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Neuro Fuzzy in Predicting the Characteristics of Some Nanomaterials

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Abstract:- Unveiling the impressive capabilities of the Adaptive Neuro-Fuzzy Inference System (ANFIS), this study effectively predicts key properties of engineered nanomaterials, opening doors to innovative applications across various industries. We initially investigate the cytotoxic effects of TiO_2 and ZnO nanoparticles on immortalized human lung epithelial cells, employing ANFIS to establish correlations between nanoparticle size and behaviour in different media and the resulting cellular membrane damage, quantified by lactate dehydrogenase release. Next, to predict the compressive strength of geopolymers, analysing over previous experimental datasets focused on critical chemical ratios. This model demonstrates its capability to optimize formulations for enhanced mechanical performance in sustainable construction materials. Additionally, we apply ANFIS to evaluate the size of silver nanoparticles in montmorillonite/starch bio nanocomposites, identifying significant factors such as AgNO3 concentration. The ANFIS models achieved high accuracy across all applications, underscoring their utility in predicting material behaviour and optimizing formulations for improved performance and safety. Collectively, these findings illustrate the potential of ANFIS as a robust tool in nanomaterial research and development.

I. INTRODUCTION

The rapid advancement of nanotechnology has opened new avenues for the development of innovative materials with exceptional properties, paving the way for applications in fields ranging from medicine to sustainable construction. [1] Understanding and predicting the behaviour of engineered nanomaterials is crucial for ensuring their efficacy and safety. [2] Among the various computational techniques available, the Adaptive Neuro-Fuzzy Inference System (ANFIS) stands out as a powerful tool for modelling complex, nonlinear relationships in data.

ANFIS combines the strengths of fuzzy logic and artificial neural networks, enabling it to handle uncertainties and variability in experimental data effectively.[3] This approach is particularly beneficial in materials science, where the interactions between various factors often lead to intricate outcomes. By integrating qualitative and quantitative information, ANFIS facilitates the optimization of material properties based on key parameters. [4]

In this study, we leverage ANFIS to explore the predictive capabilities across three distinct areas: the cytotoxic effects of titanium dioxide (TiO2) and zinc oxide (ZnO) nanoparticles on human lung epithelial cells, the compressive strength of geopolymers influenced by critical chemical ratios, and the size determination of silver nanoparticles within montmorillonite/starch bionanocomposites. Through these investigations, we demonstrate the versatility and reliability of ANFIS in modelling and predicting the behaviour of engineered nanomaterials, ultimately contributing to safer and more efficient applications in diverse fields.

II. DATA COLLECTION.

Silver nanoparticles (Ag-NPs) are recognized for their exceptional antibacterial properties, making them valuable across diverse fields such as medicine, textiles, electronics, and food safety. [5] Their advantages include strong antibacterial activity, biocompatibility, versatility, and enhanced material properties. [6] Ag-NPs can be synthesized using various methods, including chemical reduction with agents like sodium borohydride, physical methods such as UV irradiation, [7] and green synthesis using natural polymers like starch. [8] Key input parameters influencing the final size of Ag-NPs include the concentration of silver nitrate ($AgNO_3$), which affects ion availability [9]; reaction temperature, where higher temperatures may lead to larger particles; [10] the weight percentage of starch, which stabilizes the nanoparticles; and the concentration of sodium borohydride, impacting the reduction rate. [11] By optimizing these factors, the size and characteristics of Ag-NPs can be tailored for specific applications.

