Application of data driven modeling for MARS-KS code constitutive equation

Doh Hyeon Kim [a], Jeong Ik Lee [a]*
[a]Department of Nuclear and Quantum Engineering, Korea Advanced Institute of Science and Technology (KAIST)
[*]Corresponding author: jeongiklee@kaist.ac.kr

1. Introduction

Accurate safety analysis of a reactor accident scenario is based on the accuracy of the safety analysis code and how the code is utilized. Among many factors affecting the accuracy of the code, the user effect and the physical model of the constitutive equation are dominant. Therefore, to improve the accuracy of the system code from the code developer's point of view, it is necessary to develop more accurate constitutive equation based on physical model. In addition, in order to improve the physical model of safety analysis codes, various institutes in each country are continuously conducting integral effect test (IET) and separate effect test (SET) for various scenarios and thermal hydraulic conditions. However, due to the complexity of two phase flow and the difficulty of modeling, there are still cases which the experiments and code calculated results do not exactly match when IET or SET is performed. In particular, interfacial heat transfer among the constitutive equations has higher uncertainty than near-wall terms because it is difficult to measure directly in the experiment. Recently, a research work founds that predicted rate of bubble growth by various interfacial heat transfer models varies greatly from model to model [1].

In the feedforward network, although each layer is linearly coupled, it uses nonlinear activation function so that it can accurately regress various types of complex nonlinear function. In this study, SUBO experiment conducted by KAERI selected as the reference experiment that the original system code cannot accurately predict experimental void fraction. In this study, it was evaluated how accurately interfacial heat transfer coefficient could be trained by feedforward network in SUBO thermal hydraulic condition to demonstrate the potential of further improvements in the constitutive relations. In addition, it was confirmed that the same code calculation results are obtained after the constitutive equation is replaced with feedforward network in the safety analysis code, MARS-KS. Also, feedforward network was optimized to match the experimental data by applying randomness to the weight and bias values with the simulated annealing method.

2. Methods and Results

2.1 Target experiment

In this study, it is needed to find experiments with thermal hydraulic range that were not too wide and which MARS-KS did not predict accurately. Therefore, SUBO (Subcooled Boiling) experiment conducted by KAERI was selected as the target experiment since it has a suitable thermal hydraulic range and MARS-KS cannot accurately predict the void fraction of the experiment. In the SUBO facility, the subcooled boiling test was performed to extend the database for a higher mass flux and heat flux conditions under atmospheric pressure in a long test channel. In short, subcooled water is injected from the bottom, vapor is generated through the heated pipe, and the local void fractions were measured radially in the annulus at each height. The test section of SUBO facility is shown in Figure 1.

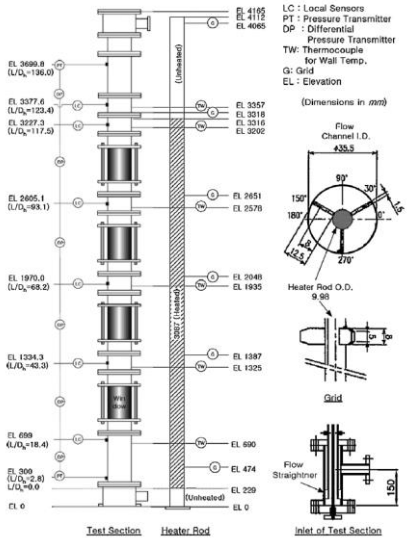

Fig. 1. Test section of SUBO facility

2.2 Feedforward network input parameter

The interfacial heat transfer equation of MARS-KS is calculated through 10 input variables. Among them, pressure, liquid temperature, vapor temperature, liquid velocity, vapor velocity, and void fraction are selected as input parameters. As output parameters of feedforward network, two coefficients, Hif and Hig, which are used to calculate interphase mass transfer in interfacial heat transfer were used. Since the feedforward network training was conducted in MATLAB, 'refprop' file provided by NIST was used for water property file for the feedforward network training. In the case of MARS-KS, the 'tpfh2o' file is used as the property file. The vapor temperature in the

