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Optimal Design of Process Equipment Through Hybrid Mechanistic-ANN Models: Effect of Hybridization

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ABSTRACT

Artificial neural networks (ANNs) have gained popularity in the last years as tools to develop data-driven models of chemical process units. However, representing a system only with such artificial intelligence models may lead to a loss in the comprehension of the occurring phenomena. Hybrid models allow combining the predictive capabilities of ANNs with the foundational knowledge of rigorous models. This study explores the impact of hybridization in designing and optimizing shell-and-tube heat exchangers, comparing a full ANN-based model with a hybrid model. The hybrid model incorporates ANN predictions for highly nonlinear components, such as heat transfer coefficients, while other calculations are performed using the rigorous Bell-Delaware model. To generate the necessary data, the rigorous model is solved under randomly selected conditions. Using Python, one ANN predicts the exchanger's cost, while another predicts the heat transfer coefficients. Both models are optimized using the differential evolution algorithm. The results indicate that the hybrid model produces designs with an approximately 67% lower standard deviation compared to the full ANN-based model when compared to the rigorous model's cost predictions. This highlights the hybrid model's ability to balance computational efficiency and accuracy, offering a promising approach for process design applications.

Keywords: artificial neural networks, hybrid models, optimal design.

INTRODUCTION

Heat exchangers are essential components in the chemical industry. Among the various types of exchangers, shell-and-tube heat exchangers stand out for their broad acceptance due to their balance between volume and heat transfer area, as well as their ability to operate over a wide range of pressures and temperatures [1]. The design of these exchangers is typically performed using the Bell-Delaware method, a methodology based on highly nonlinear mathematical relationships that involves managing both discrete and continuous variables [2]. Due to the nature of equations that compose Bell-Delaware method, it represents a non-trivial optimization problem [3].

In recent years, artificial intelligence, particularly artificial neural networks (ANNs), has gained relevance in modeling and analyzing industrial process units. Artificial neural networks are data-driven structures widely used to model chemical process units, such as reactors [4] and separation units [5]. These tools allow the prediction of system behavior from data, analyzing how input variables affect system responses. Nevertheless, developing ANN-based models requires training data, which poses challenges in process design where the equipment does not yet exist and real-world data is unavailable. On the other hand, it is crucial to emphasize the importance of avoiding reliance solely on data-based models, as this might overlook the fundamental principles governing system behavior [6]. Hybrid models address this issue by combining the predictive capabilities of ANNs for complex interactions with the foundational knowledge of mechanistic models.

In this context, this work develops an ANN model to predict the cost of a shell-and-tube heat exchanger. Furthermore, a hybrid ANN model (ANN-H) is implemented, combining predictions of heat transfer coefficient generated by an artificial neural network with the remaining design calculations, represented with the rigorous Bell-Delaware model.

This work focuses on the development and implementation of ANN and ANN-H models for the design and optimization of shell-and-tube heat exchangers. The goal is to explore methodologies for accurately predicting key parameters such as heat transfer coefficients and equipment costs based on design variables. To achieve this, ANN models are trained to analyze and predict complex relationships within the heat exchanger design, while a ANN-H model is developed to integrates the strengths of ANNs with traditional rigorous calculation techniques, such as the Bell-Delaware method. This hybrid approach leverages the ability of ANNs to predict highly nonlinear behaviors while maintaining the fundamental principles provided by mechanistic models, improving the overall accuracy of predictions.

Moreover, the study employs Bayesian optimization algorithms to determine the optimal architecture of the ANN models, ensuring accurate and reliable predictions. Subsequently, metaheuristic optimization algorithms are applied to identify the optimal values of design variables that minimize the heat exchanger cost, providing a comprehensive approach for cost-efficient design.

The results obtained from the ANN and ANN-H models are compared with the outputs of rigorous models to validate the effectiveness and reliability of the proposed methodologies. By integrating advanced machine learning techniques with traditional engineering approaches, this work seeks to bridge the gap between computational efficiency and the accuracy in heat exchanger design, offering an innovative path for process optimization in the chemical industry.

