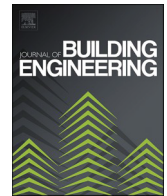




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Estimating cooling loads of Arizona State University buildings using microclimate data and machine learning

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ABSTRACT

In hot arid urban climates, building cooling equipment consumes the greatest share of energy out of all building end-use equipment. For existing buildings, dynamic system-based building energy simulation tools have provided valuable information on the impact of microclimates on cooling energy use. However, such models require in-depth information on building model parameters and often suffer from modeler bias even when sufficient calibration indices are satisfied. This study presents a data-driven approach for predicting the cooling loads of three university buildings in Arizona using simulated microclimate data. A microclimate model ENVI-met generated the input micro-scale weather data for each building. The ENVI-met simulation was validated using in-situ observations during the summer of 2018. Multiple machine learning algorithms were implemented. A final model was selected and used as baseline to predict cooling loads for each building in the dataset. The model predicts chill water tons per square meter using microclimate variables that include mean air temperature, mean absolute humidity, shading levels, and direct shortwave radiation. The black-box model was explained using an advanced machine learning model interpretation library in Python: SHAP. The baseline model predicted cooling loads with a prediction accuracy score of 0.98 using the tree-based algorithm Random Forest. Sensitivity analyses and scenario results showed that cooler microclimates reduced cooling loads for the modeled buildings. The developed framework will be used in future study extensions to explore the impacts of simulated microclimate scenarios generated by ENVI-met.

Nomenclature

Abbreviations

ASHRAE American Society of Heating, Refrigerating and Air-Conditioning Engineers

BES Building Energy Simulation

CFD Computational Fluid Dynamics

CHWTON Chill Water Ton

DUE-S Data-driven Urban Energy Simulation

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MAE	Mean Absolute Error
MAPE	Mean Absolute Percentage Error
MBE	Mean Bias Error
ML	Machine Learning
mmBTU	Million British Thermal Units
RMSE	Root Mean Square Error
SQM	Square Meter
UWG	Urban Weather Generator
UHI	Urban Heat Island

Symbols

X	Input
Y	Output
kW	Kilowatt
W	Watt
m	Meter
R^2	Coefficient of Determination
$f()$	Function
y	Sample Output
x	Sample Input
$\bar{y}$	Mean of All Samples
n	Total Number of Sample Data

Subscripts

w	Microclimate Variables
e	Energy Variables
kW	Kilowatt
b	Building Variables
i	Sample Data Point

1. Introduction

The past decades have experienced rapid population growth. In dense urban developments, ambient air temperatures are higher than rural areas driven by land cover changes and anthropogenic heat, a phenomenon known as the Urban Heat Island (UHI) effect [1]. With climate change on the rise, the UHI effect will increase in magnitude in the coming decades. The impact of UHI on building cooling energy consumption must be addressed for arid regions.

Buildings contributed 30% to global energy demand in 2019 and are responsible for one third of global greenhouse gas emissions, making them a focal point for efficiency improvements [2,3]. With global warming increasing air temperatures, cities that experience extreme heat will face many challenges in decreasing their carbon footprint while meeting cooling energy demands. The most recent data from 2009 show that cooling accounts for 25% of residential energy consumption in Arizona, compared to the 6% national average [4].

Building energy efficiency strategies are typically modeled using Building Energy Simulation (BES) tools. Such models require great attention to detail to avoid high uncertainty in the model outputs. Although BES models provide extensive knowledge of the underlying mechanisms and system dynamics of the model providing the opportunity to explore different design elements and scenarios, most BES models rarely consider the modeled building's microclimate weather parameters [5]. Instead, typical BES models use nearby weather station data, usually airport data, to simulate hourly energy consumption of the modeled building. Weather station data captures regional weather patterns but are not representative of the microclimatic conditions the buildings are embedded in.

In addition to the use of inaccurate weather data, BES models significantly suffer from bias errors that are evident when results are compared to actual data [6]. Many sources of bias stem from the complexity of buildings and how they are represented in BES models. Configuration of a BES model requires detailed information about the modeled building and how it operates daily and seasonally. Alternatively, energy predictions can be generated using Machine Learning (ML) algorithms that use statistical methods to find relationships between dependent and independent variables [7].

A ML model requires input data known as features to predict the output known as response. The design of an ML algorithm involves data processing, selection of an appropriate algorithm, feature engineering, and assessment of model accuracy using prediction scores and other indices usually applied on a separate testing dataset. Feature engineering is one of the most important steps throughout the process, requiring the selection of features that will provide the best results. For building energy predictions, modelers have tested a variety of different features such as outdoor weather conditions (dry-bulb temperature, solar radiation), indoor environmental conditions (room temperature, room relative humidity), building characteristics (geometry, orientation), time (type of day, type of hour), and operation characteristics (building use schedule, number of occupants) [8]. The selection of features depends on the magnitude of

their impact on the model's response as well as the purpose of the model. For example, to investigate the impact of occupant behavior, features related to occupants should be included.

Multiple ML algorithms have been developed, and selecting an appropriate algorithm depends on the type of data and the prediction type (numerical or categorical). In terms of learning style, ML algorithms fall under the following categories: supervised learning, unsupervised learning, and semi-supervised learning. Supervised learning happens when each data point in the training data has a known output. For unsupervised learning, the output is unknown, and for semi-supervised learning, the training data consist of a mixture of known and unknown output.

Microclimatic conditions are impacted by the configuration and composition of urban features including buildings, plants, and roads. Accurate microclimate conditions surrounding a specific building can be obtained through in-situ observations, but most buildings do not have outside sensors, and building modelers rely on available weather station data closest to the building. Alternatively, microclimate data can be simulated using Computational Fluid Dynamics (CFD) models. CFD models simulate flow by numerically solving governing equations of fluid flows. For microclimate simulations, CFD models replicate the flow of air and heat in neighborhood-sized study areas. The most popular and frequently used CFD model in urban climate studies is ENVI-met [9]. The model has been used to investigate the impact of urban form and landscaping on microclimate [10,11], the temperature amelioration by trees [12,13], effects on outdoor water use [14], and human thermal comfort [15,16].

This paper presents a novel framework to investigate the microclimate effect on three university buildings in Arizona using the CFD model ENVI-met to simulate microclimate coupled with a supervised ML algorithm to predict building cooling energy. Specifically, tree-based ML models were explored due to their interpretability using SHAP analysis. SHAP analysis provides local interpretation of the impact of different features on the model's output and are highly compatible with tree-based algorithms such as Random Forest, XGBoost, and LGBM [17]. Features included microclimate variables local to the modeled buildings.

The structure of the paper is as follows: Section 2 reviews the literature. Section 3 covers the methodology and modeling overview. Section 4 displays the results of the modeled buildings and their interpretations using SHAP. Section 5 presents a sensitivity analysis where variations of the microclimate were modeled to understand their impact on cooling energy. Section 6 discusses the results from section 4 and 5. Section 7 concludes the study.

2. Literature review

Building energy consumption varies significantly from one building to another. In terms of cooling loads, some buildings have high correlation with exterior air temperature and other weather parameters, while other buildings are not greatly affected by weather and are dominated by interior heat transfer from occupants and/or devices. Cooling loads are also influenced by thermal comfort requirements of a building, which varies based on building type, location, and operations. Heidarinejad et al. [18] studied university buildings and classified them based on their energy consumption in response to outdoor weather conditions. Buildings were classified as (1) externally-load dominated, (2) internally-load dominated, and (3) mixed-load dominated. Externally-load dominated buildings, which are also called envelope-dominated, or skin-load dominated, are those which are directly correlated with outdoor weather conditions. Internally-load dominated buildings on the other hand are influenced more by internal loads from equipment and occupants. Finally, mixed-load dominated buildings are influenced equally by outdoor weather conditions and internal loads.

