Machine Learning-Driven Optimization of Building Enclosures for Moisture Durability and Thermal Performance

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ABSTRACT

The design of moisture-durable building enclosures often involves an iterative process of selecting the materials for the specific exposure conditions to meet the performance requirements. While hygrothermal simulations are commonly used to evaluate moisture durability, they often require advanced expertise for proper implementation. Machine learning (ML) provides a promising alternative by streamlining the design process and minimizing the reliance on complex simulations.

This study presents a machine learning-based approach for predicting moisture durability in residential wall assemblies. The ML model was trained to estimate the mold index and maximum moisture content of various layers under typical exposure conditions. The model achieved a high predictive accuracy, with a coefficient of determination (R^2) exceeding 0.90 when compared to traditional hygrothermal simulations on materials that were not part of training the ML model.

Building on these results, the ML model was developed into a practical tool for optimizing wall assembly designs. This tool allows users to automatically optimize material selections based on energy, moisture, cost and other performance criteria. By incorporating multi-objective optimization, the tool identifies configurations that minimize the cost function while maintaining moisture safety and code-compliant thermal performance. Additionally, it provides insights into how material choices influence assembly durability, and moisture and thermal performance. The tool will be implemented in the Building Science Advisor (BSA), a free online too, to enhance its performance and provide more granularity on the results.

This research highlights the potential for ML-driven tools to simplify the design of high-performance building enclosures, offering architects and engineers a faster, more efficient way to balance critical performance factors.

INTRODUCTION

The construction industry faces increasing challenges in achieving high-performance building enclosures that balance

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moisture durability, thermal performance, and resource intensity. Though effective, traditional methods, including hygrothermal simulations, are complex and time-consuming. The application of machine learning (ML) offers a streamlined alternative that can simplify the design process and improve outcomes.

Machine Learning (ML) enhances building design by optimizing materials and performance. Researchers have applied ML techniques to model hygrothermal performance, as demonstrated by Tzuc et al., who trained a neural network using weather data to predict vegetative façade behavior (Tzuc et al. 2021). Similarly, Tijskens et al. evaluated different neural networks to predict masonry wall hygrothermal performance, identifying convolutional neural networks as the most effective approach (Tijskens et al. 2019, I; Tijskens et al. 2019, II). Salonvaara et al. (2021) implemented ML models, such as artificial neural networks and gradient-boosted decision trees, to simulate moisture durability in building materials with high accuracy. Beyond hygrothermal performance, Kim et al. (2018) leveraged ML to optimize double-skin façades for both thermal performance and aesthetics, demonstrating its versatility in architectural design. Additionally, ML has been used to select phase change materials (PCMs) for thermal storage, reducing the time and effort required for material selection (Bhamare et al. 2021). These studies highlight how ML enables architects and engineers to streamline complex analyses, making it an invaluable tool for optimizing building enclosure performance.

ML can significantly enhance the design process of high-performance buildings by reducing reliance on time-intensive simulations and expert-driven iterative design. Traditional building simulation methods require expert knowledge and extensive computing time to evaluate the effects of materials and climate conditions on performance. ML, however, can recognize patterns in vast datasets and quickly generate optimized material and system configurations that balance moisture durability, thermal efficiency, and other performance targets. Unlike conventional simulations, which require predefined material properties before evaluating system performance, ML can work in both directions – either by analyzing the performance with existing material properties or by defining performance requirements first and identifying suitable materials to meet the performance requirements accordingly. This capability enables a more flexible and efficient design workflow, allowing designers to explore a broader range of material combinations and building envelope solutions while ensuring compliance with performance criteria. The option to identify suitable materials to meet the performance criteria could be used to determine material properties that the scientists and engineers need to aim for.

