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AI-Driven Material Selection.

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ABSTRACT

Material choice is a vital aspect of engineering design, and it directly impacts the performance, longevity, and cost of products in various industries. For improving decision-making in this area, artificial intelligence methods are utilized to provide recommendations on appropriate materials against both quantitative and qualitative inputs from users. The system combines machine learning models with natural language processing for understanding the requirements of the user without compromising the precise design purpose or data details. With a distributed learning environment, a universal model is trained using structured datasets of mechanical properties like yield strength, tensile strength, elongation, hardness, elastic modulus, shear modulus, Poisson's ratio, and density. Random Forest and natural language processing are used in combination, and Support Vector Regression and natural language processing are used to assess and provide material recommendations based on input patterns. The system maintains user privacy while allowing effective material prediction in various application contexts. This method enhances material selection accessibility and reliability, fostering well-informed design decisions without compromising data confidentiality and interpretability through natural language incorporation.

Keywords: *Material Selection, Artificial Intelligence, Machine Learning, Natural Language Processing, Random Forest, Support Vector Regression, Mechanical Properties, Federated Learning, Explainable AI, Data Privacy*

1. Introduction

Material selection is one of the most important aspects of engineering design, impacting performance, cost, and sustainability. Classical rule-based systems are constrained in dealing with dynamic and complex inputs. The application of Artificial Intelligence (AI) and Machine Learning (ML) has revolutionized this task by making it data-driven, flexible, and scalable. Modern systems such as MechProNet exhibit high prediction accuracy for material properties but suffer from computational cost and narrow applicability.AI models today incorporate Natural Language Processing (NLP) to handle descriptive and imprecise inputs, making them more user-friendly and transparent in their decision-making. The applications range from construction to sustainable concrete design, biomaterials, and medicine, demonstrating the adaptability of AI. New methods involve Large Language Models (LLMs), Generative Adversarial Networks (GANs), Reinforcement Learning (RL), and incorporation with IoT and quantum computing, which make it more adaptable, sustainable, and able to discover new materials .These advances highlight the necessity of strong, interpretable, and secure AI systems in enabling next-generation material selection across various industries.

1.1 Problem Statement

Material selection is an essential part of engineering design, where material selection has a direct influence on the performance, cost, and sustainability of a product. Conventional approaches to material selection are unable to effectively handle large datasets or include both quantitative material properties and qualitative user preferences, resulting in suboptimal 3 solutions. These approaches are also non-transparent, so engineers cannot clearly see the reasons

behind material suggestions. The project seeks to build an AI-material selection system using machine learning algorithms to make correct and actionable material suggestions based on both user input and material attributes. The system will incorporate high-level AI techniques to make the decision-making

process transparent, such that engineers can verify and believe the suggestions. Through enabling quicker, more trustworthy, and transparent material selection, the system will streamline design workflows, lower costs, and improve product performance, all while preserving privacy and security of sensitive material information.

1.2 Proposed System

The envisaged AI-driven material selection system merges Machine Learning (ML) and Natural Language Processing (NLP) to provide exact, user-oriented material suggestions. It takes into account both quantitative information (e.g., tensile strength, yield strength, density) as well as qualitative inputs (e.g., design criteria or user preferences) to provide more customized and credible decisions. Random Forest and Support Vector Regression (SVR) will process structured data, whereas NLP will understand text-based inputs. Explainable AI functionalities will be incorporated into the system to give accurate, understandable reasons behind each suggestion in order to build greater user confidence and transparency. To guarantee data security and privacy, the system will implement Federated Learning for collaborative model training without sharing sensitive data. With this combination of ML, NLP, and explainable AI, a secure, interpretable, and flexible material selection tool that is appropriate for current engineering applications emerges.

2. Literature Survey

[1] Parand Akbari, Masoud Zamani, Amir Mostafaei, "Machine Learning Prediction of Mechanical Properties in Metal Additive Manufacturing",2024.
Introduces MechProNet for predicting properties in MAM using explainable ML. Validated on 1600+ datapoints across PBF and DED, with SHAP-based insights for properties like yield and tensile strength**.**

[2] Andi Prasetiyo Wibowo, "Unveiling the Potential of AI Assistants: A Review of AI in Building Materials Selection," 2024.
Reviews 168 papers on AI's role in construction material selection, highlighting benefits in cost, time, and sustainability.

