

IRUG 2021

The 2021 International RELAP5-3D Users Group Seminar

No. 5

Application of Surrogate Models for Best Estimate Plus Uncertainty Analysis by RELAP5 Code

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Ikuo KINOSHITA



Institute of Nuclear Safety System, Inc. (INSS)

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1. Introduction

In recent years, **Best Estimate Plus Uncertainty (BEPU) methodology** has been improved to better deal with a loss of coolant accident (LOCA) analysis.

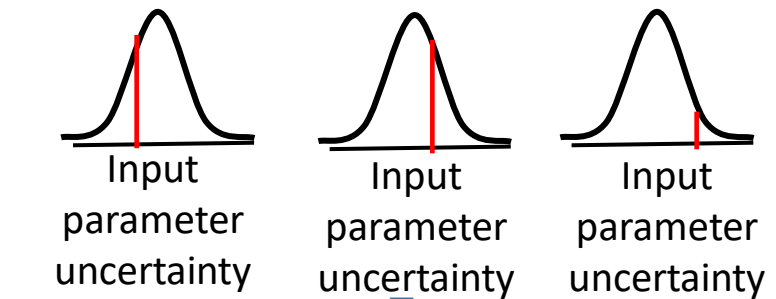
■ Procedure of BEPU analysis

- ① Verification and Validation of best estimate code (RELAP5)
- ② Uncertainty quantification of input parameters
- ③ Input uncertainty propagation analysis via Monte Carlo sampling
- ④ Statistical evaluations for FOM

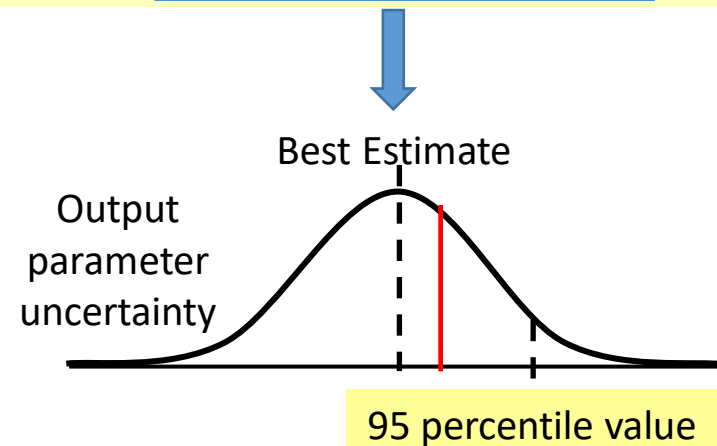
■ Problems in BEPU analysis

- RELAP5 code is computationally expensive.
- Therefore, it takes too long to perform the BEPU analysis, which limits the use of the BEPU analysis in nuclear safety activities such as sensitivity analysis, optimization, and others.

Specification of uncertain input parameters and sampling



Combination of uncertain parameters for RELAP5 code calculations



1. Introduction

An accurate and inexpensive **surrogate model** is expected to be used for rapid determination of the uncertainties on the FOM.

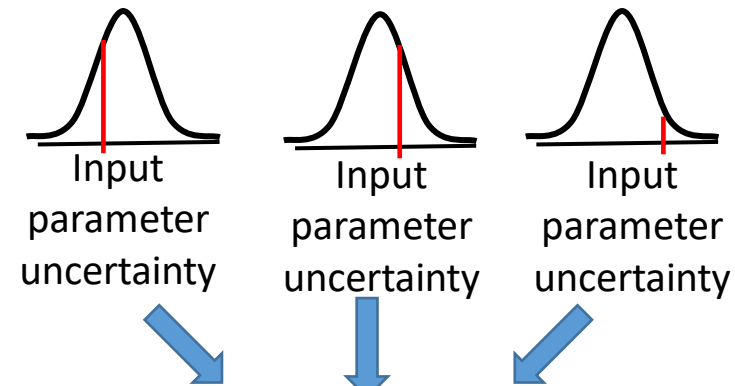
■ Surrogate Models

- A surrogate model is a mathematical representation to capture the relationships between the system (computer code) inputs and outputs.
- The key issue here is the accuracy of the uncertainty quantification predicted by the surrogate model.

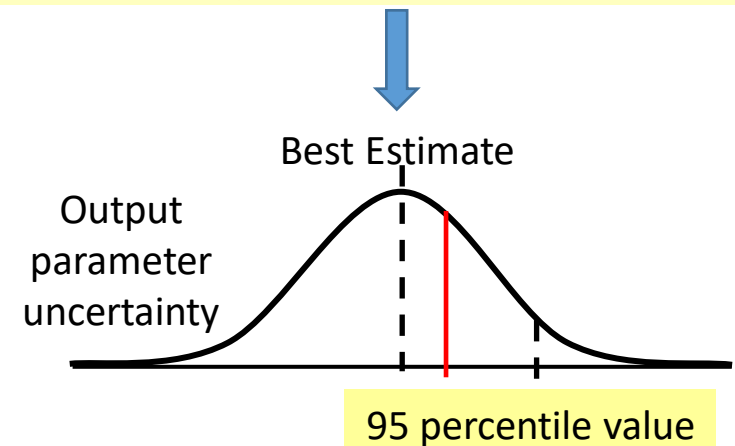
■ Case Study

- A surrogate model is generated from RELAP5 code uncertainty analysis on peak cladding temperature (PCT) for **a small break LOCA scenarios in PWRs**.
- The accuracy of uncertainty quantification of PCT by the surrogate model is investigated by comparing its results with the RELAP5 analysis results.

