Validating TRACE Void Fraction Predictive Capability Using the Quantitative Area Validation Metric

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INTRODUCTION

The work presented in this summary primarily focuses on using **quantitative validation metrics** to perform model validation. **Validation** is the process of determining the degree to which a model is an accurate representation of the real world from the perspective of the intended uses of the model [1]. Even though there is a growing interest in performing validation and a sizeable literature on this topic among the nuclear community, most of them often did little more than "we found that the model output agrees well with measurement data by plotting them together". Such an approach is often referred to as "**graphical validation**". However, graphical comparison is insufficient for assessing the accuracy of computer models because it is only qualitative. For model validation, a general applicable quantitative metric is preferred which quantifies the degree of accuracy of the computer model.

Validation metrics should be used to replace graphical comparisons for a more rigorous validation process. **Validation metrics** are quantitative measure of the level of agreement, or consistency, between computational results and experimental data. Ferson and colleagues [2] proposed the "**area validation metric**", which considers uncertainties in both computational results and measurement data. The area metric is objective, robust, unbounded, and applicable even when the data is very sparse and retains the physical units of the data. In this paper, the area metric will be used to validate the void fraction predictive capability of nuclear reactor system thermal-hydraulics code TRACE [3], using experimental data from the OECD/NEA NUPEC BFBT benchmark [4].

THE AREA METRIC

The **area validation metric** [2] uses the "area" between the Cumulative Distribution Functions (CDFs) of computational results and experimental data as a measure of the disagreement between model and data. Consider a general computer model $y = y^{\mathrm{M}}(\mathbf{x}, \boldsymbol{\theta})$ where y is the output, $\mathbf{x}$ is the vector of design variables, and $\boldsymbol{\theta}$ is the vector of calibration parameters. The CDF of computer simulations can be directly achieved by the forward Uncertainty Quantification (UQ) process, in which the uncertainties in either $\mathbf{x}$ or $\boldsymbol{\theta}$, or both are propagated to the outputs via the computer model using techniques like Monte Carlo sampling. The CDF of measurement data is usually constructed by the empirical CDF of the observation data points.

Define the CDFs for **m**odel and **e**xperiment as $F^{\mathrm{M}}(y)$ and $F^{\mathrm{E}}(y)$ respectively. The area metric $d(F^{\mathrm{M}}, F^{\mathrm{E}})$ is defined as:

$$d(F^{\mathrm{M}}, F^{\mathrm{E}}) = \int_{-\infty}^{\infty} \left| F^{\mathrm{M}}(y) - F^{\mathrm{E}}(y) \right| dy \quad (1)$$

The resulting metric $d(F^{\mathrm{M}}, F^{\mathrm{E}})$ has the same physical unit with y. Therefore it can be viewed as a direct measure of the model prediction error. Given the same observation data, a smaller area metric value means a more accurate prediction of the data. Figure 1 demonstrates the area metric for cases when the measurement data is sufficient, limited and minimum (a point value). As the CDF of the model simulation is calculated based on forward uncertainty propagation, we usually have enough samples to achieve a smooth CDF for the outputs.

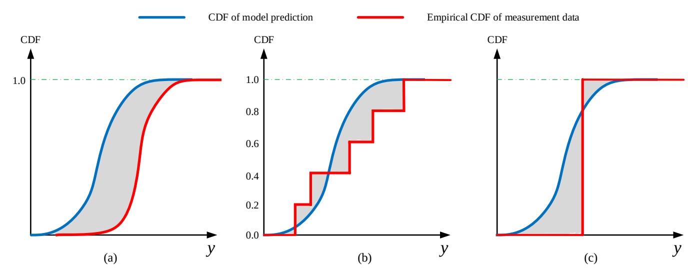

Fig. 1: Demonstration of area metric when (a) experimental data are sufficient and the empirical CDF is smooth; (b) experimental data are limited; (c) only one experimental data point is available.

THE "U-POOLING" METRIC

The area metric also includes a "**u-pooling**" method [2] which is designed for cases when data are measured at multiple validation sites (input settings). Note that the validation sites are defined by the design variables. The original area metric as shown in Figure 1 is defined for a single validation site. In presence of multiple validation sites, each validation site will result in an area metric value. These values can be very distinct in magnitude, making it difficult to draw a conclusion about the "**global**" validity of the computer model that can account for contributions from all the validation sites.