The Building Science Advisor (BSA) (Boudreaux et al., 2018, Desjarlais et al., 2021 and 2022) allows users to evaluate thermal and moisture performance of wall assemblies without needing hygrothermal simulation expertise. The user selects layers and thicknesses from drop-down menus. The results are displayed immediately with written guidance about thermal and moisture performance. The tool allows for designing walls for new construction and buildings that need to be retrofitted and provides building science knowledge and advice. If the performance is unsatisfactory the tool provides reasons why and guides the user with suggestions to improve the assembly.

The current version of the Building Science Advisor (BSA) includes a database of previously simulated cases but is limited in the range of materials and layer thicknesses it can evaluate. Figure 1 shows the user interface of BSA with inputs and performance outputs options. If users select materials or configurations outside the pre-simulated dataset, BSA cannot provide results. To overcome this limitation, an ML-powered optimization tool has been developed to enhance BSA by automating material selection based on energy efficiency, moisture durability, and life cycle impact, and even cost if data are available. Instead of relying solely on predefined simulations, the ML approach uses material properties as inputs to predict performance for various configurations. This enables multi-objective optimization, allowing the tool to identify wall assemblies that balance moisture safety, thermal compliance, and other user's requirements. By integrating ML, BSA can offer architects and engineers more precise and adaptable recommendations, improving the design of high-performance enclosures for both new construction and retrofits. While the existing BSA tool relies on a database of pre-run simulations, which can be viewed as a simple look-up table, this approach is inherently limited to the exact configurations in the database. Any deviation in material type or thickness requires a new, time-consuming hygrothermal simulation. This research addresses this gap by developing a predictive model that generalizes across a continuous/discrete space of material properties. The Artificial Neural Network (ANN) provides a powerful and flexible alternative to basic look-up tables by learning the complex, non-linear relationships between wall assembly inputs and performance outputs. This allows for rapid performance prediction for designs and enables a robust optimization framework, significantly accelerating the design process compared to traditional simulation-based approaches.