METHODOLOGY

The study focuses on a heat exchanger with methanol in the shell and seawater in the tubes [5]. Methanol flows with inlet/outlet temperatures of 95 °C and 40 °C, respectively, and a mass flow rate of 27.8 kg/s. Seawater flows through the tubes with inlet/outlet temperatures of 25 °C and 40 °C, and a mass flow rate of 68.9 kg/s. The shell and tubes are made of carbon steel.

The methodology is developed in three main stages: data generation, model development, and optimization.

Data Generation

To generate the necessary data for the artificial neural network, a shell-and-tube heat exchanger model was developed with 11 decision variables, each bounded by specific lower and upper limits. Among these, four variables are discrete, with their allowable values listed in Table 1, and seven are continuous, as detailed in Table 2.

Table 1. Allowed values for discrete design variables.

Design variable		Allowed value
Tube pitch	P_t	$[1.25d_o, 1.5d_o]$
Tube layout angle	TL	$[30°, 45°, 90°]$
Baffle cut	B_c	$[25\%, 30\%, 40\%, 45\%]$
Number of tube passes	N_p	

Table 2. Upper and lower limits for continuous variables.

Design variable		**Lower limit**	**Upper limit**
Shell diameter	D_s	0.3 m	1.5 m
Spacing in central baffle	$L_{b,c}$	0.2 D_s	0.55 D_s
Initial and final baffle spacing	$L_{b,i}, L_{b,o}$	1 $L_{b,c}$	1.6 $L_{b,c}$
Diametrical distance of the hole between the shell and baffles	δ_{sb}	0.01 d_o	0.1 d_o
Diametrical distance between tubes and baffles	δ_{tb}	0.01 D_s	0.1 D_s
Beam tubes diameter	D_{otl}	0.8 (D_s - δ_{sb})	0.95 (D_s - δ_{sb})

The design process incorporated five constraints, including operational limits such as maximum pressure drops on both the tube and shell sides, maximum and minimum fluid velocities on the tube side, and a geometric constraint, as outlined in Table 3.

Table 3. Constraints used for the STHE design.

Variables		**Constraint**
Pressure drop in tubes	Pa	≤ 70,000
Pressure drop in shell	Pa	≤ 70,000
Flow rate in tubes	m/s	≤ 0.5
		≥ 3
L/D Ratio		≤ 15

A total of 50,000 designs were generated randomly by assigning values to the decision variables within their defined ranges for continuous variables and selecting from the permissible values for discrete variables. Of these, only 11,643 designs satisfied the operational and geometric constraints established for the heat exchanger model. The remaining designs, which failed to meet these constraints, were discarded during the data cleaning to ensure the dataset's reliability.

ANN Model Development and Implementation

The valid dataset comprising 11,643 designs was utilized to train and validate the ANN. In this context, constraint variables served as input features, while the total equipment cost, calculated based on the methodology outlined in [3], was the output target.

The development of the hybrid model involved replacing the three traditional equations used to calculate the heat transfer coefficient on the tube side with a neural network model. Specifically:

- Equation 1 applies to the laminar flow regime ($Re_t < 2300$).
- Equation 2 is used for the transitional regime ($2300 \leq Re_t \leq 10{,}000$).
- Equation 3 corresponds to the turbulent regime ($Re_t > 10{,}000$).

$$h_t = \frac{k_t}{d_i}\left[1.86\left(\frac{Re_t Pr_t d_i}{L}\right)^{\frac{1}{3}}\right] \tag{1}$$

$$h_t = \frac{k_t}{d_i}\left[\frac{\frac{f_t}{2} Re_t Pr_t}{1.07 + 12.7\left(\frac{f_t}{2}\right)^{0.5}\left(Pr_t^{\frac{2}{3}} - 1\right)}\right] \tag{2}$$

$$h_t = \frac{k_t}{d_i} Re_t^{0.8} Pr_t^{\frac{1}{3}}\left(\frac{\mu_t}{\mu_w}\right)^{0.14} \tag{3}$$

These traditional equations introduce discontinuities at the transitions between Reynolds number domains. To address this, an ANN was employed to provide a smooth and continuous approximation of the overall heat transfer coefficient on the tube side.