The underlying idea of "u-pooling" is univariate Probability Integral Transformation (PIT), which states that any continuous random variable Y can be converted to a standard uniform random variable U using the CDF of Y: $U = F_Y(Y) \sim \mathrm{Uniform}(0, 1)$. If the computer model is perfectly accurate, then the measurement data can be treated as random samples drawn from the probability distribution of computed outputs. Therefore, PIT of an observation data point using the corresponding computational output CDF will produce a sample from Uniform(0, 1). Here by "corresponding" we mean that the measured and computer output are from the same validation site. If we repeat the process for many observation data points, we get a collection of transformed, or "pooled" samples that should all follow Uniform(0, 1). The empirical CDF of these "pooled" samples and the CDF of Uniform(0, 1) can be compared to produce a single aggregate metric, which includes contributions from every validation site.

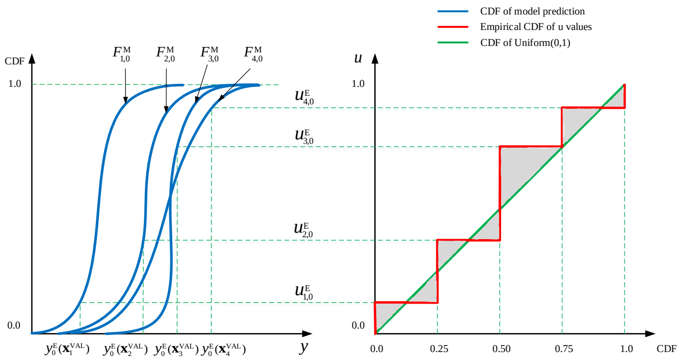

Fig. 2: Demonstration of "u-pooling" area metric evaluation at four validation sites.

Figure 2 demonstrates an example using the "u-pooling" process. Given observation data points at four input settings $\left\{y_0^{\mathrm{E}}(\mathbf{x}_i^{\mathrm{VAL}}), i = 1, 2, 3, 4\right\}$, each input setting has only one observation data. The subscript "0" stands for single output. The corresponding CDF of model outputs are $\left\{F_{i,0}^{\mathrm{M}}, i = 1, 2, 3, 4\right\}$. For each of the observation data points, we calculate a u-value:

$$u_{i,0}^{\mathrm{E}} = F_{i,0}^{\mathrm{M}}\left[y_0^{\mathrm{E}}(\mathbf{x}_i^{\mathrm{VAL}})\right], i = 1, 2, 3, 4 \tag{2}$$

The area between the empirical CDF of these u-values and the CDF of Uniform(0, 1) is calculated as the aggregated validation metric, as shown in the shaded area of Figure 2. Such a metric value accounts for the overall discrepancy between model and experiment from multiple validation sites. After "u-pooling", the area metric value is no longer unbounded. The minimum value of the validation metric is 0, indicating a perfect match, while the maximum value is 0.5, indicating the worst agreement.

APPLICATION TO TRACE

In BFBT benchmark assembly 4, cross-sectional averaged void fractions were measured at four different axial locations, hereafter referred to as `VoidF1`, `VoidF2`, `VoidF3` and `VoidF4` respectively from lower to upper positions. The design variables $\mathbf{x}$ consists of four parameters: pressure, mass flow rate, power and inlet temperature. The calibration parameters $\boldsymbol{\theta}$ consists of five physical model parameters, including `P1008`, `P1012`, `P1022`, `P1028` and `P1029`, as shown in Table I.

TABLE I: Selected TRACE physical model parameters

Parameter (multiplication factors)	Symbol
Single phase liquid to wall HTC	`P1008`
Subcooled boiling HTC	`P1012`
Wall drag coefficient	`P1022`
Interfacial drag (bubbly/slug Rod Bundle - Bestion) coefficient	`P1028`
Interfacial drag (bubbly/slug Vessel) coefficient	`P1029`

All of the five calibration parameters are multiplicative factors with nominal values of 1.0. Note that TRACE includes user access to 36 physical model parameters [5]. Those reported in Table I are selected after dimensional reduction using local/global Sensitivity Analysis (SA). The removed 31 physical model parameters are either inactive or have negligible importance for BFBT benchmark. See [6] for the detailed dimensional reduction process. In an earlier work (chapter 7 of [5]), the uncertainties associated with these five physical model parameters were inversely quantified in an inverse UQ process under the Bayesian framework. The posterior distributions (inversely quantified input uncertainties) are shown in Figure 3. The prior distributions are chosen as uniform distributions over the range of (0, 5) for all the parameters.

The validation data from BFBT are included in Table III. Note that there are 86 test cases in BFBT test assembly 4. In our earlier work [5], 59 tests are selected for validation following a sequential test source allocation algorithm. All the measurement data are treated to have 2% measurement noise relative to the provided void fraction values. Negative void fractions (non-physical) are treated as zero in validation.

