## 3.1 Machine learning methods

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  |  | **Mean** | |  |
|  |  | **Microfin tube h** | **Plain tube h** | **Deviation** |
| **Input Raw** | Mass flux | 282.678974 | 287.516213 | 0.016824 |
| Saturation pressure | 546880 | 533260.976 | 0.025539 |
| Heat flux | 12442.84554 | 12606.37154 | 0.012972 |
| Quality | 0.505296 | 0.494793 | 0.021227 |
| Pressure drop | 11966.44706 | 7230.353147 | 0.655029 |
| **Input Calculated** | Reynolds number | 5715.992018 | 5786.624969 | 0.012206 |
| Two-phase multiplier | 0.22905 | 0.233213 | 0.017847 |
| Froude number | 0.66961 | 0.687362 | 0.025827 |
| Weber number | 67.137622 | 68.23943 | 0.016146 |
| Bond number | 0.165302 | 0.167358 | 0.012288 |
| **Output** | Heat transfer coefficient | 5855.256499 | 4170.965336 | 0.403813 |
|  |  |  |  |  |

Table - Input and output statistics by tube type

### 3.2.1 Artificial Neural Network (ANN)

### 3.2.2 Locally Weighted Linear Regression (LWR)

### 3.2.3 Other Model Considerations

Tree based regression models are not considered in this work due to search for a model that is capable of extrapolating and extraction of analytical relationships between input and output variables.

### 3.2.4 Evaluation metrics

Different metrics are used to evaluate models’ predictive performances to capture different abilities of models. Used evaluation metrics are score, mean absolute error (MAE), root mean squared error (RMSE), mean absolute percentage error (MAPE) and weighted absolute percentage error (WAPE). Calculation methods of each performance metric are given below. In all metric calculations, is the actual heat transfer coefficient (or pressure drop) for the test sample, is the predicted heat transfer coefficient (or pressure drop) for the test sample, and is the mean heat transfer coefficient (or pressure drop) of all samples in the test set.

is a statistical measure of how close the data are to the fitted regression line. It is also known as the coefficient of determination, or the coefficient of multiple determination for multiple regression. In this study, we use the following definition of :

Mean absolute error (MAE) is a measure of difference between two continuous variables. For two vectors and , MAE is defined as:

Root mean squared error (RMSE) is a quadratic scoring rule that also measures the average magnitude of the error. It is defined as:

can be driven up by outliers and does not indicate under- or over-estimation. To address this issue, we use the mean absolute percentage error (MAPE) and weighted absolute percentage error (WAPE) scores whose details are given below that penalize errors relative to the true value.

Mean absolute percentage error (MAPE) is a measure of prediction accuracy of a forecasting method in statistics. MAPE is defined as:

Weighted absolute percentage error (WAPE) is a measure of prediction accuracy of a forecasting method in statistics. WAPE is defined as:

Weighted percentage bias is a measure of systematic error in regression models. Weighted percentage bias is defined as:

### 3.3 Sampling for extrapolation performance

In this section, we demonstrate the selected models' strength for making accurate estimations outside observed ranges during the experiment.

Extrapolation performance analysis is conducted by following approach: clusters are identified in principal component space through fitting a Gaussian Mixture Model (GMM), and a Ledoit-Wolf (LW) covariance estimator is fitted separately to each identified cluster again in principal component space.

Samples to be used for extrapolation are then determined by Mahalanobis distance estimations coming from LW estimators fitted on each cluster. 10 samples with the highest Mahalanobis distance are then held out for test and the rest of the samples are used for training the models.

