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Toward the application of a machine learning framework for building life cycle energy assessment

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ABSTRACT

The construction industry in the United States consumes more than 50% of the global energy supply per year, suggesting that significant efforts may be needed to reduce building energy demand and its carbon footprint. During their lifespans, buildings consume embodied energy (EE) and operational energy (OE). Building professionals, therefore, conduct life cycle energy assessments (LCEA) to quantify and understand the paradox and interconnectedness between EE and OE. Traditionally, simulation-based optimization techniques were used for design space exploration to identify a building design with the fewest energy implications. However, literature shows these data-driven approaches are often error-prone, time-consuming, and computationally expensive, and they fail to provide real-time feedback to the user. Moreover, EE and OE assessment tools are disjointed and suffer from interoperability issues. These limitations restrict design space exploration, which eventually hinders the design decision-making process. Over the last few years, the increased availability of building data has made machine learning (ML) techniques a popular choice for building performance assessments. Several articles have developed prediction models to assess or optimize OE. While this work is significant, studies utilizing ML techniques for building LCEA are lacking, mainly due to the unavailability of a large-scale LCEA database. In this paper, we propose a methodology to (1) generate a simulation-based building energy dataset for different building typologies using a parametric framework, (2) utilize the synthetically generated database to develop an ML-based prediction model to predict EE and OE, and (3) test the model using a case study. The case study results show that the model achieves high prediction performance using minimal inputs available during the early design phase. The results further indicate that ML techniques can be used by building designers with no or limited LCE expertise to instantaneously estimate building LCE performance and help them select design options with minimal LCE consumption.

1. Introduction

Every year, the construction industry in the United States consumes over 50% of the global energy supply and is also responsible for over 40% of greenhouse gas emissions [1]. Related to this, governments all over the world have announced several initiatives to reduce life cycle energy (LCE) and carbon emissions produced by the built environment [2–4]. To quantify building energy performance, building professionals use whole building life cycle energy assessments (LCEA). LCE consists of embodied energy (EE) and operating energy (OE) [5]. Most often, utilizing energy-intensive materials/processes to reduce OE creates a dichotomy between the energy spent to construct vs operate the building [6,7]. Therefore, evaluating both EE and OE is imperative for overall LCE reduction [8].

Mandatory laws and ambitious sustainability targets to decarbonize the built environment have led to a growing interest in evaluating both components of building LCE [9]. Existing simulation-based modeling methodologies to conduct LCEA are time-consuming, suffer from issues of interoperability, and are not very user-friendly [10]. As a result, industry professionals are motivated to develop innovative tools that would assist individuals with LCE-based design decisions in a fast and seamless manner. In this context, the increased availability of building data over the last few years has made machine learning (ML) based methodologies popular as an alternative to physics-based engineering

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methodologies [5,11,12]. Several studies showcasing the application of building energy consumption prediction models have been published recently [13–23]. While this work is significant, studies utilizing prediction models for building LCEA are lacking, mainly due to the unavailability of a large-scale LCE dataset [19]. Collecting real-world building energy data, especially EE data, is extremely time-consuming and impractical [8,24]. Eventually, these issues restrict the development of prediction models, specifically for the purpose of conducting building LCEA. Therefore, the application of ML-based techniques, specifically for evaluating EE and OE, is still an open research problem. In this study, we developed a simulation-based parametric framework to synthetically generate a building LCE dataset. This dataset was then used to train and test an ML-based prediction model that would assess building energy from a life cycle perspective.

2. Literature review

2.1. Challenges of using simulation-based approaches for LCEA

The literature shows that various building performance simulation (BPS) tools and technologies exist to evaluate the OE and EE of a building [25]. Some commonly used OE tools are e-Quest, IES-VE, and EnergyPlus, whereas Athena Impact Estimator, SimaPro, Tally, and One Click LCA are LCA tools used for EE calculations [26,27]. Despite the availability of these tools, building professionals still hesitate to incorporate LCE-based design decisions due to the lack of expertise or data (information) [28]. For example, a simple energy simulation run generates large volumes of information, making it difficult for a novice designer to compare and correlate different combinations of energy-saving factors [14]. Similarly, tools that simulate OE require information such as material thermal properties, HVAC specifications, occupancy schedules, etc., whereas EE tools require material quantities, construction specifications, and systems/equipment information. These data (information) are usually unavailable during the early design phase [11].

BPS tools are not well integrated into the design platforms and do not provide immediate feedback to designers [10,27–29]. EE and OE tools are not well integrated with each other which forces the designer to switch among multiple tools to holistically evaluate building LCE [30]. This workflow is not very user-friendly; ultimately, designers are reluctant to utilize these tools [27,31–35]. In addition, BPS tools need to be integrated with other optimization algorithms using other parametric modeling tools or custom scripting, which limits design space exploration [36–38]. This workflow is computationally expensive, and time-consuming, and it requires significant experiential knowledge [37,38]. As a result, building professionals evaluate a limited set of design options before selecting the optimal design. These issues with existing practices hinder the systemic reduction of building LCE. To address these issues, numerous studies have developed ML-based prediction models to improve the decision-making process associated with building energy performance assessment [39].

2.2. Ml-based approaches for building performance assessment: Current state of research

ML has become popular in today's digital society due to ever-increasing data availability, cheap data storage costs, and improved computational power [40]. These ML algorithms use computational methods to automatically analyze, recognize, and learn patterns from existing data to provide future predictions [41,42]. Within ML exist two conventionally used training approaches: supervised learning and unsupervised learning [43]. Supervised learning approaches utilize labeled datasets (i.e., input features are mapped to exact output labels). These approaches are mostly used in classification and regression tasks. Unsupervised learning approaches utilize unlabeled/raw data [41]. In this approach, the algorithm recognizes inherent trends in the input features of the dataset to predict the outcome without any human supervision [36]. Unsupervised learning methods are typically used for tasks related to clustering, dimensionality reduction, and association [36].

