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Towards Interpretable Thermal Load Predictive Models: A Systematic Review

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Abstract

Buildings are major consumers of energy; therefore, making accurate thermal load predictions is essential for improving operational efficiency and annual planning. Although machine learning (ML) has enhanced predictive capabilities, most models remain difficult to understand and explore by engineers and other stakeholders. This research presents a systematic review focusing on the role of interpretable models, specifically rule-based classifiers, decision trees, and post hoc feature attribution and interaction approaches such as Explainable AI (XAI), as design-relevant approaches for energy efficiency optimisation. Through screening and analysis, 39 of the 138 identified studies were retained. The review synthesises evidence across several key dimensions such as building envelope and material factors, spatial and geometric design, building typology, climate adaptability, occupancy behaviour, sustainable building system integration, and other related themes. The major contribution is a practice-oriented approach grounded in these themes, thus demonstrating how interpretable models reveal physical dependencies, expose model-to-reality gaps, and improve applicability across diverse building contexts. The findings highlight the need for models that are context-sensitive, easy to understand, cost-effective, and modifiable to guide engineers, designers, managers, and operators in developing thermal load modelling practices.

Keywords: building energy; civil engineering; cooling load; heating load; machine learning; artificial intelligence

1. Introduction

Buildings account for around 40% of worldwide energy usage and are one of the leading contributors to greenhouse gases; thereby, reducing energy demand in the built environment is a key climate change strategy [1,2]. There is a growing interest in predicting thermal loads (heating and cooling loads) under various conditions, specifically in relation to residential buildings with heating, ventilation and air conditioning (HVAC). Thermal load predictions are valuable not only for the operation of buildings but can also be utilised early in the design process [3–5].

Conventional thermal load modelling has been done using experience- and knowledge-based methods and physical modelling, which can be, in some cases, computationally intensive and often not transferable to many other building categories and operations [5,6]. But with data availability and computing capacity, the field of artificial intelligence (AI), especially machine learning (ML) techniques, provides promising alternatives for solutions related to energy estimates for buildings at a scale

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and accuracy exceeding traditional techniques [3,4,7,8]. Predicting thermal load is a typical supervised learning task where predictive models are developed by training on labelled input data (weather, building geometry features, etc.) to a target attribute (heating/cooling load), and then forecasting future loads [9]. Since heating and cooling loads are continuous variables, the problem is regression in nature; however, if these loads are converted into categories (low, medium, high), the problem becomes a classification task in data science. Section 2.2 provides more information.

The use of AI for thermal load forecasting is recognised for optimising the energy efficiency of building operations. In the past, a focus on attaining adequate accuracy in data modelling was assessed through the application of classification algorithms to generate models without a focus on the model's content and exploration. However, the end-user demands an understanding of the underlying rationale for the model's outcomes, which can be provided by rule-based classification, decision trees and XAI techniques. For example, XAI techniques reveal feature interactions of the model to provide more insights to the end-user, and rule-based classifiers provide rules understandable by the end-user.

There is a need for models with rich knowledge that elaborate on reasons behind outcomes for automated decision-making processes [10]. There is some evidence in the recent literature for the application of ML and XAI methods like SHapley Additive exPlanations (SHAP) and Local Interpretable Model-agnostic Explanations (LIME) in the energy efficiency domain, such as [11–14]. Model interpretability includes not just transparency but also an understanding of correlations among dissimilar features, at least from an XAI perspective. For example, even though insulation thickness, glazing configuration, and occupancy rates may influence energy demand, the interactions among these attributes are not always revealed [15]. Furthermore, some studies illustrate how data-driven models may capture different subsets of the physical and operational factors governing building loads, depending on the available data [16,17].

This research aims to systematically review interpretable classifiers and XAI approaches for thermal load prediction by identifying important themes. First, we examine interpretability to emphasise model content and the flow of decision logic that stakeholders can use. Second, we consider model-to-reality alignment and transferability to show, for example, how cross-climate deployment can degrade validity if not carefully adapted. Third, we discuss human factors related to occupancy dynamics, and we address governance and deployment to highlight alignment so that ML models translate into trustworthy decision support for design and operations. This research explores additional themes, thus extending the review in [18] from a broad survey to a practice-ready synthesis on ML techniques including XAI.

Unlike other related studies (e.g., [14,19,20]) that centre on just XAI, our systematic review is organised around several new themes. Ref. [14] surveys XAI tools around ML models for building-energy management; ref. [19] maps methods to modelling "connections and gaps"; ref. [20] emphasises sparse, transparent hybrids for predictive control. Table 1 shows the difference between this research and other thermal load reviews that separately emphasise energy-efficient design, broad data-driven energy prediction, building simulation, optimisation, passive strategies, or sensitivity analysis, e.g., [5,21–25]. The present review offers a new perspective with regard to an interpretable thermal load approach with a focus on classification rules, decision trees, and XAI. In this context, while refs. [18,25] focus more directly on heating and cooling prediction using ML techniques, their emphasis remains largely on forecasting performance and conventional data-driven models. Similarly, ref. [14] concentrates on interpretability techniques but not specifically on rule- or decision tree-based thermal load classification.

Table 1. The differences between this review paper and other available reviews.

Review	Scope	Review Approach	Interpretability Focus	Practical Contribution
[5]	Energy-efficient residential design	Narrative review of design variables affecting heating/cooling demand	Centred on physical design strategies	Guides design strategies for reducing heating and cooling demand
[21]	Data-driven building-energy prediction across building types, time scales and energy uses	Structured review of datasets, ML algorithms and performance	Emphasis is on prediction and algorithm performance	Provides a taxonomy of prediction studies and research gaps
[22]	BIM-supported dynamic thermal simulation	Review of BIM workflows and simulation tools	Focused on BIM and tools	Shows how BIM supports thermal simulation
[25]	Residential heating/cooling forecasting using ML	Comparative analysis of conventional ML approaches	Conventional ML comparison	Identifies high-performing residential thermal load forecasting models
[14]	Interpretable ML across building-energy-management applications	Explainable approaches comparison	Strong XAI focus	Clarifies interpretable techniques and challenges
[18]	Residential thermal prediction using ML	Comparative review of datasets, platforms, algorithms and performance	It includes interpretability as one of the criteria	Highlights the need for interpretable models
[23]	Thermal-performance evaluation using energy simulation	Review of simulation methods, standards, software and validation	No central ML/XAI interpretability focus	Provides best-practice guidance for thermal simulation studies
[24]	Sensitivity analysis of factors affecting building thermal performance	Review of sensitivity methods, tools, climate and typologies	Focuses on parameter sensitivity	Guides selection of parameters and sensitivity methods

Compared with existing reviews, the present systematic review provides a more focused synthesis of interpretable thermal load prediction. Earlier studies have largely concentrated on physical design strategies for reducing building-energy demand [5], broad data-driven energy prediction and algorithmic performance [21], BIM-supported thermal simulation [22], or residential heating and cooling forecasting using classic ML approaches [25]. Other reviews have examined interpretable ML mainly through XAI techniques [14] or residential thermal prediction using conventional data-driven methods [18]. Reviews of simulation methods and standards [23] and sensitivity analysis of building thermal performance [24] have also contributed methodological guidance. In contrast, the present review integrates these perspectives while placing greater emphasis on rule-based classification, decision tree logic, model interpretability, post hoc XAI, and the classification of thermal loads into interpretable states. It therefore extends

beyond performance or sensitivity analysis by focusing on human-readable model knowledge and its potential use in engineering design, operational decision-making, and stakeholder-oriented decision support.

The novelty of the present review is therefore its broader synthesis of rule-based classification, decision trees, interpretable ML, and XAI, together with the transformation of continuous heating/cooling prediction into different load classification states that enable human-readable knowledge. It further introduces cross-cutting themes spanning model-to-reality alignment, envelope and material effects, spatial and geometric design, climate and typology transferability, occupancy dynamics, multi-source datasets, simulation tool interoperability, and operational applicability. This research adds:

(1) PRISMA-driven screening focused on interpretable model content, not just feature interactions like in typical XAI approaches or other conventional ML
(2) Elevation of classification for thermal load categories
(3) Deeper discussion of design features and their impact on energy optimisation in buildings (envelope materials, spatial/geometry, Building Information Modelling (BIM)/IoT linkage)
(4) Typology, climate adaptability, and occupancy dynamics as key themes
(5) Tool interoperability (EnergyPlus/TRNSYS/IES-VE) implications.

Studying energy efficiency using ML creates value for stakeholders across the construction environment. For decision makers, models provide evidence that supports energy regulations. For industry practitioners and designers, these models highlight which building features most influence energy demand, thus guiding more cost-effective approaches and design decisions. For utility providers, accurate and explorable forecasts improve management and demand response planning. Finally, for occupants, the resulting models may enhance comfort and reduce utility expenses by promoting more tailored energy use and sustainability [26]. These themes go beyond prior review papers that primarily report XAI importance for opaque models and rarely operate rules for early-stage design or controls.

Section 2 highlights some background on the problem under consideration, and Section 3 discusses the methodology used to conduct this systematic review paper and identify the themes. Section 4 discusses in depth the diverse themes considered, and lastly, in Section 5, we provide the conclusions and possible research directions, as well as the limitations of the study.

2. Background

2.1. Building Energy Efficiency

Energy efficiency in buildings involves reducing the energy required to maintain appropriate indoor conditions through effective building design, including orientation, building form, envelope systems, glazing, shading, passive strategies, and efficient heating, cooling, and ventilation systems [5]. Because HVAC typically represents the largest end-use share, efficiency gains drive operating cost and carbon reductions [27]. In practice, heating raises indoor air temperature, ventilation exchanges air to maintain quality, and air conditioning cools with dehumidification; equipment performance is benchmarked by coefficients of performance for heating and energy efficiency ratio for cooling, indicating output per unit of energy consumed. In general, Figure 1 shows some of the factors that impact thermal loads in a residential building.

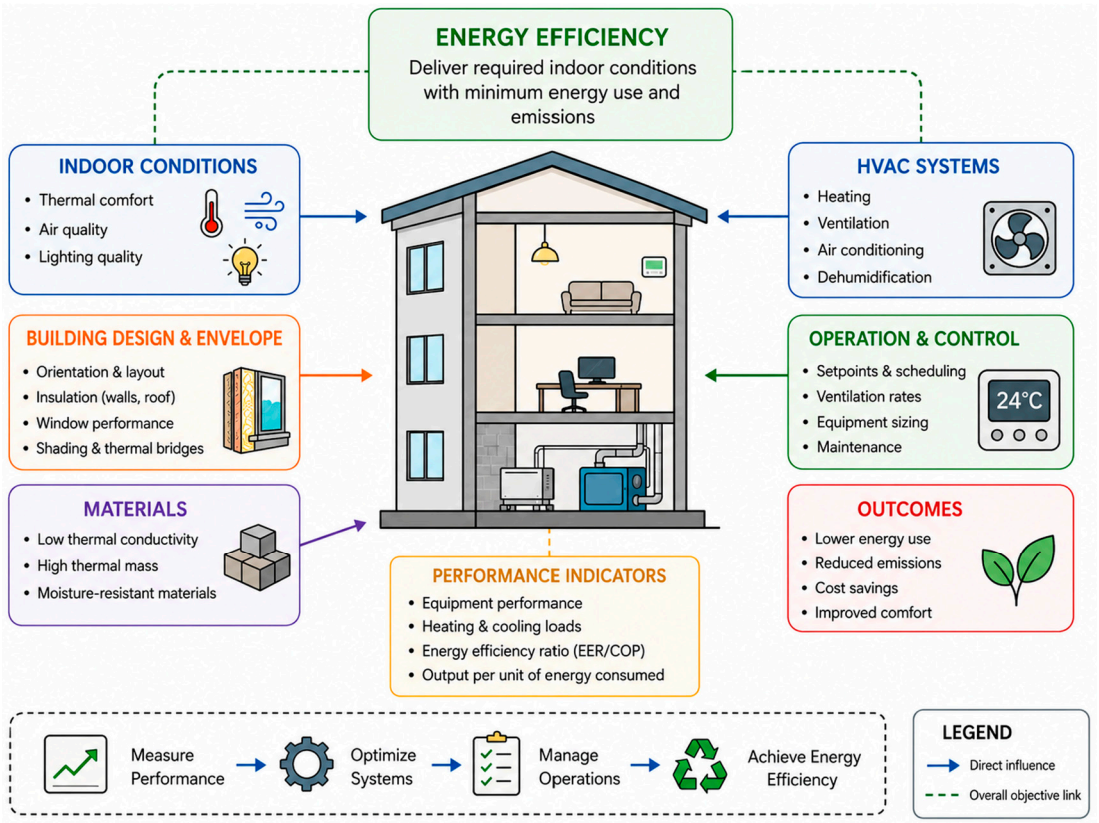

Figure 1. Residential building thermal load factors.

