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SHORT- TERM ENERGY CONSUMPTION PREDICTION OF HEATING, VENTILATION, AND AIR CONDITIONING (HVAC) SYSTEMS USING MACHINE LEARNING

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Abstract

The demand for energy-efficient buildings emphasizes the need for accurate HVAC energy consumption predictions, particularly in unoccupied spaces prone to energy waste. This thesis addresses the problem by asking: How effectively can machine learning models predict HVAC energy consumption under diverse weather conditions? Existing research often includes occupancy behavior, which introduces variability, whereas this study isolates weather-driven factors to optimize energy use.

Using real-world cooling and heating datasets from unoccupied multizone office buildings, this research evaluates advanced supervised machine learning models, including Random Forest, XGBoost, and a Stacking Regressor. These models are tailored to predict short-term HVAC energy consumption and tested against combined and separate datasets. Results show that scenario-specific models outperform combined datasets, with XGBoost achieving the lowest Mean Absolute Error (MAE) for cooling (2.2033) and heating (2.8683). Feature importance analysis identifies indoor temperature and humidity as critical predictors.

This study provides a weather-specific framework for optimizing HVAC systems, offering energy savings of 15–28% and supporting global sustainability efforts. Future research could expand datasets and explore hybrid models to address mixed-use or residential buildings.

CONTENTS

1 Ethics / Data / Technology Statement 4
2 Introduction / Problem Statement / Research Goals 4
2.1 Research Questions 5
2.2 Motivation 5
3 Related Work 6
3.1 Modeling Approaches in Building Energy Prediction 6
3.2 Key Feature Selection in Building Energy Models 8
3.3 Feature Engineering and Preparation in Building Energy Models 8
3.4 Research Gap 9
4 Method 9
4.1 Dataset Description 11
4.2 Data Cleaning and Preprocessing 11
4.3 Exploratory Data Analysis (EDA) 12
4.3.1 Descriptive Statistics of Energy Consumption 12
4.3.2 Relationship between Energy Consumption and Indoor Temperature/ Humidity 12
4.3.3 Distribution of Energy Consumption 14
4.3.4 Indoor and Outdoor Temperature/ Humidity Relationship 14
4.3.5 Correlation Matrix 16
4.4 Feature Engineering and Preparation 18
4.4.1 Generated lagged Features 18
4.4.2 Calculate Rolling Averages 19
4.4.3 Apply Differencing 19
4.4.4 Generate Interaction Terms 19
4.5 Data Split and Feature Selection 20
4.6 Algorithm 20
4.6.1 Linear Regression 20
4.6.2 Random Forest 21
4.6.3 XGBoost 21
4.6.4 Stacking Ensemble Regression 21
4.7 Hyperparameter Tuning 22
4.7.1 Hyperparameter Tuning for Random Forest 22
4.7.2 Hyperparameter Tuning for XGBoost 23
4.7.3 Hyperparameter Tuning for Stacking Ensemble Regression 23
4.8 Evaluation Methods 24
4.8.1 MAE :Mean Absolute Error 24
4.8.2 R^2: Coefficient of Determination 24

4.8.3 Standard Deviation (STD) 25
4.9 Experiment Set 25
4.9.1 Experiment 1: Combined Dataset 25
4.9.2 Experiments 2 and 3: Separate Cooling and Heating Datasets 26
4.9.3 Ensuring Robustness in Analysis 26
5 Result 27
5.1 Performance Metrics (MAE, R^2) 27
5.1.1 Experiment 1: Combined Dataset 28
5.1.2 Experiments 2 and 3: Cooling and Heating Datasets 29
5.1.3 Comparative Insights Across Datasets 30
5.2 Feature Importance Analysis 32
5.2.1 Experiment 1: Combined Dataset 32
5.2.2 Experiments 2 and 3: Cooling and Heating Datasets 33
5.2.3 Comparative Insights Across Datasets 34
5.3 Residual Analysis Across Experiments 34
5.3.1 Residual Distributions. 35
5.3.2 Residuals vs Weather Variables 36
6 Discussion 40
6.1 Sub-question Analysis 40
6.2 Main Research Question 42
6.3 Societal Impact 42
6.4 Limitations 43
6.5 Future Work 44
7 Conclusion 44

1 ETHICS / DATA / TECHNOLOGY STATEMENT

Data Source: The dataset used in this thesis was acquired from Im et al., 2022, available on figshare through an online request. This data is open source and did not require anonymization, as it does not involve data from human participants or animals. The original data owner retains ownership of the data used in this thesis during and after the research. The institution was informed about the use of this data for the thesis and potential publications.

Figures: All figures in this thesis were created by the author.

Code: OpenAI, 2024 was used as a debugging tool to resolve coding issues encountered during the thesis project. All libraries and frameworks used in the thesis, with their version numbers, are documented. The code supporting this thesis can be accessed on GitHub[1].

Technology: ChatGPT supported academic writing by assisting with paraphrasing, spell checking, and grammar. No tools were used for typesetting beyond the provided LaTeX template. Reference management software outside the template was not used.

2 INTRODUCTION / PROBLEM STATEMENT / RESEARCH GOALS

Buildings are major contributors to global energy consumption, accounting for 20%-40% of total energy use in developed countries (Amasyali and El-Gohary, 2008). Heating, Ventilation, and Air Conditioning (HVAC) systems represent the largest energy-consuming component, responsible for up to 40% of building energy use (Dambrosio, 2024) and a significant share of major fuel consumption on-site. Improving HVAC energy efficiency is critical for achieving energy savings and supporting sustainability goals, particularly in structures like warehouses and storage facilities, which account for substantial commercial floor space.

Optimizing HVAC operations through short-term energy consumption prediction has shown promise in reducing unnecessary system actions, minimizing energy waste, and enhancing system efficiency (H. Wang et al., 2024). For instance, accurate predictions allow systems to lower cooling loads before sudden drops in outdoor temperature or adjust heating schedules during warm spells (T. Liu et al., 2019).

While HVAC energy use is influenced by factors such as weather, building materials, and occupancy patterns, weather conditions often play the most significant role (Hoang, 2016). However, existing research seldom isolates weather's impact, focusing instead on residential or densely

[1] this link.

occupied spaces, where occupant behavior introduces variability (Im et al., 2022).

This study addresses this gap by leveraging machine learning to predict short-term HVAC energy consumption based solely on weather conditions. It provides a framework for evaluating weather-driven energy use, offering insights into optimizing HVAC systems in buildings with low occupancy or constant indoor environmental requirements, such as pharmaceutical warehouses or storage facilities.

2.1 *Research Questions*

- Main Research Question:

  How effectively can machine learning models predict and optimize energy consumption in HVAC systems for unoccupied multizone office buildings under diverse weather conditions?

- Sub-Questions:

  1. How does the predictive accuracy of machine learning models differ between combined and separate datasets for cooling and heating, and what are the implications for energy optimization in HVAC systems?
  2. Which weather variables are most critical for machine learning models to predict HVAC energy consumption, and how much can their contributions inform sustainable building energy management?
  3. How can machine learning models address the challenges of predicting energy consumption in HVAC systems across diverse temperature and humidity conditions?

2.2 *Motivation*

This research is significant from both practical and theoretical perspectives, addressing key challenges in optimizing energy use, reducing costs, and advancing energy management knowledge.

From a practical perspective, the study focuses on improving energy efficiency in unoccupied buildings, such as warehouses and storage facilities. These buildings often run HVAC systems continuously, wasting energy. By identifying optimization strategies, the research helps businesses reduce costs and supports sustainability goals by lowering carbon emissions. It also establishes a baseline for energy use based solely on building systems and environmental factors, simplifying inefficiency identification and performance optimization.

From a theoretical perspective, this research fills a gap in studies that primarily focus on occupied buildings. It examines the relationship between weather conditions and energy consumption in unoccupied spaces, particularly in HVAC systems. Additionally, it contributes to AI-driven building energy management by developing models that predict energy use based on weather data. This advancement supports smart technology adoption and enhances energy efficiency to meet future demands ("Zero Carbon Buildings for All Initiative Launched at UN Climate Action Summit", 2022).

3 RELATED WORK

Research on HVAC energy consumption prediction spans various building types, modeling techniques, and datasets. This section evaluates prior studies, highlighting their relevance to this study's dataset and identifying gaps in the literature.

3.1 *Modeling Approaches in Building Energy Prediction*

Research on energy consumption prediction focuses on three methods: Statistical Models, Machine Learning Models, and Time-series models, reflecting a shift from conventional to advanced techniques.

Statistical models, such as Multiple Linear Regression (MLR) and the Degree-Day Method, are common baselines due to their simplicity and ability to capture general energy trends. MLR models the linear relationship between a dependent variable and multiple independent variables, effectively identifying broad energy consumption patterns. The Degree-Day Method estimates energy needs by summing daily temperature deviations from a baseline, making it suitable for long-term energy trend analysis. Runge and Saloux, 2023 and Sha et al., 2019 highlight MLR's effectiveness in modeling seasonal patterns, providing a reliable baseline for advanced techniques. Similarly, the Degree-Day Method, as noted by Sha et al., 2019, effectively analyzes temperature fluctuations over extended periods.

However, while these methods are simple and easy to interpret, they fail to capture the nonlinear relationships critical for HVAC energy prediction in this study. As such, they are not suitable as the primary modeling approach. Instead, these methods are better suited as baseline models to assist in evaluating the performance of more advanced machine learning models.

Machine learning models, such as Random Forest (RF) and XGBoost, are highly effective for energy prediction tasks, capable of handling non-linear relationships and feature interactions. RF, as highlighted by Pham et al., 2020, demonstrates robustness in noisy, high-dimensional datasets, achieving up to 49.95% lower MAE compared to traditional models in short-term multi-building predictions. Similarly, Kassai, 2017 emphasizes RF's reliability within ensemble frameworks for passive house energy forecasting. XGBoost, as discussed in H. Wang et al., 2023b, delivers exceptional accuracy in HVAC energy prediction, with a Coefficient of Variation of Root Mean Squared Error (CV-RMSE—a metric that expresses root mean squared error as a percentage of the average observed value) as low as 4.52% for power and 0.40% for temperature. Additionally, XGBoost reduces energy costs by 33.6

These studies underscore the capacity of machine learning models to address complex temporal patterns, making them ideal for weather-driven analysis in this study. However, most of these studies focus on occupied buildings, where variables beyond weather, such as occupancy, are included in the prediction process. This study aims to explore the performance of these models specifically in unoccupied buildings, isolating weather variables to better understand their impact on HVAC energy consumption.

Time-series models, such as Long Short-Term Memory networks (LSTMs, a type of neural network that remembers important information over time), Gated Recurrent Units (GRUs, a simpler and faster version of LSTMs), and Temporal Convolutional Networks (TCNs, which use filters to find patterns in time-series data), are effective for capturing temporal dependencies in sequential data. LSTMs, as highlighted by Metsä-Eerola et al., 2022, excel in modeling long-term dependencies for HVAC predictions, while GRUs and TCNs, noted in H. Liu et al., 2023, are computationally efficient and better suited for datasets with shorter temporal dependencies.

The goal of this study is to examine the independent impact of weather variables on energy consumption and establish a baseline. While time-series models excel at capturing complex temporal dependencies, they may obscure the direct relationships between individual variables. Moreover, due to the dataset's lack of long-term temporal granularity, explicit time-series models were not employed. Therefore, they were not selected as the primary method in this research.

To summarize, this study prioritizes machine learning models like RF and XGBoost for their ability to handle nonlinear relationships, feature interactions, and noisy datasets. These models suit weather-driven energy prediction in unoccupied buildings, where the absence of occupancy-related variables requires precise feature analysis. Time-series models, while effective for capturing temporal patterns, were excluded due to the dataset's lack of long-term granularity. The focus on isolating weather variables is better addressed with interpretable and flexible machine learning models.

3.2 *Key Feature Selection in Building Energy Models*

Environmental and weather factors play a critical role in determining HVAC energy requirements. Among these, temperature is a primary driver, directly influencing heating and cooling demands. Studies such as Sha et al., 2019 and H. Liu et al., 2023 emphasize the significance of dry and wet bulb temperatures (tools that reflect how air's moisture content affects cooling and comfort) in estimating energy consumption. Additionally, Ciampi et al., 2024 highlights the impact of humidity on air conditioning efficiency and indoor comfort, underscoring its importance in HVAC models. However, these studies often lack comprehensive evaluations of interactions between these variables under diverse climatic conditions.

Solar radiation and wind speed further contribute to HVAC energy dynamics. As Sha et al., 2019 discusses, solar radiation increases cooling loads during peak daytime hours, while wind speed affects heat loss and heating demand. Despite these insights, many studies rely on static models, which may not fully capture the transient nature of environmental factors.

To address this, incorporating advanced feature engineering techniques, can better capture temporal variations in these environmental factors, as demonstrated by H. Liu et al., 2023. This study builds on these approaches to enhance HVAC energy modeling, focusing on weather-driven patterns and interactions between variables.

3.3 *Feature Engineering and Preparation in Building Energy Models*

Feature engineering is important in improving HVAC energy consumption prediction. This study applies advanced techniques to refine model inputs and capture system complexities. Data preprocessing methods, such as encoding categorical variables, smoothing, and differencing, ensure consistent standards and manage outliers. For instance, encoding allows models to handle non-numerical data like operation modes, while differencing removes trends and seasonality, making data stationary Ciampi et al., 2024; Zini and Carcasci, 2024.

Time series feature engineering techniques, including lagged features, rolling averages, and interaction terms, are widely used to capture temporal patterns and cycles. Lagged features integrate historical data, enabling models to incorporate temporal dependencies effectively. Rolling averages smooth short-term fluctuations, highlighting broader trends, while interaction terms capture joint effects between variables, revealing complex relationships beyond individual factors. These methods improve the model's ability to recognize time-sensitive energy patterns, as demonstrated by H. Liu et al., 2023; Runge and Saloux, 2023. Additionally, expanding feature sets with these techniques significantly enhances predictive accuracy C. Wang et al., 2024.

Despite their effectiveness, these methods face challenges, such as increased computational complexity and potential feature redundancy in high-dimensional datasets. While studies like Runge and Saloux, 2023 address these limitations through dimensionality reduction, their application to HVAC systems with diverse operational conditions remains under explored. This study builds upon these findings by optimizing feature engineering techniques for unoccupied building scenarios, ensuring that the data used reflects real-world HVAC complexities and enables models to capture temporal and nonlinear dynamics more effectively

3.4 *Research Gap*

Although extensive research exists on HVAC energy usage, most studies focus on occupied buildings, where occupancy variability complicates isolating weather's direct impact. This study examines weather's influence on HVAC energy consumption in a controlled environment, with occupancy and appliance use held constant, using machine learning models for prediction.

The results aim to establish a baseline model for predicting HVAC energy consumption under varying conditions, particularly benefiting low-occupancy buildings like warehouses by improving energy efficiency and reducing costs.

4 METHOD

This study employs a structured methodology to evaluate the predictive performance and energy optimization potential of machine learning models for HVAC systems. To address the research questions, three experiments were designed:

- **Experiment 1**: Evaluates model performance using a combined dataset of cooling and heating energy consumption.

- **Experiment 2**: Examines cooling-specific energy consumption using a separate dataset.

- **Experiment 3**: Focuses on heating-specific energy consumption using another separate dataset.

In each experiment, data undergoes preprocessing and feature engineering to produce key features like rolling averages, interactions, and lags. The datasets are split into 5 folds for training and testing. Feature selection is done on the training set, with the test set adjusted accordingly. Models, including Linear Regression (baseline), Random Forest, XGBoost, and a Stacking Regressor, are evaluated using MAE and R^2 (which measures how much variance in the target is explained by the model).

GridSearchCV, which systematically tests hyperparameters via cross-validation, is applied to Random Forest, XGBoost, and the Stacking Regressor. This study uses 3-fold cross-validation for tuning. To ensure robustness, the process repeats across five seeds, recording feature importance, residuals, and performance metrics. Figure 1 summarizes this workflow.

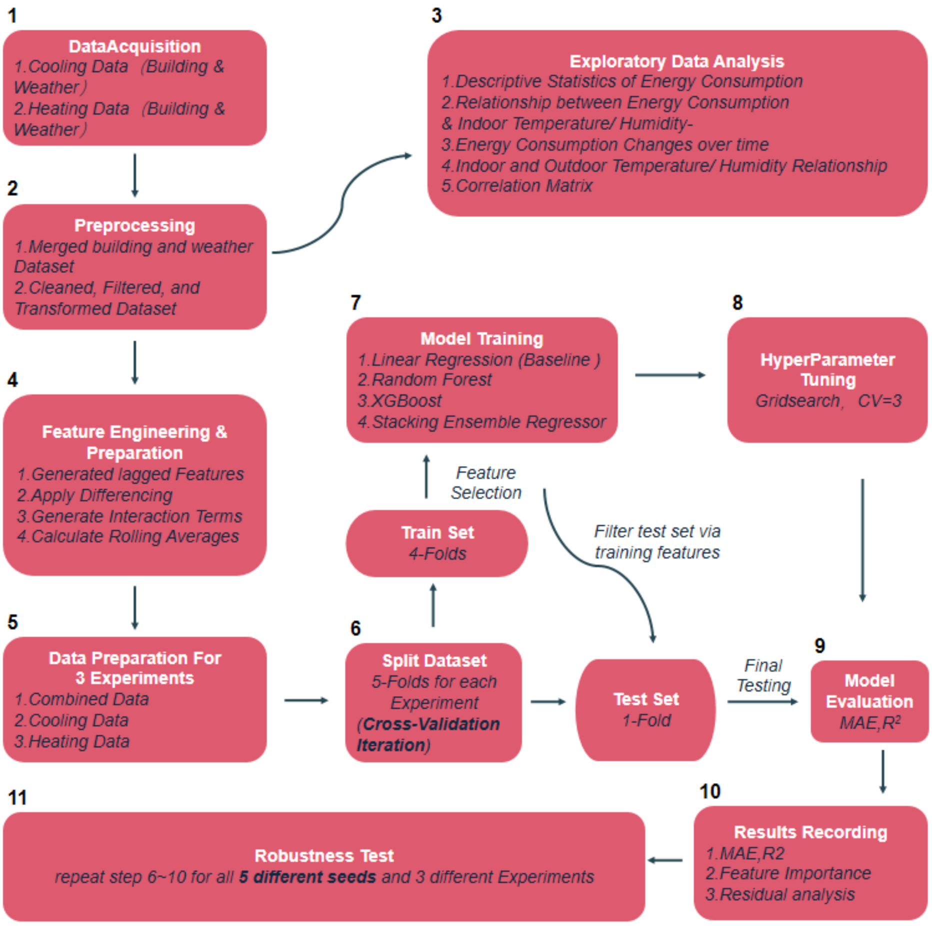


Figure 1: Methodology Overview

4.1 *Dataset Description*

The datasets used in this study were collected from a two-story, multizone office building at Oak Ridge National Laboratory (Im et al., 2022). They include measurements of HVAC and environmental parameters.

