Uncertainty Quantification for Multi-Scale Reflood Tests Using Neural Network Based Surrogate Models

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1. Introduction

The uncertainty quantification and sensitivity analyses have been widely conducted for computational codes. For evaluation of uncertainties of the code analysis, the data assimilation [1], a methodology of model calibration, is needed to refine the parameters of physical model, initial conditions and boundary conditions, which are thought to have major contributions to the response uncertainties. For a highly nonlinear problem that cannot be solved analytically, sampling approaches are effective ways to perform the data assimilation and quantify the uncertainty of the important parameters. As a representative methodology, Markov Chain Monte Carlo (MCMC) algorithm [2,3], which can find the parameter distributions via constructing Markov chains of random samples, is quite useful, in particular for the simulation of the nonlinear problems. Recently, MCMC was utilized in uncertainty estimation for thermal hydraulic system calculation by Heo et al. (2018) [4]. Based on the MCMC method with Bayes' theorem, they conducted data assimilation using 1D small scale tests, FEBA [5,6] and refined the 32 important physical models and 5 boundary conditions. Subsequently, based on the calibrated parameter distributions, a posteriori distributions for large scale (FLECHT-SEASET) [7] and multi-dimensional (PERICLES) tests [8] were obtained. The uncertainty bands for the FLECHT-SEASET and PERICLES mostly covered the experimental data. It was a successful application of MCMC to the uncertainty quantification for thermal hydraulic system code, but it required substantial CPU time to conduct the data assimilation.

In this study, to reduce the computing demand for thermal hydraulic system calculation during the MCMC simulation, the machine learning was used to develop surrogate models for the complex system. The machine learning has been recently used in many fields of engineering. A key methodology of the machine learning is the neural network. The neural network is a useful modeling tool to solve a complex problem of multi-physics and multi-system via deep learning and deep network.

In this study, the data assimilation methodology using machine learning models was suggested for the thermal hydraulic system to determine the uncertainties of the modeling parameters and the boundary conditions and uncertainties on the code simulation results. As the first step, the machine learning models were developed by learning the calculation results for the scattered conditions. Using the machine learning models, a posteriori distributions were obtained using 1D FLECHT-SEASET reflood tests and subsequently blind calculations were conducted to examine whether the calibrated parameter distributions simulate multi-dimensional PERICLES tests.

2. Construction of Neural Network Based Surrogate Model

To develop the neural network based surrogate model, the Tensorflow code [9] developed by Google was used. In the Tensorflow code, it is easy to adjust the number of neurons and hidden layer and to select the activation function. In this study, ReLU function [10] was selected as the activation function in order to make deep neural networks.

The neural network consists of an input layer, hidden layers and an output layer. In an input layer and an output layer, the input and the output variables for code calculations should be chosen properly. 5 boundary conditions and 30 physical variables which are important for the quenching phenomenon were selected as the input variables. In addition to that, the variables for the time and the location should be selected. However, the location variable was not considered in the input layer because there were difficulties for constructing the surrogate model applicable to all locations. Thus, the constructed neural network model had the total 36 input variables and predicted the wall temperature as the output.

The neural network should be trained by using the database for the target problem. In this study, the database of SPACE calculation results for Run number 31302 of the FLECHT-SEASET experiments was used. The database consists of 6 uncertainty bands with respect to the axial location (2, 4, 6, 8, 10 and 11 ft). An uncertainty band includes 10000 wall temperature profiles for 10000 distributed cases. A profile includes the wall temperature during 255 time steps (5-259 sec). Thus, there are 2550000 data for one location.

Based on that database, the six neural network models were trained and constructed for six axial locations. In order to obtain the best accuracy, the numbers of neurons and hidden layers were optimized and seven hidden layers having twenty neurons were given in every network models. All six models have good accuracies less than the root-mean-square (RMS) error of 10 % in comparison with the database of SPACE calculation results. The detail information for the constructed surrogate models is shown in Table 1.

Table 1. Neural network based surrogate models

Index	Location	Hidden layers × Neurons	RMS error
1	2 ft	7 × 20	1.6 %
2	4 ft	7 × 20	4.3 %
3	6 ft	7 × 20	8.9 %
4	8 ft	7 × 20	9.9 %
5	10 ft	7 × 20	7.7 %
6	11 ft	7 × 20	6.3 %

3. Data assimilation

To consider scaling problems when performing model calibration, two different reflood test data were used for the following two step analysis. In the first step, the model calibration was performed using FLECHT-SEASET test data. In the second step, uncertainty estimation was conducted for the cladding temperature for 2D PERICLES test using the model distributions obtained in step 1.

For the step 1 above, the neural network based surrogate model was utilized when performing the MCMC simulation. The surrogate model generates chains of parameter samples with a tremendous reduction in the computational demand. To perform data assimilation by calibrating models in the simulation code, the results of FLECHT-SEASET experiments were used. Figure 1 shows the a posteriori distribution of selected parameters obtained by MCMC simulation with neural network based surrogate models. The experimental data and the nominal values of wall temperatures produced by reference calculations at the axial level of the measuring position 8 ft for the FLECHT-SEASET obtained using the surrogate models are presented in Figures 2. The refined temperature distributions computed using about 10,000 a posteriori parameter samples at the same axial level for the FLECHT-SEASET test is also presented in the figure. As shown in the Figure 2, it was observed that the fuel rods were quenched earlier for the SPACE reference calculation. However the prediction of the wall temperatures is improved after refining the parameter distributions such that the adjusted distributions of the simulation output cover the entire experimental data sets. This confirms the parameters selected for this analysis are the major sources of the modeling uncertainties for reflood tests, and an effective algorithm for a nonlinear system is used to calibrate the parameter distributions.