Building energy efficiency improvement is an active area of research. In the United States, The American Society of Heating, Refrigerating and Air-Conditioning Engineers (ASHRAE) Standard 90.1 provides a benchmark for commercial building energy codes. These guidelines are updated every three years. Standard 90.1 covers building envelope, heating, ventilating, and air conditioning, service water heating, power, lighting, and other equipment. For each component, minimum compliance requirements are outlined in detail. Some requirements, such as building envelope, depend on the specific climate zone within which a building is located. Furthermore, Standard 90.1 includes a performance-based rating method, Appendix G, that provides an alternative compliance method. In this approach, simulation tools are necessary to compare baseline and proposed design energy consumption. Building efficiency rating systems such as LEED utilize Appendix G in their certification process.

In practice, building energy reduction strategies are tested using BES models, which utilize physics-based dynamic computations [19]. Meeting ASHRAE Appendix G requirements for example, demands the use of BES tools for compliance. The impact of occupancy behavior on a building's energy consumption is one of the major challenges for physics-based dynamic models and introduces high uncertainty in the model's time variant occupancy related parameters which translates to uncertainty in the model's outcomes [20]. Occupant behavior is often oversimplified and is not well understood, leading to significant gaps between simulated and actual energy use [21]. In a typical BES model, occupant behavior inputs are deterministic, which does not fully capture the stochasticity of occupant behavior. He et al. [22] defined three occupant behavior patterns (austerity, normal, and wasteful) and used the BES simulation tool EnergyPlus to quantify the differences in their energy consumption for a medium office building. They conclude that stochastic occupant behavior significantly impacts building energy consumption. For wasteful occupant behaviors, a 36% increase in energy consumption was observed. Amasyali et al. [8] found that occupant behavior made a difference of over 7 times in building energy consumption.

The effect of occupants, however, may not significantly alter cooling consumption patterns in externally-load dominated buildings that have consistent cooling consumption intensities irrespective of the number of occupants and their activities in a building. The outdoor design and structure of an urban development influences the surrounding microclimatic conditions which, as a result, impacts cooling energy consumption levels for externally-load dominated buildings. Mixed-load dominated buildings can also be impacted by the surrounding microclimate, however, the impact will be less. For hot climate regions, the addition of vegetation, high albedo material, and urban shade to building facades could potentially reduce cooling energy use [23].

The availability of local weather data is highly beneficial for modeling a building's energy consumption. Hong et al. [24] used local weather observations over a span of 10 years to study the effect of microclimate on energy patterns and indoor air temperature. The availability of historical microclimate data allows for the analysis of the UHI effect on building energy with less uncertainty depending on the resolution of the available data (density of measured microclimate weather data at a specific site location). However, not many regions collect high resolution microscale weather data and as such, researchers rely on simulated weather data using CFD or other simplified calculations such as the Urban Weather Generator (UWG) [25–27].

Past studies have investigated the effect of microscale weather conditions on a building's cooling/heating energy consumption using a coupled simulation approach by integrating a CFD model with a BES model such as eQuest or EnergyPlus [23,28–32]. Sedaghat et al. [23] combined ENVI-met simulations with EnergyPlus models and found that the UHI intensity varied from 3 °C to 6 °C during summer in Tehran. Using a combination of high-albedo material and added vegetation, energy savings ranged from 11% to 29% for residential buildings. Hadavi et al. [30] investigated the effects of urban configuration and density on urban climate and building energy consumption by combining OpenFOAM, a CFD simulation tool, and EnergyPlus. They found that decreasing urban compactness mitigates UHI intensity providing up to 16.4% energy savings. Zhang et al. [32] combined ENVI-met with EnergyPlus to investigate the effect of urban form on microclimate and building energy loads for eight generic residential district prototypes in Nanjing, China. They found that the use of microclimate data compared to EPW data, collected from a weather station, resulted in a difference of up to 23.4%. One of the limitations mentioned in the study is the lack of validation between simulated and actual energy and microclimate data.

Mosteiro-Romero et al. [5] coupled ENVI-met with a district scale energy simulation tool, City Energy Analyst, to investigate the effect of the microclimate on district scale energy consumption. They found that considering local microclimate conditions led to an increase of 5% in cooling demand. One of the limitations mentioned in the study, which is also evident in the previously mentioned BES-CFD coupling methods, lies in the assessment of the UHI effect. The comparison of baseline conditions using rural weather station data to microclimate conditions using CFD based simulation data may not fully capture the impact of microclimates on building energy consumption. Using rural weather data to represent baseline conditions would likely result in higher variations of cooling loads when compared to simulated microclimate data. A better approach would be to compare simulated microclimate data, validated by actual measured data, with simulated microclimate scenarios by modifying the validated microclimate model. The baseline microclimate simulation results would be used to simulate baseline building energy consumption. The baseline energy consumption would then be compared to energy consumption results under simulated microclimate scenarios, such as increased vegetation and added shade. Skelhorn et al. [33] followed this approach by using ENVI-met for microclimate simulations and IES-VE as the BES tool to measure these impacts for three commercial buildings in Manchester, UK. They found that adding 5% mature trees reduced cooling loads by 2.7% in July.

Results from these studies may be highly influenced by potential bias that exists within BES models that might not be evident [6]. For example, a modeled building could be validated with actual data using statistical indices, but the model might inaccurately simulate wall/roof insulation or air ventilation. The model may also underestimate equipment loads and overestimate HVAC loads. In such scenario, simulated results might match actual energy data, but the model would be highly influenced by a change in external weather conditions.

In recent years, statistical ML methods have been widely used in engineering applications related to building energy. Engineers and researchers use ML techniques to find relationships between building parameters for different applications including efficient building operation, efficient building design, occupancy estimation, fault detection, and energy forecasting [8,34–38]. However, ML modeling for building energy management is a relatively new field that has limited publications compared to conventional approaches. The advantage of using black-box ML models is that they require relatively little modeling effort and can capture relationships between model parameters with great precision. For some problems, the level of detailed data required to build white-box models, such as BES tools, make their usage infeasible.

Nutkiewicz et al. [31] proposed a Data-driven Urban Energy Simulation (DUE-S) framework to study the inter-building energy dynamics and urban microclimate factors that impact building energy use. The framework, which incorporates ML, was applied to 22 university buildings in California. The study utilizes BES models simulated with typical building parameters obtained from the DOE archetype models corresponding to different building types. The framework generalizes these building parameters for the selected buildings and models the geometry of the buildings using GIS data. The results of the BES simulations were then used as inputs to an ML neural network architecture ResNet to learn the relationships between simulated and metered energy data. The authors conclude that the ResNet model captures uncertainty introduced by BES simulations related to inter-building dynamics and microclimate factors. Although the proposed BES-ML framework captures these differences due to microclimate impacts, utilization of such framework to explore different microclimate scenarios is limited.

