

Article

Research on Performance Prediction of Chillers Based on Unsupervised Domain Adaptation

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Abstract

The prediction of chiller performance parameters is crucial for optimal control and fault diagnosis. Numerous efficient and accurate data-driven models have been developed and implemented. These models are normally trained on historical operational data of chiller units. However, the distribution of operational data may shift due to accumulated operating hours or changes in control strategies. Under new operating conditions, models trained on historical data often generalize poorly, leading to prediction deviations. To address this issue, this study integrates a one-dimensional convolutional neural network with a domain adaptation method that extracts features from both the source and target domains and aligns their inverse Gram matrices in terms of angle and scale. A predictive model applicable to multiple chiller performance parameters is established using limited historical data, enhancing the model's generalization ability. Compared to the baseline model (MLP), the proposed method achieves an average reduction of 74.3% in mean absolute error (MAE) and 76.1% in root mean square error (RMSE), while the R^2 values exceed 0.96 (for certain scenarios). Additionally, this paper analyzes the data distribution between the source and target domains, investigates key factors affecting the model's generalization capability, and provides insights for evaluating the quality of modeling data.

Keywords: chiller; domain adaptation; generalization ability; performance prediction

1. Introduction

Heating, Ventilation, and Air Conditioning (HVAC) systems account for a significant portion of building energy consumption, approximately 65%, with chiller units contributing about 40% of the total energy use within HVAC systems [1]. Studies indicate that a substantial amount of energy is wasted due to factors such as performance degradation, improper control strategies, and faults in chiller units [2]. Therefore, it is imperative to conduct research on performance monitoring methods for chillers to ensure they operate under optimal conditions and minimize energy consumption. Whether for fault diagnosis or optimal control, it is essential to predict key performance parameters of chillers, such as energy consumption and the coefficient of performance (COP) [3].

Prediction methods can be categorized into three primary types: white-box models, gray-box models, and black-box models. White-box models simulate chillers based on actual physical formulas and thermodynamic laws, providing a strong theoretical foundation. However, they require numerous parameters and involve complex, time-consuming



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modeling processes, which can make them challenging to apply in practical engineering scenarios [4]. Gray-box models simplify the actual physical processes to enable faster calculations of chiller performance parameters. An example of this is the Gordon-Ng method [5]. The main drawback of gray-box models is their relatively low computational efficiency [6]. Black-box models, on the other hand, adopt a data-driven approach for prediction. While they do not explain the internal workings of the model and only establish mapping relationships between inputs and outputs, they exhibit high accuracy and strong robustness. This has led to their widespread application in current research [6]. Reddy et al. conducted a comparison between gray-box and black-box models for chiller performance prediction, finding that black-box models, such as artificial neural networks, demonstrate superior performance [7]. With technological advancements, various methods, including support vector regression [8–10], convolutional neural networks [11,12], long short-term memory networks [13–15], and ensemble learning [16–18], have been applied to chiller performance prediction, all achieving high accuracy.

Data-driven models are constructed using historical operational data. Previous studies commonly utilize parameters such as cooling capacity, evaporator outlet water temperature, and condenser inlet water temperature as input features [19], while performance metrics like power consumption and coefficient of performance (COP) serve as prediction targets. The distribution of these input features significantly influences the predictive performance of the model. Research indicates that historical data from chillers often fails to encompass the full range of potential input features [20]. For example, the evaporator outlet water temperature of a chiller may be consistently maintained around 7 °C for extended periods. Models developed from such limited historical data are only applicable to operating conditions within this specific temperature range. Consequently, if the control strategy is optimized, the original model may not adequately support the new operating conditions introduced by the optimization. This issue is common in building energy system retrofits. Models constructed on historical data demonstrate insufficient robustness under cross-condition scenario. Therefore, developing chiller performance prediction methods with improved generalization is essential.

Transfer learning offers an effective solution to various challenges in machine learning [21]. The fundamental principle of transfer learning is to extract knowledge from a source domain and apply it to a target domain. The source domain consists of a dataset used for training the model, which includes complete data labels. In contrast, the target domain refers to a new dataset where the model will be applied post-training; this dataset may contain only a few or even no labeled data, and its input feature distribution can significantly differ from that of the source domain.

A commonly adopted strategy in transfer learning research is the “pre-training + fine-tuning” approach [22]. This method involves pre-training a model on the source domain data and then fine-tuning it on the target domain. This process facilitates knowledge transfer by adjusting the model parameters with minimal training data. Transfer learning has been successfully applied in various fields, including thermal comfort prediction [23,24] and air quality monitoring [25,26]. Moreover, transfer learning has been utilized in building energy systems to predict energy consumption across different systems or buildings. For example, Dou et al. implemented transfer learning to achieve cross-system predictions of chiller energy consumption [27]. Similarly, Fan et al. adopted this strategy for building energy consumption analysis, enabling cross-building energy predictions based on limited data samples [28]. Dou et al. tackled data scarcity in building model predictive control (MPC) by developing a transfer learning framework that pre-trains models on simulated data and fine-tunes them with limited real measurements. This approach significantly enhanced forecasting accuracy for HVAC energy demand and indoor air temperature [29].

Despite the success of these studies in achieving knowledge transfer, they still rely on a small amount of labeled data from the target domain. In practical scenarios, however, complete labels for target domain data are often missing or unavailable. Therefore, there is a need to develop novel methods to address this challenge.

Unsupervised domain adaptation (UDA) has recently demonstrated superior performance. UDA trains a model on a labeled source domain and aligns source and target distributions in the absence of target labels. Du et al. introduced the concept of domain adaptation into chiller fault diagnosis to enhance diagnostic performance under both cross-operational conditions and cross-control strategies [30]. Chen et al. developed an interpretability evaluation framework that validates the ability of Domain-Adversarial Neural Networks (DANN) to improve cross-condition fault diagnosis accuracy for chillers by 25% [31]. However, this method treats fault diagnosis as a classification task, where each fault type serves as a data label. In contrast, performance prediction for chillers involves data labels represented as specific numerical values, constituting a regression task, which precludes the direct application of the aforementioned method. Fang et al. proposed a combined LSTM-DANN model for cross-building energy consumption prediction [32], achieving promising predictive results even in the absence of labeled data in the target domain. This demonstrates that unsupervised domain adaptation can be effectively applied to regression prediction problems.

Currently, a research gap still exists in predicting chiller performance parameters under conditions where labeled target domain data is scarce. Existing studies focus on parameters such as energy consumption and energy efficiency, often neglecting other thermodynamic parameters such as subcooling degree and log mean temperature difference in condenser (LMTD), which also reflect the operational state of chillers and can serve as performance indicators for fault diagnosis [33]. Therefore, this paper develops a domain adaptation model (CNN-GRAM) suitable for predicting multiple chiller performance parameters by integrating a one-dimensional convolutional neural network for feature extraction with a domain adaptation approach. To validate the model's generalization capability, this study follows the methodology outlined by Liang et al. [19], using the evaporator outlet water temperature, the condenser inlet water temperature and the load ratio as the criterion for dataset partitioning to ensure a distinct data distribution between the source and target domains.

Section 2 of this paper presents the methodological framework, including the model structure, the selection of evaluation metrics and baseline model. Section 3 analyzes the data of ASHRAE RP-1043 and proposes a new method for data preprocessing. Section 4 compares the prediction results of the baseline and CNN-GRAM model. Correlation between prediction deviation and data distribution is presented in Section 4 as well. Section 5 summarizes the conclusions.

2. Methodology

2.1. Feature Extraction

A Convolutional Neural Network (CNN) is utilized for feature extraction, followed by a fully connected network that serves as the regression head to output the predicted values, as illustrated in Figure 1. Recent advances in deep learning have produced powerful feature extraction architectures, including DeepLab [34] for semantic segmentation and EfficientNet [35] for efficient image classification. However, these architectures are primarily designed for high-dimensional grid data (e.g., images) and may not be directly applicable to the low-dimensional feature vectors in chiller performance prediction. Since the input in this study consists of steady-state physical parameters rather than image data or temporal sequences, a specialized four-layer one-dimensional convolutional neural network (1-D

CNN) is employed. This architecture is specifically designed to extract the local non-linear coupling patterns among these physical features. The CNN extracts local features from the input data, and the feature outputs are generated through convolutional computations and activation functions, with the calculation formula provided in Equation (1).

$$x_j^k = f\left(\sum_{i \in M_j} x_i^{k-1} \cdot W_{ij}^k + b_j^k\right) \quad (1)$$

where x_j^k and x_i^{k-1} denote the output feature of the k -th layer and the input feature of the previous layer, respectively, W_{ij}^k represents the weight matrix of the convolution kernel, b_j^k denotes the bias and f indicates the activation function.

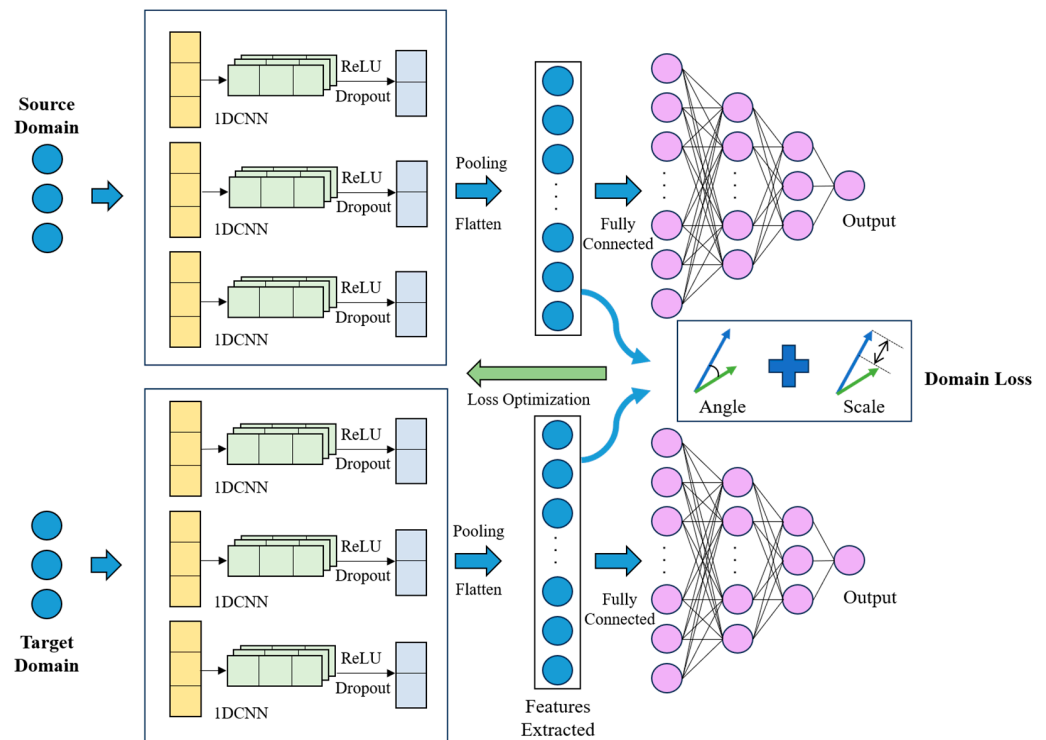


Figure 1. Schematic diagram of the prediction model structure.

A one-dimensional adaptive average pooling layer is adopted following the convolutional layer. This layer compresses the feature sequence of each channel into a fixed-length vector by averaging over the temporal dimension, thereby preserving essential information.

In this study, a four-layer convolutional network is configured with a kernel size of 3, and the ReLU function is utilized as the activation function. Additionally, dropout regularization is incorporated after the convolutional layers to mitigate the risk of model overfitting.

