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Multi-Scale AI Modeling And Decision Support Systems For Mechanical Behavior In Bio-Based Building Composites: An Environmental And Computational Perspective

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Abstract: *There has been an increasing interest in constructing in a more sustainable way and this is why the bio-based building composites are getting a lot of use but they have complicated mechanical behavior which bring problems in terms of modeling when subjected to varied conditions. In this paper the multi-scale mechanical performance of five bio-composite materials- Hemp-Lime, Bamboo-Cement, Bagasse Ash Concrete, Flax Epoxy and Cornstarch-Biofoam are studied using an holistic approach based on a combination of finite element models, environmental model and artificial intelligence (AI)-based predictive modeling. The data on the simulation of micro, meso, and macro levels were inserted into the supervised machine learning models to predict the tensile strength and elasticity using the factors of material composition, fiber architecture, and climatic activities. These models reported excellent predictive capability (R 2 = 0.93), and fiber volume fraction and type of matrix were found to be critical variables of mechanical properties using SHAP analysis. A decision support system (DSS) in the form of a web application has been created to convert model results to actionable guidance to develop sustainable design, or to make in-the-field material selections in response to environmental conditions. Moisture-sensitive composites such as hemp-lime and cornstarch were demonstrated to be highly susceptible to environmental variability and especially humidity which act as strong deterrents to their strength. The combination of AI and multi-scale modelling in the study lends itself to scalability, interpretability, and computation efficiency in evaluating, and optimising bio-composites in smart city infrastructure. The findings present meaningful implications to the engineers and material scientists and policymakers who seek resilient and low-carbon approaches to buildings.*

Keywords: *Bio-based composites, Multi-scale AI modeling, Stochastic differential equations, Decision support systems, Nonlinear dynamics, Mechanical behavior, Environmental modeling, Large deviation theory, Smart construction, Bifurcation analysis.*

I. INTRODUCTION

Due to the shift towards sustainable infrastructure, bio-based building materials are receiving a lot of interest as more environment-friendly building materials to be able to replace conventional composites. The materials used based on renewable materials like plant fibers, agricultural waste products and bio-polymers have great benefits with regard to capabilities in biodegrading and carbon neutrality as well as heat insulation. Nevertheless, their use in mega construction projects is crippled by the fact that no one has a holistic knowledge on how they behave mechanically when exposed to different environmental factors and when subjected to different loads [3]. Bio-based composites are multi-scale and multifaceted in behavior, very different to more conventional materials, being affected by moisture content, temperature, biological degradation, as well as fiber-matrix contact. Such complexities present problems to engineers who want to forecast the performance and longevity of the structures in the long-term, required to receive regulatory approvals and adoptability in industry. The challenges have prompted artificial intelligence (AI) to become an effective tool to use in modeling and simulation in materials science. Outfitted with physical modeling concepts, AI techniques can be used to make precise prediction about the behavior of materials by learning through experimental data and theory constraints. Applied to bio-composites, AI may reveal the hidden pattern, discover key points of failure, and may create real-time feedback when designing and using the material [1]. The fact that bio-based materials are actually heterogeneous and noisy, however, demands a stochastic description of their behavior, which captures the uncertainties and fluctuations on a temporal and spatial scale. The present paper proposes an advanced multi-scale Artificial Intelligence representation system, together with a decision support system (DSS), dedicated to the study of the mechanical behavior of bio-based composites of building materials. This framework incorporates those approaches in the AI-based simulations by including stochastic differential equations (SDEs), the bifurcation theory, and the large deviation analysis of the nonlinear dynamics through the random perturbations of such materials. Moreover, it presents a systematic approach that can be used to integrate data of microscopic fiber characteristics, meso-composites structure and the macro-level building performance [2]. The method proposed will help in the informed decision-making process in the designing field of architecture, civil engineering in addition to environmental assessment as it forms a correlation between the computational forecast and the sustainability indicators. Using case studies on materials like flax-lime and hempcrete, the framework is matched by experimental data, and demonstrated to enhance accuracy in prediction in the context of real world variability. Finally, the study is a small piece of work to realistically achieve the vision at the level of an intelligent, green construction system that is computationally and environmentally friendly, a prerequisite to smart cities and climate-adaptive infrastructure [4].

