Development of constitutive equations in reactor safety analysis code with data-based modeling using artificial neural network

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1. Introduction

In a nuclear reactor safety evaluation process, it is too costly to experiment in the same scale with a commercial nuclear power plant. Therefore, the safety evaluation of a nuclear reactor relies on a safety analysis computer code substantially, whose accuracy directly affects the nuclear safety. The reactor safety analysis code is consisted of governing equations and constitutive equations. The constitutive equations in a reactor safety analysis code has high accuracy for simulating a separate effect test (SET). They are typically a result of experimental data regression with a mathematically limited form. Furthermore, SET can be deliberately used for improving constitutive relations' accuracy. The code validation process also includes comparison of the code result with an integral effect test. If there is a mismatch between experiment results and simulation results, quantifying the cause and using the information to improve constitutive relations are not straightforward. Therefore, if a methodology which the accuracy of the constitutive relations is improved as the number of experimental data increases is developed, one can expect that the safety analysis code's accuracy will automatically improved as more data is accumulated. This methodology can be developed using an artificial neural network that enables data-driven modeling and has less mathematical limitations.

In the previous studies [1, 2], artificial neural networks were applied to replace the wall heat transfer coefficient, and wall friction coefficients in thermal hydraulic (TH) conditions. In this study, artificial neural networks (ANN) that substitute constitutive equations including interfacial heat transfer, interfacial friction are trained on the range that can cover wider TH conditions for analyzing design basis accidents. Methodology for the training data generation is developed to capture the two-phase flow characteristics as much as possible. Also, the methodology for increasing the model accuracy is newly tested for wall heat transfer. The reference nuclear safety analysis code used in this study is MARS-KS.

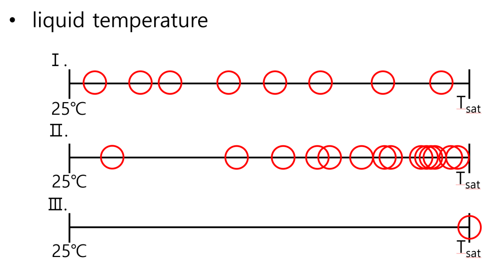
2. Data generation

The constitutive equation modules in the MARS-KS code calculate wall heat transfer coefficient, wall friction coefficient, interfacial heat transfer coefficient, interfacial friction coefficient as a function of thermal hydraulic and geometrical conditions. As the main objective of this study is generating an artificial neural network whose performance is equivalent to the constitutive equations in MARS-KS code first, output parameters of the ANN are constitutive equations, and input parameters are the TH and geometrical conditions. In the process of generating the training data for ANN, it is necessary to determine the range of TH and geometrical conditions. It is important to cover the wide range of conditions for increasing the reliability of the developing ANN. In this study, the range was selected to include the design basis accidents of the APR 1400. For the design basis accidents, LOCA, SGTR, LOOP are considered. Table I shows the conditions covering the selected DBAs.

Table I. Range of training data generation

Input parameters	Range
Pressure	0.09 – 19 MPa
Fluid Temperature	25 – (Tsat+ 50) K
Wall Temperature	25 – 1184 K
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 – 2.0E-4

TH variables except for temperatures are sampled from uniform random function in the given range. In the case of temperatures, it is not proper to sample with uniform distribution for representing two-phase phenomenon correctly. Two-phase flow occurs near the saturation temperature and using the uniform random function for sampling will not sample many data having saturation temperature of fluids. Therefore, three different sampling method is used for selecting the fluid temperature: uniform random distribution (I), log uniform random distribution (II), and single value of saturation temperature (III).



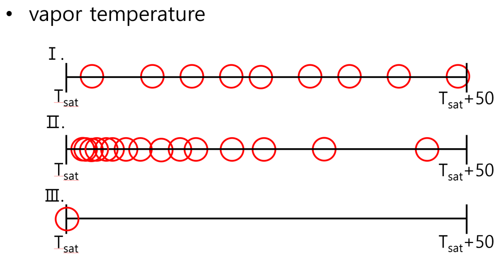


Fig. 1. Fluid temperature sampling method

Nucleate boiling regime is selected in the safety analysis code when the wall temperature is slightly higher than the saturation temperature. To capture this phenomenon, data are generated in different way with respect to the wall temperature. Log uniform random function is used when the wall temperature is higher than the saturation temperature, and uniform random function is used in other cases.