Thermal loads are the heating or cooling energy required to maintain target indoor conditions in response to external and internal drivers [28]. Loads are commonly decomposed into sensible (temperature-related) and latent (moisture-related) components. Reducing both at the source is the first step to efficiency: better insulation layout and thickness and shading lower sensible gains/losses, while designed ventilation strategies help manage latent moisture [29]. Correct placement of insulation in walls or roofs and attention to thermal bridges materially shift peak demands, thus enabling rightsizing of HVAC equipment, improved run-time efficiency, and more stable indoor conditions.

From an engineering perspective, the hierarchy is clear: (1) reduce loads via envelope and measures; (2) select high-performance HVAC to the actual heating and cooling loads; and (3) operate systems for proper ventilation rates and humidity control. Accurate load estimation must reflect weather, occupancy, and internal gains; neglecting temporal features can bias sizing and control strategies, especially in climates with variations [30]. Optimising energy around rigorous load reduction and HVAC sizing ensures durable savings and comfort, and it can be independent of particular control technology.

Reducing thermal loads contributes to energy efficiency at least from an energy reduction standpoint. Using some combination of building envelopes, insulation, and people can affect the overall energy performance of the building. For example, reducing sensible loads by improving insulation to reduce the transfer of heat through the envelope or controlling the latent moisture loads via the ventilation design to mitigate moisture in the first place [29]. Today, new forecasting methods use ML to process historical or live data to model building thermal loads, thus accounting for the complex, time-dependent interactions between the properties of the building [30]. The data-driven models are flexible to real-time changes in occupancy schedules or availability of climate data [31].

2.2. Classification Process and Explainable Classifiers

Figure 2 depicts the process of an application of machine learning, in particular explainable classification algorithms, on thermal load analysis of residential buildings. The process starts with historical data related to thermal loads, along with building features, occupancy, HVAC, climate variables, etc., which are initially preprocessed to deal with data-related issues. Then the processed data is used to train a classification algorithm to construct a model. The model is then evaluated using ML metrics and passed to the user along with feature interactions (when XAI is present as a layer) that explain important factors in the model. In our case, the model will also comprise rules, which further gives the end user rich knowledge that can be used in actionable decisions related to energy efficiency.

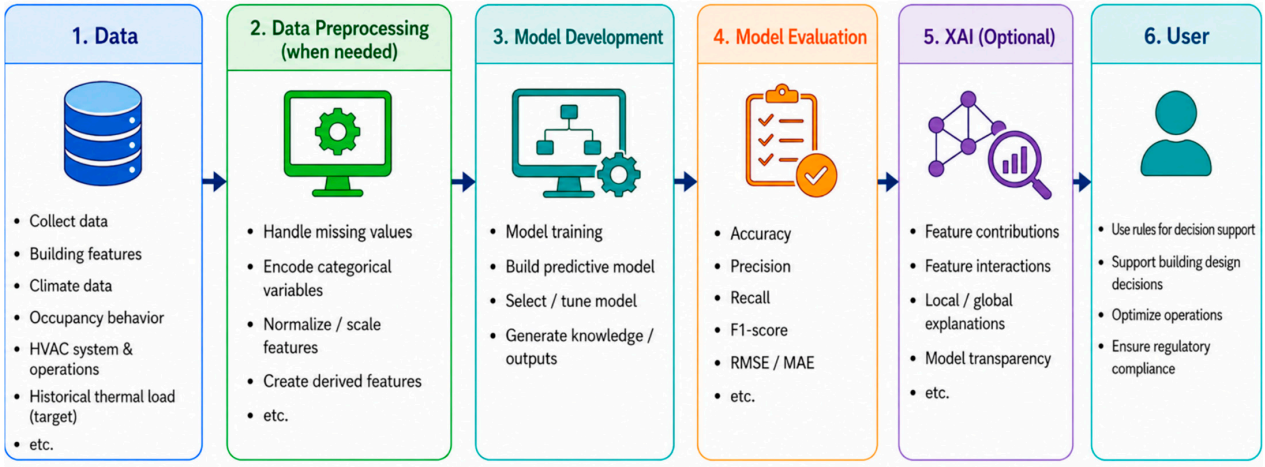

Figure 2. Explainable classification process for thermal load.

Transforming thermal load prediction from a regression-based problem into a classification task can provide an additional decision support layer rather than replacing continuous load prediction. While regression models estimate continuous heating and cooling loads, classification approaches, such as decision trees or rule-based classifiers, can assign buildings or cases to interpretable categories such as Low, Medium, or High thermal load. These categories can support easier comparison, prioritisation, and decision-making specifically for energy efficiency applications. The classification thresholds may be defined empirically from the training data, for example using percentile-based cut-off points, where the lower, middle, and upper portions of the load distribution represent Low, Medium, and High classes, respectively. Alternatively, thresholds may be established using domain-specific benchmarks, regulatory standards, or statistically derived cut-off values where appropriate. Importantly, threshold values should be determined using the training data only and then applied unchanged to the validation and test datasets to avoid any possible data leakage.

The value of discretisation is that it enables interpretable, simple knowledge extraction by the classification algorithm, thus linking combinations of climate, building features, and HVAC characteristics to thermal load states. This can support engineering design decisions by identifying combinations associated with high loads and highlighting alternatives involving material, insulation, infiltration, building form, or HVAC selection. It can also support operational decisions involving setpoints, ventilation, and system efficiency.

The XAI layer further strengthens this process by showing which features and interactions contribute most strongly to a prediction and in what direction. For engineers, this provides a transparent explanation of why a building is classified as Low, Medium, or High load, thus helping them identify the most influential and adjustable parameters for

thermal load optimisation. Because discretisation reduces numerical resolution, regression can be retained alongside classification to provide heating or cooling-load estimates, while classification provides explorable knowledge for engineers.

Rule-based classification represents one of the intuitive forms of ML, dating back to expert systems of the 1970s and 1980s where domain experts manually recorded knowledge in the form of rules. Over time, data-driven approaches such as inductive learning replaced domain expert rule acquisition with rule-based induction algorithms capable of discovering rules directly from input data. Modern rule-based models have evolved and use search strategies, rule pruning mechanisms, and probabilistic scoring to extract specific and accurate rules from large datasets [32,33]. These rule-based models are used in domains where explainability is critical, such as energy efficiency, medical diagnosis, and regulatory auditing, because they retain a logic structure that mirrors human reasoning. Rule induction algorithms, including Repeated Incremental Pruning to Produce Error Reduction (RIPPER) [34] and CN2 [35], serve as explainable models to preserve clarity of the output.

In the rule induction process, the learning algorithms automatically generate a series of rules from labelled datasets to classify new test data [36]. Each rule represents a relationship between features and class labels, and it is identified through evaluation measures like the rule's expected accuracy to reflect its accuracy in prediction [37]. These rules are extracted by searching for combinations of feature values that can distinguish one class from another and are presented as a list of conditions paired with class labels. The output is a simple human-readable set of rules that can easily be reviewed or managed [38].

A decision tree organises data into a hierarchical tree structure to perform prediction for classification tasks and can be considered part of rule-based classification approaches in ML [39,40]. The decision tree algorithm divides the training data into parts recursively based on criteria like information gain and others to identify the best input feature at each node [40–42]. The process continues until all nodes are pure or other stopping conditions are reached. To avoid model overfitting, the decision tree algorithm uses pruning techniques to stop tree growth early or trim tree branches [42]. Once constructed, each path from root to leaf can be converted into a rule describing the classification decision, and the tree or its equivalent rule set can be used to predict outcomes for new data.

Interpretability is one of the important advantages of rule-based classification models for end users. Because the structure visually mirrors human reasoning, stakeholders can easily trace how input variables influence the final decision [43]. This transparency enhances credibility and supports practical decision-making, thus allowing managers to verify that model logic aligns with real-world processes. Moreover, the rule-based model makes it straightforward to identify and communicate which factors are most important in driving outcomes, thereby facilitating compliance with audit requirements and encouraging model adoption in sensitive or regulated environments where explainability is essential.

Recently, XAI has emerged to bridge the gap between applied AI algorithms and reasoning understandable to humans. XAI consists of a family of methods that can explain complex models of deep neural networks in transparent terms [11]. The core principle of XAI is to provide explanations by identifying which input features most influence predictive decisions for specific data instances or across the model as a whole [44,45]. For stakeholders, XAI systems enhance usability by enabling engineers, in the case of thermal load prediction in buildings, to justify automated decisions and integrate them into workflows. Further, XAI models can generate visual explanations like feature rankings, saliency maps of deep learning algorithms, and decision rationale, thereby making it accessible across technical and managerial audiences.

Interpretability is a defining strength of classification models and a key reason for their appeal to non-technical stakeholders. Because each decision outcome is expressed through explicit conditions, stakeholders can understand and audit how the model reached a specific classification. This clarity builds confidence and trust while supporting accountability in domains like construction and civil engineering where decisions must be traceable and justifiable. Rule-based models thus enable stakeholders to explore, validate, and manage the rules.

While both XAI and rule-based classification models aim to promote interpretability, they differ in scope and mechanism. Rule induction and decision tree models are inherently explainable as their structure and logic are built into the model itself. In other words, the predictive model developed by the algorithm from the training dataset is explorable, as it contains simple chunks of knowledge. In contrast, XAI approaches are typically post hoc, and thus are applied to explain complex models (like deep learning systems) that are not naturally explainable. Thus, rule-based and decision tree models are "white boxes" by design, while XAI serves as an explanatory layer for otherwise opaque algorithms. Together, they represent two complementary paths toward XAI models.

3. Methodology and Search Process

The introduction of the XAI approach has become a development in the study of energy efficiency, particularly in thermal load prediction for buildings [46]. Recent advances in ML have allowed models to predict heating and cooling loads with notable accuracy but without providing further information [47,48]. Rule-based classification algorithms address this gap by producing models that are not only predictive but also understandable. This interpretability is essential for stakeholders like architects since it ensures that data-driven models' outcomes can be justified and operationalised.

After reading a large number of research papers within the scope of this research, we have identified a number of themes to discuss in this systematic review (Section 4). The research papers considered in this review were identified through a systematic selection process that drew from several databases. In this section, the methodology followed to identify, screen, and analyse the studies is detailed.

A structured literature search was conducted in accordance with PRISMA principles to identify empirical, data-driven studies concerning interpretable ML approaches for building thermal load prediction, modelling, classification, forecasting, and optimisation. The principal electronic information sources were Scopus, Web of Science Core Collection, IEEE Xplore Digital Library, and ScienceDirect. These sources were selected to provide coverage of building engineering, civil engineering, computer science, energy, HVAC, AI, and applied ML literature. Scopus and Web of Science provide broad multidisciplinary journal and conference coverage, while IEEE Xplore provides more specialised coverage of engineering and computing research. Supplementary research was undertaken through relevant publisher platforms, particularly when potentially eligible publications were identified through citation searching. Google Scholar was used only as a citation-searching source, including backward reference searching, forward citation tracing, and identification of potentially relevant studies not retrieved through the principal database searches. Records identified through supplementary searches were subjected to the same eligibility, peer-review, and duplicate screening requirements as records obtained from the principal databases.

The search strategy was organised around three main concept groups and combined using Boolean AND/OR operators. The first group represented thermal load outcomes: ("thermal load" OR "thermal load prediction" OR "thermal energy load" OR "heating load" OR "cooling load" OR "heating demand" OR "cooling demand" OR "HVAC load" OR

"building energy load"). The second group represented ML and interpretability approaches: *("machine learning" OR "artificial intelligence" OR "explainable AI" OR "explainable artificial intelligence" OR XAI OR "interpretable AI" OR "interpretable machine learning" OR SHAP OR Shapley OR LIME OR "decision tree" OR "rule induction" OR "rule-based classification" OR "rule-based model" OR "interpretable classifier" OR "random forest" OR "boosting decision tree" OR "fuzzy rule")**. The third group represented the built-environment and application context: (building OR residential OR commercial OR office OR HVAC OR "building envelope" OR insulation OR glazing OR materials OR geometry OR orientation OR occupancy OR climate OR weather OR "building operation" OR "Building design" OR "Engineering design"). These groups were combined with task-related terms (prediction OR forecasting OR modelling OR classification).