Specification of uncertain input parameters
and sampling



Combination of uncertain parameters for
Surrogate model calculations

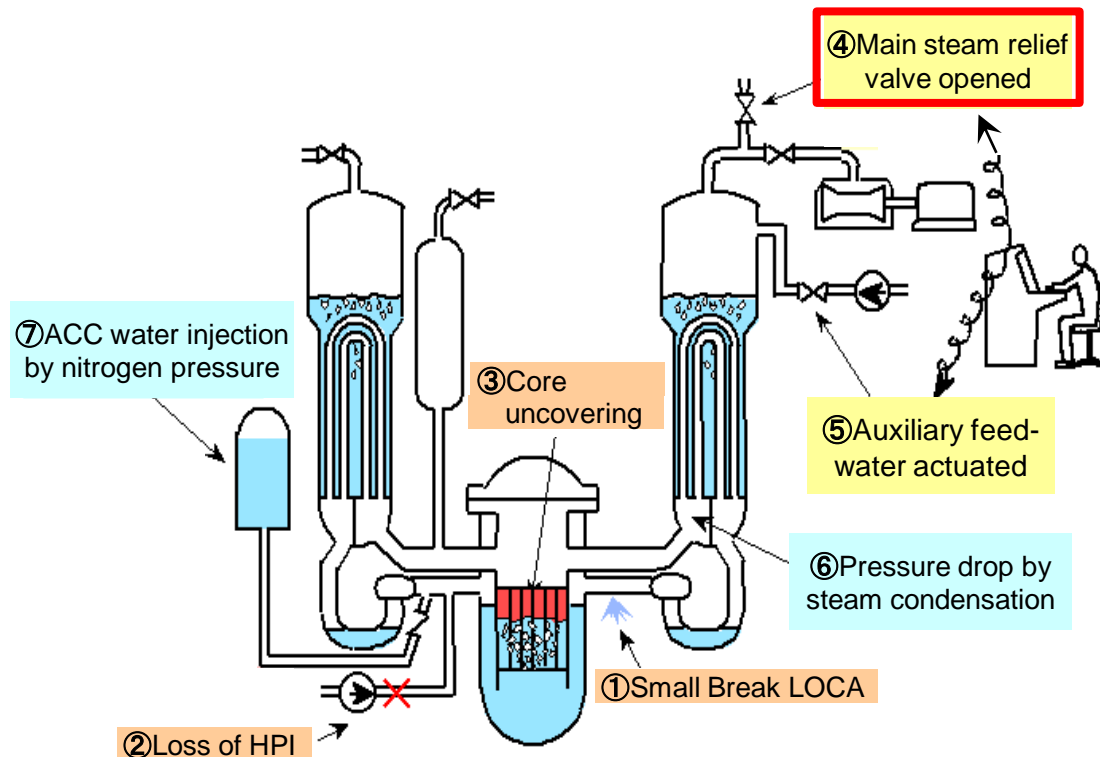


2. Reference Analysis by RELAP5 Code

(1) Analysis Object

■ Accident Management in SBLOCA with HPI failure in PWRs

LPI by intentional depressurization of SG secondary-side

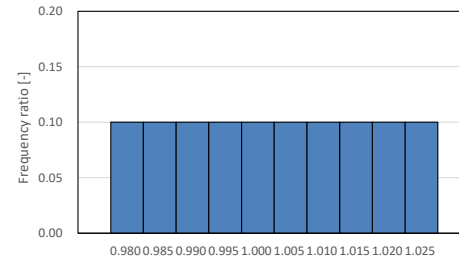


Device operation	Analysis conditions
Initial core power	Rated power
Reactor trip	Pressurizer pressure low
Turbine trip	At the same time as reactor trip
Safety injection signal	Pressurizer pressure low
PCP coast down	At the same time as safety injection signal
Main feedwater stop	At the same time as reactor trip
Auxiliary feedwater	60s after break, All loops
Main steam relief valve	Automatic operating
Initiation of HPI system	Inoperative
Initiation of ACC injection	All loops
Initiation of LPI system	All loops
Initiation of SG secondary-side depressurization	2 minutes after the CET reached 350° C, full opening of atmospheric relief valves of all loops

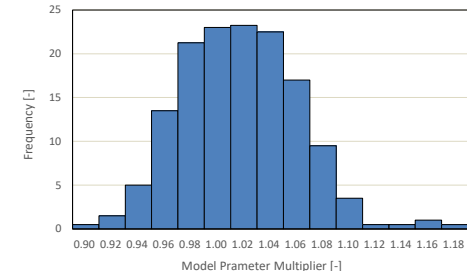
2. Reference Analysis by RELAP5 Code

(2) RELAP5 model uncertainties

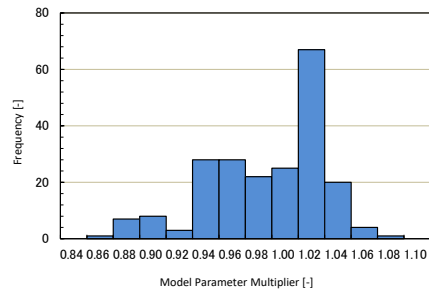
■ RELAP5 model uncertainties were quantified regarding the important phenomena by fitting experimental data from rerated separate effect tests



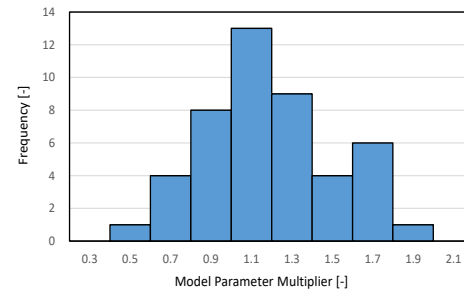
① Decay heat



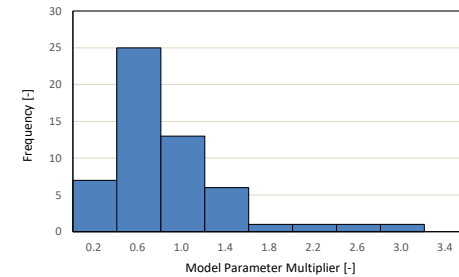
② Fuel clad oxidation



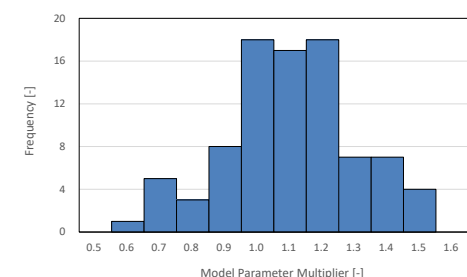
③ Fuel clad deformation



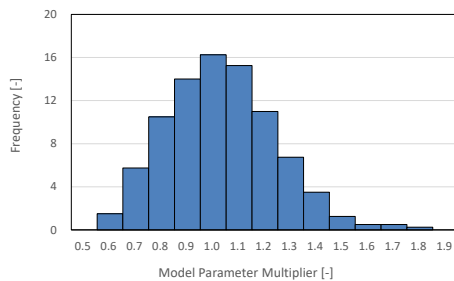
④ Uncovered core heat transfer



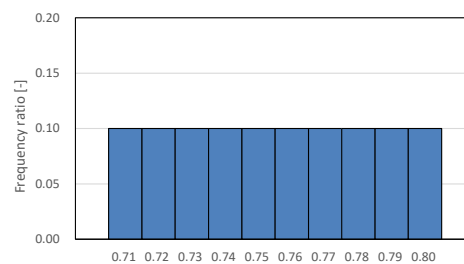
⑤ Interphase friction in the core



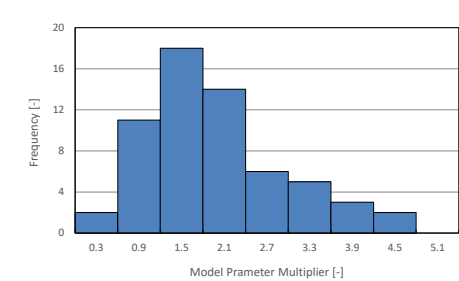
⑥ Condensation at U-tube (Nusselt)



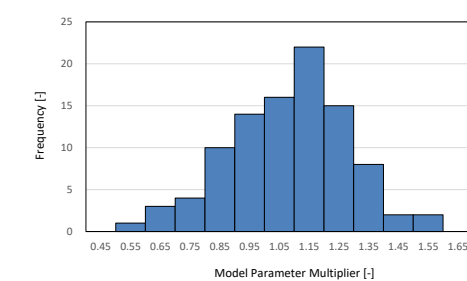
⑦ Condensation at U-tube (Shah)