Increasingly recognized as a sustainable alternative to Portland cement [12] due to their lower carbon footprint, [13] resource efficiency, and enhanced durability, making them suitable for applications like construction materials, waste encapsulation, [14] and infrastructure repair. Key inputs for geopolymer production include aluminosilicate sources (such as fly ash or slag), [15] alkali activators (like sodium hydroxide or sodium silicate), [16] water, and sometimes additives to enhance specific properties. The composition and ratios of these inputs significantly influence the mechanical properties, workability, setting time, and overall performance of the final product. [17] Predictive modelling plays a crucial role in optimizing these formulations by enabling systematic exploration of different material combinations, ensuring cost efficiency, maintaining quality control, and assessing environmental impact. [18]

Moreover, nanomaterials at the nanoscale exhibit distinct chemical and physical properties compared to their macro sized counterparts, leading to varied biological responses influenced by factors such as the route of exposure and target tissues [19]. As these engineered nanomaterials are increasingly applied in industries like food packaging, cosmetics, and electronics, there is an urgent need to evaluate their safety to protect human health and the environment. Current studies indicate that specific features of metal oxide nanomaterials, including size, surface charge, and solubility, significantly impact their biological interactions and potential toxicity. This study aims to investigate the relationship between the physicochemical properties of titanium dioxide (TiO_2) and zinc oxide (ZnO) nanoparticles and their effects on human tissues, particularly focusing on cellular membrane damage. Key inputs considered include engineered size, size in various biological media, particle concentration, and zeta potential, which influence how nanoparticles interact with cells. Understanding these interactions is critical, given the increasing use of nanomaterials in consumer products. Predictive modelling is vital in establishing correlations between specific nanoparticle properties and biological responses, streamlining risk assessments, and guiding experimental designs to identify key variables for further investigation.

Ultimately, this study underscores the importance of evaluating nanomaterial safety to safeguard human health and the environment while promoting effective applications of Ag-NPs and geopolymers in various industries.

III. ANFIS

The ANFIS (Adaptive Neuro-Fuzzy Inference System) controller is a sophisticated multilayered system that integrates fuzzy logic with neural network components. [20] Its architecture comprises five distinct layers, each fulfilling a specific role. [21] In the first layer, input variables are processed through fuzzy membership functions, transforming crisp inputs into fuzzy values. The second layer assesses the degree of membership for each rule based on these fuzzy inputs. In the third layer, the outputs of each rule are calculated by combining the fuzzy values with their respective weights, enabling the application of fuzzy rules. The fourth layer aggregates all rule outputs to generate a single fuzzy output. Finally, the fifth layer performs defuzzification, converting the fuzzy output back into a crisp value. [22] This multilayered framework allows ANFIS to effectively learn from data while leveraging the adaptability of fuzzy logic, making it an effective tool for complex modelling tasks. [23]