Multiple studies in the literature have explored the use of ML to predict building energy consumption using different features. Dong et al. [39] and Hong et al. [40] used climate related features to predict energy consumption. Zhang et al. [41] used dry-bulb temperature to predict hot water energy rate. Ascione et al. [42] predicted energy consumption using geometry, envelope, building operation, and HVAC-related features. Rastogi et al. [43] used a combination of building characteristic and climate related features to predict heating loads. Some studies used previous loads to forecast building energy consumption [44–46]. Amasyali et al. [47] used occupant behavior to predict cooling energy consumption in buildings. Acceptable accuracies were achieved using ML techniques in these studies. Different ML algorithms were used to generate these predictions, most notably deep learning approaches and ensemble approaches [47]. Each approach has its advantages and limitations. In this study, tree-based algorithms, which fall under ensemble approaches, were used for their ability to be interpreted using SHAP analysis. Multiple models were tested and compared for the final model selection. The final model was used to predict cooling loads and used to perform a sensitivity analysis in which microclimate

variables were modified to observe changes in response.

To date, no studies have used CFD based microclimate simulated data as features in an ML algorithm to predict building cooling loads. To fill this gap, this paper explores a simulation based and data driven approach by integrating a CFD model, ENVI-met, with a ML algorithm to predict cooling loads of three Arizona State University buildings in Tempe, Arizona. The novelty in this approach lies in the ease of use compared to BES tools and the ability to use different microclimate scenarios to predict energy consumption. Simulated microclimate data was used as input to the machine learning model in which the model learns the relationship between microclimate variables (air temperature, absolute humidity, shading, and direct shortwave radiation) and the building's measured cooling loads collected for each building in the study. A baseline ML model was developed to predict building cooling loads under the current simulated microclimate condition. A sensitivity analysis was performed for the baseline model where weather parameters were altered to observe impact on model predictions. The baseline ML model will be used to assess the impacts of ENVI-met simulated microclimate scenarios in future extensions of this work.

3. Methodology and model overview

The focus of this study is to understand the impact of the microclimate on externally-load or mixed-load dominated university buildings in Arizona State University (ASU). ASU provides a database of energy consumption for all campus buildings. University buildings include laboratories, offices, classrooms, and other research related facilities. Examining ASU's building energy dataset showed that most of the buildings on campus are internally-load dominated. This was identified by the lack of trends in cooling loads compared to weather parameters. Most buildings are clearly unaffected by changes in weather conditions, and it is assumed that cooling loads are impacted by other factors such as building operation patterns and internal heat gains. As such, only three buildings were identified as either mixed-load or externally-load dominated based on correlations between cooling energy and ambient air temperature and absolute humidity. Since correlations did not exceed a value of 0.76, it is likely that these buildings are not fully

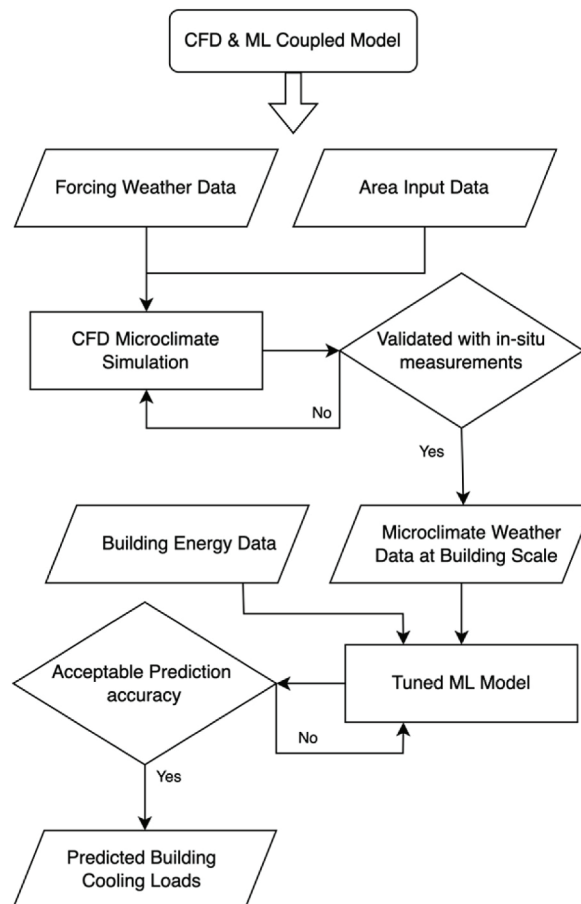


Fig. 1. Flow chart of Coupled Computational Fluid Dynamics (CFD) and Machine Learning (ML) Algorithm. The following is a summary of the above flow chart: 1. Generate the area input data for the modeled area. 2. Obtain weather forcing data from the closest weather station. 3. Run the CFD simulation with (1 and 2) as inputs and validate results with actual measurements. 4. Generate simulated microclimate data for each building from the CFD model. 5. Obtain each building's energy consumption data for the same timestamps as simulated microclimate data. 6. Tune a ML model and test results on testing dataset. 7. Predict cooling loads using the tuned model.

dominated by external loads.

The approach used in this analysis combines a CFD simulation model with a tree-based ML model. The two models are not directly linked. The microclimate data from the CFD simulation was used as input variables or features to the ML model. A flow chart of the proposed coupling method is shown in Fig. 1.

The data used to build the ML model were collected from two main sources: (1) ENVI-met microclimate simulations, and (2) ASU's campus metabolism website for building energy data [48]. The ENVI-met model was validated for the study area for a hot summer day in a prior study [15]. The simulated timeframe was from 5am to 8pm for 12 days in summer of 2018 (4 days in May, 8 days in June, and 1 day in July) using hourly local airport weather data (Sky Harbor) as forcing. The 12 simulated days were combined with available building energy data at 15-min timestamps from the campus metabolism website. The modeled area includes the following ASU buildings: Psychology, ISTB 4, and Psychology North. Table 1 contains information on the coordinates and area distribution for each building. Fig. 2 shows a map of the buildings and the ENVI-met domain, which spans $210 \times 250 \times 33$ grid cells at 2-m resolution.

Statistical machine learning models find relationships between input (X) and output (Y). For the developed model, the output (Y) was the chill water ton per square meter ($CHWTON/SQM$) of the building at a specific time. Data for the model output was collected from ASU's campus metabolism database. The raw data was in units of $CHWTON$ which was then divided by the conditioned area of each building obtained from ASU's facilities management database resulting in units of $CHWTON/SQM$ [49]. Dividing by the conditioned area allows for comparisons of the cooling intensities of each building.

The input data set (X) includes some of the outputs generated by ENVI-met for each building including mean air temperature and mean absolute humidity around the building surfaces, shading at each façade, and direct shortwave radiation at each facade including the top surface of the building. The input data set (X) also includes kW electricity usage and heating energy in $mmBTU$ which was collected with the $CHWTON$ data for each building from the campus metabolism website. Finally, building names were one-hot encoded and included in the training process as part of the input data. This will allow the model to distinguish between the different buildings in the dataset allowing for a single combined model using tree-based regression algorithms. Table 2 below shows a summary of the input variables (X) and the output variable (Y) of the predictive model.

The included microclimate parameters were based on the output of the validated ENVI-met model, which provides microscale weather data for each building. Air temperature and humidity data were simulated for each facade of the building and were averaged since the variations were relatively small between the building facades. ENVI-met also provides shading and radiation levels, which are quite different on each facade due to the orientation and design of each building. Since we are interested in the intensity within which cooling reductions can be achieved by design modifications, all facades were included for shading and direct shortwave radiation. Direct shortwave radiation data was also available for the top facade, which reflects the intensity of radiation in W/m^2 on the roof of the building.

In terms of energy input parameters, the kW data collected for each building could explain the internal heat gain in the building resulting in higher cooling requirements and might also explain the occupancy levels since an increase in occupancy usually results in more electricity consumption. As such, this feature was added as part of the input dataset. Furthermore, heating energy was included as input data to the model since it could have a direct relationship with cooling energy especially since ASU buildings use terminal reheating to balance temperatures at the zone level. This also explains why heating energy consumption was observed in the modeled summer period between May and July of 2018.

