that the most extreme model output value (i.e. worst-case scenario) can be certified to be represented beyond a specified tolerance limit of all infinite possibilities of random samplings with a certain level of confidence.

The original Wilks formula determines the sample size n for a single first-ordered statistic (e.g. a maximum or minimum) of the figure-of-merit quantity. For a one-sided first-order statistic tolerance limit, the necessary sample size n for a given tolerance limit (percentile) α at a confidence level (stability) β is defined in eq. 1 for the first-order:

$$1 - \alpha^n \geq \beta \tag{1}$$

Beyond the first-ordered statistic (e.g. maximum), the additional r-th order minimum sample size n (e.g. 2nd-maximum value) is defined by eq. 2:

$$1 - \sum_{k=0}^{n} {}_nC_k \alpha^{n-k} \left(1-\alpha\right)^k \geq \beta \tag{2}$$

For the two-sided centered tolerance limit, where the confidence interval α is centered along the continuous variation of the sample (the interval between (1- α)/2 and (1+ α)/2), the minimum sample size n is defined in eq. 3 [5]. This method would be used in the case where the output parameter has both a minimum and maximum limit.

$$1 + \alpha^k - 2a^n \sum_{k=0}^{n} {}_nC_k \left(\frac{1-\alpha}{2\alpha}\right)^k \geq \beta \tag{3}$$

In practice, the most pertinent methods for nuclear regulatory licensing is defined by eq. 1 and 2 for the one-sided tolerance intervals, as most quantities of interest have a specified maximum regulatory criterion (e.g. peak cladding temperature, cladding oxidation level, etc.)

2. SVEA Spray Cooling Experiment

The experiment modeled in this work was performed by ASEA-ATOM as a joint project with the Swedish Nuclear Power Inspectorate and the Swedish State Power Board to evaluate and license BWR spray cooling systems in a simulated full-size SVEA-64 fuel assembly [2]. The test bundle consisted of 64 Inconel-clad nichrome coil heater rods each equipped with thermocouples at 5 axial locations, and were arranged in standard SVEA spacers (Figure 1). The spray system consisted of 6 individual spray lines: one spray nozzle for each sub-bundle of the assembly (four total), one spray distributor for the water cross, and one line for the bypass region. Test 012 [2] had each of the four 4x4 sub-bundles receiving 40 g/s of spray flow injection, the bypass receiving 130 g/s of spray, and the water-cross receiving 10 g/s of spray flow.

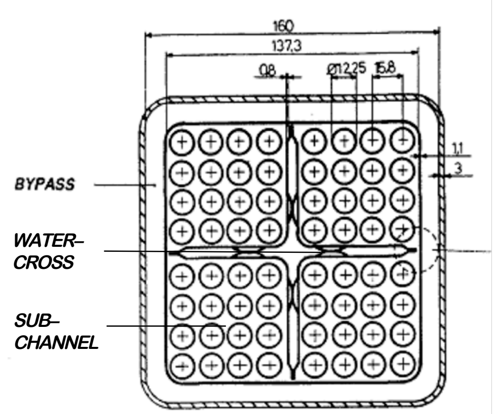

Fig. 1. Test bundle simulating a SVEA-64 assembly [2].

3. Development of the Uncertainty Quantification Model

The SVEA spray cooling experiment was modeled with a best-estimate plus uncertainty approach by using available codes suitable for this methodology. The thermal-hydraulics modeling was developed using the U.S. NRC-supported code TRACE version 5.0 Patch 4. Dakota version 6.2 from Sandia National Laboratory was chosen as the code driver for the uncertainty analysis of the developed TRACE model. Forward UQ was performed by propagating the specified TRACE model input uncertainties through the code and measuring the response on an output parameter, which is the peak cladding temperature (PCT) in this study (Figure 2). For the developed SVEA spray cooling experiment TRACE model, 31 total sensitivity parameters were identified and their uncertainties appropriately determined from original literature or from similar uncertainty quantification studies. Eight parameters were related to thermal-hydraulics parameters from the experiment (pressures, temperatures, and mass flows), sixteen parameters were related to user-defined model parameters (geometries and models for radiation heat transfer and counter-current flow limiting), and seven parameters were related to physical closure laws for heat transfer and drag relevant to TRACE reflood simulation [3].

Table 1. Uncertainty quantification parameters [3].