⑧ CCFL at inlet of U-tube



⑨ Horizontal stratification at cold leg



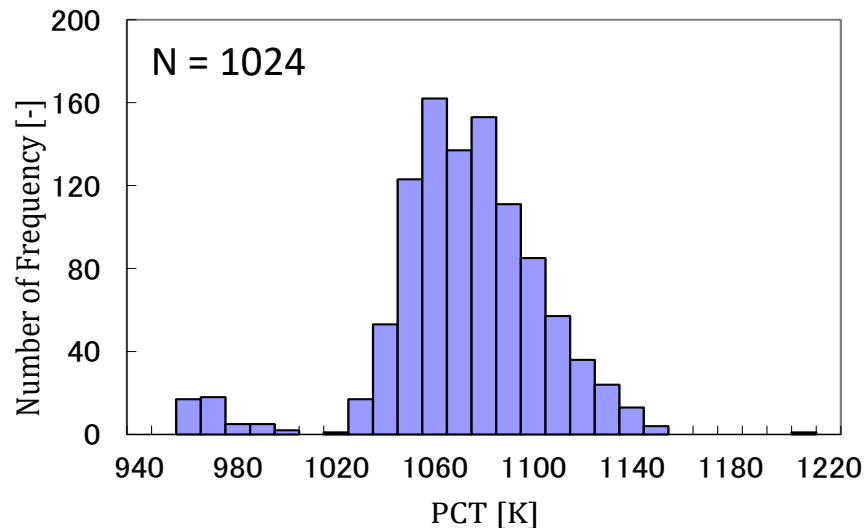
⑩ Interphase friction in downcomer

2. Reference Analysis by RELAP5 Code

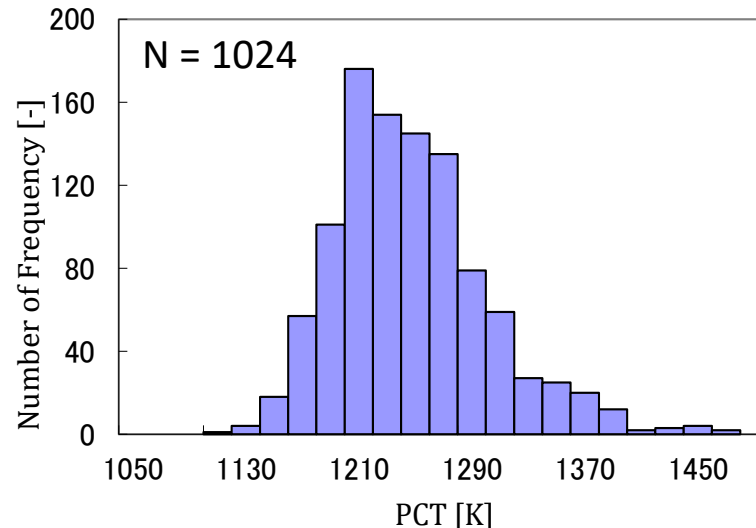
(3) Uncertainty Analysis Results

■ Uncertainty distributions of PCTs

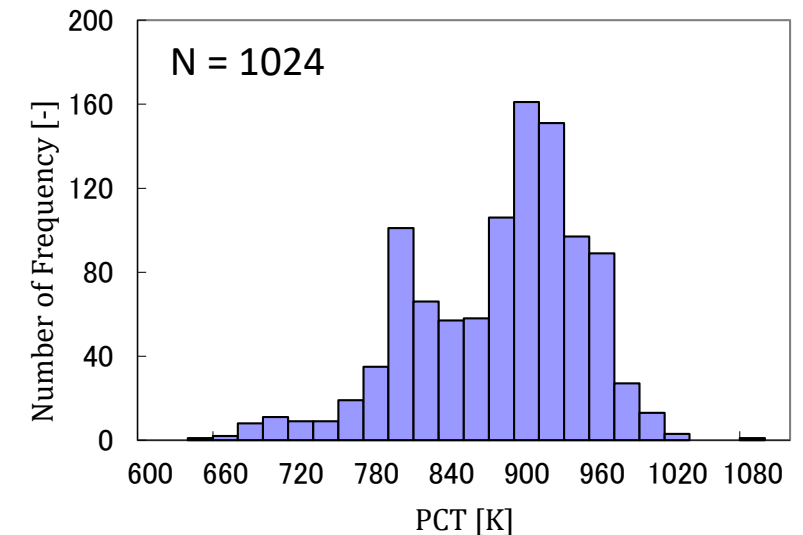
- The RELAP5 model uncertainty analysis was conducted with 1024 random sampling of the model uncertainty parameters.
- Break Sizes were 1 inch, 3 inch and 5 inch.



1 inch break



3 inch break



5 inch break

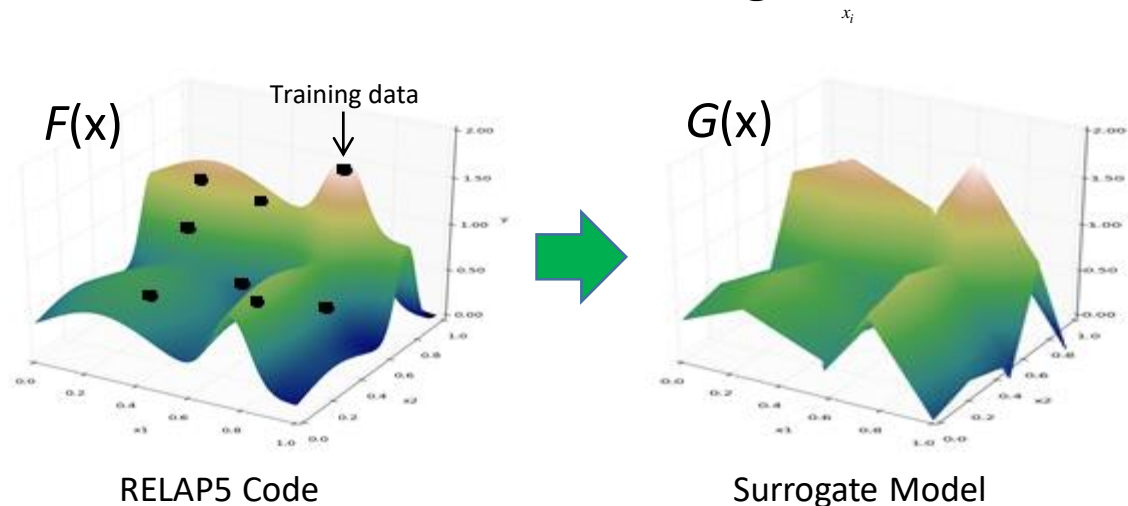
- The resultant uncertainty distributions of PCTs did not follow the normal distributions. It is important to construct the appropriate surrogate model depending on the complexity of the uncertainty analysis.

3. Uncertainty Analysis by Surrogate Models

(1) Uncertainty Analysis by Surrogate Models

■ Surrogate Models

- A surrogate model is generated to approximate the response of the computer code based on a small number of training runs.



$$F(x_i) \simeq G(x_i) \quad (x_i: \text{training data})$$

- ① Polynomial Regression
- ② Gaussian Process Model (GP)
- ③ Support Vector Machine (SVM)

■ Procedure of uncertainty Analysis by Surrogate Models

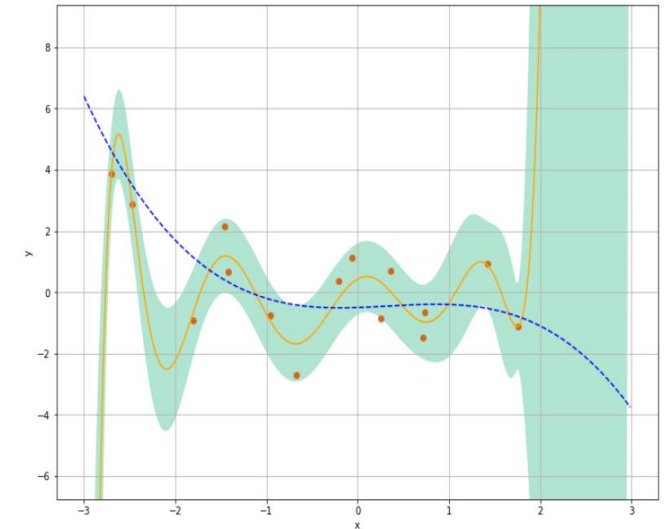
- ① Sampling training data form RELAP5 uncertainty analysis
- ② Training the surrogate model
- ③ Perform uncertainty propagation analysis using the surrogate model

3. Uncertainty Analysis by Surrogate Models

(2) Problems in Surrogate Model Application

■ Overfitting

- **Overfitting** occurs depending on the degree of freedom in a surrogate model and the number of its training data.
- The degree of freedom in a surrogate model is
 - ✓ large → the model requires a lot of training data.
 - ✓ small → the model has a poor ability to predict.