Four unique tree-based algorithms were tested: Random Forest [50], XGBoost [51], LightGBM [52], and CatBoost [53]. The Random Forest algorithm is an ensemble of decision trees that are averaged to compute the final output. The collection of decision trees makes up the random forest. The algorithm uses the bagging approach, also known as Bootstrap Aggregation, as opposed to gradient boosting, another ensemble technique used in XG Boost, LightGBM, and CatBoost. Bagging is the process of creating different training subsets sampled from the training dataset with replacement. Boosting uses a weighted average of results at each step of the iteration process. Incorrectly predicted cases from a given step are given increased weight during the next step. Boosting is an iterative procedure which is significantly different from bagging, that uses simple averaging of predictions from the sampled trees [54].

The dataset was split into training, validation, and testing. The testing day, June 9, 2018, was removed from the dataset. Then, the remaining dataset was split 70/30 for training and validation, respectively. For hyperparameter tuning, the Sklearn's RandomizedSearchCV [55] method was implemented, in which a combination of hyperparameter ranges were used to train models, and the best hyperparameters were selected based on cross-validation results. For cross validation, three folds were fitted.

4. Model results and interpretation

Results from the ENVI-met simulation were used as input to the tuned ML model. These results included diurnal microclimate

Table 1
Coordinates and area information of modeled buildings on Arizona State University's Tempe campus.

Building	Coordinates	Conditioned SQM	Classroom net SQM	Office net SQM	Research net SQM	Laboratory net SQM
Psychology	33° 25' 11" N, 111° 55' 46" W	5976	155	1392	1505	199
Psychology North	33° 25' 14" N, 111° 55' 46" W	3998	0	1191	1306	255
ISTB 4	33° 25' 4" N, 111° 55' 42" W	21521	237	3552	7685	0

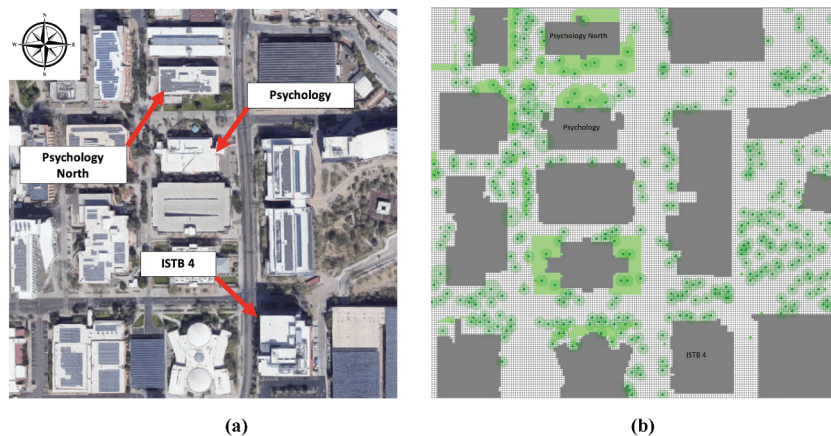


Fig. 2. (a) Satellite image of modeled buildings and (b) modeled area in ENVI-met (location of buildings, grass, and trees in the domain).

Table 2
Variables used in ML model.

Variable Type	Variable List
Building Input Variables (X_b)	Building Name (One-Hot-Encoded)
Energy Input Variables (X_e)	Electricity Consumption (kW)
	Heating Energy (mmBTU)
Microclimate Input Variables (X_w)	Mean Air Temperature (Celsius)
	Mean Absolute Humidity
	Direct Shortwave Radiation (W/m^2)
	Shade level on each facade (0–1)
Model Output (Y)	Chill water ton per square meter (CHWTON/SQM)

variables, which are presented in Table 2 as (X_w). From Fig. 2 we know that the three modeled buildings are close to each other in terms of distance. Psychology North and Psychology buildings are adjacent, and ISTB 4 is farther by approximately two buildings to the south. However, the diurnal microclimate variables were not similar due to the surrounding urban landscape and shade provided by adjacent buildings.

The most notable difference is the absolute humidity of ISTB 4 being much lower in the early hours of the morning compared to the

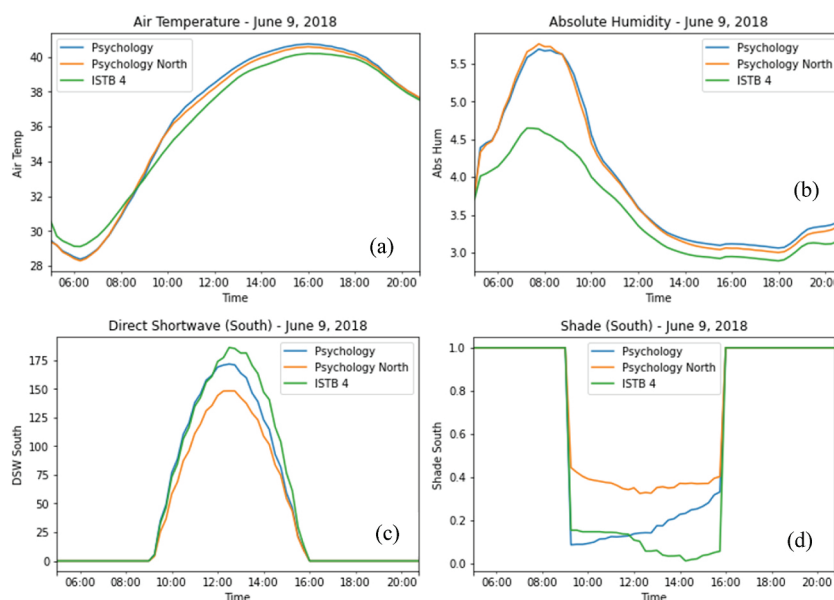


Fig. 3. Microclimate variables from ENVI-met simulation for June 9, 2018. (a) Air Temperature, (b) Absolute Humidity, (c) Direct Shortwave Radiation on South Façade, and (d) Shading Level on South Façade.

other two buildings. We note that ISTB 4 has less vegetation surrounding the building. Furthermore, the amount of solar irradiance incident on each façade is also different. Fig. 3c and Fig. 3d show the direct shortwave and shade levels respectively on the southern facades of each building. We observe an inverse correlation between these two variables whereby an increase in shade decreases direct shortwave radiation. Moreover, it is evident that sunlight exposure of each building is not the same, which could have a significant impact on cooling loads.

In supplementary data Figs. S1–S3, a timeseries is shown for the three modeled buildings on June 9, 2018. This day was removed from the training set and was used to test the ML model where the model's predictions for that date were compared to the actual data. This confirms whether the model can accurately predict an entire day, within the range of dates, without seeing the data during training. As seen from the graphs, the Psychology North building does not use heating energy on June 9, 2018. In fact, the building only uses heating on two out of the 12 modeled days. Furthermore, from Figs. S4–S6 of supplementary data, we observe that air temperature and absolute humidity have high correlations with cooling energy for all three buildings on this specific day. We also see that the Psychology building had the highest kW electricity correlation with cooling energy.

