

Iterative Classification Method for Evaluating Absolute and Relative Uncertainties of Reactivity Worth

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1. Introduction

In the validation of reactor physics parameters, the deviations between calculated and experimental values exhibit distinct statistical behaviors depending on the magnitude of the reactivity worth. Specifically, the absolute deviation (C-E) tends to be distributed within a specific range when the worth is small, but the deviation increases as the worth becomes larger. Conversely, the relative deviation (C/E-1) settles within a certain range for large worths, but significantly fluctuates due to error amplification for small worths.

In accordance with these characteristics of the deviations, uncertainties for setting acceptance criteria for reactor physics tests and safety analyses must be evaluated separately by dividing them into absolute and relative uncertainties based on a specific threshold value. For instance, the acceptance criteria for individual rod worth measurements in commercial pressurized water reactors (PWRs) are empirically established as an absolute deviation of 100 pcm for control rod worths (CRWs) less than 666 pcm and a relative deviation of 15% otherwise [1].

However, for advanced core designs lacking established criteria, such as the Sodium-cooled Fast Reactor (SFR)-based Transuranic (TRU) burner, a systematic approach is required to rigorously evaluate the reactivity worth uncertainties. Therefore, this study proposes an iterative method to systematically classify validation data and evaluate both relative and absolute uncertainties based on the magnitude of the reactivity worth, and demonstrates its applicability.

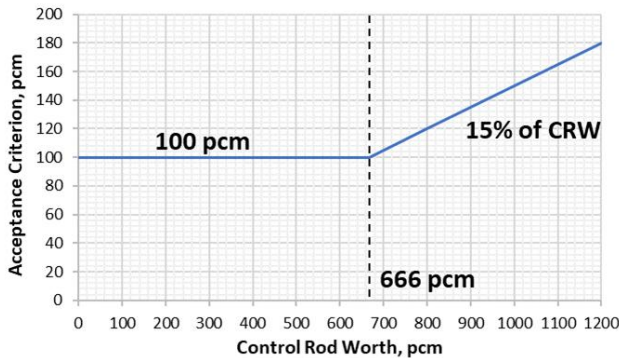


Figure 1. Acceptance criterion for deviation (C-E) in control rod worth in commercial PWRs.

2. Methodology

2.1. Iterative Classification Method

The basic relation between the absolute uncertainty, U_{abs} (in pcm), and the relative uncertainty, U_{rel} (in %), can be written as:

$$U_{abs} = \Delta\rho_{thres} \times \frac{U_{rel}}{100}, \quad (1)$$

where $\Delta\rho_{thres}$ is the threshold reactivity worth (in pcm) at which the two uncertainties become equal.

From Eq. (1), an algorithm is devised to iteratively determine $\Delta\rho_{thres}$ as follows:

$$\Delta\rho_{thres}^{(i+1)} = \frac{U_{abs}^{(i)}}{U_{rel}^{(i)}} \times 100, \quad (2)$$

where i indicates the iteration index, $U_{abs}^{(i)}$ and $U_{rel}^{(i)}$ are the absolute and relative uncertainties evaluated using the subsets of validation data with reactivity worths less than and greater than $\Delta\rho_{thres}^{(i)}$, respectively. By utilizing the updated threshold, $\Delta\rho_{thres}^{(i+1)}$, to classify the validation data, both the absolute and relative uncertainties are iteratively re-evaluated until they converge. Since this iterative process requires an initial guess for $\Delta\rho_{thres}^{(0)}$, its selection and subsequent impact on the final uncertainties will be discussed later.

Through this iterative classification effectively filters out amplified deviations in the small-worth region, while the large biases in the large-worth region is excluded from the absolute uncertainty evaluation.