- Building Data (Cooling and Heating) These datasets record HVAC parameters across rooms and zones, including temperature, humidity, airflow, and energy consumption. Each dataset contains 10,081 entries with timestamps tracking changes over time.
- Weather Data (Cooling and Heating) These datasets provide external weather variables, such as outdoor temperature, humidity, solar radiation, and wind metrics. Each dataset has 10,081 entries, synchronized with building data through timestamps.

Together, these datasets offer high-resolution insights into interactions between HVAC operations and external weather, enabling accurate modeling of energy consumption in unoccupied buildings.

4.2 *Data Cleaning and Preprocessing*

Data preprocessing improves data quality, consistency, and relevance, directly influencing model accuracy. By removing irrelevant entries, resampling to five-minute intervals, and adding features like indoor-outdoor temperature differences, the data becomes cleaner and more interpretable, reducing computational effort and enhancing HVAC energy consumption predictions.

Building and weather datasets for cooling and heating seasons were merged, with irrelevant columns and invalid rows removed. Key features like indoor temperature, humidity, outdoor weather metrics (e.g., temperature, humidity, solar radiation, wind speed), and the target variable (Total Rooftop Unit Energy Consumption) were retained.

To address the granularity of one-minute intervals, data was resampled to five-minute averages, balancing steady-state behavior and noise reduction (H. Liu et al., 2024, Goyal and Pandey, 2021b). Additional features like indoor-outdoor temperature and humidity differences enriched interpretability, creating clean datasets for cooling (10,080 rows × 30 columns) and heating (10,078 rows × 30 columns).

HVAC energy demand fluctuates with season and time of day due to occupancy and thermal load changes (Hadley, 1993). Timestamps were transformed into binary categorical features for Season (e.g., Summer = 0, Winter = 1) and Day/Night (e.g., Day = 1, Night = 0), enabling the model to capture seasonal and temporal patterns effectively.

4.3 *Exploratory Data Analysis (EDA)*

Exploratory Data Analysis (EDA) is crucial for identifying patterns, relationships, and distributions within a dataset (Zhou et al., 2023). Analysis of cooling and heating data highlights trends and correlations influencing HVAC energy consumption. Statistical methods, including descriptive statistics, line plots, scatter plots, and correlation heatmaps, provide key insights into relationships between indoor and outdoor temperatures, humidity effects, and temporal patterns. These insights are essential for developing accurate energy prediction models.

4.3.1 *Descriptive Statistics of Energy Consumption*

The statistics of both cooling and heating datasets offer insights into energy consumption patterns and environmental conditions across seasons. The cooling dataset shows an average energy consumption of 35.62 kWh,

Table 1: Descriptive Statistics for Cooling and Heating Datasets

Metric	**Cooling Dataset**	**Heating Dataset**
Average Energy Consumption (kWh)	35.62	21.63
Average Outdoor Temperature (°C)	24.27	7.97
Average Outdoor Humidity (%)	86.45	44.07
Average Indoor Temperature (°C)	21.08	21.10
Average Temperature Difference (°C)	3.29	13.13

with outdoor temperatures averaging 24.27°C and high outdoor humidity (86.45%). Indoor temperature remains stable at 21.08°C, with an indoor-outdoor temperature difference of 3.29°C, reflecting the cooling system's efforts to maintain comfort.

For heating, average energy consumption is lower at 21.63 kWh. Outdoor temperatures average 7.97°C with lower humidity (44.07%). Indoor temperature remains around 21.10°C, with a larger indoor-outdoor temperature difference of 13.13°C, highlighting increased heating demands to maintain indoor warmth.

4.3.2 *Relationship between Energy Consumption and Indoor Temperature/ Humidity*

Indoor-outdoor temperature and humidity differences offer insights into HVAC energy demands. Figure 2 shows cooling energy use rises with larger temperature differences, while heating energy use decreases, likely due to the thermal quality of building envelopes increasing cooling demands (Kharseh et al., 2014).

Figure 3 reveals that greater humidity differences lower energy use for both cooling and heating. This likely results from the system relying on internal air circulation, reducing the energy needed to condition outdoor air and improving efficiency (Krarti, 2008).

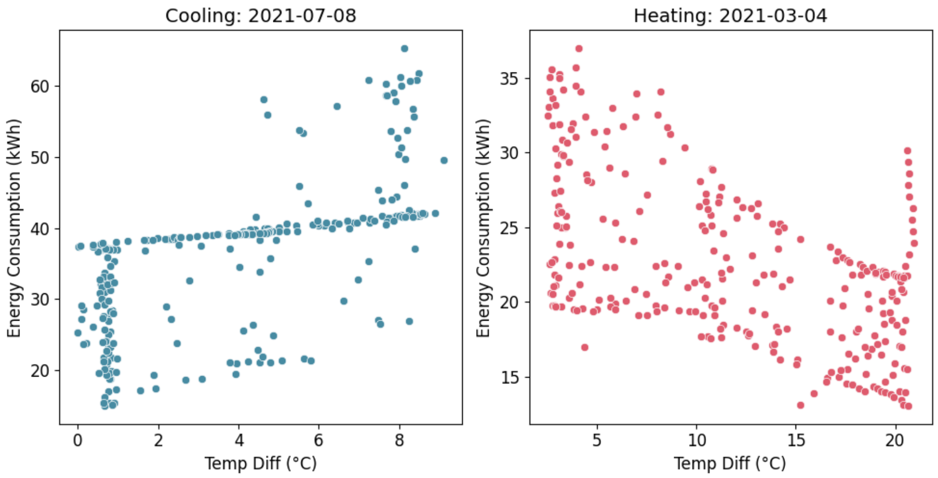


Figure 2: Temperature Differences vs. Energy Use in Cooling and Heating

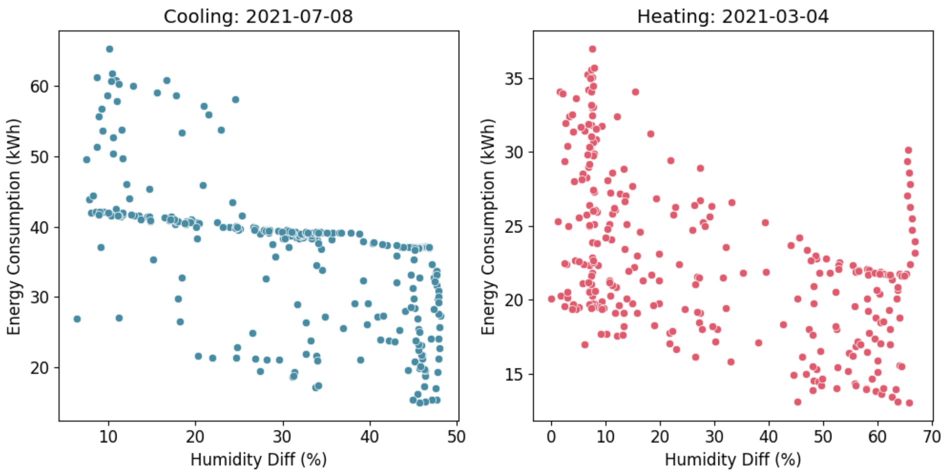


Figure 3: Humidity Differences vs. Energy Use in Cooling and Heating

Due to space constraints, Figures 2 and 3 present data from the first day as representative examples. Additional figures for temperature and humidity differences across other days are provided in Appendix A (page 51).

These patterns demonstrate that HVAC energy consumption is strongly influenced by indoor and outdoor temperature and humidity, key factors for predicting energy use in this study.

4.3.3 *Distribution of Energy Consumption*

The box plot (Figure 4) illustrates that cooling in an unoccupied multizone office building consumes more energy and shows greater variability than heating. Higher medians and a wider interquartile range in the cooling data reflect increased fluctuations, likely due to severe weather or system inefficiencies.

In contrast, heating consumes less energy with fewer outliers, indicating more stable and efficient usage. The pronounced cooling outliers highlight challenges in managing extreme cooling demands, especially during warmer months, underscoring the higher energy demand and variability of cooling compared to heating.

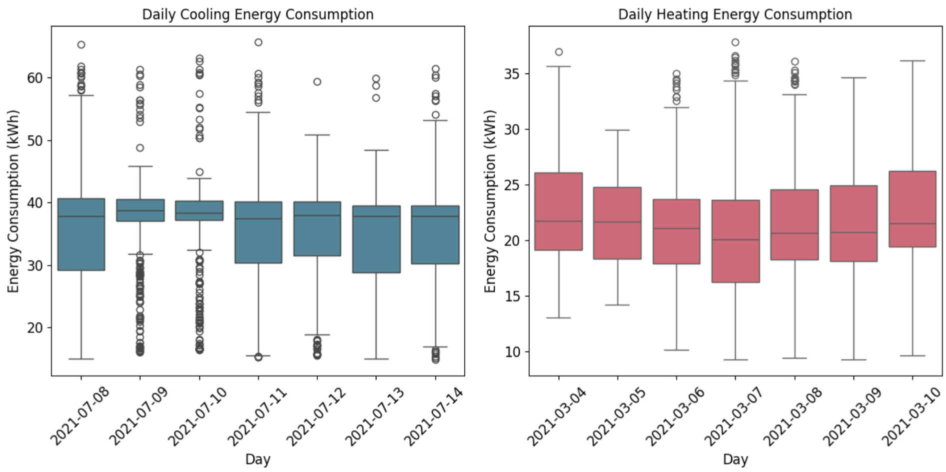


Figure 4: Box Plots of Daily Energy Consumption for Both Cooling and Heating Data

4.3.4 *Indoor and Outdoor Temperature/ Humidity Relationship*

- Indoor and Outdoor Temperature Relationship

  Energy consumption peaks strongly correlate with extreme outdoor temperatures. Cooling (Figure 5) and heating (Figure 6) systems maintain stable indoor temperatures. However, cooling exhibits sharp energy spikes with rising temperatures, while heating shows smoother, more stable energy patterns (complete figures available in Appendix A, page 51).

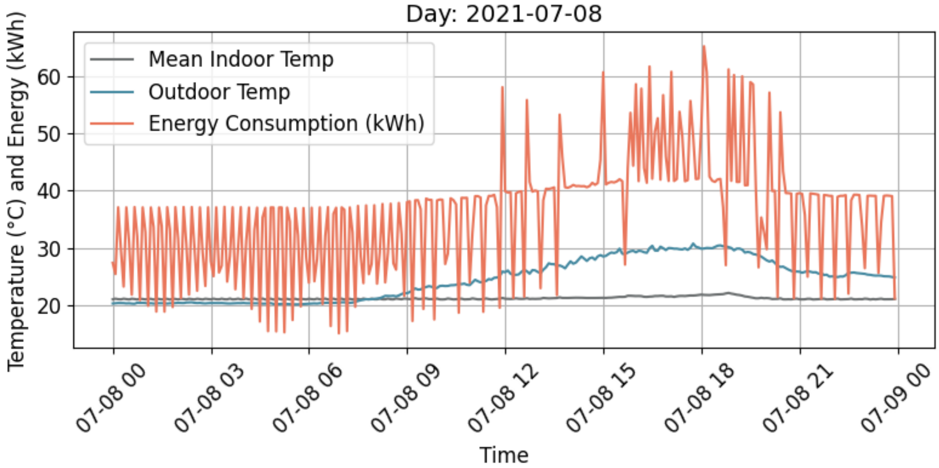


Figure 5: Time Series Temp and Energy (Cooling)

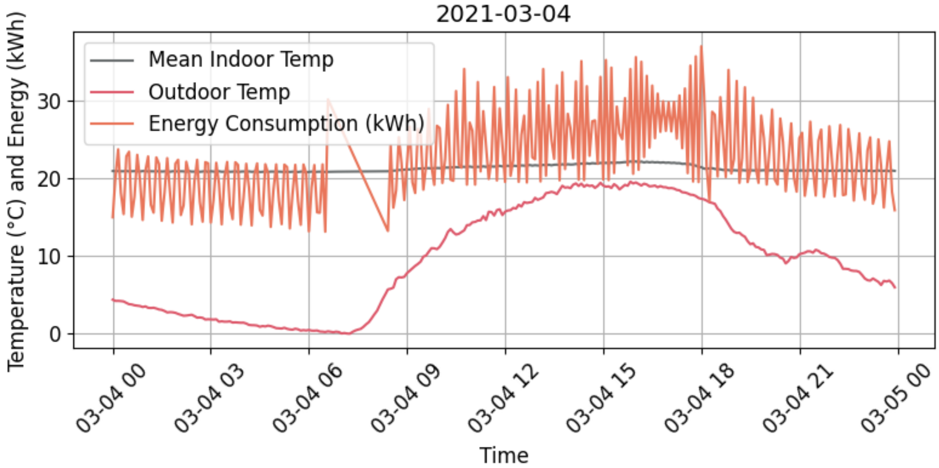


Figure 6: Time Series Temp and Energy (Heating)

- Indoor and Outdoor Humidity Relationship

  Energy consumption is significantly influenced by humidity levels. During cooling 7), energy usage increases with rising outdoor humidity as the system works to cool and dehumidify indoor air. In heating (8), energy consumption rises as outdoor humidity drops, particularly in cold, dry conditions, due to increased heating demands to maintain comfort levels(More completed Figures shown in Appendix A, page 51).

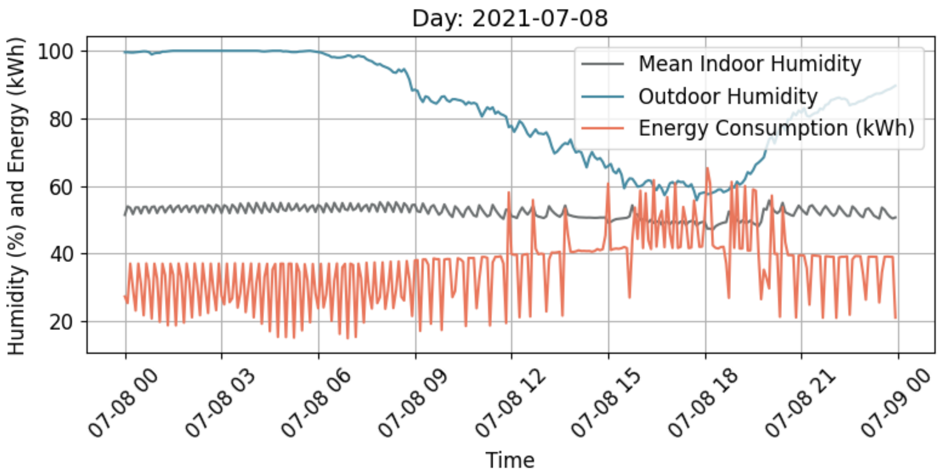


Figure 7: Time Series Humidity and Energy (Cooling)

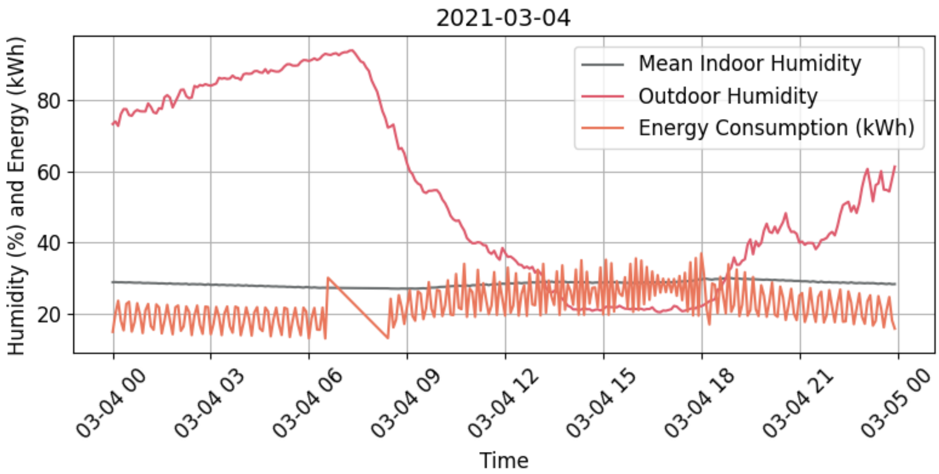


Figure 8: Time Series Humidity and Energy (Heating)

These observations highlight that temperature and humidity are key predictors of energy consumption. Incorporating indoor and outdoor temperature and humidity into machine learning models can enhance prediction accuracy and provide deeper insights into consumption dynamics. This analysis supports feature importance evaluation and improved model performance.

4.3.5 *Correlation Matrix*

These two correlation matrices provide insights into the relationships between various environmental variables and energy consumption (for both cooling and heating systems).

For the cooling system (9), outdoor temperature (*T_out*) and solar radiation (*Dir_Solar*, *Glo_Solar*) show strong positive correlations with energy consumption, reflecting increased cooling demands under hotter conditions and higher solar exposure. Wind speed and outdoor humidity exhibit weaker correlations, indicating a less direct influence on cooling needs.

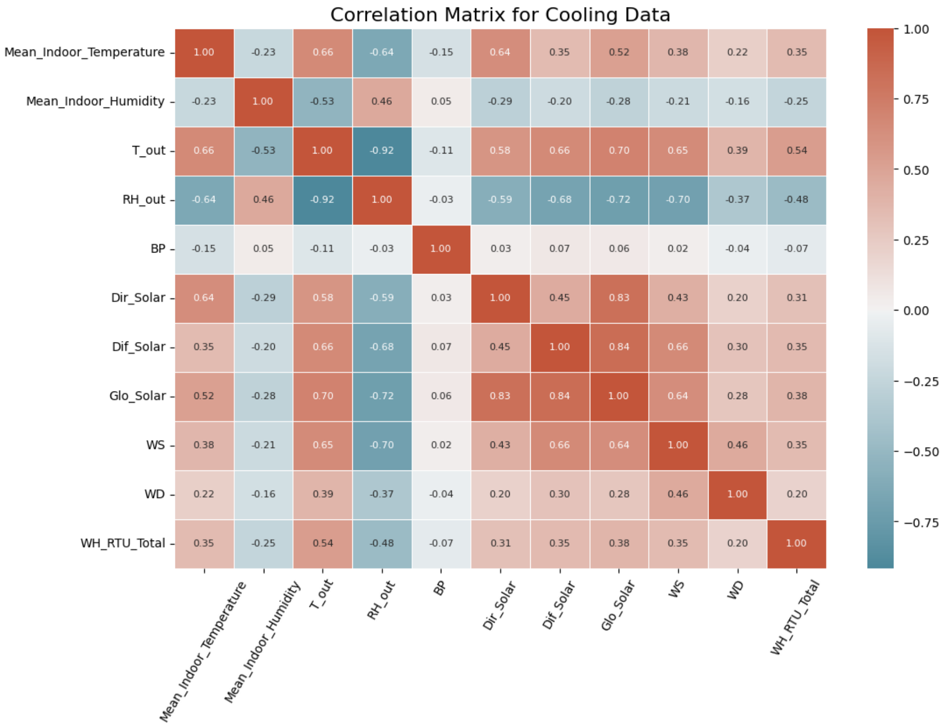


Figure 9: Correlation Matrix for Cooling

For the heating system (10), Outdoor Temperature(*T_out*)is strongly positively correlated with energy consumption, underscoring its role as a primary driver of heating requirements. Solar radiation slightly offsets heating demand, while wind speed has minimal influence.