Overall, high accuracy levels were obtained using all four ML models with the selected features. The following evaluation metrics were used to compare model predictions on the testing dataset: coefficient of determination (R^2) (equation (1)), Root Mean Square Error (RMSE) metrics (equation (2)), Mean Bias Error (MBE) (equation (3)), Mean Absolute Error (MAE) (equation (4)), and Mean Absolute Percentage Error (MAPE) (equation (5)). R^2 explains how much the variation in the dependent variable is predictable from independent variables [56]. RMSE provides a measure between model predicted values and the actual values. MBE is used to observe the direction in which errors occur and captures the average bias in predictions. MAE measures the average of the absolute difference between predicted and actual values [57]. MAPE measures the proportion of the average absolute difference between predicted and actual values divided by the actual value [58].

$$R^2 = 1 - \frac{\sum_{i=1}^n (y_i - f(x_i))^2}{\sum_{i=1}^n (y_i - \bar{y})^2} \quad (1)$$

$$RMSE = \sqrt{\frac{\sum_{i=1}^n (f(x_i) - y_i)^2}{n}} \quad (2)$$

$$MBE = \frac{\sum_{i=1}^n (f(x_i) - y_i)}{n} \quad (3)$$

$$MAE = \frac{\sum_{i=1}^n |f(x_i) - y_i|}{n} \quad (4)$$

$$MAPE = \frac{100}{n} \sum_{i=1}^n \left| \frac{y_i - f(x_i)}{y_i} \right| \quad (5)$$

Where n is the total number of sample data points, y_i is the true value of a sample data point (i), $\bar{y}$ is the mean value of all samples, and $f(x_i)$ is the predicted value of a sample data point (i).

The results of the four modeled ML algorithms are reported in Table 3 for the testing day June 9, 2018. All models performed well with small differences as shown by the R^2 , RMSE, and MBE results. MBE values were positive for all models, indicating that the models overestimate CHWTON/SQM. XGBoost was the fastest algorithm without tuning, completing training in 0.2 s. All untuned models completed training in less than 2 s for a training dataset with 2107 samples. For the untuned models, CatBoost had the highest R^2 value of 0.983, confirming CatBoost's claim of great precision without parameter tuning [53].

The tuning time for each model highly depends on the number of hyperparameters selected for tuning and the number of values included in RandomizedSearchCV for each parameter. As such, a direct comparison between the tuning time of the models would be

Table 3

Results of four tree-based algorithms on testing data using base hyperparameters and tuned hyperparameters using RandomizedSearchCV.

Model	R^2	RMSE (CHWTON/SQM)	MBE	Training Time (s)
Random Forest	0.968	0.00160	0.000829	0.42
Random Forest (Tuned)	0.979	0.00130	0.000510	246.45
XGBoost	0.980	0.00127	0.000668	0.20
XGBoost (Tuned)	0.980	0.00126	0.000482	9.83
LightGBM	0.975	0.00142	0.000737	0.89
LightGBM (Tuned)	0.981	0.00125	0.000442	5.53
CatBoost	0.983	0.00118	0.000506	1.20
CatBoost (Tuned)	0.983	0.00117	0.000521	475.16

irrelevant. Overall, training time was acceptable and was not a factor in the selection of the final model.

From these scores alone, one would assume that CatBoost is the best selection for the baseline model. However, these results are for the testing data of all three buildings combined. Further investigation of error metrics was applied for each building using the tuned models shown in Table 4.

Excluding R^2 , a lower value is preferred for all used error evaluations. Results in Table 4 show that although the CatBoost algorithm had the highest overall R^2 score for all buildings combined, it was not predicting the Psychology North building as accurately as Random Forest or XGBoost. LightGBM also had a low R^2 score for Psychology North predictions. MAPE values for Catboost and LightGBM indicate significant differences between Psychology North predictions compared to ISTB 4 and the Psychology building. Although CatBoost had more balanced MAE values, there is strong indication that it underperforms in predicting the Psychology North building. Both CatBoost and LightGBM were ruled out as baseline models.

Comparing XGBoost and Random Forest we note that only ISTB 4 predictions had higher R^2 score for Random Forest. RMSE values for the two algorithms were similar, however Random Forest had a relatively lower RMSE value for ISTB 4 predictions. XGBoost has higher MBE values for all buildings except for Psychology. MAE and MAPE scores were similar for the two models.

From analyzing prediction results for each building, we conclude that the Random Forest algorithm, which uses the bagging technique, is more suitable for this timeseries dataset. The selection of algorithm highly depends on the given dataset, and no single model works best for all datasets. In general, bagging helps decrease the model's variance, whereas boosting helps improve model bias. High bias is usually the result of oversimplified models that do not learn the patterns in the training dataset well. On the other hand, high variance is when a model overfits and learns well on the training dataset but is unable to generalize predictions for unseen data [59]. If a single decision tree model has low performance because of high bias, then boosting algorithms can be useful to increase performance. By contrast, if a single model overfits because of high variance, bagging can help reduce variance [60]. For the dataset used in this analysis, there was no issue with model performance. From the prediction plots of boosting models on the testing dataset, we observe unsmooth patterns that could be the result of overfitting. Random Forest prediction plots were relatively smooth and yielded overall better results upon evaluation of error scores on single building predictions.

The tuned Random Forest model was selected as the final baseline model and was used to perform the sensitivity analysis. Fig. 4 shows the tuned model predicted cooling energy for the test day of June 9, 2018, compared to the actual cooling data with an average difference between the two shown at the top of each graph. We note that all percent differences are positive, further indicating that the model tends to overestimate, and confirming the results of the MBE. ISTB 4 predictions were the most accurate, with an average difference of approximately 0.4%. Both Psychology and Psychology North predictions were off by around 3%. These results are satisfactory for the purpose of this analysis.

A benefit to using tree-based algorithms is the ability to display the most important features that have the highest impact on the model outcomes. The feature importance values from highest to lowest are shown in Fig. 5 for the tuned model. The feature importance value for each feature is shown in the supplementary data Table S1. We note that kW was the most important feature followed by air temperature, then heating energy. The global feature importance results provide further evidence that the modeled buildings are likely mixed-load dominated. Absolute humidity turned out to be less important to the model than air temperature but was still more important than shading and radiation. The one-hot encoded building indicators also had relatively high feature importance, proving that the modeled buildings are unique and that it is important for the ML model to identify which building the predictions are being generated for.

The feature importance results are unique to how the tree was designed for this dataset using the Random Forest algorithm. Feature importance results from other models were similar with minor differences in the order of features. Air temperature, heating energy, and kW energy were all at the top of the list. From these results, we conclude that (1) the modeled buildings are likely mixed-load dominated and (2) air temperature dominates all other climatic features.

Feature importance is a global interpretation. SHAP, a python library, provides local interpretation using shapley values and works well with tree-based algorithms. SHAP allows interpretation of a single data sample as well as all samples in different plot types. It also allows interpretation of model predictions, for instance of the testing data, as opposed to interpretation solely on the training set. Fig. 6 shows the impact of different features and the direction of impact each feature had on the outcome of a single data sample from the testing data. For this sample, kW pushed the prediction towards higher values, while air temperature pushed the outcome towards

Table 4
Prediction evaluation of four tuned tree-based algorithms on testing data for each building.