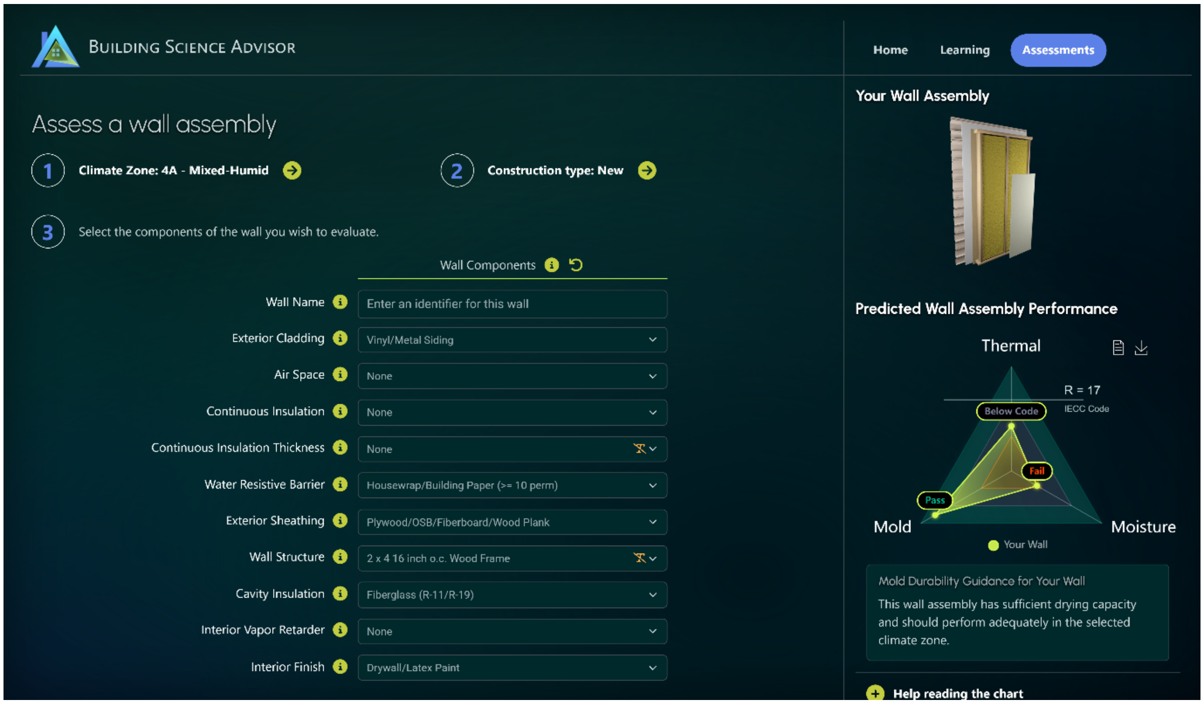


Figure 1. Building Science Advisor with user input and performance outputs.

MACHINE LEARNING INTEGRATION

Tool implementation

The developed tool is designed to be user-friendly, allowing designers and engineers to input project-specific data and receive optimized material and assembly recommendations. The tool provides visualizations of performance trade-offs and sensitivity analyses, offering insights into how different material choices impact overall performance. Integrating this tool into the Building Science Advisor (BSA) platform enhances its utility, providing a holistic view of building enclosure performance.

Data collection and pre- and post-processing

The foundation of any ML model lies in the quality and extent of the data used for training. For this study, an extensive dataset of residential wall assemblies was compiled, capturing various parameters, including material properties, indoor and outdoor climatic conditions, and moisture performance data. The data set originated from hygrothermal simulations that were pre-processed to provide descriptive properties of assembly set up for each simulated case. The simulations were post-processed to provide information that designers would use to decide whether the wall assembly is acceptable and well-performing. Permutations of different cladding, continuous insulation, water-resistive barrier, exterior sheathing, cavity insulation, and vapor retarder options were used to create about 60 000 simulation cases. The materials were selected such that the range of properties would cover typical materials in construction. Post-processing outputs were mold growth index (Ojanen et al., 2010) at critical layers of the walls, and the maximum annual moisture content of the exterior sheathing. Additionally, the U-value of the simulated wall assemblies was calculated to help evaluate code compliance or user's requirements for thermal efficiency.

ML Model Architecture

As shown in Figure 2, the primary inputs to the model are the physical properties of the materials in each layer of the wall assembly. These include such as material type, thickness, thermal conductivity, and vapor resistivity. The model also considers climatic conditions for different geographic locations. The model is trained to predict two key moisture durability indicators: the Mold Index (MI) at critical material interfaces and the maximum Moisture Content (MC) of the exterior sheathing. These outputs were selected as primary metrics used by building scientists to assess moisture-related risks.

