E3S Web of Conferences **552**, 01025 (2024) https://doi.org/10.1051/e3sconf/202455201025
ICMPC 2024

Multi-Variate Analysis of Shell & Tube Heat Exchanger using Principal Component Analysis

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Abstract. Shell & Tube Heat Exchangers (STHEs) are a critical component for various industrial applications such as chemical, oil & gas, power, etc. Due to their complex design and high manufacturing cost, the efficient operation and optimum design are quite important for overall cost minimization. Multivariate Analysis (MVA) is a technique used for analysing data with more than one type of measurement. In this paper, MVA of STHEs is carried out using Principal Component Analysis (PCA). 12 variables which predicts the Thermo-Hydraulic Performance & the costs for STHEs are considered. In total, 100 data points are generated and analysed. Two Principal Components (PCs) are adopted and scores & loadings plots are plotted. It is concluded that the first principal component primarily measures design and flow characteristics of STHE while the second principal component has negative coefficients for the factors Res, Nt, Ret, L, do, di and A_t which signifies the inverse relationship between PC2 and these factors. The current work can be extended further with applications of Partial Least Square Regression and various Machine Learning algorithms.

1 Introduction

Over the last few decades, Heat Exchangers (HXs) plays a vital role in the field of chemical, marine, Power, refrigeration and air conditioning, biomedical and electronics industry. HXs are the devices which transfer heat from one fluid to another fluid with or without mixing of those fluids. HXs can be classified in various categories based on design/construction, fluid contact type, flow arrangements, pass arrangements, fluid phases, etc. [1]. Owing to the space constraints, industries are moving towards the micro sized HXs [2]. Furthermore, now-a-days polymers are taking place of metals for various applications including HXs because of the offerings such as higher corrosion resistance, higher strength to weight ratio and budget friendliness. In past two decades, rapid growth is observed in the field of new polymer development, techniques for improving the heat transfer with polymers and hence the applications of polymers for HXs and now extensive research is going on to build HXs with polymer materials [3,4].

Shell & tube HXs (STHE) are the most prominent type of heat exchangers which have been widely used across industrial sectors such as in power generation, petroleum refinery,

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chemical industries, and process industries. The typical applications of STHE include oil coolers, condensers, feed water heaters, food processing, etc. Though the application of other types of heat exchangers is increasing, the shell and tube heat exchanger will continue its popularity for a long time, largely because of its versatility [5]. The major components of a shell and tube exchanger are tubes, baffles, shell, front head, rear head, and nozzles [6]. Other components include tie-rods and spacers, impingement plates, sealing strips, supports, and lugs. The selection criteria for a proper combination of these components are dependent upon the operating pressures, temperatures, thermal stresses, corrosion characteristics of fluids, fouling, cleanability, and cost. There are various design standards adopted for STHE design such as TEMA, ANSI/AEI [7,8].

Several parameters have to be considered for the effective design of STHE, there exist various design constraints which must be met in order to practically implement the design. The common design parameters are Baffle spacing (B), Shell diameter (D_s), tube inner & outer diameter (d_i & d_o), Reynold's number at shell side and tube side (R_{es} & R_{et}), Heat transfer coefficient on shell side and tube side (h_s & h_t), heat transfer surface area (A_t), Overall heat transfer coefficient (U), Tube length (L), number of tubes (N_t), Prandtl number (Pr), Friction factor, Mass flow rate, temperature etc. Moreover, it is proved now that these parameters are interdependent and their interaction affects the thermo- hydraulic performance of STHE [9]. This makes the design of STHE a complex problem. The aim of any system with STHE is to improve the thermal performance and simultaneously contributing to the bottom level margin by decreasing the power consumption and design & operational costs. Traditionally, Numerical approaches based on experimentation and experience (judgment) were adopted for designing of STHE. Nevertheless, it is evident from the literature that aforementioned approaches are not adequate to tackle the advancements in complexity of design and materials. In the recent past, several conventional and contemporary optimization algorithms have been applied in order to minimize the cost & pressure drop and to maximize over all heat transfer coefficient & effectiveness [10,11].