Tuned Model	Building	R^2	RMSE (CHWTON/SQM)	MBE	MAE	MAPE
CatBoost	Psychology	0.938	0.00117	0.000369	0.000966	0.0289
CatBoost	ISTB 4	0.963	0.00075	0.000165	0.000617	0.0245
CatBoost	Psychology North	0.785	0.00129	0.000687	0.000924	0.0731
Random Forest	Psychology	0.860	0.00177	0.000914	0.001410	0.0418
Random Forest	ISTB 4	0.967	0.00071	0.000075	0.000602	0.0236
Random Forest	Psychology North	0.839	0.00111	0.000390	0.000755	0.0615
XGBoost	Psychology	0.878	0.00165	0.000748	0.001397	0.0401
XGBoost	ISTB 4	0.947	0.00090	0.000291	0.000751	0.0295
XGBoost	Psychology North	0.843	0.00110	0.000408	0.000753	0.0594
LightGBM	Psychology	0.914	0.00139	0.000604	0.001167	0.0344
LightGBM	ISTB 4	0.936	0.00098	0.000120	0.000833	0.0326
LightGBM	Psychology North	0.765	0.00135	0.000602	0.000915	0.0754

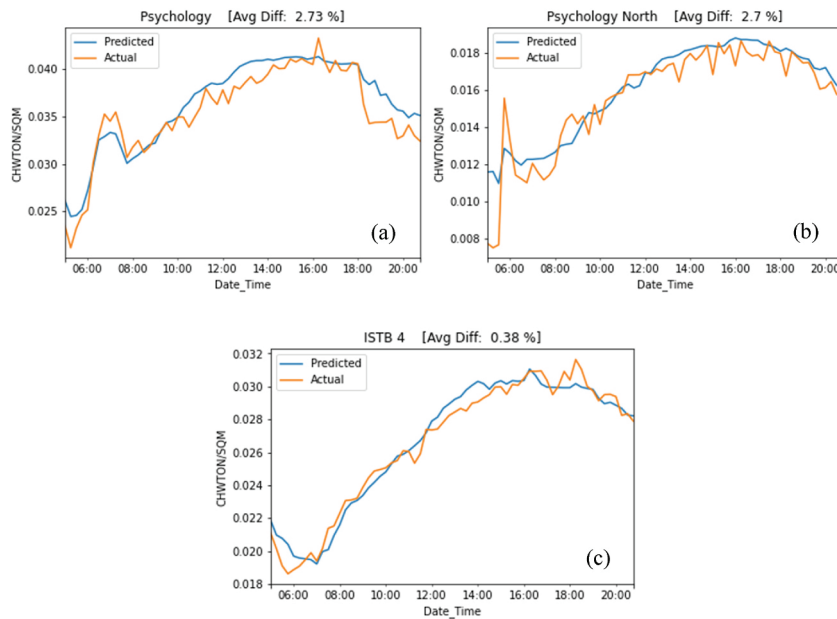


Fig. 4. Actual vs model predicted results for test day (June 9, 2018) for (a) Psychology, (b) Psychology North, and (c) ISTB 4.

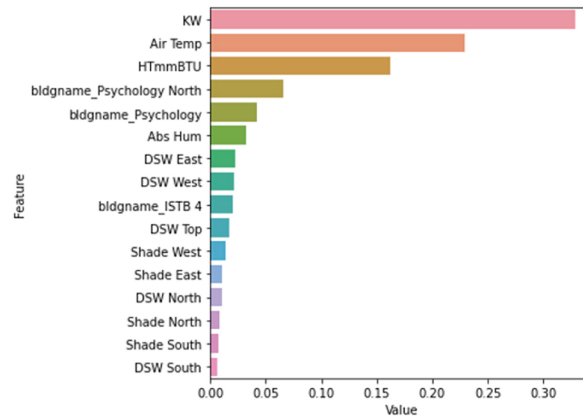


Fig. 5. Global feature importance values for tuned Random Forest model.

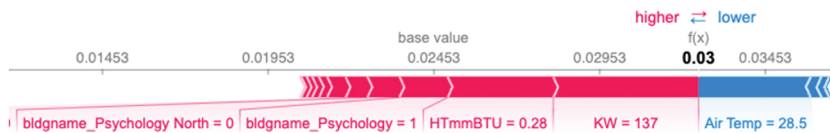


Fig. 6. SHAP force plot showing impact of features on single prediction.

lower values. Overall, the combined impact of the features pushed the outcome towards higher values compared to the base value.

Fig. 7 shows similar information for all testing data samples ordered from higher output values to lower output values. We note that for higher values starting from the left side of the graph, air temperature had the most impact in pushing the outcome towards higher values, followed by kW and heating energy. For lower output values, kW had the most impact in lowering the model output while air temperature again pushed output towards higher values.

A SHAP summary plot shown in Fig. 8 indicates how different feature values impacted the model's output. A low SHAP value below 0 had a negative impact on the model predictions, and a high SHAP value had a positive impact. The features are also ranked based on their importance level, which has similar order to the global feature importance plot in Fig. 5 with small differences.

Some of the lower kW and most of the lower air temperature values had a negative effect on the model's predictions, while higher

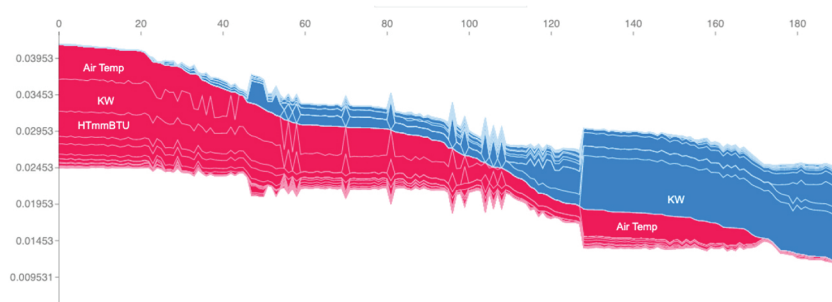


Fig. 7. SHAP force plot showing impact of features on all predictions ordered by output value.

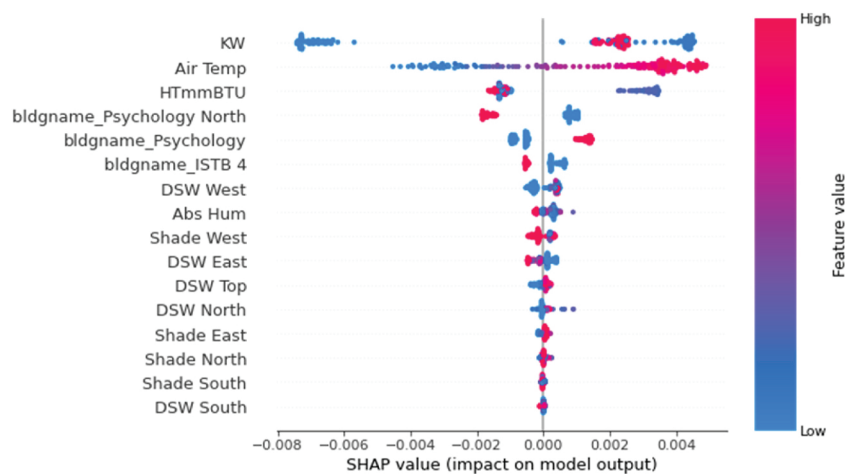


Fig. 8. SHAP summary plot for all features [KW: kW electricity, Air Temp: microclimate air temperature in celsius, HTmmBTU: heating energy in mmBTU, bldgname.: building identifier, DSW: direct short-wave radiation, Abs Hum: absolute humidity, Shade: shade level from 0 to 1]. (For interpretation of the references to colour in this figure legend, the reader is referred to the Web version of this article.)