2.2. Fully Connected Regression

Following adaptive average pooling and flattening, the network generates the feature vector. A three-layer fully connected network is employed to predict the performance parameters. The architecture of the network is optimized using a grid search method to ensure optimal performance. The underlying principles are described by Equations (2) and (3).

$$H = \sigma_1(X \cdot w_h + b_i) \quad (2)$$

$$Y = \sigma_2(X \cdot w_0 + b_h) \quad (3)$$

where X is the input feature matrix, w_h and w_0 denote the weight matrices from the input layer to the hidden layer and from the hidden layer to the output layer, respectively. σ_1 and σ_2 are the activation function. b_i and b_h represent the bias for the input and hidden layers, respectively.

2.3. Domain Adaptation Method Based on Inverse Gram Matrix Alignment Loss

Nejjar et al. proposed the DARE-GRAM method, which aligns the inverse Gram matrix subspaces rather than directly aligning the input features [36]. In relation to its domain adaptation component, this study incorporates the distributional discrepancy in chiller operational data as a loss function within the performance prediction model. The specific procedure is described as follows.

The Gram matrix is a symmetric matrix constructed from the inner products of a set of vectors in an inner product space, mathematically expressed as Equation (4).

$$Gram(Z) = Z^T Z \quad (4)$$

where Z is the input feature matrix. For chiller units, three variables—chilled water return temperature, condenser water outlet temperature, and cooling capacity—are selected as the input features, collectively forming the input matrix Z .

Performing Singular Value Decomposition (SVD) on the feature matrix and substituting the result into Equation (4) produces Equation (5).

$$Gram(Z) = Z^T Z = (UDV^T)^T (UDV^T) = VPV^T \quad (5)$$

where V is an orthogonal matrix, and P is a diagonal matrix. Their specific representations are given in Equation (6).

$$P = \begin{bmatrix} \lambda_1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \lambda_p \end{bmatrix}, \quad \lambda_1 > \cdots > \lambda_k > \cdots > \lambda_p \quad (6)$$

where λ_p represents the square of the p -th eigenvalue of the matrix Z .

Since not all basis vectors contribute equally, with those corresponding to the largest eigenvalues exerting the greatest influence, only the dominant basis vectors are considered. By discarding singular values below λ_k and treating them as zero, the Moore–Penrose pseudo-inverse can be obtained [37], as expressed in Equations (7) and (8).

$$(Z^T Z)^+ = VP^+ V^T \quad (7)$$

$$P^+ = \begin{bmatrix} 1/\lambda_1 & \cdots & 0 & \cdots & 0 \\ \vdots & \ddots & \vdots & \ddots & \vdots \\ 0 & \cdots & 1/\lambda_k & \cdots & 0 \\ \vdots & \ddots & \vdots & \ddots & \vdots \\ 0 & \cdots & 0 & \cdots & 0 \end{bmatrix} \quad (8)$$

According to reference [36], the value of k is determined by Equation (9).

$$\frac{\sum_{i=0}^k \lambda_i}{\sum_{i=0}^p \lambda_i} = Threshold \quad (9)$$

When the calculated result exceeds the preset threshold, it indicates that the first k eigenvalues have become dominant. In this study, the threshold is set at 0.9.

By performing the aforementioned calculations separately on the source and target domain data, two pseudo-inverse matrices, IG_s^+ and IG_t^+ are obtained. Based on these matrices, cosine similarity alignment is applied to the target and source domain data, resulting in the construction of a new loss function, as shown in Equations (10)–(12).

$$S_i(IG_{s,i}^+, IG_{t,i}^+) = \frac{IG_{s,i}^+ \cdot IG_{t,i}^+}{\|IG_{s,i}^+\| \times \|IG_{t,i}^+\|} \quad (10)$$

$$S = (S_1, S_2, S_3 \dots S_p) \quad (11)$$

$$L_{cos} = \|I - S\| \quad (12)$$

where IG_s^+ and IG_t^+ denote the i -th feature vector in the source domain and target domain, respectively. S is a vector composed of the cosine similarity for each column, and I represents an all-ones vector. A smaller L_{cos} indicates a smaller angular deviation between the domains. By minimizing the angular deviation between the pseudo-inverse Gram matrices of source and target domains, the subspaces spanned by their dominant eigenvectors remain consistent, thereby addressing the feature correlation mismatch induced by domain shifts [36].

Furthermore, Equation (13) is utilized to align the scale of the matrices. The Euclidean distance of the k -th order diagonal matrix is employed as the scale loss function. A smaller L_{scale} indicates a reduced scale discrepancy between the domains, where $\sqrt{\lambda_{s,i}}$ denotes the i -th eigenvalue of the Gram matrix. By minimizing the discrepancy in the magnitudes of principal eigenvalues, L_{scale} preserves the feature scale across domains, which is essential for maintaining regression stability [38]. Without L_{scale} , the aligned features may exhibit different variances, leading to biased regression coefficients.

$$L_{scale} = \|\sum_{i=0}^k \sqrt{\lambda_{s,i}} - \sum_{i=0}^k \sqrt{\lambda_{t,i}}\| \quad (13)$$

The two aforementioned loss functions are combined with the mean squared error (MSE) loss between the predicted and actual values to formulate the final loss function, as expressed in Equations (14) and (15).

$$L_{DomainLoss} = \alpha_1 L_{cos} + \alpha_2 L_{scale} \quad (14)$$

$$L = \alpha_3 L_{DomainLoss} + L_{MSE} \quad (15)$$

where α_1 , α_2 and α_3 are hyperparameters, set to ensure that the magnitudes of the respective loss terms are approximately balanced. In this paper, they are configured as 0.05, 0.001, and 0.1, respectively. Hyperparameter selection was performed using a grid search strategy. As shown in Figure 2, the model exhibits robust overall performance despite small variations in hyperparameter values.

2.4. Evaluation Metrics and Baseline Models

The coefficient of determination (R^2), mean absolute error (MAE), and root mean square error (RMSE) are adopted as evaluation metrics for model prediction, as defined in Equations (16)–(18).

$$R^2 = 1 - \frac{\sum_i (y_{pred,i} - y_i)^2}{\sum_i (\bar{y}_i - y_i)^2} \quad (16)$$

$$MAE = \frac{1}{m} \sum_1^m |y_{pred,i} - y_i| \quad (17)$$

$$RMSE = \sqrt{\frac{1}{m} \sum_i (y_{pred,i} - y_i)^2} \quad (18)$$

where y_i represents the actual value, $y_{pred,i}$ denotes the predicted value and $\bar{y}_i$ is the mean of the actual value. Multilayer perception is selected as the baseline model. It has frequently been used as baseline model in previous studies [20].

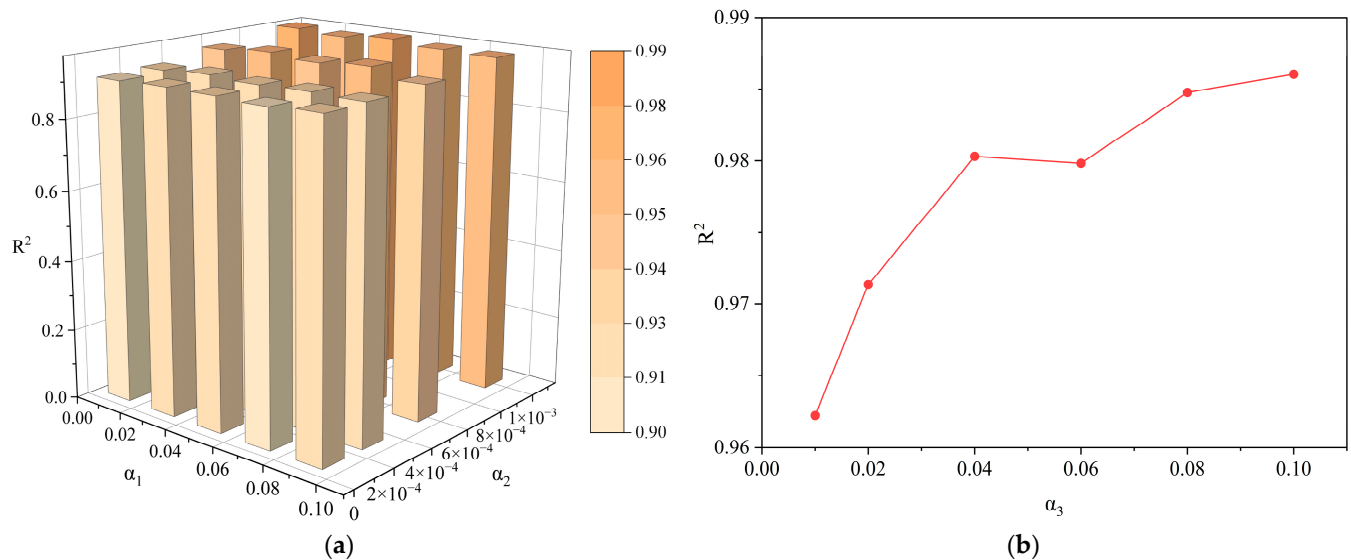


Figure 2. R^2 metrics of different hyperparameters in scenario A (Source data): (a) α_1 and α_2 ; (b) α_3 .

3. Data Analysis and Preprocessing

3.1. Data Partitioning

The ASHRAE RP-1043 experimental dataset is utilized to validate the generalization capability of the chiller performance prediction model. ASHRAE RP-1043 conducted experiments on a centrifugal chiller unit with a rated cooling capacity of 316 kW. Operational data were obtained across 27 distinct steady-state conditions by systematically varying the evaporator outlet water temperature, the condenser inlet water temperature, and the load ratio. In accordance with Liang et al. [19], this study uses the evaporator outlet water temperature, the condenser inlet water temperature, and the load ratio as the criterion for partitioning the dataset to ensure a distinct data distribution between the source and target domains. The data are divided into five operational scenarios, as detailed in Table 1.

Table 1. Partitioning results.

Scenario	Datasets	Evaporator Outlet Water Temperature (°C)	Condenser Inlet Water Temperature (°C)	Load Rate (%)
A	Source data	5~7	17~29	25~100
	Target data	10	17~29	25~100
B	Source data	5~10	17~23	25~100
	Target data	5~10	17~29	25~100
C	Source data	5~10	23~29	25~100
	Target data	5~10	17~29	25~100
D	Source data	5~10	17~29	60~100
	Target data	5~10	17~29	25~100
E	Source data	5~10	17~29	25~60
	Target data	5~10	17~29	25~100

As shown in Table 1, Scenario A simulates the distributional shift caused by varying evaporator outlet water temperature. Increasing the evaporator outlet water temperature is a common retrofit measure for improving energy efficiency. Scenarios B and C simulate shifts caused by changing condenser inlet water temperature, which depends on both control logic and wet-bulb conditions. The two scenarios validate the cross-condition generalization under complex operating conditions. Scenarios D and E simulate shifts caused by changing load rate. These two test scenarios are designed to verify whether the domain-adaptation approach can build a predictive model from a limited operating range and then apply it to full-range operating conditions.

Power consumption (kW), logarithmic mean temperature difference (LMTD) of the condenser, and subcooling degree (T_{sub}) are selected as prediction targets. Among these, power prediction has been widely studied in the context of model predictive control [39], while the latter two parameters serve as critical indicators for chiller fault diagnosis [33].

3.2. Data Preprocessing

During startup, shutdown, and transitions between operational conditions, chillers operate in non-steady states. The operational data collected during these periods can introduce interference into the prediction model. Therefore, it is essential to apply steady-state filtering and outlier removal to the raw data. This study utilizes the steady-state data filter proposed by Zhao et al. [2]. A moving time window of specified length is employed, and the slope of the regression line within each window is calculated using the least squares method. An operational state is identified as steady when the absolute value of the slope falls below a predefined threshold. Steady-state filtering is conducted on three parameters: evaporator outlet water temperature, evaporator inlet water temperature and condenser water inlet temperature, with the slope threshold set at 0.03. The threshold was determined to achieve an optimal compromise between model predictive precision and data preservation. As illustrated in Figure 3, taking T_{sub} prediction as a representative case, setting the threshold at 0.03 maintains R^2 performance without increasing MAE while preserving the majority of acquired data samples. Taking the evaporator inlet water temperature as an example, the results of the steady-state filtering are illustrated in Figure 4.