Data for training the ANN were generated by randomly sampling values for tube length and diameter, resulting in 13,127 data points. These variables are fundamental inputs to the traditional correlations, ensuring comprehensive coverage of the Reynolds number ranges and enabling the ANN to capture system behavior across all operational domains.

ANN Architecture Optimization

The optimal ANN architecture was determined using Bayesian optimization, exploring a predefined search space based on the parameters listed in Table 4. This optimization aimed to identify the configuration that maximizes the ANN's performance in terms of accuracy. The same optimization approach was applied to both the traditional and hybrid models to ensure consistency.

Table 4. Selection Parameters for ANN Architecture

Parameter	Values
Number of Layers	1 to 4
Number of Neurons per Layer	1 to 16
Activation Function	ReLU, ELU, Leaky ReLU
Optimizer	Adam, SGD

Once the optimal architecture was established, the ANN model was implemented in Python, leveraging machine learning libraries to construct and train the network. The model was designed to process the filtered dataset and predict the total equipment cost based on specific input variables for each design scenario.

Training and Validation

The dataset was partitioned into training and validation sets, with 80% allocated for training and 20% for validation. This split ensured that the ANN could generalize effectively to unseen data. The training-validation process was conducted independently for each modeling approach, reinforcing robust performance and adequate generalization capability.

In the hybrid model, the ANN replaced the segment of the Bell-Delaware model responsible for calculating convective heat transfer coefficients. The ANN's predictions were seamlessly integrated into the overall cost estimation of the heat exchanger, enhancing the model's continuity and accuracy.

Metaheuristic Optimization of Design Variables

Metaheuristic algorithms were employed through the MEALPHY library to identify the optimal values of the 11 design variables that minimize the heat exchanger cost. These algorithms iteratively explored the design space to converge on the most cost-effective configurations. The optimized design variable values were subsequently utilized in both the traditional and hybrid models to compute and compare heat exchanger costs, facilitating an evaluation of each methodology's predictive capabilities.

Analysis and Validation

The performance of the ANN and hybrid ANN-H models was assessed by analyzing the accuracy and standard deviation of their predictions. Additionally, the costs calculated for the optimal design variables were compared between both models and validated against the rigorous Bell-Delaware model. This validation ensured that the proposed methodologies are applicable under real-world conditions, demonstrating their reliability and effectiveness in optimizing heat exchanger design.

RESULTS

This section presents a comparative analysis of the outcomes derived from the two models developed in this study: the Artificial Neural Network (ANN) model and the Hybrid ANN-H model, which integrates the ANN with the rigorous Bell-Delaware model.

Performance of the ANN Model

The ANN model was trained using a filtered dataset comprising 11,643 entries. The optimal architecture identified consists of an input layer with 16 neurons, followed by two hidden layers containing 10 and 16 neurons, respectively, and an output layer.

Table 5 illustrates selected cost predictions from the ANN model alongside the corresponding values obtained from the rigorous Bell-Delaware model.

Table 5. Heat Exchanger Cost Comparison: Rigorous Model vs. ANN Predictions.

Rigorous Model Cost [USD/year]	ANN Predicted Cost [USD/year]
22,973.88	24,521.90
29,617.20	33,566.61
20,656.89	18,239.29
17,710.37	17,322.07
23,430.10	24,415.09
24,726.01	23,447.56
27,128.27	26,297.71
31,251.74	31,865.45
21,422.44	23,961.10
37,979.40	38,219.78

Figure 1 presents a scatter plot comparing the rigorous model costs against the ANN-predicted costs. The average standard deviation between the ANN predictions and the rigorous model costs is 1,079.591 USD/year, indicating a notable variability in the ANN's cost estimations relative to the rigorous model.