[3] Daniele Grandi et al., "Evaluating Large Language Models for Material Selection", 2024.

Assesses LLMs in material selection, focusing on prompt engineering and challenges in consistency.

[4] Yash Patawari Jain et al., "MSEval: A Dataset for Material Selection in Conceptual Design to Evaluate Algorithmic Models", 2024.
Presents MSEval dataset for benchmarking AI material selection models in conceptual design.

[5] Lipichanda Goswami et al., "Artificial Intelligence in Material Engineering", 2023.

Covers AI methods like GANs for material design, prediction, and discovery across research and industry.

[6] Omid Aghababaei Tafreshi et al., "Machine Learning-Based Model for Predicting the Material Properties of Nanostructured Aerogels", 2023.

Uses ML to predict aerogel properties (density, strength) for insulation and filtration applications.

[7] Jerzy Roslon, "Materials and Technology Selection for Construction Projects Supported with the Use of Artificial Intelligence," 2022.
Proposes AI and metaheuristic-based method (AMTANN) for material and tech selection in building projects.

[8] Fei Zhu et al., "Intelligent Design of Building Materials: Development of an AI-Driven Method for Cement-Slag Concrete Design," 2022.
Applies RF, DT, SVM, and optimization techniques (MOBAS, TOPSIS) for sustainable concrete mix design.

[9] Sanket Kadulkar et al., "Machine Learning-Assisted Design of Material Properties", 2022.

Explores ML tools for efficient material design and optimization, especially for custom applications.

[10] Andrij Vasylenko et al., "Element Selection for Functional Materials Discovery", 2022.

Uses interpretable ML to rank elemental contributions for novel material discovery (semiconductors, catalysts).

[11] Hengrui Zhang et al., "Uncertainty-Aware Mixed-Variable Machine Learning for Materials Design", 2022.

Discusses Bayesian methods for alloy/composite selection under uncertain data.

[12] Joseph B. Choi et al., "AI Approaches for Materials-by-Design of Energetic Materials", 2022.

Reviews deep learning and generative models for designing propellants and explosives; highlights data challenges.

[13] Stella Hrehova, Lucia Knapcikova, "ML-Assisted Design of Selected Composites Properties", 2022.

Predicts properties of composites using fiber orientation and matrix data to optimize design.

[14] Rajesh Jha, Bimal Kumar Jha, "AI-Aided Materials Design: Algorithms and Case Studies", 2022.

Explores decision trees, ANNs, and GA for alloys, with industry applications and challenges.

[15] Xianglin Liu et al., "Machine Learning for High-Entropy Alloys", 2022.

Reviews ML models for predicting behaviors of complex alloys, stressing need for physics-informed data.

[16] Ijaz Ahmad et al., "AI Techniques for Selection & Evaluation", 2021.

Surveys ML models (SVM, fuzzy logic, RF) for materials across aerospace, auto, and biomedical sectors.

[17] Aaditya Chandrasekhar et al., "Integrating Material Selection with Design Optimization via Neural Networks", 2021.

Applies neural networks for joint optimization of materials and geometry in truss structures.

[18] K. Guo et al., "AI and ML in Design of Mechanical Materials", 2021.

Reviews ML methods for predicting mechanical behaviors; discusses application challenges.

[19] Sanket Kadulkar et al., "Inverse Design of Polymer Cloud Points Using ML", 2021.

Uses neural networks for cloud point prediction in polymers, integrating design constraints.

[20] D. Merayo et al., "Prediction of Physical and Mechanical Properties for Metallic Materials", 2020.

ANN-based tool trained on 43,000+ entries predicts material properties with high accuracy using Ashby charts.