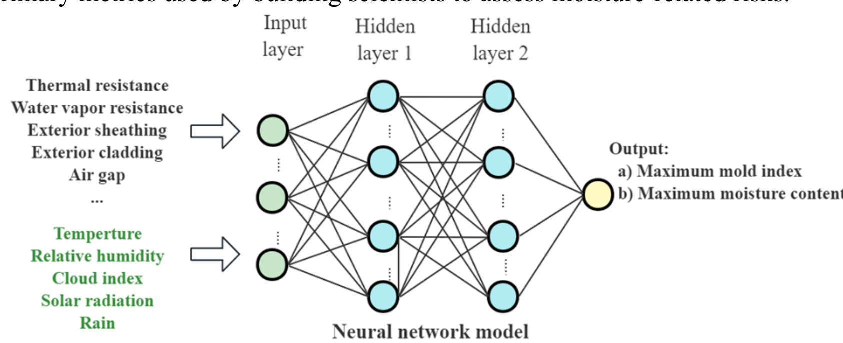


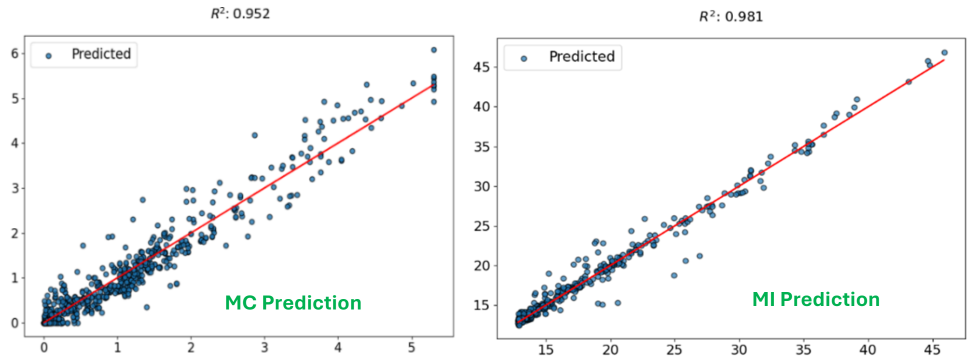
Figure 2. Neural network model

An Artificial Neural Network (ANN) was selected as the predictive model due to its proven ability to approximate complex, non-linear relationships. An ANN provides superior generalization across the continuous space of input variables, making it more suitable for an optimization-focused tool in this study. The ANN architecture consists of an input layer, two hidden layers, and an output layer that predicts the MI and MC values. This multi-layer structure allows the model to learn hierarchical features from the input data, leading to more accurate predictions. Two separate ANN models were trained: one for predicting the mold index and another for predicting moisture content.

ML Model training and validation

The models were trained on the simulation dataset and validated using a 10-fold cross-validation technique to ensure robustness and prevent overfitting. This process involves partitioning the dataset into ten subsets, training the model on nine of them, and testing it on the remaining one, repeating this process until each subset has been used for testing.

The model's predictive accuracy is high, with an average coefficient of determination (R^2) exceeding 0.95 across the validation folds. Figure 3 shows scatter plots comparing the model's predictions for Mold Index and Moisture Content against the actual values from the hygrothermal simulations. The tight clustering of points around the diagonal line (representing perfect agreement) demonstrates the model's ability to accurately replicate the simulation results. These results confirm that the trained ANN models are reliable surrogates for the time-consuming hygrothermal simulations, enabling the rapid performance predictions for the optimization framework.



Fold	R^2
1	0.974
2	0.957
3	0.985
4	0.986
5	0.992
6	0.989
7	0.995
8	0.981
9	0.974
10	0.983
Average	0.981

Figure 3. Example machine learning (ML) model testing results through a 10-fold cross-validation on training dataset

Multi-objective optimization

The optimization framework integrates the ML model with Particle Swarm Optimization (PSO) techniques to identify optimal configurations for wall assemblies. PSO efficiently explores various material selections, balancing durability and thermal performance based on machine learning predictions. Each particle represents a potential wall assembly configuration, exploring multiple design choices iteratively. By managing both continuous and discrete variables, the optimization process reflects real-world constraints, ensuring adaptable and applicable design solutions.

This approach allows for the rapid evaluation of thousands of potential wall assembly configurations to find solutions that balance multiple performance objectives. Mathematically, the multi-objective optimization problem can be stated as:

$$\text{Minimize } F(x) = [f_1(x), f_2(x), \ldots, f_k(x)] \tag{1}$$
$$\text{s.t. } g_j(x) \leq 0,\ j = 1,2,\ldots,m$$
$$x_{min} \leq x \leq x_{max}$$

Where x is a vector of design variables (e.g. choice of materials, thickness for certain layers,), $f_i(x)$ are the objective functions for different terms such as mold index, maximum moisture content, U-value, and cost and other performance targets. $g_j(x)$ are constraints (e.g., upper limit on mold index, maximum moisture content, or minimum U-value requirement), x_{min} and x_{max} denote allowable bounds for each design variable.