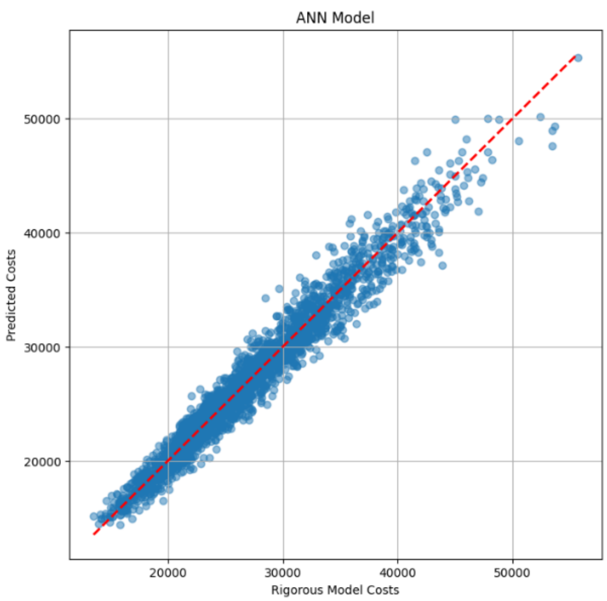

Figure 1. Comparison of rigorous model costs and ANN-predicted costs.

Prediction of Convective Heat Transfer Coefficient

A separate ANN was trained to predict the convective heat transfer coefficient in the tubes using a dataset of 13,125 entries. The optimal architecture for this ANN comprises an input layer with 8 neurons, followed by three hidden layers with 14, 7, and 16 neurons, respectively, and an output layer.

Table 8 provides representative data used for training the ANN predicting the convective heat transfer coefficient.

Table 6. Sample Data for ANN Predicting Convective Heat Transfer Coefficient

L_t [m]	d_i [m]	Flow rate in tubes [m/s]	h [W/m²]
1.00	0.19	0.51	1662.47
2.12	0.40	0.92	2304.77
4.75	0.62	1.75	3519.76
7.37	0.92	2.57	4430.22
9.62	1.83	2.98	4346.38

Table 7 compares the convective heat transfer coefficients predicted by the ANN-H model with those calculated using the rigorous model. Figure 2 illustrates the relationship between the rigorous model's convective coefficients and those predicted by the ANN-H model. The average standard deviation between the two sets of values is 5.942 $W/m^2 \cdot K$, suggesting a closer alignment between the ANN-H predictions and the rigorous model compared to the ANN model's performance in cost predictions.

Table 7. Convective Heat Transfer Coefficient Comparison: Rigorous Model vs. ANN-H Predictions

Rigorous model convective coefficient [W/m²]	Predicted convective coefficient [W/m²]
335.99	334.28
1 662.47	1 667.45
13 044.61	13 033.72
10 297.55	10 290.20
10 726.66	10 720.97
2 652.72	2 648.79
335.99	329.62
10 199.32	10 196.65
8 840.98	8 836.88
9 709.29	9 695.50

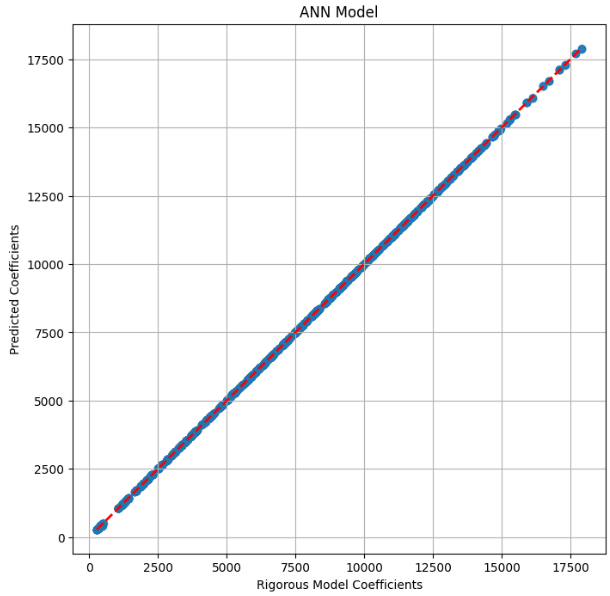

Figure 2. Comparison of rigorous model convective coefficients and ANN-H predicted coefficients.