The original area metric and the "u-pooling" technique are applied for TRACE model using prior/posterior distributions of $\boldsymbol{\theta}$. Since the prior has much larger uncertainties than the posterior, the results can be used to investigate that whether these validation metrics are capable of differentiating models containing more (prior) and less (posterior) uncertainties.

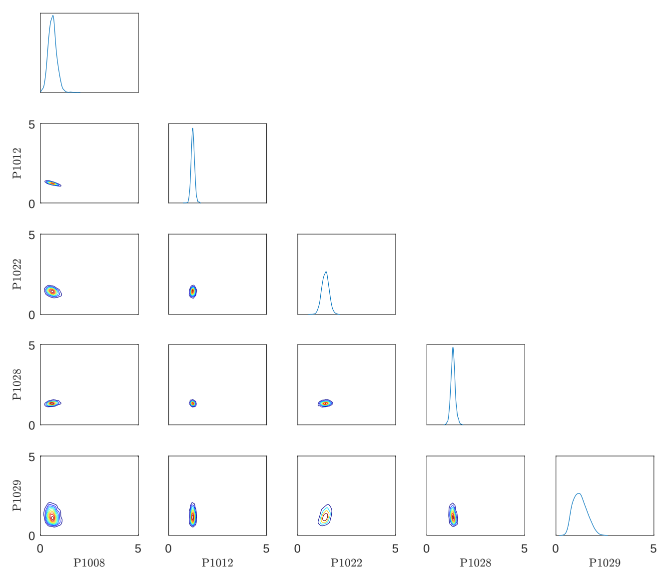

Fig. 3: Posterior joint and marginal densities of $\boldsymbol{\theta}$.

Table III shows the validation results for each of the 4 outputs at each of the 59 validation sites, using the original area metric. Figure 4 visualizes the results. It is demonstrated that the metric values for TRACE using posterior is smaller than TRACE using prior. Therefore, it can be concluded that the original area metric is capable of differentiating models containing more and less uncertainties.

Table II shows the validation results for each of the 4 outputs using the "u-pooling" method, which have contribution from all of the 59 validation sites. However, it shows the TRACE with prior is more "accurate" (smaller metric values) than TRACE with posterior. The reason is that, transformed

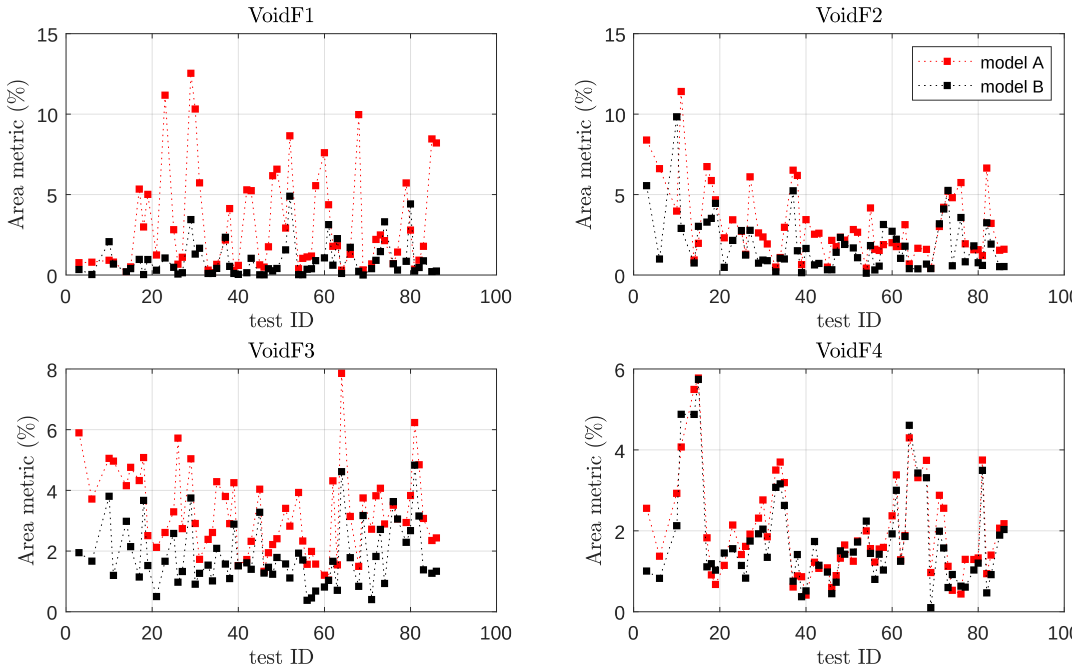

Fig. 4: Validation results at each validation site for each output using the area metric (model A/B are TRACE with prior/posterior).

data samples on the U-space do not necessarily produce small area metric values even when the computer model is very accurate. If the accurate model contains small input uncertainties, the model prediction uncertainties ranges will also be small, which are unlikely to "envelop" the observation data points. Consequently, the "pooling" process by univariate PIT using the CDF of such outputs will produce a large amount of 0's and 1's on the U-space. Therefore, the area between empirical CDF of these values and the CDF of Uniform(0, 1) will be large.