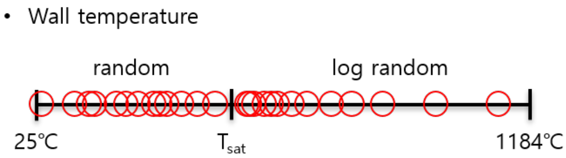
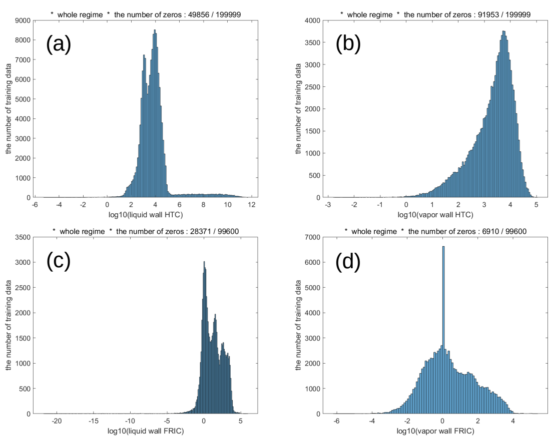


Fig. 2. Wall temperature sampling method

Hydraulic diameter, volume length, roughness is included in the geometrical conditions. Geometry information of APR1400 [3], and ATLAS instrument of DSP-04 [4], and DSP-05 [5] is used to generate training data. In case of geometrical conditions, it is not uniformly distributed, and it is distributed as several discrete values in the code inputs. Therefore, both methods are used to sample the training conditions: uniform distribution and existing discrete value.

The number of training data is more than hundred thousand for each constitutive relation and consists of the same number for each regime. Figure 3 shows the histogram of training data outputs.



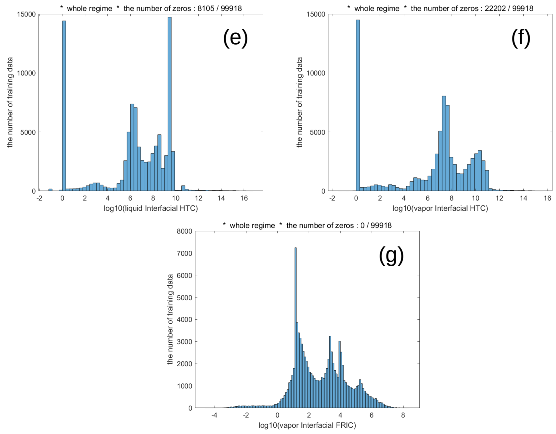


Fig. 3. Training data (a~g: coefficient of liquid wall HTC, vapor wall HTC, liquid wall FRIC, vapor wall FRIC, liquid interfacial HTC, vapor interfacial HTC, interfacial FRIC)

3. Model description

The structure of the artificial neural network should be determined before the training process begins. When performing a safety analysis with MARS-KS code, numerous iterative calculations are performed, and the code calls constitutive relations module many times per iteration. If the calculation time using the ANN takes longer time than the existing constitutive relation module, the calculation time of safety analysis increases substantially. Therefore, simple structure of artificial neural network is first preferred. Table II shows the time of calculating the wall heat transfer coefficient for ten thousand times. The number next to the ANN in Table II is (the number of node) $\times$ (the number of hidden layer).

Table II. Constitutive equation calculation time

	MARS-KS	ANN(50×4)	ANN(100×4)
Time [sec]	0.3045	0.1554	0.6909

Multi-layer perceptron is used for data regression frequently, and has a simple structure. Hyperparameters are variables that should be determined before training the artificial neural network, which includes the number of node, the number of hidden layer, activation function, learning rate, batch size, and so forth.

Table III. Range of ANN hyperparameters

Hyperparameters	
The number of node	$1 - n^2$
The number of hidden layer	2 – 4
Learning rate	1E-3 – 5E-2
Batch size	2000 – 20000
Activation function	Sigmoid, ReLU, SeLU, ELU
Loss function	Mean Squared Error (MSE)
Training and validation	75% / 25%
Optimizer	Adam optimizer

Table III shows the range of the hyperparameters. In order to select optimal hyperparameters, training was performed under the conditions given in Table III, and an ANN structure with high accuracy was selected among them. Table IV is the optimized hyperparameters for each constitutive equation which the ANN has high performance.