A graph of red and blue dots

Description automatically generated

Figure 7 - Training and extrapolation samples in principal component space

## 4. Results and Discussion

A collage of blue dots

Description automatically generated

Figure 1- Input and output interaction plots of the system

### 4.1. Validation

A screen shot of a graph

Description automatically generated

Figure 2- Finned vs plain tube samples in principal component space

|  |  |  |  |
| --- | --- | --- | --- |
|  | **PC1** | **PC2** | **PC3** |
| **Mass flux** | 0.3564 | 0.3828 | -0.1576 |
| **Saturation pressure** | 0.0366 | 0.0390 | 0.8466 |
| **Heat flux** | -0.0334 | 0.0465 | 0.0043 |
| **Quality** | -0.3549 | 0.3716 | -0.0112 |
| **Pressure drop** | 0.0005 | 0.3995 | 0.4582 |
| **Reynolds number** | 0.4600 | -0.0307 | -0.0279 |
| **Two-phase multiplier** | 0.3643 | -0.3642 | 0.1199 |
| **Froude number** | 0.3647 | 0.3765 | -0.1162 |
| **Weber number** | 0.3658 | 0.3783 | -0.0437 |
| **Bond number** | 0.3653 | -0.3656 | 0.1333 |

Table - Projection axes for principal components across input variables

|  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | **Mass flux** | **Saturation pressure** | **Heat flux** | **Quality** | **Pressure drop** | **Reynolds number** | **Two-phase multiplier** | **Froude number** | **Weber number** | **Bond number** | **Heat transfer coefficient** |
| **Category** |  |  |  |  |  |  |  |  |  |  |  |
| **0** | 190.394 | 553191.000 | 12336.142 | 0.482 | 5589.500 | 3998.390 | 0.253 | 0.284 | 28.588 | 0.181 | 5487.154 |
| **1** | 380.788 | 539760.556 | 12318.045 | 0.425 | 16670.167 | 8900.799 | 0.310 | 1.129 | 112.751 | 0.216 | 6434.455 |
| **2** | 286.271 | 539451.905 | 12924.940 | 0.518 | 12422.381 | 5496.968 | 0.208 | 0.638 | 63.710 | 0.152 | 5679.046 |
| **3** | 191.584 | 540143.645 | 12098.984 | 0.499 | 3007.376 | 3821.949 | 0.227 | 0.286 | 28.543 | 0.164 | 3717.482 |
| **4** | 380.550 | 536835.695 | 12763.618 | 0.441 | 10515.500 | 8496.691 | 0.283 | 1.127 | 112.227 | 0.200 | 4578.828 |
| **5** | 289.702 | 532606.721 | 12729.166 | 0.521 | 7815.455 | 5295.849 | 0.201 | 0.653 | 64.865 | 0.146 | 4238.314 |

Table - Input variable statistics by clusters identified in principal component space

### 4.2. Heat transfer coefficient

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | **Selected ANN config** | **R2** | **RMSE** | **MAE** | **MAPE** | **Bias%** | **WAPE%** | **Pearson-R** |
| **Fold ID** |  |  |  |  |  |  |  |  |
| **0** | ((128, 64, 32, 16, 8), 'relu') | 72.6% | -842.61 | -443.99 | -7.4% | 2.1% | -8.0% | 80.5% |
| **1** | ((128, 64, 32, 16, 8), 'relu') | 56.9% | -759.76 | -430.31 | -8.2% | -2.7% | -9.8% | 75.9% |
| **2** | ((128, 64, 32, 16, 8), 'relu') | 44.7% | -700.55 | -368.63 | -7.1% | -1.1% | -8.9% | 75.3% |
| **3** | ((128, 64, 32, 16, 8), 'relu') | 56.8% | -793.18 | -508.60 | -8.8% | 1.5% | -9.4% | 62.0% |
| **4** | ((128, 64, 32, 16, 8), 'relu') | 55.4% | -725.95 | -505.13 | -9.0% | 4.5% | -9.4% | 59.8% |