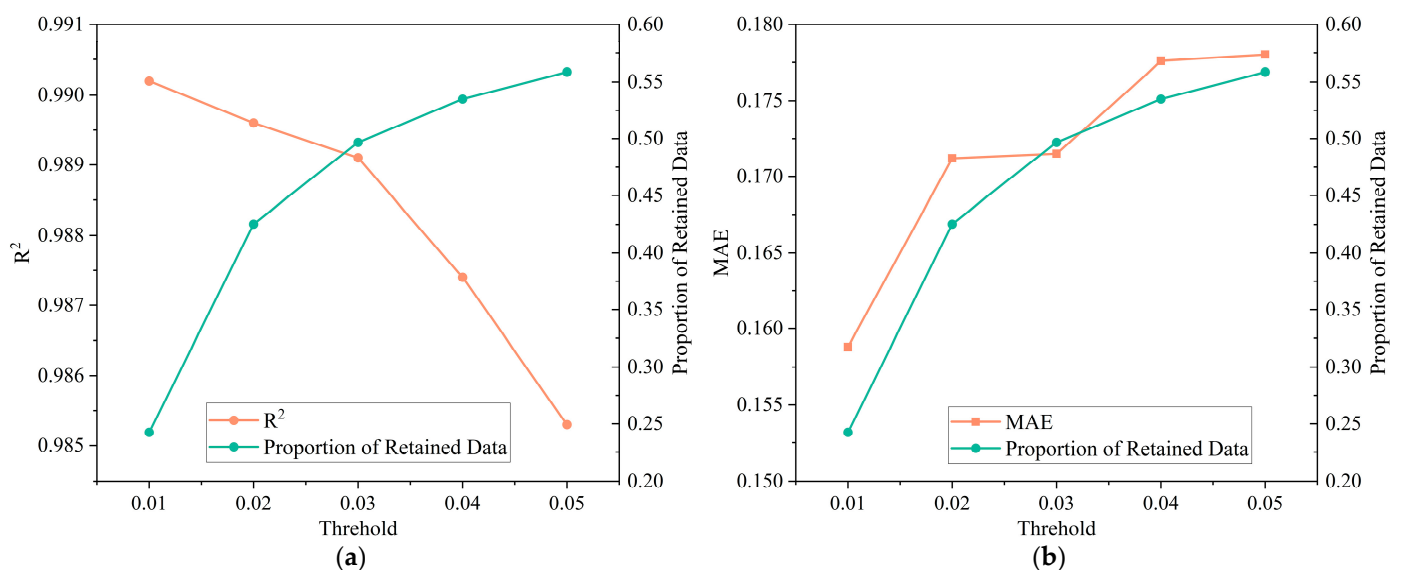


Figure 3. Threshold analysis: (a) R^2 ; (b) MAE.

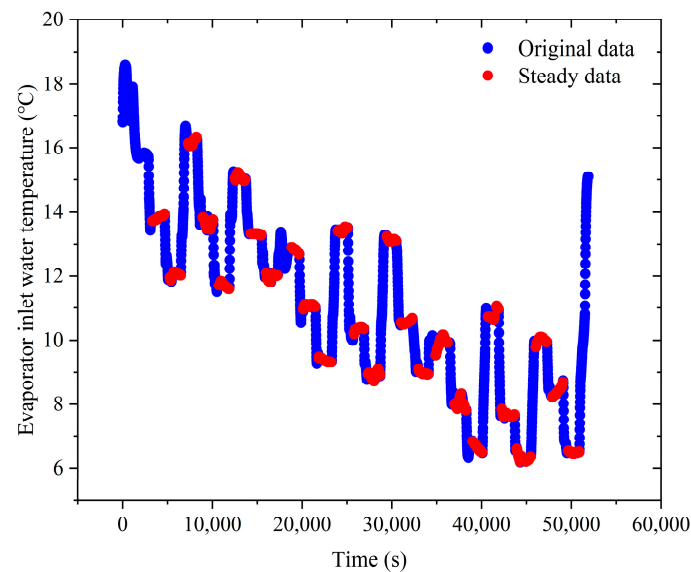


Figure 4. Steady-state data filtering.

Outliers in the data can significantly impair the performance of the prediction model. An excessive number of outliers may lead the model to learn incorrect mapping relationships, necessitating their removal. Previous studies have commonly employed the interquartile range (IQR) rule for outlier removal, limiting its application to the three aforementioned water temperature parameters to maximize the retention of the original dataset. Comprehensive outlier processing across all parameters would substantially reduce the volume of filtered data, thereby undermining the development of robust data-driven models [40]. However, this basic data processing approach inevitably results in undetected outliers within certain parameters, consequently compromising the predictive performance of the resulting models. Taking the subcooling degree as an example, as illustrated in Figure 5, subcooling under steady-state conditions tends to form clusters, yet many scattered points deviate significantly from these clusters. In such cases, identifying outliers based on data point isolation is better suited to the clustered distribution characteristic of this data.

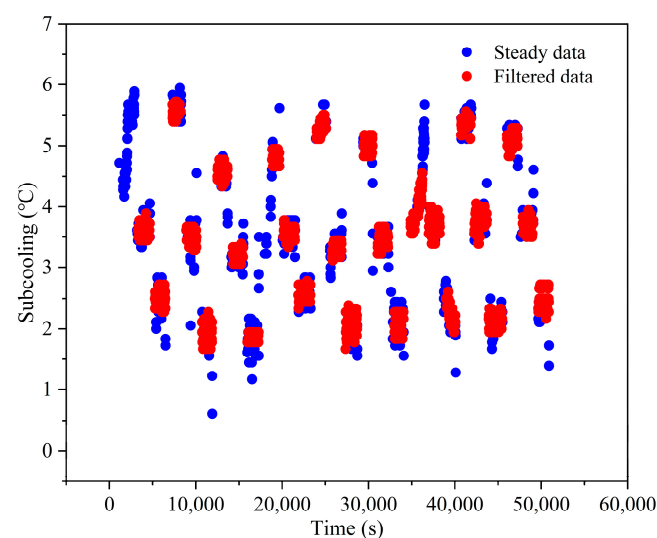


Figure 5. Outlier filtering.

To address this issue, two algorithms—Local Outlier Factor (LOF) and Isolation Forest (IF)—were employed separately to detect and remove outliers. Data points retained by

both methods were preserved, effectively filtering out isolated outliers and transient points exhibiting rapid, short-term fluctuations. The results are presented in Figure 4. These algorithms assess the degree of isolation between data points, thereby enhancing data quality. According to statistics, approximately 50% of the original data was retained after this cleaning process. In contrast, the method proposed by Zhao et al. [2] retains a maximum of 40% of the original data. This demonstrates that slightly increasing the slope threshold and supplementing it with more appropriate outlier handling algorithms can enhance the utilization rate of the raw data while simultaneously improving its quality.

4. Results and Discussion

4.1. Prediction Results of the Baseline Model

First, the predictive performance of the baseline model (MLP) in a cross-domain task is examined. Five-fold cross-validation method is employed during this process. A model is trained using the training set data, and the trained model is subsequently applied to both the validation set and the target domain data. Figure 6 presents the prediction results of the baseline model on the validation set and the target domain data in scenario A. The model demonstrates satisfactory predictive performance on the source domain data. However, when the operating conditions of the chiller change (i.e., when the evaporator outlet water temperature setpoint is altered), the original model fails to adapt to the new conditions, resulting in a significant deterioration in predictive performance, as illustrated in Figure 6d.

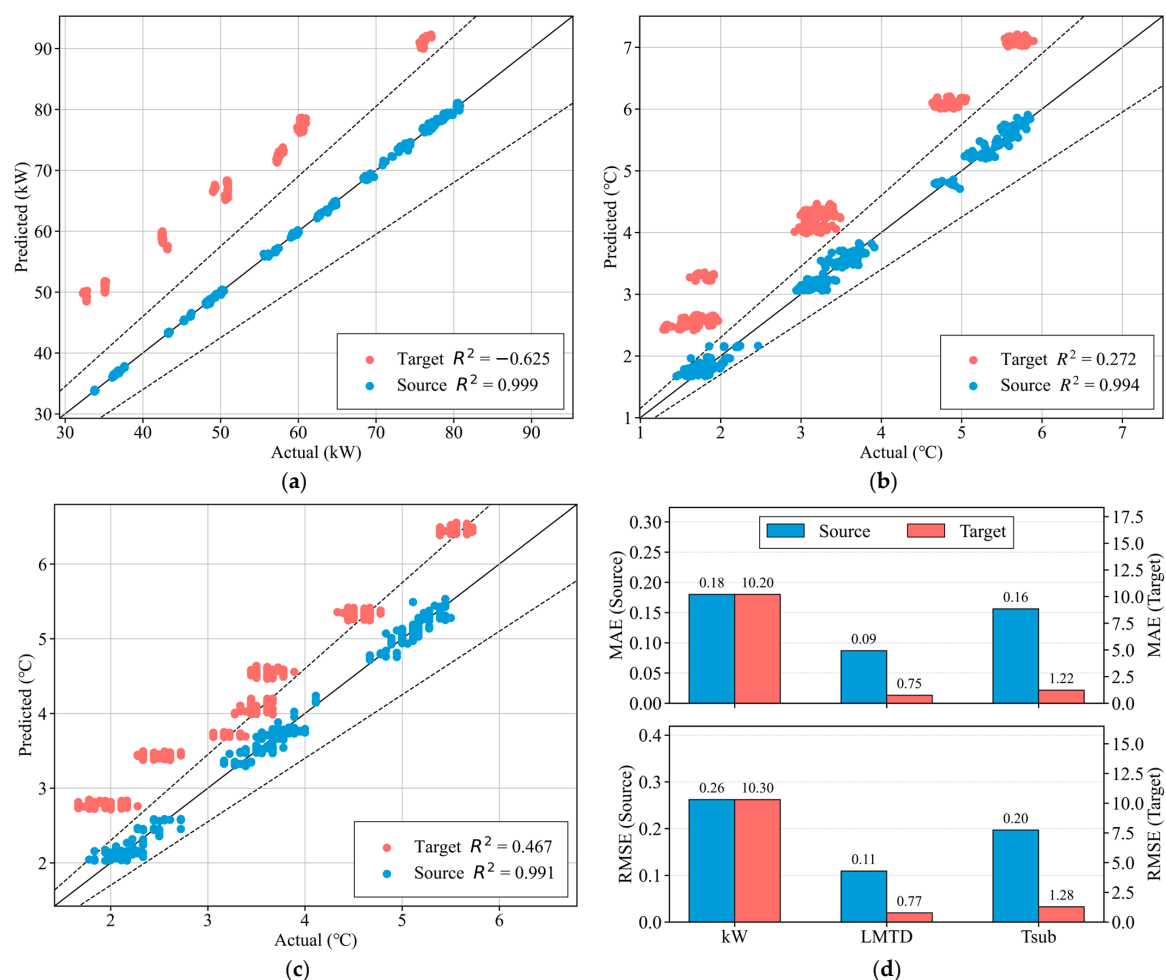


Figure 6. Prediction results of MLP in scenario A: (a) Power consumption; (b) LMTD; (c) Tsub; (d) Evaluation metrics.

