**Derivation of a Condensation Heat Transfer Model for Light Water Reactor Applications using Artificial Neural Networks**

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**Abstract:** In this study, we develop a model that can predict the condensation heat transfer coefficient (HTC) during condensation on external surfaces of the vertical tube in the presence of Non-Condensable Gases (NCG). The aim is to compile a comprehensive database that includes a wide range of geometric values and operating conditions. The study is specifically motivated by the need to establish a generalized model/correlation that can predict the condensation heat transfer performance of the passive containment cooling system used in nuclear power plants [1] [2]. This passive cooling system is driven by gravity forces to eliminate heat from the containment vessel in the event of an accident by condensing water vapor. To develop the model, we used MATLAB’s neural network toolbox to build an Artificial Neural Network (ANN) model, specifically a Multi-Layer Perceptron (MLP) network. The model predicts the HTC during the condensation process of two types of NCGs (Air and Nitrogen) as well as pure steam. The dataset used for the model was constructed from 1,613 data points obtained from various experimental sources. The input layer receives various parameters, including$ P\_{tot}, ∆T\_{sub},W\_{nc},L,D\_{h}$. The output data is the condensation HTC. The input data underwent normalization through min-max scaling, which confined each feature's values within the 0 to 1 range. On the other hand, the output data was transformed using the natural logarithm. The resulting machine learning model exhibited outstanding performance when predicting the condensation HTC. The findings of this study will represent a significant advancement in the analysis of large amounts of data from experiments and simulations, enabling the identification of complex patterns and relationships. Findings from the present study would serve as tools for the nuclear industry for designing and modelling Design Basis Accident (DBA) and Design Extension Conditions (DEC) scenarios.

**Keywords:** Artificial neural networks, condensation heat transfer coefficient, machine learning, multi-layer perceptron, non-condensable gases, Steam condensation.

I. Introduction

During a Loss-of-Coolant Accident (LOCA) or Main Steam Line Break (MSLB) in a pressurized water reactor, a large amount of steam is rapidly released into the containment building [3]. This can lead to over pressurization, over-heating and the damage to the building. One of the primary methods for reducing containment pressure and preventing gas release is by condensing steam in the gas space. For this reason, the third-generation NPPs use a Passive Containment Cooling System (PCCS) for long-term cooling and depressurization of the containment building [4]. The PCCS is a passive mechanism that employs natural forces such as gravity, natural circulation, and phase-change heat transfer to remove heat from the containment [4]. This system employs tube-and-shell heat exchangers located within the containment, which are linked to an external cooling water tank positioned outside the containment. The PCCS functions by utilizing a buoyant flow driven by gravity to circulate water coolant within the tubes, with the flow propelled by the increasing temperature of the water. Outside the tubes, the process of condensation takes place [5]. The presence of NCGs influences the rate at which heat is transferred through condensation on the outer surface of the tube. NCGs like Air or Nitrogen can detrimentally impact the condensation process, resulting in safety hazards and decreased efficiency. These gases have a tendency to build up within the passive cooling system of a reactor, diminishing the effectiveness of heat transfer and resulting in reduced power output and increased operational costs [6]. To access the heat transfer surface, steam must diffuse through the layer of NCGs. If these gases are not removed, the NCG layer adjacent to the liquid film will lack steam, causing a significant reduction in the condensation rate. Research findings have indicated that the HTC for steam condensation can undergo a reduction of up to 50% when the air concentration reaches 0.5% [7]. In a numerical analysis conducted by Bian et al.[8] the thickness of the air layer was investigated, and it was observed that the highest concentration gradient occurred at a distance of roughly 6 mm from the condensation wall. This study offers strong evidence indicating that the air layer adjacent to the condensation wall plays a pivotal role in diminishing heat transfer efficiency. On the other hand, Ma et al. [9], conducted a study to investigate steam condensation across a range of pressures, from 0.516 to 5.10 MPa, while varying the nitrogen mass fractions from 5% to 85%. The findings revealed a decrease in the condensation HTC from 1.393 to 0.165 kW/(m2·K) at a pressure of 0.517 MPa, with nitrogen mass fractions ranging from 9.03% to 75.76%.

