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Integrating experimental analysis and machine learning for enhancing energy efficiency and indoor air quality in educational buildings

Seyed Hamed Godasiaei [a], Obuks A. Ejohwomu [b,c,*], Hua Zhong [d], Douglas Booker [e]

[a] School of Chemical Engineering and Technology, Xi'an Jiaotong University, Xi'an, China
[b] Department of Mechanical, Aerospace and Civil Engineering, University of Manchester, Engineering Building A, Booth Street E, Manchester, M13 9PL, United Kingdom
[c] CIDB Centre of Excellence, University of Johannesburg, Johannesburg 2092, South Africa
[d] School of Built Environment and Architecture, London South Bank University, United Kingdom
[e] School of Civil Engineering, University of Leeds, United Kingdom

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A B S T R A C T

Ensuring energy efficiency and maintaining optimal indoor air quality (IAQ) in educational environments is vital for occupant health and sustainability. This study addresses the challenge of balancing energy consumption with IAQ through experimental analysis integrated with advanced machine learning (ML) techniques. Traditional methods often fail to optimise both simultaneously, necessitating innovative solutions leveraging real-time data and predictive models. The research employs ML models, including Recurrent Neural Networks (RNN), Long Short-Term Memory Networks (LSTM), Gated Recurrent Units (GRU), and Convolutional Neural Networks (CNN), using a dataset of over 35,000 records. Parameters such as CO_2 levels, particulate matter (PM), temperature, humidity, and exogenous variables (e.g., time, date, and rain sensor) were analysed to identify environmental factors influencing HVAC system efficiency. Predictive models achieved over 92 % accuracy, enabling precise real-time HVAC control to balance energy use and IAQ. Key findings highlight GRU and LSTM models' effectiveness, with scalability across educational institutions showing potential for reducing energy costs and improving indoor environments. Validation with diverse datasets demonstrated robustness, while SHAP (Shapley Additive exPlanations) values provided enhanced interpretability, helping policymakers and managers implement effective strategies. This research underscores the transformative role of ML in optimising HVAC efficiency and IAQ management, offering scalable, data-driven strategies to reduce carbon footprints, improve occupant well-being, and align with global sustainability goals. By overcoming traditional limitations, the study presents a systematic approach for integrating empirical data with AI, advancing smarter, healthier, and more sustainable learning environments.

1. Introduction

Energy optimization and indoor air quality (IAQ) management are critical considerations in modern building systems, particularly given the rapid pace of urbanisation and the global push for sustainability [1]. IAQ and thermal comfort significantly impact human health and productivity, as people spend the majority of their time indoors [2]. Poor IAQ is associated with respiratory diseases, cognitive impairments, and general discomfort [3], while inefficient energy consumption leads to high operational costs and substantial greenhouse gas emissions [4]. Designing environments that prioritise both health and energy efficiency is essential, especially for students, who represent the future generation [5]. Balancing IAQ management with energy optimisation remains challenging [6]. Traditional systems often rely on static controls with limited capacity to respond dynamically to indoor and outdoor conditions [7]. These systems, although functional, cannot adapt to real-time changes, resulting in inefficient energy use and compromised IAQ [8]. This is particularly problematic in buildings, where energy for heating, cooling, and ventilation comprises a significant portion of overall energy use, while occupant health and comfort are adversely affected [9]. Recent advancements in sensor technology and the Internet of Things (IoT) have revolutionised the monitoring of environmental conditions. Sensors now measure particulate matter ($PM_{2.5}$, PM_{10}), carbon dioxide (CO_2), temperature, formaldehyde, and volatile organic compounds (VOCs), providing real-time data on IAQ [10,11]. However, translating

* Corresponding author at: Department of Mechanical, Aerospace and Civil Engineering, University of Manchester, Engineering Building A, Booth Street E, Manchester, M13 9PL, United Kingdom.

E-mail addresses: obuks.ejohwomu@manchester.ac.uk, obuksejohwomu@yahoo.co.uk (O.A. Ejohwomu).

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Nomenclature

f_h	Activation function
b	Bias term
H	*Heat transfer foil with Thickness* [μm]
α	Neurone
$g_0^{(t)}$	Output gate
$h^{(t)}$	Output hidden state
$ux^{(t)}$	Represents the weighted sum of the input features
$wh^{(t-1)}$	Represents the weighted sum of the previous hidden state
T	Temperature [K]
β_j	the coefficient of predictor *j*
x_i	The input to the *i th* training example
β_0	The intercept term
μ	Mean of feature mean
$\hat{y}_i$	The predicted target value of the *i th* training example
λ	The regularisation parameter
σ	Standard deviation
y_i	True target value of the *i th* training example
x_{ij}	The value of predictor *j* for observation *i*
w_f, u_f, b_f	Weights and bias terms associated with the forget gate
w_i, u_i, b_i	Weights and bias terms associated with the input gate
W	Weights
t	Time
Z	Resulting values
x_{scaled}	Resulting values
$\min(X)$	The minimum value
$\max(X)$	The maximum value
CO_2	Carbon dioxide
CO	Carbon Monoxide
IAQ	Indoor Air Quality
LSTM	Long Short-Term Memory
GRU	Gated Recurrent Unit
ReLU	The Rectified Linear Unit
SMR	Steam Methane Reforming
CNNs	Convolutional Neural Networks
RNNs	Recurrent Neural Networks
HCHO	Formaldehyde
TVOC	Total volatile organic compounds
GEP	Genetic programming
SHAP	SHapley Additive exPlanations

Greek symbol

θ	The model parameters are represented

Subscript

avg	Average
n	Number of observations

these data into effective real-time decisions for environmental control remains a challenge [12]. Such data demand robust systems capable of processing and interpreting information quickly and accurately to optimise building operations in real time [13,14].

Machine learning (ML) offers a transformative solution by enabling the development of intelligent systems that learn from data and make optimal predictions for IAQ and energy efficiency [15]. ML algorithms applied to sensor data facilitate the creation of predictive models to adjust ventilation, heating, and cooling in real time based on changing environmental conditions [16]. These models balance energy use with IAQ, improving occupant comfort and reducing operational costs [17,18]. Additionally, ML algorithms dynamically update predictions based on historical data and external factors, such as weather conditions [19,20]. For example, predictive models can optimise ventilation rates for CO_2 and humidity without sacrificing comfort [21], while temperature control systems can be tailored to occupancy patterns for significant energy savings [22]. Notable studies have explored various aspects of IAQ and energy management. Kumar et al. [23] investigated real-time IAQ and energy monitoring in commercial buildings, addressing challenges in managing large datasets for responsive systems. Li et al. [24] developed a BPNN-based AMOPSO-GWO algorithm to predict and optimise IAQ, thermal comfort, and energy consumption, achieving over 90 % accuracy. Woloszyn et al. [25] examined relative-humidity-sensitive ventilation, demonstrating its ability to smooth RH fluctuations and save energy. Cheng et al. [26] studied outdoor air conditioning systems with stratified ventilation, achieving a mean absolute error of 1.9 % for CO_2 concentration and reducing energy consumption by 6.4 % while maintaining IAQ standards. Giliket et al. [27]. investigated pollutant levels in Istanbul, Kocaeli, and Barcelona, achieving significant improvements using the LSTM algorithm. Their results showed a 20–31 % enhancement for ozone, 11–53 % for particulate matter, 18–46 % for sulphur dioxide, and 9–47 % for nitrogen oxides. Shin et al. [28]. employed deep learning regression using fully convolutional network (FCN) and DNN architectures to predict mean air age (MAA) efficiently while preserving spatial information. Their findings demonstrated that the FCN model outperformed the DNN in accuracy and performance. Zeng et al. [29]. used a new prediction model that integrates the extended stationary wavelet transform (ESWT) and the nested short-term memory neural network (NLSTM) to predict $PM_{2.5}$ in this study. Their results show that the new methods outperform traditional methods. Despite significant advancements, existing systems lack the adaptability and integration necessary for real-time IAQ management and energy optimisation in dynamic indoor environments. The reliance on static or semi-dynamic methods limits efficiency and scalability across diverse settings. Furthermore, integrated empirical investigations and algorithms specifically tailored for schools and educational environments have received limited attention, highlighting a notable gap in the research. Addressing these limitations could lead to more effective, scalable, and context-sensitive solutions for IAQ and energy management in educational settings.

Despite advancements in energy optimization and IAQ management, a significant research gap persists in the development of dynamic, real-time solutions tailored to educational environments. Traditional approaches often rely on static or simplistic empirical models that fail to adapt to the complex and fluctuating conditions of educational settings, such as varying occupancy patterns, seasonal weather changes, and diverse IAQ parameters. These limitations result in inefficient energy consumption and suboptimal IAQ, which can adversely affect the health, productivity, and well-being of students and staff. Furthermore, existing systems lack the ability to integrate and analyze real-time data from multiple sources, such as window controls, rain sensors, and indoor/outdoor air quality metrics (e.g., $PM_{2.5}$, CO_2, Temperature, HCHO (Formaldehyde), Total volatile organic compounds (TVOC)), to make informed decisions. Additionally, the absence of interpretability and transparency in decision-making processes hinders stakeholder trust and adoption of these systems. This study addresses these critical gaps by introducing an innovative framework that leverages advanced ML models, including RNN, LSTM, CNN, and GRU, to dynamically optimize energy use and IAQ in real-time. By incorporating SHAP (SHapley Additive exPlanations) values, the framework also enhances model transparency, enabling stakeholders to understand and trust the decision-making processes. This approach not only bridges the gap between theoretical research and practical application but also provides a scalable solution for sustainable building operations in educational environments.