The literature shows that supervised learning approaches are commonly used to develop prediction models for BPA [14,44]. Two ML algorithms used widely in the building industry for supervised learning are support vector machines (SVM) and artificial neural networks (ANN) [45,46]. These algorithms are used for energy prediction because of their ability to handle complex non-linear data and large datasets [17,47]. For example, Shao et al. [48], Jain et al. [49], Zhao and Magoules [50], Lai et al. [51], Zhang et al. [52], Fan et al. [43], and Dong et al. [53] forecasted energy consumption using an SVM-based prediction model. Other studies, such as Ciulla et al. [54], Lei et al. [55], Yan et al. [56], and Singaravel et al. [57], used ANN-based prediction models. A few studies, such as Deng et al. [58], Setiawan et al. [59], and Amber et al. [60], compared the performance of the SVM-based and ANN-based prediction models to identify the best algorithm suited for building energy forecasting. However, it is important to note that the performance of an algorithm depends on several factors such as the size of the dataset, quality of data, model parameters, etc., [45,61]. Therefore, the results of these studies are not comparable, and we cannot conclude that one algorithm is better than the other [45,61]. More recently, ensemble-based learning methods have become popular since they combine a myriad of base models to obtain a single optimal prediction model. Some studies, such as Chou and Bui [62], Jovanovic et al [63], and Singaravel et al. [57], used ensemble-based prediction models to estimate the heating and cooling loads of buildings. The findings of their studies indicate that ensemble-based prediction models have better performance accuracy and generalization ability compared to a singular model. For instance, Chou and Bui [62] found that the mean absolute percentage errors (MAPE) for the ensemble model and singular model are 14.4% and 18.3%, respectively.

Our review of relevant literature shows that ML algorithms are used to predict heating and cooling loads, electricity consumption, energy use intensity, and energy demand [47]. However, there is insufficient focus on the energy consumed during the construction phase, due to the lack of reliable LCA data [64]. These data quality issues are mainly caused by unstandardized methodologies/protocols and inconsistent system boundary definitions when collecting LCA data [65–68]. In certain cases, primary LCA data are inaccessible; as a result, researchers rely on secondary data sources to obtain information [69,70]. In addition, LCA data lack temporal relevance since the United States Bureau of Economic Analysis (USBEA) publishes input–output data only once every five years [71–73]. These data are then adjusted to the present day using an energy inflation factor [74–76]. The above-mentioned issues introduce high levels of uncertainty in LCA data compared to OE data. As a result, developing an ML-based prediction model for evaluating energy from a life cycle perspective has been difficult.

3. Research goals, and objectives

The goal of this study is to develop an ML-based method to quickly estimate EE and OE intensities using a few known inputs in the early design phase. This goal would be achieved by pursuing the following research objectives:

(1) Develop a framework to generate a simulation-based building energy dataset for different building typologies.
(2) Develop, train, and test a building ML-based prediction model using the simulation-based dataset to predict EE and OE intensities.
(3) Demonstrate the application of the ML-based prediction model using a case study of two commercial buildings.

4. Research scope and limitations

4.1. Synthetic building energy dataset

The scope of this dataset was defined in terms of climate zone, building type and form, design parameters, and building loads.

Climate zone: The simulation-based building energy dataset was generated for climate zones 2A and 5A.

Building type and form: According to the Energy Information Administration (EIA), the residential and commercial sectors consumed 21 quadrillion British Thermal Units (Btu) of energy in 2019 [1]. Therefore, we generated synthetic data for commercial building typologies with a simpler rectangular design. Considering other building types, forms, and taxonomies is beyond the scope of this study; the dataset created in this study does not represent the diversity of the entire building stock.

Design parameters: The design parameters considered were categorized into two groups: (i) geometry parameters, and (ii) construction parameters. Geometry parameters include orientation, length, and width of the building, number of floors, and window-to-wall ratio (WWR). Construction parameters consist of ten different types of wall assemblies and three different types of glazing systems.

Building loads: We only considered building envelope loads such as heating, cooling, lighting, and equipment loads since they contribute approximately 75% of total OE use. Moreover, factors such as occupancy loads, type of HVAC system, and schedule are unavailable to designers during the early design phase [77]. Since life cycle embodied energy consists of a negligible proportion of demolition energy [8], we included only the initial embodied energy and recurrent embodied energy of building materials.

4.2. Building LCE prediction model

We defined the scope of the ML model in terms of data used, type of model (static vs dynamic), purpose of prediction, and performance.

Data: The study utilizes synthetic data generated using building energy simulations. The data generated in this manner may be limited (i.e., representative of only certain scenarios) in comparison to real-world building energy data, which is far more complex since it accounts for daily changes in occupancy, HVAC system schedules, etc. That said, the simulation-based approach is advantageous because it allows researchers to build unlimited building models to obtain a wide range of synthesized data for ML. Moreover, the study does not include weather parameters and utilizes the location parameter as a categorical variable.

Type of model: The building LCE prediction model developed in our study follows a supervised learning approach. Moreover, it utilizes static learning, i.e., it does not consider variation in, for instance, economy, energy production, or climate.