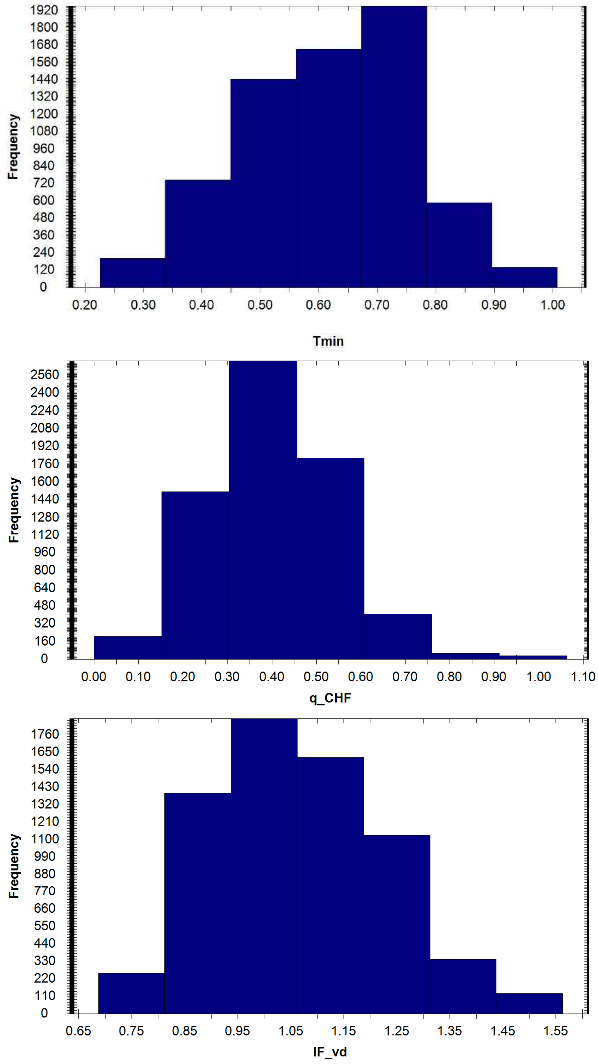

Figure 1. A posteriori distribution of the most influencing parameters obtained by MCMC simulation with neural network based surrogate models.

PERICLES experiments has been conducted to investigate multi-dimensional effects which can occur in the reactor core. For the step 2 of this analysis, a simulation was conducted in order to perform best-estimated prediction for 2D PERICLES experiments with thermal hydraulic parameters obtained via model calibration using 1D FLECHT-SEASET experiments. The experimental data and the posterior wall temperature distributions, i.e., the temperature distributions calculated by completing uncertainty propagation for the calibrated parameter samples, for the PERICLES test no. 64 are presented in Figure 3. The figure shows that the adjusted distributions of the SPACE simulation sometimes do not cover the experimental data, but overall the wall temperature is well predicted by SPACE code.

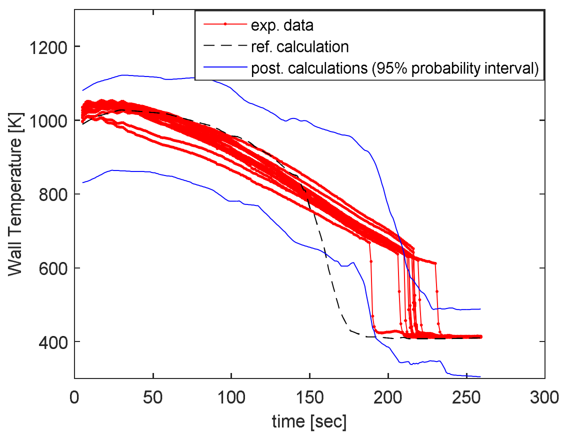

Figure 2. Uncertainty bands of the calibrated wall temperature at the axial location of 8 ft along with the experimental data for the FLECHT-SEASET run no. 31302

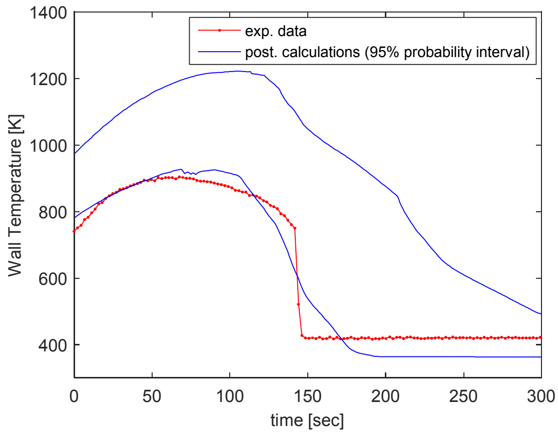

Figure 3. Uncertainty bands of the calibrated wall temperature along with the experimental data for the PERICLES run no. 64

4. Conclusion

The goal of this study is to quantify the uncertainties on the parameters via conducting data assimilation with a minimum computational demand accomplished by developed neural network models. For this analysis, first of all, the Bayesian approach was used to determine the a posteriori distributions of the parameters for the FLECHT-SEASET test data. The neural network model provided an alternative solution with a tremendous reduction in the computational demand for the calculation. For the forward uncertainty propagation performed as a blind calculation, parameters' uncertainty bands were mapped through the computational model to assess the uncertainty bands of the calculation results for the PERICLES. The result shows that the adjusted distributions of the simulation output mostly cover the experimental data. Based on the calibrated parameter uncertainties, each model's impact to the system was identified to determine the major sources of the modeling uncertainties. That will be used to discuss further model development.

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