■ Assessment of generalized performance

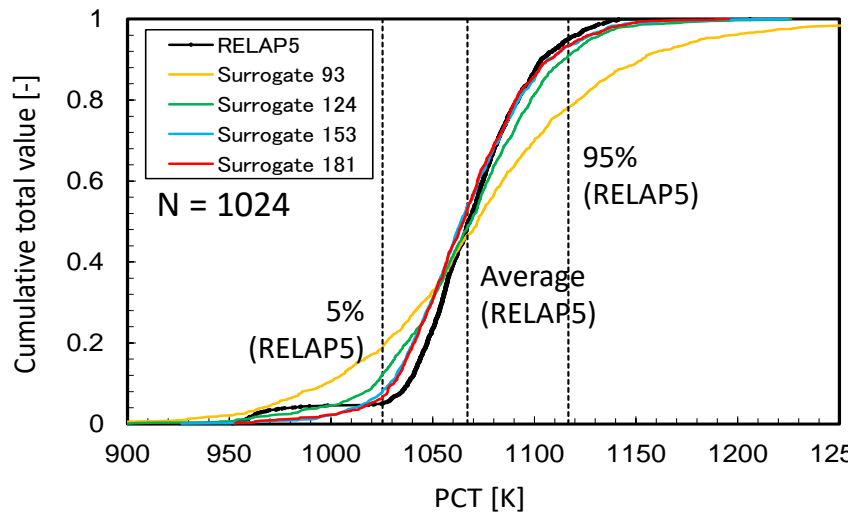
- In order to be confident with the model prediction, it is crucial to assess the generalized performance of the surrogate model.
- In this study, **cross validation** technique was applied to verify the prediction capability of the surrogate model for the 95th percentile values of the peak cladding temperature (95% PCT).

4. Results and Discussion

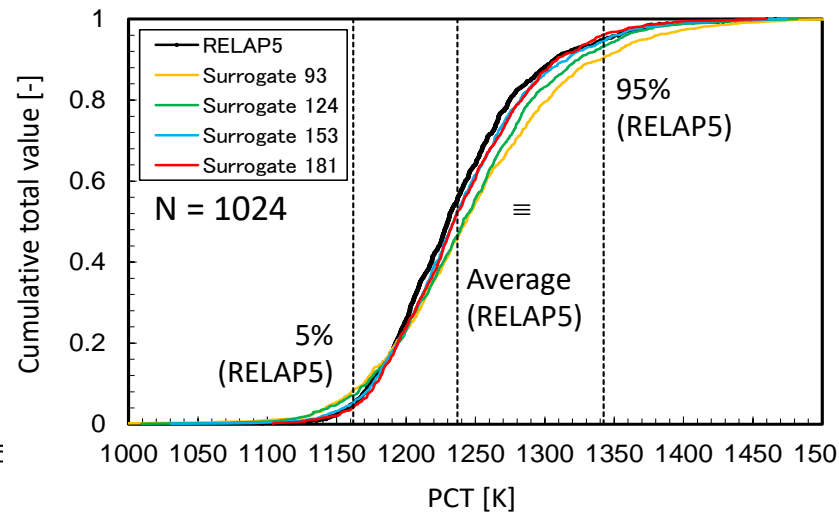
(1) Uncertainty Analysis by Surrogate Models

■ Surrogate model construction

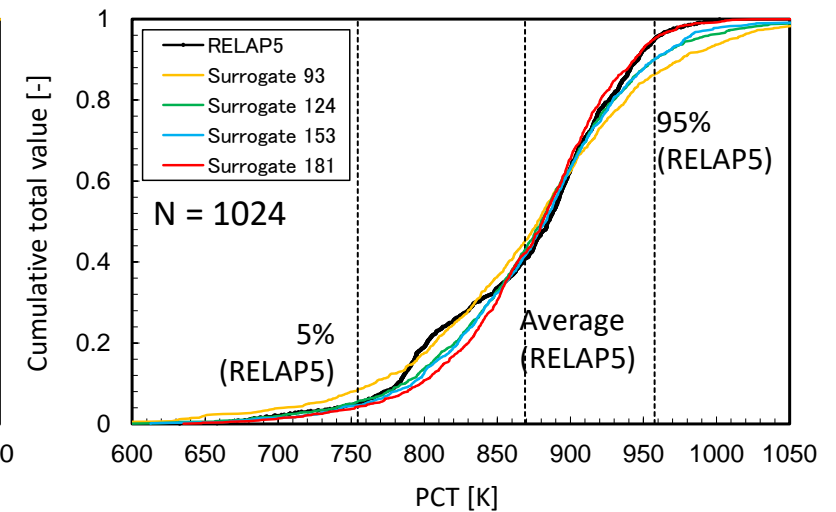
- $RELAP(x_i) \simeq Q(x_i)$, Q : Second order polynomial regression
- $Q(x_i) - RELAP(x_i) \simeq G(x_i)$, G : Gaussian process regression (squared exponential kernel)
- $Surrogate(x) := Q(x) + G(x)$
- x_i : training data, $N = 93, 124, 153, 181$ samples



1 inch break



3 inch break



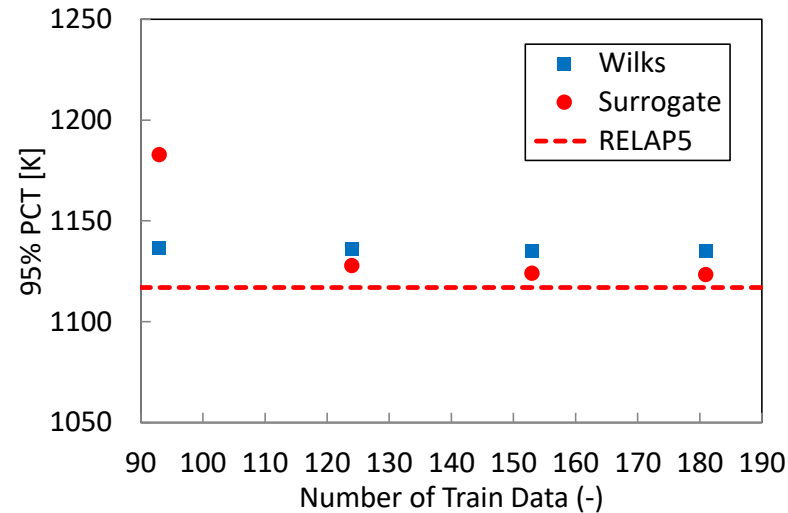
5 inch break

- The surrogate model with training data of $N = 93$ and 124 samples over-estimated the 95th percentile values of PCTs because of overfitting to the training data.