Purpose of prediction: The ML model predicts OE and EE using limited information available in the early design phase. Predicting the impact of other environmental indicators such as embodied carbon, global warming potential, carbon emissions, acidification potential, eutrophication potential, etc., is beyond the scope of this paper.

Performance: First, this model's performance was validated using a synthetic dataset that represents a subset of commercial rectangular buildings. While this is significant, other parameters (e.g., location, weather, building types and forms, internal loads, schedules, systems, and construction assemblies) need to be integrated with the developed framework to generalize and validate the performance of this building LCE prediction model. Therefore, certain inconsistencies in the model's performance may occur if the characteristics of the building are different from the dataset used to create the model. Second, comparing the effectiveness of different ML models in terms of computational time and predictive accuracy is outside the scope of this research. Lastly, this study used mean square error (MSE) and mean absolute percentage error (MAPE) for performance verification. It is important to note that the MSE loss approach is sensitive to outliers, and we acknowledge the limitation of using this metric for performance verification.

5. Research design and methods

The study design's framework has three interdependent parts closely tied to the research objectives mentioned earlier. Each part has several sub-tasks which are elaborated in separate sub-headings. The brief outline of the overall study design is shown below (Fig. 1):

5.1. Synthetic data generation: Basic framework

5.1.1 Description of building characteristics

The medium office building (a simple rectangular building) from DOE's commercial reference building models was selected as the prototype model for this framework [78]. The building has steel frame walls (2x4 16IN OC) with various exterior finishes. The thermal properties of the building envelope (walls, roof, windows, and first floor) as well as other parameters such as the HVAC specifications, occupancy schedules, and thermostat settings were in accordance with the ASHRAE 90.-2019 standards (as seen in Table 1).

5.1.2 Define design space and input features

Because it is impractical to generate data representing the entire building stock in the United States, prior to generating the building dataset, we defined certain design constraints for the geometry and construction parameters based on recommendations from similar studies as shown in Table 2. Building dimensions of 13 ft (4 m) might be too narrow and render a space non-functional. Therefore, we selected building dimensions that range from 30 ft (10 m) to 265 ft (80 m) for this study. This implies that the maximum floor area of the buildings generated in this study will be 70,000 ft^2 (6500 m^2). According to the commercial buildings energy consumption survey (CBECS) conducted by EIA in 2012, nearly 93% of the commercial buildings in the United States have an area less than 50,000 ft^2 (4625 m^2).

In terms of height, the studies conducted by Elbeltagi et al. [34], and Li et al. [79] considered buildings between one and three stories high. In addition, according to the CBECS, 97% of buildings located in the midwestern and southern regions of the United States are less than 3-stories high [80]. The building length, width, and height parameters [81]are automatically in compliance with the slenderness ratio (height: width = 10: 1). This ratio is usually measured to ensure that the building is structurally stable [82].

For this study, we selected climate zone 2A (Houston, Texas) and climate zone 5A (Chicago, Illinois) due to differences in the number of heating degree days and cooling degree days. The construction assemblies of all building envelope components are in accordance with the ASHRAE 90.1–2019 standards [85] as seen in Table 3. Table 4 lists the input and output features with their corresponding range values.

5.1.3 Granularity of the simulated dataset

Commonly used time steps in literature are 1-minute [86], 5-minutes [59,87], 15 min [88], 30 min [89], hourly [55,90], daily [60,91], monthly [92] and yearly [93]. According to the literature review conducted by Venkatraj and Dixit [47], simulation-based datasets utilize long-term (yearly) intervals whereas historic datasets utilize short-term (hourly, daily, monthly) intervals. Simulating OE for hourly/daily/monthly prediction intervals will make the process of calculating LCE computationally expensive and time-consuming. Therefore, we use yearly timesteps in this study.

5.1.4 Generate simulation-based building energy dataset using a parametric framework

Fig. 1. Conceptual study design highlighting implementation steps.

Table 1
Building characteristics.

Load parameters	Setting
Thermostat setpoint	75°F Cooling/70°F Heating
Thermal zoning	Perimeter zone depth: 15′
HVAC system	Packaged air-conditioning unit
Lighting power density	0.79 W/ft^2
Equipment power density	0.75 W/ft^2

Table 2
Range values for building dimensions obtained from literature.

Study	Range values for building length/width (m)
Singaravel et al. [57]	4 to 80 / 1 to 80
Fang and Cho [83]	9 to 17.3
Khalil et al. [84]	10 to 30
Elbeltagi et al. [34]	10 to 30
Attia et al. [27]	10 to 12
Li et al. [79]	20 to 80

Table 3
ASHRAE 90.1–2019 building envelope requirements.

Climate zone	2A – Houston **Assembly U_{max}** (Btu/hr.ft^2.°F)	5A – Chicago **Assembly U_{max}** (Btu/hr.ft^2.°F)
Walls	0.077	0.052
Windows	0.500	0.380
Roof	0.039	0.032
Floor	0.107	0.074

The building energy dataset was generated using a parametric approach which allows us to change the building geometry and construction parameters to create several variations of the prototype model (see Fig. 2). These variations were generated using Grasshopper (GH) extension in Rhinoceros 3D, a design platform.

The Galapagos add-on within the GH environment acts as a parametric controller for the input features mentioned in Table 4. This evolutionary solver was used to manipulate the input parameter sliders based on the previously defined constraints to generate several design options of the prototype model within the design space.

Operating energy: Each design iteration was assigned appropriate thermal zones and scheduling conditions which were sent to energy simulation plugins (Ladybug and Honeybee) for OE calculations. These plugins utilize EnergyPlus, considered the most robust and reliable energy simulation engine in the building industry. The OE result for each iteration was saved in a Microsoft Excel file using the TT Toolbox plugin available in GH.