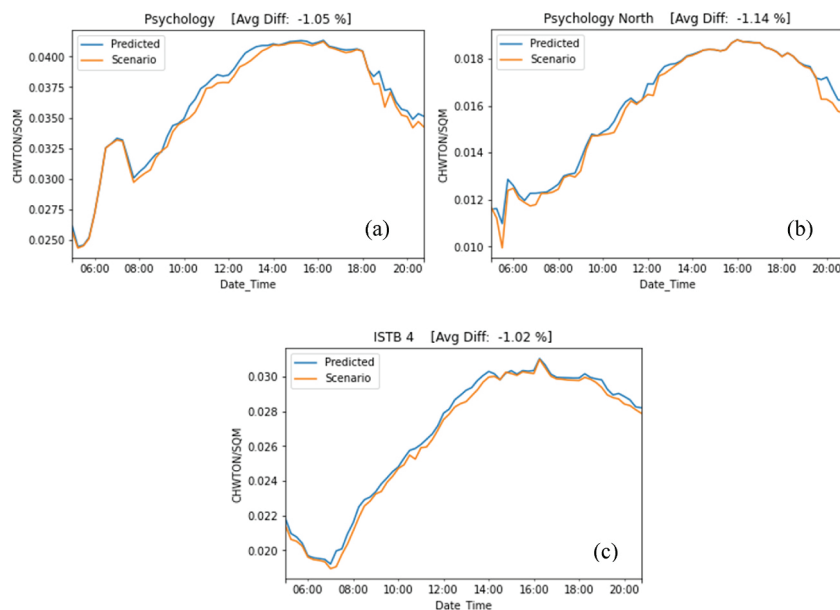


Fig. 9. Scenario predictions for 0.5 °C reduction in air temperature for (a) Psychology, (b) Psychology North, and (c) ISTB 4.

values for both had a positive effect on predictions. The opposite was observed for heating energy ($HTmmBTU$) where most higher values had a negative impact on predictions. The rest of the climatic and energy related features had a balanced effect on model predictions.

For some predictions, high and low feature values had a negative effect on some predictions and a positive effect on other predictions. This can be seen for kW and $HTmmBTU$. Some of the low kW values had a negative effect on the model, however, some also had a positive effect as indicated by their SHAP values. The SHAP value for each prediction is likely influenced by other feature values for the same sample point prediction. For instance, low air temperature at a specific sample point prediction could have a negative effect, while a low kW value for that same sample point could have a positive effect. This is also evidence that the modeled buildings are not fully externally-load dominated and that cooling loads are also influenced by building operations, including kW consumption. The combination of feature values determines how each feature impacts the model predictions. Overall, the SHAP summary plot shows that higher air temperature had a positive effect on the model and pushed the output to higher cooling load predictions.

5. Sensitivity analysis

A sensitivity analysis was conducted where small changes were made to microclimate parameters to observe their impact on model predictions. These predictions were compared to baseline predictions on June 9, 2018 for all three buildings. The sensitivity analysis includes the following scenarios: (1) reducing air temperature by $0.5\text{ }^{\circ}\text{C}$, (2) reducing absolute humidity by a value of 0.5, (3) increasing shade for each facade by 20%, and (4) combining all three scenarios.

Fig. 9 show the difference between baseline predictions and predictions with $0.5\text{ }^{\circ}\text{C}$ reduction in air temperature. Overall, this change had a clear reduction in cooling energy with an average reduction of -1% . However, a reduction in absolute humidity did not yield the anticipated reduction in cooling energy and had no significant impact on predictions.

For part (3) of the sensitivity analysis, where an additional 20% shade was added to specific facades, only the Psychology building had significant reductions in cooling loads. Specifically, increasing shade on the west facade had the highest impact in reducing cooling loads for afternoon hours shown in Fig. 10. Increasing shade on the east facade by the same amount reduced cooling energy in the early hours with less impact as shown in Fig. 11. Our sensitivity analysis also indicates that both the Psychology North and ISTB 4 buildings had no significant reductions in cooling loads from 20% added shade.

The Psychology North building has a unique design that reduces sunlight exposure to interior surfaces. This analysis only investigates added shade to the entire building facade and does not consider interior irradiation exposure. As such, we note that some buildings do not benefit greatly from overall added shade due to their unique design features that incorporates shading strategies to interior spaces. The lack of cooling reductions from added shade to ISTB 4 building for example is likely due to the exterior shading louvers that the building is equipped with. The ISTB 4 building is a relatively newer building commissioned in 2012 and has a LEED Gold certification.

Results of the combined microclimatic changes are shown in Fig. 12 for all three buildings. Up to approximately -2% cooling energy reductions were observed for the Psychology and Psychology North buildings under the modeled microclimate input data. The ISTB 4 building had the lowest reductions at approximately -1% .

6. Discussion

Our sensitivity analysis provided insights into the magnitude of cooling energy reductions that could be achieved under cooler microclimates. We note that the western facade had the biggest impact in terms of added shade for the Psychology building. Donovan et al. found similar results where they estimated the effect of shade trees on summertime electricity use of 460 single-family homes in Sacramento, California [61]. They conclude that trees on the southern and western sides of a house reduce electricity use. However, this analysis is specific to university buildings, which are designed and operated much differently than residential buildings. This was evident in our analysis of the Psychology North and ISTB 4 buildings which were not greatly impacted by added shade due to their unique design features.

Some studies implement specific design strategies such as the addition of urban shade and vegetation to the surrounding building exterior, but only quantify the impact of these specific microclimate designs on cooling energy consumption levels. Sedaghat et al. [23] found that with high-albedo materials and vegetation, air temperature drops of $2.1\text{ }^{\circ}\text{C}$ were achieved in Tehran, Iran, consequently reducing residential cooling energy by 29%. Using weather data collected from 27 stations over a span of 10 years and a BES simulation tool, Hong et al. [24] found that microclimate impacts are less than 5% of cooling and heating loads for large hotel and office prototype buildings in San Francisco, CA. Huang et al. [27] found that cooling demand increases by up to 15% in the dense city of Hong Kong. Using a BES simulation tool, Boccalatte et al. [25] compared an efficient urban design configuration to the reference case for 3 European climate zones. They found that using rural weather data, annual air condition requirements are underestimated by 10% for the modeled residential building. Moreover, they conclude that the enhanced urban design configuration was able to reduce annual energy consumption by 2.2%. Palme et al. [62] found that different urban configurations could reduce cooling energy by 2–50% for residential buildings in Italy, with an average of 15%. Hadavi et al. [29] found that decreasing urban compactness provided up to 16.4% energy savings.

Results reported in prior studies are mostly higher than what was found in this analysis, which did not exceed 2% in the combined scenario case and could be the result of differences in building types. Large university buildings are unique and are occupied much differently compared to other building types. University buildings are also less likely to be externally-load dominated, which reduces the effect that the microclimate has on building cooling loads.

Our results are based on a hypothetical sensitivity analysis with small changes in microclimate variables compared to actual

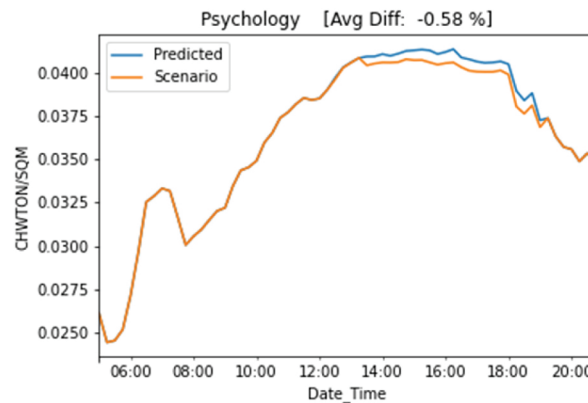


Fig. 10. Predictions for 20% increase in west shade for Psychology building. (For interpretation of the references to colour in this figure legend, the reader is referred to the Web version of this article.)

