# Improvement Methodology of Constitutive Equations in Safety Analysis Code using Integral Effect Test Data

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# 1. Introduction

Accidents in nuclear power plants are investigated with the safety analysis code since experimental approach is often too challenging. Thus, as the accuracy of the safety analysis code increases and the uncertainty of code result is reduced, nuclear power can become safer and more economical. Accordingly, research works to improve the accuracy of the safety analysis code have been conducted for several decades, and experiments to improve the safety analysis code capability are still in process. There are several factors affecting the accuracy of the safety analysis code: user effect, constitutive equation, input nodalization, numerical errors, etc. Most of the constitutive equations are empirically developed correlations such as models for heat transfer and friction at wall and interface of phases.

In the past, separate effect tests were conducted to observe the local phenomena. Recently, integral effect tests (IETs) are conducted to observe the overall phenomena of a nuclear reactor. As the IETs are conducted, there are cases where the code and the experimental results show differences. In this case, the constitutive equation is modified after minimizing the user effect. However, it is very difficult to improve the constitutive equation directly by using the IET data as it is not focused on the local and isolated phenomenon. Therefore, a methodology to improve constitutive equation is presented by directly using experimental data.

This study consists of the following: generation of constitutive equation data, sub-division of constitutive equations, and application of multiplier coefficients to the values from constitutive equations. First, the constitutive equation values according to the thermal-hydraulics and geometric conditions within a wide range are generated. Second, the thermal hydraulic conditions are sub-divided by using the generated data with machine learning technique. Lastly, the multiplier coefficients are applied to the values of constitutive relations with respect to the sub-divided thermal hydraulic regime. The multiplier coefficients are then optimized to reduce the error of the code results to the experiment data.

In the previous studies, this methodology is applied to the SET experiment. It was applied to the steady state experiment, SUBO [1], and to the transient experiment, MIT pressurizer [2]. In this study, it is applied to the integral effect test that can observe various phenomena. The DSP-05 experiment is selected for this purpose, and an error calculation methodology was developed for a multi-variable transient calculation.

### 2. Data Clustering

In order to sub-divide the thermal hydraulic conditions for optimizing constitutive equations, it is necessary to generate constitutive equation data in the wide range. The generated data are the values of the constitutive equations with respect to various thermal-hydraulic and geometric conditions. Since the data was generated in the previous studies [1,2] the same data is used in this study. The range of the generated data is shown in Table I, and the generated data is shows in Figure 1.

Table I. Range of training data generation [1]

Input parameters	Range
Pressure	0.09 – 19 MPa
Fluid Temperature	25 – (Tsat+ 50) °C
Wall Temperature	25 – 1184 °C
Void Fraction	0-1
Mass Flux	3 - 150%
Slip Ratio	1 – 3
Hydraulic Diameter	8E-4 – 12 m
Volume Length	0.01 – 550 m
Angle	0 or 90
Roughness	0 - 2.0 E-4





Fig. 1. Training data (from left top: coefficient of liquid wall HTC, vapor wall HTC, liquid wall FRIC, vapor wall FRIC, liquid interfacial HTC, vapor interfacial HTC, interfacial FRIC)

The clustering of the thermal-hydraulic conditions is proceeded by following the methodology and results reported in the previous studies [1, 2]. The thermalhydraulic conditions were sub-divided using the selforganizing map (SOM) clustering method [3]. The SOM clustering method creates a prototype of the raw data to be clustered through mapping. By using SOM methodology, a benefit in computational cost can be obtained. To find the optimal clustering number, gap statistics [4] and silhouette method [5] were applied. Also, in this study, the cluster number is selected in the constraint that the clustering number is larger than the value that corresponds to the all regimes being divided more than twice. This is the minimum clustering number which is presented in Table II alongside with the optimal clustering number obtained from the previous process. Selected clustering results are shown in Figure 2.

Table II: Minimum group number of clusters [2]

	Minimum clustering number	Optimum clustering number
Wall Heat Transfer	71	109
Wall Friction	55	55
Interfacial Heat Transfer	49	83
Interfacial Friction	51	60



regime [2]

# 3. Multiplier Coefficient Optimization

In this study, the following method is used to the optimization of multiplier coefficients. First, the experiment is simulated with a set of multiplier coefficients extracted with 95% confidence interval within the range of minimum 95% values using the KREM method. The minimum error set can be obtained from the calculation. Second, optimization is performed using the multiplier coefficient set as an initial set. A conjugate gradient method is applied to find the optimal set of multiplier coefficients.

# 3.1. KREM method

The KEPRI realistic evaluation model (KREM) is a methodology developed by the Korean nuclear industry and uses non-parametric statistical methods [6]. In order for the maximum value to exceed the p percentile of the population with a confidence level of q% among n value randomly selected, the number of samples, n, should satisfy the following inequality.

$$1 - \left(\frac{p}{100}\right)^n \ge \frac{q}{100} \tag{1}$$

For the minimum error to exceed 95% of the total population with 95% confidence level, at least 59 samples must be extracted. Therefore, in this study, 59 multiplier coefficient sets were created and applied to each sub-regime, and the set with minimum error is found.

