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Study on the Application of Machine Learning in Computational Fluid Dynamics

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1. INTRODUCTION

Experimenting hypothetical nuclear power plant accidents is very challenging, thus many computational studies are being conducted. However, there are limitations to severe accident simulation using CFD (Computational Fluid Dynamics). Especially for two-phase flow, improving prediction accuracy of CFD requires special effort due to complexity and non-linearity. However, a CFD approach to modeling complex two-phase flows is becoming important for predicting the consequences of severe accidents. In order to overcome the existing limitations of CFD, more and more efforts are being made to apply machine learning to CFD. Kwon et al. [1] made a machine learning approach for heat transfer correlation. Maulik et al. [2] applied deep leaning to OpenFOAM and confirmed the possibility of using complicated neural architectures for practical CFD problems. Machine learning-based data analysis can predict outputs based on existing data, which can contribute to accurately predicting two-phase flows.

Therefore, this study presents an attempt to develop a physical model for CFD simulation using machine learning techniques. In particular, by applying the developed model to a subcooled boiling CFD simulation, the physical model of CFD is evaluated and machine learning applicability is reviewed. This will lead to the development of better prevention and mitigation strategies for serious accidents in nuclear power plants.

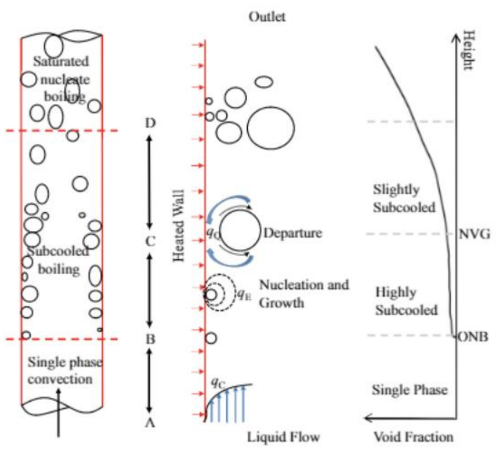

Fig 1. Illustration of subcooled boiling flow in a vertical uniformly heated tube [3].

2. METHODOLOGY

2.1 Methodology

First, a target physical model is selected. The wall heat transfer model used in the CFD code is generally RPI model [4]. Then, it is necessary to generate data for model training. ANN (Artificial neural network) is used as the machine learning technique. The ANN consists of an input layer, hidden layers, and an output layer. This has the advantage that even if each input parameter has a non-linear relation it can be expressed as a relational expression. An appropriate parameter selection for input is important to improve the accuracy of machine learning model. As the number of parameters increases, the amount of data and time required for learning increases. In addition, parameters correlated with output should be selected. Therefore, the appropriate range of parameters and datasets must be determined. After setting the input parameter and range, data was generated through numerical simulations. Random data is generated via MATLAB and REFPROP by setting an appropriate range of parameters. Based on this data, model training was proceeded. Model training improves accuracy while adjusting the hyperparameter. Lastly, the machine learning model will be validated and evaluated through the test set.

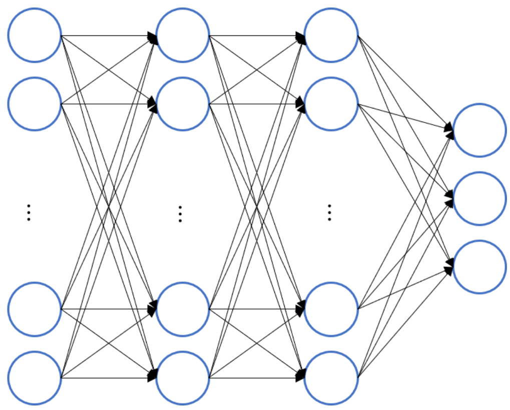

Fig 2. ANN model structure

2.2 RPI wall boiling model

The Rensselaer Polytechnic Institute(RPI) wall boiling model proposed by Kurul and Podowski [4] describes the wall boiling of subcooled boiling and is mainly used in commercial CFD code. The RPI wall boiling model is based on the heat flux partitioning model, and the total heat flux from wall to the fluid (q_w'') is consisted of convective heat flux (q_c''), quenching heat flux (q_q'') and evaporative heat flux(q_e'').