TABLE II: Validation results for each output using the "u-pooling" area metric.

outputs	TRACE using prior	TRACE using posterior
`VoidF1`	0.1256	0.2049
`VoidF2`	0.0438	0.2108
`VoidF3`	0.1696	0.2471
`VoidF4`	0.0812	0.2384

CONCLUSIONS

In this summary, we applied the area metric and the "u-pooling" metric [2] for the validation of TRACE based on BFBT steady-state void fraction data. Posterior distributions (with smaller uncertainties) from an earlier inverse UQ work [5] are used as input uncertainties for TRACE. TRACE using prior distributions (with larger uncertainties) is also considered for comparison. The validation results shows that the original area metric is capable of differentiating models containing more and less uncertainties, while the "u-pooling" metric fails to do so. In this work, the four outputs are all validated separately, without considering their dependence. In the future, the area metrics will be improved for multiple correlated outputs.

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TABLE III: Void fraction measurement data, and validation results at each validation site for each output using the area metric.

test ID	Void fractions measurement data				Validation results: TRACE with prior				Validation results: TRACE with posterior			
	VoidF1	VoidF2	VoidF3	VoidF4	VoidF1	VoidF2	VoidF3	VoidF4	VoidF1	VoidF2	VoidF3	VoidF4
3	-0.40	31.92	59.27	71.40	0.77	8.39	5.90	2.56	0.34	5.55	1.95	1.01
6	-0.90	7.00	48.42	66.80	0.80	6.61	3.71	1.37	0.03	1.00	1.67	0.83
10	-0.70	2.50	44.58	70.10	0.92	3.97	5.05	2.93	2.07	3.83	3.81	2.13
11	-1.00	12.30	59.08	76.60	0.80	11.41	4.96	4.07	0.68	2.90	1.20	4.88
14	-0.10	0.90	19.70	30.40	0.19	0.94	4.15	5.49	0.20	0.75	2.98	4.88
15	0.00	17.20	35.95	47.30	0.51	1.97	4.76	5.78	0.40	3.03	2.15	5.74
17	6.90	42.62	60.62	67.40	5.34	6.74	4.32	1.83	0.97	3.29	1.15	1.11
18	19.30	55.73	67.51	75.50	2.99	5.87	5.08	0.91	0.03	3.52	3.67	1.19
19	32.10	65.66	76.17	81.00	5.01	4.68	2.51	0.68	0.96	4.45	1.52	1.03
21	0.30	19.57	44.11	56.20	1.24	2.31	2.12	1.15	0.30	0.48	0.50	1.45
23	14.30	51.73	69.56	74.50	11.18	3.43	2.61	2.14	1.06	2.15	1.66	1.56
25	40.66	74.78	83.26	84.70	2.82	2.72	3.29	1.42	0.48	2.76	2.58	1.14
26	-1.00	-0.60	19.20	36.90	0.67	1.29	5.72	1.62	0.06	1.24	0.97	0.83
27	-0.70	19.00	45.79	57.70	1.10	6.10	2.74	1.92	0.14	2.78	1.33	1.75
29	15.20	55.54	72.61	75.70	12.54	2.62	5.04	2.31	3.45	0.74	3.75	1.93
30	25.30	65.85	77.76	82.10	10.32	2.37	2.91	2.76	1.30	0.93	0.91	2.04
31	37.06	72.41	81.46	86.10	5.73	1.93	1.73	1.85	1.66	0.89	1.27	1.34
33	-0.20	0.20	12.20	21.20	0.30	0.50	2.39	3.50	0.10	0.20	1.54	3.07
34	0.00	8.00	24.85	35.60	0.15	1.09	2.61	3.70	0.10	1.04	1.02	3.16