The PRISMA process [49], shown in Figure 3, was applied to ensure transparency in study selection. The initial database search identified 138 records. After removing 10 duplicate records, 128 records remained for title and abstract screening. At this stage, 49 records were excluded, leaving 79 reports sought for retrieval. The retained reports were successfully retrieved and assessed for full-text eligibility. Following the inclusion and exclusion criteria presented in Tables 2 and 3, 40 reports were excluded: 11 were not focused on building thermal load prediction, 20 did not include a relevant interpretability or XAI component, and 9 provided insufficient methodological information or did not meet the data-driven thermal load prediction criteria. Consequently, 39 studies were included in the systematic review.

Table 2. Inclusion criteria.

Criterion	Description	Justification
Publication Type	Peer-reviewed journal articles or conference proceedings	Ensures scholarly quality control and contribution to the academic literature
Timeframe	Studies published primarily between 2020 and 2025, with earlier highly relevant studies included where directly related to the review scope	Captures recent developments in interpretable ML while retaining seminal relevant studies
Domain Focus	Studies on building-energy efficiency focusing on heating, cooling, or thermal load prediction, forecasting, modelling, classification, or optimisation	Ensures direct relevance to thermal load prediction and building-energy applications
Methodology	Studies using rule-based classification, decision trees/tree-based models, interpretable ML, XAI methods, or related approaches that provide explicit model interpretation, feature attribution, decision logic, or rule extraction	Ensures that studies provide predictive/XAI/interpretable analysis
Empirical Analysis	Studies presenting quantitative analysis using measured, operational, experimental, or simulated building-related data	Ensures that the synthesis is based on empirically evaluated models rather than purely conceptual discussions
Methodological Rigour	Studies must clearly report some information on the dataset or data source, method, or analysis, and quantitative model evaluation or validation results	Provides a consistent minimum standard for assessing the reliability and interpretability of the included evidence
Language	English-language publications	Allows consistent screening, coding, and synthesis
Peer-reviewed Status	Must be published in a peer-reviewed venue	Ensures academic quality and reliability

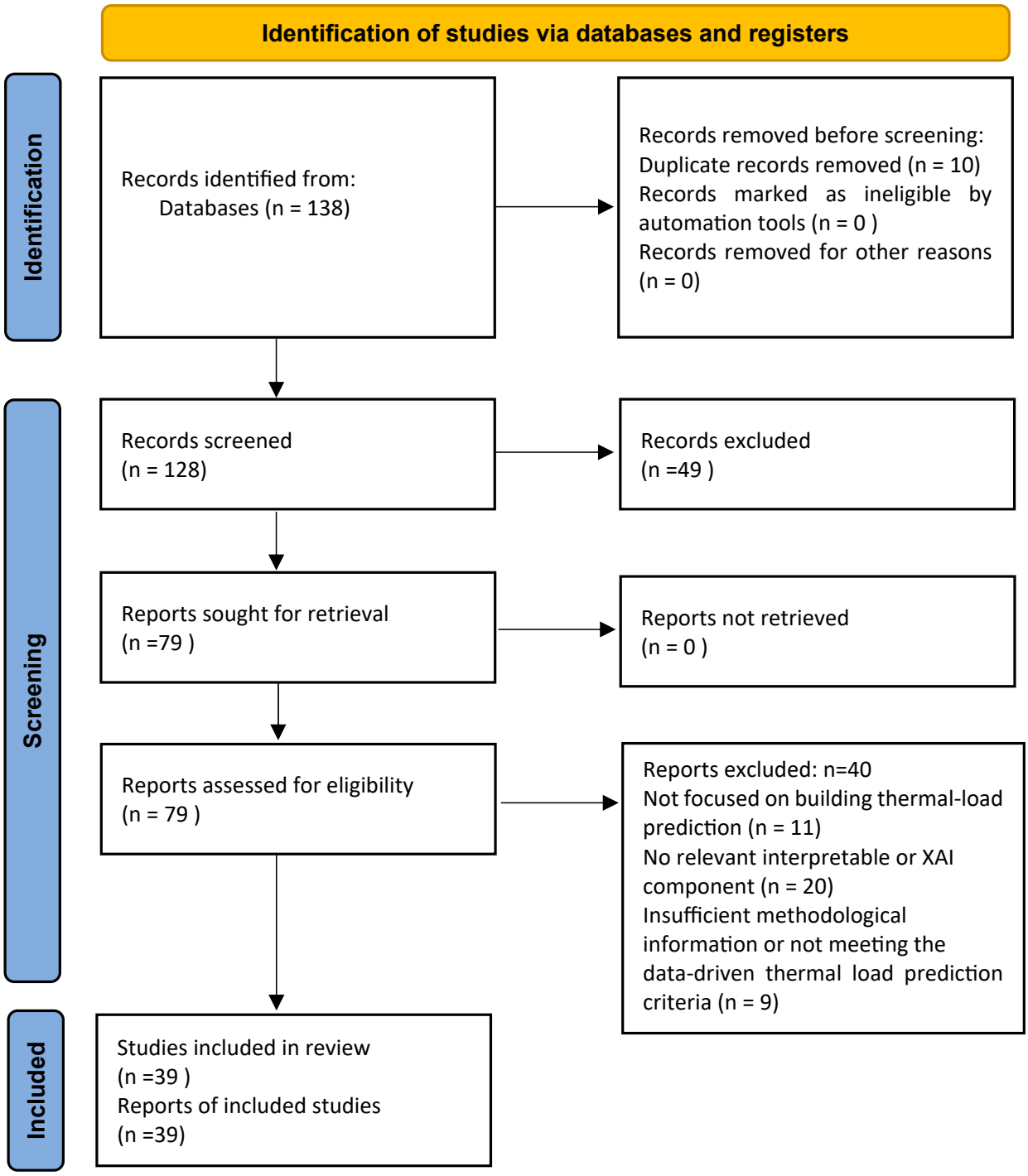

Figure 3. PRISMA process followed.

Table 3. Exclusion criteria.

Criterion	Description	Justification
Domain Irrelevance	Studies not focused on heating, cooling, or thermal load prediction, modelling, classification, forecasting, or optimisation.	Keeps the review centred on building-related thermal load applications.

Table 3. *Cont.*

Criterion	Description	Justification
Simulation Only	Pure engineering or physics-based simulation studies without ML or interpretable ML.	Excludes studies that do not contain the data-driven dimension required by the review.
Lack of Relevant Interpretability/Related Approach	Studies using ML without rule-based classification, decision trees/tree-based models, interpretable ML, XAI, feature attribution, rule extraction, or another clearly explanatory approach.	Operationalises "related approaches" and ensures that included studies contribute interpretable or explanatory information.
Insufficient Empirical Analysis	Studies without measured, operational, experimental, or simulated building-related data used for quantitative model development or evaluation.	Ensures that the evidence base is empirically grounded
Insufficient Methodological Rigour	Studies that do not clearly report essential information such as the dataset or data source, methods used or quantitative evaluation/results.	Provides a minimum standard for assessing the reliability and reproducibility of the included evidence.
Non-peer-reviewed/Inaccessible	Reports, opinion papers, duplicate records, non-English studies, or publications for which the full text could not be assessed.	Ensures that the final evidence base is accessible, peer-reviewed, and suitable for systematic assessment.

During the identification stage, all retrieved publications were screened, with earlier studies included only when they demonstrated significant relevance to rule-based classification or decision tree or ensemble with decision tree or XAI in building-energy domains. Other regulation-based websites were, in some cases, included to provide factual information in sections like the introduction. The screening stage applied the inclusion criteria to retain peer-reviewed papers that focused on heating and cooling-load prediction using at least one tree-based or rule-based algorithm, or an XAI-driven approach. Some studies reporting broader energy-load outcomes were retained where the analysis had a direct and substantive relationship to heating, cooling, HVAC demand, or building thermal performance.

At the eligibility stage, exclusion criteria were applied to remove non-relevant domains and studies without ML components, and data-driven models lacking explainability. Non-peer-reviewed materials, duplicates, or inaccessible papers were also excluded. Finally, during the inclusion stage, only English-language, peer-reviewed studies demonstrating methodological rigour and contextual relevance were retained. This process ensured that studies were reliable and empirically grounded.

The themes reported in Section 4 were derived through the structured thematic procedure described later in this section. The resulting categories represent recurring patterns identified across the study-level evidence rather than topics selected a priori. These themes emerged after reviewing the retained studies, and they collectively provide an approach for understanding both the technical and social dimensions of energy efficiency in the context of thermal load analysis. These themes are not independent but interconnected aspects of how thermal loads function in real contexts with respect to the energy efficiency of buildings. For example, data gaps in building features limit model performance, yet rule-based classifiers and XAI approaches can reveal their relative importance and guide better

strategies. Further, features such as geometry and orientation are well established [16], but data-driven models make the magnitude of their influence visible across different typologies [50].

Furthermore, occupancy dynamics have long been recognised as a factor in optimisation [31], and the distinction between rule-based application and XAI has not been well explored in data-driven studies related to thermal load analysis. Finally, building systems expand the relevance of load prediction to financial impacts [51]. By situating all these themes, and others, within an AI approach, the review ensures that the analysis does not stop at the technical performance of ML models but connects directly to engagement and collaboration among stakeholders.

To elaborate further on the process of identifying the themes by categorising the papers during full-text selection and analysis, the retained studies were systematically analysed for this review. For each study, information was extracted on the study context, thermal load target, dataset and data source, ML method(s), interpretability/XAI approach, feature types, and principal findings. The thematic analysis was then conducted inductively from these extracted study-level data. In the first stage, recurring concepts were identified across the evidence table, including model interpretability, data characteristics, physical building features, contextual variables, and operational applications. Related concepts were subsequently grouped into higher-order thematic categories by combining conceptually similar codes. For example, insulation, glazing, wall properties, and thermal characteristics were grouped under Building Envelope and Materials, while orientation, compactness, floor layout, and geometric characteristics were grouped under Spatial and Geometric Design Factors.

Similarly, recurring evidence concerning climate zones and building types formed Building Typology and Climate, while occupancy schedules and behavioural variables formed Occupancy Behaviour. The resulting themes were then reviewed against the included studies to confirm that each theme was supported by multiple papers and reflected recurring evidence rather than isolated observations. Studies were permitted to contribute to more than one theme because several studies examined overlapping building, data, and interpretability factors. This iterative grouping process produced the thematic structure used in Section 4, and the mapping between them and the retained studies.

Lastly, it should be noted that the exact dates of the original searches, database-specific retrieval counts, and archived database-specific search histories were not retained during the process of searching and retaining the studies. The thematic synthesis and quantitative mapping presented in Section 4 are based on with additional support citations that are relevant but not part of the systematic evidence base.

4. Themes and Discussion

4.1. Interpretability

XAI models do not represent standalone algorithms; instead, they are approaches designed to interpret the internal logic of complex models, particularly deep learning and artificial neural network (ANN) structures after training [52,53]. Typically, an XAI process involves three main stages: (1) the development of a predictive model, usually based on neural networks or other classification algorithms; (2) the application of post hoc interpretability techniques to identify how specific input features influence outputs; and (3) visualisation or ranking of these features to provide insights [54,55]. This workflow allows analysts to understand parts of the deep learning "black box" without modifying its architecture.

However, unlike rule-based classifiers, XAI mechanisms do not inherently generate new rules from data. Instead, they study the relationships already encoded within opaque

models. While XAI helps to explain a trained black-box model, rule-based classifiers inherently create logical structures (IF–THEN rules) during model generation. These rules inherently provide direct traceability between input features and predictions [10,34].

Recent advances in XAI demonstrate increasing efforts to enhance interpretability in data-driven thermal analysis. For instance, ref. [52] introduced an attention-based neural network for cooling-load prediction, where attention weights highlighted influential features such as occupancy and ambient temperature. Similarly, ref. [53] employed XAI to analyse the importance of input parameters for deep learning-based building load prediction across five climate zones, demonstrating that the types and number of essential input variables varied according to climatic conditions. These studies illustrate the growing role of XAI as a feature-attribution mechanism for exposing drivers of thermal load predictions rather than generating explicit model knowledge.