The mathematical optimization techniques are proved to be effective as compared to the traditional design methods. Genetic Algorithm (GA) is widely applied for the design optimization of HXs such as for design improvement considering pressure drop as a constraint by Selbas et al.,2006 [12]. Minimization of investment & operating cost of the pumps is achieved with GA by Caputo et al., 2008 [13]. Also, design optimization of STHE is performed with GA by Ponce-Ortega et al., 2009 [14] and Costa and Queiroz, 2008 [6]. Babu and Munawar, 2007 [15] applied Differential Evolution (DE) algorithm along with modified GA for optimal design of STHE. Along with GA, Particle Swarm Optimization (PSO) algorithm is also applied for design improvement with minimum cost by Patel and Rao, 2013 [16]. Sahin et al., 2011 [17] optimized the design with Artificial Bee Colony (ABC) algorithm. Biogeography-Based Optimization (BBO) algorithm was found to be effective for the design of STHE [18]. Intelligent Tuned Harmony Search (ITHS) algorithm and Improved ITHS (IITHS) algorithms were applied for the economic optimization of the STHE by [19]. Socio-Inspired optimization methodology referred to as cohort Intelligence (CI) [20] and its hybrid version with GA known as Adaptive Range Genetic Algorithm (ARGA) [21] are applied for design and economic optimization of STHEs. In the above context, the Multi-Objective Optimization of STHEs have also been performed [22-25]. Furthermore, along with design optimization economic cost optimization is also performed by [13, 26-27].

However, a few research material is available for Multi-Variate Analysis (MVA) of STHE [28,29]. The current work focusses on MVA of STHE using Principle Component Analysis

(PCA). 12 variables such as Baffle spacing (B), Shell diameter (Ds), tube inner & outer diameter (di & do), Reynold's number at shell side and tube side (Res & Ret), Heat transfer coefficient on shell side and tube side (hs & ht), heat transfer surface area (At), Overall heat transfer coefficient (U), Tube length (L), number of tubes (Nt) which predicts the Thermo-Hydraulic Performance & the costs for STHEs are considered. In total, 100 data points are generated and analysed. Two Principal Components (PCs) are adopted and scores & loadings plots are plotted.

The remainder of the paper is organized as follows: Section 2 describes the adopted methodology including PCA. The problem formulation has been presented in Section 3. The results are discussed in Section 4 along with graphical representations. The conclusions and future directions are given in section 5.

2 Methodology

As discussed in Section 1, In this work MVA of STHE is performed using PCA. In data analytics the interactions amongst variables and to the responses are analysed. Three types of analysis are generally carried out viz. univariate, bi variate and multi-variate. In univariate analysis only one variable at a time considered; two variables are considered in bivariate analysis; whereas the investigation in which more than two variables are considered is referred to as multi-variate analysis. The main aim of MVA is to find patterns and correlations between several variables considered simultaneously. The majority of real world problems are with more than one variable and having multiple responses and hence MVA is applied across the domains [30]. The common examples are weather forecasting, health care analysis, economic predictions, pharmaceutical applications, behavioural investigations etc. In the literature, MVA is classified into five categories. The first category is data reduction in which higher dimensional data patterns are presented in a lower dimensional space. PCA falls into this category which has been applied in the current work. Data sorting is the second category in which classification of data instances based on similar characteristic is performed. Cluster analysis is the common example of this category. Techniques such as redundancy analysis forms the third category of MVA in which investigations for dependencies among variables and responses are carried out. Prediction and multivariate analysis of variance (MANOVA) are the fourth and fifth categories inch predictive and exploratory analysis are performed respectively [31].

PCA is a statistical technique for reducing the dimensionality of a data set. Its origin is through [32] and a complete guide to PCA is provided by [33]; However, its modern formulations are presented by [34] who also coined the term "principal component". In PCA the original raw data is transformed into a new coordinate system with which the maximum variation can be explained with fewer dimensions as compared to the initial data. It is a popular technique for analysing big datasets with higher number of dimensions [35]. PCA is considered as an unsupervised learning algorithm in which data points are orthogonally transformed in new features [36]. These new transformed features are referred to as Principle Components (PCs). With PCA, the interpretability of the data is increased with visualising multidimensional data on coordinate system. Typically, in PCA the first two PCs are used to plot the data in two dimensions and to further analyse it [37]. The typical applications of PCA include quantitative decisions in finance [38], image processing [39], recommendation systems, face and speech recognition [40] and data correlation applications [41] across various industrial sectors.