Embodied energy: The surface areas of different building components (e.g., walls, floors, roofs, and windows) were calculated using mathematical formulas and custom scripting in GH. Next, the surface area information for each iteration was exported into a Microsoft Excel file using the TT Toolbox. From the surface area information, we derived material quantities and converted them into cost information using National Construction Estimator (2017) data. Because we used input–output-based hybrid (IOH) data referred from [94], we needed quantities in terms of cost. The total cost of repair and maintenance for a 60-year building lifespan was sourced from the White Stone Cost Report (2009–2010). This cost information was then disaggregated based on the material groups of the IOH model as per [94]. The material-specific energy intensity and fuel-specific primary energy factors were applied to

Table 4
Input (I/P) and output (O/P) features with potential range values.

Number	I/P feature	Range values	Parameter type
1	Climate zone	2A - Houston 5A - Chicago	Categorical
2	Orientation	0° – 360°	Continuous
3	Length	30 ft – 265 ft	Continuous
4	Width	30 ft – 265 ft	Continuous
5	Number of stories	1–3	Continuous
6	Height of each floor	10 ft to 15 ft	Continuous
7	Window-to-wall ratio	10% – 90%	Continuous
8	Glazing system	Climate zone 2ASingle pane glass (U = 0.050 Btu/hr.ft^2.°F)Double pane glass (U = 0.40 Btu/hr.ft^2.°F)Triple pane glass (U = 0.35 Btu/hr.ft^2.°F) Climate zone 5ADouble pane glass (U = 0.40 Btu/hr.ft^2.°F)Triple pane glass (U = 0.35 Btu/hr.ft^2.°F)	Discrete
9	Wall type	Climate zone 2A Stucco + Fiberglass (U = 0.075 Btu/hr.ft^2.°F) Brick + Mineral wool (U = 0.066 Btu/hr.ft^2.°F) Concrete panel + Mineral wool (U = 0.052 Btu/hr.ft^2.°F) Stucco + Fiberglass (U = 0.051 Btu/hr.ft^2.°F) Concrete panel + Expanded polystyrene (U = 0.047 Btu/hr.ft^2.°F) Climate zone 5A Stucco + Fiberglass (U = 0.051 Btu/hr.ft^2.°F) Concrete panel + Expanded polystyrene (U = 0.047 Btu/hr.ft^2.°F) Brick + Cellulose (U = 0.040 Btu/hr.ft^2.°F) Brick + Extruded polystyrene (0.039 Btu/hr.ft^2.°F) Stone veneer + Extruded polystyrene (0.036 Btu/hr.ft^2.°F)	Discrete
Number	**O/P target**		
1	Operating energy intensity		
2	Embodied energy intensity		

the disaggregated cost to estimate EE as shown in Fig. 3. A more detailed description related to the EE calculation method is available in Venkatraj and Dixit [95] and Kumar et al. [94]. These EE calculations were performed using the IOH methodology which is considered a more complete and reliable methodology for EE calculations since it covers a larger system boundary [95].

5.1.5 Size of the dataset

Generating a large dataset increases computational cost, processing, and resources, while a small dataset might reduce the representation of the search space [14]. In this study, we utilized analogies from similar parametric simulation-based studies [11,15,39,96] to determine the size of our dataset. Ultimately, we generated a dataset with 6000 samples.

5.2. ANN model development: Basic framework

5.2.1 Feature selection and engineering

To determine the input features of the ML model, we conducted an initial study [10] to quantify the variation in EE and LCE caused by the implementation of OE-reducing measures. The findings of this study showed that all the input features (ex: climate zone, orientation, glazing system, WWR, etc.,) play an important role in predicting the output (LCE). Therefore, we retained all 12 input features.

The previously generated sample dataset consists of data in its raw form, i.e., it was not prepared for the ML algorithm, and therefore, could not be used. Discrete categorical variables must be transformed into a representative numerical format using an encoding scheme before using them in the ML model. This process is commonly referred to as feature engineering. The discrete categorical variable (climate zone) has two distinct levels (2 and 5), and each climate zone was mapped to binary (0 or 1) values using functions available in the Pandas library.

5.2.2 Data pre-processing

After feature engineering, we ensured that missing, repeated, or invalid values were eliminated from the dataset and that the data were transformed into a suitable format for the ML algorithm. This study utilized the MinMaxScaler function from the Scikit Learn package to normalize the data. Data normalization is essential since some of the study's input features do not have units (e.g., location, number of stories), some have different units (e.g., orientation, length, width, etc.), and some have percentages (e.g., WWR). In addition, data normalization prevents certain features with a larger range from overcompensating for features with a smaller range (i.e., length ranges between 32ft – 265ft,

Fig. 2. Framework to generate simulation-based building dataset.

Fig. 3. IOH disaggregated approach for EE assessment.

whereas floor height ranges between 10ft – 16ft) [39]. Data normalization unifies and scales all the input features, therefore preventing an overflow error in the input value. During the process of normalization, original values are rescaled and shifted to a new range between 0 and 1. This also helps reduce dependency on feature selection and improves training performance.

5.2.3 Train-test split

This study split 70% of the data for training, 15% for validation, and the remaining 15% for testing using the train_test_split function available in the Scikit Learn package.