SUBO thermal hydraulic condition is very close to the saturation temperature because SUBO experiment was conducted in two-phase flow. In addition, the difference between the saturation temperature and the vapor temperature is used during the calculation of the interfacial heat transfer constitutive equation. However, even if the saturation temperature was predicted differently by 0.01 degree Celsius, calculated tsg is nearly 10 times different between two property files. Therefore, the liquid temperature and the gas temperature of the input parameters were changed to tsf, and tsg, which are the difference from the saturation temperature, respectively.

Table I: Input parameter thermal hydraulic condition

Input parameter	Unit	Value
P (Pressure)	kPa	150-200
Tsf (Tf – Ts)	K	-30 – 0
Tsg (Tg – Ts)	K	-0.01 – 0.01
vl (liquid velocity)	m/s	1.0 – 3.0
vg (vapor velocity)	m/s	0.0 – 5.0
ag (void fraction)		0.0 - 0.7

2.3 Feedforward network training

Using MATLAB, separate platform that performs the same calculations as the original MARS-KS constitutive equation was used to randomly generate input output datasets for feedforward network. The thermal hydraulic conditions used to generate random datasets are shown in Table 1. In the case of vapor temperature, the subcooled vapor temperature exists because it is a process of subcooled boiling. Sigmoid function and ReLu were used as the activation functions, and the number of hidden layers was 2 with 20 to 30 nodes for the given datasets. The input parameters were normalized between -1 and 1, and the output parameters were trained by taking logarithmic values of the original values because the range of interfacial heat transfer coefficients was too wide. By changing the node number and the log base number, feedforward network with the least error was found. As a result of finding the feedforward network with the smallest error through 50,000 data sets, the smallest error was found when the node number is 28 and the log base number is 1.5. In addition, as a result of re-training by increasing the data sets to 100,000 for the smallest error condition (node number: 28, log base number: 1.5), Hig showed 2.98% and Hif showed 2.75% error of MAPE (mean absolute percentage error) compared with original MARS-KS constitutive equation.

2.4 Modified MARS-KS for feedforward network

MARS-KS code has been modified to read the weight and bias values of the neural network by additional input file and to perform the same calculations as the neural network during the code calculation. Figure2 shows the code progress of the modified MARS-KS.

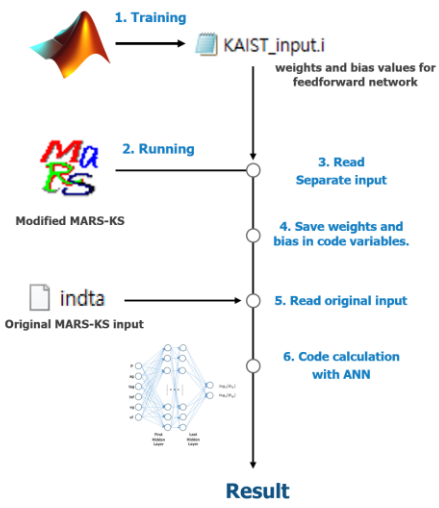

Fig. 2. Code progress of modified MARS-KS code

The weight and bias values of the trained feedforward network were saved as separate input files, and the MARS-KS has been modified to read both input files for the original simulation and feedforward network simultaneously. Modified MARS-KS code and original MARS-KS were used for calculating SUBO BaseRB case. Figure 3 shows calculated void fraction of Original MARS-KS and Feedforward network MARS-KS. The error of the calculated void fraction of two codes is 0.0011%. In the case of the liquid temperature and the vapor temperature, the same results were obtained on the significant figures number output from two MARS-KS code. Accordingly, it is confirmed that the same results are obtained when the interfacial heat transfer coefficient is replaced by the feedforward network in original MARS-KS.

