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Study on the Application of Machine Learning in Computational Fluid Dynamics

NQe KAIST Nuclear & Quantum Engineering

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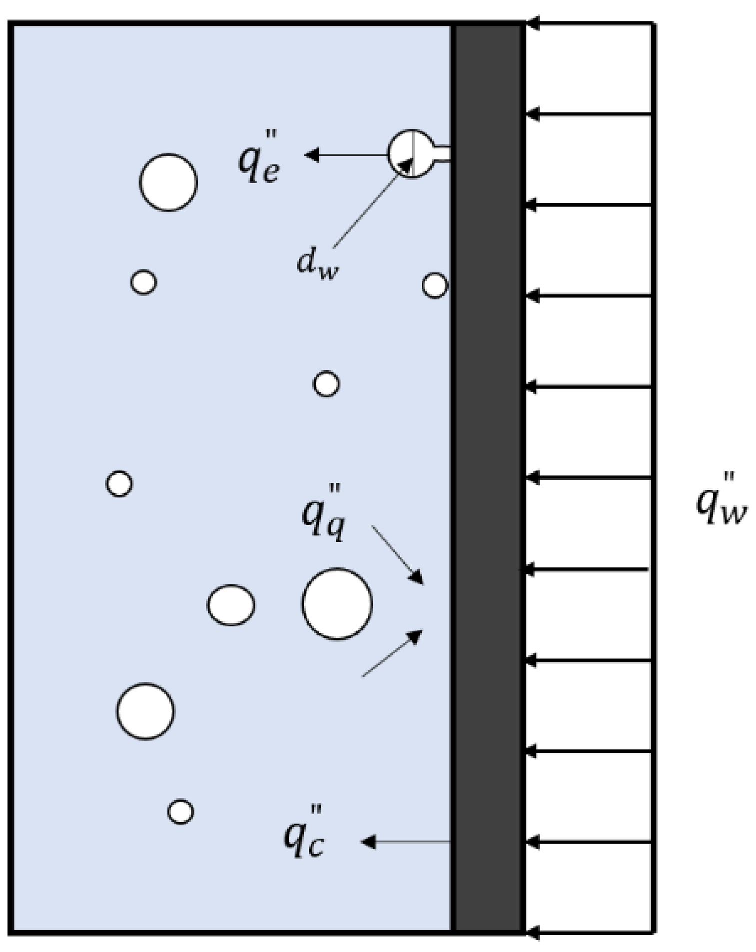
Introduction

- ✓ For nuclear power plant accident simulation, using CFD are being conducted, but in two-phase flow, it has lower prediction accuracy of CFD relatively due to complexity and non-linearity.
- ✓ Accurate modeling of two-phase flows via CFD is becoming important for predicting the consequences of nuclear power plant severe accidents.
- ✓ Machine learning-based data analysis can predict outputs based on existing data, which can contribute to accurately predicting two-phase flows.

Methodology

RPI wall boiling model

- ✓ RPI wall boiling model 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'').



$$q_w'' = q_c'' + q_q'' + q_e''$$

- convective heat flux (q_c'')
  - $q_c'' = h_c(T_w - T_l)(1 - A_b)$
    - $A_b = \min\left(1, K\frac{N_w \pi d_w^2}{4}\right)$
    - $K = 4.8\exp\left(-\frac{\rho_l c_{p,l}(T_w - T_l)}{80\rho_g h_{fg}}\right)$
    - $N_w = 210^{1.805}(T_w - T_l)^{1.805}$
    - $d_w = \min\left(0.0006e^{\left(-\frac{\Delta T_{sub}}{45.0}\right)}, 0.0014\right)$
- quenching heat flux (q_q'')
  - $q_q'' = \frac{2\sqrt{k_l \rho_l c_{p,lf}}}{\sqrt{\pi}}(T_w - T_l)$
  - $f = \sqrt{\frac{4g(\rho_l - \rho_g)}{3d_w \rho_l}}$
- evaporative heat flux (q_e'')
  - $q_e'' = V_d N_w \rho_g h_{fg} f$

Fig. RPI heat flux partitioning model

Artificial Neural Network

- ✓ ANN (Artificial neural network) is used as the machine learning technique.
- ✓ This has the advantage that even if each input parameter has a non-linear relation it can be expressed as a relational expression.
- ✓ the appropriate range of parameters and datasets must be determined. After setting the input parameter and range, data was generated through numerical simulations.
- ✓ physical model of CFD wall heat transfer for two phase flow simulation, is expressed as an ANN model.
- ✓ The loss function of the ANN model is Mean Square Error (MSE), and the evaluation is represented by the R^2 score.