On the source domain data, both MAE and RMSE are maintained within relatively small ranges. Among these, the two metrics for power are slightly larger than those for subcooling degree and logarithmic mean temperature difference, primarily because the numerical scale of power is significantly larger than that of the other two parameters. Furthermore, the R^2 values for all three parameters exceed 0.99, indicating strong model fitting performance. In contrast, on the target domain data, MAE and RMSE increase substantially, while R^2 decreases. The model almost completely fails to make accurate predictions. This demonstrates that when the distribution of the chiller's operational data shifts, conventional neural network models cannot maintain their excellent performance.

A similar pattern was observed in scenarios B and C. When the range of the condenser inlet water temperature varied, the accuracy of the MLP declined significantly. Figure 7 presents the prediction results in scenarios B and C.

Figure 8 presents the evaluation metrics of baseline model in scenario B and C. As shown in the figure, the model achieves very low error rates in the source domain, indicating good fitting capability on the training data. However, a significant decline in performance is observed when the model is applied to the target domains. Specifically, the prediction error for power consumption increases dramatically in both scenarios. This substantial discrepancy confirms that the baseline model lacks sufficient generalization ability and fails to provide accurate predictions when the condenser inlet water temperature changes.

Scenarios D and E exhibit a more severe performance degradation under data distribution shifts. Figure 9 indicates that the two scenarios show a strong correlation between chiller power consumption and load rate. Under high load conditions, the chiller operates at higher power levels, while under low load conditions, the power consumption decreases. This relationship is consistent across different operating scenarios.

In Scenario D, the target domain operates at significantly higher power and load rate levels compared to the source domain. Conversely, in Scenario E, the target domain operates at lower power and load rate levels than the source domain. In both cases, the target domain values completely exceed the numerical range of the source domain. This result indicates that the model trained on the source domain data fails to generalize accurately when applied to operating conditions outside its training range. Evaluation metrics of baseline model in scenario D and E are demonstrated in Figure 10.

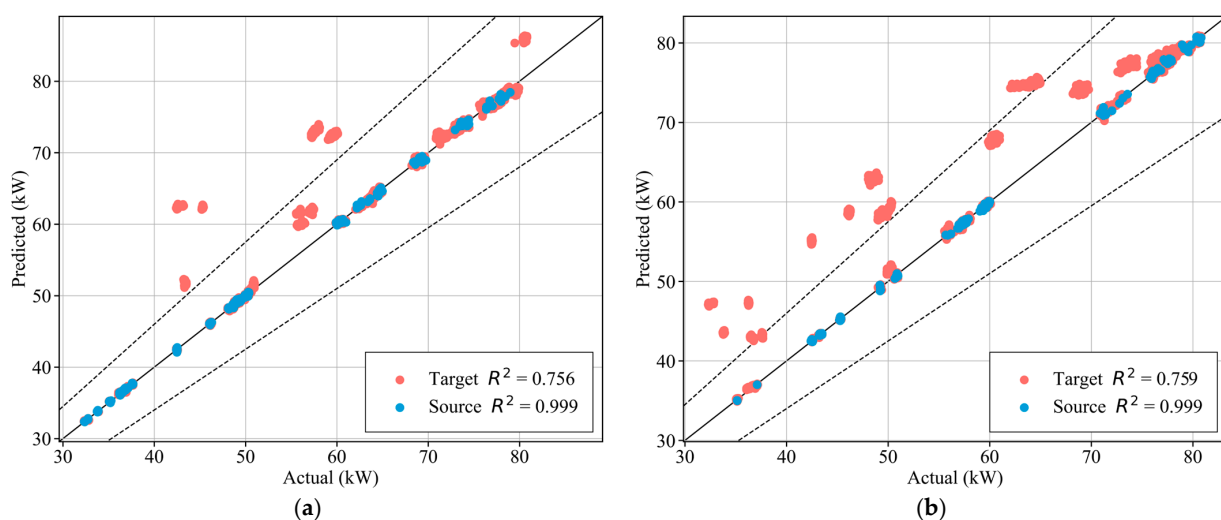


Figure 7. Cont.

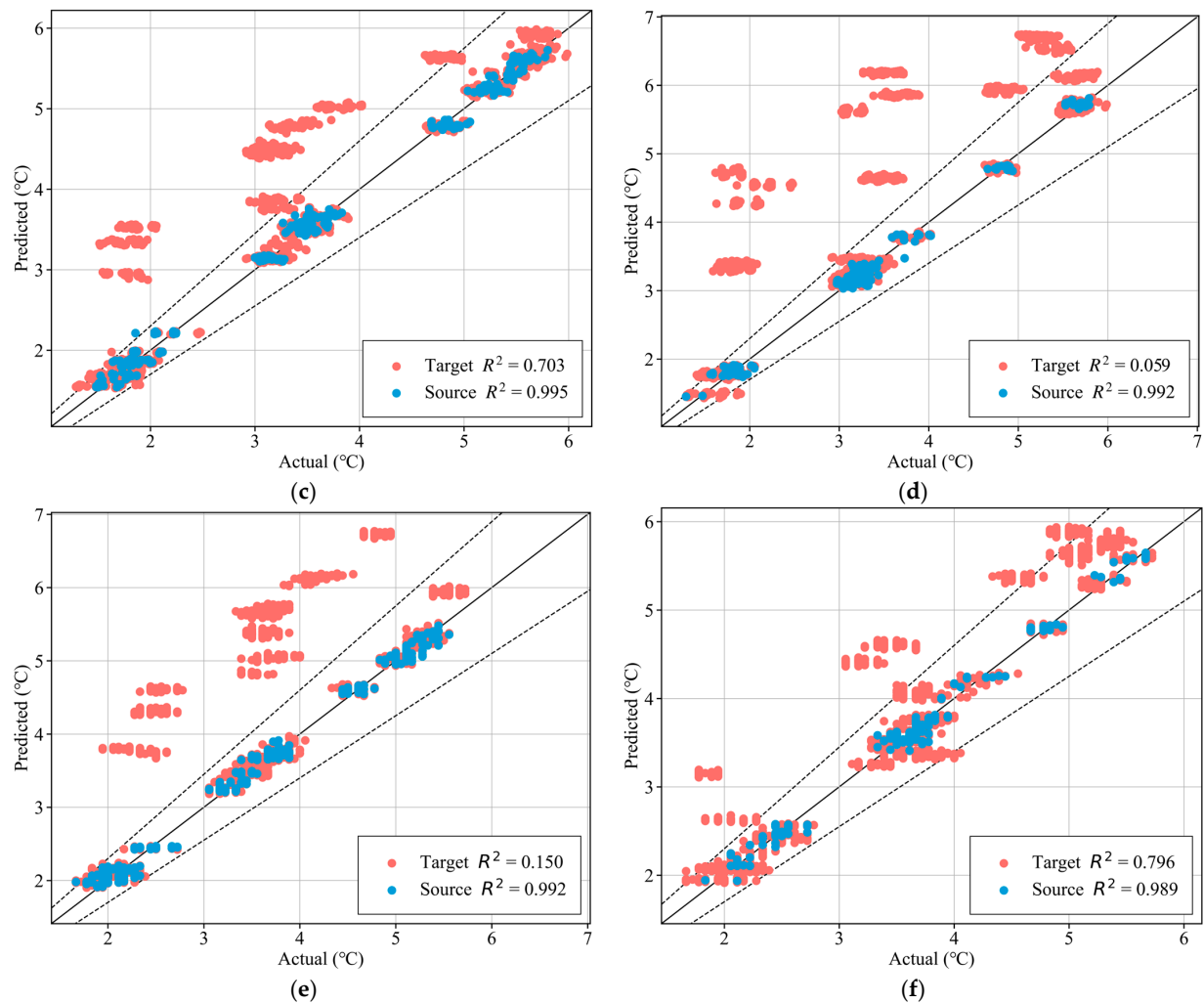


Figure 7. Prediction results of MLP in scenario B and C: (a) Power consumption in scenario B; (b) Power consumption in scenario C; (c) LMTD in scenario B; (d) LMTD in scenario C; (e) T_{sub} in scenario B; (f) T_{sub} in scenario C.

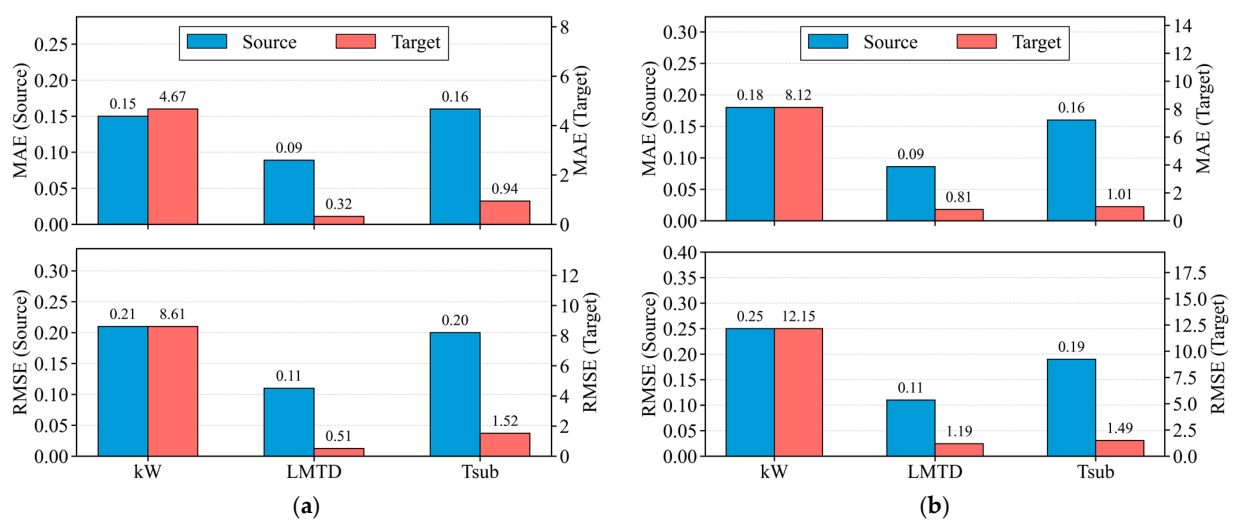


Figure 8. Evaluation metrics of baseline model: (a) Scenario B; (b) Scenario C.