2. Advances in predictive modelling and environmental sensor integration: experimental insights and strategies

The interaction between energy efficiency and IAQ is a very complicated issue in educational facilities, where the optimization goal is to make the built learning environment healthier and sustainable [30]. Most educational institutions face a big challenge in maintaining indoor environments free from contaminants to ensure good IAQ for students and staff while at the same time minimising energy use. Adequate ventilation is important for thermal comfort and pollutant removal, but it often results in increased energy consumption [31]. This research explores solutions that respond to these competing priorities by using data-driven strategies and practical interventions. The case study used in this research is a Primary School in Codsall, Staffordshire, United Kingdom. Codsall is a quite village that is situated very close to Wolverhampton. It offers semi-rural surroundings with both residential and greenery settings. Although the place carries a placid and quite environment, the situation of the school at Wolverhampton Road exposes it to urbanisation process and environmental problems. Proximity to high-traffic commuter routes, railway lines and stations, town centre, shopping area parking and petrol stations introduces a complex mix of air pollution from vehicular emissions, PM and VOCs. Thus, the current site is an excellent location for studying the impacts of external environmental factors on IAQ and energy use in educational settings. This study specifically focuses on two classrooms within the school, selected as they are similar in all respects, have the same dimensions, identical window sizes and usage patterns. Each classroom is occupied by 35 students of both sexes, all within the primary school age group; this demographic is particularly sensitive to air quality, as children's developing systems are more susceptible to air pollutants. Kids' health and well-being take precedence, which explains the urgency to understand and find solutions to challenges in IAQ at schools. Indeed, active school hours (from 9:00AM to 3:15PM) are critical periods within which this research endeavour conducts pollutant-level monitoring in classrooms over several months. The key parameters based on the sensitivity analysis of the parameters affecting IAQ as reviewed in Fig. 1 were time, date, rain sensor, $PM_{2.5}$, PM_{10}, outdoor temperature, CO_2, indoor temperature, formaldehyde and TVOCs with the aim of understanding their impact on optimization strategies. These pollutants were selected based on their strong health effects and potential to vary with occupancy, outdoor air conditions, and ventilation practises. Real-time sensor data were collected to track variations in pollutant levels, thereby providing a thorough understanding of how IAQ changes throughout the day. The experimental design of this study also considered natural ventilation as one of the key parameters for balancing IAQ and energy efficiency. The windows in both classrooms served as the major ventilation source. The research aim was to create window-opening percentages that would maintain pollutant levels within safe limits while preventing excessive energy loss or temperature instability. The predictive model developed for this purpose incorporates integrated data on outdoor air conditions, indoor temperatures, and pollutant concentrations. The equipment and materials used in this study are listed in Table 1, comprising high-precision environmental sensors and data logging systems. Such a set of tools gives the capability to measure and analyse IAQ parameters and environmental conditions with accuracy, thus forming the basic data set for model development that leads to an intelligent system able to suggest or even automate strategies for ventilation. The system would then, by using predictive algorithms, advise on the optimal percentages of opening windows in real time to maintain air quality and temperature within set ranges. This is important beyond the primary school used in this case study because this research tackles the twin challenges of energy efficiency and IAQ in its findings, hoping to provide solutions scalable for educational institutions across the UK and beyond. Since children spend most of their day inside school facilities, improving IAQ is more likely than not lead to better cognitive performance, better health, and better long-term development. Further, optimization of energy efficiency in schools contributes to broader sustainability goals and reduces carbon emissions while lowering operating costs.

The NAQTS V2000 is an air quality monitoring system designed to measure a wide range of air quality and environmental parameters with high precision. It utilizes both a condensation particle counter to measure ultrafine particles (UFPs), expressed as a particle number concentration (PNC) and an optical particle counter (OPC) to measure $PM_{2.5}$ and PM_{10}. It also includes an NDIR CO_2 sensor, electrochemical sensors for CO and NO_2, and metal oxide sensors for dual measurements of CO, NO_2, and VOCs. Additionally, the system is equipped with sensors for temperature, pressure, and relative humidity, along with a 3D accelerometer and a 3D gyroscope to monitor vibrations. External noise levels, measured in decibels (dBA), can be assessed through the integrated USB ports, and an optional configuration to integrate four thermal desorption tubes to enable comprehensive VOC speciation analysis. To ensure the accuracy and reliability of data, co-located measurements were conducted using three primary sensors deployed in both a dynamic classroom and a control classroom. This strategic placement ensured alignment of outputs from different devices, allowing for consistency in recorded data across multiple measurement points. By positioning the sensors in close proximity, both indoors and outdoors, cross-referencing of measurements taken simultaneously within the same environment was facilitated, which is a crucial step in data validation. Any discrepancies in sensor readings were carefully identified and addressed to

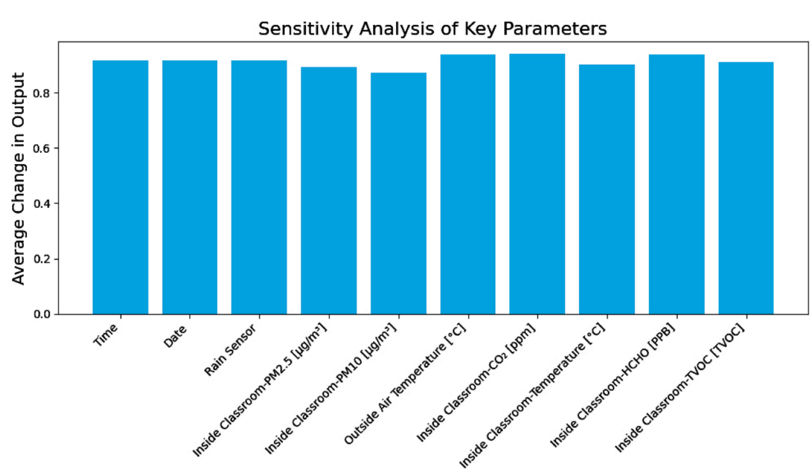

Fig. 1. A Comprehensive study for sensitivity analysis of key parameters in indoor air quality optimization in educational buildings.

Table 1
NAQTS V2000 system specifications for monitoring IAQ and environmental conditions.

Category Particulates	Specification Particle Number	Details Particle Mass
Technology	Mixing CPC with embedded diluter	Laser-based
Concentration Range	0 - 1000,000 cm^3	0 – 1000 $\mu g/m^3$
Concentration Accuracy	± 10 % compared to reference CPC	± 15 $\mu g/m^3$
Operating Temperature	0 to 35 °C	0 to 35 °C
Operating Humidity	0 to 95 %	0 to 95 %
Response Time	<3 secs (T10-T90)	<6 secs (T10-T90)
Working Fluid	IPA	—
Gases	**Carbon Dioxide (CO_2)**	**Electrochemical Sensors**
Technology	NDIR	Electrochemical
Range	0 to 10,000 ppm	CO: 0–1000 ppm, NO_2: 0–5 ppm
Resolution	—	CO: 0.5 ppm, NO_2: <20 ppb
Accuracy	±30 ppm or ±3 % reading (whichever is larger)	—
Operating Temperature	0 to 50 °C	—
Operating Humidity	0 to 95 %	—
Response Time	<10 secs	<15 secs
Supplier	—	SPEC Sensors
Metal Oxide Sensors	**Environmental**	**Details**
Technology	Metal Oxide	—
CO/VOCs Range	1 to 1000 ppm	—
NO_2 Range	0.01 to 10 ppm	—
Operating Temperature	−10 to 50 °C	—
Response Rate	<15 secs	—
Pressure	800 to 1100 hPa, ±0.25 %	—
Humidity	±3 % RH	—
Supplier	SGX Sensortech	—
Miscellaneous	**Unit Specifications**	**Details**
Power	<100 W, 12 V DC	—
Noise	~55 dBA	—
Data Storage	SD Card, Local MySQL, optional Cloud Storage	—
Data Acquisition Rate	1Hz	—
Communications	WiFi, Web-based GUI, GSM	—