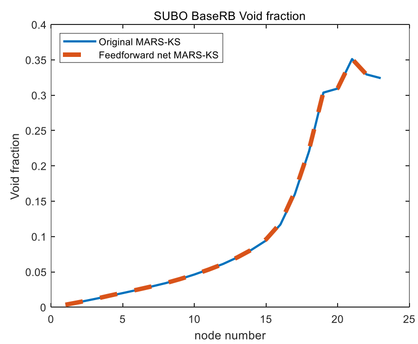

Fig. 3. Calculated Void fraction of Original MARS-KS and Feedforward net MARS-KS

2.5 Feedforward network optimization

In this study, ~~it is needed to modify~~the pre-trained feedforward network was attempted to evolve ~~by~~ from ~~using~~ a small number of experimental data. Therefore, a different method from the conventional neural network optimization was needed.

The proposed preliminary method is ~~Random~~ randomizing values ~~were used~~ in the weight and bias values of the feedforward network, and a minimum error set was obtained by applying simulated annealing method. Simulated annealing is a probabilistic technique for approximating the global maximum of a given function. It is useful to approximate global optimization in a large search area for an optimization problem.

The detailed optimization process is as follows. First, a wide range of random variable was multiplied at the weight and bias values of the feedforward network, which the original values can calculate almost the same values as the original MARS-KS interfacial heat transfer constitutive equation does. Among several random combinations, some combinations of small errors with the experimental data were selected. For each selected combination, the narrow and wide ranges are multiplied with a probability and the minimum error sets are updated whenever the error is reduced. Finally, the least error combination was found among each selected and optimized combinations. Figure 4 shows the flowchart of weight and bias values optimization.

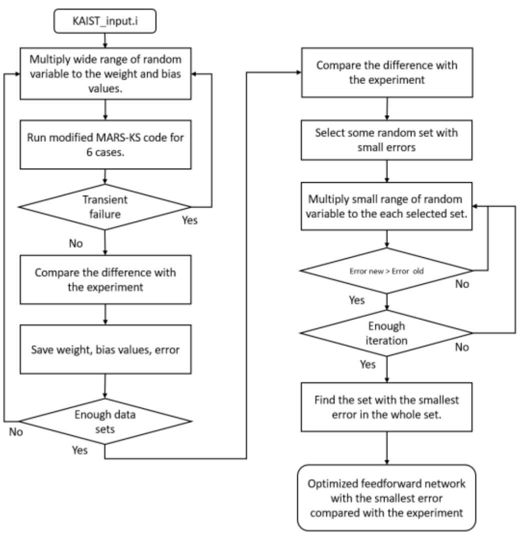

Fig. 4. Flowchart of weight and bias optimization

2.6 Results

It is confirmed that random perturbation of the weight and the bias values of the feedforward network change the predicted void fraction of the modified MARS-KS code. Figure 5 shows the change in the predicted void fraction of the MARS-KS code. The thick purple line in the middle of ~~the~~ Figure 5 represents the experimental results of SUBO BaseRB case.

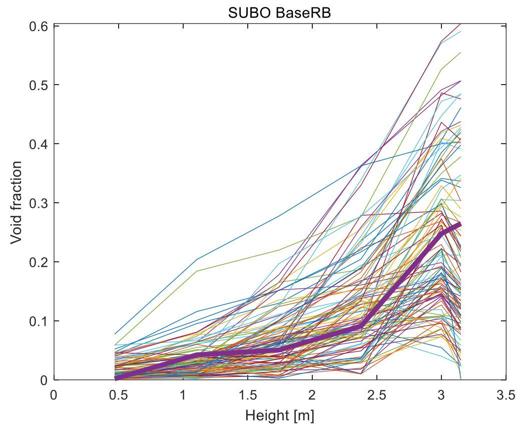

Fig. 5. Modified MARS-KS calculated void fraction by perturbing weight and bias values

Figure 6 shows the calculated results of the modified MARS-KS with the least-error-set. Original MARS-KS has a total void fraction error of 0.1821, and the modified code shows a total void fraction error of 0.0473, which shows the modified MARS-KS code predicts the experimental data much better than the original MARS-KS code.