2.2. Tolerance Limit Method

For the uncertainty evaluation, the two-sided parametric tolerance limit method [2] was applied. This method defines an interval that covers at least (100P)% of future observations y with a confidence of $(1 - \alpha) \times 100\%$ as follows:

$$\Pr(\Pr(y \in \bar{y} \pm S_p k_2(\alpha, P, N)) \geq P) = 1 - \alpha. \quad (3)$$

where the weighted mean, \bar{y} , and the pooled standard deviation, S_p , are calculated as follows:

$$\bar{y} = \frac{\sum_{i=1}^N y_i / \sigma_i^2}{\sum_{i=1}^N 1 / \sigma_i^2}, \quad (4)$$

$$S_p = \sqrt{s^2 + \frac{N}{\sum_{i=1}^N 1 / \sigma_i^2}}, \quad (5)$$

$$s^2 = \frac{\frac{1}{N-1} \sum_{i=1}^N (y_i - \bar{y})^2 / \sigma_i^2}{\frac{1}{N} \sum_{i=1}^N 1 / \sigma_i^2}, \quad (6)$$

and y_i is the deviation for i -th validation datum, σ_i^2 is the variance of deviation combining experimental and calculational uncertainties, N is the number of validation data.

The two-sided tolerance factor, $k_2(\alpha, P, N)$, in Eq. (3) is calculated as:

$$k_2(\alpha, P, N) = uvw, \quad (7)$$

$$u = z_{(1+P)/2} \sqrt{1 + \frac{1}{N}}, \quad (8)$$

$$v = \sqrt{\frac{N-1}{\chi_{\alpha}^{2, (N-1)}}}, \quad (9)$$

$$w = \sqrt{1 + \frac{N-3 - \chi_{\alpha}^{2, (N-1)}}{2(N+1)^2}}, \quad (10)$$

where $z_{(1+P)/2}$ is the $(1+P)/2$ -th quantile of the standard normal distribution, $\chi_{\alpha}^{2, (N-1)}$ is the α -th quantile of the chi-square distribution with $N-1$ degrees of freedom.

The final uncertainty incorporating both the bias and its uncertainty is evaluated as:

$$U = \sqrt{\bar{y}^2 + (S_p k_2(\alpha, P, N))^2}. \quad (11)$$

In this study, both the coverage fraction, P , and the confidence level $(1 - \alpha)$ is set to 0.95 to evaluate the 95/95 tolerance limit. It should be also noted that this method requires a normal distribution. Therefore, when the null hypothesis of a normality test, such as the Shapiro-Wilk [3], is rejected for a dataset, the non-parametric tolerance limit method should be applied. However, in such cases, the parametric approach was maintained, as the primary objective of this study is to demonstrate the conceptual framework of the iterative classification method.

3. Results

3.1. Selection of Validation Data

The target core for this uncertainty evaluation is an SFR-based TRU burner loaded with metallic fuels consisting of 25 wt% TRU. To construct a validation dataset, reactor physics experimental data from the ZPR and ZPPR facilities [4,5] were selected based on similarity coefficients exceeding 0.8 with respect to the target core. The similarity coefficients and corresponding reactivity worths were calculated using the SANDY/NJOY/McCARD code system [6] with the ENDF/B-VII.1 [7]. Consequently, 31 and 50 validation cases were selected for CRW and sodium void reactivity worth (SVRW), respectively.

Figure 2 shows the absolute and relative deviations for the CRW while Figure 3 shows those for the SVRW. In both figures, the shaded regions highlight data points prone to overestimating uncertainty, specifically due to noise amplification in relative deviations and significant biases in absolute deviations. To prevent these points from distorting the results, the proposed iterative classification method systematically determines a threshold to exclude such anomalies.