maintain data integrity, ensuring that the recorded air quality parameters were both accurate and comparable. IAQ was monitored continuously for one month in both the dynamic classroom, where the air quality monitoring system was actively in use, and the control classroom, which remained unmodified for comparative purposes. The sensors captured fluctuations in key air quality parameters such as $PM_{2.5}$, CO_2, VOCs, temperature, and humidity, providing insights into how IAQ naturally varies throughout different periods of the day, including class transitions and ventilation periods. This monitoring process aimed to establish a baseline understanding of how IAQ is influenced by typical classroom activities, occupancy levels, and external factors. Special attention was given to CO_2 concentrations, which serve as a critical indicator of ventilation efficiency and overall air quality, as well as $PM_{2.5}$ levels, which are directly associated with particulate pollution and its potential impacts on respiratory health. VOC concentrations were also closely monitored, as these pollutants originate from various indoor sources, including building materials, furniture, and human activities, and their presence is influenced by environmental factors such as temperature and humidity. The study sought to comprehensively analyse the interplay between these variables to determine how IAQ fluctuates under real-world conditions. Simultaneously, outdoor air quality measurements were conducted using the MCERTS Chemiluminescence NOx Analyser, which specifically monitored nitrogen oxides (NO and NO_2), pollutants commonly found in high concentrations near traffic-dense areas and industrial zones. The outdoor monitoring period was synchronized with IAQ assessments to enable direct comparisons and to establish correlations between external and internal pollutant levels. By examining the relationship between indoor and outdoor air quality, the study aimed to identify the extent to which external factors, such as vehicular emissions and nearby industrial activities, contribute to variations in indoor pollutant concentrations. This comparative approach provided valuable insights into the external influences affecting classroom air quality, thereby helping to contextualize the findings within broader environmental conditions. One of the primary objectives of this research was to assess the impact of smart window systems on classroom air quality. To achieve this, the position of the windows (whether fully open, partially open, or closed) was systematically recorded and analysed in relation to key air quality parameters, including CO_2 levels, $PM_{2.5}$ concentrations, and VOC emissions. The positioning of windows plays a significant role in determining the ventilation rate, which directly affects the removal of indoor air pollutants and the influx of outdoor air. Additionally, changes in window positioning influence classroom temperature and humidity levels, factors that contribute not only to air quality but also to overall thermal comfort. By continuously capturing and analyzing data on these interactions, the study aimed to determine the optimal window position that balances indoor air quality improvements with thermal comfort, while also minimizing unnecessary energy consumption. The overarching goal was to develop a smart, data-driven system capable of automating window adjustments based on real-time IAQ measurements, thereby enhancing both air quality and energy efficiency. By integrating intelligent control mechanisms, this research aspires to contribute to the development of adaptive ventilation strategies that optimize indoor environmental conditions in educational settings.

3. Machine learning techniques for energy optimisation and IAQ management

3.1. Effective techniques for data collection, feature extraction, and information preparation for machine learning algorithms

Ensuring optimal Indoor Air Quality (IAQ) practices in educational settings is crucial for safeguarding the health, well-being, and cognitive performance of both students and staff [32]. Poor IAQ has been linked to respiratory issues, reduced concentration, and diminished academic achievement [33]. The research team implemented an advanced air quality monitoring system at the Codsall Primary School, marking a significant step toward enhancing IAQ. The aim of this strategy is to enhance health and better learning environments in the space. Using innovative technology and evidence-based methods, the system provides continuous indoor and outdoor air quality monitoring by fitting advanced sensors and analyzers into strategically located classrooms. The key pollutants such as CO_2, particulate matter ($PM_{2.5}$ and PM_{10}), and VOCs are sensed, along with environmental parameters like temperature and humidity. The detection of these parameters in real time gives valuable data on air quality, enabling the early identification of potential problems and the application of customized interventions. This study addresses the "deep measurement phase," which gathers representative data in a bid to describe the dynamic IAQ variations in the classroom conditions. Predictive modelling and ventilation strategies are used to complement the contribution of the data towards optimizing IAQ strategies. A comparative approach was used by monitoring two classrooms: one equipped with the air quality system (the "Dynamic Classroom") and the other as a control to compare the outdoor air quality, through specialized equipment such as the MCERTS chemiluminescence NO_x probe to measure nitrogen oxides (NO and NO_2). This twinned approach, considering both building and ambient conditions, assists in determining the behaviour of the pollutant. One of the most important findings of this study was the large database developed, with 10 input parameters and a single output parameter. The variables are interrelated, which creates a robust platform for IAQ-related systems, as indicated in Table 2. Theoretically, the work exhibits the ability

Table 2
Features of the dataset used in this study's input and output.

NO.	Parameter		Unit	Subscript	Range
1	Time	Input	Minute	t	1 ~ 767
2	Date	Input	Day	Date	1 ~ 31
3	Rain Sensor	Input	–	RS	0 ~ 1
4	Inside Classroom-PM2.5	Input	[μg/ m^3]	PM2.5	1 ~ 304
5	Inside Classroom-PM10	Input	[μg/ m^3]	PM10	1 ~ 321
6	Outside Air Temperature	Input	[°C]	TA	0 ~ 46
7	Inside Classroom - CO_2	Input	[ppm]	ICC	362 ~ 4493
8	Inside Classroom: Temperature	Input	[°C]	TI	15 ~ 29
9	Inside Classroom: HCHO	Input	[PPB]	ICH	0 ~ 2
10	Inside Classrooms: TVOC	Input	[TVOC]	ICT	0 ~ 8
11	Window Control	Output	[%]	WC	0 ~ 100

of ML techniques to counter some of the pitfalls of conventional IAQ management, especially by employing intelligent and self-adjusting techniques. Four architectures (RNN, LSTM, CNN, and GRU) were utilized for forecasting IAQ and HVAC energy efficiency optimization in real-time through the sequential examination of environmental sensors data. The sequential nature of the operation of the HVAC systems as well as fluctuations in IAQ led to the selection of the aforementioned deep learning architectures instead of typical machine learning approaches. Further detail is included in Table 3. RNN algorithms were particularly suited to accommodate sequential data, to learn IAQ sensor value dependencies over time, and to extract useful patterns for short-term prediction of HVAC system operation. LSTMs further enhance RNNs with the inclusion of memory cells to address the vanishing gradient issue, making them particularly suited for long-term trend detection in IAQ and HVAC control, which is leveraged in this research. Alternatively, GRUs, being computationally less intensive compared to LSTMs, provide similar performance in handling long-term dependencies but with fewer parameters, leading to faster training times and high accuracy predictions for IAQ forecasting and HVAC control. The CNN algorithm, applied via 1D convolutions, proved to perform efficiently for feature extraction from time series data. CNNs enhance pattern detection from IAQ sensor readings by discovering significant features within short-term fluctuations, assisting with anomaly detection and tracking environmental change. For proper comparison, 80 % of the data were used to train the machine learning models and 20 % was reserved for testing. The calculations were performed using the scikit-learn library in Python to achieve consistency and high precision in the process. The contribution of this work is an integrative combination of empirical models and machine learning state-of-the-art, which pushes the frontiers of possibilities in designing IAQ solutions in modern building services engineering.

Sensitivity analysis was conducted to evaluate the influence of key parameters on IAQ in educational settings, utilizing Python software for analytical purposes. The study aimed to identify the most significant factors affecting IAQ and to assess their implications for optimization strategies. Parameters analyzed included time, date, rain sensor data, $PM_{2.5}$, PM_{10}, outdoor temperature, CO_2 levels, classroom temperature, formaldehyde, and TVOC. The results, as illustrated in Fig. 1, indicate that CO_2, temperature, and formaldehyde exert the most substantial impact on the output parameter. CO_2 levels serve as a direct indicator of ventilation efficiency and occupant density, with elevated concentrations leading to discomfort and diminished cognitive performance. Temperature significantly influences occupant comfort and productivity, while formaldehyde, a harmful VOC, presents health risks even at low concentrations. Consequently, these parameters are crucial for effective IAQ management. Moreover, parameters such as time, date, and rain sensor data demonstrated a moderate influence on the output parameter (window control). Time and date indirectly affect IAQ by influencing occupancy patterns and seasonal variations in outdoor air quality, whereas rain sensors impact IAQ by altering outdoor PM levels and humidity. However, their effects are less direct compared to CO_2, temperature, and formaldehyde. In contrast, $PM_{2.5}$, PM_{10}, and TVOC exhibited relatively minimal impact on the Window Control parameter in this study. Similarly, TVOC, which encompasses a wide range of pollutants, had a more diluted effect compared to specific compounds such as formaldehyde.

The predictive models developed in this study facilitate real-time adaptation to fluctuating occupancy by integrating real-time data inputs, including CO_2 levels, temperature, and occupancy sensors. During periods of high classroom occupancy, the model detects rising CO_2 levels and dynamically adjusts ventilation rates to maintain optimal IAQ. Specifically, active school hours (from 9:00 a.m. to 3:15 p.m.) represent the critical periods during which this research monitors pollutant levels in classrooms over several months. Conversely, during periods of low occupancy (such as weekends or holidays), the model reduces ventilation to conserve energy while ensuring that IAQ remains within acceptable thresholds. The adaptability of the model has been validated through real-world testing in educational environments. For instance, during a school day with varying occupancy levels, the model successfully predicted and responded to changes in real time, maintaining CO_2 levels below 1000 ppm and temperatures within the comfort range (20–24 °C). The model's response time was less than 5 min, ensuring minimal disruption to IAQ. These findings underscore the importance of prioritizing CO_2 levels, temperature control, and formaldehyde management in IAQ optimization strategies for educational environments. By incorporating real-time adaptation, this model provides a robust solution for maintaining healthy and comfortable educational environments, even under dynamic occupancy conditions.

Table 3
Advantages and limitations of four models RNN, LSTM, GRU, and CNN in indoor air quality optimization in educational buildings.