$$q_w'' = q_c'' + q_q'' + q_e'' \qquad (1)$$

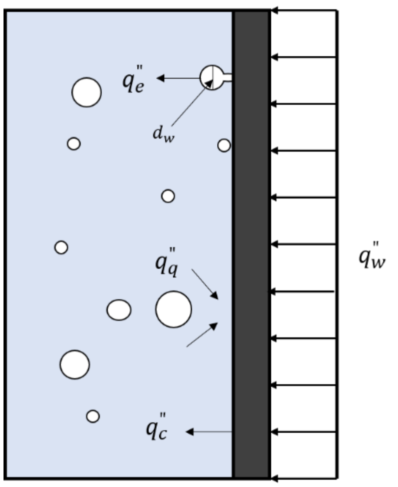

Fig 3. RPI partitioning model

The convective heat flux, $q_w^{''}$ is quantified by the convective heat transfer between single liquid phase and heated wall surface that is not covered by the attached nucleating bubbles [3]. The $q_c^{''}$ is expressed by

$$q_c^{''} = h_c(T_w - T_l)(1 - A_b) \tag{2}$$

Where the T_w is the wall temperature, T_l is liquid temperature, h_c is single phase heat transfer coefficient, and A_b is the proportion of heated wall covered by nucleating bubbles, estimated by

$$A_b = \min\left(1, K\frac{N_w \pi d_w^2}{4}\right) \tag{3}$$

where K is an empirical constant estimated by Del Valle and Kenning equation [6]

$$\mathrm{K} = 4.8\exp\left(-\frac{\rho_l c_{p,l}(T_w - T_l)}{80\rho_g h_{fg}}\right) \tag{4}$$

N_w is the active nucleate site density, and given by Lemmert and Chawla model [7]

$$N_w = 210^{1.805}(T_w - T_l)^{1.805} \tag{5}$$

d_w is the bubble departure diameter, and given by Tolubinsky- Kostanchuk model [8]

$$d_w = \min(0.0006e^{\left(-\frac{\Delta T_{sub}}{45.0}\right)}, 0.0014) \tag{6}$$

where $\Delta T_{sub} = T_{sat} - T_l$, T_{sat} is saturated temperature, ρ_l is liquid density, ρ_g is vapor density, $c_{p,l}$ is the specific heat of liquid and h_{fg} is the latent heat.

The quenching heat flux, $q_q^{''}$ is defined as the process of liquid cooling due to flow induced by bubbles departing from the wall. The $q_q^{''}$ is expressed as

$$q_q^{''} = \frac{2\sqrt{k_l \rho_l c_{p,l} f}}{\sqrt{\pi}}(T_w - T_l) \tag{7}$$

f is the frequency of bubble departure, given by Cole correlation [9]

$$f = \sqrt{\frac{4g(\rho_l - \rho_g)}{3d_w \rho_l}} \tag{8}$$

where k_l is the thermal conductivity of liquid phase, and g is the gravitational acceleration.

The evaporative heat flux, $q_e^{''}$ is defined in the process of phase change from liquid to vapor. The $q_e^{''}$ is expressed as

$$q_e^{''} = V_d N_w \rho_g h_{fg} f \tag{9}$$

where $V_d = \frac{\pi d_w^3}{6}$ is the volume of the bubbles based on the departure diameter.

3. RESULT AND DISCUSSION

Main variables of the RPI wall boiling model are P, T_w, T_l, v_l, and T_{sat}, and those are the input parameters of the ANN. Output parameter is the total wall heat flux, $q_w^{''}$. The range of parameters are determined by experimental condition of B.J. Yun et al. [5], SUBO(Subcooled Boiling) experiment.

Table 1. Range of input parameter (Case 1) [5]

Parameters	value	Unit
Pressure (P)	185-196.8	kPa
Wall temperature (T_w)	400-450	K
Liquid temperature (T_l)	363-423	K
Liquid velocity (v_l)	1.1415-2.1675	m/s

In the RPI model, parameters and heat fluxes are related mostly non-linear. The total wall heat flux is proportional to the temperature difference, such as (T_w – T_l), (T_w – T_{sat}), and (T_l - T_{sat}) than using each temperature directly. Therefore, a model with P, v_l, (T_w- T_l), (T_w- T_{sat}), (T_l- T_{sat}) as input parameters is developed and trained. The information of the ANN model is shown in Table 2.