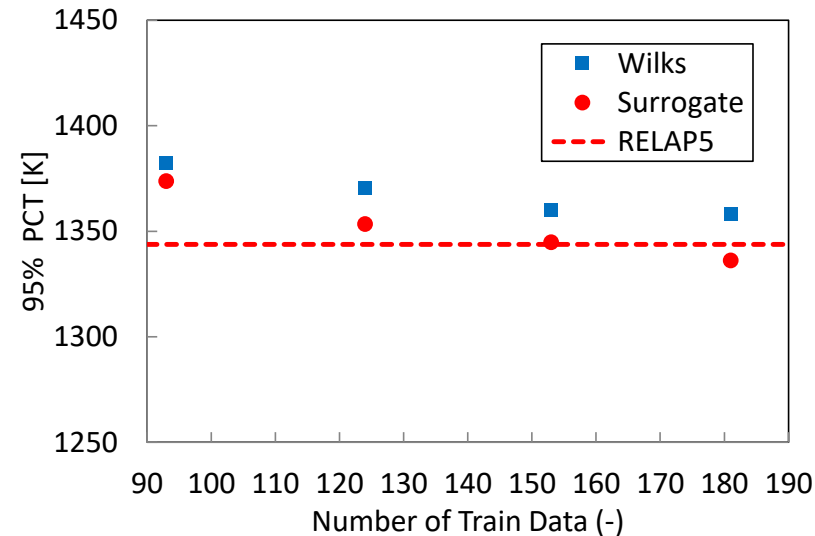
4. Results and Discussion

(1) Uncertainty Analysis by Surrogate Models

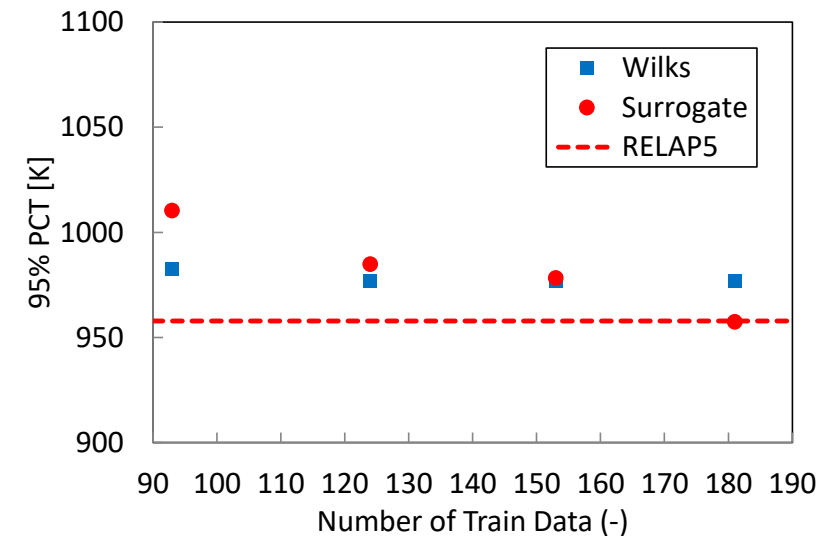
■ Comparison with Wilks formula method



1 inch break



3 inch break



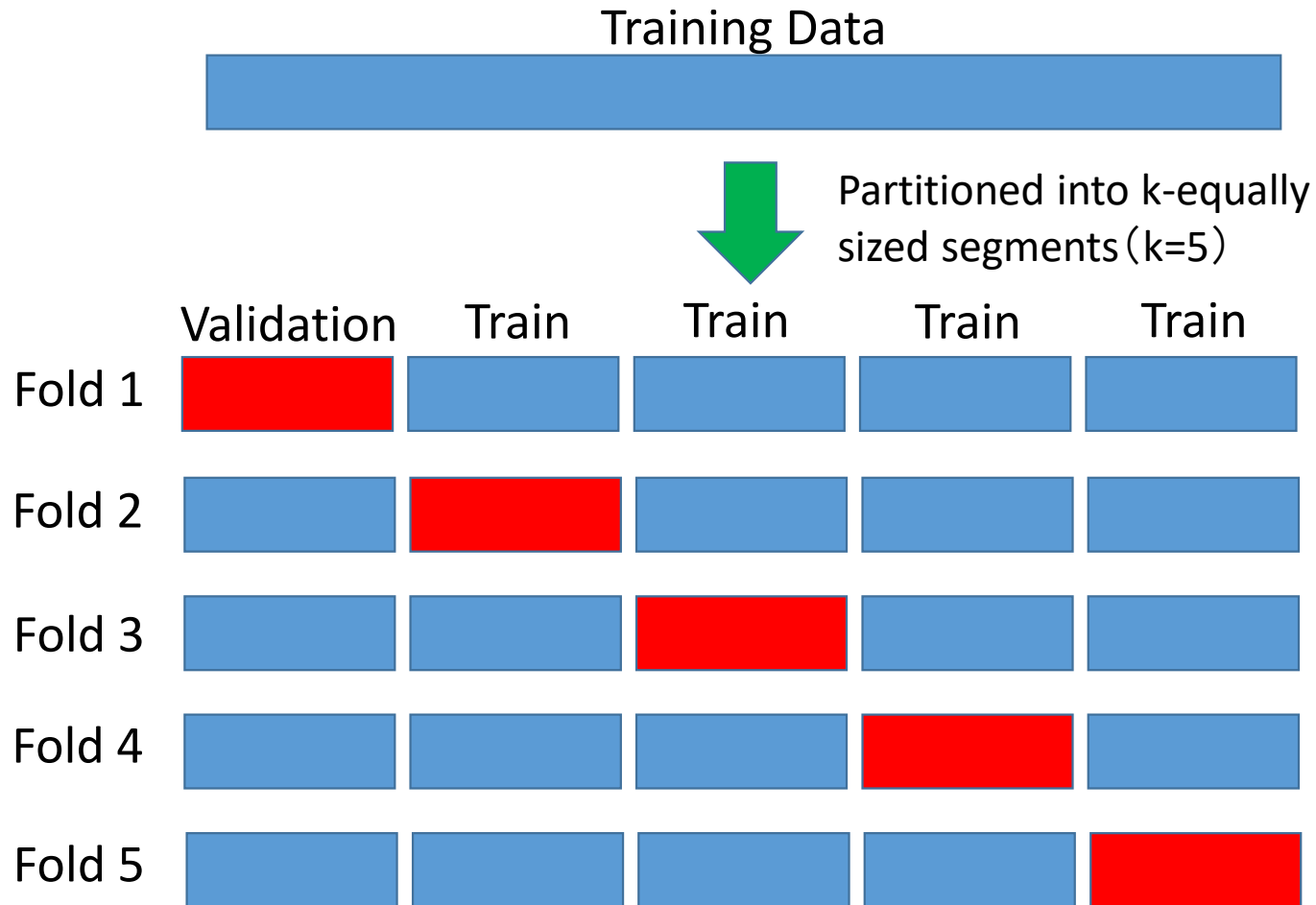
5 inch break

- The prediction accuracy was improved of the surrogate model for the 95% PCT by increasing the number of the training data.
- The prediction accuracy was lower than the Wilks method in the cases when the training data were 93 samples for 1 inch breaks as well as 93 and 124 samples for 5 inch break. The poor accuracy was due to the overfitting of the surrogate model to the training data.

4. Results and Discussion

(2) Cross Validation

■ K-Fold Cross Validation



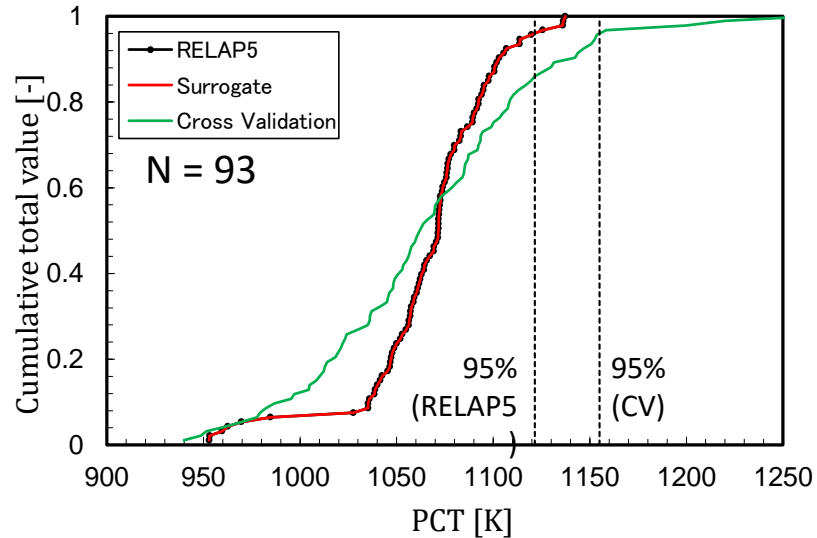
■ LOOCV

- Leave-One-Out Cross Validation (LOOCV) is a special case of k-fold cross validation.
- k equals the number of instances in the training data.