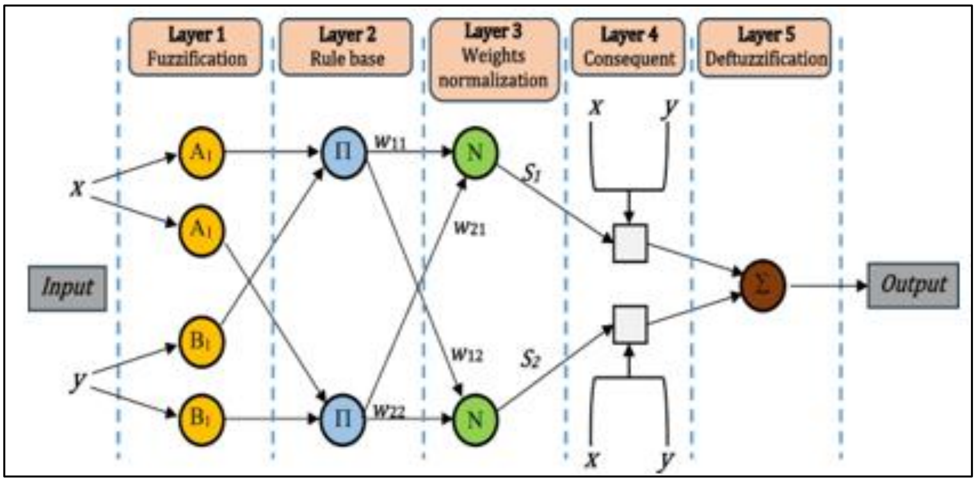

Fig 1: Architecture of ANFIS

IV. DATA ANALYSIS

We commenced our investigation by analysing 24 datasets from the pioneering research of Christie Sayes et al. (2010), [24] focusing on the physical characteristics of TiO2 nanoparticles, including their engineered size in both water and phosphate-buffered saline (PBS), zeta potential, and the resulting cellular membrane damage values. We further incorporated 40 datasets from Dali Bondar's (2014) study, [25] which detailed critical chemical ratios such as Al_2O_3/SiO_2, Na_2O/Al_2O_3, Na_2O/H_2O, and Na/[Na+K], along with their corresponding compressive strength (CS) values. To further enrich our analysis, we examined 30 datasets from P. Shabanzadeh et al. (2014) [26] to explore various experimental conditions affecting the size of silver nanoparticles, concentrating on key parameters including AgNO3 concentration, reaction temperature, starch percentage, and NaBH4 concentration. Throughout this comprehensive study, we employed the Adaptive Neuro-Fuzzy Inference System (ANFIS) as a powerful tool for determining the properties of nanoparticles, enabling accurate predictions and enhancing our understanding of their behaviour in diverse applications.

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V. RESULT AND DISCUSSION

The Adaptive Neuro-Fuzzy Inference System (ANFIS) networks were designed to predict various outcomes based on different input variable ratios across three distinct datasets.

In the first model, five input variables—engineered size (nm), size in water (nm), size in PBS (nm), concentration (mg/L), and zeta potential—were employed to predict membrane damage values between 0.02 and 1.4. Using 18 samples for training and 6 for testing, the training occurred over 150 epochs, resulting in an overall RMSE of 0.6762, indicating consistent accuracy across the dataset.