Table - Cross validation results for ANN configurations -

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Score** | **Average** | **Std** | **Min** | **25%** | **50%** | **75%** | **Max** | **Test Score** |
| **Test R2** | 57.3% | 9.9% | 44.7% | 55.4% | 56.8% | 56.9% | 72.6% | **76.3%** |
| **Test RMSE** | -764.41 | 55.95 | -842.61 | -793.18 | -759.76 | -725.95 | -700.55 | **571.15** |
| **Test MAE** | -451.33 | 58.11 | -508.60 | -505.13 | -443.99 | -430.31 | -368.63 | **385.29** |
| **Test MAPE** | -8.1% | 0.8% | -9.0% | -8.8% | -8.2% | -7.4% | -7.1% | **7.3%** |
| **Test Bias%** | 0.8% | 2.8% | -2.7% | -1.1% | 1.5% | 2.1% | 4.5% | **0.6%** |
| **Test WAPE%** | -9.1% | 0.7% | -9.8% | -9.4% | -9.4% | -8.9% | -8.0% | **7.7%** |
| **Test Pearson-R** | 70.7% | 9.2% | 59.8% | 62.0% | 75.3% | 75.9% | 80.5% | **76.4%** |

Table - Cross validation and test score statistics -

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Fold ID** | **Selected LWR config** | **Test R2** | **Test RMSE** | **Test MAE** | **Test MAPE** | **Test Bias%** | **Test WAPE%** | **Test Pearson-R** |
| **0** | (1, 20) | 73.5% | -828.87 | -453.28 | -7.8% | 3.2% | -8.2% | 83.8% |
| **1** | (1, 20) | 68.6% | -675.94 | -464.50 | -9.4% | 0.5% | -8.8% | 73.1% |
| **2** | (0.7, 20) | 56.3% | -765.69 | -476.13 | -9.6% | -5.1% | -10.8% | 70.5% |
| **3** | (0.7, 20) | 34.9% | -760.23 | -406.56 | -8.5% | -2.7% | -10.0% | 77.6% |
| **4** | (0.7, 20) | 23.4% | -951.70 | -583.23 | -10.3% | 3.1% | -11.3% | 38.5% |
| **Test Set** | **(0.7, 20)** | **64.5%** | **698.13** | **461.61** | **8.9%** | **4.6%** | **10.0%** | **76.4%** |

Table - Cross validation and test scores for LWR configurations -

A graph with red and blue dots

Description automatically generated

Figure 3 - Actual vs predicted heat transfer coefficients for plain tube

A graph with a line and dots

Description automatically generated with medium confidence

Figure 4- Actual vs predicted heat transfer coefficients for micro finned tube

### 4.3. Pressure drop

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Fold ID** | **Model type** | **Configuration** | **Test R2** | **Test RMSE** | **Test MAE** | **Test MAPE** | **Test Bias%** | **Test WAPE%** | **Test Pearson-R** |
| **0** | ANN | ((128, 64, 32, 16, 8), 'relu') | 94.6% | -1208.29 | -873.77 | -9.4% | 7.8% | -9.3% | 97.3% |
| **1** | ANN | ((128, 64, 32, 16, 8), 'relu') | 66.8% | -3196.07 | -1723.78 | -14.9% | -14.7% | -21.5% | 91.3% |
| **2** | ANN | ((128, 64, 32, 16, 8), 'relu') | 86.1% | -2639.49 | -1348.12 | -12.5% | 6.8% | -12.1% | 89.2% |
| **3** | ANN | ((128, 64, 32, 16, 8), 'relu') | 88.6% | -1864.51 | -1250.50 | -13.1% | -0.3% | -13.1% | 88.6% |
| **4** | ANN | ((128, 64, 32, 16, 8), 'relu') | 87.1% | -1834.56 | -1361.69 | -21.9% | -3.7% | -18.5% | 87.5% |
| **0** | LWR | (2, 20) | 92.9% | -1381.97 | -1012.09 | -12.9% | 0.5% | -11.5% | 92.9% |
| **1** | LWR | (2, 20) | 91.1% | -1521.85 | -1184.95 | -29.6% | -3.7% | -21.3% | 91.8% |
| **2** | LWR | (0.7, 20) | 88.8% | -1847.06 | -1197.47 | -12.3% | 3.0% | -11.8% | 89.5% |
| **3** | LWR | (1, 20) | 85.0% | -2740.48 | -1313.47 | -13.2% | 6.1% | -12.4% | 87.1% |
| **4** | LWR | (0.7, 20) | 63.8% | -3336.76 | -1937.61 | -17.8% | -5.5% | -21.2% | 72.7% |