5.2.4 Setting up the multi-output ANN model

The ANN model is preferred for solving interdependencies among multiple parameters [36,97,98]. The basic processing unit in an ANN model is referred to as a neuron/node. Each neuron holds the real-value representation of an attribute and is interconnected to neurons in the next layer of the network through weighted association lines [99]. To further explain, each node in the hidden layer is a weighted sum of the input nodes, while the output node is the weighted sum of the hidden nodes [100]. A simple mathematical representation of the summation process is shown using Equation (1) and Fig. 4, where x, w, b, and y refer to the raw input features of value, weight, bias, and model output, respectively.

$$y = \sum_{i=1}^{n} x_i w_i + b_i \tag{1}$$

$$R(z) = \max(0, z) \tag{2}$$

The output value from each hidden layer neuron is then transformed using an activation function to limit its range and set boundaries. In this study, the rectified linear unit (ReLu) was used as the activation function for the hidden layer. The ReLu activation function is defined using Equation (2), where z is the weighted sum of the input node.

Next, we determined the number of nodes in the hidden layer using Equation (3), which is the most common approach in neural network design [29,45]. Here, n_h, n_i, and n_o represent the number of hidden layer nodes, input layer nodes, and output layer nodes, respectively.

$$n_h = \frac{n_i + n_o}{2} \tag{3}$$

Therefore, we began the iterative training process with 7 nodes in the hidden layer. The goal of the training process is to minimize the loss function and reach the point of convergence, thereby ensuring that the model fits the problem correctly (Fig. 5). In this study, we utilized mean squared error (MSE) as the loss function and the Adam optimizer to adaptively adjust the learning rate of the model. The MSE is calculated using Equation (4), where n is the number of samples, $\hat{y}$ is the prediction output, and y is the true value.

$$Costfunction = MSE = \frac{1}{n}\sum_{i=1}^{n}(\hat{y} - y)^2 \tag{4}$$

Fig. 4. Mathematical representation of the hidden layer neuron.

Fig. 5. Flowchart of the iterative training process.

This iterative process of training continues until it is terminated by early stopping, which is a regularization technique to prevent the model from overfitting. The patience criterion for early stopping was set to 20 in this study, i.e., if the loss increases for 20 consecutive iterations, the training process would be terminated (see Fig. 6).

Subsequently, we performed several experiments to improve the performance of the ML model. Certain parameters of the initial ML model (number of hidden layer nodes, network architecture, learning rate, and activation function), were modified to improve the accuracy of the model. The ML model was created using the TensorFlow, Keras, and Scikit Learn packages.

5.2.5 Performance evaluation of the ANN model

To evaluate the performance of the developed model, we compared the output targets generated from the model and the true value from the test dataset. This study used the coefficient of determination (R^2) and mean absolute percentage error (MAPE) to evaluate model performance. These performance metrics are calculated using Equations 5–6 shown below:

Fig. 6. Loss curve for early stopping.

$$R^2 = 1 - \frac{\sum(\hat{y} - y)^2}{\sum(y - \bar{y})^2} \tag{5}$$

$$MAPE(\%) = \frac{1}{n}\sum_{i=1}^{n}\left|\frac{\hat{y} - y}{y}\right| \times 100 \tag{6}$$

where:
'n' is the total number of data points,
'$\hat{y}$' is the predicted output,
'y' is the actual output,
'$\bar{y}$' is the mean of the actual output.

5.3 Test case

We tested the generalization ability of the developed ML model on two test cases described in Table 5.

The OE intensity and EE intensity of the test cases were evaluated using both the traditional and data-driven approaches. In the traditional approach, the geometry of the test cases was modeled on Rhino. Then the Ladybug and Honeybee plugins available in the Grasshopper environment were used to simulate OE intensity. For EE, we first disaggregated the information obtained from the contractor's schedule of values into different material groups. After that, the IOH-disaggregated approach described was utilized to calculate EE intensity.

In the data-driven approach, we deployed the ML model developed in this study to estimate building energy. Here, we provided information for the previously defined input fields. After entering the input parameters, the prediction method was called to estimate OE intensity and EE intensity. Finally, we determined and compared the variation in results between both approaches.

6. Main assumptions

We make the following assumptions in this study:

- The useful life span of a building is 60 years.
- The default assumptions for thermostat setpoint, thermal zoning, HVAC system type, lighting power density, equipment power density, and occupancy schedules are compliant with ASHRAE 90.1–2019 standards.
- A packaged air conditioning unit which used energy sources such as natural gas (furnace) and electricity (air-conditioner) was used as the HVAC system in the simulations.
- The parameters associated with climate, energy supply mix, and economy remain constant over 60 years.
- The building is a stand-alone structure i.e., the influence of the surrounding buildings is not considered for OE calculations.
- The EE of materials is the same across different geographic locations.
- The change in structural systems based on building height is ignored for simplicity.

7. Results

7.1. Performance evaluation of the developed multi-output ANN model

The final network architecture of the ML model developed in this study is illustrated in Fig. 7. This model has 12 nodes in the input layer, 17 nodes in the first hidden layer, 10 nodes in the second hidden layer, and 2 nodes in the output layer. The model summary indicates three dense layers (i.e., nodes of the dense layer are connected to all the nodes of the preceding layer). Each dense layer transforms the input it receives based on the network's weights and biases. In total, the model has 423 trainable parameters. Table 6 shows the setting of the model's hyperparameters used during the training process.

During an epoch, the model evaluates its performance on the training

Table 5
Characteristics of test cases.