3. Methodology

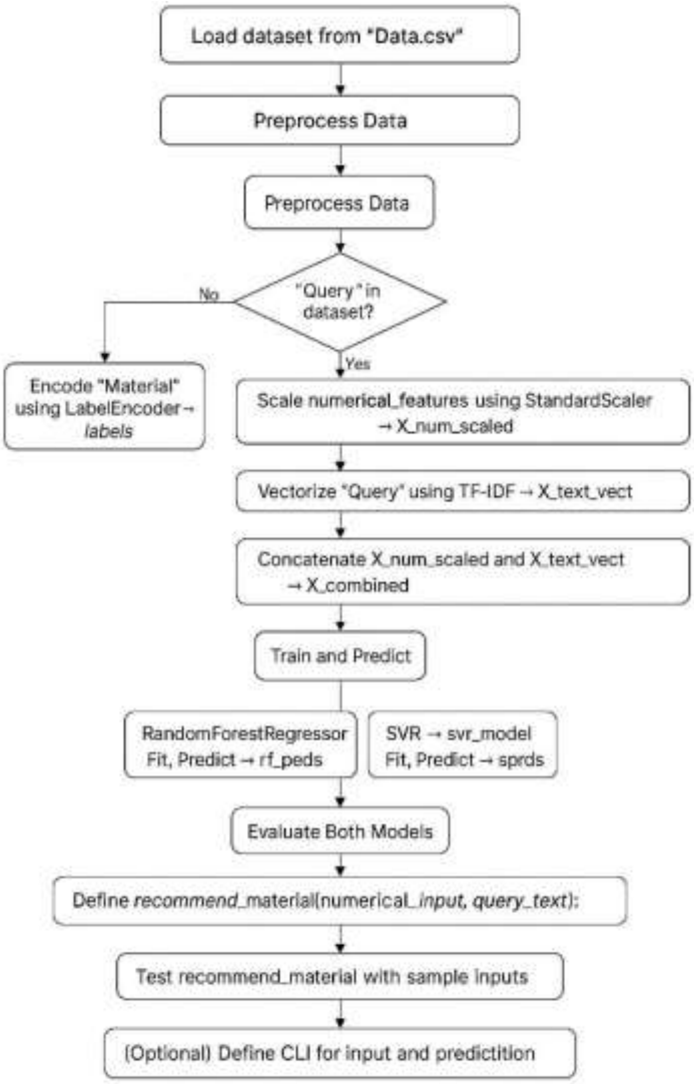

Figure 1: Flow Diagram for AI-Driven Material Selection

The design of the AI-driven material selection system follows a structured development process aimed at accurately recommending materials based on both numerical data and descriptive user inputs. From Figure 1 it begins with data collection, where material property datasets containing key mechanical and physical attributes such as tensile strength, yield strength, density, and elastic modulus are sourced from verified repositories. This raw data is then preprocessed through steps such as cleaning, normalization, and transformation to make it suitable for machine learning applications. Both numerical features and textual inputs are processed, with the latter being handled using Natural Language Processing (NLP) techniques to extract meaningful parameters from user-defined requirements or design constraints. Following preprocessing, two predictive models are trained: one using Random Forest in combination with NLP, and the other using Support Vector Regression (SVR) integrated with NLP. These models are selected for their ability to process structured numerical data as well as interpret descriptive language inputs. The models are evaluated using key performance metrics, including the R^2 score, Mean Absolute Error (MAE), and Root Mean Square Error (RMSE). These metrics offer comprehensive insight into the model's performance by measuring prediction accuracy and error magnitude. The Random Forest model with NLP integration demonstrates superior performance in terms of higher R^2 and lower MAE and RMSE values and is thus chosen for deployment. In the deployment phase, the selected model is integrated into a user interface that allows engineers and designers to input material requirements in both numerical and descriptive forms. The interface is designed to be robust and adaptable, capable of handling incomplete or loosely defined input while still delivering accurate and relevant material recommendations. This design ensures that the AI system is not only data-driven but also responsive, interpretable, and secure for real-world engineering applications.