Hence, the importance of addressing condensation in the presence of NCGs cannot be overstated as we strive for the safe and efficient operation of NPPs. Traditional modelling techniques face challenges in accurately capturing this complex process due to multiple interacting factors. However, the utilization of soft computing approaches through machine learning (ML) algorithms offers a promising solution. ML has the capability to analyze vast datasets derived from experiments and simulations, uncovering intricate patterns and relationships that may not be easily discernible using conventional methods. By applying ML to model condensation in NPPs, engineers can unlock significant potential [10]. It allows for the optimization of reactor design and operation, the enhancement of safety measures, and the maximization of overall efficiency. Furthermore, gaining a deeper understanding of this process plays a critical role in managing the risks associated with NPPs and ensuring a reliable and sustainable energy source for future generations.

For instance, Balcilar et al. [11] conducted a study on the condensation HTC and pressure drops of R134a in a small vertical tube. They employed various ANN methods, including MLP, radial basis networks, generalized regression neural networks, and an adaptive neuro-fuzzy inference system. The results showed that the MLP method with a 5-13-1 structure and RBFN exhibited a good correlation with the experimental data, with only a minor deviation. Similarly, Azizi et al. [12] utilized an ANN with 440 experimental data points to analyze the condensation HTC in an inclined tube, achieving a mean absolute error (MAE) of less than 2%.

Cho et al. [13] and Lee et al. [14] employed ML models to predict condensation heat transfer rates. Cho et al. [13] used a MLP neural network model, surpassing previous correlations with a MAE of 4.2%. Similarly, Lee et al. [14] utilized a CNN-based DenseNet architecture, demonstrating superior predictive capabilities compared to existing correlations. Lee et al. [15] trained their neural network model using 3,000 pseudo-data points generated from ten existing condensation models. The model, consisting of a fully connected layer and a CNN-based DenseNet, underwent validation through hold-out cross-validation and evaluation using separate experimental data. The results showcased excellent performance in predicting condensation heat transfer coefficients, as the model effectively learned the strengths of each correlation. A new empirical correlation was proposed based on the parametric analysis, accounting for the effects of relevant variables. This new correlation exhibited a mean absolute percentage error (MAPE) of 13.6%, a root mean square error (RMSE) of 18.0%, and an MAE of 133.8 for the 868 experimental data points. Moreover, it consistently displayed improved results with similar error levels across all experiments, showcasing the efficacy of the generated data during the evaluation process.

The researchers have successfully examined the heat transfer characteristics during condensation when NCGs are present. However, there is currently a lack of a comprehensive model or correlation that can accurately predict the HTC for condensation with NCGs, mainly due to previous studies being limited to specific geometric and operational variations. This study aims to address this gap by developing universal models that can predict the HTC of condensation heat transfer on the outer surfaces of vertical tubes of PCCS when NCGs are present, considering a wide range of geometric and operational conditions. To achieve this, we compiled a database comprising 1,613 data points of condensation heat transfer on external surfaces of the vertical tube, considering both NCGs and pure water vapor. Then, we analyzed the effects of various geometric and operational variables. Additionally, we proposed new predictive tools based on a multilayer perceptron to enhance the accuracy of predicting condensation HTC when NCGs are present.

II. Methods

This study utilizes the MATLAB neural network toolbox to implement the ANN model. Specifically, a MLP network is utilized to forecast the HTC during the condensation process of two NCGs -Air and Nitrogen- and pure steam. The effectiveness of the MLP network is influenced by the amount of data utilized, thus, a dataset consisting of 1,613 data points is employed. Table 1 presents the sources of the data. These data points are obtained from various experimental research studies and cover specific ranges as described below.