Extending this direction, ref. [54] combined SHAP-based feature analysis with temporal attention mechanisms for multi-step heating-load forecasting, demonstrating that interpretability can also reveal the relative importance of historical time steps as well as conventional input features. This is particularly relevant for thermal load forecasting, where temporal dependencies are central to model behaviour. However, such explanations remain dependent on the underlying predictive architecture and therefore do not provide the explicit decision rules associated with interpretable models. Ref. [55] extended explainability to district-heating systems by developing a framework for heat-load prediction, although the authors emphasised that preprocessing and feature-normalisation requirements may constrain scalability.

Further evidence of this trend is seen in hybrid intelligent approaches that integrate interpretability into load prediction. For example, ref. [9] proposed a hybrid model combining integral feature selection with ML for low-energy buildings, while ref. [56] explored feature-importance measures to improve the trustworthiness of heat demand forecasting. In a related development, ref. [57] introduced data-driven control methods for air-conditioning systems in which interpretability and reliability were treated as important design considerations for operational decision-making. These approaches demonstrate that interpretability is increasingly being incorporated not only at the explanation stage but also into feature selection, control, and model design processes.

Other recent studies further refine explainability within complex prediction settings. For instance, ref. [58] proposed a deep learning strategy for predicting the thermal conductivity of porous materials, while ref. [59] developed interpretable models using both public and internal laboratory datasets to identify influential predictors of material conductivity. In addition, ref. [60] advanced this direction through large language model (LLM)-based methods capable of explaining thermal-control logic in building systems. Moreover, ref. [61] optimised heat-load prediction using rolling-average outdoor temperatures and interpretable models, providing another direction toward explainable thermal forecasting. Collectively, these studies indicate that explainability is being extended across material-level prediction, building load forecasting, and operational control; however, the form of explanation differs substantially across these applications, ranging from feature rankings to natural-language explanations and temporal attention.

At the household level, ref. [12] demonstrated the value of SHAP in energy forecasting by identifying influential current and lagged consumption variables. Similarly, ref. [62] combined XGBoost with multiple post hoc explanation techniques, including SHAP and LIME, for multi-scale household energy forecasting. The use of several explanation methods within the same framework provides a broader view of model behaviour and allows local and global explanations to be compared. Nevertheless, this also illustrates a continuing methodological issue in XAI: different explanation techniques may describe the same

predictive model from different perspectives, making interpretation dependent on the selected explanatory method rather than solely on the underlying model structure. In addition, ref. [11] applied ML and XAI approaches to predict residential heating and cooling loads using building design features, linking model interpretation with sustainable architectural design and energy-performance assessment. A recent study by [63] used the DRIVE-XAI framework on smart-meter data from 10,000 households and reported strong alignment with regulatory benchmarks.

Despite these promising advances, XAI models face important limitations, such as many XAI techniques remaining fundamentally post hoc, meaning that explanations are constructed after model training and may not fully represent the internal reasoning of the predictive model [64]. The increasing use of combinations of several explanation methods, as demonstrated in [54,62], strengthens the visibility of influential features and time-dependent relationships but does not eliminate this distinction between explanation and model logic. Second, interpretability still lacks a standardised metric or universally accepted definition. As refs. [14,19] emphasise, interpretability is often qualitative and context-dependent, with evaluation based on cognitive simplicity, perceived usefulness, or user trust rather than common quantitative measures. Some studies associate interpretability with how intuitively users can understand model outputs, whereas others emphasise the stability and reproducibility of feature rankings [19,20].

Although interpretability in XAI is often treated qualitatively, some researchers have attempted to develop quantitative measures. For example, ref. [65] introduced indicators such as rule count, feature usage, and explanation stability to assess the complexity and consistency of model explanations. Further, ref. [66] proposed the "Co-12" framework, which defines 12 conceptual properties of interpretability, including compactness and correctness. Similarly, ref. [67] developed metrics that compare explanation outputs against known neural-network triggers to evaluate how accurately XAI methods recover underlying model reasoning. These efforts demonstrate progress toward measurable interpretability, although no standardised evaluation framework has yet emerged.

Computational efficiency also remains an important constraint. Ref. [68] showed that increasing model and explanation complexity can limit practical implementation, particularly when additional environmental or operational considerations are incorporated. Similarly, ref. [55] noted that extensive feature normalisation and post-model analysis may hinder the scalability of XAI in district-heating applications, while ref. [69] observed that even interpretable control systems often require model simplification to support real-time operation. The multi-step forecasting framework in [54] further illustrates this trade-off: additional explanation mechanisms such as SHAP-based feature analysis and temporal attention can improve understanding of model behaviour, but they also introduce additional analytical layers that must be balanced against computational and operational requirements.

These concerns parallel those raised in hybrid models, which seek to balance predictive accuracy and transparency. Refs. [58,59] demonstrate that explainability can be incorporated at the material or feature level, but its reliability depends on appropriate data treatment and model design. Similarly, refs. [9,60] indicate that global feature rankings can strengthen confidence in predictive results, particularly when their interpretation is validated against domain knowledge. The broader evidence, including [54,62], therefore suggests that XAI is becoming increasingly sophisticated and multi-layered, but greater explanatory complexity does not necessarily translate directly into greater interpretability for engineering stakeholders. This reinforces the importance of distinguishing between post hoc explanation and intrinsically transparent rule- or tree-based models when evaluating the practical usefulness of interpretable thermal load prediction.

4.2. Rule Model Scarcity in Thermal Load Prediction

Rule-based classifiers have become increasingly relevant in thermal load prediction, particularly as researchers seek models that provide further knowledge beyond predictive accuracy. Compared to complex deep learning models, rule-based approaches yield outcomes that are explicit and easier to understand. Ref. [10] demonstrated that classification models with rules could accurately predict residential thermal loads while providing human-readable insights into how building factors contribute to cooling or heating demand. This level of interpretability supports building operators in understanding not just what the load will be, but why it behaves as such under different conditions. Similarly, ref. [70] combined zone-level neural networks with rule-based control to improve operational optimisation, thereby illustrating how human rules can explain complex prediction systems by logical constraints and safety conditions that align with expert knowledge.

Furthermore, rule-based classification methods naturally produce transparent knowledge structures that can encode expert knowledge and physical constraints into model logic. This capability enhances operational usability and turns model transparency into insights rather than retrospective descriptions. As ref. [71] noted, such interpretability promotes improved communication and knowledge sharing among technical and non-technical stakeholders.

Several studies exemplify the progression of explainable and tree-based models within the energy domain. Ref. [13] combined clustering decision trees with adaptive Multiple Linear Regression to produce an interpretable building-energy load prediction method with accuracy comparable to more complex models. Their approach achieved cooling-load prediction accuracy comparable to more complex learning techniques while retaining interpretable decision structures. This trend is also evident in [72], where a Gradient Boosting Decision Tree (GBDT) model was applied to cooling-load prediction for an ice-storage air-conditioning system. Although the ensemble structure improved predictive performance, its interpretability remains less direct than that of a single decision tree because the final prediction is distributed across multiple trees.

Similarly, ref. [73] combined discrete wavelet transform with tree-based ensemble learners for residential heat-load forecasting, demonstrating that tree ensembles can effectively capture temporal and nonlinear thermal load patterns. However, the added preprocessing and ensemble complexity reduce the immediate transparency of the model compared with simpler rule-based classifiers. In contrast, ref. [74] applied a decision tree model directly to building heating-load prediction, illustrating the advantage of a simpler tree structure in providing traceable decision paths while still achieving strong predictive performance. These studies therefore demonstrate a continuum between predictive accuracy and interpretability across single-tree, ensemble-tree, and rule-based approaches.

Similarly, ref. [10] analysed residential building samples containing features such as glazing ratio, wall type, orientation, and insulation thickness. By transforming the regression problem into a classification task through discretisation and sensitivity analysis, the authors employed rule-based algorithms to achieve high prediction accuracy for heating- and cooling-load categories while producing human-readable decision rules. Unlike ensemble approaches such as [72,73], this type of classification provides explicit conditional knowledge that can be examined directly by engineers and other stakeholders.

The outcomes of rule-based models generally focus on conditional relationships between building characteristics and thermal responses. For instance, ref. [75] applied an optimised M5Rules-GA approach to heating-load prediction using geometric and design variables. Earlier work by [76] similarly demonstrated the value of decision tree approaches for building-energy demand modelling, particularly because their hierarchical structures make the basis of individual predictions more visible than conventional statistical or black-box models. More recent evidence from [74] reinforces this advantage by showing that

decision tree methods can retain strong heating-load predictive capability while preserving a model structure that can be inspected and translated into decision logic. By comparison, tree-based or rule-based classifiers such as those used in [75,77] may provide higher robustness or predictive accuracy, but their aggregation of multiple trees can make the resulting reasoning less straightforward to communicate to practitioners.

The content of the model therefore remains a key advantage of rule-based classifiers and individual decision trees over post hoc XAI and more complex ensemble approaches. While XAI techniques can provide explanations for opaque models, their outputs may still require technical expertise to interpret. As ref. [78] noted, simpler model structures allow stakeholders to inspect, manage, and potentially embed model logic into operational decision processes. Decision tree and rule-based approaches used by [77,79,80] further illustrate how explicit decision paths can support communication among engineers, operators, and sustainability specialists. In contrast, ref. [73] demonstrates that ensemble-tree methods occupy an intermediate position: they retain a tree-based foundation but sacrifice some direct interpretability in exchange for stronger predictive modelling of nonlinear and temporal relationships.

To further improve the application of rule-based classifiers in thermal load prediction, future studies could incorporate richer data representations, such as thermal imagery or 3D spatial occupancy maps, to capture spatial dynamics that are often absent from conventional tabular datasets. Integrating such information into interpretable frameworks could enable models to generate spatially dependent rules for energy zoning and HVAC control. Hybrid approaches may also provide a productive research direction, where the predictive strength of trees or tree-based ensembles such as those demonstrated in [73,74] is combined with explicit rule extraction or XAI mechanisms to recover more accessible decision logic. Likewise, extending single-tree approaches such as [74] with carefully controlled optimisation or explanation techniques may improve predictive performance without substantially compromising model transparency.

4.3. Multi-Source Data

Thermal load data quantify the heating and cooling demands of indoor environments and are used to optimise energy efficiency. These datasets capture interactions between different features, including occupancy patterns and behaviour [81]. Thermal load estimation is critical as energy systems transition toward higher efficiency targets and data-driven operational strategies [21]. Since heating and cooling fluctuate over minutes or hours, temporal resolution becomes a defining dimension of thermal data, introducing a new challenge to the problem [82].

District heating and cooling systems operate through centralised plants that distribute thermal energy to multiple buildings via interconnected pipelines [83]. Thermal load readings in these networks are obtained using energy metres placed at substations, recording mass flow, supply and return temperatures, and instantaneous thermal power. Their temporal nature and system-wide diversity make district datasets operationally complex [84]. In contrast, building-level datasets rely on local instrumentation such as sensors, thermostats, and smart metres to capture indoor temperatures, humidity, and equipment cycles. Simulated datasets complement real measurements by offering controlled, noise-free environments for modelling and are often produced via simulation tools such as EnergyPlus or finite element thermal solvers [85].

Table 4 shows a few different datasets related to residential buildings, commercial facilities, district-heating networks, and machine-level thermal simulations. These datasets differ in temporal resolution, physical scale, feature richness, and sensor modalities. Building datasets such as UCI's Energy Efficiency, Building Data Genome Project (BDG2) or

NREL-ResStock emphasise envelope, operational, and meteorological contributions to heating and cooling demands. District datasets by Geysen et al. [82] illustrate the operation of network-level thermal variations. Machine tool thermal datasets demonstrate the value of high-frequency thermal sensing for ML prediction.

Table 4. Thermal load prediction datasets.