4. Results and Discussions

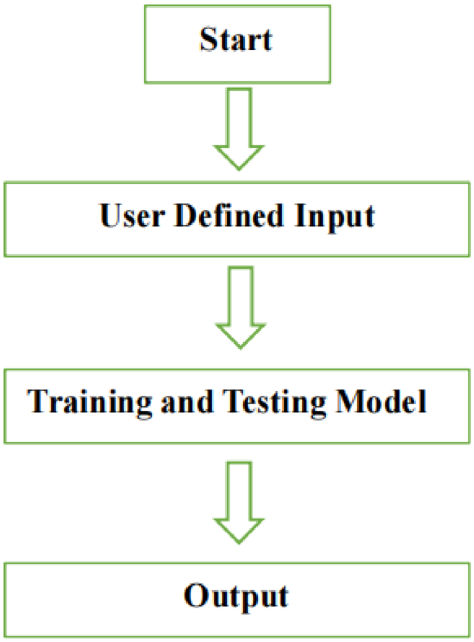

Figure 2: Flow Diagram for Implementation of AI-Driven Material Selection Model

Figure 2 represents the constructed AI-Driven Material Selection tool integrates Natural Language Processing (NLP) and a Random Forest (RF) model to recommend appropriate engineering materials as a function of user-specified requirements. The tool can handle numerical inputs for primary mechanical properties as well as additional optional text descriptions for flexible and natural interaction. The model accurately predicts partial or full datasets and applies imputation methods to manage missing values to make continuous predictions. This allows engineers to operate effectively even without all material parameters. The RF model categorizes materials according to patterns learned from a varied dataset, giving material recommendations based on user specifications. While the system attains rudimentary functionality and provides material-relevant prediction, its accuracy at present demonstrates the necessity of further improvement. Prediction accuracy depends on factors such as dataset size, feature quality, and balance of material classes. In spite of this, the tool presents the capability of AI in facilitating automation and acceleration of material choice, reducing human error, and enhancing decision-making in engineering design. Further development, such as dataset growth and model adjustment, will enhance its predictive power and practical application

4.1 Training and Testing Model

The training and testing process comprised comparing various machine learning models for the identification of the most appropriate model to apply for AI-assisted material selection. Two were initially tested: Random Forest merged with NLP (Natural Language Processing), and independently, Support Vector Regression (SVR) and NLP. Both the models were analyzed according to how well they predict material properties. Following a comparative study, Random Forest with NLP was chosen because it is more accurate and performs better in both numerical and descriptive input handling. The model can accept user-supplied inputs in two forms: numerical ranges or text description. Even when the user omits certain parameters or supplies incomplete data, the model can still make correct predictions by understanding the input provided using NLP methods. In testing, the model was able to return correct material recommendations when offered various kinds of input, exhibiting flexibility and strength in real-world scenarios.

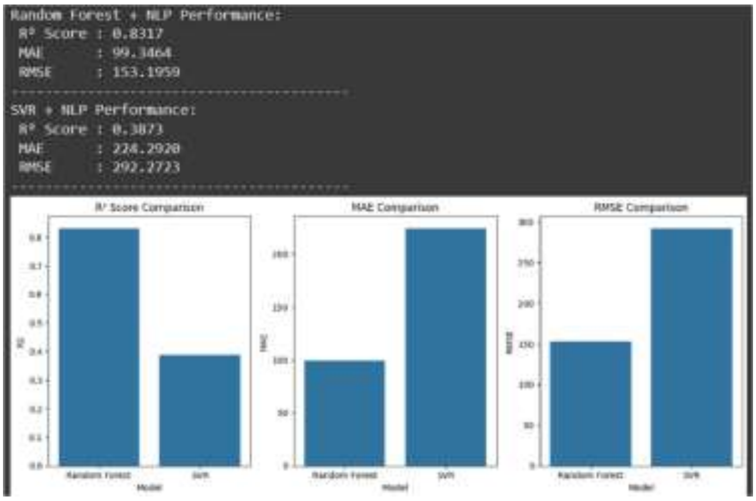

Figure 3: Comparison between the Random Forest and Support Vector Regression models.

Figure 3 describes the comparison between the Random Forest and Support Vector Regression (SVR) models, both integrated with Natural Language Processing (NLP), highlights the superior performance of the Random Forest model across key evaluation metrics. The performance was assessed using R-squared (R^2), Mean Absolute Error (MAE), and Root Mean Squared Error (RMSE). The Random Forest model achieved an R^2 score of 0.8317, significantly higher than SVR's 0.3873, indicating a much stronger correlation between the predicted and actual values. Additionally, the Random Forest model exhibited lower error rates, with an MAE of 99.3464 and an RMSE of 153.1959, compared to SVR's MAE of 224.2920 and RMSE of 292.2723.These metrics collectively demonstrate that Random Forest delivers more accurate and reliable predictions. The visual representation through bar charts further reinforces this conclusion, showing clear advantages of the Random Forest model over SVR in all aspects. Therefore, the Random Forest model, in combination with NLP, is concluded to be the more effective approach for this AI-driven material selection task.