* Mass fraction of NCG: $w\_{nc}$= 0–0.9;
* Total pressure $P\_{tot}$ = 0.1–2.0 MPa
* Wall subcooling temperature $ΔT\_{sub}$ = 1.7–125.5 K;
* Tube length$ L$ = 0.3–3.5 m;
* Hydraulic diameter of tube $D\_{h}$ = 10–46 mm;

**II.A. The ANN model development**

In order to create and fine-tune the MLP model using the training data, it is crucial to allocate a significant portion of the data to the training set. Nonetheless, to prevent the network from overtraining, it is necessary to have a validation set, and to evaluate the model's predictive capabilities, a testing set is required. To ensure the reliability of the MLP model, the data was divided randomly into three sets: 70% for training and 15% each for the validation and testing sets. It is of utmost importance that the validation and testing sets be sufficiently large to yield precise outcomes.In order to prevent data loss during machine learning caused by significant variations in input data, it is vital to normalize the data as an important part of preparing the dataset.

Table 1. Consolidated database of the test conditions of the condensation heat transfer experiments.

|  |  |  |
| --- | --- | --- |
| **No** | **Author (year)** | **Data point** |
| **Air** |
| **1** | Dehbi (1991) [16] | 216 |
| **2** | Liu et al. (2000) [17] | 25 |
| **3** | Kawakubo et al. (2009) [18] | 46 |
| **4** | Su et al. (2013)[19]  | 148 |
| **4** | Su et al. (2014) [20] | 19 |
| **5** | Tong et al. (2015) [21] | 62 |
| **6** | Lee et al. (2017)[22] | 43 |
| **7** | Fan et al. (2018a) [23] | 209 |
| **8** | Fan et al. (2018b) [24] | 64 |
| **9** | Jang et al. (2018) [25] | 18 |
| **10** | Kim et al. (2020) [26] | 48 |
| **11** | Niu et al. (2021) [27] | 105 |
| **12** | Kang et al. (2021) [27]  | 45 |
| **13** | Cao et al. (2021) [29]  | 72 |
| **14** | Bian et al. (2021) [30] | 179 |
| **15** | Zhang et al. (2021) [31] | 54 |
| **16** | Hwang and Jerng (2022) | 7 |
| **17** | Park et al. (2022) [32]  | 74 |
| **18** |  |  |
| **Total** | **1424** |
| **Nitrogen** |
| **1** | Ahn et al. (2007) [33] | 9 |
| **2** | Kim (2009) [34] | 68 |
| **Total** | **81** |
| **Pure steam** |
| **1** | Kawakubo et al. (2009) [18] | 14 |
| **2** | Tong et al. (2015) [21] | 19 |
| **3** | Fan et al. (2018a) [23] | 14 |
| **4** | Kang et al. (2021) [28] | 15 |
| **5** | Bian et al. (2021)  | 19 |
| **6** | Zhang et al. (2021) [31] | 13 |
| **8** | Niu et al. (2021) [28] | 11 |
| **Total** | **108** |

This normalization process ensures that all features have a similar scale or range, making them more compatible with specific machine learning algorithms. In this current study, the input data was subjected to min-max scaling for normalization, limiting the values of each feature within the range of 0 to 1. Conversely, the output data underwent a transformation utilizing the natural logarithm. The input layer of the model receives the following parameters: $P\_{tot}, ∆T\_{sub},w\_{nc},L,D\_{h}$. The output data represents the condensation HTC ($h$).

The network was trained for 30,000 epochs, but to prevent overtraining, an early stopping mechanism was applied at the 15,000th epoch. This mechanism was activated when the validation error did not decrease for 10 consecutive epochs. The MLP architecture was subjected to a model selection process, wherein various configurations were evaluated. These configurations included 2-10 hidden layers and 2-40 nodes for each hidden layer. A total of 100 combinations of hyperparameters were tested using the same training dataset and conditions as shown in Table 2.

Table 2. The results of the quantitative assessment are presented in terms of the mean absolute percentage error.