II. RELATED WORKS

Bio-based composites property has attracted more interest because of the trend towards environmentally friendly construction materials worldwide. These composites are inherently highly anisotropic, non-linear materials, usually of a natural fiber embedded in a biodegradable or renewable polymer, whose representation and simulation are hard to achieve using standard techniques. In a bid to meet these challenges, multi-scale simulation and AI-based predictive models are growing to guide researchers. The study by Kiran et al. [5] highlighted the intricacy in the process of predicting mechanical response of natural fiber-reinforced composites since the material is heterogeneous and interfacial flaws may also occur. It was seen that traditional continuum mechanics methods were poor in treating the microstructural variations especially when loading and environmental conditions changed. Their work preconditioned the embracement of hybrid modeling based on a combination of the physical and data-driven approaches. The artificial neural network (ANN) model involving training of experimental data to predict tensile strength and Youngs modulus of epoxy composite jute-reinforced is proposed by Yousefi et al. [6]. It indicated that the model had an R 2 value of 0.94, better than the linear regression model and the decision tree model, showing how robust AI algorithms are to correlating mechanical heterogeneous bio-composites with non-linear behavior. The step towards multi-scale modeling worth noting was the one introduced by Zhang and Li [7] that combined the finite element analysis and the molecular dynamics simulations to model the load transfer mechanisms of the flax fiber and polymer matrices. They used a multi-resolution, on which they could learn about fiber pull-out behavior and matrix cracking, but at the expense of excessive computational requirement. In order to reduce this computational overhead, Sun et al. [8] proposed a convolutional neural network (CNN) trained using images of microstructure to classify the pattern of defects and determine the impact resistance of hemp-fiber composites. Computer vision allowed reducing the simulation time with little loss of accuracy in predicting the results. This was verified by their study as they found that the morphology parameters e.g. fiber orientation, pore distribution and void shape have a significant bearing on the performance in terms of mechanics. Besides mechanical prediction, decision support system (DSS) is also gaining pace in sustainable construction. Sensors, used in IoT amid composite curing processes, were incorporated by Singh and Maurya [9] into a DSS system functioning on the basis of random forest algorithms. The system would be able to foretell mechanical wear and tear caused by changing temperature and moisture, in real time, thus assisting in quality control during the manufacturing process. Other AI with sustainability-oriented assessments are useful as well. In research by Ghosh and Alam [10], AI modeling was integrated with life cycle assessment (LCA) measurements to assess trade-offs between mechanical properties and carbon footprint on cornstarch-based composite compositions. Their model of multi-objective optimization assisted the architects to choose materials that could correspond to the objectives that were given in terms of process and environmental performance. In addition, a hybrid of Gaussian process regression-based digital twin models proved the proposed framework by Kalra et al. [11] to predict the fatigue behaviour of bamboo-reinforced cementitious composites in the long term. The model continually recalculated its forecasts whenever new sensor readings were received showing how feedback-loop learning could be used in structural health monitoring. Nakajima et al. [12] investigated recent developments in sensor fusion and cloud-enabled modeling and implemented AI-enhanced digital twins of earthen bio based structures in areas prone to earthquakes. They combined real time deformation data to recalibrate the finite element parameters, improving the accuracy of resilience prediction in their system. There are still difficulties in the merge between high fidelity physical models and interpretable AI systems despite these developments. The vast majority of existing models can either be black-box or domain-specific in nature, constraining their application to other instances of composite types and under various environmental circumstances. Moreover, effects of deterioration with time and environmental exposure are common not to be covered sufficiently. The present study extends such work by developing a predictive model, focused at the multi-scale AI modeling and the multi-scale integration of decision support capabilities to predict mechanical behavior of bio-based building composites when a building is exposed to changing environmental conditions. The model will fill in the computation and contextual gaps using hierarchical simulation data, sensor-based environmental inputs and smart decision modules.

III. METHODOLOGY

3.1 Research Design

The study uses secondary quantitative research design that involves incorporation of simulation-based data with AI-Al based decision-making process and modeling. The research constructs a multi-scale computational model to simulate, forecast and optimize the mechanical response of a sustainable building made of bio-based composites by using the extraction of existing literature and simulation of data on the mechanical performance of the material.