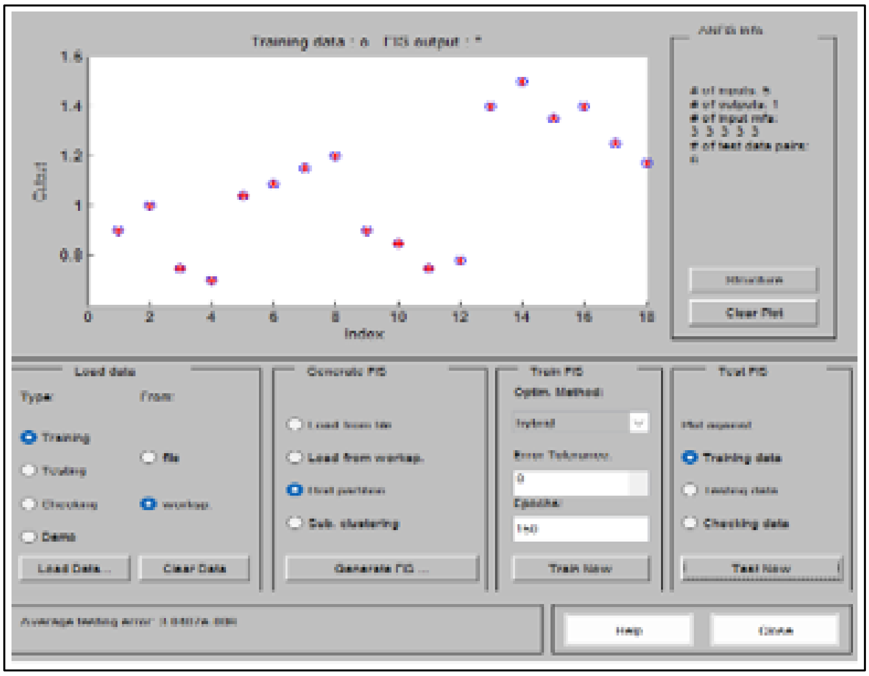

Fig 2: Training Plot: ANFIS Model for Predicting Membrane Damage

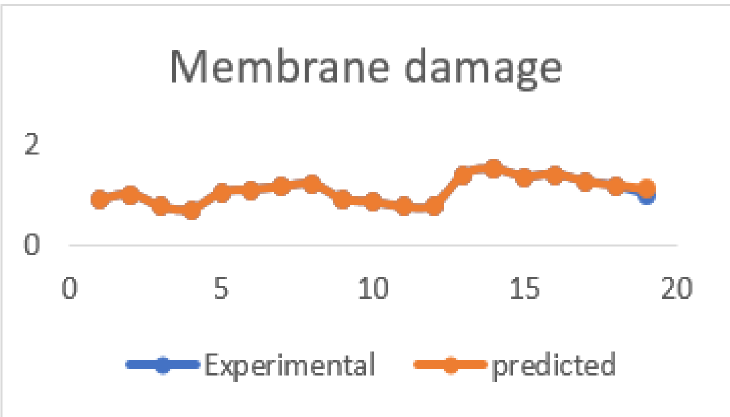

Fig 3: Response plot

The second model utilized four input variables—Al_2O_3/SiO_2 (V), Na_2O/Al_2O_3 (X), Na_2O/H_2O (Y), and Na/[Na+K] (Z)—to predict compressive strengths ranging from 2.85 MPa to 70.86 MPa. With 30 samples for training and 10 for testing, this model achieved strong predictive accuracy after 100 epochs, yielding an overall RMSE of 0.8716 and an average predicted compressive strength of approximately 36.47 MPa.

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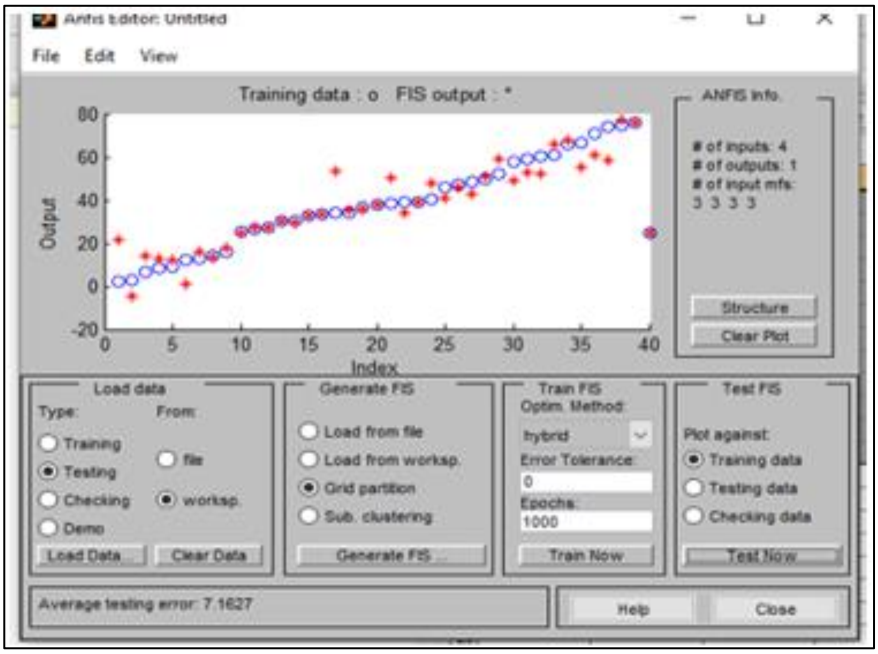