Table IV. ANN Hyperparameters

	Node number	Hidden layer number	Activation function
Wall HTC ($T_w > T_{sat}$)	90	3	ReLU
Wall HTC ($T_w < T_{sat}$)	60	2	ReLU
Wall FRIC	44	3	ReLU
Interfacial HTC	40	3	Sigmoid
Interfacial FRIC	30	3	ReLU

4. Results and Discussion

Table V shows the training accuracy, and validation accuracy. This training and validation accuracies are in logarithmic values. The accuracy decreases in the process of changing the logarithm to original value but due to the large span of data it is inevitable to use logarithmic transfer of the original data.

Table V. Accuracy of the artificial neural network

	MSE (training)	MSE (validation)	R^2
Wall HTC ($T_w > T_{sat}$)	1.796E-3	2.156E-3	0.9677
Wall HTC ($T_w < T_{sat}$)	2.330E-3	2.362E-3	0.8999
Wall FRIC	3.245E-3	3.188E-3	0.9076
Interfacial HTC	5.206E-3	5.843E-3	0.9001
Interfacial FRIC	9.785E-4	1.035E-3	0.9417

Table VI shows the accuracy of the ANN in wall heat transfer coefficients. R^2 decreased significantly when the logarithm values change to the original values. Most result shows that the error is not negligible compared to the existing constitutive relation, and two reasons can be inferred which lower the model accuracy. The constitutive equations in MARS-KS code are composed of different correlations according it is selected by choosing heat or flow regime first. The data complexity increases due to the logical statement used for the regime selection and the number of different correlations used in the constitutive equations. Also, in the MARS-KS code, there are non-physical values programmed in constitutive equations to increase the stability of the code.

Table VI. Result of Liquid Wall Heat Transfer Test

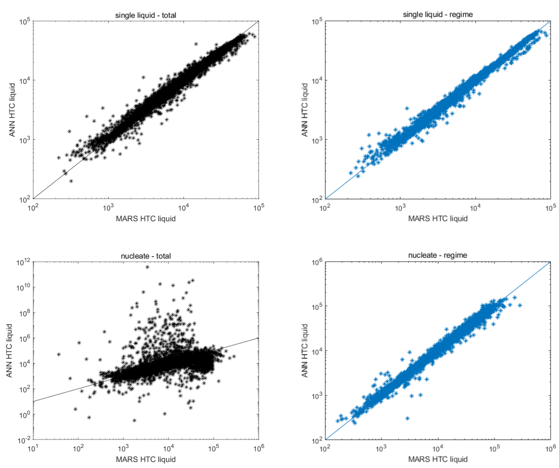
	MAPE (%)	MAXE (%)	R^2
Single Vapor	490.61	1.49E+04	-1.2585
Nucleate	9.46E+05	1.10E+10	0.3022
Transition	2.88E+03	3.54E+07	0.9019
Film	1.11E+03	1.15E+07	0.7504
Single Liquid	7.20	371.74	0.9823
Condensation	89.92	1.38E+04	0.6473

For increasing the accuracy of the model, different artificial neural network is used for each regime. Also, an artificial neural network that classifies the regimes according to the TH conditions is combined to the constitutive equation module. Lastly, non-physical values are excluded in the training process. In the single vapor regime, void fraction of the most data has unity value, which denotes that the fluid is only consisted of vapor. However, in the MARS-KS code, there is a few cases that void fraction is not unity. If the wall temperature is higher than the saturation temperature and the fluid temperature, and total heat flux value is negative at the same time, MARS-KS code considers this case as the single vapor regime. These data are also excluded as this condition is not necessarily the single vapor state. Similarly, there is a few cases that vapor heat transfer coefficient is not zero in nucleate boiling regime, and this data is also excluded.