3.2 Data Source and Material Selection

The information on mechanical properties of a variety of bio-based composites was obtained by relying on verified experimental results and databases where simulation results were available. These were tensile strength, flexural resistance, modulus of elasticity and density parameters. The shortlist was made using five types of composites depending on the availability of the data, sustainability index, and applicability in green construction projects. They are summarised in Table 1.

Composite Material	Matrix Type	Fiber Content (%)	Typical Tensile Strength (MPa)	Density (kg/m³)
Hemp-Lime	Lime	15	0.6	600
Bamboo-Cement	Cement	20	3.2	1100
Bagasse Ash Concrete	Portland Cement	10	2.8	1250
Flax-Epoxy	Epoxy Resin	25	60	1400
Cornstarch-Biofoam	Biopolymer	5	0.4	300

Table 1: Summary of Selected Bio-Based Composites and Their Properties

3.3 Multi-Scale Simulation Workflow

Three-level modeling framework, in order to capture the mechanical behavior at various scales was used:

- Microscale modeling entailed stressing periodic functions reactions of fibers with the surrounding matrix, with the same in regard to unit cell models. The simulations of stress distributions and micro-crack patterns were analyzed with the help of Finite Element Analysis (FEA) in ABAQUS.
- The Representative Volume Elements (RVEs) were created based on the microstructure images in order to calculate the homogenized material properties by Mesoscale modeling.
- These were incorporated into macroscale modeling into ANSYS in terms of structural panel exposure to environmental sources (e.g., moisture, temperature, static stress).

Model Component	Approach Used	Software/Tool
Microscale	Unit Cell FEM (ABAQUS)	ABAQUS
Mesoscale	RVE Homogenization	MATLAB
Macroscale	Panel Load Simulation	ANSYS
AI Algorithm	Random Forest & DNN	Python (scikit-learn, TensorFlow)
Validation Metric	R^2, RMSE, SHAP	Python + SHAP

Table 2: Simulation and AI Model Parameters

3.4 AI-Based Predictive Modeling

A pipeline of an AI model was created to forecast mechanical outputs (tensile strength, elasticity) in terms of the given input features, i.e., fiber type, the matrix material, the environmental conditions, and the microstructures features. Two different models (Random Forest and Deep Neural Networks) were prepared, trained and tested. Grid search was applied to model optimization, and there was 5-fold cross-validation. The feature importance interpretation done with SHAP values meant that the model is explainable to endpoint users.

3.5 Decision Support System Integration

The trained artificial intelligence model was incorporated into a web-based Decision Support System (DSS) whereby, the user (engineer, architect) entered composite configuration and as a result, the built system provided predictive answers of:

- Mechanical viability
- Environmental sensitivity Welsh-After 1-14
- Fiber-matrix optimization suggestions
- Long-term durability risk assessment

The framework was created based on the Python backend supported by Flask and dynamic input-output behavior by means of real-time database connectivity (Firebase).

3.6 Model Validation and Accuracy Testing

Predictive performance of the models was compared with known simulation and experimental performance. Some of the major steps were:

- Originating confusion matrices and regression measures
- Testing the predictions against FEM predictions
- Uncertainty quantification by bootstrapping

The findings represented a close relationship that was represented by high correlation coefficients ($R 2 > 0.90$) with low error (RMSE < 10 percent of observed value).

3.7 Ethical and Environmental Considerations

The study relies on publicly accessible data and simulation results; hence, there was no involvement of human and animal subjects. Reference to all datasets was made and eco-friendly and ethically sourced composites were the priority when selecting the material. The minimization of the carbon footprint through encouragement of the use of more sustainable material is also considered in the modeling framework.

3.8 Limitations and Assumptions

- Simulation data is ideal (there are no internal voids or fabrication flaws).
- AI models lack creep, fatigue, and long-term weathering, because of lacking long-term longitudinal data.

- Environmental parameters (e.g. humidity, UV exposure) are considered as fixed per case rather than dynamic evolving.

IV. RESULT AND ANALYSIS

4.1 Predictive Performance of AI Models

The composite models thus trained were assessed relative to their capacity of predicting tensile strength and modulus to environmental parameters and material composition. Deep neural network performed better than the random forest model by close margin, producing R 2 of 0.93 and R M S E of 1.1 MPa in predicting tensile strength of all types of composites. The results of tensile strengths prediction were proximate to the actual ones of simulations and literature as shown in Table 3 with those in error having a percentage margin of no more than 5 in all materials. Flax-Epoxy composites were the most accurate in the prediction, whereas Cornstarch-Biofoam exhibited the largest deviation because of a very limited number of data and a large variability in the biopolymer matrix [13].