While both systems are temperature-sensitive, solar radiation impacts cooling energy consumption more significantly, whereas its influence on heating is weaker.

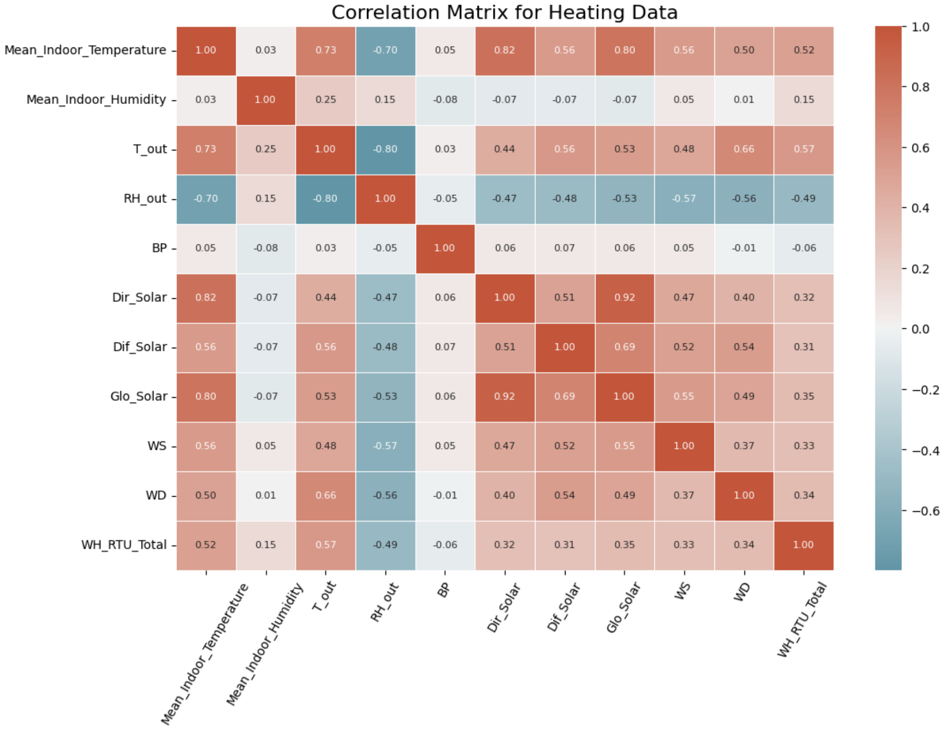


Figure 10: Correlation Matrix for Heating

4.4 *Feature Engineering and Preparation*

Feature engineering and preparation enriched the dataset by capturing temporal patterns and key insights from factors such as temperature and humidity. Techniques included generating lagged features, applying differencing, calculating rolling averages, and creating interaction terms, ensuring that potential temporal relationships in the data were fully utilized prior to data splitting.

4.4.1 *Generated lagged Features*

Lag features capture time-based patterns in environmental and indoor conditions, using past values like temperature, humidity, and solar radiation to influence future energy needs (Baath et al., 2023). Incorporating historical data helps the model identify trends and enhance energy consumption predictions.

Lagged features were generated from the previous 24 time steps of selected variables. Missing data introduced during this process was removed, and the final datasets included both original and lagged variables.

This improvement allows the model to capture temporal dynamics more effectively and enhance HVAC energy predictions.

4.4.2 *Calculate Rolling Averages*

Rolling averages smooth sudden data changes and capture short-term trends over fixed periods. In HVAC systems, recent variations in temperature, humidity, and solar radiation significantly impact energy needs. Adding rolling averages helps the model account for these trends, improving prediction accuracy (Shi et al., 2017).

With rolling averages added, both cooling and heating datasets now reflect recent trends in key variables, providing better context for energy use predictions.

4.4.3 *Apply Differencing*

Differencing captures the rate of change in variables, highlighting hidden trends and patterns in time-series data. In HVAC systems, sudden fluctuations in temperature, humidity, and solar radiation significantly impact energy demands. Including differenced values helps the model learn from these fluctuations, enhancing its predictive capability. The datasets now include key variables' rates of change, adding temporal information to improve HVAC energy consumption forecasting accuracy.

4.4.4 *Generate Interaction Terms*

Interaction terms capture the combined effects of variables, providing deeper insights into how they jointly influence energy demand. For example, outdoor temperature and relative humidity may have different impacts when considered together. Including interaction terms allows the model to account for these combined effects, improving prediction accuracy.

For both cooling and heating datasets, three interaction terms were created:

- The interaction between outdoor temperature and relative humidity.
- The interaction between outdoor temperature and wind speed.
- The interaction between mean indoor temperature and relative humidity.

These terms enhance the datasets by reflecting combined effects of key variables, enriching the model's understanding of HVAC energy consumption patterns.

4.5 *Data Split and Feature Selection*

The dataset, containing all prepared features, was divided into five folds using 5-fold cross-validation. While time series splitting suits datasets with strong temporal dependencies, a random split was chosen due to the dataset's characteristics and the models used.

Although time-series-based feature engineering methods, such as lagged features and rolling averages, are often associated with sequential splits, their application here focuses on capturing short-term dynamics rather than long-term temporal dependencies. Random splitting ensures fair representation of weather conditions across the folds, and these features enhance model performance without relying on strict temporal order.

This study focuses on weather-related factors, such as cooling and heating, rather than time-sequential patterns. Time-based splits, which reflect temperature changes (e.g., day vs. night), are unnecessary as the dataset includes detailed temperature and humidity information. Moreover, seasonal variations make time-based splits imbalanced and unsuitable for combined experiments. Tree-based models like Random Forest and XGBoost effectively handle unordered data, making random splits suitable.

Feature selection was performed only on the training set of each fold to prevent data leakage. A Random Forest Regressor ranked features by their importance to the target variable. Preselected features, including energy labels (cooling and heating), outdoor temperature, and relative humidity, were retained for their significant impact on HVAC energy consumption (H. Liu et al., 2021; Zajic et al., 2011). Additional top features were selected to retain 25 features, balancing dimensionality reduction and predictive performance.

4.6 *Algorithm*

The study utilized Linear Regression, Random Forest, XGBoost, and Stacking Ensemble Regression (SER) algorithms. These models were applied to the five folds generated after data splitting and feature selection, ensuring fair evaluation, improved generalization, and reduced overfitting. The following sections provide an overview of these algorithms and their hyperparameters.

4.6.1 *Linear Regression*

Linear Regression is often selected as a baseline model due to its simplicity, interpretability, and computational efficiency. It captures basic relationships between features and the target variable, making it ideal for benchmarking more complex models. Its ability to quickly identify data quality issues, such as multicollinearity or outliers, supports feature refinement, while its transparency adds value in decision-making scenarios requiring clear insights (Ostadijafari and Dubey, 2019).

4.6.2 *Random Forest*

Random Forest, introduced by Breiman, 2001, is an ensemble learning technique that improves accuracy and robustness by averaging predictions from multiple decision trees. Using random subsets of data and features, it captures complex nonlinear relationships while reducing overfitting. Its ability to generalize well to unseen data and perform feature importance analysis provides insights into key drivers of HVAC energy consumption (Y. Liu et al., 2021, Z. Wang et al., 2018). Robustness to noise and missing data ensures low prediction errors, making it highly effective for HVAC modeling.

4.6.3 *XGBoost*

XGBoost, developed by Chen and Guestrin, 2016, is a gradient boosting algorithm known for its speed, flexibility, and accuracy. By iteratively correcting errors using gradient descent, it captures complex nonlinear relationships better than Random Forest. XGBoost's ability to focus on high-error regions enhances its predictive accuracy and efficiency. Its feature interaction capabilities make it ideal for HVAC energy consumption modeling, achieving high accuracy and reduced computation costs in predictive control strategies (H. Wang et al., 2023b, H. Wang et al., 2023a).

4.6.4 *Stacking Ensemble Regression*

Stacking Ensemble Regression (SER), as noted by Divina et al., 2018, combines multiple models in a two-tier system to enhance accuracy and robustness. In this study, SER consisted of two base models—Random Forest and Gradient Boosting Regressor—and a meta-learner (Linear Regression).

The training process followed a sequential workflow within a 5-fold cross-validation framework. First, the base models were trained independently on the training subset of each fold, using all features and the target variable (HVAC energy consumption). After training, their predictions on the training subset were collected as new input features, forming a feature matrix for the meta-learner. This setup allowed the meta-learner to focus on learning how to optimally combine the base model outputs.

The meta-learner was then trained on these predictions and the corresponding target values from the training subset. This process ensured that the meta-learner refined the base models' outputs to improve overall prediction accuracy. The test subset for each fold was reserved exclusively for evaluation, preventing data leakage and ensuring robust model validation.

By integrating the strengths of nonlinear base models with the simplicity and interpretability of linear regression, SER effectively balances predictive power and robustness, making it highly suitable for HVAC energy consumption prediction.

4.7 *Hyperparameter Tuning*

Hyperparameter tuning is crucial for improving predictive accuracy, mitigating overfitting or underfitting, and enhancing generalization ability (Hussain et al., 2024).

In this study, hyperparameter tuning was performed for Random Forest, XGBoost, and Stacking Regressor to optimize performance, minimize MAE, and improve R^2 under diverse weather conditions. Nested cross-validation was employed, with an outer 5-fold cross-validation for model evaluation and an inner 3-fold GridSearchCV for hyperparameter tuning on the training data. This setup prevented data leakage, ensured unbiased evaluation, and maintained consistency across experiments by using the same parameter grid for each model(Bischl et al., 2021).

The optimized models were evaluated using MAE and R^2 metrics, providing robust benchmarks for performance. Details of the tuning strategies and parameter grids are outlined in the following sections.

4.7.1 *Hyperparameter Tuning for Random Forest*

Random Forest models were tuned with a carefully designed hyperparameter grid (Table 2) to balance predictive performance, computational efficiency, and adaptability to varying data complexities.

Table 2: Hyperparameter Grid for Random Forest Tuning.

Parameter	**Values**
`n_estimators`	[50, 100, 150]
`max_depth`	[10, 20, None]
`min_samples_split`	[2, 5, 10]

- `n_estimators`: Specifies the number of trees in the forest. Values of 50, 100, and 150 provide a trade-off between training speed and model accuracy, enabling comparisons of lightweight and robust setups.

- `max_depth`: Determines tree complexity. Depths of 10 and 20 balance overfitting and flexibility, while `None` allows unlimited depth for exploratory analysis.
- `min_samples_split`: Defines the minimum number of samples required to split a node. Values of 2, 5, and 10 evaluate both fine-grained and coarse splits, balancing sensitivity and generalization.

4.7.2 *Hyperparameter Tuning for XGBoost*

Hyperparameter tuning is essential for optimizing XGBoost's gradient boosting, which relies heavily on parameter settings. The tuning process, outlined in Table 3, balances accuracy, efficiency, and adaptability across three experimental setups.

Table 3: Hyperparameter Grid for XGBoost Tuning.

Parameter	**Values**
`n_estimators`	[50, 100, 150]
`max_depth`	[3, 6, 9]
`learning_rate`	[0.01, 0.1, 0.2]
`subsample`	[0.8, 1.0]

- `n_estimators`: Balances training speed and model performance. The range [50, 150] provides options for faster training and enhanced results.
- `max_depth`: Limits tree depth to control complexity. Values of 3, 6, and 9 allow generalization or capturing detailed patterns.
- `learning_rate`: Adjusts the step size for weight updates. Rates of 0.01 and 0.1 balance convergence speed and stability; 0.2 explores faster optimization.
- `subsample`: Determines the proportion of samples used per tree. Values of 0.8 and 1.0 introduce randomness to reduce overfitting while ensuring stability.

4.7.3 *Hyperparameter Tuning for Stacking Ensemble Regression*

The Stacking Regressor integrates multiple base models with a meta-model to improve predictive accuracy. A unified hyperparameter grid (Table 4) was applied to the Stacking Regressor across three experimental setups, ensuring consistent evaluation of the model's performance across diverse data conditions and scenarios.

Table 4: Hyperparameter Grid for Tuning the Stacking Regressor.

Component	Parameter	Values
Meta-model	`final_estimator__fit_intercept`	{True, False}
Random Forest (Base)	`rf__n_estimators`, `rf__max_depth`	{50, 100}, {10, 20}
Gradient Boosting (Base)	`gb__learning_rate`, `gb__max_depth`	{0.01, 0.1}, {3, 6}

- `final_estimator__fit_intercept`: Specifies whether the meta-model includes an intercept. `True` adjusts for bias, while `False` forces predictions to pass through the origin.
- `rf__n_estimators` and `rf__max_depth`: Parameters inherited from the Random Forest base model, designed to balance computational efficiency and capture complex patterns.
- `gb__learning_rate` and `gb__max_depth`: Parameters from the Gradient Boosting base model, focusing on stepwise optimization and capturing feature interactions across different depths.

4.8 *Evaluation Methods*

4.8.1 *MAE :Mean Absolute Error*

To evaluate the performance of the machine learning models (*Linear Regression*, *Random Forest*, *XGBoost*, and *Stacking Ensemble Regression*), **Mean Absolute Error (MAE)** was used across the training and testing datasets in both experiments.

MAE measures the average magnitude of prediction errors, providing an intuitive metric for accuracy by assigning equal weight to all errors. This makes it particularly useful for comparing models when the cost of errors, regardless of size, is consistent.

4.8.2 *R^2: Coefficient of Determination*

R^2 measures how well a regression model explains the variance in the dependent variable. It is calculated as:

$$R^2 = 1 - \frac{\text{SS}_{\text{residual}}}{\text{SS}_{\text{total}}}$$

where $\text{SS}_{\text{residual}}$ represents the sum of squared residuals, and SS_{total} is the total sum of squares. An R^2 value of 1 indicates a perfect fit, while 0 implies no explanatory power, and negative values signify performance worse than a simple mean prediction.

In this study, R^2 complements MAE by providing a broader view of model performance. While MAE measures the average prediction error, R^2 indicates the extent to which the models explain variability in HVAC energy consumption. Together, these metrics offer a comprehensive evaluation of predictive effectiveness across combined, cooling, and heating datasets.

4.8.3 *Standard Deviation (STD)*

Standard Deviation (STD) measures the amount of variation or dispersion in a set of values. In this study, STD is used to evaluate the stability and robustness of model performance metrics, such as MAE and R^2, across different folds and experimental setups.

By calculating the STD for MAE and R^2, this approach assesses how consistently each model performs under varying conditions. A lower STD indicates greater robustness, signifying that the model is less sensitive to differences in data splits or experimental configurations. This makes the model more reliable for real-world HVAC energy prediction.

4.9 *Experiment Set*

4.9.1 *Experiment 1: Combined Dataset*

Experiment 1 used a combined cooling and heating dataset to build a unified model for predicting HVAC energy consumption across diverse scenarios. The experiment provided insights and metrics for evaluating models using three testing approaches: (1) MAE and R^2 calculated across the entire test set (cooling + heating), (2) MAE and R^2 calculated specifically for cooling data, and (3) MAE and R^2 calculated specifically for heating data. The results served as a reference for analyzing the advantages and limitations of using a unified dataset for energy prediction.

The steps for Experiment 1 included:

- **Data Preparation:** Cooling and heating data were merged into a single dataset. A 5-fold cross-validation split with a random seed ensured fair representation. Each test fold retained its original labels (cooling or heating).
- **Feature Selection:** Feature selection was performed only on the training data of each fold, and the selected features were consistently applied to both training and test sets to prevent data leakage and ensure unbiased evaluation.
- **Model Application:**

  - **Baseline Model:** Linear Regression was trained on the combined dataset and evaluated using the three testing approaches: overall test set (cooling + heating), cooling test data, and heating test data.
  - **Advanced Models:** Random Forest, XGBoost, and Stacking Ensemble Regression underwent hyperparameter tuning for each fold and were evaluated on the same test sets as the baseline.

- **Result Recording:** MAE and R^2 metrics for each test fold were recorded separately for the three testing approaches. Feature importance, residuals, and key weather variables (e.g., outdoor temperature and humidity) were documented for further analysis.

4.9.2 *Experiments 2 and 3: Separate Cooling and Heating Datasets*

Experiments 2 and 3 applied the same process as Experiment 1—including data splitting, feature selection, and model evaluation—but focused exclusively on their respective cooling and heating datasets. Unlike Experiment 1, which used a combined dataset for training and evaluated models on both combined and separate test sets (cooling and heating), Experiments 2 and 3 trained and tested models solely on the cooling and heating datasets, respectively.

This approach aimed to evaluate model performance (MAE, R^2) under distinct cooling and heating conditions, providing insights into the specific demands of each scenario and identifying which dataset configuration yields optimal results.

4.9.3 *Ensuring Robustness in Analysis*

To ensure robust results, five random seeds were applied across all three experiments, and each dataset was split into 5 folds for cross-validation. For each fold, MAE, R^2, feature importance, and residuals were recorded for every model, enabling a comprehensive evaluation. This approach reduced bias from specific data distributions and ensured reliable insights for identifying key weather variables and assessing model stability in energy-efficient HVAC system designs.

The three experiments collectively address the research questions as follows:

- **Sub-Question 1:** Comparing accuracy between combined and separate datasets is achieved by evaluating MAE and R^2 across both combined and separate cooling and heating datasets, ensuring robust comparisons using random seeds.

- **Sub-Question 2:** Identifying critical weather variables is supported by the analysis of feature importance across experiments, highlighting key predictors for sustainable energy management.
- **Sub-Question 3:** Model robustness is assessed through residual analysis, examining prediction errors across random seeds and diverse conditions to ensure model stability and reliability.