Dataset Name	Source	Type of Features Used	Dataset Size	Temporal	System Type
Energy Efficiency Dataset (UCI)	https://archive.ics.uci.edu/dataset/242/energy+efficiency	Building geometry, envelope, glazing	768 simulated building cases; 8 input features	No	Building
Operational Thermal Load Forecasting—District Heating Networks	https://www.sciencedirect.com/science/article/pii/S0378778817312070	Thermal load, climate, temporal	27 months from 10 residential buildings in Rottne, Sweden	Yes	District heating
Temperature Modelling in Machine Tools	https://arxiv.org/abs/2509.16222	Thermal, material, spatial, simulation	29 probe locations × 1800 time steps × 17 simulation runs	Yes	Mechanical thermal system
Residential Cooling Load Case-Study Dataset	https://www.sciencedirect.com/science/article/pii/S2590123025029354	Indoor climate, outdoor climate, cooling load	One year of hourly environmental data from two monitored residential rooms (C1 and C3)	Yes	Building
Hourly Load Profiles for 24 Facilities	https://data.mendeley.com/datasets/rfnp2d3kjp/1	Energy load, building type	24 facilities × 8760 hourly values; 6 EnergyPlus reference buildings and 18 simulated buildings	Yes	Building
ASHRAE Great Energy Predictor III Dataset	https://www.kaggle.com/c/ashrae-energy-prediction	Building, energy, HVAC/metre, climate	More than 20 million training observations from 2380 m in 1448 buildings across 16 sources	Yes	Building
Building Data Genome Project 2 (BDG2)	https://arxiv.org/abs/2006.02273	Building, energy, HVAC/metre, climate	3053 m from 1636 non-residential buildings at 19 sites; 2016–2017; approximately 53.6 million measurements	Yes	Building
End-Use Load Profiles for the U.S. Building Stock (ResStock/ComStock)	https://data.openei.org/submissions/4520	Building, envelope, HVAC, energy, climate	Very large building-stock dataset; calibrated and validated 15 min profiles for major U.S. building types.	Yes	Building

A challenge in thermal load analysis application is obtaining comprehensive thermal-related features, whether from real measurements or synthetic simulation tools. Real-world data collection is limited by privacy concerns, sensor calibration errors, and high

installation and maintenance costs, especially when multiple environmental features such as temperature, humidity, solar radiation, and occupancy must be continuously monitored across building zones. Collecting this data also involves additional expenses for BIM integration, IoT sensor networks, and data synchronisation systems, which can make large-scale studies financially unfeasible.

On the other hand, generating synthetic datasets through simulation requires domain knowledge, model calibration, and computational resources to represent the diversity of real-world conditions. Accurate prediction of thermal loads depends on numerous interacting features, including geometry, building envelope properties, orientation, occupancy, operational schedules, and local weather dynamics, among others. Many existing buildings still lack standardised digital twins or complete material specifications, which further complicate data collection and feature extraction. Consequently, the development of rich, representative datasets for energy optimisation remains a complex and costly process that continues to limit real-world deployment of predictive models.

The complexity of the thermal load prediction process lies not only in the methods used but also in the heterogeneity and interaction among the elements of the data sources. Robust data-driven models need a diversity of features. However, challenges related to multi-source data availability, data collection, data integration, and data preprocessing to support model construction are still areas that require further attention. For instance, ref. [10] indicated that the absence of humidity data from residential cooling demand models caused a decrease in performance. In a similar context, ref. [30] highlighted that the inclusion of time and other related factors, such as day type and hour of the day, could contribute to the performance of cooling predictions when using ML techniques.

Moreover, a study by [14] showed a strong case for how some building and material factors impact model performance for thermal load prediction. More importantly, including more features like those based on a building's structure and envelope can impact predictive accuracy for models that estimate heating and cooling loads. Studies such as [86,87] illustrate how thermal load prediction often relies on data from relatively limited and predefined sets of building descriptors, which highlights a broader multi-source data limitation, as datasets collected from different sources may vary considerably in their feature coverage and may not consistently capture the entire characteristics of real buildings. While this allows the analysis to continue, it may minimise the validity and the generalisability of the results.

Many ML algorithms, including ensemble learning methods, showed good performance in thermal load prediction applications. However, their effectiveness is dependent on the quality of the data, the preprocessing phase, and the features selected [88,89]. For instance, ref. [88] achieved adequate accuracy in prediction using the LightGBM algorithm based on data through the use of feature selection methods. Nevertheless, such results are not always reproducible for systems that have incomplete data or data quality issues.

The use of the IoT is being promoted as a means for real-time data collection and integration into BIM systems to track and optimise energy use. For example, ref. [90] pointed out that while IoT allows data acquisition in real-time, most systems utilised in buildings use static historical databases to train predictive models. In this approach, real-time flexibility is not achieved because it is imperative to consider short-term changes in weather and occupancy rates, among other energy-related factors. In addition, dynamic learning models involving real-time data streams are still not widely used in this important domain. An issue related to data quality in thermal load analysis is handling several data types. Features such as insulation type and HVAC operation modes require encoding methods that preserve their real meaning while still being compatible with numerical

models. However, this integration step is often underestimated, leading to datasets that overrepresent continuous variables and ignore important categorical ones.

4.4. Simulation Tools

Thermal energy modelling tools are important to building design since they enable the simulation of energy consumption under different climatic and operational scenarios. Commonly adopted tools include EnergyPlus [91], CESAR-P [92], TRNSYS [93], DesignBuilder [94], and OpenStudio [95], among others, each varying in cost, file formats, process, and interoperability.

Open-source tools such as EnergyPlus are commonly used in research due to their availability, flexibility, and capability for large simulations [91,92]. In contrast, commercial tools like DesignBuilder and IES-VE [96] are favoured by practitioners for their navigable graphical user interfaces, built-in templates, and visualisation capabilities that reduce the technical complexity of energy analysis. Cost remains a factor: while open-source platforms provide customisation for free, some licenced tools offer technical support and simplified model setup. Thus, tool selection often depends on the intended use, experimentation level, industry requirement, or policy assessment.

The modelling complexity of these tools influences both synthetic data production and modelling process accuracy. Tools such as EnergyPlus and TRNSYS provide physics-based dynamic simulation engines that are capable of handling thermal variation and control systems [97]. TRNSYS, in particular, excels in transient system modelling for renewable integration. On the other hand, EnergyPlus is commonly used to generate physics-based simulated building-energy data that can subsequently support ML model development and evaluation. Meanwhile, DesignBuilder and OpenStudio are used as graphical front ends for EnergyPlus as they offer workflows that maintain physical accuracy. The IES-VE tool integrates modules for daylighting, ventilation, and comfort analysis, thereby making it a comprehensive simulation tool for professional design settings [98]. CESAR-P [92] extends these capabilities to the urban scale, supporting multi-building energy analysis and district-level analysis, which are the basis of smart city energy planning.

A crucial consideration for simulation tools is interoperability with BIM and compatibility with 2D and 3D design formats such as Revit, ArchiCAD, and IFC. As refs. [22,99] emphasised that linking BIM and simulation tools may reduce manual data entry by enabling automatic exchange of geometric and material information. However, inconsistencies in data standards can be seen as a potential limitation; many of the simulation tools rely on intermediate formats such as gbXML or IFC for translation [100]. Ref. [101] proposed using physical BIM libraries to standardise thermal parameters and facilitate model synchronisation between design and simulation environments.

Usability also varies: while open-source tools demand a higher technical level of expertise, commercial tools like IES-VE and DesignBuilder focus on automation, embedded databases, and navigable user interfaces. As simulation evolves, the integration of optimisation algorithms with building-energy modelling can strengthen the connection between energy-performance analysis and design or operational decision-making [97]. Overall, choosing the right simulation tool requires balancing cost, process complexity, interoperability, data, and accuracy to ensure technical robustness and usability.

Table 5 shows common features associated with the energy modelling simulation tools such as cost, setup requirements, input data, output data, interoperability and use complexity level.

Table 5. Summary of common energy modelling simulation tools with common features.

Tool Name	Description	Requirements	Interoperability	Input Data	Output Data
EnergyPlus	Simulation engine for detailed HVAC, lighting, and thermal load analysis	Computational resources; knowledge of building physics	Native IDF/epJSON input; can be linked with OpenStudio and other BIM/BEM workflows	Geometry, materials, HVAC, weather (EPW), occupancy	Thermal loads, HVAC performance, comfort metrics
TRNSYS	Modular transient simulation tool for thermal and renewable-energy systems	Technical setup; advanced modelling knowledge	TRNBuild and TRNSYS3D workflows; can exchange data with external tools	Component specification, solar/weather data, control logic	Transient heat flow, heating/coolig demand, energy-system efficiency
DesignBuilder	Commercial GUI for EnergyPlus with daylighting and energy-analysis capabilities	Moderate system specifications; GUI simplifies setup	gbXML and IDF import; BIM workflows with Revit, ArchiCAD and other gbXML-enabled applications	Geometry, materials, occupancy, HVAC templates	Energy use, load charts, cost and comfort metrics
OpenStudio	SDK and modelling environment for EnergyPlus enabling scripting and automated workflows	Moderate technical knowledge; supports scripting	Direct EnergyPlus integration; OpenStudio SDK/API and SketchUp-based modelling workflows	Model geometry, schedules, thermal properties, HVAC and weather	Cooling/heating loads, energy results and machine-readable outputs
IES-VE	Integrated suite for full-building energy and environmental simulation	Moderate to high technical requirements; professional modelling environment	BIM interoperability through Revit and exchange formats such as gbXML and IFC	3D BIM models, HVAC, materials, occupancy and weather	Energy KPIs, thermal loads, comfort reports and graphical outputs
CESAR-P	Dynamic urban building-energy simulation tool for district-scale applications	Moderate technical knowledge; Python 3.8/3.10-based workflow and urban/building-stock data preparation	Python-based framework coupled with EnergyPlus; supports structured urban/building-stock data workflows	Building-stock data, geometry, construction parameters, weather and energy-system parameters	Heating, cooling and electricity demand; primary energy, CO_2 and cost results
IDA ICE	Dynamic multi-zone simulation tool focusing on indoor climate and HVAC performance	Building-physics and HVAC expertise	IFC-based BIM import, including geometry, zones and selected construction/material properties	Weather, geometry, envelope data, internal gains and systems	Energy use, heating/cooling demand, air quality and thermal comfort
DOE-2/eQUEST	Established engine/interface for building-load and HVAC-performance estimation	Relatively lightweight setup; building-energy modelling knowledge required	Limited modern BIM interoperability; mainly tool-specific input/interface workflows	Simplified geometry, constructions, HVAC, schedules and occupancy data	Annual/monthly energy use and building-load summaries

Table 5. *Cont.*

Tool Name	Description	Requirements	Interoperability	Input Data	Output Data
ESP-r	Integrated airflow, moisture, thermal and energy-system simulation environment	High technical skill; building-physics knowledge	Supports external data/geometry exchange, although BIM interoperability is less direct than newer BIM-oriented tools	Material, geometry, weather, internal gains and control-logic data	Energy, airflow, thermal and environmental results
EnergyPlus	EnergyPlus integrated with optimisation algorithms for enhanced analysis	Requires optimisation knowledge and, depending on the framework, coding skills	EnergyPlus API and file-based/programmatic coupling with external optimisation tools	Simulation parameters, design variables, objective functions and constraints	Optimised energy use, objective values, Pareto fronts and KPIs

4.5. Spatial, Design and BIM Factors

A wide range of data-driven approaches focus primarily on operational or sensor-based information rather than detailed spatial and geometric representation. For example, ref. [102] proposed a rule-based system for detecting energy efficiency anomalies from building data, illustrating an operational modelling approach in which detailed building geometry was not the principal source of predictive information. In contrast, BIM-based research demonstrates the potential to represent buildings using richer geometric, spatial, and physical information. Studies such as [22,100,101] examine the use and transfer of BIM information within building-energy and thermal simulation environments, thus highlighting the potential of digital building models to provide structured geometric and physical information for performance analysis.

The integration of detailed building information with thermal-performance modelling can improve the representation of building geometry and physical characteristics [99], while ML approaches can reveal how design variables such as orientation, compactness, surface area, and glazing characteristics relate to heating and cooling loads [13,16]. A remaining challenge is therefore to connect the richer spatial information available through BIM-oriented approaches with interpretable data-driven thermal load prediction. This challenge may be particularly relevant for existing and older buildings, for which complete digital geometric and material information is not always available.

Improvements in predictive algorithms do not necessarily result in richer representations of building geometry. For example, ref. [80] used a decision tree model combined with dual metaheuristic optimisation to improve cooling-load prediction. Although such approaches can improve predictive performance, the building representation remains dependent on the predefined input variables available to the model rather than a complete representation of the building's spatial configuration. This distinction is important because a model may achieve high predictive accuracy while still providing limited information about room configuration, façade articulation, surrounding context, or other geometric relationships relevant to thermal behaviour.

Within spatial and geometric design modelling, refs. [60,103] demonstrate that data-driven models often represent buildings through a limited set of predefined geometric and design variables. These variables provide useful information for predictive modelling but represent only part of the full spatial and physical configuration of a building. As discussed more broadly in interpretable building-energy modelling [14,60], simplified representations may limit the extent to which relationships between spatial and geometric factors and predicted energy demand are fully

exposed, making it more difficult for designers and engineers to understand how combinations of design characteristics influence thermal performance.