A key feature of the framework is its adaptable objective function. Each objective is integrated into the cost function according to specific requirements. Some examples are:

- Thermal Performance (U-value): The U-value is calculated based on the cumulative thermal resistances of the wall components. Different U-value requirements are enforced for commercial and residential buildings based on different climate zones. If the computed U-value exceeds the target limit, a penalty is added proportionate to the violation magnitude.
- Moisture Performance: The machine learning model predicts the mold index (MI) and maximum moisture content (MC) for each candidate assembly. If these exceed acceptable limits (e.g., mold index > 2 or MC% > 20), a penalty is added to the cost function, or the solution is rejected. Alternatively, the user can define a soft constraint where solutions exceeding the limit are still evaluated but heavily penalized.
- Other constraints: Other cost functions can be introduced. For example, the total cost of materials can be added as another objective or as part of a weighted sum with moisture and durability goals.

The optimization tool effectively manages continuous and discrete variables, reflecting practical design constraints. Particle Swarm Optimization (PSO) is employed as the optimization engine in the designed framework. PSO uses a swarm of particles (candidate solutions) that move through the design space, guided by their own best positions and the global best position found so far. PSO can handle continuous variables (e.g., layer thickness) efficiently and can also be adapted for mixedvariable problems. In this approach, each particle represents a candidate wall assembly configuration defined by its position (i.e., the set of design variables) and a velocity vector that dictates the search direction.

Two trained neural network models serve as predictors within the framework: one estimates the mold index and the other predicts the moisture content. These models are incorporated directly into the objective function to provide immediate feedback on moisture performance for any candidate solution. As the PSO algorithm iterates, the predicted MI and MC values inform the penalty terms within the cost function, ensuring that only configurations satisfying the durability criteria are favored. This integration significantly reduces the reliance on complex simulations and expedites the iteration process.

Figure 4 illustrates the workflow for optimizing wall assemblies while allowing users to pre-select certain layers. The optimization process begins by allowing users to pre-select certain layers (e.g., specific exterior cladding, water-resistive barrier, and sheathing board types). After fixing certain layers, the user may choose which remaining parameters to optimize, such as:

- Discrete parameters: e.g., material type of the water-resistive barrier, vapor barrier, continuous insulation, cavity insulation, and exterior sheathing.
- Continuous parameters: e.g., material thicknesses for continuous insulation, cavity insulation, and exterior sheathing.

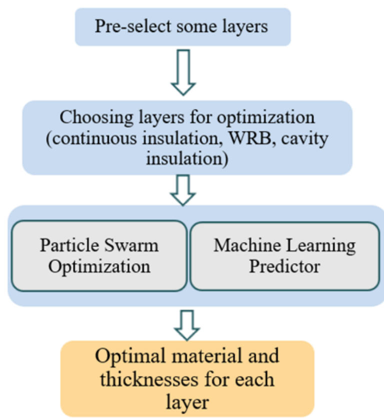


Figure 4 Example optimization workflow

Figure 5 is an example convergence plot from the PSO-based optimization process. For the selected layers, the user specifies upper and lower bounds for thickness (for continuous variables) and selects permissible material types (for discrete variables). Once these choices are made, the PSO is applied with the machine learning predictors (for mold index and moisture content) to find the optimal configuration that satisfies the performance criteria, such as limiting mold index, meeting required U-values. In this process, pre-selection of layers effectively reduces the dimensionality of the optimization problem, making it more computationally efficient and easier to focus on critical variables. The PSO algorithm utilizes machine learning predictions to efficiently navigate the search space and identify optimal solutions that balance key performance objectives. By fixing certain layers in advance, users can ensure that design elements with regulatory constraints remain unchanged, while still exploring innovative ways to improve the wall assembly's overall performance. Figure 5 shows how different design variables (e.g., thicknesses for cladding, exterior sheathing, cavity insulation, and continuous insulation) evolve over the iterations, along with the corresponding cost, mold index, moisture content, and U-values for each candidate solution (particle).