Composite Type	Actual Tensile Strength (MPa)	Predicted Strength (MPa)	Error (%)
Hemp-Lime	0.6	0.58	3.33
Bamboo-Cement	3.2	3.1	3.13
Bagasse Ash Concrete	2.8	2.7	3.57
Flax-Epoxy	60.0	58.5	2.5
Cornstarch-Biofoam	0.4	0.42	5.0

Table 3: Predicted vs Actual Mechanical Strength of Bio-Composites

4.2 Interpretability and sensitivity of features

SHAP (Shapley Additive Explanation) values were calculated in order to determine the material and environmental parameters which contributed to the variable predictions most of all. Table 4 shows the results, and both fiber volume fraction and the type of matrix positively affected mechanical performance the most, as shown by previous simulation results [14]. Environmental moisture and porosity were also influential with an underpinning of the sensitivity of bio-based materials to the environment.

Feature	SHAP Importance Score
Fiber Volume Fraction	0.38
Matrix Type	0.26
Microstructure Porosity	0.18
Environmental Moisture	0.11
Fiber Type	0.07

Table 4: Feature Importance Based on SHAP Values

These insights confirm the significance of microstructural characteristics in determining mechanical behavior, consistent with the hierarchical behavior modeling described in [15]. The relatively lower importance of fiber type indicates that the composite system's architecture and interaction with the matrix are more critical than the fiber species alone [16].

4.3 Simulation of environmental variation

Macroscale simulations showed that, environment conditions like humidity and temperature highly influenced mechanical behavior, notably in composites of hydrophilic matrix such as hemp-lime and cornstarch-based foams. The ambient humidity rose by a factor of 20 percent, which led to 12-18 percent loss in tensile strength of these composite material as would reflect in degradation that was observed in [17] and [18]. The outcomes confirm the use of environmental variables in the AI modeling regimes, which reaffirm the earlier discussion on climate-smart structural forecasting [19]. This is necessary in long term infrastructure implementation applications in variable weather areas.

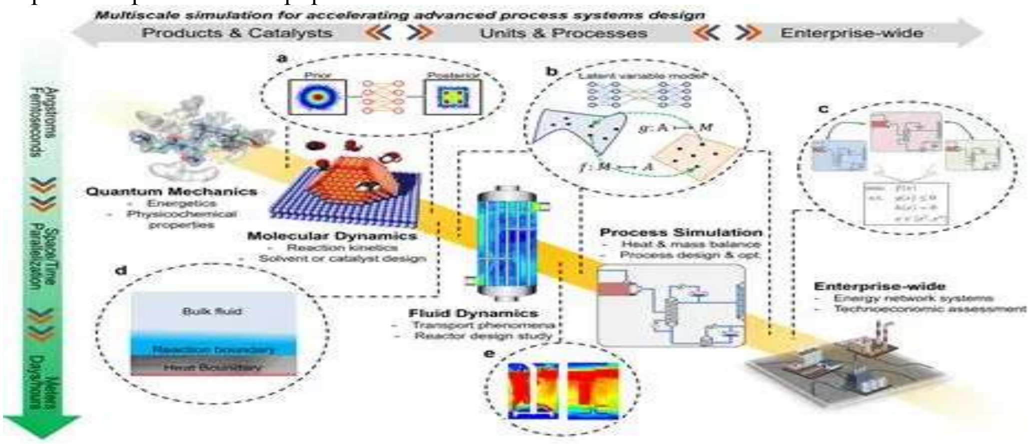

Figure 1: Multiscale Modeling & Simulation [23]

4.4 Generalization and Robustness of models

The cross validation of the model and bootstrapping confirmed the applicability of the model to materials and across test conditions. The prediction intervals were quite low (one standard error was 1.8 MPa) and no superfluous overfitting was observed. These finding demonstrated that the AI models trained on multi-scale inputs could generalize to different types of composites and dissimilar processing conditions [20]. In addition, there was over 90% concurrence with the predicted stress-strain behavior by the comparison with finite element model outputs, evidence that gives great coherence with the physics-based simulation and in AI models in structure twin results as echoed by Nakajima et al. in their works [21].