A related research opportunity concerns the integration of operational sensor information with spatial building data. IoT-enabled smart building systems can provide real-time environmental and operational information for energy management applications [27,90]. However, sensor-derived information and architectural or geometric building descriptions are often treated as separate data sources. Greater integration of these information streams could enable predictive thermal load models to associate changing indoor and operational conditions with the spatial and physical characteristics of the building. Such integration could be particularly valuable for understanding design-related thermal variability and for connecting operational building behaviour with the physical conditions established during design.

Looking toward the future, research should prioritise richer and more context-aware representations of spatial and geometric building characteristics to improve the predictive performance, interpretability, and generalisability of ML models for thermal load estimation [13,104]. Existing studies demonstrate that design and configuration variables can contribute to heating and cooling-load prediction [16,85]. However, these descriptors are commonly represented as individual numerical attributes rather than as an integrated description of the building's spatial configuration. Future research could therefore move beyond isolated geometric variables toward representations that retain relationships among building form, orientation, façade configuration, zoning, and other spatial characteristics.

Future datasets could also be expanded to incorporate more detailed geometric, façade, orientation, and spatial descriptors so that predictive models are better able to account for building design conditions and assumptions. Large-scale resources such as NREL's ResStock demonstrate the value of combining multiple categories of residential building information. However, such resources generally represent buildings through structured characteristics and archetypal attributes rather than complete architectural geometry, detailed room configuration, façade articulation, or full three-dimensional spatial relationships. Future design-oriented datasets could therefore build on the breadth of such building stock datasets while incorporating progressively richer geometric and spatial information.

This distinction is particularly important across the engineering design process because the amount and resolution of building information change as a project develops. During conceptual and early design, relatively accessible building descriptors may be sufficient to support rapid annual or seasonal thermal load estimates and preliminary comparisons between design alternatives. At this stage, ML models could provide designers and engineers with rapid feedback on how major geometric choices are associated with changes in expected heating and cooling demand. As the project progresses into schematic and detailed design, richer information becomes available, including façade configuration, glazing distribution, zoning, wall and roof assemblies, insulation placement, thermal properties, and spatial relationships. Incorporating this progressively richer information could refine thermal load predictions and provide more specific explanations of the consequences of individual design decisions.

At the operational stage, largely static design descriptors can then be supplemented with dynamic information such as weather, occupancy, HVAC operation, setpoints, indoor environmental measurements, and monitored energy or thermal load data. Developing datasets and interpretable ML models around this progressive increase in information could therefore connect early-stage architectural decision-making, detailed engineering and HVAC design, and operational thermal load forecasting. Rather than requiring the same level of information at every stage, predictive models could progressively increase

in detail as the building design develops and additional geometric, material, system, and operational information becomes available.

4.6. Building Envelope and Material

Building envelope characteristics influence heating and cooling loads, but there is a clear difference between the level of physical detail considered in thermal studies and that commonly represented in ML models. Experimental and analytical studies consider insulation thickness, material arrangement, thermal storage, and wall orientation [15,28,29,105,106], whereas ML studies frequently rely on broader descriptors such as wall area, roof area, glazing area, compactness, height, and orientation [16,85,103]. This contrast suggests that strong predictive performance does not necessarily mean that the physical behaviour of the envelope is adequately represented within the model.

Envelope variables also interact rather than operate independently. Insulation performance depends on thickness, position within the wall assembly, thermal mass, orientation, climate, and internal heat gains. Refs. [28,106] showed that optimum insulation thickness and associated energy performance vary according to wall orientation and climatic conditions, while ref. [29] demonstrated that insulation location within wall assemblies affects heating and cooling demands. Similarly, ref. [15] showed that the thermal behaviour of insulation and phase change materials is influenced by internal heat gains. Collectively, these findings indicate that envelope performance depends on combinations of material, configuration, and operating conditions rather than individual material attributes alone.

By comparison, commonly used ML thermal load models provide substantially less material detail. Refs. [16,85,103] predict heating and cooling loads using predefined variables including relative compactness, surface area, wall area, roof area, height, orientation, glazing area, and glazing distribution. Although these descriptors support effective prediction, they do not explicitly represent insulation location, material layer sequence, thermal diffusivity, or detailed thermal mass distribution considered in physical envelope studies [28,29,106]. This reveals a gap between established physical knowledge of envelope behaviour and the information represented in many data-driven thermal load models.

The importance of this gap depends on the engineering application. During early design, relatively accessible variables such as wall area, glazing, orientation, and compactness may be sufficient for rapid comparison of design alternatives [16,85]. During detailed design or retrofit assessment, however, greater material resolution becomes important because buildings with similar geometric characteristics may exhibit different thermal behaviour depending on insulation configuration and wall construction [28,29,106]. Therefore, increasing model complexity is not necessarily required at every stage; rather, the level of envelope detail should correspond to the intended design decision.

BIM-based energy modelling provides one route for incorporating richer physical information. Ref. [99] examines interoperability between BIM and thermal simulation, while ref. [101] demonstrates how BIM libraries can represent physical building information for thermal energy simulation. Together, these studies indicate that geometry, construction, and material information can be retained in structured digital building models. However, this level of representation is more established in simulation workflows than in interpretable ML thermal load modelling. A key research opportunity is therefore to identify which BIM-derived envelope and material properties provide additional predictive and explanatory value when incorporated into ML models.

Material-focused ML research further suggests that greater physical interpretability is possible. Although ref. [58] focuses on porous materials rather than whole building thermal loads, it demonstrates an interpretable deep learning approach that relates three-dimensional material structure to effective thermal conductivity. Its relevance is therefore

methodological: similar approaches could potentially be used to explore relationships between envelope structure, material properties, and building thermal performance when sufficiently detailed building data become available.

Applicability is also conditioned by climate and building type. Ref. [105] applies data-driven techniques to heating and cooling requirements of poultry buildings across different climatic conditions, while refs. [28,29,106] demonstrate that envelope performance itself varies with climate, orientation, and insulation configuration. These patterns suggest that models developed using a restricted range of envelope configurations should not automatically be assumed to generalise across different climates or building typologies.

The regulatory dimension adds another applicability condition. Ref. [107] shows that residential energy efficiency standards vary across climatic regions and place different requirements on building thermal performance. Consequently, ML models intended for practical design or retrofit support may need to account for physical, climatic, and regulatory differences rather than relying solely on fixed benchmark variables.

Overall, the literature reveals a persistent gap between physical envelope knowledge and its representation in data-driven thermal load modelling. Physical studies show that insulation thickness, insulation position, thermal mass, material configuration, orientation, climate, and internal gains interact in determining thermal performance [15,28,29,106], while ML studies often represent the envelope through broader geometric and glazing descriptors [16,85,103]. Future models should therefore incorporate envelope information progressively according to the engineering application. Early design models may rely on accessible aggregate variables, whereas detailed design and retrofit models could incorporate wall and roof assemblies, insulation characteristics, thermal conductivity, and other material information available through BIM or engineering databases [99,101].

4.7. Building Typology and Climate

Thermal load behaviour varies across building typologies and climatic conditions, which limits the assumption that a model developed for one context will transfer directly to another. Evidence from different building types shows that AI methods can perform effectively across heterogeneous buildings, but their applicability depends on differences in use, occupancy, systems, and climate. Ref. [50], for example, demonstrated energy savings across building typologies and European climate settings, indicating that shared AI-based control is feasible. However, this does not imply that building type is irrelevant; rather, the system had to accommodate different building functions, occupancy patterns, heating systems, and operating conditions.

Climate introduces a further source of variability because the importance of predictive inputs changes with environmental conditions. Using 2000 office building models in each of five climate zones, ref. [53] found that both the number and type of essential variables for load prediction differed across climates. This is important for model transferability: a feature set that is sufficient in one climate may be redundant or incomplete in another. XAI therefore has value not only for explaining predictions but also for identifying when climate-specific input selection is required.

The literature also shows a tendency toward models developed within narrowly defined climatic or typological contexts; for instance, ref. [108] developed heating and cooling-load prediction specifically for residential buildings in the hot arid climate of Dhahran, Saudi Arabia, while ref. [77] examined lightweight residential buildings under subtropical conditions. The latter showed that thermal performance depended on combinations of envelope properties rather than individual dominant variables alone. These studies provide useful context-specific models, but neither demonstrates universal performance outside the climate nor building conditions represented in its

dataset. Consequently, high within-context accuracy should not be interpreted as evidence of cross-climate generalisability. A similar limitation applies to temporal and operational heat-load forecasting, in which [73] showed that short-term heat-load prediction depends on historical load, meteorological variables, system parameters, and feature selection. Its findings support the importance of contextual inputs, but the study does not test transfer between climatic regions.

Recent work further confirms the importance of weather information, such as [109]; the authors found that residential energy performance was influenced by variables including temperature, humidity, wind speed, and solar radiation, and used SHAP to examine their contribution. However, the model was developed using residential data from York, UK. This provides detailed evidence of weather sensitivity within one location but leaves open the question of whether the same feature relationships remain stable under substantially different climatic regimes.

Building representation can also affect generalizability, as indicated by [110]; the authors incorporated both image-based floorplans and vector-based building parameters in a stacking ensemble model for residential building performance. The model showed improved accuracy and generalisation relative to the tested base models, thus suggesting that representations of building configuration can strengthen prediction. Nevertheless, this form of within-dataset generalisation is different from demonstrating transfer across fundamentally different building typologies or climate zones.

Climate dependence is also reflected in building regulations, as documented by [107], which documents separate residential energy efficiency standards for Northern, Central, and Southern China, corresponding to distinct heating and cooling conditions. This reinforces the broader modelling implication that thermal-performance requirements are geographically conditioned and that a single climatic representation may be inappropriate for models intended for wider deployment.

The evidence indicates that building typology and climate should be treated as applicability conditions rather than secondary variables, as studies demonstrate successful prediction within residential, office, lightweight, and other building contexts [50,73,77,108,110], while refs. [53,107,109] show that climate and weather alter the relevance of predictive variables and thermal requirements. A remaining gap is the limited evidence of rigorous cross-climate and cross-typology validation.

4.8. Occupancy Behaviour

Occupancy is a dynamic contributor to building-energy demand because changes in presence and use affect indoor conditions, HVAC operation, and comfort requirements. However, the evidence suggests that occupancy is represented in very different ways across data-driven models. Ref. [31] demonstrates that occupancy can be inferred from measured indoor variables including temperature, humidity, light, and CO_2. This supports the feasibility of occupancy-aware modelling, but it also shows that occupancy estimation depends on the availability and quality of indoor environmental data rather than being a universally accessible input.

A stronger operational integration is demonstrated in [50], where temperature, humidity, movement detection, occupancy, outdoor conditions, and energy consumption were continuously collected and used to update building thermal models and heating control. This contrasts with fixed scheduling approaches because occupancy information was incorporated into real-time control. However, the system required sensing infrastructure, continuous data acquisition, and computational resources, indicating that the benefits of dynamic occupancy modelling are conditional on the availability of suitable building management and sensing systems.

Occupant-related modelling also extends beyond presence or absence. Ref. [111] incorporates resident satisfaction into AI-based home energy management to illustrate that energy optimisation cannot always be separated from user comfort. This creates an important trade-off: strategies that minimise energy consumption may not produce acceptable indoor conditions, while comfort-oriented control may increase energy demand. Occupancy models intended for operational use should therefore distinguish between simply detecting presence and representing occupant preferences or comfort requirements.

Some studies which did not consider occupancy, such as [110,112,113], achieve adequate heating and cooling load prediction performance using building variables. For instance, ref. [110] integrates floor plan and building parameters for residential performance prediction, while occupant behaviour was not accounted for as a central input. Ref. [113] develops fuzzy rule-based systems that balance performance and interpretability in residential energy consumption application. These approaches demonstrate that predictive performance can be achieved for annual thermal load prediction without detailed behavioural representation, but their applicability may be weaker when operational occupancy patterns differ substantially from those embedded in the training conditions.

Overall, the evidence reveals a gap between occupancy-aware operational models and thermal load models dominated by physical or historical variables. Refs. [31,50,111] demonstrate the value of measured occupancy, indoor conditions, and resident preferences. Future work should assess when occupancy information materially improves prediction and control rather than assuming that greater behavioural detail is always necessary. For operational forecasting and HVAC control, dynamic occupancy and comfort information may be important; for early design applications, simpler occupancy assumptions may remain sufficient.