Parameter	Reference	Uncertainty*
Thermal Hydraulic Initial Parameters		
Spray system pressure	2 bar	0.1 bar
Spray system temperature	323 K	0.75%
Bundle spray mass flow	20-80 g/s	1%
Bypass spray mass flow	65-130 g/s	1%
Water cross spray mass flow	10 g/s	1%
Water drain temperature	323 K	0.75%
Steam vent temperature	393 K	0.75%
Outlet pressure	2 bar	0.1 bar
Vessel-related parameters		
Bundle wall roughness	1×10^{-6} m	30%
Bypass wall roughness	1×10^{-6} m	30%
Water-cross wall roughness	1×10^{-6} m	30%
Length of main channel	3.68 m	0.01 m
Length of bypass channel	3.68 m	0.01 m
Length of water-cross	3.68 m	0.01 m
Bundle-related parameters		
Bundle flow area	2.428×10^{-3} m^2	1%
Bundle hydraulic diameter	0.01114 m	1%
Bypass channel flow area	6.14×10^{-3} m^2	1%
Bypass hydraulic diameter	0.0884 m	1%
Water Cross flow area	1.612×10^{-3} m^2	1%
Water Cross hydraulic dia.	0.0453 m	1%
Rod emissivity	0.45	0.10
Bundle wall emissivity	0.30	0.10
CCFL slope	1.0	0.80-1.0
CCFL constant	1.0	0.88-1.0
Heat Transfer Coefficients (TRACE physical models)		
DFFB Wall-Liq. HTC	1.0	45%
Wall Liquid HTC	1.0	15%
Wall Vapor HTC	1.0	20%
DNB/CHF	1.0	8%
Interfacial Drag Coefficients (TRACE physical models)		
Annular-Mist Intf. Drag	1.0	25%
DFFB Interfacial Drag	1.0	40%
Wall Drag	1.0	5%

*Uncertainty value references can be found in [3].

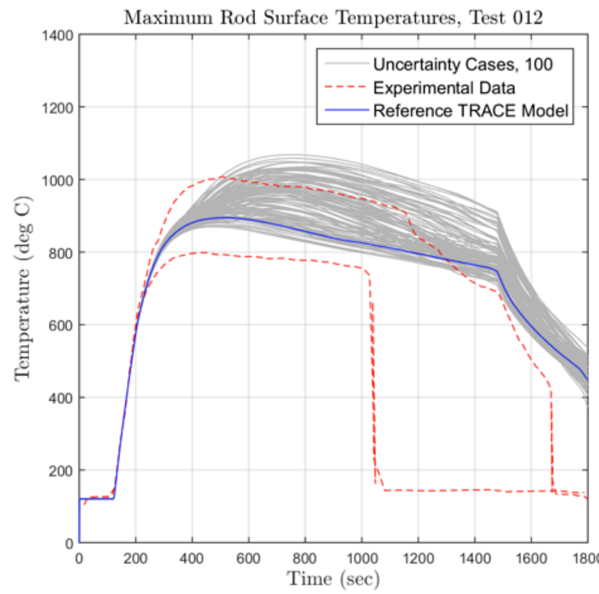

Fig. 2. Peak cladding temperatures for 100 forward-UQ sampled TRACE models of Test 012 compared to the reference model and the experiment data range [2].

The uncertainty analysis of the TRACE model using Dakota is performed in the following procedure:

1. A TRACE reference model is developed with a list of input parameters and their uncertainty distributions.
2. Dakota randomly samples each input parameter and generates a user-defined number of TRACE inputs.
3. Each generated TRACE input is executed, and the output parameters (a scalar quantity of interest) are extracted from each simulation result. Although each TRACE input must be executed in serial, multiple models can be simultaneously run in parallel according to available computational resources.
4. Dakota takes the output parameters and the sampled input parameters and returns the output parameter uncertainty distribution and the correlations and rankings of the sensitivity of the input parameter uncertainties on the output parameters.

4. Confirmation of Wilks' Method Using the Uncertainty Quantification Model

Using the validated TRACE model, the applicability of Wilks' method was assessed by performing direct Monte Carlo simulation to generate a sufficiently large sample of the propagated input uncertainties for comparison. In the original validation UQ work, the input parameters were defined with uniform distributions to assume no knowledge of the uncertainty. In order to assess Wilks' method, a second input parameter distribution defined over consistent variances was added for comparison. For each type of distribution, 1000 TRACE models were generated from random sampling of the input parameters, executed, and collected to determine the PCT (Figure 3). From the sets of 1000 PCT values, the "true" 95th percentiles (tolerance limits) were determined (Table 1). The present study only examines a single parameter (PCT) for the figure-of-merit, although multiple may be relevant for safety limits [1].