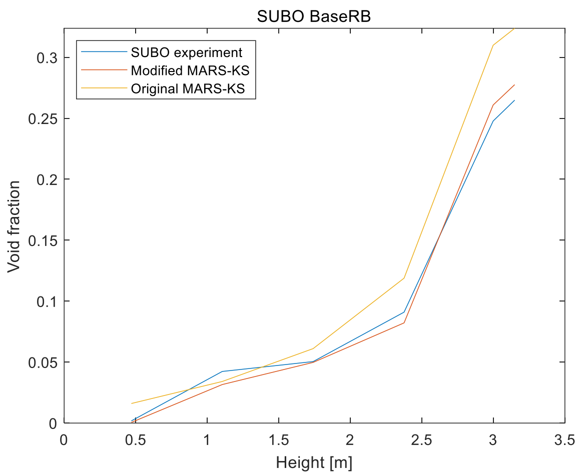

Fig. 6. Modified MARS-KS results with the smallest error-set

3. Conclusions

As a result of this study, it was possible to replace interfacial heat transfer constitutive equation with a feedforward network. Also, it is confirmed that random perturbation of the weight and the bias values of the feedforward network changes the predicted void fraction of the modified MARS-KS code successfully. By applying the simulated annealing method for optimizing random perturbations, it was possible to find the weight and bias values combination that showed the smallest error compared with ~~SUBO~~ experimental data.

Acknowledgments

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REFERENCES

[1] M.R. Abdollahi, M. Jafarian, and M. Jamialahmadi, The rate of bubble growth in a superheated liquid in pool boiling, Heat and Mass transfer, 2017

[2] S.A.Mohammadein, and K.G.Mohamed, Growth of a Vapour Bubble in a Superheated Liquid of Variable Surface Tension and Viscosity Between Two-phase Flow, Applied Mathematics & Information Sciences, Tanta University, Nov, 2013

[3] Y.Liao, Evaluation of Interfacial Heat Transfer Models for Flashing Flow with Two-Fluid CFD, Fluids, 2018

[4] B.J.Yun, B.U.Bae, D.J.Euh, and C.H.Song, Experimental investigation of local two-phase flow parameters of a subcooled boiling flow in an annulus, Nuclear Engineering and Design, 2010

[5] B.J.Yun, B.U.Bae, D.J.Euh, G.C.Park, and C.-H.Song, Characteristics of the local bubble parameters of a subcooled boiling flow in an annulus, Nuclear Engineering and Design, 2009

[6] Experimental Study of Local Bubble Parameters of the Subcooled Boiling Flow in a Vertical Annulus Channel, KAERI, 2008

[7] Integral Cooling Performance Tests for Nuclear Power Plants and Development of Advanced Safety Analysis Technology, KAERI, 2011

[8] J.J.Lee, Application of Adjoint Based Node Optimization Method to Nuclear Thermal-Hydraulic System Analysis Code, Master Thesis, Korea Adv. Inst. Science, Techn., Daejeon, Republic of Korea, 2019

[9] S.G.Shin, Analysis of Two-phase Constitutive Relation Models implemented in Thermal-Hydraulic System Analysis Codes, Master Thesis, Korea Adv. Inst. Science, Techn., Daejeon, Republic of Korea, 2019

[10] S.W.Bae, H.K.Cho, Y.J.Lee, H.C.Kim, Y.J.Jung, and K.Kim, A Summary of Interfacial Heat Transfer Models and Correlations, 2007

[11] Plesset,M. and Zweick,S., The Growth of Vapour Bubbles in Superheated Liquids, J.Appl. Phys., 1954

[12] MARS CODE MANUAL VOLUME I –V, KAERI, 2009