4.9. Sustainable Building Systems

AI-based approaches increasingly support sustainable building performance through energy prediction, design assessment, interpretation, and operational decision-making. Ref. [8] demonstrates the use of ML for improving building-energy prediction and efficiency, while ref. [11] extends this direction toward XAI for sustainable residential design. Ref. [51] further shows that XAI can connect energy-efficient building characteristics with financial outcomes. Together, these studies indicate that sustainable building intelligence can extend beyond prediction accuracy to support design and economic decision-making.

A stronger connection to sustainable operation appears when prediction is linked with interpretable control. Ref. [52] demonstrates cooling-load prediction, while ref. [69] applies interpretable ML within building-energy control to generate simple, understandable rules that are explainable in nature. Ref. [70] further integrates thermal load prediction with rule-based HVAC optimisation. These studies suggest that the value of ML for sustainable buildings increases when predictions can inform understandable operational decisions rather than remaining standalone forecasts.

Sustainability also requires consideration of objectives beyond energy consumption. Ref. [110] integrates daylighting, thermal comfort, and energy consumption, while ref. [111] considers energy efficiency together with resident satisfaction. These approaches highlight trade-offs between energy reduction, occupant comfort, and indoor environmental performance. However, they remain narrower than comprehensive sustainability assessment because carbon, life cycle impacts, and regulatory performance are generally outside their modelling scope.

At the same time, recent thermal load studies [114–117] continue to emphasise improvements in heating and cooling prediction and optimisation. This demonstrates continuing methodological progress but also reveals a gap: improved predictive performance

does not itself constitute broader sustainable building performance. More system-oriented research reflects a gradual transition toward smart building-energy management [118], with ref. [119] extending this direction through optimisation of smart building-energy management systems.

The literature shows a fragmented progression toward sustainable building intelligence. Prediction, explainability, operational control, comfort, economic outcomes, and smart energy management are increasingly represented [8,11,51,52,69,70,115–119], but generally within separate modelling frameworks. Future sustainable building systems should integrate these dimensions more coherently, while broader sustainability claims should require explicit consideration of carbon, life cycle, and regulatory performance.

Table 6 shows the mapping of the 39 studies with the identified themes, and Table 7 illustrates the details of these studies based on several different criteria. Studies in Table 6 may contribute to more than one theme; therefore, the thematic counts are not mutually exclusive.

Table 6. Mapping retained studies with the proposed themes.

Theme Title	Covered Papers	No. of Studies Mapped to Theme	Inclusion Basis
Interpretability	[10–13,17,20,52–56,60,62,69,87,104,109,113]	18	Explicit XAI or interpretability is a core method; interpretable studies are included only when interpretability is explicitly analysed.
Rule Models Scarcity in Thermal Load Prediction	[3,7,8,10,13,56,70,72–75,77,79,80,87–89,113,116,117]	20	Rule induction, fuzzy rules, regression trees, tree ensembles, or rule-based control is a substantive modelling component.
Multi-source Data	[3,7,8,10,11,17,54,55,68,72,75,80,87,89,108–110,115–117]	20	Small/benchmark or restricted datasets, multiple datasets/sources, multimodal sources, or explicit data-size/availability limitations are substantive to the study.
Simulation Tools	[9,53,60,69,77,88,105,108,110]	9	Simulation or virtual data is used directly in the study
Spatial, Design and BIM Factors	[3,9–11,75,77,80,87–89,105,108,110,115–117]	16	Geometry, orientation, floor plan, compactness, area, layout or related spatial design variables are substantive model inputs.
Building Envelope and Material	[3,9–11,75,77,80,87–89,105,108,115–117]	15	Envelope/material variables and insulation properties are substantive inputs.
Building Typology and Climate	[9,53,77,105,108,109]	6	Climate-zone comparison, climate-specific model applicability, weather/climate effects, or a distinctive building typology is a central applicability condition.
Occupancy Behaviour	[17,20,52,88,110,113]	6	Occupancy, occupant behaviour, presence, usage patterns or thermal comfort/human response is explicitly modelled or analysed.
Sustainable Building Systems	[8,11,17,20,52,55,56,60,69,70,72,73,80,110]	14	Operational energy management/control, HVAC/district-heating operation, integrated comfort/energy performance, or sustainable design/management is a substantive application.

Table 7. Summary of the retained papers.

	Study	Year	Target	Dataset Source	ML Methods	XAI/ML	Type of Features	Main Finding
1	Chaganti et al. [3]	2022	Thermal load	UCI Machine Learning Repository; Ecotect simulations	MLP, k-NN, linear regression, Random Forest, GAM; proposed three-Random-Forest voting ensemble (3RF)	ML	Building design/geometry; Envelope/glazing	The proposed ensemble achieved high R^2 for heating and cooling load
2	Benavente-Peces & Ibadah [7]	2020	Other	Public data repositories including UCI, DOE OpenEI, Data.world, Kaggle, World Bank and EU Open Data	Decision tree, Gaussian Naive Bayes, k-NN, LDA, SVC, Logistic Regression and other classifiers	ML	Building characteristics; Climate/location; Energy-use	Decision tree gave the strongest average classification performance
3	El Mghouchi & Udristioiu [9]	2025	Thermal load	Simulated with TRNSYS (Type 155) coupled to MATLAB R2023a for Meknes, Ifrane and Marrakech, Morocco	ANN, decision tree, SVM, ELM, XGBoost, Random Forest, TreeBag, GLR, GPR, linear regression, GAM, KRR and LRR	ML	Envelope/material; Glazing; Ventilation	Integral Feature Selection produced reduced input subsets. SVM was strongest in most test cases
4	Abdel-Jaber & Dirks [10]	2024	Thermal load	UCI Machine Learning Repository; Ecotect simulations	Rule-based classification models, including decision tree and RIPPER	ML	Building design/geometry; Envelope/glazing	Rule-based classification predicted heating- and cooling-load categories
5	Alotaibi [11]	2024	Thermal load	UCI Machine Learning Repository; Ecotect simulations	Elman Neural Network (ENN), Gaussian Process Regression (GPR) and Boosted Trees (BT), with M1–M3 input-feature variants	XAI	Building design/geometry; Envelope/glazing	GPR-M3 gave the strongest overall results. SHAP was used to explain feature effects
6	Zhang et al. [13]	2024	Cooling	Operational data from an office building used as the case study	Clustering decision trees combined with adaptive Multiple Linear Regression	ML	Historical load; Climate/weather; Temporal; Building operation	The interpretable method achieved accuracy comparable to Random Forest and XGBoost and improved prediction accuracy
7	Manfren & Nastasi [17]	2023	Energy load	Hourly data from Procida City Hall, Italy combined with outdoor-air temperature and calendar data	Time-of-Week-and-Temperature (TOWT) piecewise/multivariate linear regression	ML	Energy/load; Climate/weather; Temporal; Building operation	TOWT models achieved RMSE of 20.0–28.5%

Table 7. *Cont.*

	Study	Year	Target	Dataset Source	ML Methods	XAI/ML	Type of Features	Main Finding
8	Meng et al. [20]	2025	Energy load	Loughborough University	K-means and Gaussian-mixture clustering; Random Forest classification; predictive ML/DL models within the sparse interpretable approach	ML	Energy/electrical; Building/household; Occupancy; Temporal; Climate/weather	Occupancy-related household-use demonstrated how contextual household and weather information can support energy prediction
9	Li et al. [52]	2021	Cooling	Operational data from the Building of the International Commerce Centre, Hong Kong	Attention-based sequence-to-sequence Recurrent Neural Network (RNN)	DL	Historical load; Climate/weather; Temporal; Building operation/BAS	Attention-based RNN models improved 24 h-ahead cooling-load prediction over non-attention baselines
10	Chung & Liu [53]	2022	Cooling	U.S. DOE reference office-building models sampled using Latin Hypercube Sampling and simulated across five climate zones	Deep learning load-prediction models with input-importance analysis using SRC, LIME and SHAP	XAI	Building design/envelope; Climate/weather; Internal gains; Temporal	SHAP identified compact sets of influential inputs while maintaining predictive accuracy
11	Dang et al. [55]	2023	Heating	Hourly operational data from an LNG cogeneration district-heating plant in Cheongju, Korea	SVR, MLP, AdaBoost, LightGBM and XGBoost	XAI	Historical heat demand; Climate/weather; Temporal/calendar	XGBoost produced the strongest test performance; XAI highlighted temperature and temporal variables as important drivers.
12	Zdravković [56]	2025	Heating	SCADA data gathered from Substation 17 of a local district-heating system	Gradient Boosting	XAI	Historical heat demand; Climate/weather; District-heating operation; Temporal	Global-importance analyses identified previous heat demand and ambient temperature as major predictors
13	Zhang et al. [68]	2023	Thermal load	Operational data from 3 buildings in Shenzhen, China, with hourly cooling-load and weather data	Six AutoML frameworks: Auto-WEKA, H_2O, TPOT, AutoGluon, FLAML and AutoKeras	ML	Historical load; Climate/weather; Temporal; Building operation	AutoML improved prediction accuracy by 1.10–18.66% over other modelling
14	Hu et al. [70]	2021	Thermal load	Data from a 5-story office building in Tianjin, China	Measured BAS data from a five-story office building in Tianjin, China	ML	Indoor/zone conditions; Climate/weather; HVAC operation; Energy/load	The ANN achieved low RMSE for load demand and energy consumption

Table 7. *Cont.*

	Study	Year	Target	Dataset Source	ML Methods	XAI/ML	Type of Features	Main Finding
15	Bui et al. [75]	2020	Heating	UCI Machine Learning Repository; Ecotect simulations	Genetic-Algorithm-optimised M5Rules (M5Rules–GA)	ML	Building design/geometry; Envelope/glazing	The M5Rules–GA model provided the strongest heating-load prediction
16	Sun & Bi [79]	2021	Heating	Electric heating-load data from users across 12 electric-heating categories	Hybrid CART decision tree regression forecasting model	ML	Historical load; Temporal; HVAC/system; Occupant behaviour; Control/economic	A CART-based model was used for electric heating-load forecasting
17	Lin et al. [80]	2025	Cooling	UCI Machine Learning Repository; Ecotect simulations	Decision tree optimised with Giant Trevally Optimiser (GTO) and Equilibrium Slime Mould Algorithm (ESMA)	ML	Building design/geometry; Envelope/glazing	The optimised DTGT model achieved the strongest reported cooling-load performance
18	Havaeji et al. [87]	2024	Cooling	UCI Machine Learning Repository; Ecotect simulations	Support Vector Machine, Naive Bayes, linear regression and decision tree	ML	Building design/geometry; Envelope/glazing	SVM achieved the highest reported accuracy, followed by decision tree and Naive Bayes
19	Guo et al. [88]	2023	Thermal load	EnergyPlus simulations of typical residential-building cases for Hohhot, China.	LightGBM optimised using a Tree-structured Parzen Estimator (TPE)	ML	Envelope/material; Building design; HVAC/setpoints; Occupancy/behaviour	TPE-LightGBM produced the strongest heating- and cooling-load prediction results
20	Alawi et al. [89]	2024	Thermal load	UCI Machine Learning Repository; Ecotect simulations	SVR, k-NN, Random Forest, MLP, Gradient Boosting and XGBoost	ML	Building design/geometry; Envelope/glazing	Random Forest was best for heating, and XGBoost was best for cooling-load predictions
21	Manfren et al. [104]	2022	Energy load	Electric and thermal energy plus local weather data from a Passive House residential building in the Province of Forlì-Cesena, Emilia-Romagna, Italy	Interpretable regression-based data-driven building-energy models using piecewise linearization and dummy variables	ML	Energy/load; Climate/weather; Temporal; Building operation	The interpretable regression retained good predictive performance