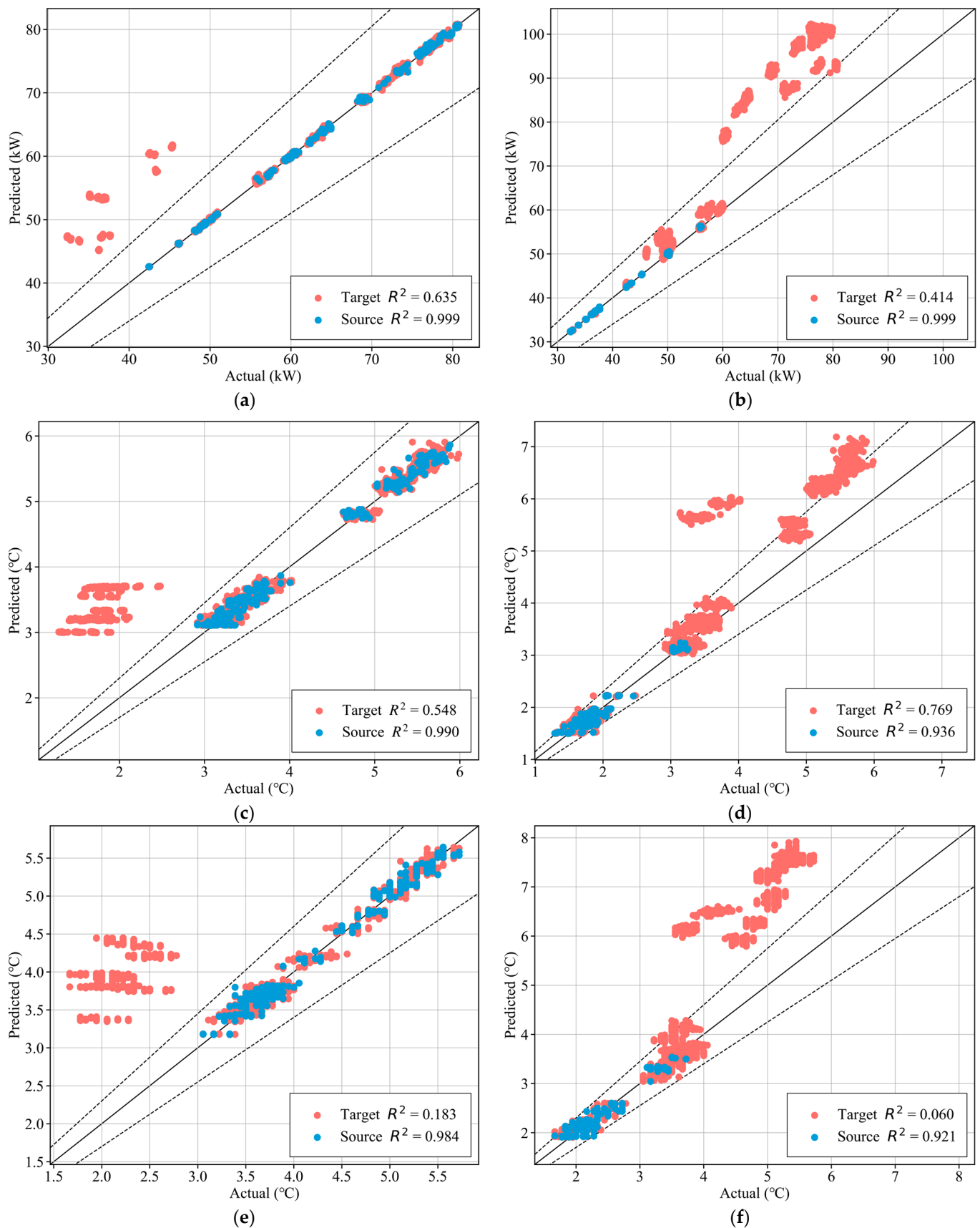


Figure 9. Prediction results of MLP in scenario D and E: (a) Power consumption in scenario D; (b) Power consumption in scenario E; (c) LMTD in scenario D; (d) LMTD in scenario E; (e) T_{sub} in scenario D; (f) T_{sub} in scenario E.

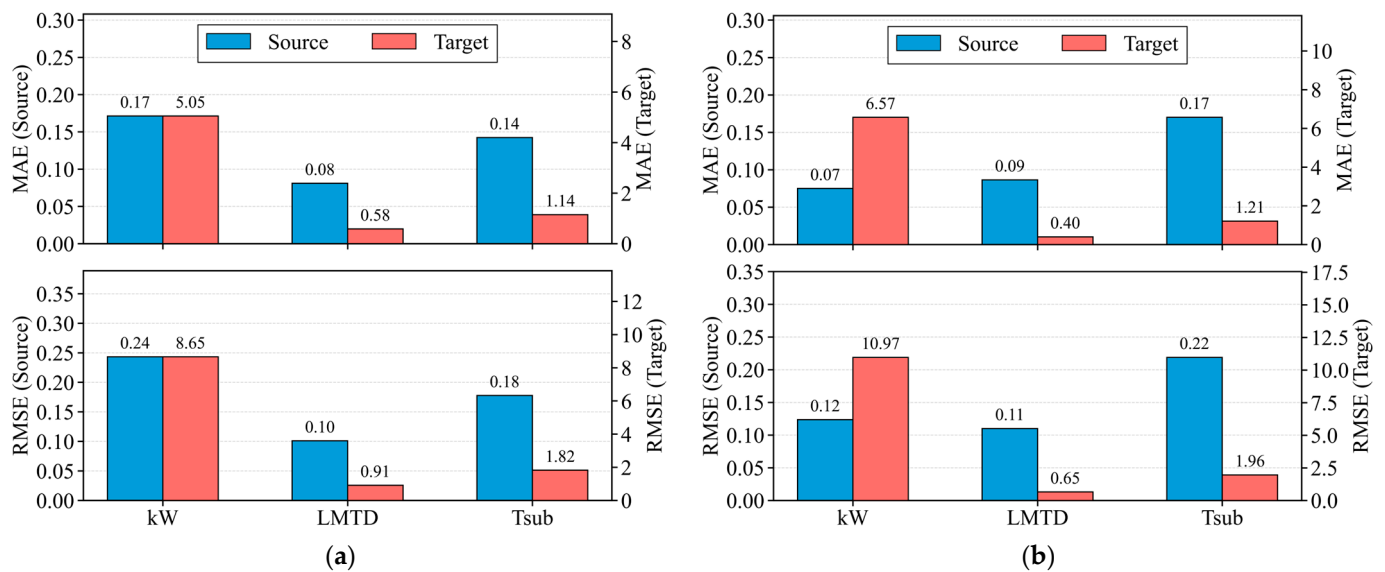


Figure 10. Evaluation metrics of baseline model: (a) Scenario D; (b) Scenario E.

4.2. Prediction Results of CNN-GRAM Model

Following the same data partitioning approach, the domain adaptation model (CNN-GRAM) method was employed to make predictions on the validation set of the source domain data and the target domain data, respectively. The results in scenario A are shown in Figure 11.

The proposed model demonstrates robust generalization capabilities on unseen data, with prediction deviations largely confined within a 15% threshold. Figure 11d presents the performance metrics of CNN-GRAM model in scenario A. The result indicates that, although the predictive performance of the domain adaptation model on the source domain dataset shows a slight decrease compared to the baseline model, it remains within an acceptable range. In addition, the model significantly improves predictive performance on the target domain data. Two metrics on both validation set and target set become closer. It indicates that the proposed model demonstrates greater robustness in cross-condition tasks. This performance is also evident in scenarios B and C, as illustrated in Figures 12 and 13. The results show that the proposed method can effectively address distribution shifts caused by changes in the condenser inlet water temperature. Although a few data points exhibit deviations, the overall performance remains satisfactory. The model achieves an average coefficient of determination (R^2) above 0.95 in the target domain.

However, the domain adaptation method is still insufficient for Scenarios D and E. As shown in Figure 14, power, LMTD, and subcooling all demonstrate a positive correlation with the load ratio. The value ranges in the target domain differ significantly from those in the source domain, leading to a shift in target domain predictions. For example, in Figure 14a, the source-domain range is approximately 43–80 kW, whereas the target domain additionally covers 30–40 kW. The model maintains good performance within the overlapping range, but shows a marked shift in the newly added interval. This result indicates that domain adaptation can correct biases caused by distribution shifts, but it cannot fully extrapolate beyond the range covered by the source domain data.

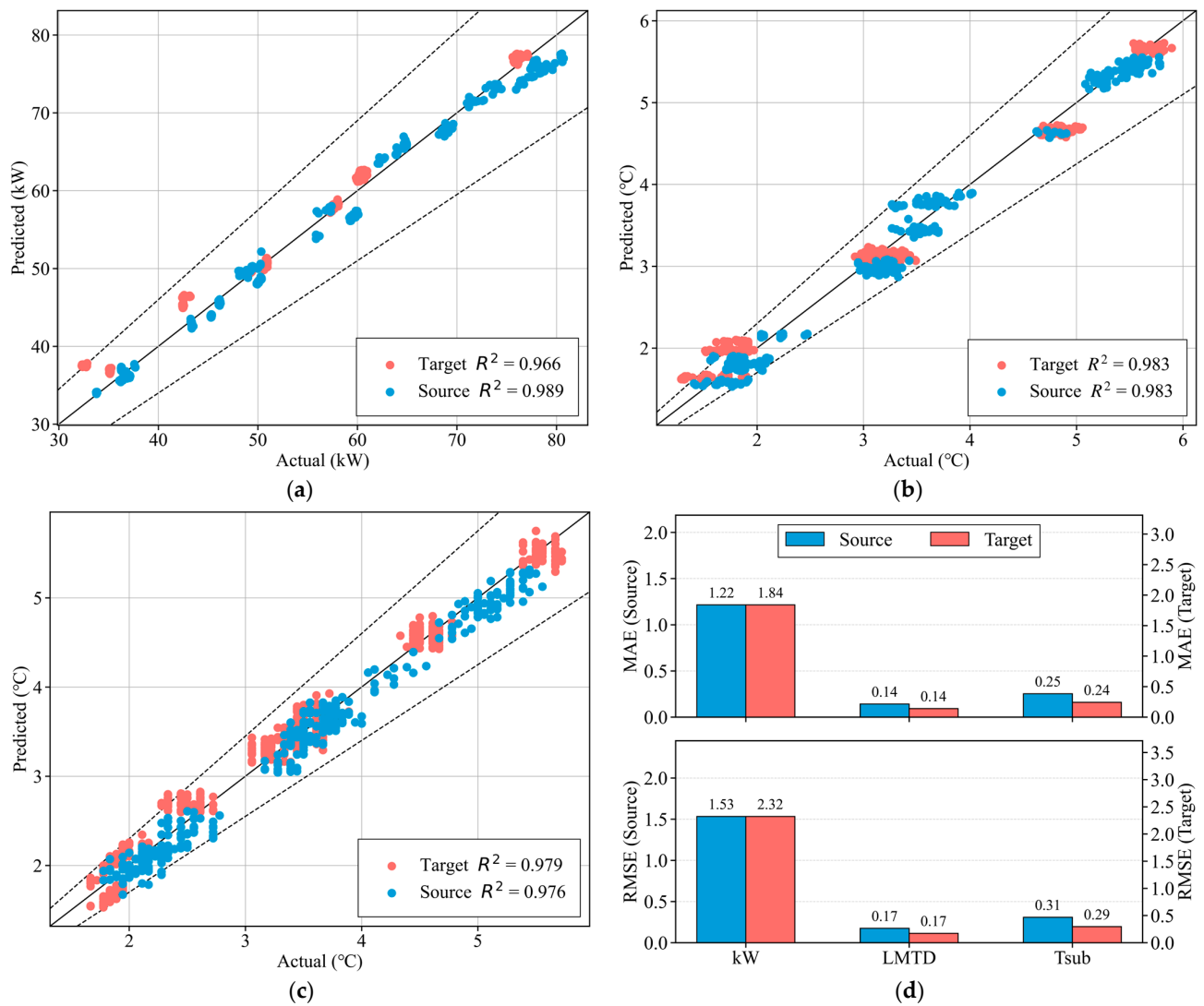


Figure 11. Prediction results of CNN-GRAM in scenario A: (a) Power consumption; (b) LMTD; (c) Tsub; (d) Evaluation metrics.