PCA algorithm is based on mathematical concept such as variance, co-variance, Eigen values and Eigen vectors. As discussed earlier PCA forms the new features named as PCs which are linear combinations of the original variables. Generally, the first PC represents the direction along which the data points exhibit the largest variation, the second PC is the direction uncorrelated to the first PC. For standardized data sets for which every data point is centred to zero, the PCs are normalized eigenvectors of the covariance matrix. Every PC which is uncorrelated to any other components, and when it is projected on the related component is construed as the direction maximizing the variance of the samples [42].
Assume, the system with n variables $x_1, x_2, x_3, \dots, x_n$.
A set of n variables is created, $C_1, C_2, C_3, \dots, C_n$ which is a linear combination of $x_1, x_2, x_3, \dots, x_n$. These $C_1, C_2, C_3, \dots, C_n$ are called the principal components which are represented in equation 1, 2 and 3 respectively.

$$C_1 = a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + \cdots + a_{1n}x_n \quad (1)$$

$$C_2 = a_{21}x_1 + a_{22}x_2 + a_{23}x_3 + \cdots + a_{2n}x_n \quad (2)$$

$$C_n = a_{n1}x_1 + a_{n2}x_2 + a_{n3}x_3 + \cdots + a_{nn}x_n \quad (3)$$

The coefficients $a_{11}, \dots\ a_{nn}$ are selected to fulfil the following constraints;
Variance of C_1 should be the maximum as shown in equation 4.

$$\text{Var}\ (C_1) \geq \text{Var}\ (C_2) \geq \text{Var}\ (C_n) \quad (4)$$

The solution to these coefficients is presented mathematically by [34]. The sum of the squares of the all the coefficients is one.
$C_1 = a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + \cdots + a_{1n}x_n$ is called the first principal component of $x_1, x_2, x_3, \dots, x_n$.

The loadings for the PC1 are given by $a_{11}, \dots\ a_{nn}$. The vector generated with these individual loadings is referred to as the principal component loading vector. Based on the loadings (a_{ij}), the principal component scores are calculated.

The first PC score for the first observation is calculated with the observed variable values:

$$C_1 = a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + \cdots + a_{1n}x_n \quad (5)$$

Since there are n observations, there will be n PC scores for the the first principal component. The mathematical concept underlying PCA is the decomposition of the data matrix into two orthogonal submatrices. The aforementioned orthogonal matrices are referred to as: Scores and Loadings. The loadings are considered as the weights for every original variable while calculating the PCs.

3 Problem Formulation

In this paper, the design of the shell and tube heat exchanger is considered with reference to the [43]. As discussed in the section 1 STHEs has been widely used in variegated domain. Several experimental, numerical simulation studies have been performed to investigate and improve the thermal performance of STHEs. Further, in the recent past optimization of STHEs have been carried out for minimizing the investment, annual operating, and energy cost. From the literature it is evident that the most significant factors influencing thermo-hydraulic performance of STHEs are mentioned in Table 1.

Table 1: Variables with symbols

Variable	Symbols
Baffle spacing (m)	B
Shell Diameter (m)	D_S
Tube outer diameter (m)	d_o
Tube inside diameter (m)	d_i
Shell side Reynold's number	Re_S
Tube side Reynold's number	Re_t
Shell side heat transfer coefficients	h_S
Total area	A_t
No. of Tubes	N_t
Tube side heat transfer coefficients	h_t
Overall heat transfer coefficients	U
Length of tube (m)	L

The current work focuses on the multi-variate analysis of the above mentioned factors. B, D_S, d_o and d_i are the independent variables on which other factors such as Re_S, Re_t, h_S ,A_t, N_t, h_t, U , L are dependant. For this analysis, the lower limit and upper limit for the independent variables are considered based on the literature. The random values are generated for each of the variables within the range and are considered for the analysis. The lower and upper limits are mentioned in the Table 2.