Table VII. Result of Liquid Wall Heat Transfer Test when using the different artificial neural network for each regime

	MAPE (%)	MAXE (%)	R^2
Single Vapor	-	-	-
Nucleate	5.76	213.74	0.9913
Transition	253.47	2.92E+06	0.9955
Film	96.99	2.98E+05	0.9287
Single Liquid	4.35	212.5	0.9932
Condensation	62.32	1.96E+04	0.7439

Table VII shows the accuracy of the ANN when using the methods mentioned above. It is clearly observed from Figure 4 that the ANN model accuracy is improved. Average accuracy increased in most regime. However, in some regimes, the average accuracy is still low.



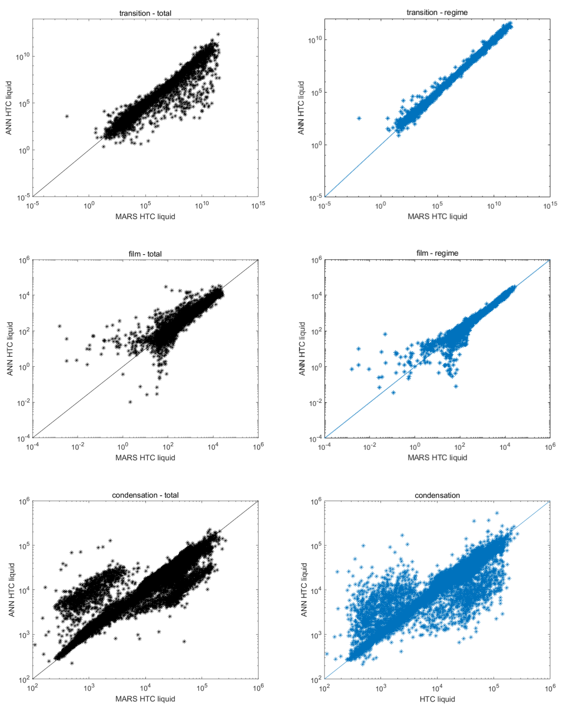


Fig. 4. MARS-KS liquid wall heat transfer coefficient versus prediction using artificial neural network (left: using one ANN for whole regime, right: using different ANN for each regime)

Figure 5 shows the accuracy of the artificial neural network that separates determines the regime. Decision tree, Naïve Bayes classifier, support vector machine, K-nearest neighbor are all tested. Support vector machine has the highest accuracy among them, and the average accuracy is 94.5 %.

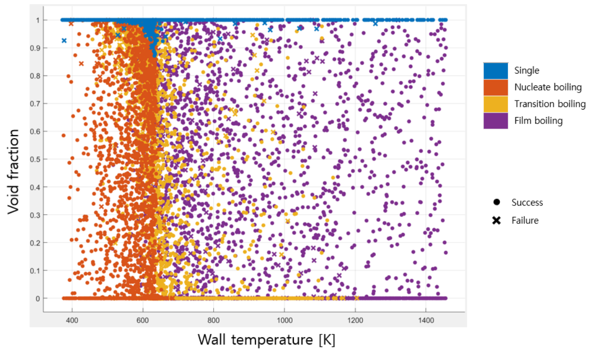


Fig. 5. Heat transfer regime classification results

5. Summary and Further works

In this study, an artificial neural network has been developed to observe the feasibility to be used for the constitutive relations in the nuclear safety analysis code. ANN enables data-driven modeling, thus the authors think that as more experimental data accumulates the code accuracy can be improved better if ANN can be used for the constitutive relations of the code. In the previous study, wall heat transfer coefficient and wall friction coefficient were trained with the artificial neural network within narrow thermal hydraulic conditions. In this study, the range is expanded that can cover the design basis accidents in a nuclear power plant. Interfacial heat transfer and interfacial friction which were not dealt in the previous study are also newly developed with ANN. In order to minimize the code calculation time, multi-layer perceptron which has a simple structure is first tested. However, the accuracy of the code is not satisfactory if the training data range covers the whole regime. Output parameters are trained in logarithmic scale due to the wide range, and errors were greatly increased in the process of transferring logarithmic value to the original value. To improve the model accuracy, training is performed using different artificial neural networks for each heat transfer regime, and artificial neural networks for determining the regime is also newly constructed. Furthermore, non-physical values are excluded from the training data. The accuracy increases for most regimes. However, accuracy is still unsatisfactory in some regimes, which should be further improved. If necessary, using more complicated artificial neural network will be used.

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