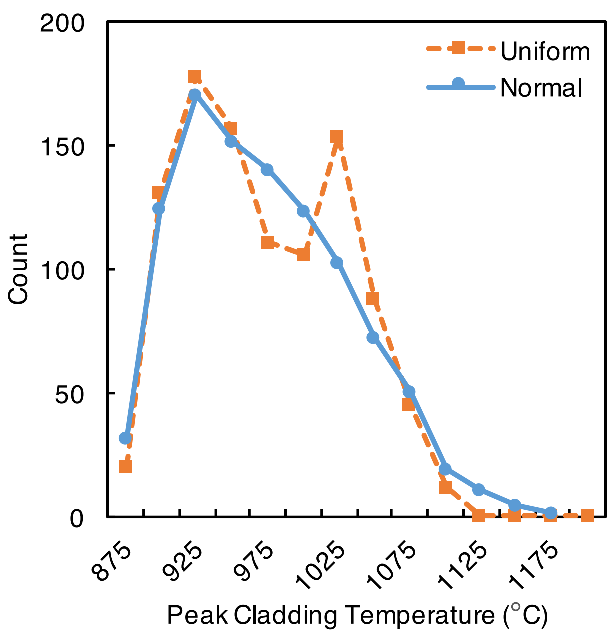

Fig. 3. Distribution of peak cladding temperatures from 1000 sampled UQ cases of the TRACE model for two different input parameter probability distributions

Using Wilks' method to determine the sample sizes for both one-sided *r*-th order and two-sided first-order at 95% tolerance / 95% confidence (as suggested by the US NRC [1]), the sets of 1000 PCT values were randomly sub-sampled 100 times, and the maximum (or minimum) values of those sub-sampled "Wilks sets" were compared to the "true" 95th percentile. The number of randomly sub-sampled "Wilks sets" that did not lie beyond the 95% tolerance limit was then compared to the 95% confidence requirement. If Wilks' theorem holds, then at least 95 of the 100 sub-sampled sets should have included at least one PCT value (or more, depending on the *r*-order) that exceeds the 95th percentile of the total set of 1000 PCT values. For the two-sided tolerance interval, at least 95 of the 100 sub-sampled sets should have included one PCT value that lies above the upper 97.5th percentile and one PCT value that lies below the lower 2.5th percentile (for a 95% tolerance interval) [4].

III. RESULTS AND DISCUSSION

The TRACE model was propagated extensively through forward UQ methods using two probability distributions, with the PCT from the whole transient collected as the output figure-of-merit. Comparing the TRACE + UQ results to the experiment data (Table 2), the simulation maximum PCT overlaps the experiment data for every distribution type to various degrees. The maximum PCT had greater over-prediction for the normal distribution, most likely due to the longer distribution tail length that had more evident effect on certain sensitive input parameters. This is also observed in the distribution of the collected PCT (Figure 3). This behavior is consistent with the present TRACE model as the simulation showed a tendency to spread towards the upper range of PCT across the transient (Figure 2). For both distributions, the mean PCT was consistently over-predicted by 70°C compared to the experiment average PCT, demonstrating that the validated TRACE model is conservative. The 95% tolerance limits were determined from these sets of data, for the one-sided upper bound and the two-sided upper and lower bounds (at the 97.5th and 2.5th percentile).

Using the two collected sets of data, the minimum meaningful sample size according to Wilks' theorem (Equations 1-3) was determined for the one-sided tolerance interval first, second, and third orders, as well as the two-sided tolerance interval first order according to the 95%/95% tolerance/confidence level required by regulation set by the US NRC. From each set of 1000 PCT values, a sub-sample was randomly collected 100 times, and the maximum PCT from that sub-sample was determined. These results are shown graphically in figures 4 and 5.

Table 2. Comparison of peak cladding temperature statistics from 1000 sample UQ cases of the TRACE model for two different input parameter probability distributions, compared to Test 012 experiment data [2].

Peak Cladding Temperature (°C)	***Test 012 Experiment***	**Uniform Distribution**	**Normal Distribution**
Max. Value	1007	1092	1173
95% T.L. (Upper)	--	1054	1065
Mean	887	960	961
Median	--	953	957
Std. Dev.	--	55	59