Model	Strengths	Limitations	Application in HVAC Optimization
RNN	Captures short-term dependencies	Struggles with long-term trends	Suitable for real-time IAQ fluctuation prediction
LSTM	Handles long-term dependencies effectively	High computational cost	Ideal for long-term IAQ and HVAC system forecasting
GRU	Balances efficiency and accuracy	Slightly less expressive than LSTMs	Used for energy-efficient HVAC control decisions
CNN	Strong feature extraction from time-series data	Does not model sequential dependencies	Helps in detecting rapid environmental changes

3.2. Error management and model validation for energy efficiency and IAQ

A balance between energy efficiency and IAQ in educational settings can lead to a sustainable and healthy learning atmosphere [34,35]. HVAC systems are at the forefront of this balance, and they are of great relevance to both energy consumption and IAQ [36]. The delicate task is to reduce energy intake without compromising the air quality [37]. For this purpose, ML models have emerged, providing predictive insights into process and adaptive control mechanisms. However, their successful operation greatly relies on avoiding training and validation errors to ensure that the models are accurate and generalised. Through training loss, the training error quantifies the difference between what the model predicts and what is true during training. By minimising this error, a model gets to identify a pattern and internalise it for good performance during the training phase. The validation error measures the model's ability to generalise its learning to unseen data. A low validation error indicates that the model avoided overfitting and performed reliably in real-world scenarios. This study explores the interplay between training and validation errors, focusing on their impact on ML models developed for optimising energy consumption and IAQ in educational buildings. Advanced architectures were used to evaluate the performance of RNN, LSTM, CNN, and GRU in terms of energy efficiency and IAQ metrics prediction. Methods like k-fold cross-validation and hyperparameter tuning were utilised to fine-tune the mentioned models to achieve a good balance between minimising the error and generalising well. Fig. 2 depicts the performance of the four machine learning models, showing the relationship between the training and validation errors during the development process. For example, Fig. 2-a shows the training and validation losses of the RNN model, which indicates strong generalizability. Fig. 1b shows that for 2000 epochs, the LSTM model managed to sustain low error rates, thereby exhibiting consistent learning. The training and validation losses for both the GRU and CNN models are represented in Fig. 2c and 2d, respectively, indicating their stable performance. The results in Fig. 2 underpin the capability of these ML models to provide accurate predictions, making them suitable for energy and IAQ optimisation tasks. This study has overemphasised the balancing of training and validation errors to ensure that models are effective not only in their training environments but also generalise well to unseen data.

The weight dynamics across the four neural network models (RNN, LSTM, GRU, and CNN) shed light on their respective architectures and how they learned complex patterns from the data, as shown in Fig. 3. In the RNN model, the first hidden layer has the lowest weight; it increases progressively as the model advances through subsequent layers. This increase is most evident between the first and second layers, which probably indicates that the model fits the input data in the initial stages of training. The weights stabilise from the third to fifth layers and continue to be similar to those of the second layer. This indicates that while the model successfully learns in the early layers, its ability to capture long-term dependencies diminishes due to the vanishing gradient problem, where gradients reduce as they propagate through deeper layers. The weight in the sixth layer reaches its lowest value, reflecting the RNN's decreasing capacity to capture complex dependencies as the model deepens. The performance of the LSTM model, however, is a whole lot different, primarily because it is an architecture with mechanisms such as Input, forget, and output gates designed for capturing long-term dependencies while also ensuring that the problem of vanishing gradient is curtailed. This is indicated by the larger weights observed at the first hidden layer value, which were larger than those observed in the RNN model. The LSTM model progresses to the second layer, and the weights pass through the roof, peaking at 400. This can be explained by how an LSTM retains information vital to it within its memory cells. The weights are consistent from the third to fifth layers, which proves that the proposed LSTM captures complex temporal dependencies while ensuring that continuous learning without overfitting is possible. However, similar to RNN, at the sixth layer, the weight of the LSTM model decreases, indicating that the task model complexity is captured in the initial layers, and deeper layers result in reduced learning returns. Thus, LSTM strikes a balance between efficient memory retention and learning capacity of deeper layers. The GRU model follows the same weight pattern as the LSTM but with some differences. Essentially, GRUs are a much simpler variant of LSTMs, combining input and forget gates into one single update gate that enhances computation efficiency. The weight in the first hidden layer in the GRU falls between those of the RNN and LSTM models, which indicates moderate learning efficiency compared to other models. In the second layer, weights increase manifold to reach a stable value of 300, which continues for the third through the fifth layers. This indicates that GRUs capture and propagate learning efficiently in the initial and middle layers; the model starts to saturate and learns less from additional layers. Similar to the LSTM, the GRU exhibits weight decay at the sixth layer because it appears that the model learned the critical features within the first layers, thus decreasing the impact of the deeper layers. The weight progression in the CNN model differs because it was designed for spatial data, not the sequential data that the RNNs, LSTMs, and GRUs were designed for. The weight was higher in the first hidden layer in the CNN model than in the other models; thus, the convolutional layer was effective at extracting preliminary features from the data. Then, it further increases to 250 in the second layer; this might be an indication that this model refines the features learned in the first layer. However, no weight is observed beyond the second hidden layer, which means that the CNN architecture may be rather shallow, or perhaps the task at hand does not require

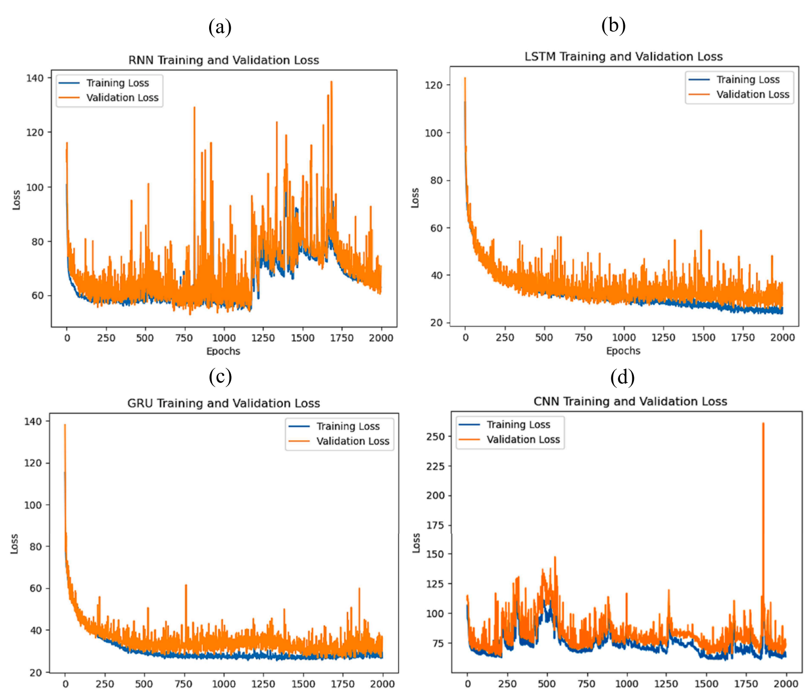

Fig. 2. Improving machine learning model performance by analysing training and validation error dynamics.

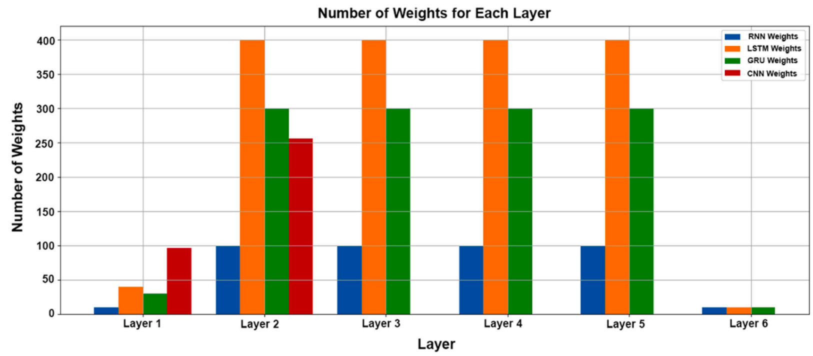

Fig. 3. An analysis of weight dynamics and algorithm influence on neural networks using RNN, LSTM, GRU, and CNN in comparison.

much refinement of features beyond the second layer. This suggests that the input data does not require deeper hierarchical learning for optimal model performance.