|  |  |
| --- | --- |
|  | ***Layer*** |
| ***Node*** | *2* | *4* | *6* | *8* | *10* |
| *2* | 11.56 | 11.54 | 11.54 | 4.81 | 11.54 |
| *4* | 4.32 | 3.90 | 3.22 | 11.54 | 3.86 |
| *6* | 3.92 | 3.26 | 3.17 | 3.154 | 3.36 |
| *8* | 3.60 | 3.08 | 2.68 | 2.84 | 4.22 |
| *10* | 3.60 | 3.16 | 3.12 | 2.91 | 3.08 |
| *12* | 3.59 | 3.09 | 2.74 | 2.95 | 2.77 |
| *14* | 3.11 | 2.71 | 2.46 | 2.33 | 2.59 |
| *16* | 3.11 | 2.53 | 2.75 | 2.53 | 2.62 |
| *18* | 3.22 | 2.54 | 1.96 | 2.29 | 2.35 |
| *20* | 3.16 | 2.45 | 2.35 | 2.35 | 2.65 |
| *22* | 2.98 | 2.54 | 2.52 | 2.33 | 2.25 |
| *24* | 2.79 | 2.52 | 2.19 | 2.04 | 2.52 |
| *26* | 2.96 | 2.34 | 2.02 | 2.07 | 2.13 |
| *28* | 2.80 | 2.38 | 2.15 | 2.02 | 2.33 |
| *30* | 2.78 | 2.24 | 2.15 | 2.14 | 2.02 |
| *32* | 3.03 | 2.42 | 2.08 | 2.43 | 2.25 |
| *34* | 2.83 | 2.38 | **1.91** | 2.40 | 2.63 |
| *36* | 2.77 | 2.26 | 2.10 | 2.19 | 2.32 |
| *38* | 2.79 | 2.00 | 2.23 | 2.12 | 2.46 |
| *40* | 2.73 | 2.25 | 2.09 | 1.94 | 2.30 |

The details and parameters of the solution models can be found in Table 2.

Table 3. A summary of the solution models along with their respective parameters.

|  |
| --- |
| **Solution models** |
| ***Machine learning model***  | Multilayer perceptron (MLP) |
| ***Tool*** | MATLAB R2022b |
| ***Input***  | $$P\_{tot},∆T\_{sub},w\_{nc},L,D\_{h}$$ |
| ***Output***  | Average heat transfer coefficient  |
| ***Activation function***  | Hyperbolic tangent sigmoid  |
| ***Initializer***  | He initializer  |
| ***Optimizer***  | Adam optimizer  |
| ***Learning rate***  | 0.001 |
| ***Layers***  | 2-10 |
| ***Nodes*** | 2-40 |
| ***Maximum training***  | 30,000 epochs |
| ***Early stopping***  | 15,000 epochs |
| ***Optimum structure***  | 6 layers, 34 nodes |

III. Development of a new condensation HTC correlation

Before building the MLP model suggested in this research, we used the Pearson correlation coefficient, referred to as “$R\_{AB}$” [35], to investigate the fundamental connections between the condensation HTC and various input parameters. The Pearson correlation coefficient analysis is a commonly employed statistical technique that measures the linear relationship between two variables and is represented as “$R\_{AB}$”:

$ R\_{AB}=\frac{\sum\_{i}^{n}(A\_{i}-̿)(B\_{i}-\overbar{B})}{\sqrt{\sum\_{i}^{n}(A\_{i}-\overbar{A})^{2}} \sqrt{\sum\_{i}^{n}(B\_{i}-\overbar{B})^{2}}}$ (1)

$R\_{AB}$, has a range of +1 to -1, indicating a complete positive or negative linear relationship between variables, respectively. The magnitude of $R\_{AB}$ reflects the strength of the association between the variables. A higher absolute value of$ R$ indicates a stronger correlation. Fig. 1 depicts the correlations between the condensation HTC and various input parameters. Among these parameters, the parameter $w\_{nc}$ demonstrates a significant correlation, having the highest absolute value of $R\_{AB}$ at 0.63. This result is consistent with physics, as it has been documented that a small mass fraction can lead to a significant decrease in the HTC for condensation. This occurs because it creates a resistance that impedes the steam from condensing on the wall. The total pressure,$P\_{tot}$, follows with a correlation coefficient of 0.16. When pressure is elevated, both the bulk and mixture average temperatures rise, leading to an increase in the term related to the mixture's molecular weight, which is positively associated with the condensation HTC. The length, $L,$ exhibits a correlation coefficient of 0.13. In contrast, the condensation HTC shows a weaker correlation with the subcooling temperature, $∆T\_{sub}$, having an absolute value of $R$ of 0.09.



Fig. 1. Evaluation of the Pearson correlation coefficients concerning the input parameters of the MLP neural network.