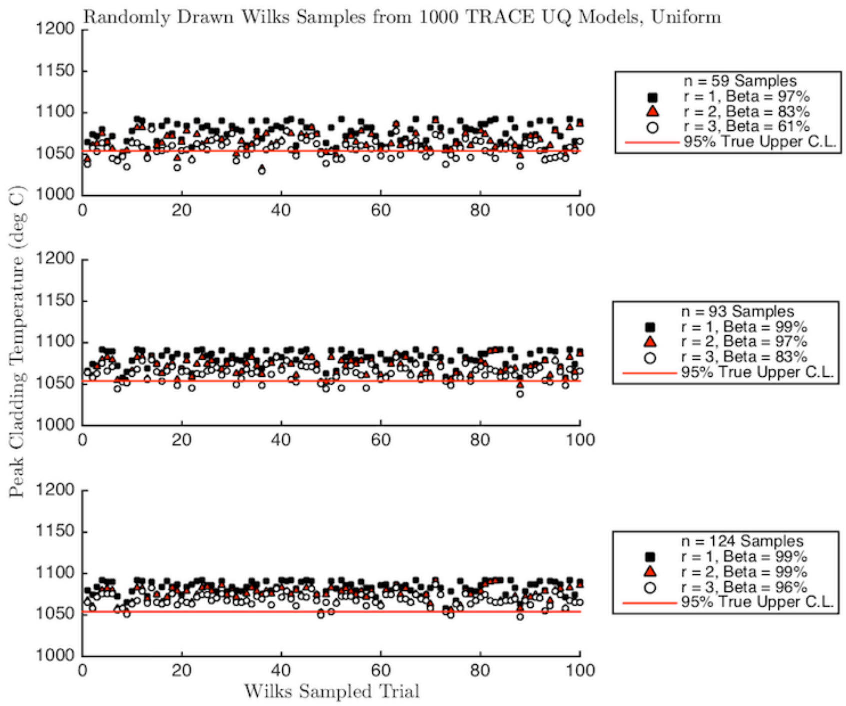

Fig. 4. Assessment of the validity of Wilks' method applied to collected sets of 1000 TRACE UQ models with assumed uniform distribution on the input parameter uncertainty. The first three ordered-statistics (peak cladding temperature) are plotted for each set of *n* samples and compared to the 95% tolerance limit from the total set of 1000 samples.

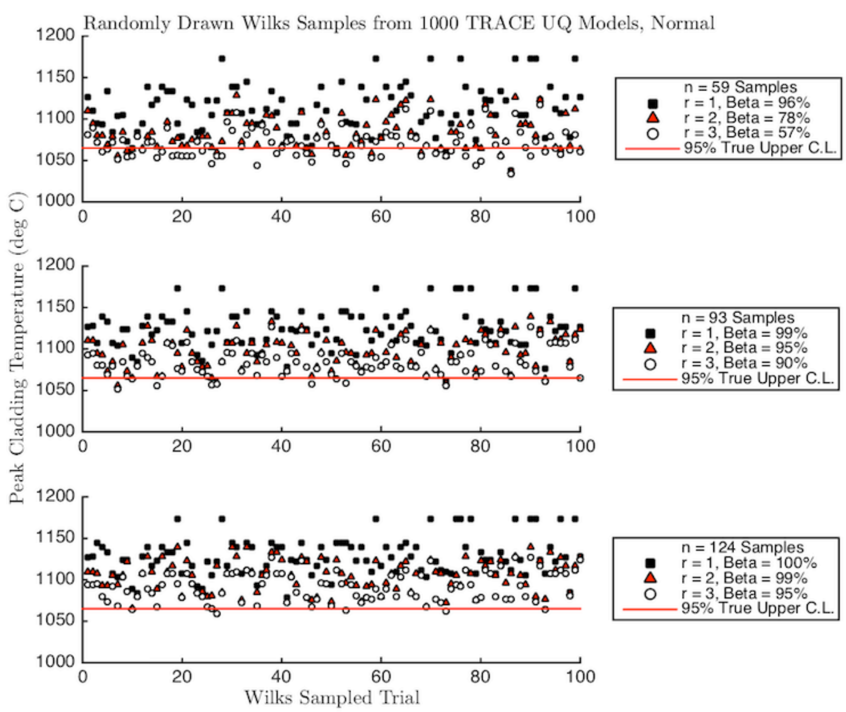

Fig. 5. Assessment of the validity of Wilks' method applied to collected sets of 1000 TRACE UQ models with assumed normal distribution on the input parameter uncertainty. The first three ordered-statistics (peak cladding temperature) are plotted for each set of *n* samples and compared to the 95% tolerance limit from the total set of 1000 samples.

Table 3. Number of Wilks' sampled cases that included *r*-th order PCT(s) beyond the 95% tolerance limit out of 1000 trials.