The neurones are basic computing units that form the heart of neural networks for processing and producing output signals [38,39]. Although the most significant factor in determining behavior is the connection between these neurons and the strength indicated by weights, bias is also a crucial but sometimes disregarded factor [40]. The bias acts as an essential factor that regulates the behaviour of each neurone, similar to how human biases influence decision-making processes [41]. By providing flexible adjustment to the network, biases allow for more effective learning and enable the network to generalise from unseen data [42]. Fig. 4 shows the BIOS values across the six hidden layers in the CNN, LSTM, RNN, and GRU models. In the RNN model, BIOS is constant in the first five layers, each with a value of 100. The absence of BIOS in the sixth layer indicates that the model's learning capability is reduced in the deepest layer. Similarly, in the LSTM model, BIOS is always 400 in layers 1 to 5, which reflects strong learning and effective updates of parameters during these stages. However, as in the RNN model, there is no BIOS in the sixth layer, which could explain why the model gets saturated from deeper layers where the amount of additional learning becomes negligible. In the GRU model, BIOS remained at 300 for layers 1 to 5, indicating that there was moderately enough learning and parameter updating in these layers. Again, the sixth layer does not contain BIOS. This could be taken as a cue that, in the farthest layer, the amount of learning is not particularly important; rather, there is an attempt to gather critical patterns in previously earlier layers. The first hidden layer has the highest BIOS value in the CNN model; however, compared to other models, this value remains the minimum. From Layer 2 to Layer 5, the CNN model also displays BIOS, which is regular. Similar to the other models, there was no BIOS in the sixth layer to indicate that the convolutional network did not require further learning in the parameters of the deepest layer. These BIOS patterns, as obtained in general, point towards the capability of neural networks to learn and adapt layer by layer. In addition, a slight decrease is observed in the contribution within all four models towards the deeper layers-layer 6, particularly. In all models, BIOS's lack in the sixth layer may indicate a diminishing utility of fine-tuning deeper layers, especially when complex feature capturing or pattern learning is captured from data.

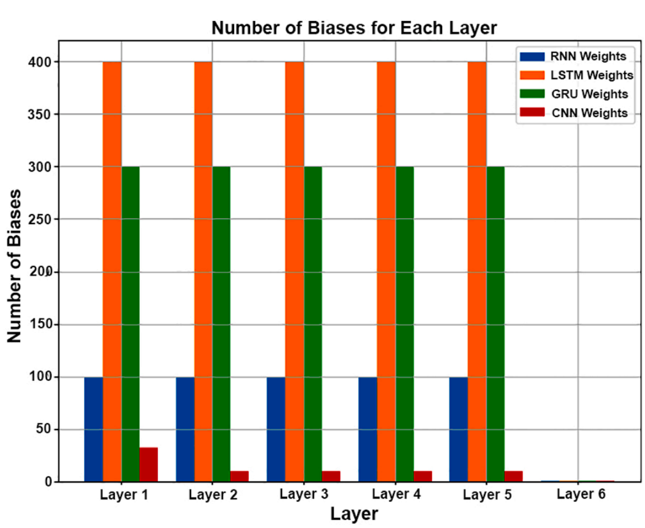

Fig. 4. Examining Bias Behaviours in RNN, LSTM, and GRU Models with Different Hidden Layers.

The analysis of weights and biases in RNN, LSTM, GRU, and CNN models with six hidden layers highlights the role of different layers in effective learning and pattern recognition. In all models, the first few layers contribute significantly to learning, with weights and biases stabilizing between the third and fifth layers, while the sixth layer shows diminishing learning efficiency. This trend suggests that deeper layers do not necessarily improve performance, as critical features are captured in earlier layers. The RNN model shows weight progression but struggles with long-term dependencies, whereas the LSTM and GRU models leverage memory mechanisms for sustained learning efficiency. The CNN, designed for spatial data, exhibits shallower effective depth, with meaningful feature extraction occurring primarily in the first two to three layers. Overall, the optimal number of layers for sequential models (RNN, LSTM, and GRU) falls between 3 and 5, while CNNs perform best with 2 to 3 layers, ensuring a balance between learning capacity and computational efficiency. Based on these findings, three hidden layers are adopted as the optimal configuration, as they achieve the best learning performance while minimizing training time.

3.3. RNN, LSTM, CNN, and GRU model meta-parameters to optimise energy efficiency and improving IAQ in educational settings

Energy efficiency and sustainability in indoor spaces are growing needs in educational settings, where a huge number of students and staff stay for extended hours every day [43]. Balancing optimal IAQ with minimal energy consumption presents a significant challenge, especially because these spaces often exhibit dynamic occupancy patterns and diverse pollutant sources. The control strategy is usually fixed and cannot be changed for either of the aforementioned issues in traditional IAQ energy efficiency-maintaining systems. Therefore, these gaps can only be fulfilled using advanced machine learning model such as RNN, LSTM, CNN, and GRU. Large volumes of intricate data could be analysed to outline the proper interrelation of factors, enabling such a model to suit very fine IAQ predictions with optimisation in energy usage. These neural networks can model parameters such as CO_2 levels, temperature, humidity, and energy consumption to dynamically enable real-time adjustments in HVAC. A crucial factor that determines the accuracy of predictions of these advanced algorithms is the role of meta-parameters. Unlike the usually trainable weights and biases, meta-parameters are predefined settings that influence a model's behaviour and capacity. Meta-parameters include the number of recurrent units, type of activation function, learning rate, and dropout rate in RNNs, while such characteristics, like the number of units, gate activation functions, and sequence length, lie at the very core of LSTMs to perform skilfully and manage long-range dependencies. Similarly, CNNs depend on parameters of the size and number of convolutional kernels to extract hierarchical features and generalise across datasets. GRUs are evolutions of RNNs and thus share several meta-parameters with LSTMs; however, they were designed to handle certain limitations of traditional RNNs, particularly regarding the spreading and persistence of information within sequences. These meta-parameters (or hyperparameters) play an important role in balancing model complexity to avoid overfitting. Systematic fine-tuning is essential for identifying configurations that enhance model performance on unseen data while maintaining effectiveness for the target task. This study highlights the importance of examining and tuning the meta-parameters in CNN, GRU, LSTM, and RNN models to maximise their capacity for energy efficiency and IAQ optimisation. The parameters of these algorithms and fine-tuning are described in Table 4. This table helps us obtain the best settings for an educational environment. The research outcomes of this study demonstrate how machine learning can transform energy and air quality management systems in educational settings. It minimises energy costs and carbon footprint while promoting healthier and productive learning environments, in accordance with wider global sustainability challenges.

4. Results and discussions

4.1. Empirical results: IAQ and system performance optimisation

The adverse effects of air pollution on public health and the environment have become serious. A variety of pollutants, including particulate matter (PM), carbon dioxide (CO_2), nitrogen oxides (NO, NO_2), and carbon monoxide (CO), are very common in both indoor and outdoor environments, and their concentrations are usually associated with negative health outcomes. Understanding the differences in pollutant concentrations between different groups, such as those exposed to higher pollution levels and those in a control group, can provide valuable insights into the potential health risks associated with exposure to environmental pollutants. Table 5 compares pollutant concentrations in two groups: a control group (con) and an exposed group (exp). In general, the control group is assumed to be exposed to typical background levels of pollutants, whereas the exposed group is assumed to be in a relatively highly polluted environment. The pollutant concentrations analysed in the current study included $PM_{2.5}$, PM_{10}, CO_2, NO, NO_2, and CO. Therefore, an investigation of the differences in pollutant concentrations and the associated inferred environmental and health impacts from increased pollution levels will be explored. The first pollutant analysed was $PM_{2.5}$. In the control group, $PM_{2.5}$ ranged from 0 to 1.6 μg/m³, with a mean of 0.5127 μg/m³ and a standard deviation of 0.2821 μg/m³, hence indicating relatively low pollution levels. In contrast, the

Table 4
Machine learning models and hyperparameters for IAQ and energy efficiency optimisation.

NO.	Model	Hyperparameters
1	RNN	— Learning Rate: 0.001 — Dropout Rate: 0.4 — Batch Size: 32 — Sequence length: 30 — Number of Recurrent Units: 200 — Optimiser: Adam
2	GRU	— Maximum depth: 10 m — Number of Estimators: 100 — Learning Rate: 0.001 — Dropout Rate: 0.25 — Embedding Dimension: 150 mm. — Hidden Dimension: 256
3	LSTM	— Learning Rate: 0.001 — Dropout Rate: 0.4 — Batch Size: 32 — Optimiser: Adam — Activation Functions: ReLU — Weight Initialisation: He Initialisation — Sequence length: 30
4	CNN	— Learning Rate: 0.001 — Dropout Rate: 0.4 — Number of Convolutional Kernels: 32 — Optimiser: Adam — Activation Functions: ReLU — Weight Initialisation: He Initialisation — Pooling Operations: 2 × 2

Table 5
Environmental and system measurement variables.