	Test case 1	Test case 2
Climate zone	5A	2A
Test cases	Prototype reference building	Real life case study building
Data source	Commercial Reference Buildings, Department of Energy, 2022	Google Earth, University architect's office
Building form		
Number of floors	4	2
Gross floor area	33,700 sqft	114,366 sqft
Exterior wall construction	Steel-framed building with 4″ stucco and fiberglass insulation (U = 0.052 Btu/hr.ft^2.°F)	Steel-framed building with 4″ brick veneer/stone cladding and mineral wool insulation (U = 0.066 Btu/hr.ft2.°F)
Exterior window construction	Double pane glass (U = 0.40 Btu/hr.ft2.oF)	Double pane glass (U = 0.40 Btu/hr.ft2.°F)

Fig. 7. Network architecture of the energy prediction model.

Table 6
Model hyperparameters.

Model hyperparameters	Setting
Batch size	32
Activation function	ReLu
Optimizer	Adam
Learning rate	0.01
Patience criteria for early stopping	20 epochs

dataset and validation dataset using the loss function. This measured performance (loss/cost) of the model is plotted in the form of a learning curve. The loss curve provides crucial information regarding the fit of the model. If the validation loss decreases to a point and then begins increasing again, then the model is overfitting, i.e., it will not generalize well. In the opposite scenario, if the model is not trained for sufficient epochs, it will not learn from the data and is said to have the problem of underfitting. During the first epoch, we note that model loss (MSE) was extremely high due to random weight initializations. This loss progressively decreased during the training process, which adjusts the weights of the network. The loss curve decreased to a point of stability during which the training process was stopped by using the early stopping callback at epoch 113 (Fig. 8). At the end of the training process, the overall loss was 0.028. The MAE for output 1 (OE intensity) was 0.92, whereas the MAE for output 2 (EE intensity) was 0.90.

Fig. 9 illustrates the correlation analysis between the actual energy intensity obtained using the parametric workflow and the model output. The predicted values (represented by the points) are very close to the regressed diagonal line for both outputs (OE intensity and EE intensity). This demonstrates a very strong correlation between the actual and predicted values. The R^2 values are also very close to 1, suggesting that the model has a good fit. It is important to note that R^2 values do not account for bias. For that reason, we also examine the residual plots to ensure that our model predictions are not biased.

The x-axis and y-axis of Fig. 10 represent the predicted values and standardized residual values, respectively. The residual value is essentially calculated as the difference between actual value and predicted value for each data point. Positive residual values indicate the prediction was low, whereas negative values indicate the prediction was too high. Residual values of zero represent a perfect prediction. We observe no specific patterns or residual outlier values in the residual plot shown in Fig. 10. In addition, we observe that the residual values are clustered and evenly distributed around the lower single digits of the y-axis. This indicates the developed model does indeed fit the data well. However, in

Fig. 8. Training loss curve.

Fig. 9. Correlation between actual and predicted energy intensity.

Fig. 10. Residual plot for predicted values of (a) operating energy intensity, and (b) embodied energy intensity.

Fig. 10-b, the plot exhibits some characteristics of heteroscedasticity. This means that the variance in the residual values is unequally distributed. From the plot, we notice the residual value increases as we progress from lower to higher values of EE intensity, indicating that further improvements can be made to the developed model. This heteroscedasticity may arise due to the right skewness of the EE intensity data.

Fig. 11 shows the comparison between the predicted values and true (simulated) values of OE intensity and EE intensity for all data points in the test dataset. In Fig. 11, data points are plotted on the x-axis while the model predictions and true values of energy intensities are plotted on the y-axis. Each point in the scatter plot represents the predicted value, whereas the continuous line represents the true value in Fig. 11-a. A more detailed version of the same plot is illustrated in Fig. 11-b. Here, the true values are represented with continuous lines, whereas the predicted values are shown using dashed lines.

This graph (Fig. 11 b), along with Table 7, demonstrates that the over or underestimated values of predicted energy intensities are negligible and very close to the simulated value. This indicates that the developed ML model has high predictive accuracy.

7.2. Test cases and results

Test cases 1 and 2 were modeled in the Rhino/Grasshopper environment (Figs. 12 and 13). The OE intensity for both case study buildings was simulated using the Ladybug and Honeybee plugins within the GH environment. These plugins utilize EnergyPlus, considered the most robust energy simulation engine in the building industry.

For test case 1, located in climate zone 5A, we calculated EE using the surface area information of different building components obtained from the prototype model. The simulation results of OE and EE intensity were 44.02 kBtu/ft^2.year and 31.02 kBtu/ft^2.year, respectively. The input parameter values shown in Table 8 were entered into the developed ML model to predict the OE and EE intensities of Building 1. The prediction results of OE and EE intensities were 45.92 kBtu/ft^2.year and 31.70 kBtu/ft^2.year, respectively. The percentage errors between the simulated and predicted values of OE and EE intensities were 4.13% and 2.14%, respectively.

For test case 2, located in climate zone 2A, the simulation output of OE intensity was 52.40 kBtu/ft^2.year. The contractor's schedule of values was used to calculate EE intensity using the IOH-disaggregated approach. The EE intensity calculated in this manner was 28.63 kBtu/ft^2.year.

Next, we entered the building parameter values (Table 9) into the developed ML model to predict its energy intensities. The predicted values of OE and EE intensities were 53.51 kBtu/ft^2.year and 30.78 kBtu/ft^2.year, respectively. The percentage errors between the simulated output and predicted output were 2.07% and 6.9% for OE and EE intensity, respectively.

8 Discussion

8.1 Overview

In this study, we developed an ML model for building energy prediction by comprehensively integrating building LCE components. The findings show that ML models can indeed simplify the process of building LCE analysis.