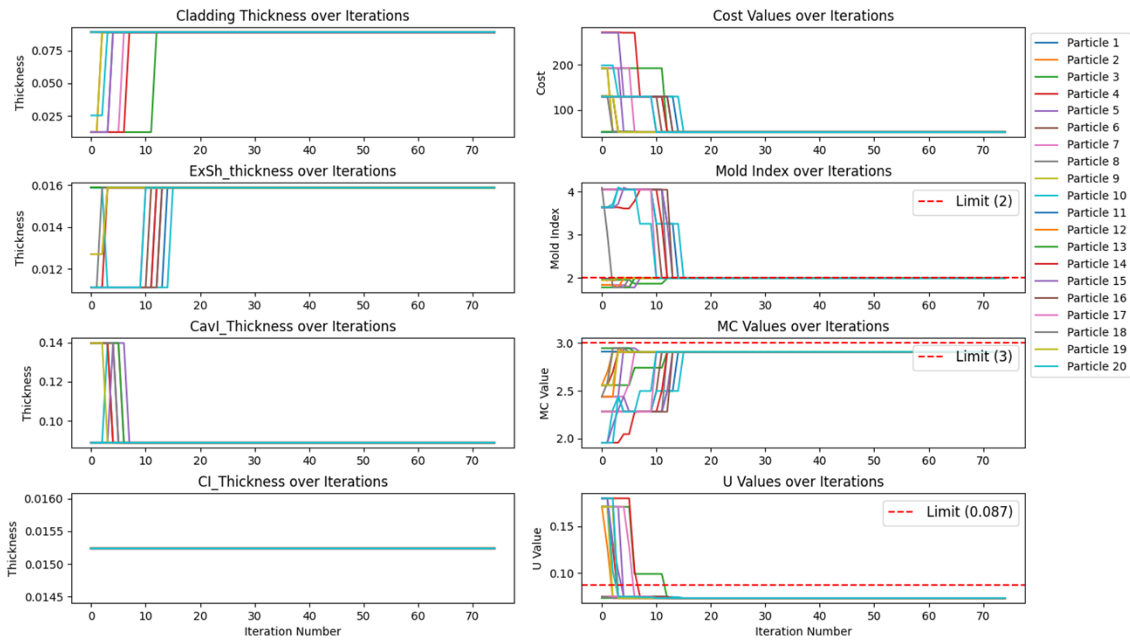


Figure 5 Example convergence process of the optimization, illustrating how variables such as thickness, cost, mold index, MC values, and U-values evolve over iterations for different particles

EVALUATION AND RESULTS

Case study analysis

Case studies across various climates demonstrated the ML tool's effectiveness, with optimized designs showing lower mold indices and moisture content. As shown in Figure 6, two case studies were conducted in two different climate zones with different U-value requirements.

Pre-selected
Original Sample
Optimized

- Pre-selected: fiber cement siding, OSB
- Selecting the right materials and thicknesses for continuous insulation, WRB, VB, and cavity insulation

Exterior Sheathing Material	WRB	VB	Continuous Insulation	Cavity Insulation	ExSh_thickness	CI_thickness	Cavl_Thickness	Mold Index	U
OSB	50 perm	None	None	fiberglass insulation	0.00952	0	0.0889	0.095	0.05927
Cladding Material	5 perm	Ploy	EPS	Air	0.011125	0.01524	0.01397	0.067	0.06335
Fiber Cement	10 perm	Kraft	XPS	Spray foam	0.0127	0.0127			
	0.5 perm	5 Perm	Min. Fiber	ConcCMU4 (ext)	0.02	0.0254			
		SVR			0.0158	0.0381			
					0.016	0.0508			
					0.019	0.0762			

Climate Zone 5A Cold
Syracuse NY
U<0.065

Exterior Sheathing Material	WRB	VB	Continuous Insulation	Cavity Insulation	ExSh_thickness	CI_thickness	Cavl_Thickness	Mold Index	U
OSB	50 perm	None	None	fiberglass insulation	0.00952	0	0.0889	0.114	0.05927
Cladding Material	5 perm	Ploy	EPS	Air	0.011125	0.01524	0.01397	0.394	0.05292
Fiber Cement	10 perm	Kraft	XPS	spray foam	0.0127	0.0127			
	0.5 perm	5 Perm	Min. Fiber	ConcCMU4 (ext)	0.02	0.0254			
		SVR			0.0158	0.0381			
					0.016	0.0508			
					0.019	0.0762			

Climate Zone 6A Cold
Minneapolis MN
U<0.057

Figure 6 Example optimization results for Syracuse, NY, (Climate zone 5A) and Minneapolis, MN (Climate zone 6A).