To evaluate the effectiveness of the trained ML model, a distinct test dataset was employed, and its results are shown in Fig. 2. The predictions made by the model were found to be accurate. I.e., the assessment of the model’s accuracy revealed a Pearson’s coefficient of 0.95, indicating a robust correlation between the predicted values and the actual experimental data.

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Fig. 2. Scatter plot of experimental condensation HTC vs the predicted condensation HTC.

The condensation HTC is directly influenced by the pressure and inversely affected by the mass fraction of NCG. To account for the impact of these factors, several correlations were examined. After a thorough investigation, it was determined that the ratio between the numerator and denominator, as defined in the Dehbi model [16], effectively captures the behavior of these variables, specifically the total pressure $(P\_{tot})$ mass fraction of non-condensable gases ($w\_{nc}$), and wall subcooling $(∆T\_{sub}$). As a result, the updated correlation incorporates both the numerator and denominator components from the Dehbi model [16], In order to encompass the influence of all the aforementioned variables, the proposed correlation expression is presented as follows:

$h=\frac{\left(\frac{L}{D}\right)^{-0.009}\left(\left(-12.437-0.01P\_{tot}^{13.36}\right)-1770.59+16.9P\_{tot}^{12.37}\right)log\_{10}w}{∆T\_{sub}^{-0.01}}$ (2)

There have been various experimental correlations proposed in prior research on steam condensation with air. These commonly cited correlations include the Uchida [36] and Dehbi [16], experimental correlations. The Uchida experimental correlation solely accounted for the impact of air mass fraction, while Dehbi’s correlation considered the effects of $P\_{tot}, w\_{nc},$and$ ∆T\_{sub}$. Its experimental condition range is available in Table 3 in addition to the current model’s experimental conditions.

**Fig. 3**, exhibits the evaluation process of the current model’s accuracy based on the outcomes of Dehbi’s correlation. The model's ability to predict condensation HTC was demonstrated in the present study with a high level of accuracy, as indicated by the percentage of data points predicted within a deviation bandwidth of ±10%, which was 100%.

Table 4. Conditions for experiment in chosen paper for comparison.

|  |  |
| --- | --- |
| **Model** | **Experimental Conditions** |
| *Dehbi (1991)* [16] | $$0.28\leq w\_{nc}\leq 0.9$$$$0.15\leq P\_{t}\leq 0.45 MPa$$$$14.7\leq ∆T\_{sub}\leq 47 K$$ |
| *Current model* | $$0\leq w\_{nc}\leq 0.9$$$$0.1\leq P\_{t}\leq 2.0 MPa$$$$1.7\leq ∆T\_{sub}\leq 125.5 K$$ |



Fig. 3. Assessment of the present correlation (equation-2) to predict Dehbi’s experimental data.

IV. Conclusions

Investigating NCG's influence on NPP condensation rates is key for safety and efficiency. While experimental and computational studies have been insightful, they face constraints like simulating realistic conditions. ML offers a more precise approach for predicting condensation HTC, promising safer, more efficient NPP operations. Therefore, in this work, we propose to use an MLP model for forecasting condensation HTC in various environments, with promising initial results. An accurate and computationally efficient predictive machine learning MLP model was developed by incorporating multiple dimensionless parameters that have a significant impact on condensation HTC. By utilizing Pearson correlation coefficient analysis and importance analysis for parameter selection, a new correlation for heat transfer was developed and evaluated. The evaluation of the mode demonstrated its reliability in providing accurate predictions for all 1,613 data points within the compiled database. Notably, the results indicated that 98.7% of the predicted data fell within the ±10% range, which represents the minimum deviation observed. Moreover, to evaluate how well the new correlation can predict the effect of helium, it was compared to the experimental investigation carried out by Dehbi [16]. The model showed a high level of accuracy by successfully predicting a percentage of data points within a deviation range of ±10%. Specifically, the results showed that the model predicted 100% of the data points within the desired deviation range for Dehbi's study. In summary, this research represents a significant step forward in the application of ML algorithms in nuclear engineering and has the potential to revolutionize the way we approach complex engineering problems in the future.

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