This study holds significant time and cost implications. The ML approach drastically reduces the amount of time and expertise required for modeling. The computer used to generate the parametric building energy dataset and develop the ML model has an Intel® Core™ i9-9980HK CPU @ 2.4 GHz processor and 64 GB RAM. Professionals and practitioners are aware that running a single traditional building energy simulation takes several hours to a day and is computationally expensive. Using this model, after setting up the parametric workflow, each run took approximately 60–90 s for the 1-story and 2-story building

Fig. 11. Scatter plot comparison between predicted and simulated values of energy intensities (a) for all the data points in the testing dataset, and (b) small sample of the testing dataset.

Table 7
Predicted vs True values for a small sample of the testing dataset.

OE intensity (kBtu/ft^2.year)			EE intensity (kBtu/ft^2.year)		
Simulated	**Predicted**	**Residual**	**Simulated**	**Predicted**	**Residual**
55.85	56.44	−0.59	38.99	38.87	0.12
63.29	60.93	2.36	34.23	34.34	−0.11
48.38	48.53	−0.15	33.16	33.18	−0.02
55.61	54.59	1.02	33.53	32.29	1.24
62.17	59.51	2.66	31.63	32.77	−1.14

Fig. 12. Energy model of test case 1 located in climate zone 5A.

models whereas, the computational time taken for the 3-story building models nearly doubled (i.e., ~120–180 s). The time taken to model the 3D geometry of the case study building on Rhino was approximately 3–4 h, after which the energy simulation took 2–3 min to run. As already mentioned, traditional energy simulation workflows are plagued by issues of interoperability. Therefore, the EE calculations for both studies were conducted on Microsoft Excel using the IOH-disaggregated approach. These EE calculations took an additional 10 min to compute. Our study overcomes time and cost challenges by utilizing the ML approach providing instantaneous results. The computational time was approximately 1 microsecond for each step during the training process. The developed model requires very few numerical inputs to perform energy assessments that closely approach the accuracy of traditional simulation results. It is important to mention that while it took approximately 12–13 min to simulate the OE and EE results of the case study buildings, the developed ANN provided results in less than 1 s. Undoubtedly, the speed of the ML approach is advantageous for generative design and optimization where millions of design options must be simulated.

Despite the availability of open-source building energy datasets, a lack of datasets containing EE information still persists. This hinders the implementation of ML-driven solutions for building LCEA. Our findings suggest that the ML model's robustness could be improved by adding more diversity to the data. Expanding the database to include EE information for different building types, shapes, materials, locations, etc. will make it more diverse and robust. In addition, we can also generate synthetic datasets by taking advantage of parametric modeling techniques and data augmentation. These findings are corroborated by studies conducted by Singaravel et al. [57], Wang et al. [101], and D'Amico et al. [64]. Furthermore, we also recommend combining real-world data with synthetic data to create a holistic dataset.

Based on the set of experiments we conducted to identify optimum

Fig. 13. Energy model of building 2 located in climate zone 2A.

Table 8
Characteristics of case study building in climate zone 5A.

Input Parameter	Value
Location	5A
Length	152ft
Width	55ft
Number of floors	4
Floor height	10ft
Wall U-value	0.051 Btu/hr.ft^2.°F
WWR-N	0.20
WWR-W	0.20
WWR-S	0.20
WWR-E	0.20
Window U-value	0.40 Btu/hr.ft^2.°F
Orientation	0°

Table 9
Characteristics of test case 2 in climate zone 2A.

Input Parameter	Value
Location	2A
Length	255ft
Width	360ft
Number of floors	2
Floor height	15ft
Wall U-value	0.066 Btu/hr.ft^2.°F
WWR-N	0.500
WWR-W	0.010
WWR-S	0.276
WWR-E	0.15
Window U-value	0.40 Btu/hr.ft^2.°F
Orientation	315°

Table 10
Experiments conducted to determine optimum network architecture.

Experiment	Model architecture	Output 1 (OE intensity)		Output 2 (EE intensity)		Epochs
		MAPE (%)	R^2	MAPE (%)	R^2	
1	12, 7, 2	3.64	0.86	3.83	0.73	175
2	12, 8, 2	3.92	0.85	4.22	0.64	89
3	12, 9, 2	3.38	0.84	4.91	0.58	113
4	12, 10, 2	2.82	0.89	3.43	0.75	61
5	12, 11, 2	3.87	0.86	4.45	0.64	50
6	12, 12, 2	2.80	0.91	4.36	0.58	54
7	12, 13, 2	3.68	0.86	3.97	0.69	225
8	12, 14, 2	3.71	0.86	4.19	0.65	84
9	12, 15, 2	3.91	0.85	4.19	0.63	63
10	12, 9, 5, 2	2.92	0.89	4.73	0.58	90
11	12, 9, 7, 2	1.73	0.96	3.85	0.73	134
12	12, 9, 9, 2	2.37	0.94	4.14	0.70	206
13	12, 11, 5, 2	2.50	0.93	2.87	0.83	116
14	12, 11, 7, 2	1.82	0.95	2.55	0.87	131
15	12, 11, 9, 2	2.95	0.90	4.30	0.68	58
16	12, 14, 5, 2	1.48	0.97	5.05	0.52	156
17	12, 14, 7, 2	2.75	0.90	3.89	0.58	48
18	12, 17, 10, 2	1.95	0.96	2.47	0.90	113
19	12, 9, 6, 3, 2	2.57	0.93	5.43	0.50	195
20	12, 10, 5, 10, 2	1.59	0.97	3.72	0.76	54
21	12, 10, 15, 10, 2	1.67	0.96	3.49	0.78	100
22	12, 12, 15, 10, 2	1.71	0.96	3.20	0.74	88
23	12, 12, 15, 12, 2	2.21	0.95	3.29	0.72	80
24	12, 14, 7, 10, 2	1.88	0.96	3.11	0.71	70
25	12, 14, 10, 7, 2	1.77	0.96	2.84	0.84	107