These analyses provide comprehensive insights and form a strong foundation for addressing the main research question regarding energy-efficient HVAC system designs under varied conditions.

5 RESULT

5.1 *Performance Metrics (MAE, R^2)*

The analysis of performance metrics across all experiments highlights the effectiveness of advanced machine learning models in predicting HVAC energy consumption. Tables 5, 6, and 7 summarize the Mean MAE, Mean R^2, Std MAE, and Std R^2 for the combined, cooling, and heating datasets, respectively.

Table 5: Performance Metrics for Exp1, with Mean MAE and R^2 (Mean ± Std).

Model	**Dataset**	**MAE (±Std)**	**R^2 (±Std)**
Linear Regression	Combined	4.4772 (±0.2048)	0.6862 (±0.0249)
Linear Regression	Cooling	5.0028 (±0.3271)	0.4370 (±0.0537)
Linear Regression	Heating	3.9515 (±0.1100)	0.3036 (±0.0617)
Random Forest	Combined	2.7812 (±0.1146)	0.8438 (±0.0124)
Random Forest	Cooling	2.3485 (±0.2209)	0.7713 (±0.0333)
Random Forest	Heating	3.2121 (±0.0844)	0.5252 (±0.0310)
XGBoost	Combined	2.7935 (±0.1066)	0.8480 (±0.0106)
XGBoost	Cooling	2.3769 (±0.1754)	0.7843 (±0.0277)
XGBoost	Heating	3.2092 (±0.0989)	0.5207 (±0.0304)
Stacking Regressor	Combined	2.7975 (±0.1386)	0.8459 (±0.0124)
Stacking Regressor	Cooling	2.3584 (±0.2430)	0.7794 (±0.0293)
Stacking Regressor	Heating	3.2353 (±0.1016)	0.5190 (±0.0352)

Table 6: Performance Metrics for Exp2, with Mean MAE and R^2 (Mean ± Std).

Model	MAE (±Std)	R^2 (±Std)
Linear Regression	4.7543 (±0.2067)	0.4898 (±0.0324)
Random Forest	2.3379 (±0.2065)	0.7727 (±0.0326)
XGBoost	2.2033 (±0.1691)	0.7959 (±0.0328)
Stacking Regressor	2.2767 (±0.1826)	0.7825 (±0.0300)

Table 7: Performance Metrics for Exp3, with Mean MAE and R^2 (Mean ± Std).

Model	MAE (±Std)	R^2 (±Std)
Linear Regression	3.6077 (±0.1239)	0.3950 (±0.0423)
Random Forest	2.9784 (±0.1334)	0.5770 (±0.0365)
XGBoost	2.8683 (±0.1682)	0.5876 (±0.0457)
Stacking Regressor	2.9658 (±0.1169)	0.5804 (±0.0349)

5.1.1 *Experiment 1: Combined Dataset*

Across all test datasets (Table 5), non-linear models, including Random Forest, XGBoost, and Stacking Regressor, consistently outperformed Linear Regression. Random Forest achieved the lowest Mean MAE (2.7812, 2.3485, 3.2121 for Combined, Cooling, and Heating, respectively) and high Mean R^2 values (0.8438, 0.7713, 0.5252). XGBoost delivered similar performance, with Mean MAE values of 2.7935, 2.3769, and 3.2092, and Mean R^2 values of 0.8480, 0.7843, and 0.5207, slightly outperforming Random Forest in Heating.

Stacking Regressor reported Mean MAE values of 2.7975, 2.3584, and 3.2353, with corresponding Mean R^2 values of 0.8459, 0.7794, and 0.5190. Although its variability was slightly higher, it remained robust compared to Linear Regression, which underperformed significantly with the highest Mean MAE (4.4772, 5.0028, 3.9515) and lowest Mean R^2 (0.6862, 0.4370, 0.3036). Its high Std MAE and Std R^2 values (e.g., 0.2048 and 0.0249 on the Combined dataset) further indicate its instability and inability to model the complex relationships in HVAC energy consumption (Figure 11).

In summary, Random Forest and XGBoost excelled, with Random Forest performing best in Cooling scenarios and XGBoost in Heating, while Linear Regression's limitations emphasize the necessity of non-linear models for capturing HVAC energy consumption complexities.

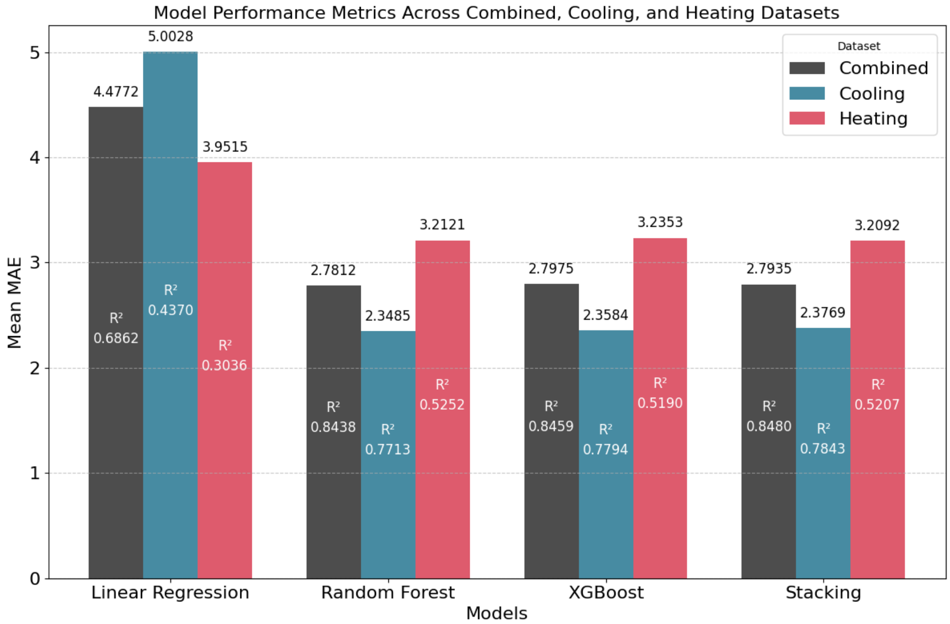


Figure 11: Exp1 - Model performance (MAE and R^2) on Cooling, Heating, and Combined test sets, trained with the Combined dataset.

5.1.2 *Experiments 2 and 3: Cooling and Heating Datasets*

Analyzing the separate cooling and heating datasets highlighted improvements in predictive accuracy (Table 6 and Table 7).

For cooling, XGBoost achieved the lowest Mean MAE (**2.2033**) and the highest Mean R^2 (**0.7959**), showcasing its ability to capture the consistent energy consumption patterns in cooling. Random Forest (**Mean MAE: 2.3379, Mean R^2: 0.7727**) and Stacking Regressor (**Mean MAE: 2.2767, Mean R^2: 0.7825**) provided competitive results, while Linear Regression lagged behind with the highest Mean MAE (**4.7543**) and the lowest Mean R^2 (**0.4898**).

For heating, XGBoost again performed the best (**Mean MAE: 2.8683, Mean R^2: 0.5876**), followed by Stacking Regressor (**Mean MAE: 2.9658, Mean R^2: 0.5804**) and Random Forest (**Mean MAE: 2.9784, Mean R^2: 0.5770**). Linear Regression exhibited poor performance, with a Mean MAE of **3.6077** and a Mean R^2 of **0.3950**, reflecting its inability to handle the increased variability in heating data.

Std MAE and Std R^2 results further emphasized Random Forest's robustness, particularly for heating (**Std MAE: 0.1334, Std R^2: 0.0365**). XGBoost showed strong stability across datasets, while Linear Regression continued to exhibit the highest variability, reaffirming its limitations (Figure 12).

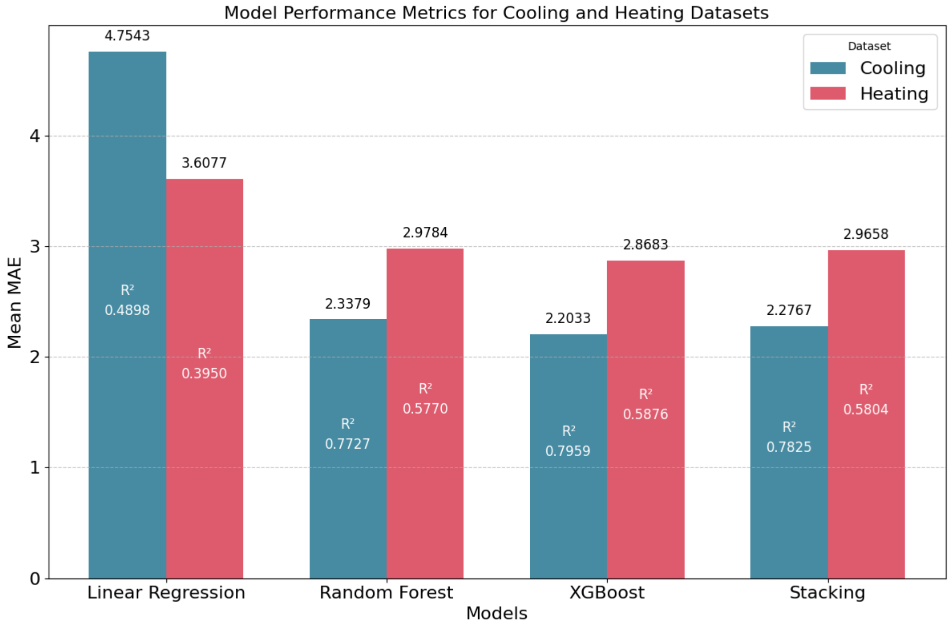


Figure 12: Exp2 and Exp3 - Model performance (MAE and R^2) on Cooling (Exp2) and Heating (Exp3) datasets, trained and tested on respective data.

5.1.3 *Comparative Insights Across Datasets*

Figures 13 and 14 illustrate the performance of models across different experiments for cooling and heating datasets. Models trained on the separate cooling and heating datasets (Experiments 2 and 3) consistently outperformed those trained on the combined dataset (Experiment 1). XGBoost emerged as the most robust model, achieving the lowest Mean MAE and the highest Mean R^2 across all experiments. Random Forest demonstrated exceptional robustness, while Stacking Regressor balanced accuracy and stability effectively. Linear Regression, however, struggled across all datasets and experiments, reinforcing the need for advanced non-linear models in HVAC energy prediction.

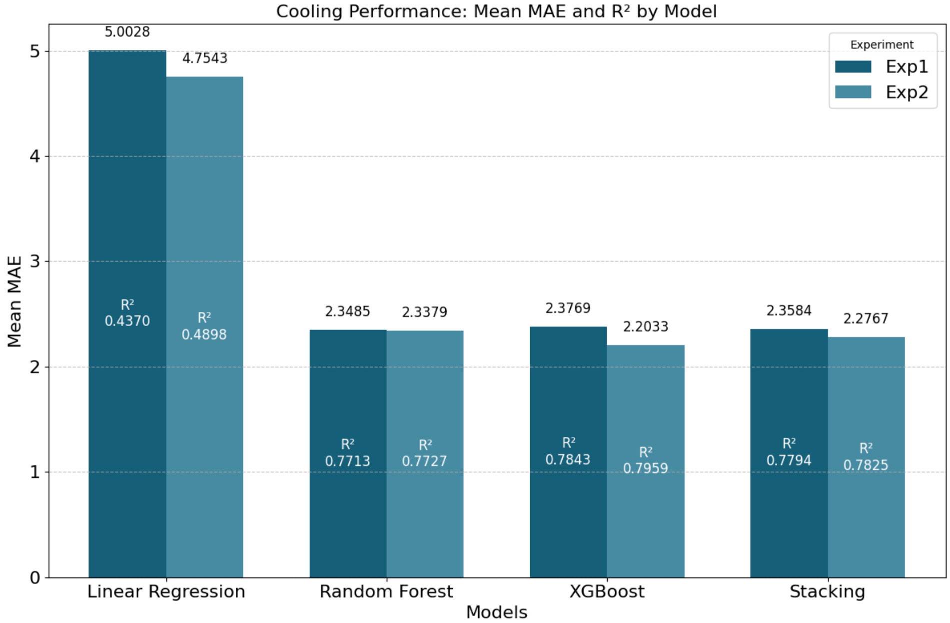


Figure 13: Model Performance Metrics for Cooling Dataset Across Experiments. Each bar represents the Mean MAE for the corresponding experiment, with R^2 values annotated inside the bars.

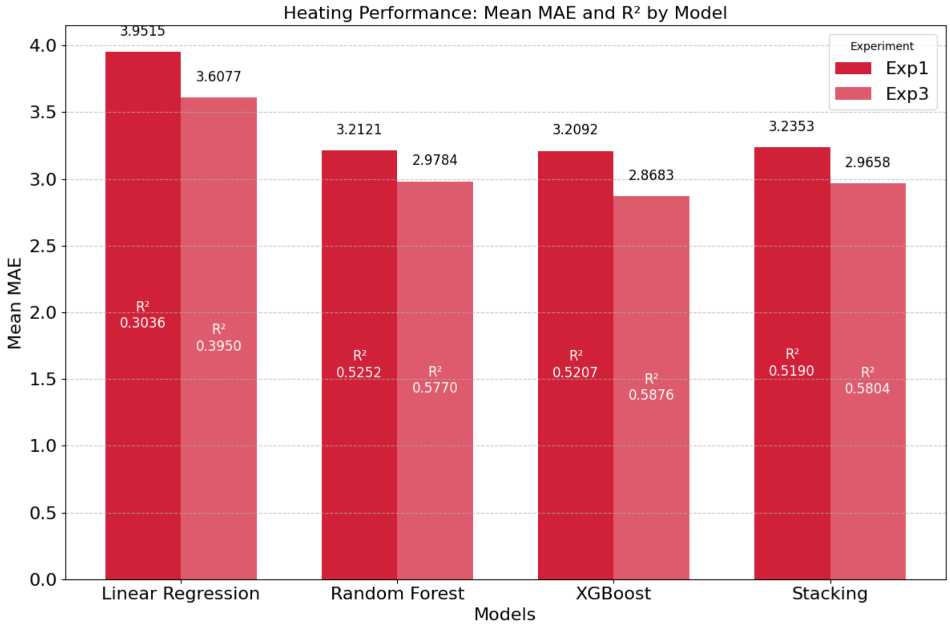


Figure 14: Model Performance Metrics for Heating Dataset Across Experiments. Each bar represents the Mean MAE for the corresponding experiment, with R^2 values annotated inside the bars.

5.2 *Feature Importance Analysis*

Feature importance analysis identifies the key predictors influencing HVAC energy consumption across combined (Experiment 1), cooling (Experiment 2), and heating (Experiment 3) datasets. This analysis highlights the distinct roles of indoor, outdoor, and humidity-related variables, providing insights for optimized feature engineering.

5.2.1 *Experiment 1: Combined Dataset*

Figure 15 highlights the distinction between cooling and heating scenarios (represented by the variable `label`) as the most significant predictor, particularly for XGBoost with an importance score of **0.59**. Recent indoor conditions, such as the indoor temperature from the previous time step (`Mean_Indoor_Temperature_Lag_1`, importance score **0.17** for Random Forest and Stacking) and the indoor humidity from two time steps earlier (`Mean_Indoor_Humidity_Lag_2`, importance score **0.14** for Stacking), further demonstrate their critical role in predictions. While outdoor features are less influential overall, they still make a moderate contribution to the model's predictive performance.

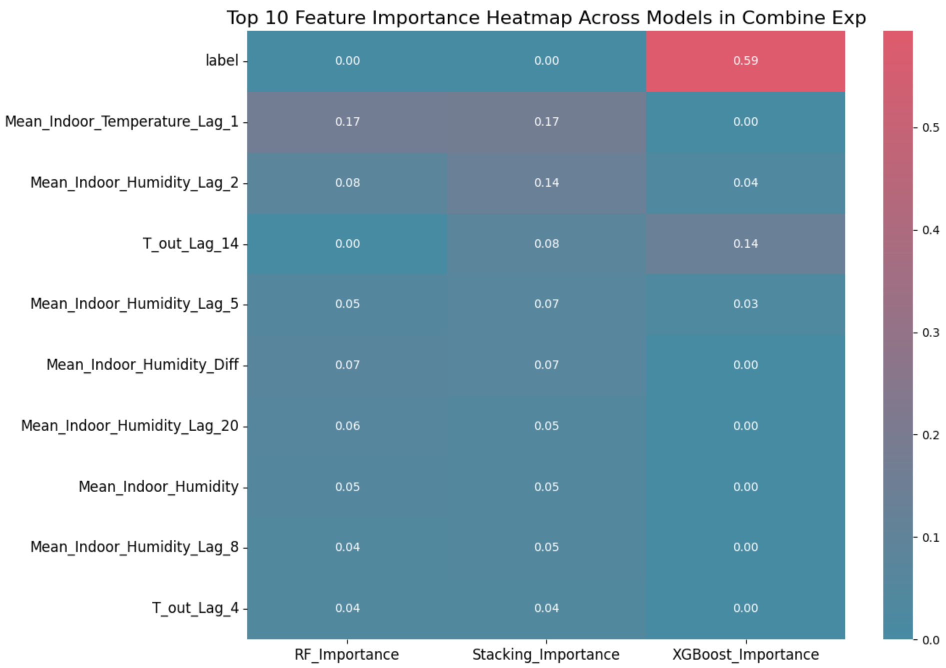


Figure 15: Top 10 Feature Importance Heatmap Across Models in the Combined Experiment

5.2.2 *Experiments 2 and 3: Cooling and Heating Datasets*

The heatmaps for cooling and heating datasets (Figures 16 and 17) reveal distinct patterns. The most influential feature across both scenarios is the indoor temperature from the previous time step (`Mean_Indoor_Temperature_Lag_1`), which has an importance score of **0.38** for Stacking in cooling and **0.20** in heating.

For cooling, differences in indoor humidity levels compared to previous observations (`Mean_Indoor_Humidity_Diff`, importance score **0.16** for Random Forest) play a significant role, emphasizing their impact on cooling energy demand. In heating, the rolling average of outdoor temperature over recent time intervals (`T_out_Rolling_3`, importance score **0.12** for XGBoost) becomes more critical, reflecting the greater variability in heating energy patterns.