$$\mathrm{MSE} = \frac{1}{N}\sum_{i=1}^{N}(y_{actual,i} - y_{pred,i})^2$$

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

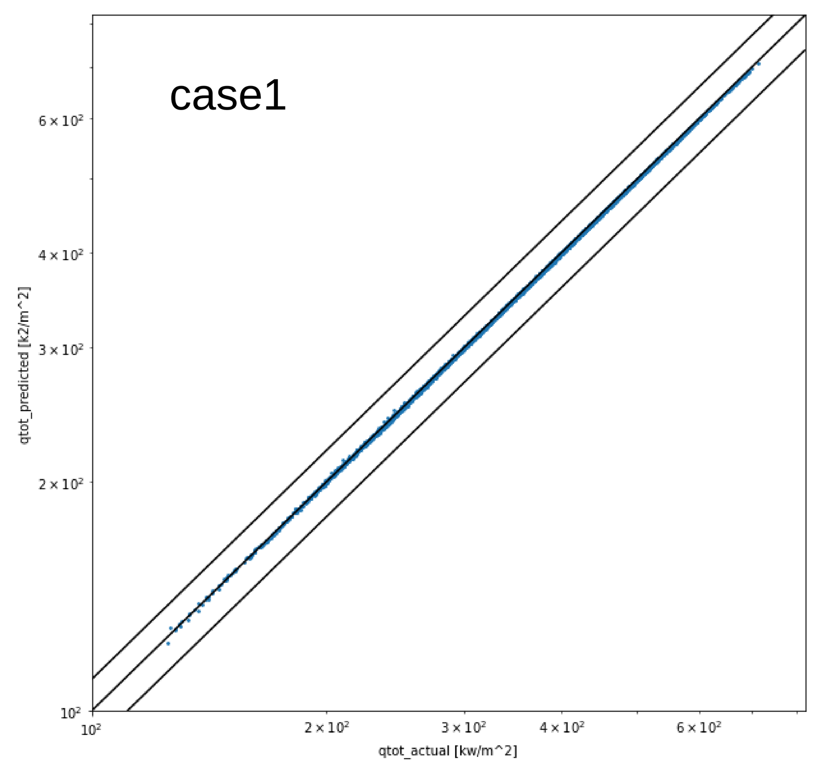
Result and Discussion

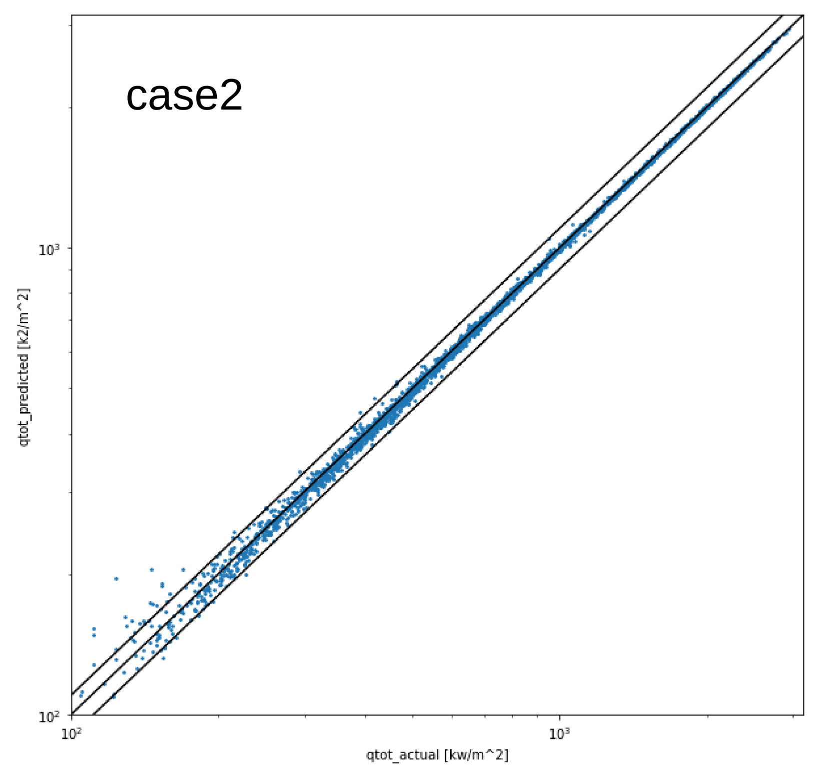
Range of input parameters

Parameters	Value		Unit
	Case 1	Case 2	
Pressure (P)	185 - 196.8	185 - 300	kPa
Wall temperature (T_w)	400 - 450	400 - 600	K
Liquid temperature (T_l)	363 - 423	363 - 450	K
Liquid velocity (v_l)	1.1415 - 2.1675	1.1415 - 2.1675	m/s

ANN model information

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





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

- ✓ 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, vl, ($T_w - T_l$), ($T_w - T_{sat}$), and (T_l -T_{sat}) as input parameters is developed and trained.
- ✓ In case 1, the model was trained with the thermohydraulic range data of the SUBO experiment, and case 2 has a wider range than that. The narrower the range, the smaller the error and the higher the R2 score. But it was confirmed that the R^2 score is above 0.99 in all cases.

Conclusion and Future work

- ✓ RPI model, which is the physical model of CFD wall heat transfer for two phase flow simulation, is expressed as an ANN model and possibility of substituting the RPI model through ANN was confirmed.
- ✓ In the future, developed ANN model will be applied to a CFD code. Connecting well-trained ANN model to CFD is expected to reduce the errors generated from real simulations.