network architecture, the model performance does not increase significantly by adding more nodes or depth to the network (Table 10). This may be due to the limited size of the synthetic dataset. Moreover, Table 10 also shows that the model's MAPE and R^2 performance for OE intensity are much better in comparison to EE intensity. This can be explained by the right skewness and variation in EE data, implying that most of the data points are distributed to the left side. The density of data on the left side may be much higher for both EE and OE intensities since we used the Galapagos (an optimization-based plug-in) to generate data. In the future, studies may consider using other simulation approaches to generate a more balanced dataset.

We also conducted ML training using the same network architecture to understand the performance difference between (i) a single output prediction model (separate training for OE and EE) and (ii) a multi-output prediction model (combined training for OE and EE). Table 11 shows the MAPE values for the single-output model as slightly higher compared to the multi-output model. Similarly, Fig. 14 illustrates that the R^2 value of the single output model is lower than that of the model simultaneously training both outputs. These results indicate that the combined ML training runs leverage the correlation between the two prediction tasks to improve model performance. Multi-output prediction models are, therefore, beneficial in terms of training time and predictive performance. Training disjoint models for each output could become computationally expensive and time-consuming, particularly for models that utilize large datasets or have complex network architecture.

Table 11
Single output vs multi-output prediction model.

	Single output prediction model			Multi-output prediction model		
	Epochs	**MAPE (%)**	**R^2**	**Epochs**	**MAPE (%)**	**R^2**
OE intensity	63	2.01	0.94	113	1.95	0.96
EE intensity	141	2.80	0.86		2.47	0.90

8.2. *Generalization ability of the developed model*

The ML model's ability to handle previously unseen data is referred to as generalization. Overfitting (overtraining the model on training data) or underfitting (not training the model sufficiently) both lead to

Fig. 14. Correlation between simulated and predicted energy intensity for a single output prediction model.

poor generalization ability of the model. In certain cases, the data collected for the training dataset might not accurately represent the entire population. As a result, the model's performance while handling unseen data decreases. To reduce sample bias in this study, we carefully selected parameter constraints to ensure that the model space is large enough to represent most of the building stock and derive energy consumption patterns. Despite these considerations, the generated sample dataset is still missing certain parts of the population. Epistemic uncertainty arises in the regions of the population lacking data. In our case, it refers to input parameters outside the range of our parametric model. For example, we have no data for instances of the parametric model with length or width values greater than 265 ft (80 m). In such cases where the input parameter value is outside the range of the training dataset, the ANN model will use extrapolation to determine the output value. Extrapolation is defined as the "prediction from a model that is a projection, extension, or expansion of an estimated model" outside the range of data that was used for model calibration.

Generally, an ANN model does not perform well in regions with no training data; this is associated with high extrapolation error costs [102]. For instance, in test case 1, the number of floors parameter is outside the training range. In addition, we assume that test case 1 has core and perimeter zoning while evaluating the OE intensity using the prediction model. Here, the percentage error for OE and EE intensities is 4.14% and 2.14%, respectively. Similarly, in test case 2, one input parameter (width = 360 ft) was out of the data range used for training the model. Moreover, the shape of the case study building is not a perfect rectangle; therefore, certain assumptions were made about the input parameters of the prediction model. Upon comparing the simulation results with the model outputs, we notice that the percentage error for the case study building was estimated to be 2.07% for OE intensity and 6.90% for EE intensity. In both test cases, the error costs are less than 10%, which is recommended for highly accurate forecasting [103]. However, the error costs are much higher than the MAPE values of the model for OE and EE intensities, which were 1.95% and 2.47%, respectively. These results show that the developed model has good generalization ability and the error cost for out-of-sample predictions is high. Since the training classifier is dependent on the function within the dataset, we can only be approximately correct for the out-of-range distribution. This data dependence on the finite dataset used for training limits the wide use and application of ANN models. We therefore recommend using input parameters within the range used for sample data generation to ensure an accurate prediction.

9. Conclusions

This study investigated the feasibility of developing an ML-based framework to predict both EE intensity and OE intensity, to address building energy from a life cycle perspective. The study generated a synthetic building LCE dataset to train and test an ML model. The developed ANN model can fairly simplify the process of LCE analysis in the design phase and has high prediction accuracy in estimating both outputs. More specifically, the study also highlights the suitability of using an ANN model to handle complex nonlinear relationships among various building parameters. The analytical results indicate the most optimum neural network architecture had a MAPE value of 1.95% and R^2 of 0.96 for OE intensity; and a MAPE value of 2.47% and R^2 of 0.90 for EE intensity. The comparison between the single output and multi output ANN model shows that combined ML training improves model performance by leveraging the correlation between the two prediction tasks. Lastly, the case study results demonstrate that the predicted and simulated values of OE and EE intensity have an error margin ranging from 2% to 7%. These results highlight the benefits of using ML-based models for building LCEA in terms of cost, time, and effort. Importantly, designers would not have to switch back and forth between several tools or deal with issues caused by interoperability. Thereby, this model could streamline the design decision-making process. Future studies can test this model on more real building energy data to assess and improve the performance of the ML model. We also suggest exploring the use of more complex neural networks such as Convolutional Neural Networks (CNN's) or Transformers and methods such as Transfer Learning to more reliably predict LCE performance.

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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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