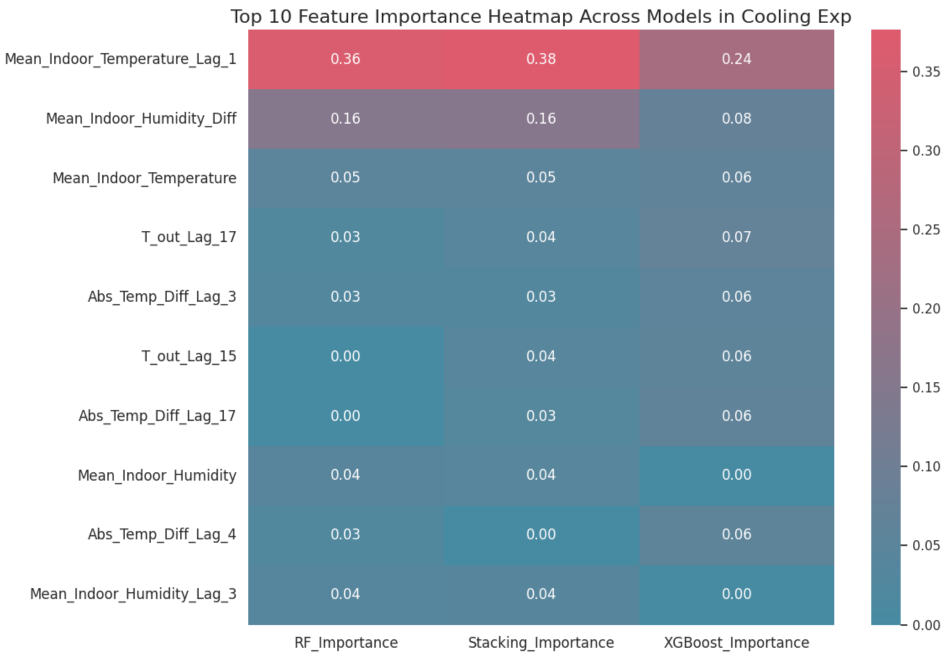


Figure 16: Top 10 Feature Importance Heatmap Across Models in Cooling Experiment

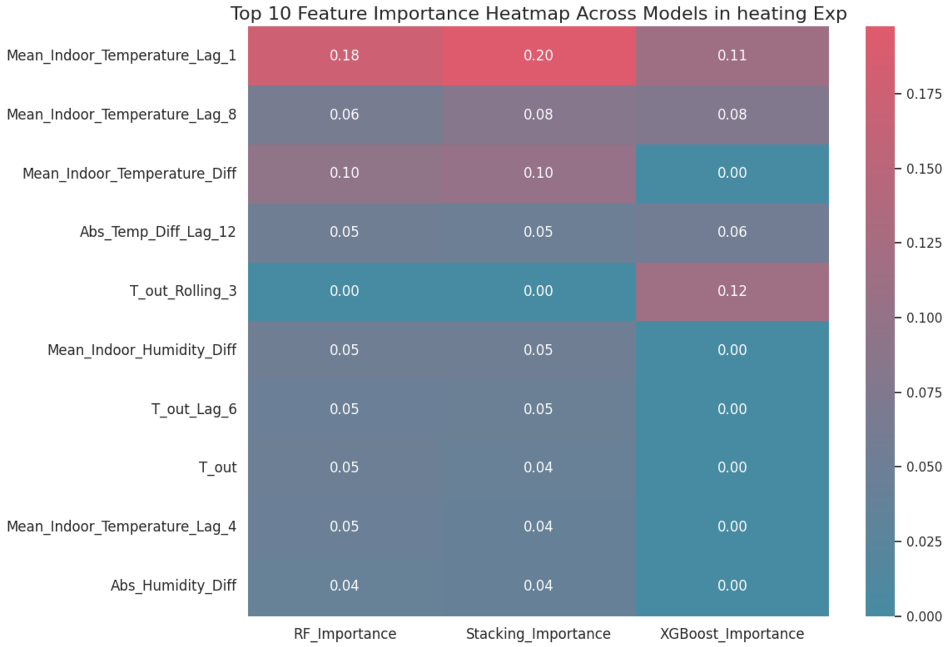


Figure 17: Top 10 Feature Importance Heatmap Across Models in Heating Experiment

5.2.3 *Comparative Insights Across Datasets*

Across all datasets, the indoor temperature from the previous time step(Mean_Indoor_Temperature_Lag_1) consistently emerges as the most critical predictor. Features related to humidity play a significant role in cooling scenarios, while heating models rely on a broader range of temperature-related variables to capture the complexity of heating energy demand. Although outdoor features are less influential overall, they still provide relevant information for the predictions.

These findings underscore the importance of tailoring feature engineering to dataset-specific dynamics. Cooling models should prioritize lagged temperature and humidity, while heating models require broader temperature-related features to address variability.

5.3 *Residual Analysis Across Experiments*

The residual distributions and weather interactions for Random Forest, XGBoost, and Stacking Regressor were analyzed across the combined (Experiment 1), cooling (Experiment 2), and heating (Experiment 3) datasets. The results reveal consistent model behaviors while highlighting dataset-specific challenges and robustness differences.

5.3.1 *Residual Distributions.*

The residuals for all models exhibit symmetric, bell-shaped distributions centered around zero (Figures 18, 19, and 20), indicating unbiased predictions. For the combined dataset (Exp1), Random Forest shows the narrowest spread, followed by XGBoost and Stacking Regressor, reflecting varying precision levels. In the cooling dataset (Exp2), Stacking achieves the narrowest spread, indicating strong robustness under consistent cooling patterns, while heating data (Exp3) introduces greater variability across all models, highlighting challenges in capturing heating dynamics.

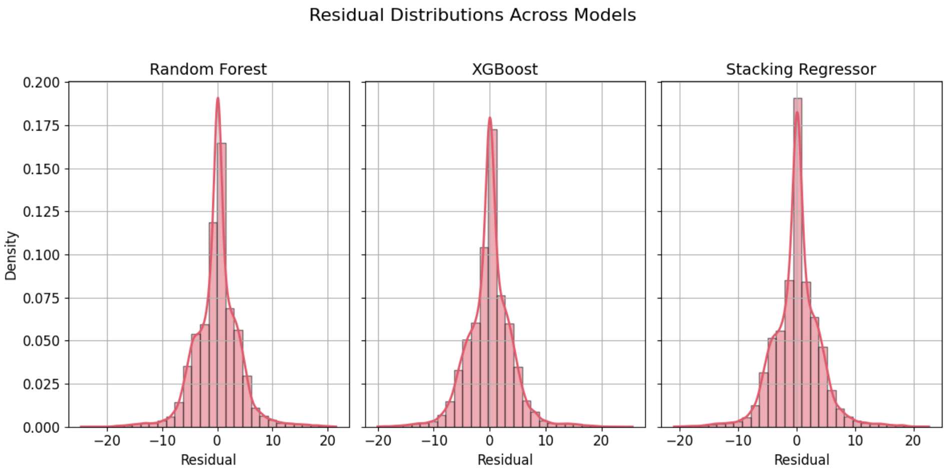


Figure 18: Residual Distributions Across Models: Combined Dataset (Exp1)

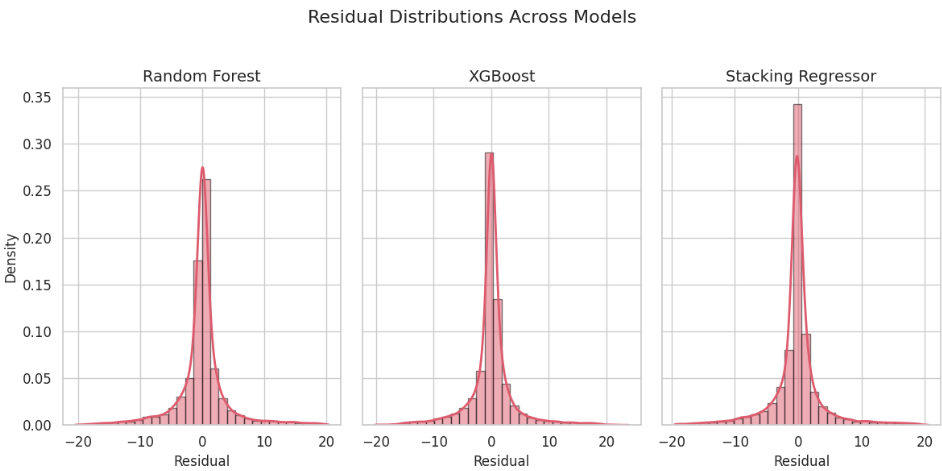


Figure 19: Residual Distributions Across Models: Cooling Dataset (Exp2)

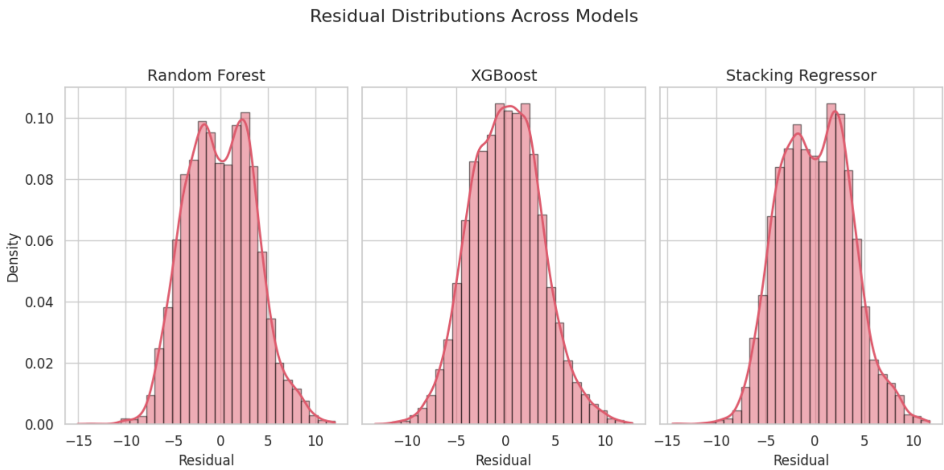


Figure 20: Residual Distributions Across Models: Heating Dataset (Exp3)

5.3.2 *Residuals vs Weather Variables*

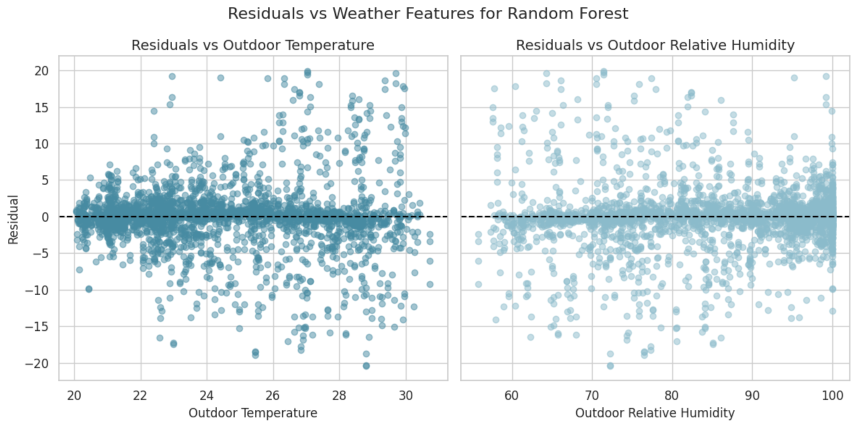
Residuals plotted against outdoor temperature and relative humidity (Figures 21, 23, and 22) reveal distinct model-environment interactions across combined (Exp1), cooling (Exp2), and heating (Exp3) datasets.

For cooling data, residuals remain closer to zero across models, showing smaller prediction errors, though more dispersed in the humidity dimension. Random Forest and XGBoost exhibit tighter residual clustering near zero for temperature-driven cooling variations, while Stacking Regressor shows larger dispersion. Humidity plays a secondary role compared to temperature. Overall, Random Forest performs best, followed by XGBoost, with Stacking trailing.

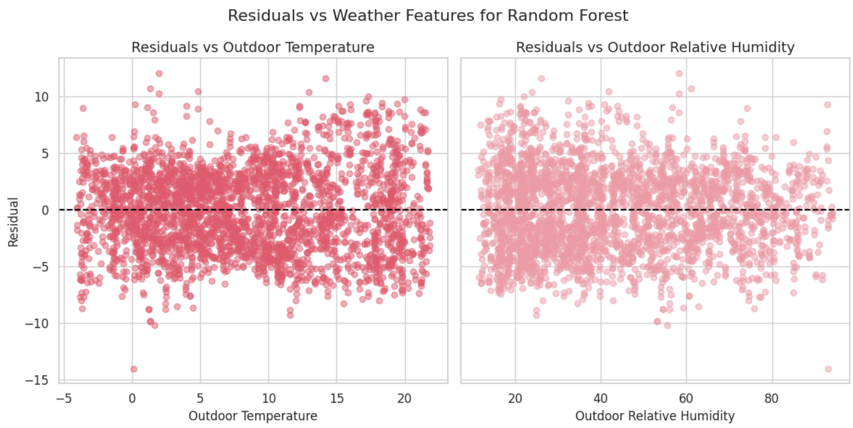
For heating data, residuals deviate farther from zero, reflecting larger biases and challenges in capturing dynamics. Temperature has a stronger impact than humidity, with Random Forest and XGBoost showing better residual compactness, while Stacking displays greater dispersion. The reduced influence of humidity emphasizes temperature-driven patterns in heating predictions. Random Forest and XGBoost outperform Stacking, though heating remains harder to model than cooling.

Residual analysis shows cooling data is more predictable, with Random Forest and XGBoost delivering better accuracy and robustness across variations in temperature and humidity. In contrast, heating data exhibits larger prediction biases, primarily influenced by temperature. These findings highlight the importance of model-specific optimization for heating scenarios to reduce errors and enhance robustness.

(a) Residuals vs Outdoor Conditions for Random Forest (Experiment 1)

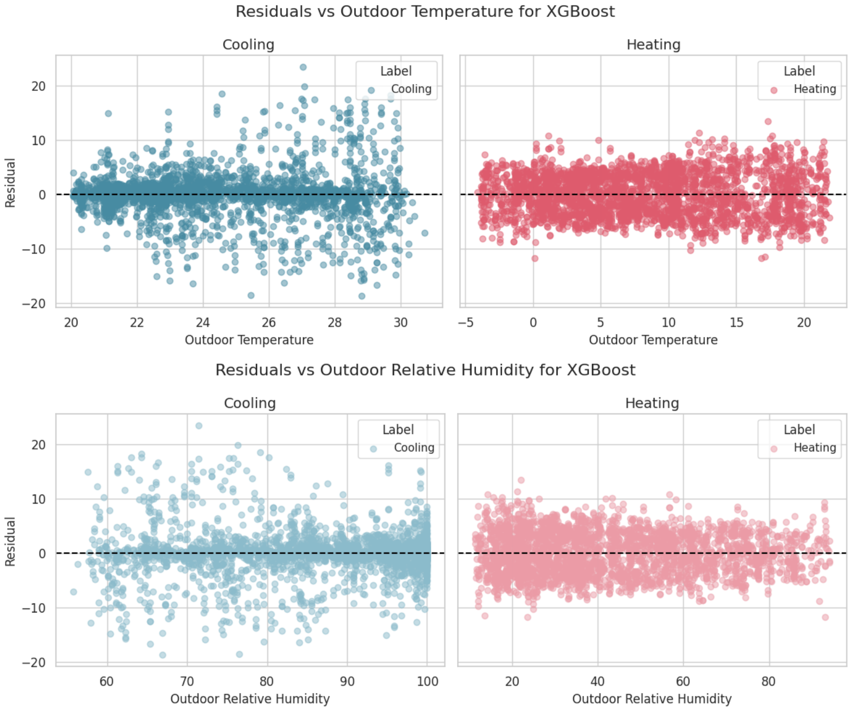


(b) Residuals vs Outdoor Conditions for Random Forest (Experiment 2)

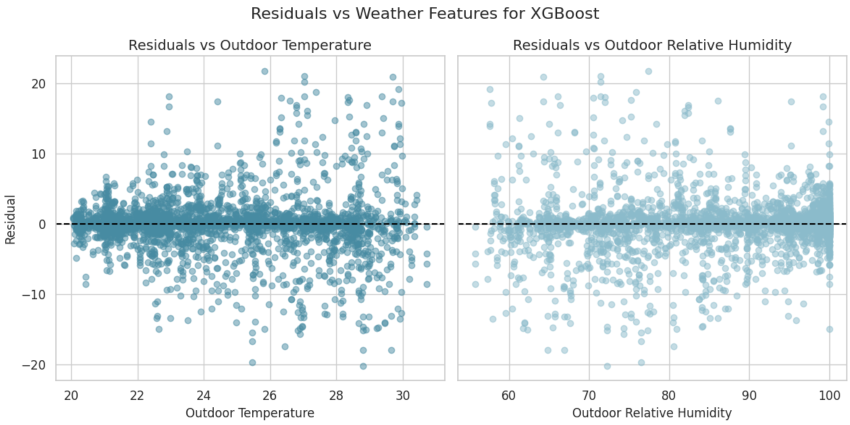


(c) Residuals vs Outdoor Conditions for Random Forest (Experiment 3)

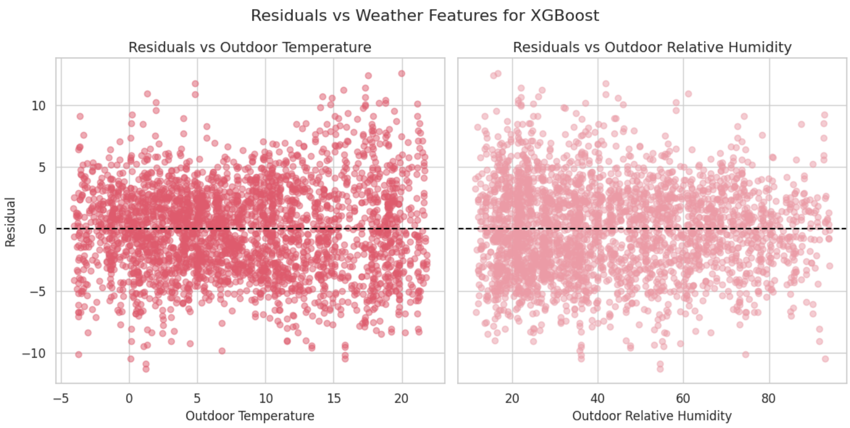
Figure 21: Residuals vs Outdoor Conditions for Random Forest Across Experiments



(a) Residuals vs Outdoor Conditions for XGBoost (Experiment 1)