Table 2: Variables with limits

Variable	Symbol	Lower Limit	Upper Limit
Baffle spacing (m)	B	0.2	0.5
Shell Diameter (m)	D_S	0.2	1
Tube outer diameter (m)	d_o	0.008	0.051
Tube inside diameter (m)	d_i	0.0064	0.0408

3.1 Data Normalization

As discussed in Section 1, PCA is a variance based technique. It projects the raw data onto the newly formed PCs which maximizes the variance. These PCs are based on the Standard Deviation (SD) of original variables. Hence, while projecting onto the PCs, variables having higher SDs are calculated with higher weight as compared to the variables having lower SDs. Moreover, variables with different units of measurement and varied range (lower & upper limits) also contributes to this bias for PCs formation. In the light of above, the raw data is normalized with mean as zero. In this way, all variables are reorganized to have the same SD; in turn the same weights for projecting onto the PCs. In the current study, it can be clearly observed from Table 2 that, variables B and Ds are having large variances when compared to the do and di. Furthermore, for variable m and Ds, the range is 0.3 and 0.8 respectively; while for do and di it is 0.043 & 0.034 respectively. Hence, data normalization is required. In this work, each of the instance (data point) for every variable is normalized by using the equation 1.

$$Normalized\ Value = \frac{Value - Mean}{SD} \tag{6}$$

4 Results and Discussion

Table 3. PCs associated with variables

Var.	PC1	PC2	PC3	PC4	PC5	PC6	PC7	PC8	PC9	PC10	PC11	PC12
B	0.102	0.081	0.040	-0.841	-0.438	-0.269	0.002	-0.085	-0.009	-0.007	-0.042	0.002
Ds	0.338	0.178	-0.232	-0.129	0.363	-0.059	0.681	-0.082	-0.194	0.182	0.320	-0.074
do	0.351	-0.004	0.421	0.045	-0.017	-0.101	0.038	0.648	0.001	0.463	-0.228	-0.018
di	0.350	-0.028	0.387	0.200	-0.041	-0.125	-0.104	-0.737	-0.063	0.301	-0.149	-0.006
Res	0.283	-0.358	-0.037	-0.129	-0.244	0.783	0.105	-0.044	0.255	0.098	0.110	0.020
Hs	0.192	0.524	0.026	0.028	-0.121	0.248	-0.478	0.077	-0.348	0.051	0.490	-0.111
At	0.370	-0.020	0.370	0.183	-0.151	-0.199	0.163	0.085	0.244	-0.667	0.302	0.021
Nt	0.153	-0.168	0.236	-0.406	0.728	0.150	-0.313	-0.004	-0.077	-0.248	-0.095	0.014
Ret	0.330	-0.297	-0.371	0.089	-0.087	-0.137	-0.158	0.052	-0.191	-0.141	-0.194	-0.714
Ht	0.231	0.516	-0.128	0.052	-0.058	0.277	0.148	-0.014	-0.105	-0.310	-0.655	0.153
U	0.303	0.221	-0.404	0.005	0.166	-0.195	-0.296	-0.012	0.709	0.163	0.031	0.110
L	0.312	-0.355	-0.325	0.086	-0.092	-0.168	-0.161	0.076	-0.395	-0.039	0.036	0.660

12 variables are considered such as B, Ds, do, di, Res, Ret, hs, ht, U, At and L. 12 variables and hence maximum 12 PCs are possible. Table 3 describes the Principal Components (PCs) associated with the 12 variables. Table 4 shows the Eigen values, Explained Variance and Cumulative Variance. It is evident from the Table 1 that 10 PCs explains 100% of the variance observed in the variables. Hence, further analysis can be performed by considering no. of PCs as 10.

Table 4: Eigen values, Explained Variance & Cumulative Variance

PC	Eigen Value	Explained Variance (%)	Cumulative Explained Variance (%)
1	4.16	34.6	34.6
2	2.47	20.6	55.2
3	2.06	17.2	72.4
4	1.03	8.6	81
5	0.93	7.8	88.8
6	0.42	3.5	92.3
7	0.38	3.2	95.5
8	0.22	1.8	97.3
9	0.17	1.4	98.7
10	0.11	0.9	99.6
11	0.07	0.6	100
12	0.003	0.0	100

Figure 1 represents the outliers observed in the data set. The reference point is considered as 4.736 and all the instances lying above this threshold value are considered as outliers. Figure 2 shows the score plot which is projection of the data points on to the principal components (PCs) in two dimensions only. It is essentially a scatter plot with PC1 on x-axis and PC2 on y- axis. It uses equal scale for both the axis. The plot contains data points that represents the original sample data. In this case, data points related to the all 12 variables are distributed in 2 PCs. It is evident in figure 2 that the data is centred around the mean.