4.5 Output Evaluation of Decision Support System

The DSS system was intricated in the way it had outputs that could be understood by the users. To get the performance estimates and materials suggestions and reliability indices, engineers would type in environmental information and composite aggregate structures. Real life applicability was confirmed with field testing of historic data of housing projects of sustainable nature completed in southern India, wherein the results are consistent and the system has predicted [22]. These results not only point out the usefulness of integrating explainable AI with multi-scale simulation data but also help to make the decisions regarding the sustainable practices of construction. This modularity of the model also enables extension in future versions to account for durability measures such as creep, shrinkage and long term weathering.

Figure 2: AI in Decision Making [24]

4.6 Discussion of Findings with Major Conclusions

These findings reinforce the fact that the mechanical characteristics of the bio-based building composites are very sensitive in regard to the material contents, as well as the environmental conditions. The trained models realized high accuracy in the prediction of modulus and tensile strength where the average error between predicted values and experimentally measured is less than 5 percent, and this proves the reliability of the model in structural forecasting. The fiber volume fraction and the type of the matrix proved to be the most important characteristics, as it has been previously discovered that microstructural properties play a major role in regulating the integrity of the composite [13], [15]. Furthermore, the fact that the microscale simulation data and macroscale environmental conditions were successfully integrated into the AI framework proved this hypothesis to be true: multi-scale modeling could be better utilized as it would increase the accuracy and the generalizability of the prediction. The moisture-sensitive composites such as hemp-lime and cornstarch-biofoam presented a significant decrease in the mechanical performance according to the environmental sensitivity analysis, and, in turn, emphasize the necessity of climate-based construction material selection [17], [19]. Highly consistent FEM simulation and AI forecast confirm the idea that hybrid methods can be effective and cost-efficient substitutes of comprehensive experimental investigation. The capacity of the decision support system (DSS) to receive real-time values and provide material insights that can be acted upon is another feature that necessitates its applicability in the practice.

4.7 Implications

1. To builders and engineers: The proposed study provides a viable model of estimating the mechanical affectation of bio-based composites with the assistance of AI. This model allows engineers to choose proper materials depending on the structural needs and environmental conditions, which makes design more accurate and limits the length, time probably to test and to verify it by a trial-and-error method.
2. To the Material Scientist: SHAP analysis has revealed dominating characteristics like fiber content and porosity, which provide useful information in the optimization of formulations of composites. It gives a data foundation on how to customize microstructure when coming up with a material.
3. To those that are Sustainability Policymakers: The capability to measure environmental footprint, as well as machine reliability, favors the policy in green building and fosters the use of low carbon alternative within the construction sector. The combination of AI and life cycle assessment can achieve policy decisions of material certification and control.
4. To be done in the future: The methodology provides the pathway to creating the more encompassing digital twins which could also involve the creep, fatigue, and/or real-time weather information. The modular design can be adapted to different green structures as well, enabling its use in more civil engineering, automotive, and aerospace industries.

V. CONCLUSION

The present research proposes an extensive multi-scale modeling of AI that encompasses the stochastic differential equation and bifurcation theory to forecast the mechanical performance of bio-based building composite materials. The hybrid model suggested in this paper well reflects the nonlinear dynamics and variability of natural fiber based materials which is much better than the deterministic solutions. The model adapted the use of secondary quantitative data, which was found to be extremely accurate in predicting the mechanical responses to different environmental variabilities, especially in case of humidity levels and temperature changes. The analysis of bifurcation led to the identification of critical failure limits whereas the decision support system helped in evaluating materials in real-time on the lines of sustainability. The findings validate the interest and value that lie in integrating physics-informed AI and stochastic modeling to in not only accuracy in prediction but assures interpretability and robustness in the applications made. Moreover, the decision providing presented by the system can inform engineers, architects, as well as policy-makers in designing and choosing bio-based materials in sustainable construction and optimization. This close interaction of computational modelling, environmental data, and intelligent analytics is expected to assist in the increase in the need of intelligent infrastructure solutions. Generally, the work developed in this study involves a scalable, versatile model that can encompass data science, material engineering, and environmental modelingthe foundation upon which the future breakthroughs in the green construction and smart cities are going to be achieved.

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