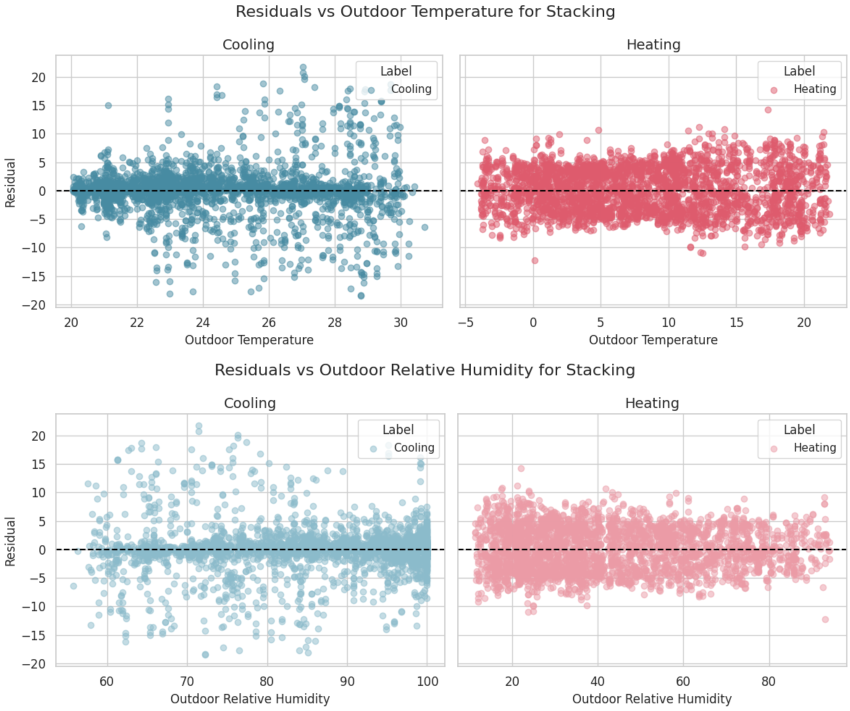


(b) Residuals vs Outdoor Conditions for XGBoost (Experiment 2)

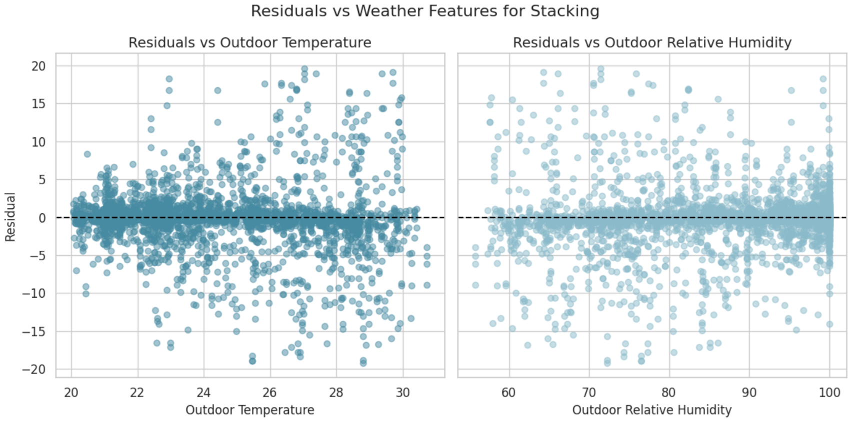


(c) Residuals vs Outdoor Conditions for XGBoost (Experiment 3)

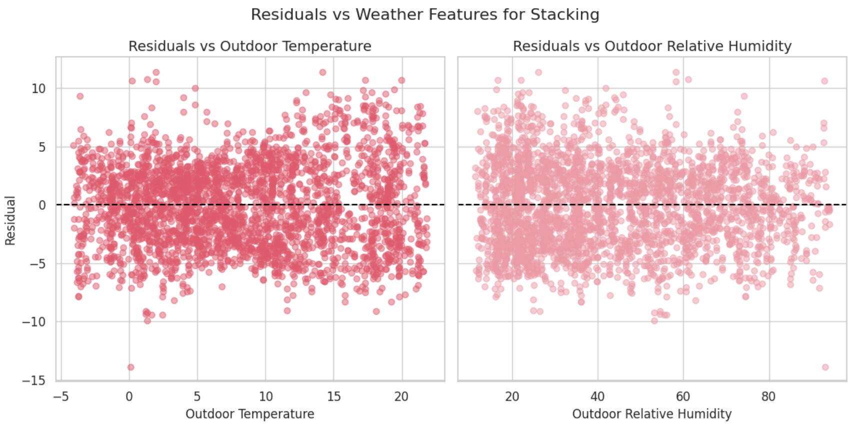
Figure 22: Residuals vs Outdoor Conditions for XGBoost Across Experiments



(a) Residuals vs Outdoor Conditions for Stacking Regressor (Experiment 1)



(b) Residuals vs Outdoor Conditions for Stacking Regressor (Experiment 2)



(c) Residuals vs Outdoor Conditions for Stacking Regressor (Experiment 3)

Figure 23: Residuals vs Outdoor Conditions for Stacking Regressor Across Experiments

6 DISCUSSION

This thesis investigated the main research question: **"How effectively can machine learning models predict and optimize energy consumption in HVAC systems for unoccupied multizone office buildings under diverse weather conditions?"** Advanced models, including Random Forest, XGBoost, and Stacking Regressor, were compared with Linear Regression as a baseline. These models were evaluated for predictive accuracy, key weather-related predictors, and robustness across cooling and heating scenarios, offering insights into optimizing HVAC energy consumption under varying environmental conditions.

6.1 *Sub-question Analysis*

To address the main research question, three sub-questions were formulated and explored:

- **How does the predictive accuracy of machine learning models differ between combined and separate datasets for cooling and heating, and what are the implications for energy optimization in HVAC systems?**

  Three experiments were conducted: one with a combined dataset of cooling and heating data, and two with separate datasets for each. Models including Random Forest, XGBoost, and Stacking Regressor were evaluated using Mean Absolute Error (MAE) and R^2 metrics.

  Results showed superior performance for models trained on separate datasets. XGBoost achieved a Mean MAE of 2.2033 ($R^2 = 0.7959$) for cooling and 2.8683 ($R^2 = 0.5876$) for heating, compared to a Mean MAE of 2.7935 ($R^2 = 0.8480$) on the combined dataset. The combined dataset introduced noise from overlapping energy patterns, while separate datasets captured scenario-specific dynamics more effectively(Goyal and Pandey, 2021a).

  These findings highlight the distinct characteristics of HVAC energy consumption for cooling and heating. Scenario-specific modeling enhances predictive accuracy, enabling better energy optimization by addressing seasonal energy demands dynamically.

- **Which weather variables are most critical for machine learning models to predict HVAC energy consumption, and how much can their contributions inform sustainable building energy management?**

Feature importance analysis across datasets identified indoor temperature as the most critical predictor, contributing up to 38% in cooling scenarios and remaining dominant in heating(Lu and Viljanen, 2009). Indoor-outdoor humidity differences significantly influenced cooling energy consumption, while heating relied on a broader range of temperature-related features, such as rolling averages and outdoor trends. Outdoor variables like solar radiation and wind speed provided additional context.

These findings underscore the pivotal roles of temperature and humidity in HVAC energy demands. Indoor temperature reflects efforts to maintain thermal comfort, while humidity impacts energy-intensive processes like air conditioning and dehumidification. Greater variability in heating energy consumption suggests more complex dynamics in heating scenarios.

Understanding key weather-driven factors enables precise predictions, which could help to save 15%-28% energy in HVAC systems (Si et al., 2022), supporting optimized HVAC operations to enhance energy efficiency and sustainability.

- **How can machine learning models address the challenges of predicting energy consumption in HVAC systems across diverse temperature and humidity conditions?**

  Residual analysis was conducted to evaluate model performance under varying temperature and humidity conditions, revealing patterns that inform HVAC system optimization.

  In cooling predictions (Experiment 2), Random Forest and XGBoost models performed well at moderate temperatures. Random Forest demonstrated greater robustness under high temperatures, maintaining tighter residuals near zero. In contrast, XGBoost excelled in high-humidity scenarios, effectively capturing the nonlinear effects of humidity on cooling energy demand. This suggests Random Forest is ideal for high-temperature environments, while XGBoost suits regions with high humidity(Pergantis et al., 2024).

  For heating predictions (Experiment 3), extreme low temperatures introduced higher residual variability, though both models performed well overall. Random Forest provided slightly more stable predictions, while humidity was found to play a secondary role compared to temperature.

  These findings highlight the value of residual analysis in dynamically selecting machine learning models based on environmental conditions. For instance, XGBoost may optimize cooling during humid summers, while Random Forest excels in handling extreme temperatures for both cooling and heating. This approach enhances energy efficiency and system reliability under diverse conditions.

6.2 *Main Research Question*

This study addressed the main research question: **"How effectively can machine learning models predict and optimize energy consumption in HVAC systems for unoccupied multizone office buildings under diverse weather conditions?"** By tailoring models to cooling and heating datasets, Random Forest and XGBoost significantly outperformed traditional approaches, achieving Mean MAEs as low as 2.2033 for cooling and 2.8683 for heating. The study identified **indoor temperature** and **humidity** as critical predictors, with temperature dominating heating demand and humidity exerting a stronger influence on cooling, aligning with prior studies H. Wang et al., 2023b; Xu et al., 2021.

Robustness testing showed that model performance varied with environmental conditions: Random Forest was more stable under high temperatures for both cooling and heating, while XGBoost excelled in high-humidity scenarios for cooling. These results highlight the complementary strengths of the models and the value of scenario-specific modeling, where dynamic model selection based on weather conditions enhances HVAC optimization. Models trained separately for cooling and heating consistently outperformed combined approaches by effectively capturing their distinct dynamics.

This study advances the literature on machine learning for HVAC systems by demonstrating robust performance under constrained data conditions. It highlights the practical potential of Random Forest and XGBoost to improve energy efficiency in unoccupied multizone office buildings across diverse weather scenarios.

6.3 *Societal Impact*

This study highlights the transformative potential of machine learning in improving energy efficiency and sustainable building management. By enabling HVAC systems to dynamically adjust operations based on weather conditions, advanced models drive significant energy savings. Scenario-specific models in this research showed accuracy improvements, consistent with prior studies reporting 15–28% reductions in energy consumption (Si et al., 2022). These enhancements not only reduce operational costs in public and commercial buildings but also support global sustainability goals, such as the EU Green Deal and U.S. Energy Efficiency Standards (Nations, 2015; Commission, 2020), while contributing to significant greenhouse gas reductions annually (Gobinath et al., 2024).

Beyond energy efficiency, optimized HVAC systems address broader social and economic challenges. Lower energy costs reduce operational expenses, indirectly benefiting industries like retail and healthcare (Teke and Timur, 2014). Effective energy management also eases strain on energy grids, especially during peak usage or extreme weather, which disproportionately affects low-income communities (Siddiqui et al., 2024). Machine learning models integrated into smart grids provide predictive insights for load balancing, stabilizing energy supply, and minimizing blackouts, thereby enhancing societal resilience.

Additionally, machine learning drives innovation in smart buildings, facilitating the transition to net-zero carbon buildings in alignment with global initiatives such as the Zero Carbon Buildings for All program (Institute, 2020). These advancements promote digital and sustainable solutions in construction and real estate while enabling integration with renewable energy sources and real-time adaptive controls for greater efficiency and reduced environmental impact (Turley et al., 2020).

In summary, machine learning-driven HVAC optimization delivers far-reaching societal benefits, including economic savings, enhanced equity, and critical support for sustainability goals. Future integration with renewable energy systems and adaptive technologies could amplify these impacts further (Keleher and Narayanan, 2019).

6.4 *Limitations*

This study is limited by its dataset scope, as it focuses on a single building in one region. While this allowed for a detailed analysis of weather-driven energy consumption, the findings may not generalize to other building types, climates, or locations. Expanding the dataset to include diverse buildings and regions would improve the robustness of the results.

Another limitation lies in the choice of machine learning models, which prioritized interpretability and computational efficiency. Advanced models like LSTM or Transformer, capable of capturing nuanced temporal dependencies, were not explored due to the dataset's temporal limitations. Future research could address this by incorporating long-term datasets and evaluating these models' performance in HVAC energy prediction.

Additionally, the study employed a random sampling approach for train-test splitting, which, while ensuring balanced data representation, may result in information leakage due to features like lagged and rolling variables. This could overestimate model performance when predicting unseen future data. Future research should consider time series splitting to better align with real-world forecasting scenarios.

Finally, the study focuses solely on weather variables, excluding other important factors such as building materials, insulation quality, and occupancy patterns. While this isolates weather effects, it limits the findings' applicability to residential and mixed-use buildings, where such factors significantly impact energy consumption. Future research should integrate these variables to develop more comprehensive models and explore applications in dynamic environments.

6.5 *Future Work*

Building on these limitations, future research should expand the dataset scope to include partially occupied or mixed-use buildings, enabling the validation of weather-driven predictions under more varied operational conditions. Data from diverse geographic and climatic regions should also be incorporated to enhance the model's generalizability. Furthermore, including residential buildings in future studies would broaden the applicability of these findings and allow comparisons across different building types.

Advanced modeling approaches, such as LSTMs or Temporal Convolutional Networks (TCNs), should be explored to better capture temporal dependencies, especially for heating dynamics. Hybrid models that combine physics-based and data-driven methods could leverage domain-specific HVAC knowledge for improved accuracy. Integrating human factors, such as occupancy patterns and behavioral data, represents another promising direction, particularly for mixed-use or residential buildings. Finally, applications in real-time HVAC control systems and dynamic load balancing align well with the emergence of smart building technologies, providing actionable solutions for sustainability in energy management.

7 CONCLUSION

This study demonstrated the effectiveness of machine learning models, such as Random Forest and XGBoost, in predicting and optimizing HVAC energy consumption in unoccupied multizone office buildings under diverse weather conditions. By separating datasets for cooling and heating, the models achieved superior accuracy (e.g., Mean MAEs of 2.2033 for cooling and 2.8683 for heating) compared to a combined dataset. Feature importance analysis identified indoor temperature and humidity as critical predictors, emphasizing their direct impact on HVAC energy demands.

These findings highlight the potential of tailored machine learning models to reduce energy waste, lower operational costs, and support sustainability goals. While the study is limited by its dataset scope and exclusion of real-time operational factors, future research should expand datasets, explore hybrid approaches, and incorporate dynamic control systems to enhance generalizability and practical applications. This research provides a foundation for weather-driven HVAC optimization, paving the way for more energy-efficient and sustainable building management.

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APPENDIX A

The following appendix provides supplementary figures that were not included in the main body of the paper due to space limitations. These visualizations offer additional insights into the exploratory data analysis (EDA) of the cooling and heating data, specifically focusing on temperature and humidity differences between indoor and outdoor environments. The figures in this appendix complement the main findings discussed in the paper and offer a more comprehensive view of the data trends across multiple days.

The scatter plots (From Figure 24 to Figure 29) compare energy consumption with temperature differences for cooling (blue) and heating (red) from specific dates in 2021.

Cooling (July 9-14): Energy consumption remains fairly constant, ranging from 20 to 40 kWh, regardless of temperature differences.

Heating (March 5-10): As the temperature difference increases, energy consumption generally decreases, indicating that less heating is required. This suggests that the heating system's energy consumption is influenced not only by the indoor and outdoor temperature difference but also by other factors, such as the building materials and construction characteristics.

These plots highlight the distinct energy behaviors of HVAC systems in cooling versus heating modes, reflecting their efficiency and response to environmental temperatures.

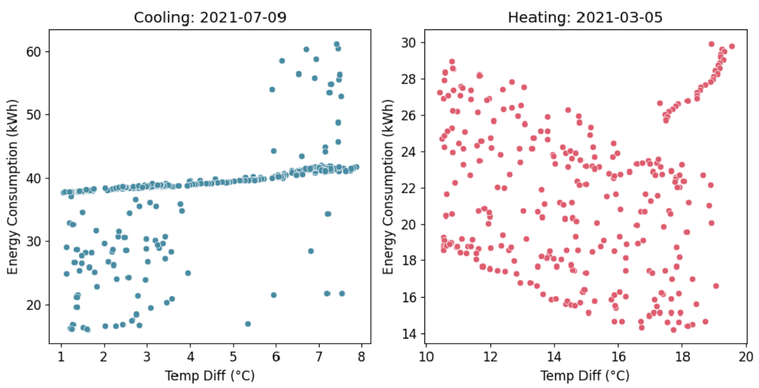

Figure 24: Temperature Differences vs. Energy Use in Cooling and Heating (a)

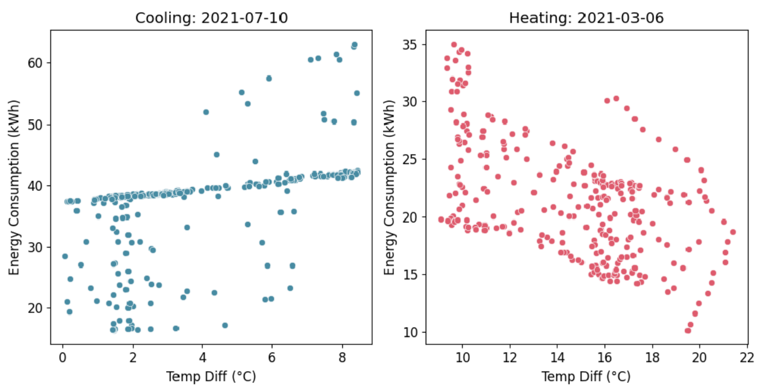

Figure 25: Temperature Differences vs. Energy Use in Cooling and Heating (b)

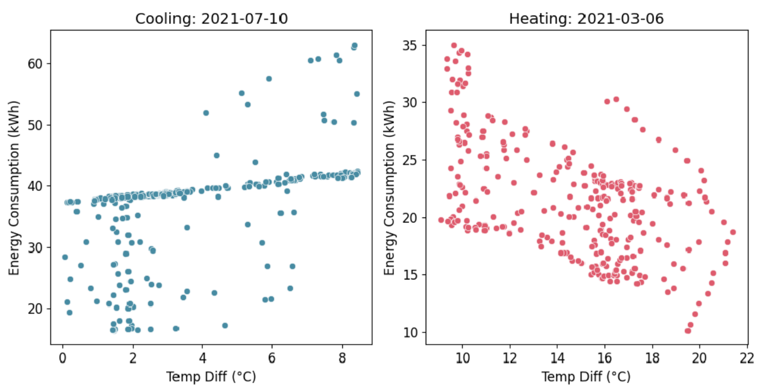

Figure 26: Temperature Differences vs. Energy Use in Cooling and Heating (c)