Table 7. *Cont.*

	Study	Year	Target	Dataset Source	ML Methods	XAI/ML	Type of Features	Main Finding
22	Irshad et al. [108]	2022	Thermal load	Simulation dataset for Dhahran, Saudi Arabia, developed in MATLAB from 70 model-building cases	Shuffled Shepherd Red Deer optimisation linked Self-Systematised Intelligent Fuzzy reasoning-based Neural Network (SSRD–SsIF–NN)	ML	Building geometry/configuration; Energy/operation	The proposed SSRD–SsIF–NN reported low MAE and RMSE for heating and cooling loads
23	Roy et al. [115]	2020	Thermal load	UCI Machine Learning Repository; Ecotect simulations	Deep neural network, Gradient Boosted Machine, Gaussian Process Regression, Minimax Probability Machine Regression and comparison models	ML/DL	Building design/geometry; Envelope/glazing	DNN produced the best cooling-load while Gaussian Process Regression produced the best heating-load predictions
24	Küçüktopcu [105]	2023	Thermal load	EnergyPlus simulations of 5 broiler-house models across four Turkish climates	Random Forest, artificial neural network and Support Vector Regression	ML	Building geometry; Envelope/material; Climate/weather; Indoor conditions	Random Forest provided the strongest results among the compared models
25	Pachauri & Ahn [116]	2022	Thermal load	UCI Machine Learning Repository; Ecotect simulations	Regression Tree Ensemble with least-squares boosting; SRTE; compared with stepwise regression and GPR	ML	Building design/geometry; Envelope/glazing	The proposed SRTE reduced RMSE for heating and cooling loads
26	Mohebbi & Afzal [117]	2024	Thermal load	UCI Machine Learning Repository; Ecotect simulations	Extra Trees Regression, decision tree regression and SVR, combined with Tyrannosaurus Rex Optimisation Algorithm (TROA)	ML	Building design/geometry; Envelope/glazing	Optimised Extra Trees produced the strongest reported heating-load
27	Iram et al. [109]	2025	Energy load	UK Government Energy Performance Certificate detached houses in York, UK	Conventional ML models plus deep neural networks, including a residual/attention-enhanced DNN	XAI	Building/EPC characteristics; Climate/weather; Energy/economic; Temporal	Random Forest was the strongest model; SHAP was used to quantify how weather variables influenced the energy-efficiency predictions

Table 7. *Cont.*

	Study	Year	Target	Dataset Source	ML Methods	XAI/ML	Type of Features	Main Finding
28	Gorzałczany & Rudziński [113]	2024	Energy load	Kaggle 'Energy Consumption Prediction' dataset	Fuzzy Rule-Based Prediction Systems with multi-objective evolutionary optimisation (generalised SPEA2)	ML	Building characteristics; Climate/weather; Occupancy; HVAC/energy systems; Temporal	The fuzzy rule-based systems improved interpretability and transparency
29	Yan et al. [110]	2024	Energy load	RPLAN dataset with energy-performance outputs using building/climate simulations	Stacking ensemble learning	ML	Spatial/layout; Building design; Envelope/glazing; Climate/weather	The stacking ensemble reduced MAPE and supported joint prediction of daylighting, thermal comfort and energy consumption.
30	Zhang & Chen [60]	2024	Cooling	Virtual building case study based on the U.S. DOE Reference Small Office Building	Machine learning-based model predictive control with Shapley-value attribution and LLM-based explanation	XAI	Building/HVAC state; Control/setpoints; Demand response/power constraints	Combining Shapley values with an LLM was useful to generate human-understandable explanations of opaque precooling-control decisions
31	Zhang et al., [69]	2024	Cooling	Virtual building co-simulated with machine-learning control for an MPC-based precooling/demand-response case study	ML integrated with Shapley-value attribution and LLM in-context learning	XAI + LLM	Building/HVAC state; Control/setpoints; Demand response/power constraints	The approach combined XAI with LLM to provide human-understandable explanations of ML control decisions
32	Bhandary et al. [12]	2024	Energy load	Smart-metre measurements collected in the authors' apartments in Bangalore, India	Multiple regression models; best-performing model interpreted with LIME and SHAP	XAI	Electrical/energy; Historical energy; Temporal	LIME and SHAP provided local and global explanations of the selected model
33	Pham et al. [8]	2020	Energy load	Building Data Genome Project	Random Forest, M5P and Random Tree	ML	Historical energy/load; Temporal	Random Forest outperformed M5P and Random Tree and provided models with low MAE

Table 7. *Cont.*

	Study	Year	Target	Dataset Source	ML Methods	XAI/ML	Type of Features	Main Finding
34	Zara et al. [77]	2025	Thermal load	Simulated dataset for lightweight buildings under a subtropical climate.	CART Decision Tree with sensitivity analysis	ML	Envelope/material; Building design/configuration	CART identified combinations of thermophysical parameters associated with heating/cooling energy performance
35	Zhang et al. [72]	2021	Cooling	Data from a commercial building with an ice-storage air-conditioning system.	Gradient Boosting Decision Tree (GBDT) with grid-search tuning; compared with SVM and DNN	ML	HVAC/system operation; Cooling-load variables	GBDT outperformed SVM and DNN with lower reported MAE
36	Gong et al. [73]	2020	Heating	Data from a heat-exchange station in Xiqing District, Tianjin, China	Discrete wavelet transform with Extremely Randomised Trees and Gradient Boosting Decision Trees; LASSO/Pearson feature selection	ML	Historical load; Temporal; District-heating operation; Climate/weather	The DWT–ETR model achieved the strongest one-hour-ahead heat-load prediction
37	Yan et al. [74]	2025	Heating	UCI Machine Learning Repository; Ecotect simulations	Decision tree with metaheuristic optimisation, including DT + FOX variants	ML	Building design/geometry; Envelope/glazing	Decision tree achieved high R^2 and low RMSE
38	Neubauer et al. [54]	2025	Heating	MFRB: measured heat-meter data from a multifamily building in Berlin, Germany, plus Open-Meteo weather. DHS: public district-heating data from Niš, Serbia	Encoder–Decoder deep learning multi-step forecasting model	XAI	Historical load; Climate/weather; Temporal	Deep SHAP feature selection reduced NRMSE and training time
39	Devanathan et al. [62]	2025	Energy load	UCI Machine Learning Repository	Holt–Winters time-series decomposition + XGBoost; baseline comparisons with Random Forest and other ML models	XAI	Electrical/energy; Temporal/time-series	The HW + XGBoost + XAI approach achieved high R^2 and low RMSE, while XAI analyses explained feature contributions across multiple forecasting scales

5. Conclusions

This systematic review shows that research on interpretable thermal load prediction is unevenly developed across the identified themes. A PRISMA-guided process was used to select the relevant studies, which were then analysed using a structured thematic approach. For each retained study, information was extracted on the building context, thermal load target, dataset and source, ML method, interpretability/XAI approach, feature domains, and main findings. Recurring concepts were grouped into higher-order themes, with studies allowed to contribute to more than one theme where appropriate. The strongest emphasis was on rule-based models, multi-source data, interpretability, and spatial and envelope-related factors. In contrast, building typology and climate adaptability and occupancy behaviour were less represented. This suggests that methodological development has progressed faster than research on human behaviour and model transferability across different building and climate contexts.

A key pattern across the Interpretability of ML models theme is the distinction between post hoc and intrinsic interpretability, together with the additional knowledge that can emerge when the thermal load prediction problem is reformulated from continuous regression into classification. XAI approaches can reveal feature interactions and temporal effects in complex classification models, whereas models with rules, like rule-based classifiers and decision trees, expose decision logic directly through explicit paths or human-readable rules. By converting continuous heating and cooling loads into meaningful thermal load levels, the ML model can reveal an additional layer of natural knowledge that is less visible in a purely numerical prediction. Engineers can then identify combinations of characteristics related to buildings, weather, HVAC, etc., associated with particular load states and use these relationships to support design decisions and optimisation. This creates a useful distinction between predicting how much thermal load is expected and explaining why a building falls into a particular thermal load level. Hybrid and deep learning models may offer predictive capability, but rule-based classifiers can provide more directly usable engineering knowledge.

A second pattern emerges from the overlap between multiple themes, including Simulation Tools, Multi-Source Data, Building Envelope and Material Factors, Spatial and Geometric Design Factors, and Building Typology and Climate Adaptability. Many studies rely on simulated or benchmark datasets because sufficiently detailed real-world data for annual thermal load estimation, as well as high-resolution operational data, can be difficult and expensive to obtain. For early design applications, this presents a particular limitation because annual or seasonal heating and cooling estimation requires comprehensive information on building configuration, geometry, envelope properties, materials, structural characteristics, climate, and building typology, while measured datasets that combine these variables with corresponding thermal load outcomes remain limited.

Simulated datasets provide an important and scalable source for model development by allowing building characteristics and operating conditions to be varied systematically. However, their applicability to real buildings depends on the accuracy and completeness of the assumptions and input parameters used in the simulation. Differences between simulated and actual buildings in envelope properties, occupancy, HVAC operation, weather conditions, controls, and other contextual factors can produce a model-to-reality gap and reduce transferability to unseen buildings. Consequently, explanations derived from models trained primarily on simulated data may accurately describe relationships within the simulated parameter space but may not fully represent the physical and operational relationships observed in real buildings.

The data challenge differs for operational thermal load analysis. Daily or hourly optimisation depends on continuous measurements of weather, occupancy, indoor conditions,

HVAC operation, setpoints, equipment states, and historical load behaviour. Collecting these data from real buildings requires sensors, metering infrastructure, calibration, maintenance, data integration, and often BIM or IoT connectivity, making large-scale operational datasets expensive to establish and maintain. Annual design-stage estimation is therefore constrained mainly by the scarcity of comprehensive real datasets linking design features to annual heating and cooling demand, whereas operational forecasting is constrained by the cost and complexity of acquiring sufficiently granular real-time data. These distinct limitations suggest that annual design estimation and operational optimisation require different data strategies rather than being treated as a single thermal load modelling problem.

The same themes also expose a generalisability problem. Climate, building typology, orientation, envelope composition, structural configuration, and HVAC characteristics alter thermal load relationships across applications. Models developed for one climate or building type may therefore lose validity when transferred elsewhere. This supports the development of climate-adaptive and typology-aware interpretable models, but such contextualisation depends on richer input data and more consistent representation of physical building characteristics across datasets.

A further gap concerns the limited use of progressive engineering design approaches. The Spatial and Geometric Design Factors, Building Envelope and Material Factors, and Building Typology and Climate Adaptability themes show that the information available to engineers changes as a project progresses. Early design decisions may initially rely on climate, building type, floor area, orientation, and form, followed by structural configuration, envelope materials, glazing, insulation, and eventually HVAC system specifications. However, much of the reviewed literature evaluates models using fully assembled feature sets rather than modelling the progressive availability of engineering information.

This is particularly important when distinguishing annual or seasonal thermal load estimation from operational thermal load forecasting. Annual design-oriented estimates can support early comparison of alternatives, envelope evaluation, and preliminary HVAC sizing before a building becomes operational. At this stage, data-driven models trained on large simulated building stocks, such as ResStock-type datasets, could offer a cost-effective alternative to repeatedly constructing detailed simulation models, particularly when only partial design information is available. Their usefulness, however, depends on whether the simulated data adequately represents the geometric, structural, material, climatic, and typological variables identified across the themes. Operational thermal load analysis addresses a different engineering objective and depends more heavily on hourly or sub-hourly weather, occupancy, setpoints, HVAC behaviour, sensor measurements, and lagged load information for forecasting, control, and day-to-day optimisation.

Other gaps are evident in the Occupancy Behaviour and Human Factors and Sustainable and Operational Building Systems themes. Occupancy remains sparsely represented despite its direct influence on internal heat gains and HVAC demand. Real-time measurements and spatial and structural information are also not yet routinely integrated well with interpretable ML. Similarly, sustainability-oriented studies remain limited in their inclusion of embodied carbon, lifecycle indicators, regulatory requirements, and measurable sustainability KPIs alongside thermal load prediction.

The evidence suggests that the main research need is not simply focused on predictive performance in thermal load prediction. A more important direction is the development of progressive and interpretable thermal load models that reflect the sequence of engineering decisions and distinguish between design-stage annual estimation and operational forecasting. Such models should incorporate progressively richer information on building configuration, structural characteristics, materials, HVAC systems, and other relevant factors while preserving transparent model logic. For early design applications, this would

allow engineers to update annual heating and cooling estimates as new design information becomes available and use the results to compare alternatives and support preliminary HVAC sizing. For operational applications, models should instead incorporate the temporal and behavioural information required for daily or hourly optimisation.

The findings suggest that the practical relevance of interpretable thermal load modelling is strongest where model transparency is linked with building design factors, envelope and material characteristics, operational data, and rule-based or XAI-supported decision processes. These findings indicate that architects and engineers may benefit from more transparent evidence on the combinations of building characteristics associated with heating and cooling demand, while utilities and building operators may gain value from interpretable operational and demand-response models.

Future research should therefore place greater emphasis on cross-typology and cross-climate validation, richer occupancy and behavioural data, and improved integration of IoT, BIM, and real data. Hybrid modelling approaches and more standardised evaluation approaches may also help strengthen the transferability and practical applicability of interpretable thermal load models across diverse building contexts.

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