Fig 4: Training Plot: ANFIS Model for Predicting Compressive strength

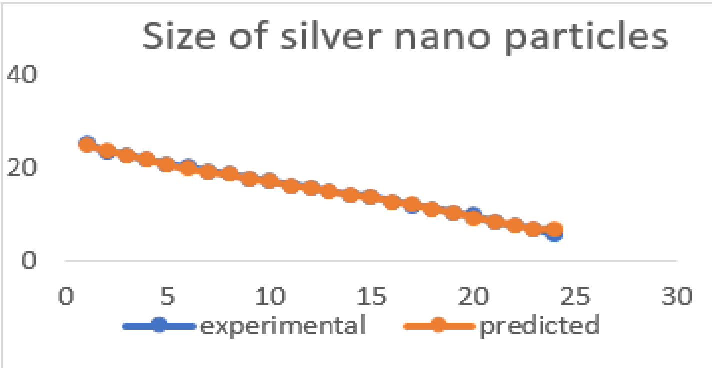

Fig 5: Response plot

The third model focused on the synthesis of silver nanoparticles, using five input variables: $AgNO_3$ concentration (M), temperature, starch, and $NaBH_4$ concentration (M). Training with 23 samples and testing with 7 over 150 epochs, this model effectively predicted nanoparticle sizes ranging from 6.6914 nm to 24.9586 nm, achieving an overall RMSE of 0.3233, which highlights its precision and reliability. Collectively, these ANFIS models demonstrate strong predictive capabilities and minimal errors across a variety of applications.

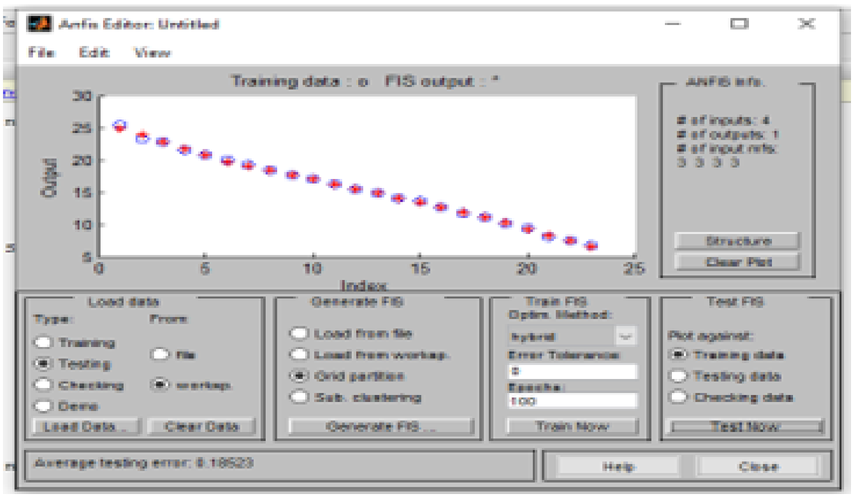

Fig 6: Training Plot: ANFIS Model for Predicting Size of silver nano particles

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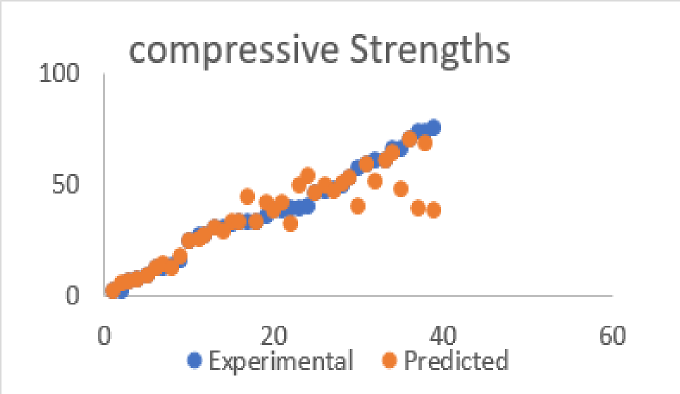

Fig 7: Response plot

VI. CONCLUSION

In conclusion, the application of Adaptive Neuro-Fuzzy Inference System (ANFIS) models across diverse datasets underscores their robustness and versatility in predictive modelling. The models successfully demonstrated strong predictive accuracy for membrane damage, compressive strengths, and silver nanoparticle sizes, each with minimal errors as indicated by their low RMSE values. The ability to utilize various input variables effectively highlights the adaptability of ANFIS in addressing complex relationships within data. Overall, these findings reinforce the potential of ANFIS as a reliable tool in materials science and nanotechnology, paving the way for future research and practical applications in the field.