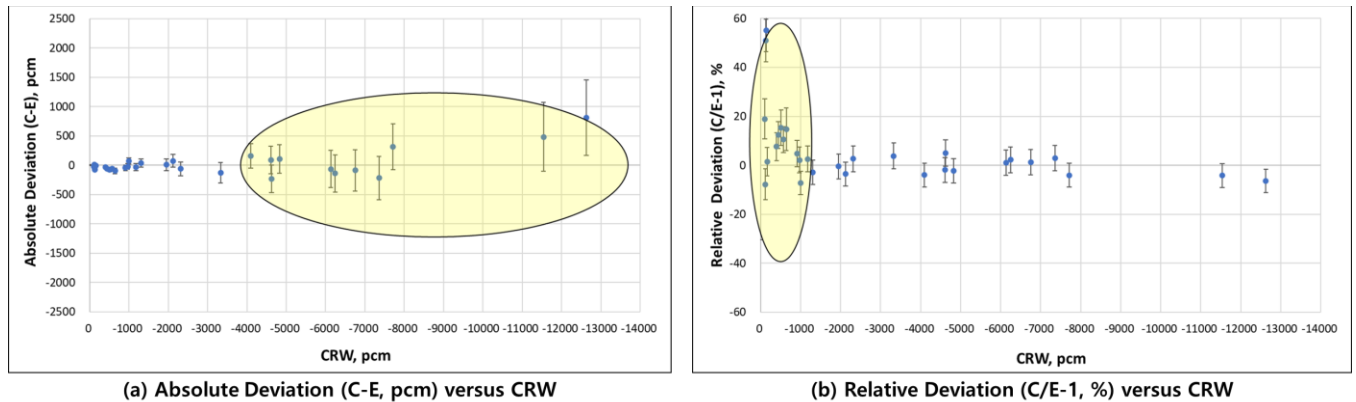


Figure 2. Absolute and relative deviations versus control rod worth (CRW). Yellow shadings indicate data points prone to overestimating uncertainty.

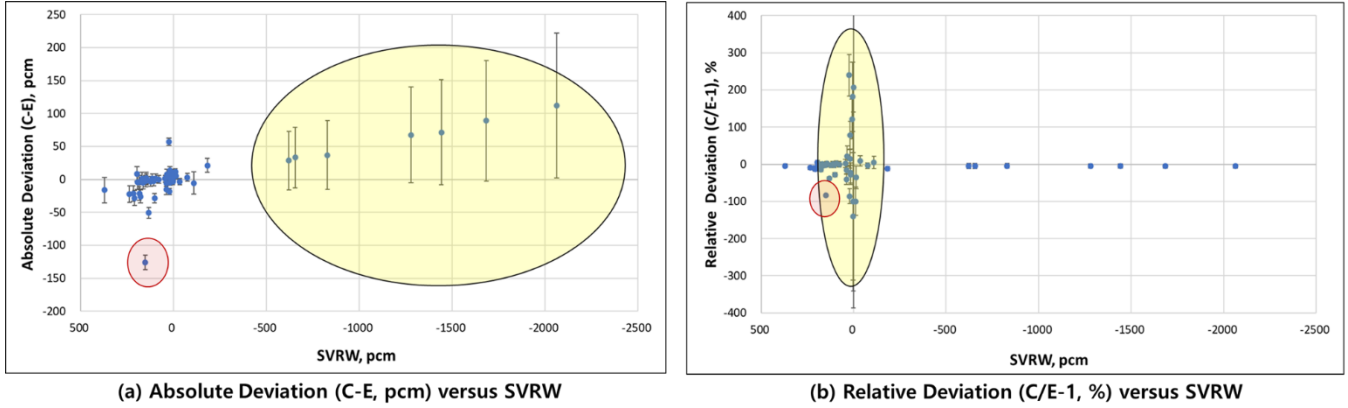


Figure 3. Absolute and relative deviations versus sodium void reactivity worth (SVRW). Yellow shadings indicate data points prone to overestimating uncertainty. Red shadings indicate the anomalous data point that leads to a bifurcated convergence of iterative classification method (refer to Section 3.2 for details).

3.2. Uncertainty Evaluation Results

The iterative classification method was applied to evaluate the uncertainties for both CRW and SVRW using the selected validation data. Furthermore, sensitivity analyses were performed to investigate the impact of the initial guess for threshold reactivity worth $\Delta\rho_{thres}$. Table I and Table II summarize the uncertainty evaluation results with various initial $\Delta\rho_{thres}$ values for CRW and SVRW, respectively.