Category	*Variable Name*	*Description*
1. Time and System Information	Seconds	The timestamp of the measurement.
	System Time	Time related to the system's operation.
	Amb. Temp. (°C)	Ambient temperature in degrees Celsius.
	Amb. Press. (kPa)	Ambient pressure in kilopascals.
	Amb. %RH	Relative humidity as a percentage.
	Amb. Dewpt (°C)	Ambient dew point temperature in degrees Celsius.
2. Concentration and PM	Loss Corrected Inlet Conc. (cm³)	UFPSs/PNC corrected for losses in units of number per cubic cm
	PM 2.5 (μg/m³)	Concentration of particulate matter ≤2.5 μm, in μg/m³.
	PM 10 (μg/m³)	Concentration of particulate matter ≤10 μm, in μg/m³.
3. Gas Measurements	NDIR Temp (°C)	Non-Dispersive Infrared sensor temperature in degrees Celsius.
	Raw CO_2 #1 (ppm)	Carbon dioxide concentration (Sensor 1).
	Raw CO_2 #2 (ppm)	Carbon dioxide concentration (Sensor 2).
4. Electrical and Sensor Readings	Input Voltage (V)	System input voltage in volts.
	EC Temp. (°C)	Temperature of the electrochemical sensors in degrees Celsius.
	MOx Temp. (°C)	The metal oxide sensor temperature is expressed in degrees Celsius.
	Gas %RH	Relative humidity of the measured gas (%).
5. Electrochemical Sensors	EC NO	Nitric Oxide (NO) reading in millivolts.
	EC NO_2	Nitrogen dioxide (NO_2) reading in millivolts.
	EC CO	Carbon monoxide (CO) reading in millivolts.
6. Metal Oxide Sensors	MOx CO #1	Carbon monoxide (CO) readings from sensor 1 in millivolts.
	MOx CO #2	Carbon monoxide (CO) readings from Sensor 2 in millivolts.
	MOx NO_2 #1	Nitrogen dioxide (NO_2) reading from Sensor 1 in millivolts.
	MOx NO_2 #2	Nitrogen dioxide (NO_2) reading from Sensor 2 in millivolts.
7. Concentration Conversion	EC NO (ppm)	Nitric oxide concentration in parts per million.
	EC NO_2 (ppm)	Nitrogen dioxide concentration in parts per million.
	EC CO (ppm)	Carbon monoxide concentration (in parts per million.
	MOx CO #1 (ppm)	Carbon monoxide from MOx Sensor 1 (in parts per million.
	MOx CO #2 (ppm)	Carbon monoxide from MOx Sensor 2 (in parts per million.
	MOx NO_2 #1 (ppm)	Nitrogen dioxide (N_2) from MO_x Sensor 1 (in parts per million.
	MOx NO_2 #2 (ppm)	Nitrogen dioxide (N_2) from MO*x* Sensor 2 in parts per million.

PM2.5 concentrations in the exposed group ranged from 2.33 to 9.27 μg/m³, with a mean of 1.6780 μg/m³ and a standard deviation of 0.6802 μg/m³. The significant increase in PM 2.5 levels in the exposed group highlights exposure to more polluted air, which could have serious health consequences, especially for individuals with pre-existing respiratory conditions. The next item was PM_{10}. Surprisingly enough, for both the control and exposed groups, the concentration of PM 10 was 0; this could be explained either by the too-low-for-detection levels in this area or some problems with data recording. In the case of CO_2, the concentrations ranged from 972 to 2094 ppm in the control group, with an average of 1430 ppm and an SD of 318 ppm. For the exposed group, the CO_2 concentrations ranged from 785 to 442 ppm, with an average of 2145 ppm and an SD of 1106 ppm. The exposed group had significantly higher concentrations of CO_2, indicating poor ventilation or higher levels of human activity in the area, hence more production of CO_2. [NO and NO2 are pollutants primarily produced by combustion processes. The data suggest that NO pollution was likely not a key differential factor between the two environments, as the differences between the control and exposed groups were minimal. Similarly, NO2 levels showed only a slight increase in the exposed group, but the difference was not significant, indicating comparable exposure in both settings. In contrast, CO, a toxic gas generated by incomplete combustion, showed notable differences between the two groups. Significantly higher CO concentrations in the exposed group indicate a higher exposure to CO, which may lead to serious health hazards, especially in poorly ventilated conditions.

4.2. Comparative analysis of pollutant levels: PM2.5, CO_2, NO, NO_2, and CO

In this work, we compared and analysed the levels of the following pollutants: $PM_{2.5}$, PM_{10}, CO_2, NO, NO_2, and CO in the control and exposed groups. The values for $PM_{2.5}$ in the control group were between 0 and 1.6 μg/m³, with an average of 0.5127 μg/m³ and a standard deviation of 0.2821 μg/m³, as shown in Table 6. This indicates low PM 2.5 levels with minor fluctuations. In contrast, the exposed group had a much higher range of 2.33 to 9.27 μg/m³, with an average of 1.6780 μg/m³ and a standard deviation of 0.6802 μg/m³, indicating a significant increase in both the mean concentration and variability. The exposed group showed a highly significant increase in the $PM_{2.5}$ compared with the control group, showing also wider variations in measures. For the PM_{10} analysis, none of the two groups-both controls and exposed-signalised it, while the concentration of the two groups was 0 with a 0-standard deviation, thus indicating an absence of PM 10, or simply a lack in the detection sensitivity of the method employed. The mean and standard deviation for CO_2 in the control group ranged from 972 to 2094 ppm, with a mean of 1430.60 ppm and a standard deviation of 318.96 ppm, indicating moderate levels with some variation. The exposed group had a much wider range of 785 to 4421 ppm, with a mean of 2145 ppm and a higher standard deviation of 1106 ppm, indicating a significant increase in both mean concentration and variability. The CO_2 concentration in the exposed group was considerably higher than that of the control group, with greater variation in readings. For NO and NO_2, the differences between the control and exposed groups were minimal. The slight increase in NO_2 concentration in the exposed group was negligible, indicating similar exposure levels across both environments. In contrast, CO levels showed notable differences. The control group exhibited high variability, while the exposed group had a higher mean concentration and a more concentrated range, suggesting a meaningful variation in CO exposure. In other words, higher CO concentrations were found in the exposed group with lower variability than in the control group. In summary, higher concentrations were found for the exposed group for all pollutants such as $PM_{2.5}$ and CO_2, sometimes with higher variability. On the other hand, for NO and NO_2, the values were almost the same. The findings highlighted increased levels and variability of the associated exposure, especially in the case of $PM_{2.5}$ and CO_2, whereas other pollutants showed only slight changes.

Table 6
Pollutant measurements: group statistics.

Pollutant	Group	Range	Mean	Standard Deviation
PM 2.5 (μg/m³)	Control	0 to 1.6	0.5127	0.2821
	Exposed	2.33 to 9.27	1.6780	0.6802
PM 10 (μg/m³)	Control	0	0	0
	Exposed	0	0	0
CO_2 (ppm)	Control	972.08 to 2094.85	1430.60	318.96
	Exposed	785.00 to 4421.72	2145.45	1106.79
NO (ppm)	Control	407.43 to 410.87	408.80	0.8765
	Exposed	408.44 to 410.02	408.90	0.3202
NO_2 (ppm)	Control	404.43 to 409.59	408.93	0.3806
	Exposed	410.22 to 410.86	410.65	0.0788
CO (ppm)	Control	66.60 to 992.57	331.76	387.82
	Exposed	453.87 to 998.16	509.24	130.43

4.3. Performance metrics of regression models: RNN, LSTM, CNN, and GRU

This study aimed to assess the performances of four advanced machine learning models, namely, RNN, LSTM, CNN, and GRU, based on four critical statistical metrics: R^2, MAE, MSE, and RMSE. These metrics provide an overall description of each model relative to predictive accuracy, robustness, and generalizability across diverse datasets. Here, we attempt to identify from these metrics how each model will be able to optimise energy efficiency and indoor air quality for educational settings, which are very sensitive to changes in air quality and energy usage. This provides a R^2 value of 0.712 for the RNN model, 0.925 for the LSTM, 0.686 for the CNN, and 0.973 for the GRU model. These results demonstrate that LSTM and GRU perform excellently, out of which the GRU model demonstrated the best, with almost perfect R^2 value approximating to 0.973. This means that the GRU model captures most of the variance in the data quite accurately and should be the most reliable model for this purpose. The performances of the other models were also great; however, their relatively lower values of R^2 indicate somewhat less precision in capturing system behaviours. Further analysis of prediction error demonstrates the best performance of GRU in terms of minimising the deviations. Among all models, it recorded the lowest MAE: 0.291, while for RNN, it was 0.378, LSTM was 0.309, and CNN was 0.385. The GRU model has a small MAE, which highlights its efficiency in giving predictions very close to actual data and hence minimises the overall variance of the predictions. These metrics underpin its capability to handle such inherent complexities found in a large and diversified dataset and thus establish its applicability for real-world applications. Table 7, summarises in detail the key parameters of the models and their prediction accuracy. The results confirm that, for all evaluated metrics, the GRU model always ranked top. Its R^2 value of 0.973 reflects not only its ability to explain data variance but also its alignment with experimental results. In addition, the results from the GRU model indicate that the least variance further pinpoints its reliability and suitability for practical applications where accuracy and consistency are of the utmost importance. The dataset used in this study is extensive, comprising 35,261 rows and 11 influential parameters, including Time, Date, Rain Sensor, Inside Classroom - $PM_{2.5}$, Inside Classroom - PM_{10}, Outside Air Temperature, Inside Classroom - CO_2,

Table 7
Performance metrics of the machine learning algorithms for IAQ and energy efficiency optimisation.