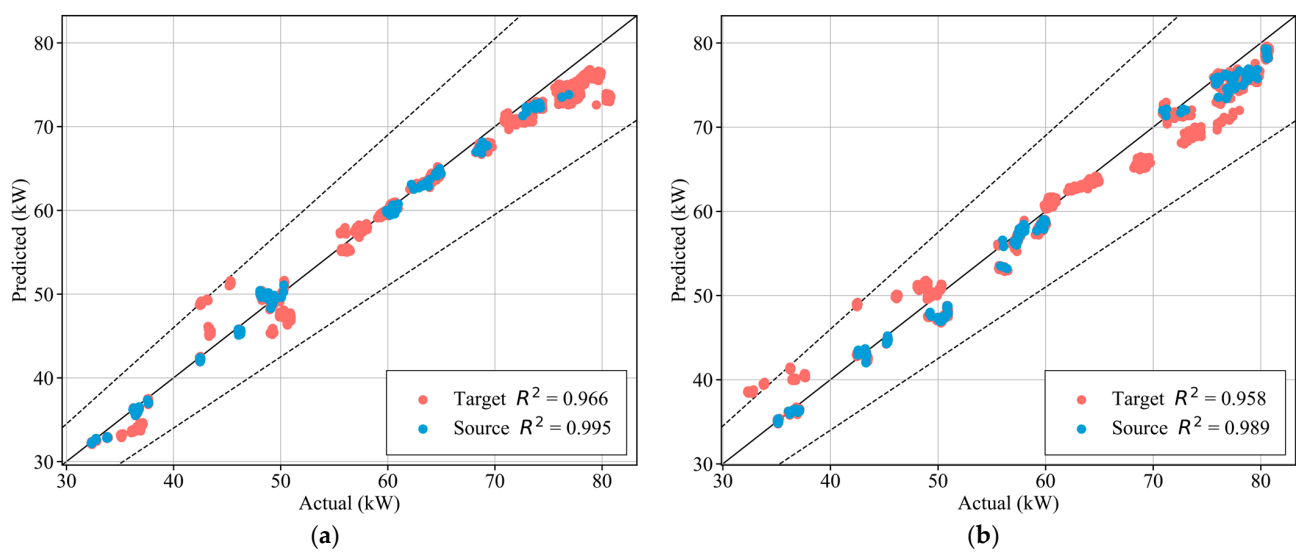


Figure 12. Cont.

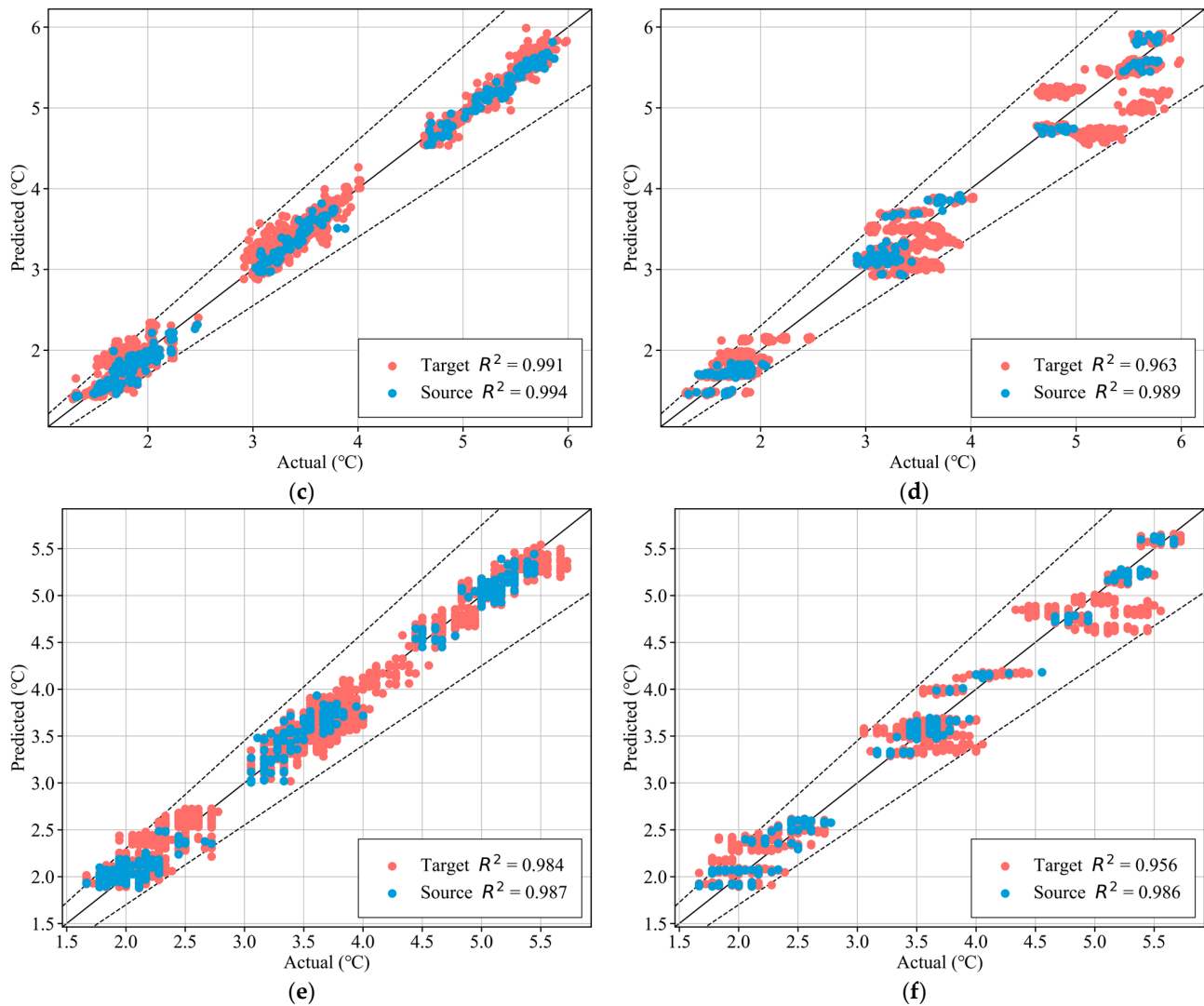


Figure 12. Prediction results of CNN-GRAM in scenario B and C: (a) Power consumption in scenario B; (b) Power consumption in scenario C; (c) LMTD in scenario B; (d) LMTD in scenario C; (e) T_{sub} in scenario B; (f) T_{sub} in scenario C.

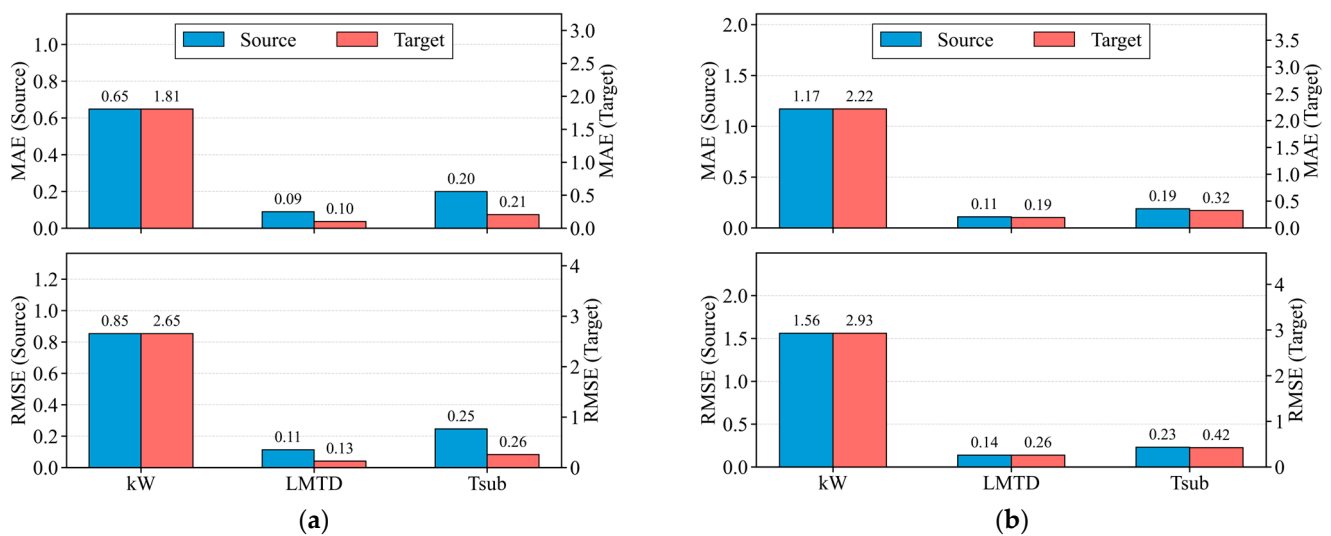


Figure 13. Evaluation metrics of CNN-GRAM model: (a) Scenario B; (b) Scenario C.

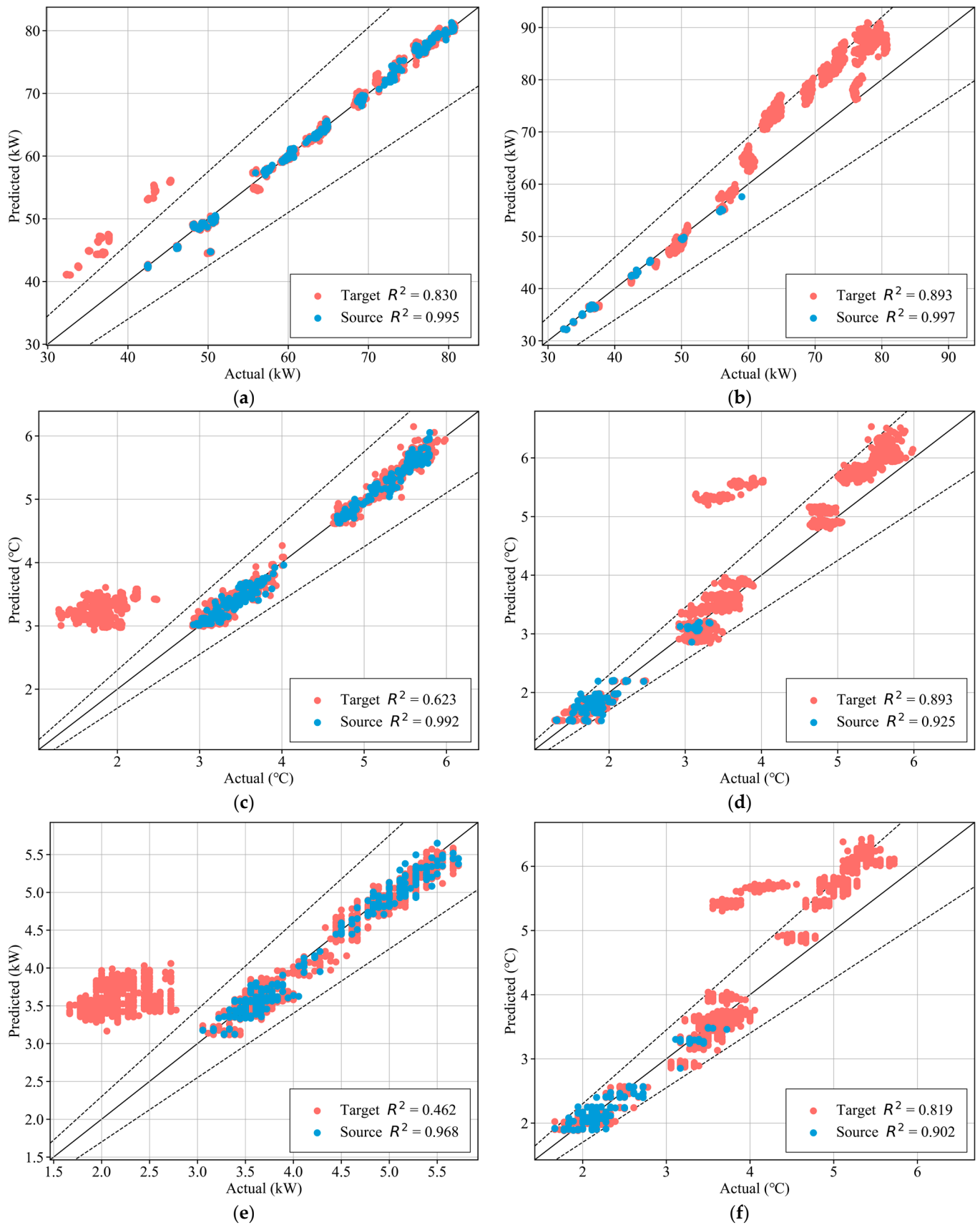


Figure 14. Prediction results of CNN-GRAM in scenario D and E: (a) Power consumption in scenario B; (b) Power consumption in scenario C; (c) LMTD in scenario B; (d) LMTD in scenario C; (e) T_{sub} in scenario B; (f) T_{sub} in scenario C.