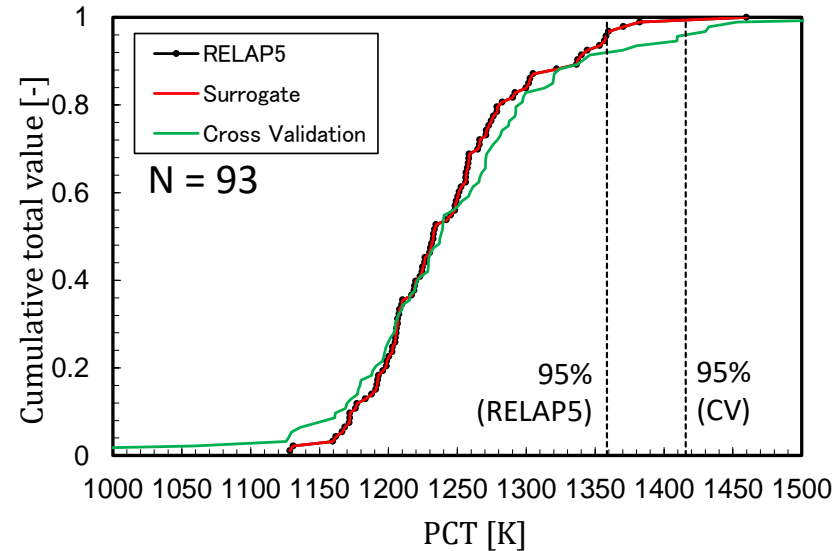
4. Results and Discussion

(2) Cross Validation

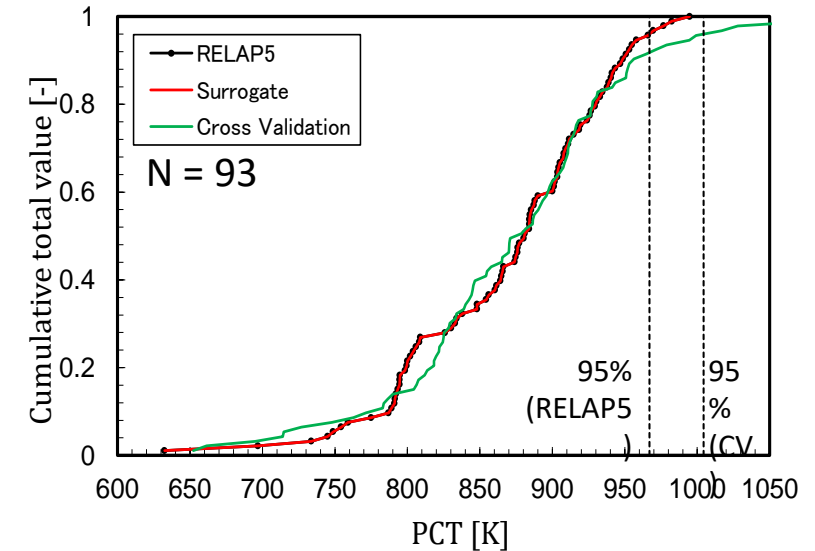
■ LOOCV (N = 93 samples)



1 inch break



3 inch break



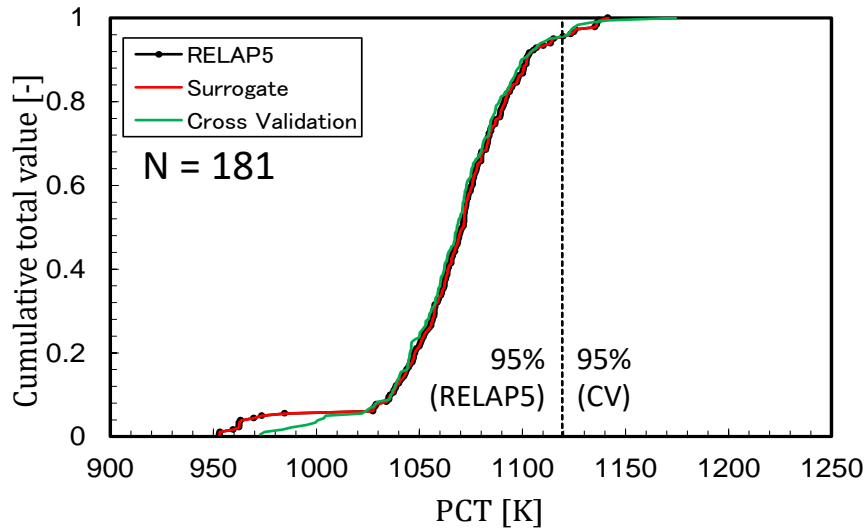
5 inch break

- The CDFs of surrogate models were in good agreement with those of RELAP5 calculations.
- The CDFs of LOOCV were different from those of surrogate models. These results indicated that the surrogate model over-fitted the training data of 93 samples.

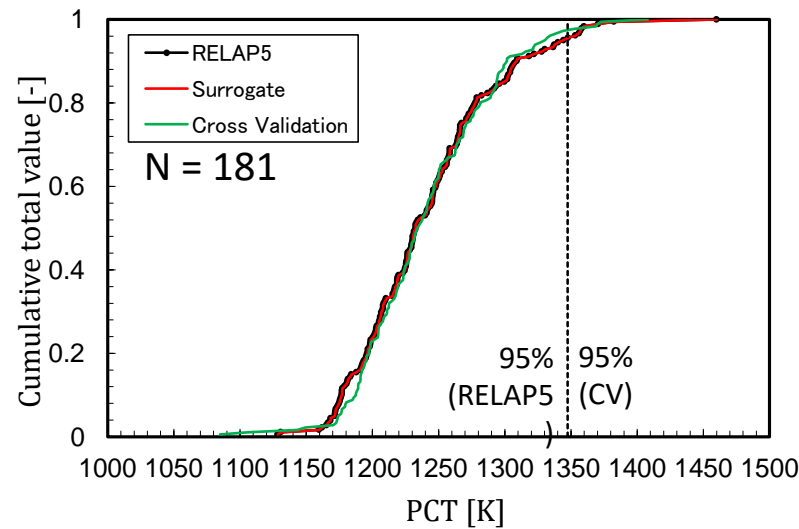
4. Results and Discussion

(2) Cross Validation

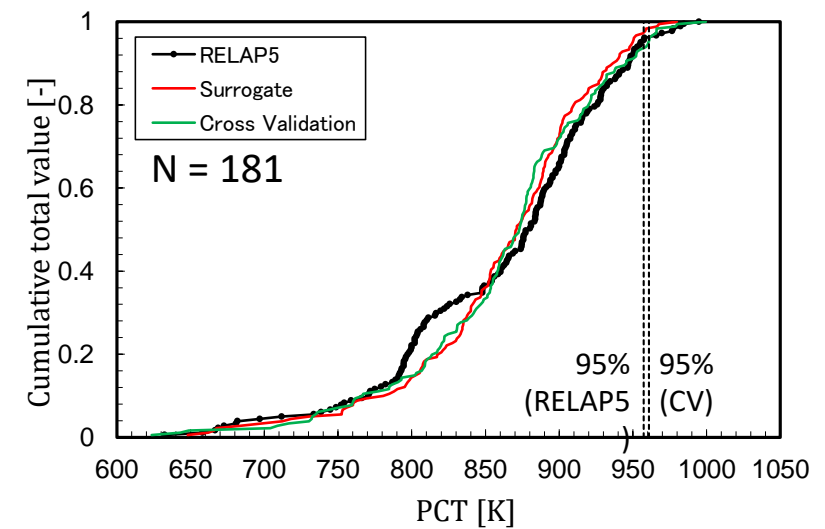
■ LOOCV (N = 181 samples)