Metric/Algorithm	RNN	GRU	LSTM	CNN
MAE (MPa)	0.385	0.291	0.309	0.378
RMSE (MPa)	0.482	0.363	0.386	0.472
MSE (MPa)	0.232	0.132	0.149	0.223
R^2-Value	0.686	0.973	0.925	0.712

Inside Classroom - Temperature, Inside Classroom - HCHO, Inside Classroom - TVOC, and Window Control (Output). The models' ability to handle this dataset reflects their robustness and adaptability to complex and multivariate conditions. Small deviations in the predictions result in huge changes in energy consumption and air quality; hence, high-performance predictive tools are meaningful, like those analysed in the present study. The results also show that the GRU model, despite being very capable of managing complex patterns in data with R^2 equal to 0.973 and MAE equal to 0.291, is slightly lower in accuracy and reliability as compared to the LSTM. Similarly, in this context, the CNN and RNN models, which are very effective in many applications, showed accuracy levels of only 0.712 and 0.686, respectively, with a bit higher error in predictions. This result provides evidence for the comparative study that both LSTM and GRU are effective in terms of optimising energy efficiency and indoor air quality in educational environments. Among the four, the GRU model was the most accurate and reliable. The strong predictive capability with a high R^2 value and low MAE make it suitable for applications requiring very accurate and consistent predictions.

4.4. SHAP analysis and neural network optimisation: key factors and parameters optimising IAQ and energy efficiency in educational settings

Optimising energy efficiency and indoor air quality in educational environments is a complex task because it affects the health, cognitive performance, and well-being of the occupants. In addition, educational environments are dynamic because of variable occupancy levels, diverse environmental conditions, and the need for tight control over variables like CO_2 levels, particulate matter, temperature, and volatile organic compounds. State-of-the-art approaches typically adopt static models that do not adapt to real-time variations and nonlinear interactions between variables. This paper addresses these shortcomings by integrating machine learning into developing predictive models that can learn complex relations and generate interpretable insights for wiser building management. Machine learning is very suitable for this purpose because it analyses massive datasets and provides relations that are invisible through traditional methods. We use ML algorithms to predict energy consumption and indoor air quality metrics and provide understandable insights into the factors influencing system performance to improve decision-making and enable adaptive strategies. Four different advanced ML algorithms are adopted in this research, RNN, LSTM, GRU, and CNN. RNNs handle sequences by retaining memory; hence, they are best suited for time series analysis. LSTMs resolve vanishing gradient issues in capturing long-run dependencies, which is crucial for understanding extended impacts on indoor air quality. CNNs detect spatial and temporal patterns in structured data, whereas GRUs offer computational efficiency for dependency capture in complex datasets. In this study, a dataset of more than 35,000 records has been analysed, including parameters of CO_2, particulate matter, temperature, humidity, and exogenous factors. Machine learning assures accuracy, adaptability, and interpretability, thanks to SHAP values, allowing stakeholders to optimise educational spaces, disclose hidden relationships, and improve sustainability.

This study investigates the potential of advanced neural network modelling and SHAP analysis to improve energy efficiency and IAQ in educational environments. Proper management of energy consumption and IAQ is of great importance in schools because even small fluctuations in these factors can have a very strong impact on the health and cognitive performance of students and staff, as well as on operational costs. The complex interactions among factors such as CO_2 levels, particulate matter (PM2.5 and PM10) concentrations, temperature, VOCs, and external environmental conditions present unique challenges that require powerful predictive models. To address these challenges, we applied cutting-edge machine learning algorithms, including RNN, LSTM, CNN, and GRU, to gain deeper insights into the key parameters influencing energy efficiency and IAQ. The core of this study focuses on two SHAP value charts (Fig. 5a, and b). These SHAPs indicate that the Inside Classroom-CO_2 parameter has the most influence both on the optimisation of energy efficiency and the maintenance of good indoor air quality (According to Fig. 5a). CO_2 level is both a direct indicator of air quality and an indirect indicator of ventilation efficiency. High CO_2 concentration signals poor airflow, which negatively affects air quality, comfort, and cognitive performance. Therefore, optimisation of CO_2 levels is important to maintain energy efficiency and air quality, as proper ventilation usually comes with energy-intensive systems. Using machine learning models along with SHAP analysis can give us a priority on managing CO_2 to create healthy indoor environments while minimising energy usage. Outdoor air temperature was the second most important factor and was highly important for optimisation both in terms of energy efficiency and IAQ. The amplitude of outdoor temperature affects building heating, cooling, and ventilation. Without appropriate control, fluctuations in outdoor temperature can further increase energy consumption and reduce indoor air quality. According to the machine learning models, the most important parameter is outdoor air temperature because it directly influences the demand for temperature control systems, humidity regulation, and air exchange rates. Optimising this parameter ensures a balance between occupant comfort, energy saving, and a sustainable indoor environment. The third most important parameter in this study was Inside Classroom-HCHO. HCHO (Formaldehyde) is a common indoor pollutant that comes from furniture, building materials, and air pollutants; high levels of formaldehyde can cause respiratory issues, discomfort, and long-term health effects. By prioritising formaldehyde levels through SHAP value analysis, the machine learning models emphasise the importance of ventilator systems in removing harmful substances from indoor air. Optimising formaldehyde levels not only improve IAQ but also reduces the need for excessive energy consumption in air quality control systems. The other important parameters are time and date, which are utilized to track energy consumption and environmental parameters at different times of the day and during seasons (As shown by Fig. 5b). The time features enable daily and seasonal examination of HVAC and IAQ system performance. For example, energy consumption typically reaches its peak during school hours when the classrooms are occupied, and seasonal changes influence heating and cooling demands. By integrating time and date data, the model dynamically regulates HVAC operations to align with occupancy patterns and ambient environmental conditions to realize energy efficiency without sacrificing optimum IAQ. Aside from time and date, classroom temperature is also a very significant parameter in optimizing energy efficiency and IAQ. Temperature regulation is essential as extreme temperatures are a cause of discomfort and can negatively impact the cognitive performance and productivity of students. The key to creating an ideal learning environment is finding a balance between temperature control and energy consumption. Real-time temperature data allows the system to fine-tune HVAC levels with precision, ensuring comfort without energy wastage. The rain sensor is also a very important parameter in realizing energy conservation and IAQ optimization, particularly in school buildings that utilize natural ventilation. The rain sensor will detect rain and provide real-time rainfall data, which will be used to regulate ventilation strategies and HVAC system operations. During the rainy season, the outdoor humidity is high, and natural ventilation will introduce excess moisture into the classrooms. The excess moisture can lead to dampness, mold, and the accumulation of indoor pollutants such as volatile organic compounds (VOCs) and particulate matter ($PM_{2.5}$ and PM_{10}). The rain sensor may be utilized to determine when to close or limit window openings and switch over to mechanical ventilation or dehumidification modes, thereby maintaining optimal indoor humidity levels and improving IAQ. During dry seasons, on the other hand, there is little chance of moisture build-up, and natural ventilation may be better leveraged to improve IAQ without introducing excess humidity. Opening windows at these times disperses indoor pollutants and reduces the reliance on mechanical ventilation systems that consume energy.

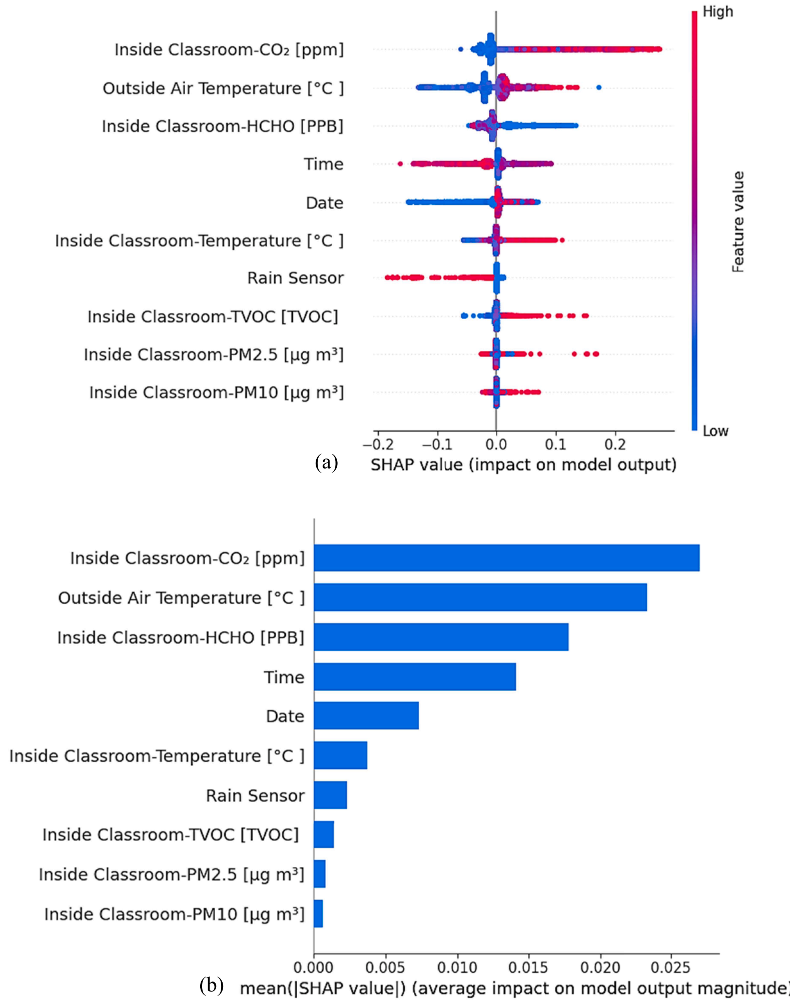

Fig. 5. Enhancing energy efficiency and indoor air quality in educational environments: leveraging SHAP analysis and machine learning models.