In the case of CRW, $\Delta\rho_{thres}$ converges to 716 pcm for various initial guesses except for the extreme values (0 and 12629 pcm). The final absolute and relative uncertainties were evaluated as 125.32 pcm and 17.51%, respectively. Note that the relative uncertainty was significantly reduced from 30.59% obtained using the entire validation datasets (i.e., initial $\Delta\rho_{thres} = 0$ pcm). This is attributed to the filtering out the datasets affected by the amplified deviation in the relative uncertainty evaluation. Meanwhile, the absolute uncertainty is slightly increased from 105.24 pcm, which is due to the larger number of validation data reducing the tolerance factor.

Furthermore, the Shapiro-Wilk test results indicate that

the non-parametric method should be applied when the entire validation datasets were used to evaluate the absolute and relative uncertainties, respectively. Conversely, the iterative classification method successfully classifies the data into a subset that fails to reject the normality. Therefore, the proposed method offers a distinct advantage by appropriately classifying data to reduce the deviation and helping the distribution follow a normal distribution.

In the case of the SVRW, $\Delta\rho_{thres}$ converges to 64 pcm when the initial $\Delta\rho_{thres}$ is less than 152 pcm, whereas it converges to 225 pcm for other tested cases (except for the extreme cases). This is due to the abnormal data point at 151.1 pcm with absolute and relative deviations of -126 pcm and -83%, respectively. This data point is also highlighted in red in Figure 3. When this specific point is included in the relative uncertainty evaluation, the relative uncertainty abruptly increases. The final uncertainties were evaluated as 42.42 pcm and 66.62% with the initial guess below 152 pcm, and 47.57 pcm and 21.11% otherwise. Unlike the CRW case, the normality test results for SVRW indicate normality was rejected for most cases. Therefore, for a rigorous evaluation of the SVRW uncertainty, a non-parametric method should be applied, which will be further investigated in future work.

Table I. Control rod worth (CRW) uncertainty using iterative classification method

Initial $\Delta\rho_{thres}$	Iteration	$\Delta\rho_{thres}$, pcm	No. of Validation Data		CRW Uncertainty		Shapiro Wilk Test	
			Absolute	Relative	Absolute, pcm	Relative, %	Absolute	Relative
0	0	0	0	31	N/A	30.59	N/A	Rejected
500	0	500	8	23	142.17	19.87	Passed	Passed
	1	715	11	20	125.32	17.51	Passed	Passed
	2	716	11	20	125.32	17.51	Passed	Passed
1000	0	1000	14	17	117.23	17.62	Passed	Passed
	1	665	11	20	125.32	17.51	Passed	Passed
	2	716	11	20	125.32	17.51	Passed	Passed

Initial $\Delta\rho_{thres}$	Iteration	$\Delta\rho_{thres}$, pcm	No. of Validation Data		CRW Uncertainty		Shapiro Wilk Test	
			Absolute	Relative	Absolute, pcm	Relative, %	Absolute	Relative
1500	0	1500	16	15	113.49	18.36	Passed	Passed
	1	618	10	21	129.17	18.32	Passed	Passed
	2	705	11	20	125.32	17.51	Passed	Passed
	3	716	11	20	125.32	17.51	Passed	Passed
3000	0	3000	19	12	109.84	20.07	Passed	Passed
	1	547	8	23	142.17	19.02	Passed	Passed
	2	748	11	20	125.32	17.51	Passed	Passed
	3	716	11	20	125.32	17.51	Passed	Passed
12629 (Max. Worth)	0	12629	31	0	105.24	N/A	Rejected	N/A

Note: Bold values indicate the final uncertainties for the initial guess.

Table II. Sodium void reactivity worth (SVRW) uncertainty using iterative classification method