The result shows the comparison of the original and the optimized wall assemblies for each climate zone. Fiber Cement Siding and OSB Sheathing were fixed in both case studies based on user's design preferences. The tool was permitted to select materials and thicknesses for the continuous insulation (CI), water-resistive barrier (WRB), vapor barrier (VB), and cavity insulation. As shown in the figure, each optimized solution features unique thicknesses and material choices for these layers, demonstrating the tool's search for an improved design tailored to each climate zone's U-value requirement. Across both zones, the predicted mold index and the maximum moisture content in the optimized designs are lower than in the original samples, indicating enhanced moisture durability. Each optimized design also meets its respective U-value limit (defined by the user for commercial buildings) (0.065 for 5A and 0.057 for 6A). The tool's adaptive feature allows it to identify optimal trade-offs among moisture durability, thermal performance, and user's other constraints for each specific climate.

Performance metrics

The performance of the optimized designs was evaluated based on several metrics, including thermal resistance, moisture content, and life cycle impact. The optimized designs consistently outperformed baseline designs balancing these performance targets. The tool's ability to provide rapid and accurate predictions significantly reduces the time and expertise required for design iterations. The integration of this ML optimization tool into the Building Science Advisor has significant implications for the construction industry. By automating the selection of wall assembly materials based on energy efficiency, moisture durability, and users' other constraints, this tool enables architects, engineers, and builders to make more informed design decisions. It modernizes the evaluation of competing objectives, ensuring that building envelopes meet thermal and moisture performance requirements while minimizing use of resources. This advancement not only enhances the efficiency of new construction and retrofit projects but also promotes the adoption of novel materials and construction practices, ultimately leading to more durable buildings with low energy cost.

DISCUSSION

Implications for the construction industry and future research directions

The adoption of machine learning and optimization fundamentally changes traditional approaches, allowing for faster, more precise, and more effective design processes that previously relied on more labor-intensive or conventional methods. The integration of this ML optimization tool into the Building Science Advisor automates the selection of wall assembly materials based on thermal, energy and moisture performance, durability and other user's constraints. This tool enables the construction industry stakeholders such as architects, engineers, and builders to make more informed designs to more durable and energy-efficient buildings. While the current study demonstrates the feasibility and benefits of ML-driven optimization, further research is needed to refine the models and expand their applicability. Future work could explore the integration of additional performance criteria, such as acoustic performance and fire safety, into the optimization framework. Expanding the dataset to include a wider variety of building types and materials will enhance the model's robustness.

CONCLUSION

The study presents a novel machine learning-driven approach to optimize building enclosure designs. The developed tool efficiently balances moisture durability, thermal efficiency, and other factors under user-defined constraints. By reducing reliance on extensive hygrothermal simulations, it rapidly provides tailored recommendations for specific climates and building requirements. The case studies demonstrate that the ML-driven optimization tool enhances wall assembly designs by improving moisture resilience, minimizing trial and error, and meeting defined thermal performance criteria. By translating advanced computational insights into practical recommendations, the tool not only streamlines decision-making but also sets a new benchmark for achieving high-performance building envelopes. Integrating this optimization tool into the Building Science Advisor provides industry professionals with an effective resource for simplifying complex trade-offs and fosters data-driven decision-making. Future developments could expand its capabilities to include cost considerations, further enhancing its value for high-performance building design.

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NOMENCLATURE

F	=	Optimized function
f	=	Objective functions for different terms such as mold index, maximum moisture content, U-value, etc.
g	=	Constraints for objective function.

Subscripts

i, j	=	index values

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