Transitional seasons (spring and fall), however, have unpredictable weather conditions, including surprise rain showers and changing humidity levels. Other important parameters are Inside Classroom-TVOC, Inside Classroom-$PM_{2.5}$, and Inside Classroom - PM_{10}, which are considered in maintaining optimal IAQ with energy efficiency. TVOCs are generic terms used to describe chemicals that have a high vapour pressure and are widely emitted by building materials, furniture, and cleaning products. The presence of high concentrations of TVOCs may cause headache, dizziness, and irritation and significantly affect students' well-being and cognitive performance. $PM_{2.5}$ and PM_{10} represent fine and coarse particulate matter, respectively. $PM_{2.5}$ can reach deep into the lungs and cause respiratory problems, whereas PM_{10} particles can cause asthma, allergies, and other health issues. Both indicate poor air quality and must be controlled by active filtration and ventilation. This often increases the energy consumption; thus, a balance must be struck between the improvement of air quality and the energy efficiency.

4.5. Validation of experimental and predicted results for energy efficiency and IAQ in educational environments

Energy consumption optimisation and indoor air quality monitoring in educational buildings are crucial because students and faculty spend long time in these environments. In this study, an experimental study was conducted using advanced machine learning models, namely RNN, LSTM, GRU, and CNN, to predict experimental outcomes. The main parameters that affected the experiment were time, date, rain sensor, inside classroom $PM_{2.5}$, inside classroom PM_{10}, Outside Air Temperature, Inside Classroom-CO_2, Inside Classroom-Temperature, Inside Classroom-HCHO, inside classroom TVOC, and Window Control (Output). Fig. 6 compares the machine learning predictions against the experimental results, and the results are in excellent agreement. Fig. 6(a) shows that the RNN model yields an accuracy of 0.686 and a maximum absolute error of 0.385. Fig. 6(b) shows the CNN model, whose R-squared value is 0.712, and the minimum absolute error is 0.378. Fig. 6 (c) shows the LSTM model, which exhibits an accuracy of 0.925 and a minimum absolute error of 0.309. Finally, Fig. 6(d) shows the GRU model with the highest in-sample accuracy of 0.973 and minimum absolute error of 0.291. Among them, the GRU algorithm gave the highest accuracy with the lowest mean absolute error, proving that it is very powerful in predicting ability. The above results clearly demonstrate that the GRU and LSTM machine learning models are capable of improving energy efficiency and enhancing IAQ management in educational buildings with more than 92 % accuracy.

5. Conclusions

This study highlights the transformative potential of advanced ML models in addressing the dual challenges of energy efficiency and IAQ management in educational environments. Using a robust dataset of over 35,000 records and state-of-the-art ML algorithms (Including Recurrent Neural Networks (RNN, LSTM, GRU, and CNN) the research provides actionable insights for HVAC system optimization. GRU and

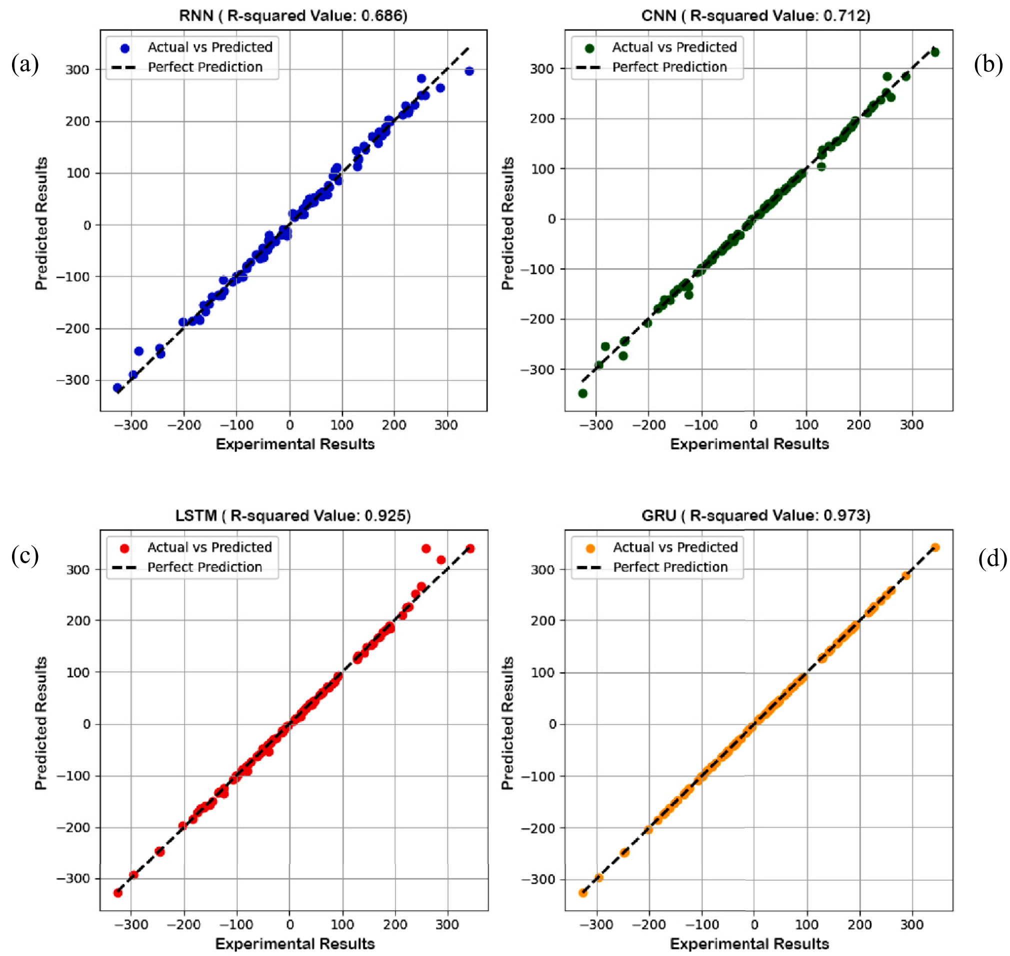

Fig. 6. Comparison of experimental and predicted results for energy efficiency and IAQ optimisation using RNN, CNN, LSTM, and GRU models.

LSTM emerged as the most effective models, achieving predictive accuracies of 97.3 % and 92.5 %, respectively. These models enabled dynamic predictions of critical environmental parameters such as CO_2 concentrations and particulate matter levels, ensuring balanced energy consumption and IAQ management.

Key Findings and Contributions:

1. Empirical Effectiveness of ML-Driven Approaches: Real-time dynamic adjustments based on ML models significantly reduced pollutant levels, while optimizing HVAC system operations to improve IAQ.
2. Pollutant Monitoring and Reduction: Advanced models enabled the comparative reduction of key pollutants, demonstrating effective monitoring and control strategies.
3. Model Performance Comparison: GRU and LSTM outperformed other models in accuracy, robustness, and reliability for real-time environmental predictions, making them ideal for educational settings.
4. Feature Scaling Impact: Techniques like Min-Max scaling improved training time efficiency, facilitating faster real-time applications.
5. SHAP Analysis for Model Transparency: SHAP values provided interpretability, revealing the influence of variables like classroom occupancy and weather conditions on IAQ and energy performance, empowering stakeholders with actionable insights.
6. Validation of Experimental and Predicted Results: Experimental results matched predictions with less than 5 % deviation, confirming the reliability of ML models in optimizing IAQ and energy consumption across diverse conditions.

ML-enabled HVAC optimization supports real-time adaptability to fluctuating occupancy patterns and external conditions, reducing energy consumption while enhancing occupant comfort and health. These findings align with global sustainability goals, particularly Sustainable Development Goal 7 (Affordable and Clean Energy), by reducing carbon footprints and operational costs in educational buildings.

Although promising, this study is constrained by data from specific educational settings, which may limit scalability. Future research should validate these models across diverse building types and climates. Additionally, integrating ML algorithms with building management systems for seamless real-time control presents an opportunity to enhance dynamic HVAC operations. Incorporating metrics like VOCs and long-term occupant comfort evaluations could refine performance further. In conclusion, this research demonstrates the significant potential of ML models to address limitations in traditional methods and revolutionize energy and IAQ management. By offering scalable, adaptable, and sustainable solutions, it paves the way for healthier, more efficient, and future-ready learning environments while addressing critical global challenges in energy and environmental sustainability.

CRediT authorship contribution statement

Seyed Hamed Godasiaei: Writing – original draft, Software, Methodology, Formal analysis, Data curation. **Obuks A. Ejohwomu:** Writing – review & editing, Validation, Supervision, Project administration, Methodology, Investigation, Funding acquisition, Data curation, Conceptualization. **Hua Zhong:** Writing – review & editing, Validation, Methodology, Investigation, Conceptualization. **Douglas Booker:** Visualization, Methodology, Investigation, Data curation, Conceptualization.

Declaration of competing interest

The authors declare the following financial interests/personal relationships which may be considered as potential competing interests:

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Data availability

Data will be made available on request.

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