1 inch break



3 inch break



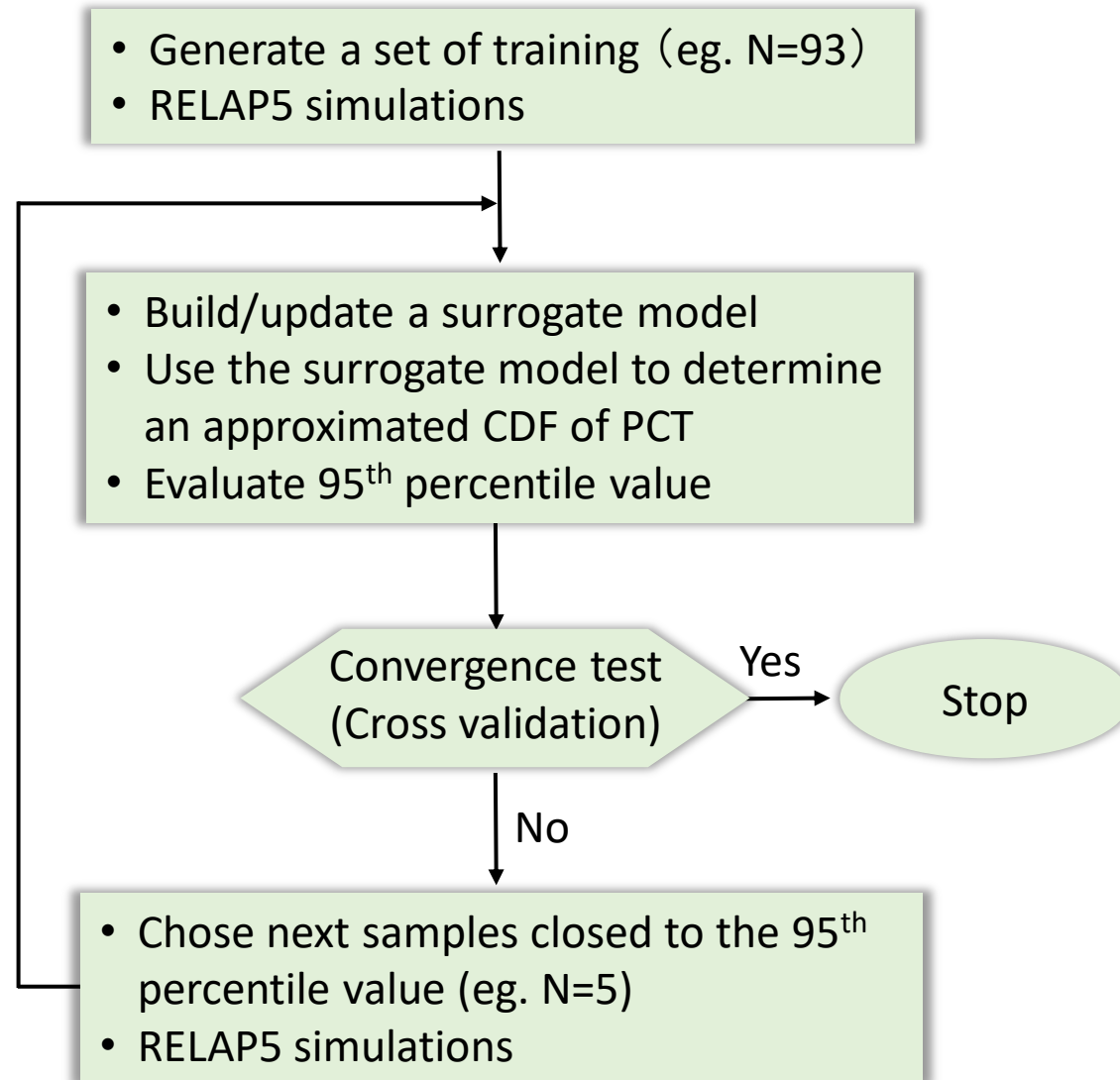
5 inch break

- The CDFs of LOOCV were in good agreement with those of the surrogate models. These results indicated that the surrogate models had the generalized performance.
- The generalized performance of the surrogate model for the 95% PCT prediction can be estimated using the cross validation on the training data set.

4. Results and Discussion

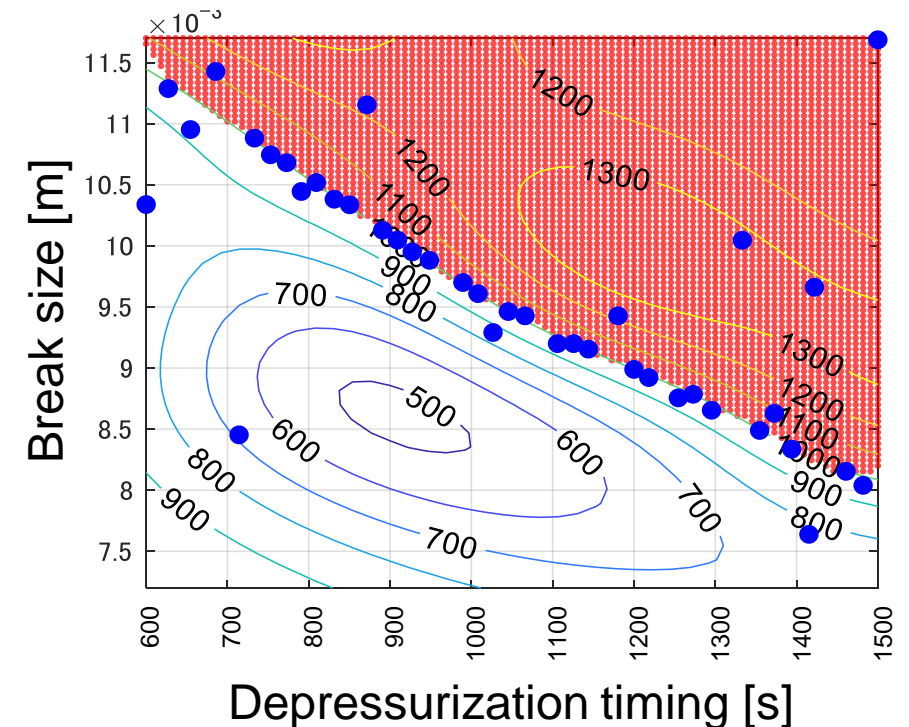
(3) Application of Adaptive Sampling

■ Adaptive sampling for 95th percentile value



■ RAVEN Limit Surface Search

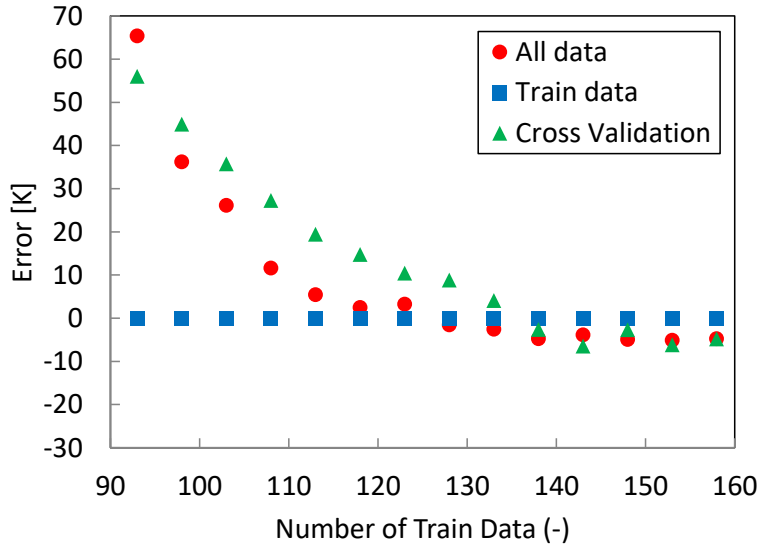
- Adaptive sampling procedure for 95th percentile values was developed based on RAVEN Limit Surface Search algorithm.