Wilks *r*-th order formula	**Determined Sample Size *n***	**Uniform distribution**	**Normal distribution**
One-sided 1st-order	59	949	948
One-sided, 2nd-order	93	955	958
One-sided, 3rd-order	124	956	965
Two-sided, 1st-order	146	968	965

Those maximum PCT values were compared to the 95% upper tolerance interval of the larger set, and the number of times the Wilks' set under-predicted the tolerance interval was counted to determine whether the confidence level β was at least 95%. For $r = 2$ and 3, the second-max and third-max values were compared. Figures 4 and 5 confirm that Wilks' method holds for the one-sided *r*-th order provided the appropriate minimum sample size *n* for that order, regardless of the input parameter probability distribution. The sampling exercise was increased to collect 1000 sub-samples in the same manner, for the one-sided and two-sided tolerance intervals, as shown in Table 3. Out of 1000 collected sub-samples, at least 950 trials should include at least one or more PCT values above the 95% upper tolerance interval (one-sided), or contain at least one PCT value above the 97.5% upper tolerance interval and one PCT value below the 2.5% lower tolerance interval (two-sided) for Wilks' theorem to be valid. In the two-sided case, this statistic will provide a tolerance limit bound for the prediction of PCT, but only the maximum value (one-sided) is relevant when performing a comparison against the regulatory acceptance criterion. For every case, the theorem holds, although to less conservative degree for lower orders.

In addition, a Spearman partial rank correlation was performed to determine the order and impact of the most sensitive input parameters. Across both distributions, the order of the seven most significant parameters was consistent, as shown in Table 4. This comparison is important for determining if a change in input parameter probability distribution also changes that parameter's impact on the output quantity significantly or adversely. In this case, changing the distribution from uniform to normal results in the higher-ranked parameters having greater impact on the prediction of peak cladding temperature, most likely due to the long tail of the distribution. All parameters maintain their monotonic relationship, which is expected.

From these observations, it is evident that the one-sided first-order equation is sufficient for a computational model to conservatively and qualitatively confirm a safety limit. If each code simulation is reasonably inexpensive, higher orders and larger sample sizes according to Wilks' theorem can be used to more accurately determine the model output parameter value at the specified tolerance level, as successive orders will yield values that are closer a model's "true" uncertainty tolerance limit (Figures 4 and 5). However, from a licensing evaluation standpoint, such higher orders would not be beneficial, as the most extreme case value of a model is the necessary value to assert that a computational model is fully conservative while also predicting that the modeled system will fall within the assessed acceptance criteria.

IV. CONCLUSIONS

The overall results of this work confirm that Wilks' method is valid and consistent not only in theory but also when applied to a validated computational simulation of a realistic scenario nuclear safety experiment. The results confirm that the number of uncertain input parameters (dimensionality) as well as the particular probability distribution of the input and output parameters do not affect the validity of Wilks' method. These qualities make this

Table 4. Comparison of Spearman ranking of the most sensitive model parameters from the sets of 1000 TRACE UQ models. Positive rank values indicate a positive increase on the modeled peak cladding temperature, whereas negative rank values indicate an inverse effect on the modeled peak cladding temperature, with 1.0 being the highest possible rank value.

Parameter	**Uniform distribution**	**Normal distribution**
Counter-current Flow Limit (CCFL) Constant	-0.96	-0.96
Rod Surface Emissivity	-0.67	-0.72
Counter-current Flow Limit (CCFL) Slope	0.63	0.70
Dispersed Flow Film Boiling (DFFB) Wall-Liquid HTC	0.59	0.62
Outlet Pressure	-0.40	-0.33
Wall Surface Emissivity	-0.37	-0.30
Wall Vapor Heat Transfer Coefficient	0.32	0.24

methodology very attractive considering the computational cost often required, establishing a reasonable amount of simulation work needed to meaningfully assess a safety limit while considering model uncertainties [1]. Furthermore, the results indicated that in typical scenarios, only the one-sided first-ordered Wilks' method is needed to make an assessment to acceptance criteria.

Although the current regulation criteria are defined by single-quantity limits for which one-sided tolerance limits are sufficient, future criteria may include limits for which a quantity must fall within a specified range of values, requiring a two-sided tolerance limit approach. In the present modeled scenario, the time-to-quench is another relevant quantity of interest that would be represented with a two-sided tolerance limit, and should be investigated further. It is also possible that other types of input distributions (log-normal, etc.) may have an impact on the validity of Wilks' method as presented and should also be considered. Arguments have been made that multiple acceptance criteria in a model should be considered simultaneously as a single output parameter [1], indicating that Wilks' method could effectively hold for any number of both input and output parameters. This would be a possible area of further study and of importance to multi-physics modeling. Lastly, further work should also investigate the possible relevance of cross-correlation between input parameters and their effect on this methodology for various models, as well as confirm this methodology for determining the minimum sample sizes for multiple output figures-of-merit.

NOMENCLATURE

α = tolerance limit (percentile)
β = confidence level (stability)
n = sample size
y = model output parameter value

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