From the loading plot which is represented in figure 3, it is clear that first principal component has large positive correlations with the variables such as Res, L, Ret, At, do, di, Ds, and ht. Moreover, we can observe from the loading plot that variables do, di and A_t are grouped together which signifies the geometrical design parameters for the tube. Also, factors Res, Ret and L are closely correlated, which represents flow characteristics of shell and tube. Hence, the first principal component primarily measures design and flow characteristics of this heat exchanger. The second principal component has negative coefficients for the factors Res, Nt, Ret, L, do, di and A_t; however, do, di and A_t can be neglected owing to the practically zero (-0.004, -0.028, -0.020 respectively) explained variance by PC2. which signifies the strong inverse relationship between PC2 and these factors. Figure 4 represents the bi-plot which combines scores and the loading vectors in a single plot. The scores and loading vectors are represented by dots and the straight lines respectively. The PC1 scores are plotted on bottom x-axis while PC2 on left y-axis. The loadings of PC1 are plotted on x-axis and on y-axis for PC2.

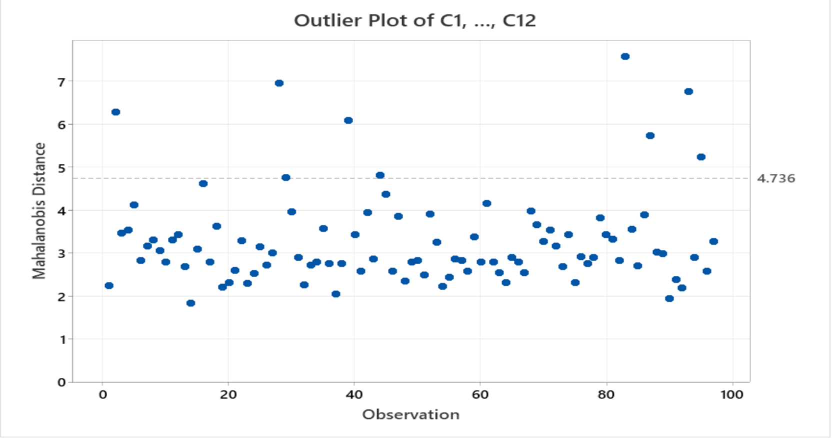

Fig. 1. Outlier Plot

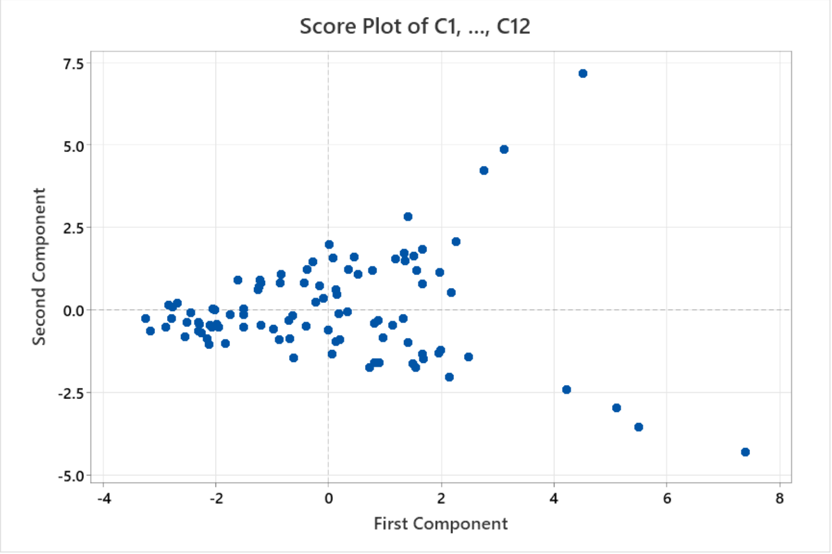

Fig. 2. Score Plot

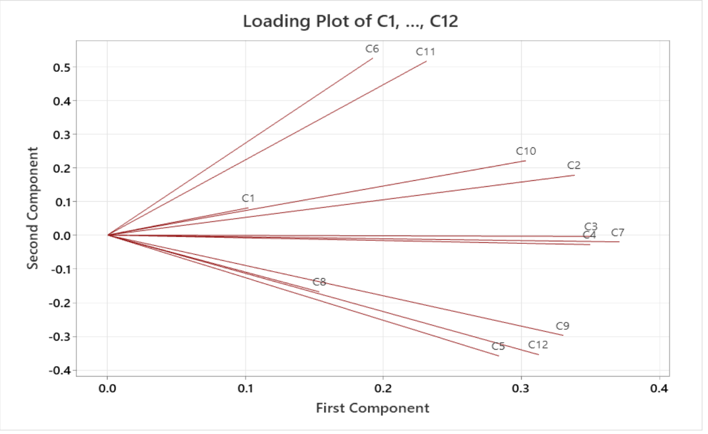

Fig. 3. Loading Plot

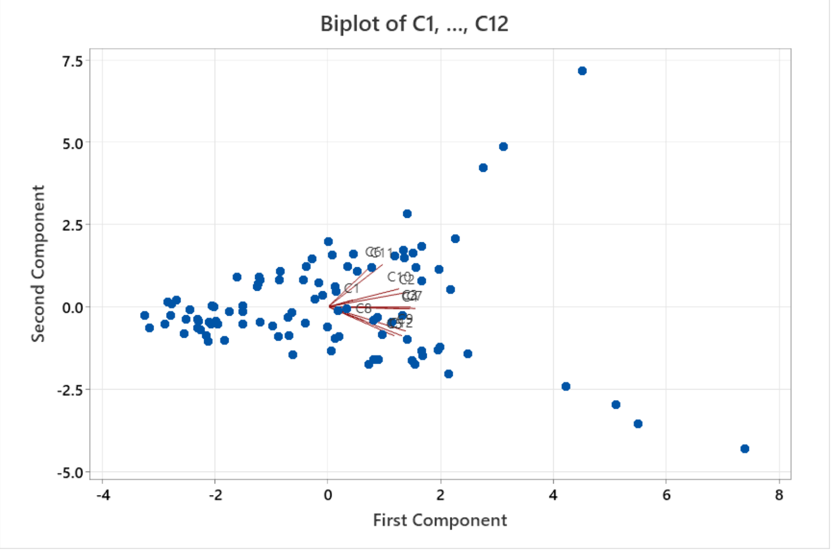

Fig. 4. Biplot

5 Conclusions & Future Directions

Shell & Tube Heat Exchangers (STHEs) have been widely applied across various industrial sectors. In the recent past, several experimental, numerical & simulation based investigations are performed to investigate and improve the thermal performance of STHEs. Further, recently, various AI based optimization algorithms have been applied for minimizing the investment, annual operating, and energy costs for STHEs. However, there is a little work available in the literature for the Multi-Variate Analysis of STHEs. In this work, Multi-Variate Analysis using Principal Component Analysis (PCA) is carried out for Shell & Tube Heat Exchanger (STHE). In total, 12 variables such as Baffle spacing (B), Shell diameter (Ds), tube inner & outer diameter (di & do), Reynold's number at shell side and tube side (Res & Ret), Heat transfer coefficient on shell side and tube side (hs & ht), heat transfer surface area (At), Overall heat transfer coefficient (U), Tube length (L), number of tubes (Nt)are considered. These variables describe the Thermo-Hydraulic performance of STHE and hence are selected. The lower and upper limits for each of the variables are chosen based on the existing literature. The random values are generated for each of the variables within the range and are considered for the analysis. In total 100 data points are generated and analysed. Outliers, Scores & Loadings, and Bi-Plots are plotted. For the 12 variables, 2 PCs are defined. It is observed that first PC has larger positive correlations with the variables Res, L, Ret, At, do, di, Ds, and ht. It is evident from the loading plot that variables do, di and A_t are grouped together emphasizing the geometrical design parameters for the tube. Moreover, factors Res, Ret and L are closely correlated, representing the flow characteristics of shell and tube. Hence, it can be concluded that the first principal component primarily measures design and flow characteristics of STHE. The second principal component has negative coefficients for the factors Res, Nt, Ret, L, do, di and A_t. However, do, di and A_t has practically zero (-0.004, -0.028, -0.020 respectively) explained variance for PC2 and hence are not considered in the analysis. PC2 loading plot signifies the strong inverse relationship between PC2 and Nt, Ret and L. The current work has opened avenues for Multi-Variate Analysis of Heat Exchangers. In the near future, authors intend to apply Partial Least Square Regression for the performance prediction of STHEs. Moreover, the Machine Learning Algorithms could be applied for evaluating and improving heat Exchanger performance.

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