Table 2. ANN model information

Input parameter number	5
Output parameter number	1
Hidden layer number	2
Node number	50
Epoch	300
Learning rate	0.01
Activate function	ReLu
Optimizer	Adam
Loss function	MSE

$$R^2 = 1 - \frac{\Sigma(y_{actual,i} - y_{pred,i})^2}{\Sigma(y_{actual,i} - y_{mean})^2} \tag{10}$$

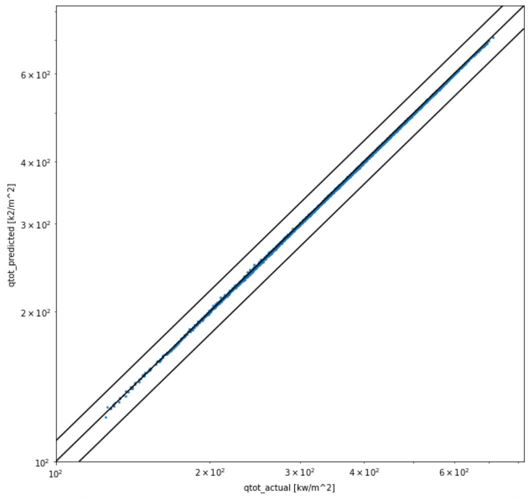

Fig 4. Total wall heat flux for test data (Case 1)

The evaluation result of the ANN model for the range of Table 1. is shown in Fig.4. The accuracy of the model can also be evaluated through the R^2 scores shown in Eq (10). As a result, R^2 score is 0.9998, Maximum Absolute Percentage Error (MAPE) is 0.2616 and Maximum Absolute Error (MAXE) is 5.4477.

Table 3. Range of input parameter (Case 2)

Parameters	value	Unit
Pressure (P)	185-300	kPa
Wall temperature (T_w)	400-600	K
Liquid temperature (T_l)	363-450	K
Liquid velocity (v_l)	1.1415-2.1675	m/s

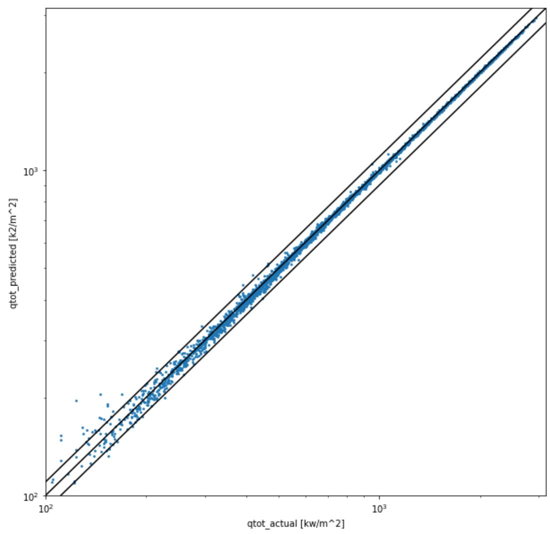

Fig 5. Total wall heat flux for test data (Case 2)

Case 2 has a wider range than Case 1. Likewise, the result is shown in Fig.5. As a result, R^2 score is 0.9997, MAPE is 1.5226 and MAXE is 98.7375. The results of each case are listed in Table 4.

Table 4. Model accuracy and result

	Case 1	Case 2
MAPE	0.2616	1.5226
MAXE	5.4477	98.7375
R^2 score	0.9998	0.9997

4. CONCLUSION AND FUTURE WORK

In this study, the RPI model, which is the physical model of CFD wall heat transfer for two phase flow simulation, is expressed as an ANN model. This is to naturally improve the model with data for the future severe accident simulation. In particular, training data was generated using the data range of the SUBO experiment to simulate the subcooled boiling regime first. The main input parameters were identified as pressure, liquid velocity, wall temperature, liquid temperature, saturation temperature, and output is the total wall heat flux. It was found from the study that temperatures should not be used directly for inputs, but temperature difference should be used for better correlation. As a result, it was confirmed that the R^2 score is above 0.99 in all cases.
In the future, the developed ANN model will be applied to a CFD code and compare it with experimental data from CFD simulation. Connecting well-trained ANN model to CFD is expected to reduce the errors generated from real simulations, and it will enable the implementation of algorithms that can improve the performance of CFD naturally from the accumulation of data. During nuclear power plant severe accidents, various phenomena occur. Thus, the developed method can be applied to these phenomena as well to further improve the prediction accuracy.

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