Figure 15 presents the evaluation metrics of the proposed model in Scenarios D and E. Compared with the baseline model in Figure 10, the results show that although the CNN-GRAM model cannot achieve accurate extrapolation, it still provides higher accuracy than the baseline model. This advantage is more evident in Scenario E. When the training data come from a low-load range, the model can still roughly estimate the performance parameters in the target domain.

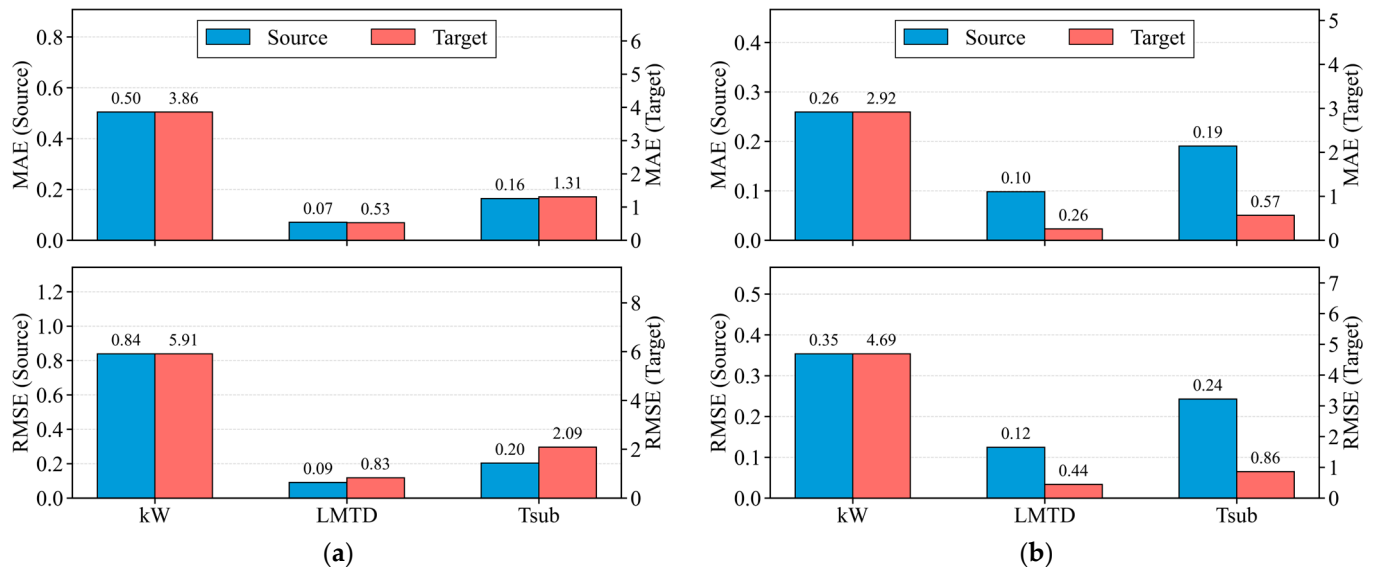


Figure 15. Evaluation metrics of CNN-GRAM model: (a) Scenario D; (b) Scenario E.

Table 2 presents a comparative evaluation of the Baseline model (MLP) and the proposed domain adaptation model (CNN-GRAM) across five cross-condition scenarios (A–E). The results demonstrate that the proposed model possesses superior generalization capabilities, particularly in Scenarios A–C. Across these three scenarios, the CNN-GRAM model achieves an average reduction of approximately 74.3% in MAE and 76.1% in RMSE, with R^2 values consistently exceeding 0.95. Although the model encounters certain extrapolation challenges in scenarios D and E, it maintains a significant performance advantage over the baseline model.

Table 2. Comparative of evaluation metrics between baseline and domain-adaptation models in target domain.

Parameters	Scenario	Model	MAE	RMSE	R^2
Power	A	Baseline	10.20	10.30	−0.63
		CNN-GRAM	1.84	2.32	0.97
	B	Baseline	4.67	8.61	0.76
		CNN-GRAM	1.81	2.65	0.97
	C	Baseline	8.12	12.15	0.76
		CNN-GRAM	2.22	2.93	0.96
	D	Baseline	5.05	8.65	0.64
		CNN-GRAM	3.86	5.91	0.83
	E	Baseline	6.57	10.97	0.41
		CNN-GRAM	2.92	4.69	0.89

Table 2. *Cont.*

Parameters	Scenario	Model	MAE	RMSE	R ²
LMTD	A	Baseline	0.75	0.77	0.27
		CNN-GRAM	0.14	0.17	0.98
	B	Baseline	0.32	0.51	0.70
		CNN-GRAM	0.10	0.13	0.99
	C	Baseline	0.81	1.19	0.06
		CNN-GRAM	0.19	0.26	0.96
	D	Baseline	0.58	0.91	0.55
		CNN-GRAM	0.53	0.83	0.62
	E	Baseline	0.40	0.67	0.77
		CNN-GRAM	0.26	0.44	0.89
T _{sub}	A	Baseline	1.22	1.28	0.47
		CNN-GRAM	0.24	0.29	0.98
	B	Baseline	0.94	1.52	0.15
		CNN-GRAM	0.21	0.26	0.98
	C	Baseline	1.01	1.49	0.80
		CNN-GRAM	0.32	0.42	0.96
	D	Baseline	1.14	1.82	0.18
		CNN-GRAM	1.31	2.09	0.46
	E	Baseline	1.21	1.96	0.06
		CNN-GRAM	0.57	0.86	0.82

4.3. Correlation Between Prediction Deviation and Data Distribution

To investigate the data distribution characteristics of the source and target domains, the t-Distributed Stochastic Neighbor Embedding (t-SNE) method was employed to map the data into a two-dimensional space, visualizing the high-dimensional data distribution (perplexity = 50, random seed = 42). Robustness was examined by varying the perplexity and the random seed. The main conclusion is stable and not influenced by specific choices of perplexity or random initialization. Figure 16 illustrates the data distribution before and after domain adaptation. As depicted in the figure, the source and target domain data are distinctly separated in the original data, indicating a significant difference in their distributions. This separation explains why traditional models experience performance degradation outside the training set; data-driven models fail to learn the correct mapping relationships under new data distributions. By applying a domain adaptation method to align the source and target domain data and calibrating model parameters based on their discrepancies, new features are ultimately obtained. The results indicate that the data distributions of the source and target domains have become increasingly similar, showing greater overlap.

However, despite the successful alignment of feature distributions, the model exhibits performance degradation in Scenarios D and E, as evidenced in Table 2. This phenomenon highlights the critical distinction between “distribution alignment” and “numerical extrapolation”. In Scenarios D and E, the datasets are partitioned based on load rates, creating a scenario where the numerical range of the target labels significantly exceeds that of the source labels. Consequently, the model struggles to extrapolate.

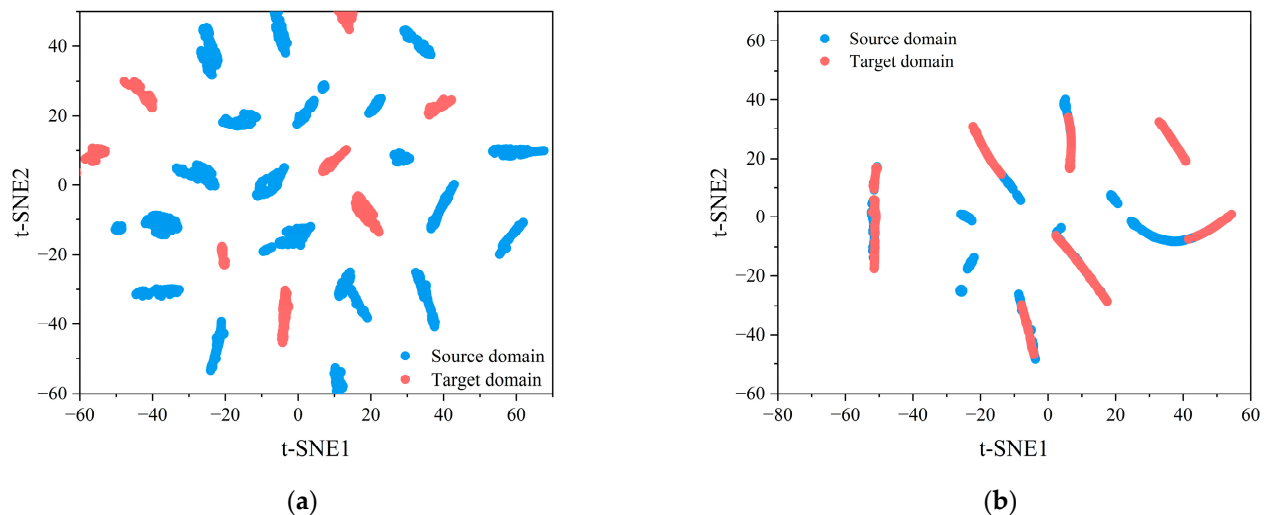


Figure 16. t-SNE data distribution in scenario A: (a) Original data; (b) Distribution of features via domain adaptation.

This finding reveals a fundamental boundary for unsupervised domain adaptation in regression tasks. While the method can effectively correct for shifts in input feature distribution, it cannot generate predictive knowledge for target values that lie completely outside the numerical support of the source domain. Therefore, ensuring that the training data covers a sufficiently broad span of operating loads is as critical as the domain adaptation algorithm itself for robust chiller performance prediction. Reliability may depend on distributional coverage, not just model complexity.

This highlights the importance of data quality in data-driven modeling, especially in a regression task. This research provides a basis for assessing model reliability to validate the applicability across the full operational range of chillers. Nevertheless, for typical energy retrofit projects, the proposed method remains applicable. For units with a well-balanced load-ratio distribution, improving chiller COP commonly relies on retrofit measures such as increasing the evaporator outlet water temperature and decreasing the condenser inlet water temperature. Consequently, the data distribution changes primarily in the input features.

4.4. Limitations and Future Work

The performance degradation observed in Scenarios D and E reflects a fundamental limitation of data-driven models, which has been extensively documented in the machine learning literature. Research indicates that feature alignment cannot guarantee correct predictions when target labels lie outside the source label space [41]. While the proposed CNN-GRAM method mitigates distribution shift via feature alignment, it cannot reliably extrapolate to operating regimes that are absent from the training data.

Future work should develop modeling frameworks with out-of-distribution extrapolation capability. Additionally, rigorous and quantifiable metrics are needed to evaluate whether historical data are adequate for training models intended for deployment under altered operating conditions.

5. Conclusions

This study proposed a robust cross-condition prediction framework for chiller performance parameters (Power, LMTD, and Subcooling) by integrating a 1-D CNN with a domain adaptation technique based on inverse Gram matrix alignment. The specific conclusions are as follows:

1. The proposed CNN-GRAM model effectively overcomes the limitations of traditional data-driven models, which typically suffer from performance degradation when operating conditions shift. By aligning the feature distributions, the model achieves high predictive accuracy on the target domain without requiring labeled data for the new operating conditions. This modeling approach is equally applicable to other tasks, such as forecasting cooling and heating loads in air-conditioning systems, as both are regression tasks that are constrained by limited and low-quality historical data.
2. Validated on the ASHRAE RP-1043 experimental dataset, the proposed model outperformed baseline methods (MLP). Specifically, in cross-condition prediction tasks (Scenario A–C), the CNN-GRAM model reduced the MAE by an average of 74.3% and the RMSE by 76.1%, while maintaining R^2 exceeding 0.95.
3. A framework that integrates a steady-state filter with outlier-detection algorithms (Local Outlier Factor and Isolation Forest) is proposed to leverage the distributional characteristics of the raw data. Results show that the framework retains more valid operational data than traditional slope-thresholding. It indicates that data processing should account for the underlying data distribution.
4. This study identifies a critical boundary condition for domain adaptation under given input features. While CNN-GRAM model is robust to shifts in the input feature distribution, its prediction accuracy degrades if the numerical range of the prediction target in the target domain falls completely outside the range observed in the source domain (Scenarios D and E). This highlights the necessity of analyzing the distribution of both input features and prediction targets to ensure model reliability in engineering applications. In retrofit projects, distributional shifts occur primarily in the input features. The proposed model is well-suited to such cases.