## 3.2. Conjugate gradient method

The conjugate gradient method is a derivative-based method. It calculates the gradient from the starting point, sets the direction, and then search the moving distance through line search. Since it is not possible to obtain the differential value of the multiplier coefficient through an analytical method, the numerical differential calculation method is used. The conjugate gradient method sets the direction using both the gradient of the previous step and the gradient of the current step, which can be calculated using the following formula.

$$d^{(k)} = -c^{(k)} + \frac{c^{(k)}}{\|c^{(k-1)}\|} d^{(k-1)}$$
(3)

#### 3.3. DSP-05 experiment

The DSP-05 experiment is performed with an ATLAS experiment facility which is a pressurized light water reactor thermal-hydraulic effect testing facility operated by KAERI. DSP-05 selected the SGTR accident as a scenario and performed an experiment by operating the SGTR break system through the disconnection and a valve on the steam generator. ATLAS experimental facility is shown in Figure 3.



Fig. 3. ATLAS experimental equipment schematic [7]

The error for IET test is newly defined in this study. In the previous study, a method based on the dynamic time warping was developed. However, since the previous study was targeting a single variable output optimization problem, it is necessary to modify the error calculation in the multi-variable optimization problem. Therefore, weights are applied to the error calculation. The modified error is shown below.

Error  
= 
$$\sum_{k=1}^{K} \beta_k \frac{\sum_{i=1}^{n} |\overline{V_{i,min}}|}{n_k (X_{max} - X_{min})(Y_{max} - Y_{min})}$$
 (4)

In this study, the same values were used for all weights, and the variables used to calculate the error are shown in Table III. Variables with noise were filtered by using time smoothing. It is noted that the measured values and errors are shown in normalized values.

Table III. IET optimization variables

Experiment	DSP-05
Variable	Primary system pressure
	SG-1 secondary pressure
	SG-2 secondary pressure,
	SG-1 secondary level
	SG-2 secondary level
	Integrated mass of MSSV discharge
	RPV core level
	RPV downcomer level
	Loop-1 flow rate
	Loop-2 flow rate
	SGTR flow rate



Fig. 4. DSP-05 optimization results

The optimization results are shown in Figure 4. Selected values used for optimization are plotted. The error for each step is shown in Figure 5. Step 1 is the result of calculating with the original MARS-KS, Step 2 is the minimum error from the KREM methodology, and Step 3 is the minimum error from the conjugate gradient method.

As a result of the optimization calculation, it can be seen that the error is reduced about 10.83%. However, the deviation of the reduced error for all variables is still substantial. SG-1 secondary level is a variable with significantly reduced error of 39.21%, while SG-2 secondary pressure shows the limited success for reducing error by 0.84%.



## 4. Summary and Further Works

In this study, a methodology for improving the accuracy of nuclear safety analysis codes is presented. It is a method of improving constitutive equations using experimental data directly, and consists of the following three steps: data generation, sub-division of thermalhydraulic conditions, and application of multiplier coefficients for optimization of the constitutive equations. SOM clustering methodology was used for clustering, and gap statistics and silhouette method were used as accuracy indices. Optimization of the constitutive equations is performed with multiplier coefficient, KREM method and conjugate gradient method. In the previous study, the similar process was applied to the steady and transient SET experiments. Therefore, in this study, it was applied to the IET experiment. An error is newly defined to reduced error of many variables simultaneously. DSP-05 experiment was selected for the demonstration of the process, and it was confirmed that the error was reduced by 10.83%. However, it was also confirmed that the errors in measurement variables are reduced non-uniformly and some variables can be better optimized than the other variables. .

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#### REFERENCES

[1] ChoHwan Oh et al., Constitutive Equations Improvement Methodology of Reactor Safety Analysis Code using Experimental Data: Application to SUBO Experiment, Transactions of the Korean Nuclear Society Spring Meeting, Jeju, Korea, May 13-14, 2021.

[2] ChoHwan Oh et al., Methodology of Constitutive Equations Improvement in Safety Analysis Code using Experimental Data: MIT Pressurizer Experiment, Transactions of the Korean Nuclear Society Fall Meeting, Changwon, Korea, Oct. 21-22, 2021.

[3] Juha Vesanto and Esa Alhoniemi, Clustering of the Self-Organizing Map, IEEE TRANSACTIONS ON NEURAL NETWORKS, Vol. 11, No. 3, pp. 586-600, 2000.

[4] Robert Tibshirani et al., Estimating the number of clusters in a data set via the gap statistic, J. R. Statist. Soc. B, Vol. 63, Part 2, pp. 411-423, 2001.

[5] Peter J. Rousseeuw, Silhouette: a graphical aid to the interpretation and avlidation of cluster analysis, Journal of Computational and Applied Mathematics, Vol. 20, pp. 53-65, 1987.

[6] S.W. Lee et al., APR1400 large break loss of coolant accident analysis using KREM methodologies, Proceedings of the KNS autumn meeting, 2003.

[7] Lee, J. B. Description Report of ATLAS Facility and Instrumentation (Second Revision). KAERI/TR-7218/2018, Korea Atomic Energy Research Institute, 2018.