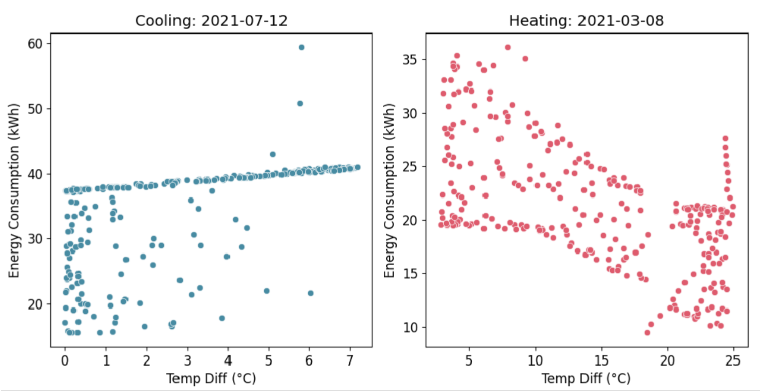

Figure 27: Temperature Differences vs. Energy Use in Cooling and Heating (d)

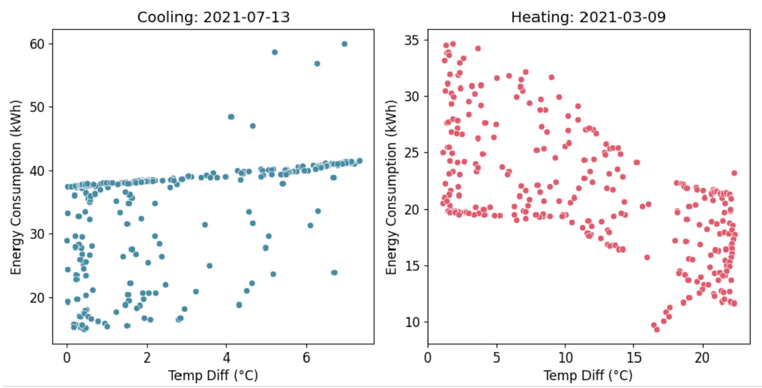

Figure 28: Temperature Differences vs. Energy Use in Cooling and Heating (e)

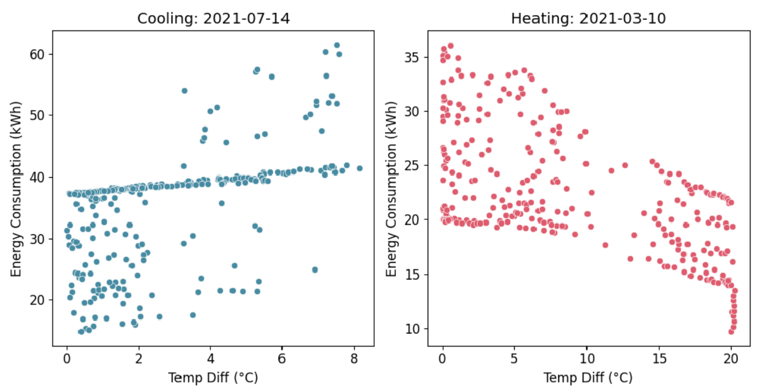

Figure 29: Temperature Differences vs. Energy Use in Cooling and Heating (f)

The scatter plots (From Figure 30 to Figure 35) showcase energy consumption related to humidity differences for both cooling (blue) and heating (red) systems from specific dates in 2021.

Cooling (July 9-14): The data points indicate that energy consumption reduced slightly as the humidity difference increased, typically ranging between 20 to 60 kWh. The trend is not as obviuos as that in heating data, suggesting that cooling systems may be efficiently managing humidity without significantly increasing energy expenditure.

Heating (March 5-10): In contrast, the heating data points show a decreasing trend in energy consumption as humidity differences increase, especially noticeable on dates like March 4 and March 10. This suggests that higher external humidity may reduce the heating load, possibly due to less air exchange.

These plots clearly differentiate the behavior of HVAC systems in response to changes in humidity during cooling and heating seasons, underlining the systems' adaptive responses to environmental conditions.

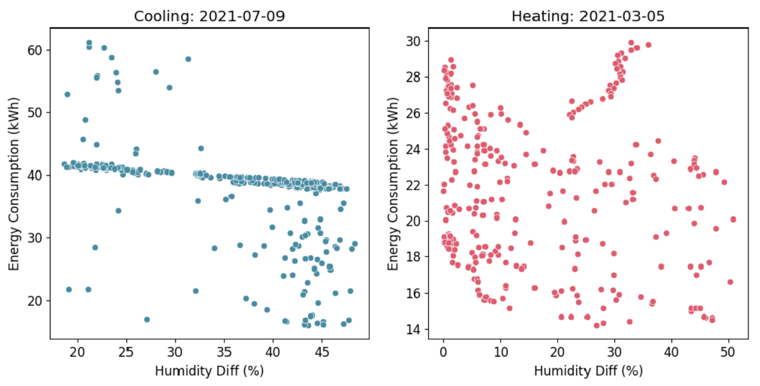

Figure 30: Humidity Differences vs. Energy Use in Cooling and Heating (a)

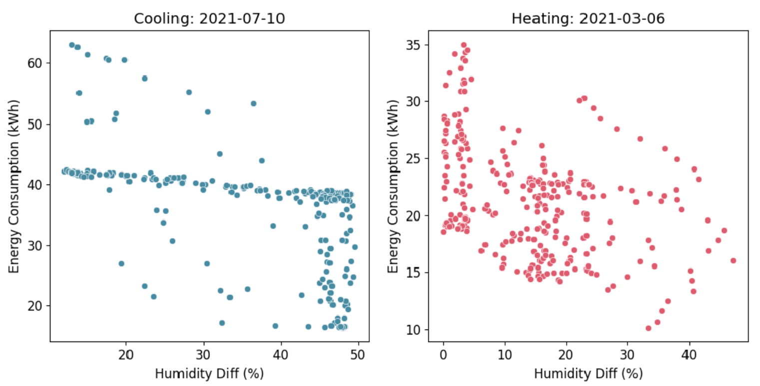

Figure 31: Humidity Differences vs. Energy Use in Cooling and Heating (b)

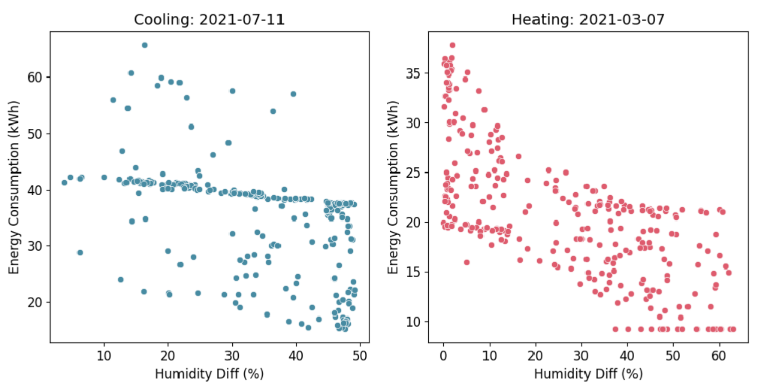

Figure 32: Humidity Differences vs. Energy Use in Cooling and Heating (c)

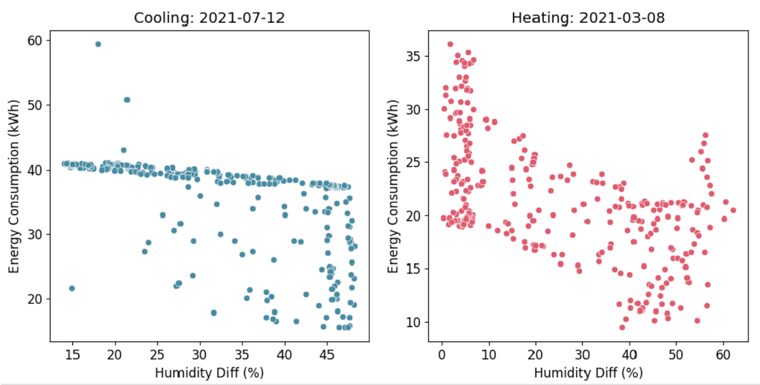

Figure 33: Humidity Differences vs. Energy Use in Cooling and Heating (d)

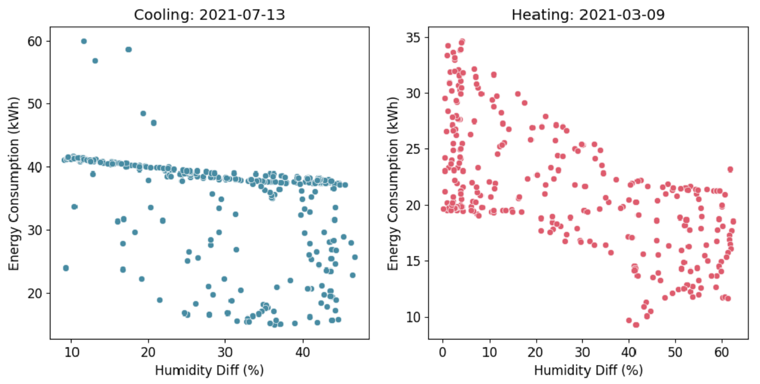

Figure 34: Humidity Differences vs. Energy Use in Cooling and Heating (e)

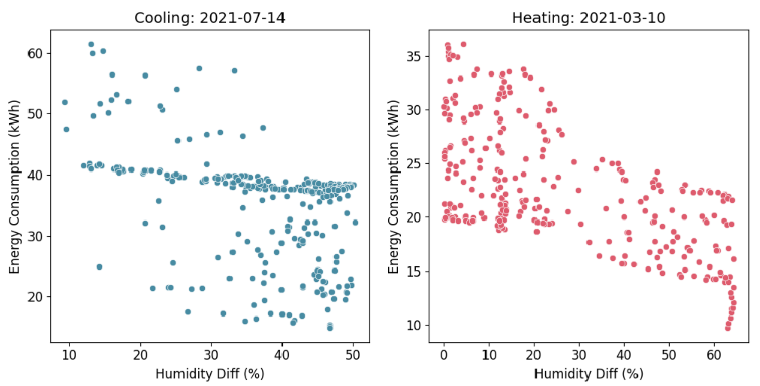

Figure 35: Humidity Differences vs. Energy Use in Cooling and Heating (f)

The provided plots (From Figure 36 to Figure 41) show daily data from July 9, 2021, to July 14, 2021, tracking mean indoor temperature, outdoor temperature, and energy consumption for cooling. A significant observation is the strong correlation between outdoor temperature spikes and energy consumption peaks, indicating increased HVAC activity on hotter days to maintain stable indoor temperatures.

Despite these trends, there are notable dips in energy usage on certain days, such as July 10 and July 14, suggesting intermittent reductions in HVAC use. These insights are essential for optimizing energy management and enhancing HVAC system efficiency in building operations.

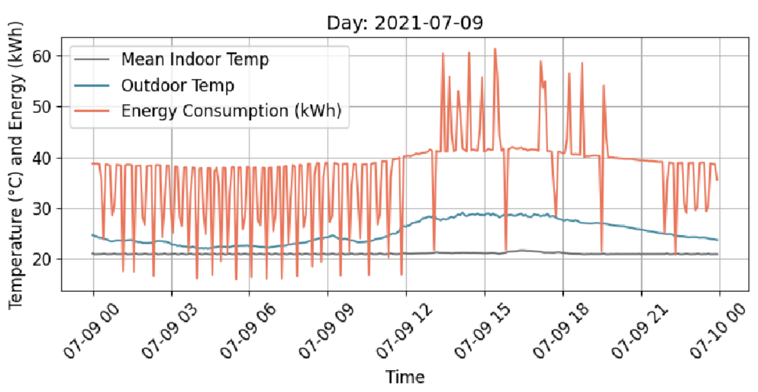

Figure 36: Time Series Temp and Energy Cooling(a)

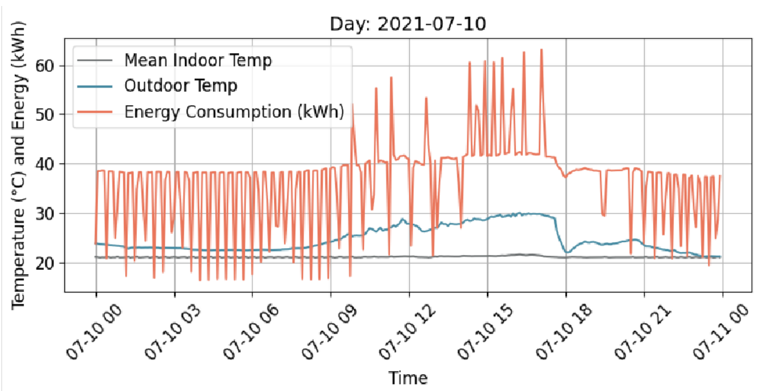

Figure 37: Time Series Temp and Energy Cooling(b))

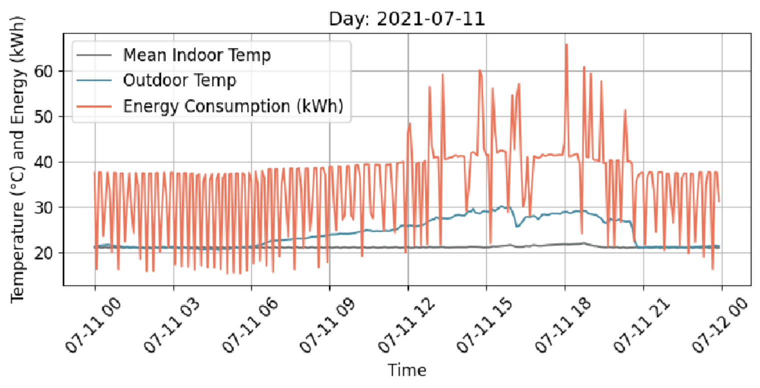

Figure 38: Time Series Temp and Energy Cooling(c)

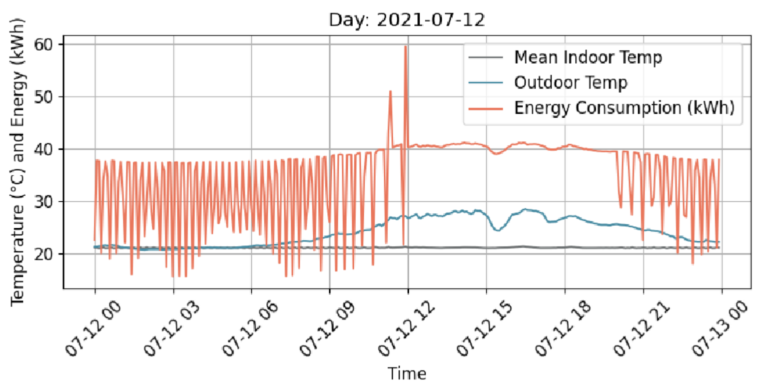

Figure 39: Time Series Temp and Energy Cooling(d))

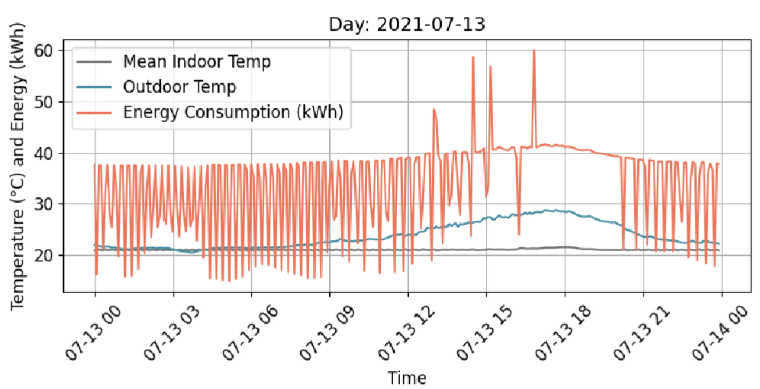

Figure 40: Time Series Temp and Energy Cooling(e)

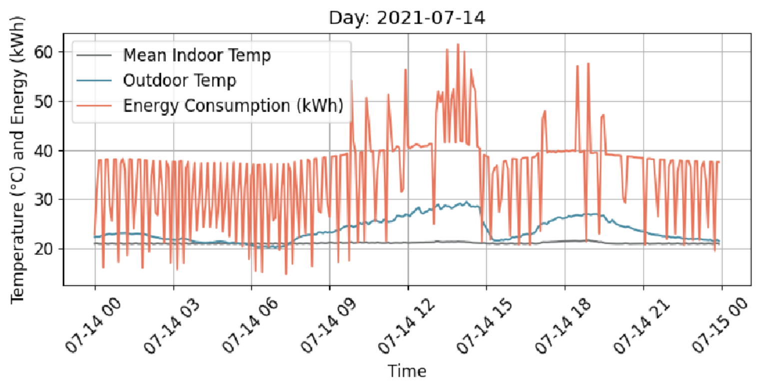

Figure 41: Time Series Temp and Energy Cooling(f))

The series of plots (From Figure 42 to Figure 47) from July 9 to July 14, 2021, illustrate the cooling data for mean indoor and outdoor humidity, alongside energy consumption. Notably, spikes in energy consumption coincide with periods of lower outdoor humidity. This suggests that the HVAC systems are working harder to exchange air when indoor and outdoor conditions are more similar, thereby conserving energy required for additional dehumidification.