Initial $\Delta\rho_{thres}$	Iteration	$\Delta\rho_{thres}$, pcm	No. of Validation Data		SVRW Uncertainty		Shapiro Wilk Test	
			Absolute	Relative	Absolute, pcm	Relative, %	Absolute	Relative
0	0	0	0	50	N/A	65.16	N/A	Rejected
50	0	50	18	32	42.42	66.62	Rejected	Rejected
	1	64	18	32	42.42	66.62	Rejected	Rejected
100	0	100	21	29	39.13	68.92	Rejected	Rejected
	1	57	18	32	42.42	66.62	Rejected	Rejected
	2	64	18	32	42.42	66.62	Rejected	Rejected
151	0	151	30	20	40.28	80.19	Rejected	Rejected
	1	50	18	32	42.42	66.62	Rejected	Rejected
	2	64	18	32	42.42	66.62	Rejected	Rejected
152	0	152	31	19	49.64	21.38	Rejected	Passed
	1	232	41	9	47.57	21.11	Rejected	Rejected
	2	225	41	9	47.57	21.11	Rejected	Rejected
200	0	200	39	11	47.56	21.67	Rejected	Rejected
	1	219	41	9	47.57	21.11	Rejected	Rejected
	2	225	41	9	47.57	21.11	Rejected	Rejected
500	0	500	43	7	47.38	23.48	Rejected	Passed
	1	202	39	11	47.56	21.67	Rejected	Rejected
	2	219	41	9	47.57	21.11	Rejected	Rejected
	3	225	41	9	47.57	21.11	Rejected	Rejected
2063 (Max. Worth)	0	2063	50	0	47.09	N/A	Rejected	N/A

Note: Bold values indicate the final uncertainties for the initial guess.

4. Summary and Conclusions

This study proposed an iterative classification method to systematically categorize validation datasets for absolute and relative uncertainty evaluations. The method was devised to enhance the uncertainty evaluation results by facilitating the dataset to follow normality, thereby justifying the use of the parametric approach. Furthermore, it effectively filters out noise-affected data in relative uncertainty evaluations and excludes largely biased data in the absolute uncertainty evaluations.

The proposed method was applied to evaluate the uncertainties of CRW and SVRW for an SFR-based TRU burner reactor using the selected validation data from the ZPR/ZPPR benchmark experiments. For the CRW, the relative uncertainty was significantly reduced compared to the result using the entire validation dataset. Moreover, the classified subsets successfully satisfied the normality assumption, validating the application of the parametric method. Notably, the threshold reactivity worth converged to a single value regardless of the initial guess. These results successfully demonstrate the effectiveness and robustness of the proposed method. However, the method exhibited limitations when applied to the SVRW.

In the SVRW uncertainty evaluation, the method exhibited a bifurcated convergence driven by an anomalous data point with exceptionally large deviation. Furthermore, the normality assumption was rejected for most cases, invalidating the application of the parametric approach. As a further study, the integration of the non-parametric tolerance limit method into the proposed framework, as well as a rigorous strategy for filtering out such abnormal data points will be investigated.

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REFERENCES

- [1] "Reload Startup Physics Tests for Pressurized Water Reactors," ANSI/ANS-19.6.1-2011, American Nuclear Society, La Grange Park, IL, USA, 2011.
- [2] W.G. Howe, "Two-sided tolerance limits for normal populations – some improvements," *J. Am. Stat. Assoc.*, vol. 64, pp. 610-620, 1969.
- [3] J. P. Royston, "Remark AS R94: a remark on algorithm as 181: the W test for normality," *Applied Statistics*, vol. 44, pp. 547-551, 1995.
- [4] OECD/NEA, "International Handbook of Evaluated Reactor Physics Benchmark Experiments," 2022/2023 Edition, NEA/NSC/DOC (2006)1, OECD/NEA, 2023.
- [5] S.J. Kim, et al., "ZPPR-15 and BFS Critical Experiments Analysis for Generation of Physics Validation Database of Metallic-Fueled Fast Reactor Systems," KAERI/RR-3621/2012, Korea Atomic Energy Research Institute, 2013.
- [6] Y.G. Jo, et al., "Uncertainty quantification based on similarity analysis of reactor physics benchmark experiments for SFR using TRU metallic fuel," *Nucl. Eng., and Technol.*, vol. 56(9), pp. 3626-3643, 2024.
- [7] M.B. Chadwick, et al., "ENDF/B-VII.1 nuclear data for science and Technology: cross sections, covariances, fission product yields and decay data," *Nucl. Data Sheets*, vol. 112, pp. 2887-2996, 2011.