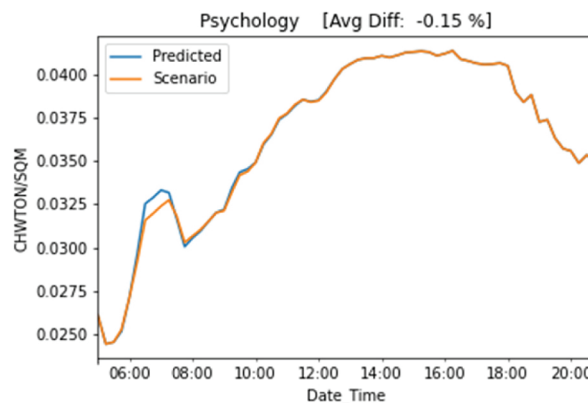


Fig. 11. Predictions for 20% increase in east shade for Psychology building. (For interpretation of the references to colour in this figure legend, the reader is referred to the Web version of this article.)

scenario modeling. This approach provided valuable insights on how cooling loads can be reduced due to these small changes. Additionally, one must consider the different climate zones within which these studies are located. One key finding of our analysis is that a 0.5°C reduction in air temperature had an average of -1% reduction to cooling energy levels of mixed-load dominated buildings in an arid region.

It should be noted that the purpose of the developed model is not to forecast cooling energy, rather it is to estimate cooling for a specific summer day to identify how the output is sensitive to changes in microclimate parameters. It is also important to note that the developed model is unable to predict cooling outside of the range of training dates. The selected days for training the model were in summer of 2018 between May and July, which have unique patterns compared to fall and spring seasons when classes are in progress. This was also evident upon examining the campus metabolism data that showed a significant energy consumption increase in August due to higher occupancy levels and modified set points and equipment operating schedules adjusted by ASU's facilities management. Including more days during the semester requires collection of sufficient data to enable the model to distinguish the buildings' behavior in certain months. Since the ENVI-met model was only validated for summer, simulation results for other days in the year were not included. This could be part of future analysis whereby microclimate simulation data can be validated for semester seasons (Fall and Spring) when students and faculty occupancy levels increase.

The decision to use the Random Forest algorithm was the result of testing multiple algorithms including XGBoost, Catboost, and LightGBM. The advantage of using a tree-based algorithms is that features do not need to be scaled for training. Most ML algorithms require scaling input parameters during the preprocessing phase for the model to perform better and converge faster. All tested algorithms performed well for the dataset with prediction accuracy above 90% for the selected testing day.

Including more features in the model might allow ML algorithms to achieve greater accuracy since the output could be influenced by multiple factors that are not fully captured in the input data. Buildings are complex systems that have unique features that change with time and could explain energy usage patterns. The operating schedule of a building and the flow of occupants in and out of a building are some examples of time varying features that could provide valuable information to the model. Moreover, data on end-use level consumption and building equipment controls such as fans, temperature set points, lighting, and other stationary equipment would provide higher accuracy and better interpretability, especially for buildings with cooling patterns that are not highly affected by

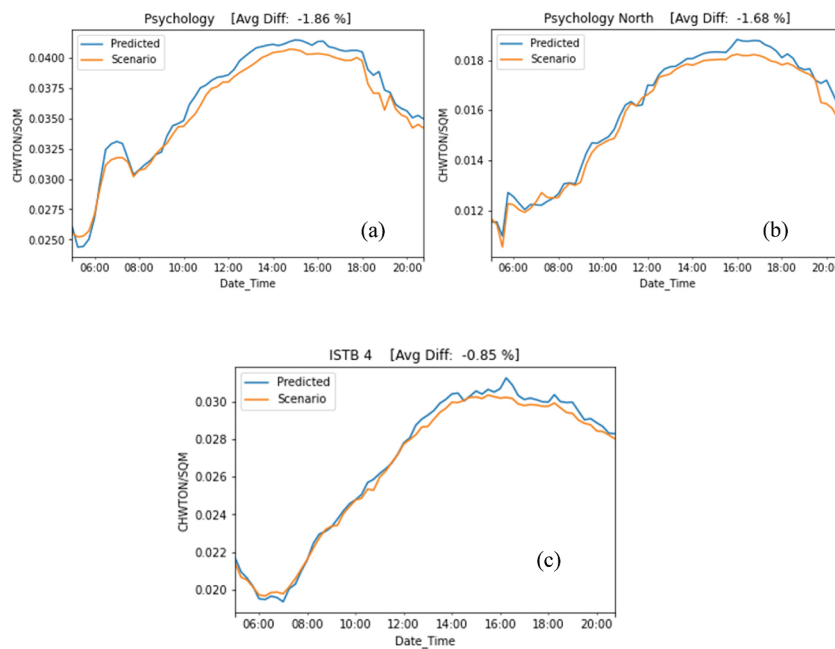


Fig. 12. Predictions for all scenarios combined for (a) Psychology, (b) Psychology North, and (c) ISTB 4.

exterior conditions and are dominated by interior loads. Sensor data capturing the heat gained from internal loads might explain the cooling loads for such buildings. Although this type of data is currently not available, we recommend the integration of sensor technology in modern buildings to leverage the utilization of machine learning algorithms that can provide valuable insights.

One of the most notable setbacks of CFD simulation software is the computational time required to run simulations for large areas and high-resolution data. This limits the data that can be used to run ML algorithms and as a result, the generalizability of the model reduces. With more data for an entire year in similar 15 min timestamps such ML models can be generalized for different seasons of the year. However, due to data limitations, the developed model is only suitable for analysis of the summer period of 2018, which is what the model was trained for. Using the model without verification data is not recommended. The purpose of this analysis is not to develop a generalized predictive model, rather it is to understand how microclimate variables influence ASU building cooling loads for the studied timeframe. Tree-based algorithms proved to be useful for this purpose, predicting the testing dataset with high accuracy.

7. Conclusions

The developed model combines both CFD based microclimate simulations and a data driven ML approach to find the relationship between microclimate and cooling loads for university buildings. The significance of using a data-driven model is to minimize the risk of modeler bias, which BES simulation tools often suffer from. Our approach is much simpler, especially in the context in which we model large university buildings. Using a BES simulation tool to develop a model for such buildings is a great challenge and has high uncertainties. The developed framework is highly beneficial for assessing the microclimate impact on complex existing buildings rather than modeled prototypes.

The proposed framework can be replicated for any type of building (residential or commercial); however, it is important to first identify if the building is externally-load dominated or mixed-load dominated. Since the aim of this framework is to understand the impact of microclimate on cooling energy use, using this approach for internally-load dominated buildings is not feasible without non-climatic features. In terms of data, a CFD simulation of the modeled area is required to generate the microclimate data. Energy consumption data is also required and should match the timestamps of the CFD simulated data. Finally, multiple ML algorithms should be tested to identify the best fit for a given dataset.

For the modeled buildings, the cooling loads were indeed influenced by microclimate conditions. Results from the sensitivity analysis show that reduction in air temperature has the highest effect. Furthermore, shading and radiation effects were also observed, and reductions occurred in meaningful periods matching the modifications made. In future extensions of this work, ENVI-met scenarios will be simulated for different microclimate designs that utilize urban shading, trees, and high-albedo material. The output of these modeled scenarios will then be used to make predictions using the baseline model, and a similar analysis can be performed.

CRedit authorship contribution statement

Ali Alyakoob: Conceptualization, Methodology, Software, Data curation, Writing – original draft, Visualization, Writing – review & editing. **Sherly Hartono:** Conceptualization, Methodology, Software, Validation, Writing – review & editing. **Trevor Johnson:** Data curation, Visualization, Writing – review & editing. **Ariane Middel:** Supervision, Resources, Software, Data curation, Writing – review

& editing.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at <https://doi.org/10.1016/j.job.2022.105705>.

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