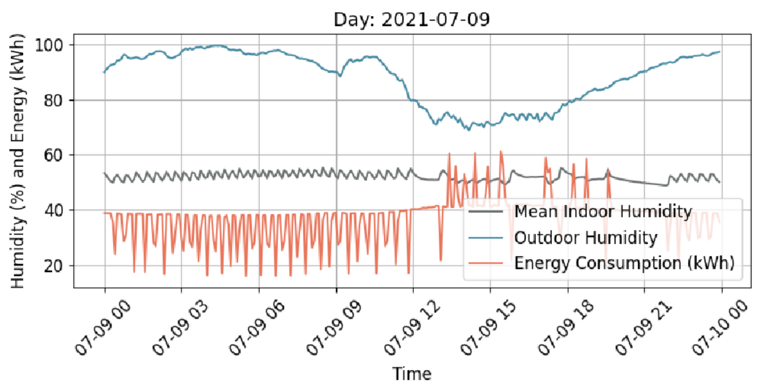

Figure 42: Time Series Humidity and Energy Cooling(a))

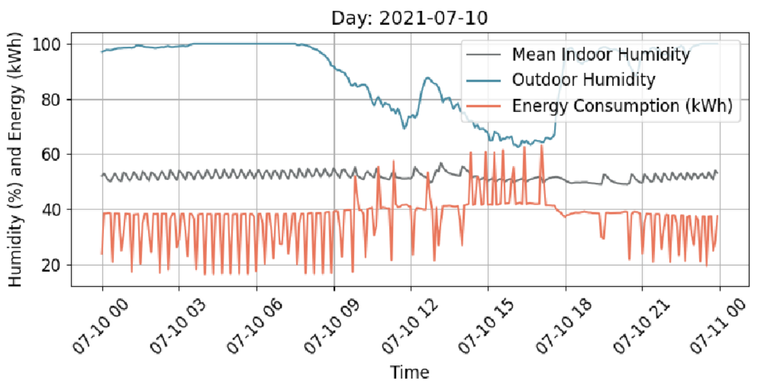

Figure 43: Time Series Humidity and Energy Cooling(b))

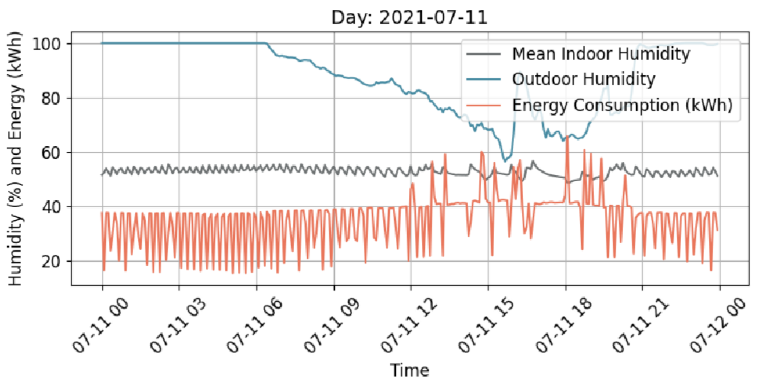

Figure 44: Time Series Humidity and Energy Cooling(c))

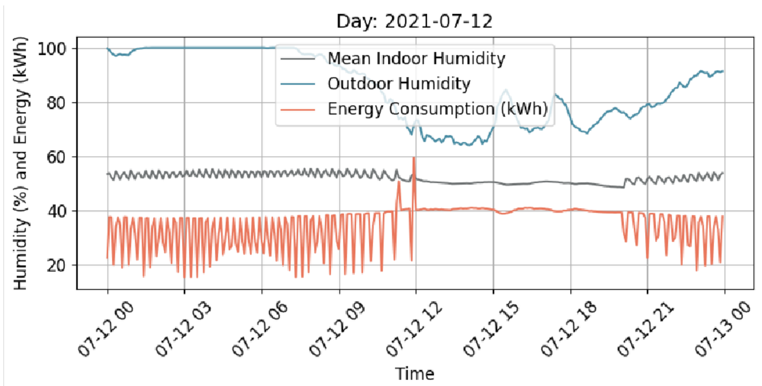

Figure 45: Time Series Humidity and Energy Cooling(d))

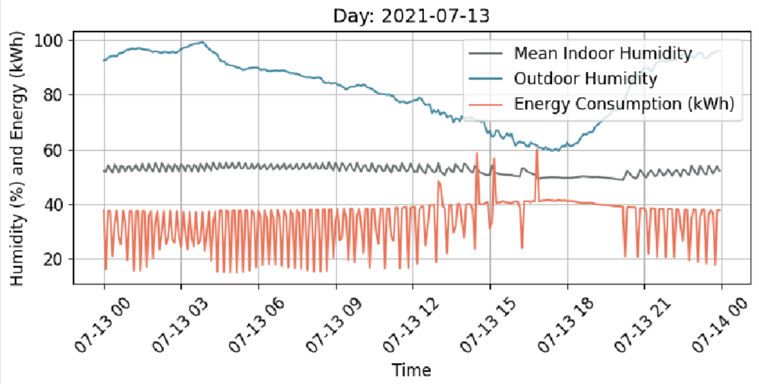

Figure 46: Time Series Humidity and Energy Cooling(e))

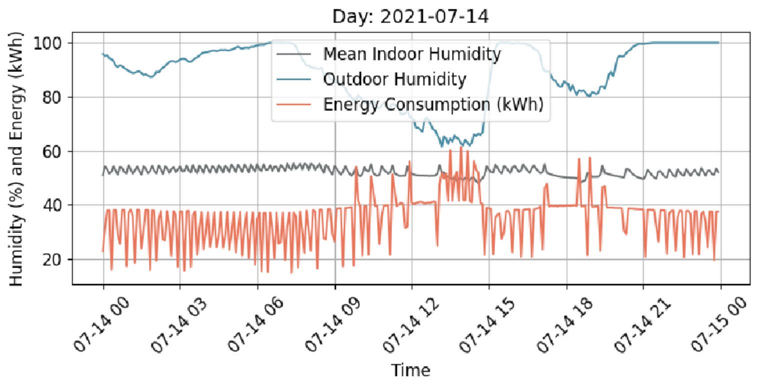

Figure 47: Time Series Humidity and Energy Cooling(f))

The plots (From Figure 48 to Figure 53) from March 5 to March 10, 2021, show that when the outdoor temperature is significantly lower than the indoor temperature, the HVAC energy consumption remains relatively stable. However, as the outdoor temperature drops further, energy consumption suddenly spikes and continues to rise even as the outdoor temperature begins to increase. This behavior contrasts with the cooling system chart, indicating that the energy consumption of the heating system is influenced by temperature changes but operates under a mechanism distinct from cooling systems. This suggests that the heating system's operation is likely affected by factors beyond just the indoor and outdoor temperature difference.

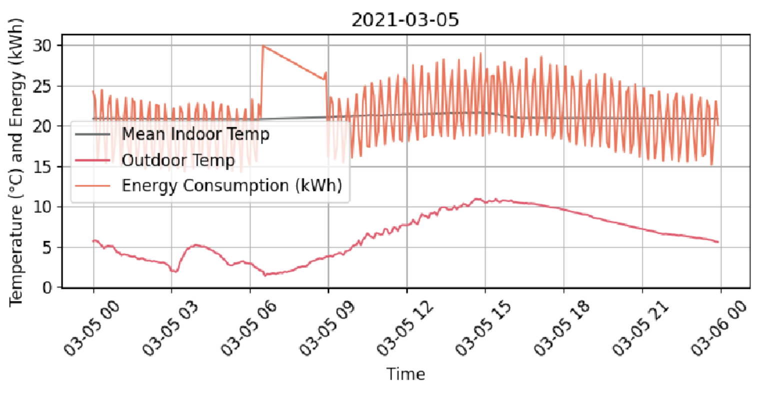

Figure 48: Time Series Temp and Energy Heating(a)

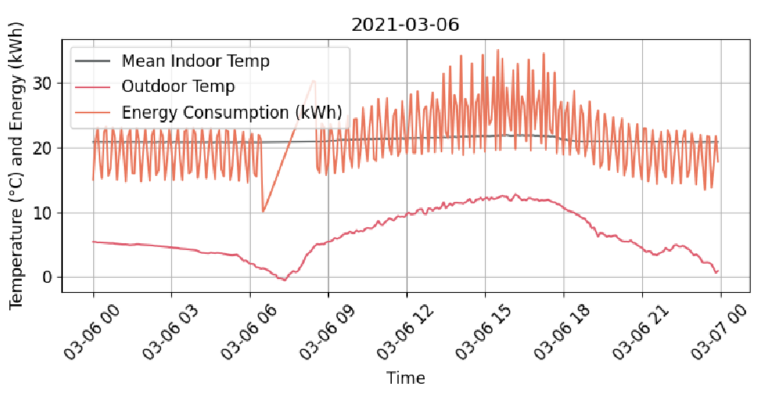

Figure 49: Time Series Temp and Energy Heating(b)

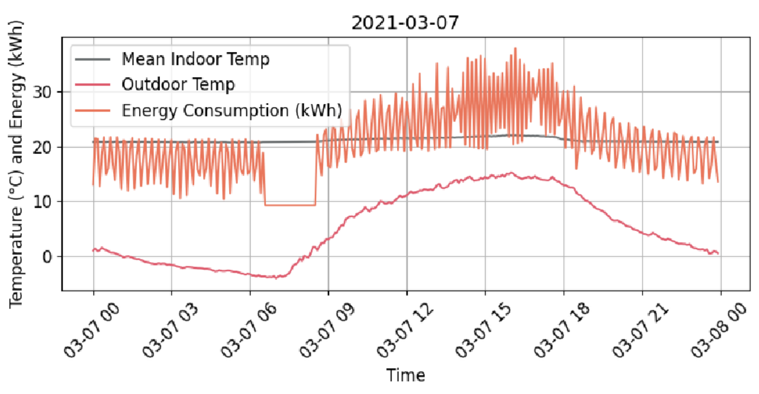

Figure 50: Time Series Temp and Energy Heating(c)

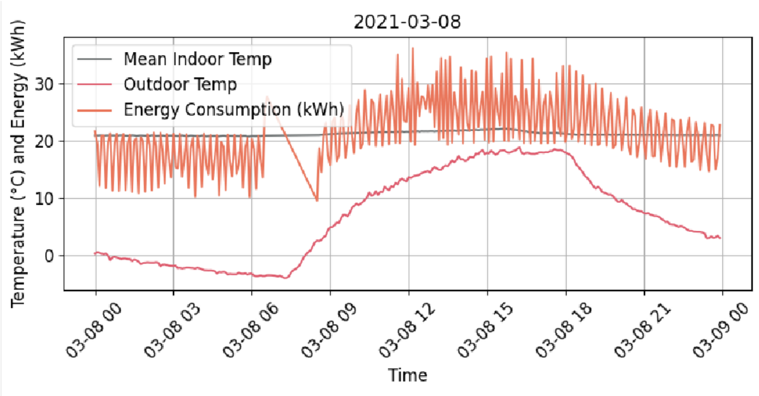

Figure 51: Time Series Temp and Energy Heating(d)

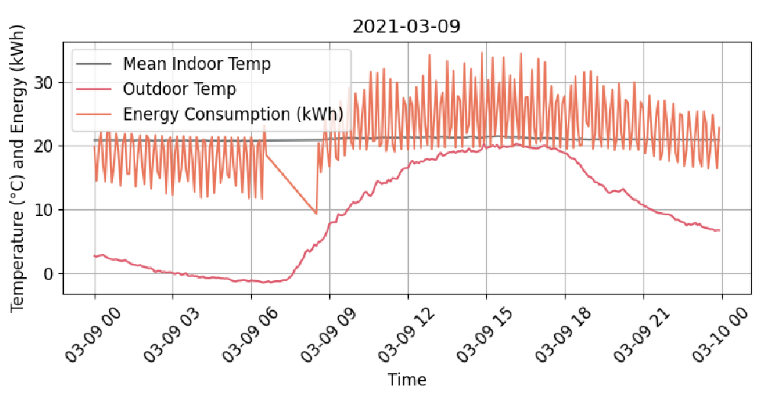

Figure 52: Time Series Temp and Energy Heating(e)

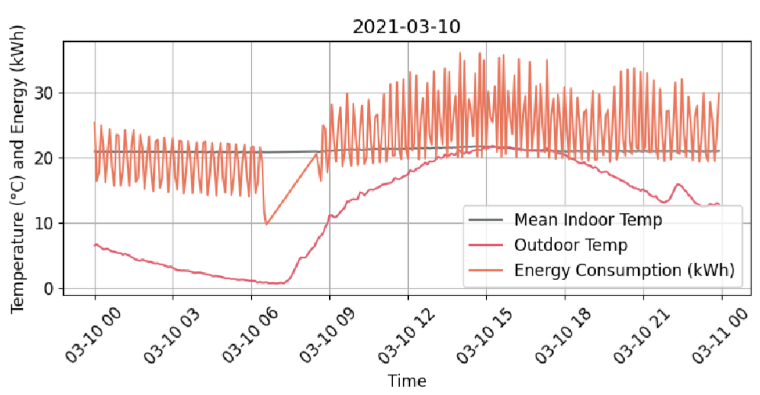

Figure 53: Time Series Temp and Energy Heating(f)

The plots (From Figure 54 to Figure 59) from March 5 to March 10, 2021, illustrate heating data for mean indoor humidity, outdoor humidity, and energy consumption. Notably, energy consumption increases when the indoor humidity relatively equal to outdoor humidity, indicating the heating system's response to maintain comfort. Days like March 6 and March 9 show this correlation distinctly. This data helps understand the impact of indoor and outdoor humidity on energy use and can guide optimization of HVAC systems.

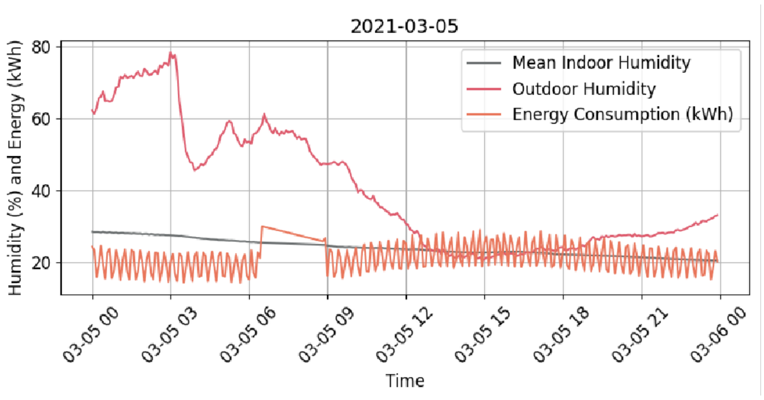

Figure 54: Time Series Humidity and Energy Heating(a)

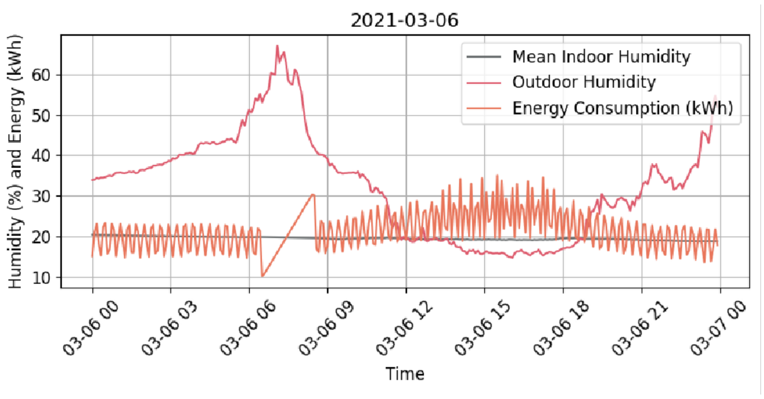

Figure 55: Time Series Humidity and Energy Heating(b)

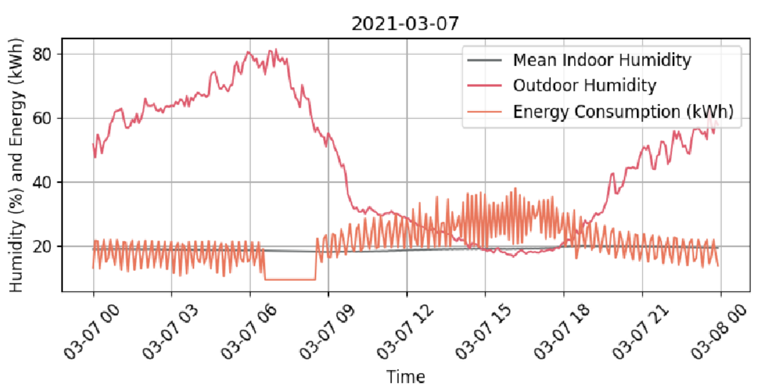

Figure 56: Time Series Humidity and Energy Heating(c)

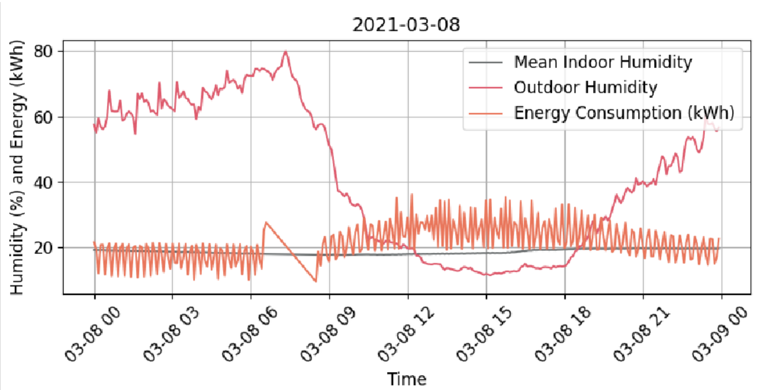

Figure 57: Time Series Humidity and Energy Heating(d)

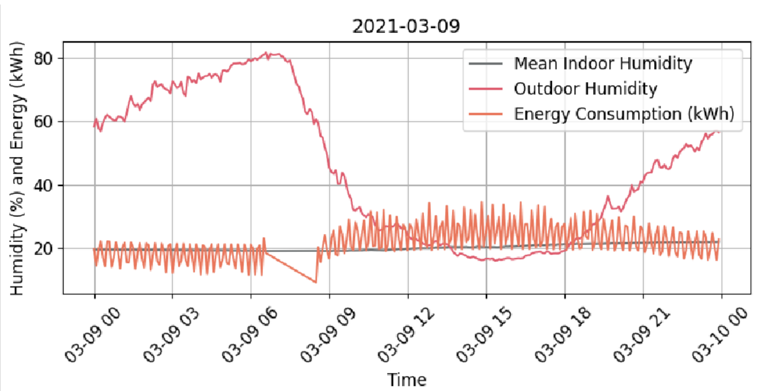

Figure 58: Time Series Humidity and Energy Heating(e)

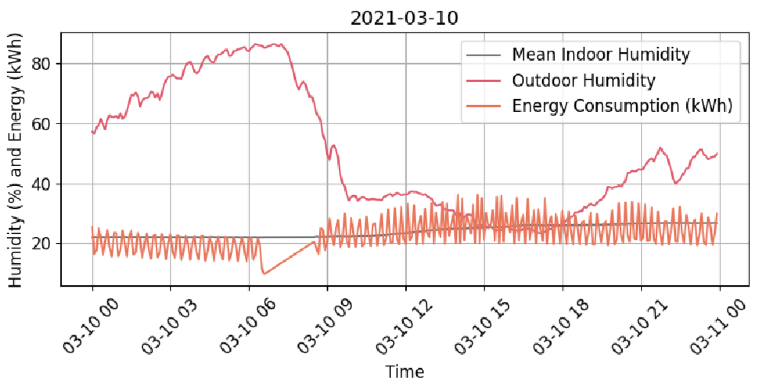

Figure 59: Time Series Humidity and Energy Heating(f)