4.2 Results

```
Enter the material description (optional):
Enter the value for Su (press enter to skip): 421
Enter the value for A5 (press enter to skip): 39
Enter the value for Bhn (press enter to skip): 126
Enter the value for E (press enter to skip): 207000
Enter the value for G (press enter to skip): 79000
Enter the value for mu (press enter to skip): 0.3
Enter the value for Ro (press enter to skip): 7860
Enter the value for Sy (press enter to skip): 314

Predicted Material: Steel SAE 1015
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Figure 4: Results of AI-Driven Material

Figure 4 describes that Material matching analysis has also confirmed Steel SAE 1015 to be the most appropriate material with reference to the given properties. Steel SAE 1015 is lowcarbon steel that contains nearly 0.15% of carbon. Steel SAE 1015 finds extensive applications wherever there is a need for optimum combination of strength, ductility, and machinability. Its ultimate tensile strength (Su) being 421 MPa, Steel SAE 1015 supports moderate loads without rupturing. Its fracture elongation at A5 of 39% reflects its high ductility, deforming markedly before breaking. Its Brinell Hardness Number (Bhn) of 126 reflects its moderate hardness, providing wear resistance while remaining fairly soft in relation to high-carbon steels. Also, its modulus of elasticity (E) value of 207,000 MPa and shear modulus (G) value of 79,000 MPa indicate its excellent stiffness and resistance to shearing stress, which are well suited for structural and mechanical uses. It has a Poisson's ratio of 0.3, meaning Steel SAE 1015 is normally behaving under stress, which spreads out laterally when under compression. The 7860 kg/m³ density is normal for steel and reflects its weight per volume, while the 314 MPa yield strength (Sy) ensures the material has enough strength to support heavy loads without permanent deformation.

5. Conclusion

The higher material selection accuracy of the Random Forest with Natural Language Processing model compared to the Support Vector Regression NLP model. The RF model, when used with NLP, is a stronger and more accurate predictor of material properties than SVR. This is primarily because RF is an ensemble learning method that can handle large datasets with high dimensional features more effectively, offering better generalization and less susceptibility to overfitting. In contrast, SVR, although effective in many regression tasks, struggles with complex, non-linear relationships, especially when the dataset is noisy or has many outliers. The Random Forest with Natural Language Processing model could produce more precise material predictions by taking advantage of both structured numerical inputs and user-provided natural language descriptions. Such integration of NLP enables flexibility in capturing qualitative user inputs, which the RF model interprets and processes more accurately. By taking into account both quantitative data and qualitative parameters, the combination of Random Forest and NLP far exceeds SVR, producing more accurate and consistent material selection outcomes. Furthermore, with all user-specified inputs, including tensile strength, elongation, hardness, and other properties of the materials, the Random Forest with NLP model's capability to incorporate these inputs and provide more consistent and accurate predictions is remarkable. This makes the entire process of material selection more intuitive and user-friendly while providing a higher level of accuracy and reliability. Finally, the RF + NLP methodology turns out to be a more efficient technique for the optimization of material selection in complex engineering applications and provides better performance compared to the conventional SVR-based models.

6. Future Scope

The future potential of this project is full of promise for further development and extension. One of the main avenues is to integrate a wider selection of materials, such as polymers, composites, and ceramics, to extend the system's application to many different industries such as aerospace, automotive, and construction. Also, in-line data integration from sensors and production processes may be able to make the process of selecting materials more dynamic and 31 situation-specific. Enhancing the system's NLP functionality to process more sophisticated and vague natural language inputs would also make the system more flexible. The model can be integrated with predictive maintenance software, employing material predictions in combination with operational data to evaluate long-term material performance. The future could also witness the integration of multi-objective optimization algorithms that trade-off material performance with cost, sustainability, and environmental considerations. Industry-specific implementations of the model may be created to specialize recommendations to specific industries, and interfacing with big databases of materials and simulation packages would enable better verification of material selections. Finally, shifting from a research-oriented model to actual implementation in businesses would make it more practically useful and open the doors for commercialization, making the system a potential tool of great power for engineers and designers to use in data driven material selection.

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