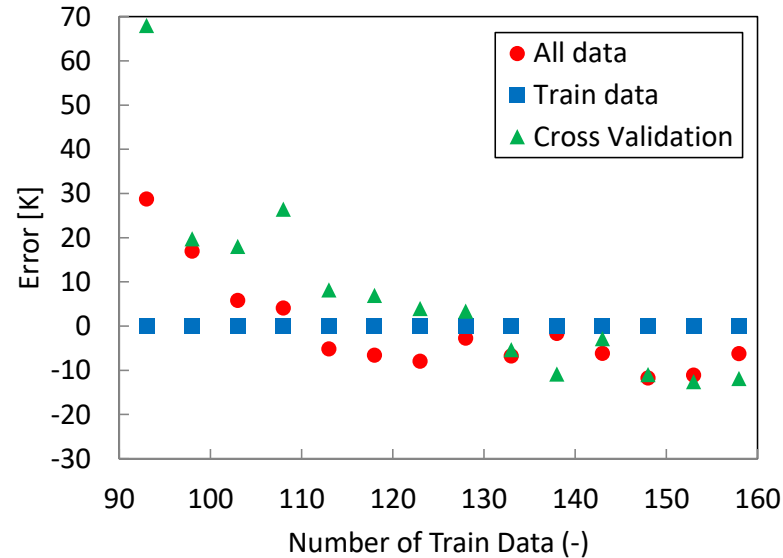
4. Results and Discussion

(3) Application of Adaptive Sampling

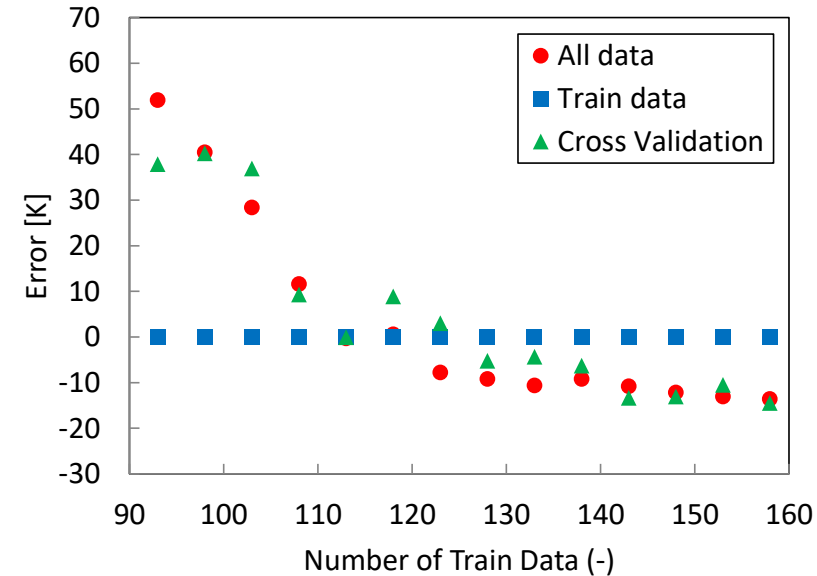
■ LOOCV for adaptive sampling



1 inch break



3 inch break



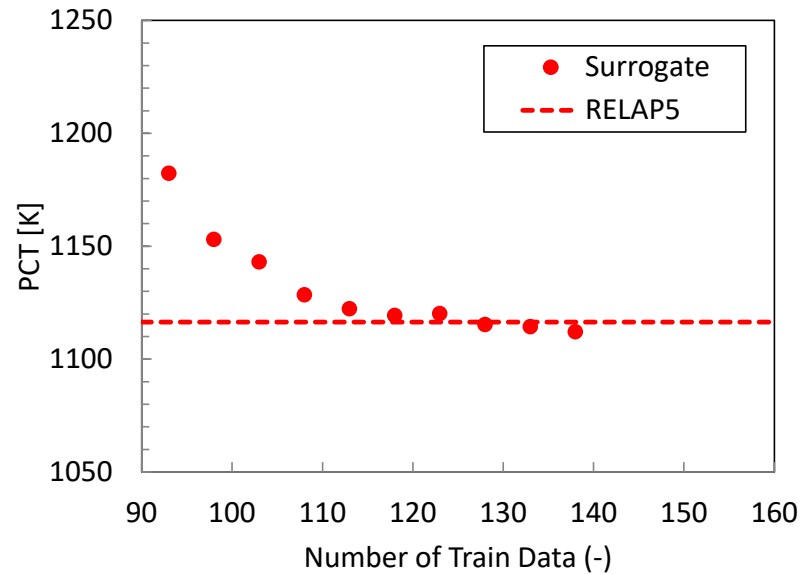
5 inch break

- By repeating the adaptive sampling, the prediction errors of the 95% PCT by the surrogate models approached zeros.
- The prediction errors of the 95% PCT were able to be estimated by the cross validation on the training data set.

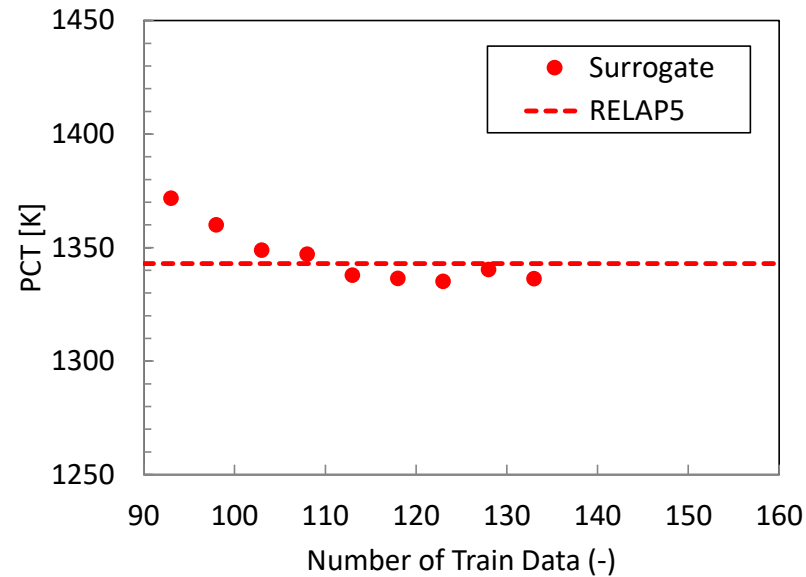
4. Results and Discussion

(3) Application of Adaptive Sampling

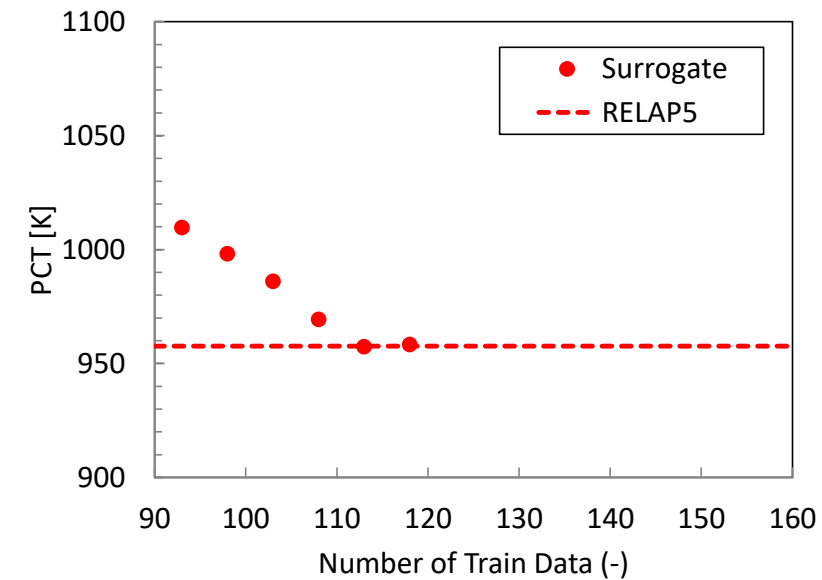
■ 95% PCT evaluation using adaptive sampling



1 inch break



3 inch break



5 inch break

■ The surrogate model with the high accuracy of the 95th percentile value prediction was able to be effectively constructed by repeating the adaptive sampling with the target of the 95th percentile values and confirming the model prediction accuracy using the cross validation on the training data set.

5. Conclusions

- Application of a surrogate model was discussed on uncertainty analysis by the RELAP5 code for a small break LOCA in PWRs.
- Comparison with the RELAP5 uncertainty analysis results confirmed that the generalized performance of the surrogate model for the 95% PCT prediction could be estimated using the cross validation on the training data set.
- The effectiveness of the adaptive sampling technique was verified to improve the prediction accuracy for the 95% PCT using a small number of training data.
- The surrogate model with high accuracy for the 95th percentile value prediction was able to be effectively constructed by improving the surrogate model using the adaptive sampling procedure with the target of the 95% PCT and confirming the model prediction accuracy using the cross validation on the training data set.

Thank you for your attention.