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Abbreviations

The following abbreviations are used in this manuscript:

MAE	Mean absolute error
RMSE	Root mean square error
R^2	The coefficient of determination
MLP	Multilayer perception
CNN	Convolutional neural network
UDA	Unsupervised domain adaptation
LMTD	Logarithmic mean temperature difference in condenser
T_{sub}	Subcooling

References

- Thangavelu, S.; Myat, A.; Khambadkone, A. Energy optimization methodology of multi-chiller plant in commercial buildings. *Energy* **2017**, *123*, 64–76. [\[CrossRef\]](#)
- Zhao, Y.; Wang, S.; Xiao, F. A statistical fault detection and diagnosis method for centrifugal chillers based on exponentially-weighted moving average control charts and support vector regression. *Appl. Therm. Eng.* **2013**, *51*, 560–572. [\[CrossRef\]](#)
- Zhao, Y.; Li, T.; Zhang, X.; Zhang, C. Artificial intelligence-based fault detection and diagnosis methods for building energy systems: Advantages, challenges and the future. *Renew. Sustain. Energy Rev.* **2019**, *109*, 85–101. [\[CrossRef\]](#)
- Yao, Y.; Shekhar, D. State of the art review on model predictive control (MPC) in Heating Ventilation and Air-conditioning (HVAC) field. *Build. Environ.* **2021**, *200*, 107952. [\[CrossRef\]](#)
- Gordon, J.; Ng, K.; Chua, H.; Lim, C. How varying condenser coolant flow rate affects chiller performance: Thermodynamic modeling and experimental confirmation. *Appl. Therm. Eng.* **2000**, *20*, 1149–1159. [\[CrossRef\]](#)
- Wei, Y.; Zhang, X.; Shi, Y.; Xia, L.; Pan, S.; Wu, J.; Han, M.; Zhao, X. A review of data-driven approaches for prediction and classification of building energy consumption. *Renew. Sustain. Energy Rev.* **2018**, *82*, 1027–1047. [\[CrossRef\]](#)
- Reddy, T.A.; Niebur, D.; Andersen, K.K.; Pericolo, P.P.; Cabrera, G. Evaluation of the Suitability of Different Chiller Performance Models for On-Line Training Applied to Automated Fault Detection and Diagnosis (RP-1139). *HVACR Res.* **2011**, *9*, 385–414. [\[CrossRef\]](#)
- Yang, Y.; Xu, L.; Han, H.; Ren, Z.; Wu, K.; Liu, F. Soft measurement and prediction of refrigerant leakage based on SVR-LSTM. *Int. J. Refrig.* **2023**, *152*, 303–314. [\[CrossRef\]](#)
- Tang, C.; Li, N.; Bao, L. Predictive Control Modeling of Regional Cooling Systems Incorporating Ice Storage Technology. *Buildings* **2024**, *14*, 2488. [\[CrossRef\]](#)
- Zhu, X.; Zhang, S.; Jin, X.; Du, Z. Deep learning based reference model for operational risk evaluation of screw chillers for energy efficiency. *Energy* **2020**, *213*, 118833. [\[CrossRef\]](#)
- Fan, C.; Chen, H. Research on eXplainable artificial intelligence in the CNN-LSTM hybrid model for energy forecasting. *J. Build. Eng.* **2025**, *111*, 113150. [\[CrossRef\]](#)
- Zhang, X.; Li, X. Chiller load prediction based on CEEMDAN-BiLSTM-Attention model for sufficient data and small sample data cases. In Proceedings of the IEEE 12th Data Driven Control and Learning Systems Conference (DDCLS), Xiangtan, China, 12–14 May 2023; pp. 1634–1639.
- Wang, J.; Du, Y.; Wang, J. LSTM based long-term energy consumption prediction with periodicity. *Energy* **2020**, *197*, 117197. [\[CrossRef\]](#)
- Yu, C.; Chen, J.; Chen, Y. Enhanced LSTM framework for water-cooled chiller COP forecasting. In Proceedings of the IEEE International Conference on Consumer Electronics (ICCE), Las Vegas, NV, USA, 10–12 January 2021; IEEE: Piscataway, NJ, USA, 2021.
- Wang, Y.; Cheng, H.; Chen, H.; Ye, M.; Ren, Y.; Yang, C. A hybrid model based on wavelet decomposition and LSTM for short-term energy consumption prediction of chillers. *J. Build. Eng.* **2025**, *99*, 111539. [\[CrossRef\]](#)
- Chakraborty, D.; Elzarka, H. Early detection of faults in HVAC systems using an XGBoost model with a dynamic threshold. *Energy Build.* **2019**, *185*, 326–344. [\[CrossRef\]](#)
- Yao, W.; Li, D.; Gao, L. Fault detection and diagnosis using tree-based ensemble learning methods and multivariate control charts for centrifugal chillers. *J. Build. Eng.* **2022**, *51*, 104243. [\[CrossRef\]](#)
- Rizi, B.; Faramarzi, A.; Pertzborn, A.; Heidarinejad, M. Forecasting operation of a chiller plant facility using data-driven models. *Int. J. Refrig.* **2024**, *167*, 70–89. [\[CrossRef\]](#)
- Liang, X.; Zhu, X.; Chen, S.; Jin, X.; Xiao, F.; Du, Z. Physics-constrained cooperative learning-based reference models for smart management of chillers considering extrapolation scenarios. *Appl. Energy* **2023**, *349*, 121642. [\[CrossRef\]](#)
- Guo, F.; Li, A.; Yue, B.; Xiao, Z.; Xiao, F.; Yan, R.; Li, A.; Lv, Y.; Su, B. Improving the out-of-sample generalization ability of data-driven chiller performance models using physics-guided neural network. *Appl. Energy* **2024**, *354*, 122190. [\[CrossRef\]](#)
- Pan, S.J.; Yang, Q. A Survey on Transfer Learning. *IEEE Trans. Knowl. Data Eng.* **2010**, *22*, 1345–1359. [\[CrossRef\]](#)
- Chaudhary, G.; Johra, H.; Georges, L.; Austbo, B. Transfer learning in building dynamics prediction. *Energy Build.* **2025**, *330*, 115384. [\[CrossRef\]](#)
- Gao, N.; Shao, W.; Rahaman, M.; Zhai, J.; David, K.; Salim, F. Transfer learning for thermal comfort prediction in multiple cities. *Build. Environ.* **2021**, *195*, 107725. [\[CrossRef\]](#)
- Somu, N.; Sriram, A.; Kowli, A.; Ramamritham, K. A hybrid deep transfer learning strategy for thermal comfort prediction in buildings. *Build. Environ.* **2021**, *204*, 108133. [\[CrossRef\]](#)
- Yadav, N.; Sorek-Hamer, M.; Von Pohle, M.; Asanjan, A.; Sahasrabhojane, A.; Suel, E.; Arku, R.; Lingenfelter, V.; Brauer, M.; Ezzati, M.; et al. Using deep transfer learning and satellite imagery to estimate urban air quality in data-poor regions. *Environ. Pollut.* **2024**, *342*, 122914. [\[CrossRef\]](#)
- Middya, A.; Roy, S. Pollutant specific optimal deep learning and statistical model building for air quality forecasting. *Environ. Pollut.* **2022**, *301*, 118972. [\[CrossRef\]](#)

27. Dou, H.; Zmeureanu, R. Transfer Learning Prediction Performance of Chillers for Neural Network Models. *Energies* **2023**, *16*, 7149. [[CrossRef](#)]
28. Fan, C.; Sun, Y.; Xiao, F.; Ma, J.; Lee, D.; Wang, J.; Tseng, Y.C. Statistical investigations of transfer learning-based methodology for short-term building energy predictions. *Appl. Energy* **2020**, *262*, 114499. [[CrossRef](#)]
29. Dou, H.; Zhang, K. Transfer learning for cross-building forecasting of building energy and indoor air temperature in model predictive control applications. *J. Build. Eng.* **2025**, *111*, 113341. [[CrossRef](#)]
30. Du, Z.; Liang, X.; Chen, S.; Li, P.; Zhu, X.; Chen, K.; Jin, X. Domain adaptation deep learning and its T-S diagnosis networks for the cross-control and cross-condition scenarios in data center HVAC systems. *Energy* **2023**, *280*, 128084. [[CrossRef](#)]
31. Chen, Z.; Rezgui, Y.; Zhang, R.; Zhang, X.; Zhao, W.; Li, Y. Feature-level interpretability in transfer learning-based chiller fault diagnosis. *Build. Environ.* **2025**, *285*, 113527. [[CrossRef](#)]
32. Fang, X.; Gong, G.; Li, G.; Chun, L.; Li, W.; Peng, P. A hybrid deep transfer learning strategy for short term cross-building energy prediction. *Energy* **2021**, *215*, 119208. [[CrossRef](#)]
33. Tran, D.; Chen, Y.; Chau, M.; Ning, B. A robust online fault detection and diagnosis strategy of centrifugal chiller systems for building energy efficiency. *Energy Build.* **2015**, *108*, 441–453. [[CrossRef](#)]
34. Song, Z.; Zou, S.; Zhou, W.; Huang, Y.; Shao, L.; Yuan, J.; Gou, X.; Jin, W.; Wang, Z.; Chen, X.; et al. Clinically applicable histopathological diagnosis system for gastric cancer detection using deep learning. *Nat. Commun.* **2020**, *11*, 4294. [[CrossRef](#)]
35. Kabir, H.; Wu, J.; Dahal, S.; Joo, T.; Garg, N. Automated estimation of cementitious sorptivity via computer vision. *Nat. Commun.* **2024**, *15*, 9935. [[CrossRef](#)]
36. Nejjar, I.; Wang, Q.; Fink, O. DARE-GRAM: Unsupervised Domain Adaptation Regression by Aligning Inverse Gram Matrices. In Proceedings of the 2023 IEEE/CVF Conference on Computer Vision and Pattern Recognition (CVPR), Vancouver, BC, Canada, 18–22 June 2023; pp. 11744–11754.
37. Penrose, R. A generalized inverse for matrices. *Math. Proc. Camb. Philos. Soc.* **2008**, *51*, 406–413. [[CrossRef](#)]
38. Chen, X.; Wang, S.; Wang, J.; Long, M. Representation Subspace Distance for Domain Adaptation Regression. In Proceedings of the International Conference on Machine Learning (ICML), Online, 18–24 July 2021.
39. Nisa, E.; Kuan, Y. Comparative Assessment to Predict and Forecast Water-Cooled Chiller Power Consumption Using Machine Learning and Deep Learning Algorithms. *Sustainability* **2021**, *13*, 744. [[CrossRef](#)]
40. Liu, J.; Shi, D.; Li, G.; Xie, Y.; Li, K.; Liu, B.; Ru, Z. Data-driven and association rule mining-based fault diagnosis and action mechanism analysis for building chillers. *Energy Build.* **2020**, *216*, 109957. [[CrossRef](#)]
41. Gong, B.; Grauman, K.; Sha, F. Learning Kernels for Unsupervised Domain Adaptation with Applications to Visual Object Recognition. *Int. J. Comput. Vis.* **2014**, *109*, 3–27. [[CrossRef](#)]

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