REFERENCES

[1]. **Md Kazi Rokunuzzaman,** The Nanotech Revolution: Advancements in Materials and Medical Science, June 2024.

[2]. **S. Ahmad**, Engineered 'Nanomaterials by design' theoretical studies experimental validations

[3]. current and future prospects, 2018.

[4]. **Vasileios D. Sagias et al**., Adaptive Neuro-Fuzzy Inference System-Based Predictive Modeling of Mechanical Properties in Additive Manufacturing,2024.

[5]. **DV Dao et al**., Artificial intelligence approaches for prediction of compressive strength of geopolymer concrete,2019

[6]. **Guangyu Zhang et al.,** Synthesis of silver nanoparticles and antibacterial property of silk fabrics treated by silver nanoparticles,2014

[7]. **Baker, C et al.,** Synthesis and Antibacterial Properties of Silver Nanoparticles,2005

[8]. **Ngoc Phuong Uyen Nguyen et al.,** Synthesis of Silver Nanoparticles: From Conventional to 'Modern' Methods—A Review, 2023

[9]. **Sobhy M Yakout et al.,** A novel green synthesis of silver nanoparticles using soluble starch and its antibacterial activity,2015

[10]. **Essam Elatafi et al.,** Effect of Silver Nitrate ($AgNO_3$) and Nano-Silver (Ag-NPs) on Physiological Characteristics of Grapes and Quality during Storage Period.2022

[11]. **Hongyu Liu et al.,** Effect of temperature on the size of biosynthesized silver nanoparticle: Deep insight into microscopic kinetics analysis, 2020.

[12]. **Umme Thahira Khatoon et al.,** Sodium borohydride mediated synthesis of nano-sized silver particles: Their characterization, anti-microbial and cytotoxicity studies. 2023

[13]. **N.B. Singh et al.,** Geopolymers as an alternative to Portland cement: An overview 2020.

[14]. **Benjamin C. McLellan et al.,** Costs and carbon emissions for geopolymer pastes in comparison to ordinary Portland cement. 2011

[15]. **D. C. Southam et al.,** Towards more sustainable minefills - Replacement of ordinary Portland cement with geopolymer cements. 2007.

[16]. **Amalina Hanani Ismail et al**., A review of aluminosilicate sources from inorganic waste for geopolymer production: Sustainable approach for hydrocarbon waste disposal. 2024

[17]. **LN Tchadjie et al.**, Enhancing the reactivity of aluminosilicate materials toward geopolymer synthesis. 2018

[18]. **Chandani Tennakoon** et al., Influence and role of feedstock Si and Al content in Geopolymer synthesis.2014

[19]. **Mostafa jalal et al**., RETRACTED ARTICLE: A new nonlinear formulation-based prediction approach using artificial neural network (ANN) model for rubberized cement composite. 2022

[20]. **Xi-Qiu Liu** et al., Biological responses to nanomaterials: understanding nano-bio effects on cell behaviors.2017

[21]. **Christie Sayes et al**., Comparative Study of Predictive Computational Models for Nanoparticle-Induced Cytotoxicity, 2010.

[22]. **Johanna M. Orozco-Castañeda et al**. Evaluating Volatility Using an ANFIS Model for Financial Time Series Prediction, September 2024.

[23]. **In Lih Ong et al.,** A Five-Layered Business Intelligence Architecture.2011.

[24]. **A. Ellery et al.,** Artificial intelligence through symbolic connectionism—A biomimetic rapprochement,2015

[25]. **Yaw Opoku Mensah Sekyere et al.** A Novel ANFIS Controller for LFC in RES Integrated Three-Area Power System, 30 July 2024.

[26]. **Dali Bondar**, The use of neural network to predict strength and optimum composition of natural alumina-silica based geopolymers, 2013.
[27]. **P. Shabanzadeh et al.,** Neural network modelling for prediction size of silver nanoparticles in montmorillonite/starch synthesis by chemical reduction method, 2014.