35	0.20	19.13	36.32	46.90	0.66	2.97	4.29	3.19	0.41	1.00	2.09	2.63
37	9.90	41.69	59.27	66.40	2.18	6.52	3.80	0.61	2.35	5.24	1.57	0.75
38	19.66	52.49	68.39	73.90	4.13	6.19	2.90	0.89	0.54	1.51	1.09	1.41
39	0.10	0.50	11.70	23.00	0.29	0.65	4.25	0.87	0.10	0.15	2.89	0.37
40	0.00	11.90	30.55	41.00	0.60	3.44	1.52	0.41	0.04	1.65	1.51	0.52
42	6.40	36.87	56.01	62.20	5.29	2.54	1.72	1.22	0.14	0.63	1.61	1.74
43	17.50	50.69	67.22	70.20	5.24	2.60	2.32	1.07	1.04	0.72	1.40	1.15
45	-1.10	-0.90	11.90	24.10	0.63	0.49	4.04	1.09	0.02	0.33	3.28	0.98
46	-0.90	11.20	31.74	42.10	0.49	2.15	1.33	0.60	0.01	0.33	1.28	0.45
47	1.50	25.03	46.17	53.60	1.76	1.76	1.94	0.89	0.39	1.41	1.47	0.73
48	7.00	38.35	57.83	63.30	6.17	2.36	2.21	1.32	0.27	2.34	1.24	1.51
49	18.10	51.26	67.80	72.00	6.58	2.17	2.41	1.65	0.41	1.90	1.79	1.42
51	3.20	22.34	37.79	43.70	2.92	2.83	3.41	1.25	1.56	1.68	1.58	1.47
52	19.80	45.79	59.56	64.50	8.65	2.66	2.82	1.75	4.90	1.08	1.11	1.72
54	-1.60	-1.50	10.00	24.20	0.39	0.43	3.93	2.00	0.02	0.11	1.93	2.24
55	-1.20	10.80	32.38	43.80	1.04	4.17	2.33	1.56	0.02	1.83	1.71	1.44
56	-0.30	23.59	45.61	54.40	1.12	1.60	1.56	1.23	0.36	0.31	0.38	0.80
57	-0.30	23.77	45.89	55.00	1.18	1.53	1.99	1.55	0.39	0.55	0.45	1.42
58	5.80	38.63	57.45	64.50	5.55	1.89	1.57	1.59	0.89	3.14	0.68	1.03
60	17.30	51.16	67.02	74.00	7.60	2.01	1.20	2.37	1.07	2.72	0.82	1.93
61	25.48	60.62	73.40	80.70	4.37	1.77	1.05	3.38	3.13	2.22	1.03	3.00
62	0.10	0.40	22.79	43.50	1.79	1.78	4.31	1.29	0.61	1.04	1.66	1.25
63	0.00	20.19	52.68	64.50	1.82	3.13	1.55	1.88	2.26	1.79	0.71	1.86
64	0.10	0.40	12.90	26.30	0.31	0.69	7.85	4.30	0.10	0.40	4.62	4.61
66	0.90	23.86	46.82	57.10	1.29	1.66	3.14	3.31	1.72	0.39	1.78	3.43
68	14.90	50.88	66.44	75.10	9.97	1.59	1.50	3.74	0.23	0.68	0.84	3.31
69	-0.10	0.40	9.40	18.20	0.32	0.42	3.75	0.97	0.00	0.40	3.17	0.10
71	0.00	19.90	32.93	42.00	0.69	3.02	2.72	2.88	0.40	3.18	0.40	1.99
72	1.90	26.75	43.73	52.30	2.21	4.21	3.82	2.56	0.91	4.10	1.82	1.58
73	8.50	38.90	55.06	62.70	2.49	5.21	4.07	1.12	1.46	5.26	2.71	0.60
74	18.60	49.08	64.39	69.50	2.14	4.81	2.89	0.53	3.31	0.58	0.93	0.92
76	0.70	10.60	28.10	36.50	0.71	5.75	3.51	0.44	0.70	3.57	3.63	0.63
77	1.30	21.00	41.59	47.00	1.43	1.94	3.05	1.30	0.31	0.82	3.06	0.61
79	13.60	46.73	64.30	67.90	5.72	1.57	2.94	1.29	0.85	1.81	2.29	1.03
80	21.80	57.64	72.91	75.00	2.79	1.58	3.83	1.33	4.42	0.77	2.67	1.20
81	-0.10	0.30	11.10	22.60	0.37	1.21	6.23	3.75	0.26	0.60	4.83	3.49
82	0.60	11.40	30.19	37.60	0.92	6.65	4.84	0.94	0.47	3.25	3.16	0.47
83	1.40	21.80	41.59	49.90	1.78	3.21	3.07	1.40	0.88	1.92	1.38	0.92
85	13.90	47.39	63.52	69.70	8.46	1.54	2.35	2.07	0.21	0.52	1.27	1.89
86	13.50	47.39	63.52	69.80	8.21	1.60	2.43	2.18	0.25	0.53	1.33	2.03