Table - Cross validation results for pressure drop models

A graph of a graph with a number of points

Description automatically generated with medium confidence

Figure 5 - Actuals vs predictions for pressure drop in plain tube

A graph of a graph with blue and red dots

Description automatically generated

Figure 6 - Actuals vs predictions for pressure drop in micro finned tube

### 4.4. Extrapolation performance

A screen shot of a graph

Description automatically generated

Figure 8 - Actual vs prediction plots for extrapolations on plain tube heat transfer coefficients

A graph with red dots

Description automatically generated

Figure 9 - Actual vs prediction plots for extrapolations on micro finned tube heat transfer coefficients

|  |  |
| --- | --- |
| **Score** | **Value** |
| R2 | 61.65% |
| MAPE | 9.06% |
| RMSE | 915.4918 |

Table - Performance metrics for extrapolation of on Plain tube

## 5. N/a

In the existing work, detailed comparative research has been undertaken to evaluate the predictive capabilities of four prominent ML techniques. These techniques include linear regression, which establishes a linear relationship between variables for prediction; SVM, a powerful classifier that can regress or maximize the margin between classes or fitting points; DTR, which employs recursive splitting to model non-linear relationships; and ensemble-based RF, which associations multiple decision trees to enhance forecast accurateness and mitigate overfitting. The forthcoming sections delineate the distinctive mechanisms and performance traits of each method, offering a comprehensive understanding of their applicability and effectiveness across various scenarios.

LR is a statistical method employed for modeling the relation between a dependent variable and one or more independent ones by fitting a linear equation to the spotted data points. The formula for simple linear regression can be represented by Eq. 6.

(6)

where is the dependent variable, is the independent one, is the y-intercept, is the slope coefficient, and represents the error term accounting for the variability not explained by the model. The objective of LR is to estimate the values of and that minimize the sum of squared differences between the real and guessed values of the dependent variable, thus establishing a linear relationship that allows for prediction and inference based on the independent variables [23].

SVM is a ML method employed for classification and regression tasks. In classification, SVM aims to obtain a hyperplane that best separates different classes by maximizing the margin between them. The equation for a linear SVM can be written as:

(7)

Here, represents the predicted output, w denotes the weight vector, x is the input feature vector, and is the bias term. The objective is to learn the optimal values of and that minimize the regression error while allowing for a specified tolerance margin. The regression SVM formula is:

(8)

In both cases, SVM can be extended to handle non-linear relationships employing kernel functions, which implicitly map the input data into a higher-dimensional space. This capability enables SVM to effectively capture complex patterns and make accurate predictions for various types of data. [24].

DTR is a non-linear regression algorithm used in ML. It predicts a continuous target variable by recursively splitting the feature space into subsets based on the input variables' values. Each split represents a decision node in the tree, leading to terminal nodes where predictions are made. The formula for DTR involves creating a tree structure that predicts the target variable by averaging the target values of the training samples within each terminal node. Mathematically, the DTR model can be represented as:

(9)

Here, represents the predicted target variable, is the target value of the training sample within the terminal node, and is the number of samples in the terminal node. DTR can capture complex relationships in data and handle non-linear patterns effectively. However, it can also be prone to overfitting if not appropriately controlled through hyperparameters or ensemble techniques like Random Forest or Gradient Boosting [25].

RF is a powerful ensemble ML algorithm that relates multiple decision trees to enhance prediction accuracy and decrease overfitting. It can be used for both classification and regression tasks. The formula for RF involves creating a gathering of decision trees, where each tree is trained on a subset of the data and potentially with different subsets of features. The predictions of individual trees are then combined through averaging (for regression) or voting (for classification) to obtain the final prediction. In the context of regression tasks, the formulation for aggregating predictions within a RF can be represented as:

(10)

where represents the number of individual trees within the Random Forest ensemble [19].

A group of blue dots

Description automatically generated

A group of blue dots

Description automatically generated