Performance of the Hybrid ANN-H Model

The Hybrid ANN-H model integrates the ANN to predict the convective heat transfer coefficients, thereby replacing the traditional equations in the rigorous Bell-Delaware model. The cost predictions from the ANN-H model are presented alongside the rigorous model costs in Table 8.

The ANN-H model exhibits an average standard deviation of 348.55 USD/year when compared to the rigorous model, which is significantly lower than the 1,079.59 USD/year observed in the ANN model. This reduction in variability indicates improved consistency and accuracy in cost predictions when utilizing the hybrid approach.

Table 8. Heat Exchanger Cost Comparison: Rigorous Model vs. ANN-H Predictions

Rigorous model cost [USD/year]	ANN- H predicted cost [USD/year]
29,617.20	30,038.76
20,656.88	21,333.41
17,710.36	18,678.41
23,430.09	23,815.72
24,726.01	25,351.33
27,128.27	27,346.88
31,251.73	31,655.29
21,422.44	21,903.92
37,979.39	38,235.07

Optimization of Design Variables

Table 9 summarizes the optimal values of the design variables obtained through metaheuristic optimization for both the ANN and ANN-H models, along with the corresponding total costs.

Table 9. Optimal Design Variables and Costs: ANN vs. ANN-H Models

Design variable	Optimal value (ANN)	Optimal value (ANN-H)
Shell diameter	0.3 m	0.3 m
Tube diameter	d_o-0.25in, d_i-0.194in	d_o-0.25in, d_i-0.194in
Tube pitch	1.25 do	1.25 do
Tube arrangement	45°	90°
Number of passes in the tubes	1	4
Baffle cut percentage	25%	45%
Spacing in central baffle	0.2 D_s	0.2 D_s
Initial and final baffle spacing	1 $L_{b,c}$	1.036 $L_{b,c}$
Diametrical distance of the hole between the shell and baffles	0.01 d_o	0.1 d_o
Diametrical distance between tubes and baffles	0.01 D_s	0.09 D_s
Beam tubes diameter	0.948 (D_s - δ_{sb})	0.95 (D_s - δ_{sb})
Cost (USD/year)	13437.20	13 404.28

Both models suggest similar optimal values for most design variables, with notable differences in the tube arrangement angle and the number of tube passes. Specifically, the ANN model favors a 45° tube arrangement with a single tube pass, whereas the ANN-H model recommends a 90° arrangement with four tube passes. These variations reflect how the ANN-H model's integration of convective coefficient predictions influences the optimization process to achieve lower cost outcomes.

The comparative analysis indicates that the Hybrid ANN-H model consistently demonstrates lower variability in cost predictions compared to the standalone ANN model. The reduced standard deviation in the ANN-H model suggests a closer alignment with the rigorous Bell-Delaware model, thereby enhancing prediction reliability.

Furthermore, the optimization results reveal that while both models converge towards similar solutions for most design variables, the ANN-H model achieves marginally lower total costs. This outcome underscores the potential benefits of integrating ANN with traditional modeling approaches, particularly in achieving more accurate and reliable cost estimations.

CONCLUSIONS

This study compared an Artificial Neural Network (ANN) model with a Hybrid ANN-H model for the design and cost optimization of shell-and-tube heat exchangers. The results indicate that the Hybrid ANN-H model achieves more accurate cost predictions, evidenced by lower average standard deviations than the standalone ANN model. This improvement is attributed to effectively integrating the rigorous Bell-Delaware model with the ANN, balancing accuracy and computational efficiency.

Despite these advantages, the Hybrid ANN-H model does not consistently match the computational efficiency of the rigorous model across all scenarios. In some cases, it may require additional computational resources, limiting its applicability where rapid calculations are necessary. Nevertheless, the Hybrid ANN-H model remains a viable alternative for scenarios where both predictive accuracy and computational efficiency are critical.

Overall, the findings demonstrate the potential of combining artificial neural networks with traditional engineering methodologies to enhance the design and analysis of industrial process units. This integration offers a balanced approach to managing computational costs while improving prediction accuracy, paving the way for more effective optimization in thermal system design.

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