

AI-driven process–structure modeling of sonochemically synthesized composite materials using machine learning and computer vision

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Abstract. The development of advanced composite materials requires a comprehensive understanding of the relationships between processing conditions, microstructural evolution, and resulting material properties. However, optimization of synthesis parameters remains challenging due to the complex and nonlinear interactions governing composite fabrication. This study presents an AI-driven computational framework that integrates machine learning and computer vision for process–structure modeling of sonochemically synthesized TiO₂–cotton composites. Experimental datasets were generated by systematically varying key sonication parameters, including horn power, sonication time, sonication cycles, precursor concentration, and processing temperature. Computer vision techniques were employed to quantitatively characterize nanoparticle size, surface loading, and dispersion behavior from microscopic observations, while machine learning models were developed to establish predictive relationships between processing variables and composite characteristics. The developed models successfully captured the nonlinear dependencies between sonication parameters and material responses, enabling accurate prediction of composite morphology and nanoparticle distribution. ANN achieved the highest R² for nanoparticle size (0.990) and TiO₂ loading (0.912), whereas GBR achieved the highest R² for dispersion index (0.759), with an RMSE of 0.025. These results indicate that predictive performance depends on the target characteristic.

1. Introduction

Materials informatics uses experimental and computational data to establish relationships among material composition, processing conditions, structure and properties. Previous studies have applied machine learning to materials processing and the prediction of functional and mechanical properties of nanoparticle-coated textiles [1–5]. Recent developments extend predictive modeling toward materials design. Ma et al. [14] introduced the MLMD platform, integrating property prediction, surrogate optimization and active learning to guide materials exploration, including under limited data availability. However, reliable predictions depend on the design of the complete modeling workflow. Ma et al. [15] highlighted how dataset construction, feature selection, data partitioning and model evaluation can substantially affect materials machine-learning results. These considerations are particularly relevant to process–structure modeling of sonochemically synthesized composites using relatively small experimental datasets.

Titanium dioxide (TiO₂) nanoparticles have attracted considerable attention because of their excellent photocatalytic activity, ultraviolet (UV) shielding capability, antimicrobial performance, and chemical stability. Consequently, TiO₂-based composites have been widely investigated for functional textile applications including self-cleaning fabrics, antimicrobial surfaces, environmental remediation, and protective clothing [7–10]. Among the available synthesis techniques, sonochemical processing offers an environmentally friendly and efficient approach for depositing nanoparticles onto textile substrates. Ultrasonic cavitation generated during sonication enhances nanoparticle dispersion,

improves adhesion to fiber surfaces, and promotes uniform coating formation. Nevertheless, the final characteristics of TiO₂-coated fabrics are highly dependent on multiple interacting processing variables such as horn power, sonication time, precursor concentration, processing temperature, and sonication cycles, making process optimization particularly challenging [7–10].

Artificial neural networks (ANNs) have demonstrated excellent capability for modeling nonlinear engineering problems where conventional statistical methods often fail. In addition, regression-based machine learning algorithms, including Gradient Boosting Regression (GBR), Support Vector Regression (SVR), Linear Regression (LR), and Bayesian Ridge Regression (BR), provide valuable alternatives for predicting material behavior and evaluating model robustness [11–13]. Simultaneously, computer vision techniques enable quantitative characterization of microscopic images by automatically extracting particle size, morphology, and dispersion information, reducing subjectivity associated with manual image analysis.

Computer vision provides complementary tools for extracting quantitative structural information from electron microscopy images. Rettenberger et al. [16] developed uncertainty-aware Mask R-CNN models for particle segmentation in SEM images, addressing challenges associated with image blur, particle agglomeration and different magnifications, and evaluating the results against expert annotations. Day et al. [17] combined computer vision and unsupervised learning to automate nanoparticle image segmentation and generate acquisition coordinates for subsequent STEM characterization. These studies demonstrate advances in automated microscopy while emphasizing the importance of task-specific validation. In the present study, conventional image processing, SVM classification and the Circular Hough Transform are applied to characterize TiO₂ particles on cotton surfaces alongside predictive modeling of synthesis conditions.

Despite significant progress in applying artificial intelligence to materials engineering, relatively few studies have integrated machine learning and computer vision within a unified framework for process–structure modeling of sonochemically synthesized TiO₂-based composite materials. Establishing reliable predictive relationships between synthesis parameters and composite morphology remains an important challenge for intelligent manufacturing and advanced functional textile design.

Therefore, this study presents an AI-driven framework that combines machine learning and computer vision for modeling the process–structure relationship of sonochemically synthesized TiO₂–cotton composites. Experimental datasets generated under different sonication conditions were employed to train predictive models capable of estimating nanoparticle size, surface loading, and dispersion characteristics. Furthermore, computer vision techniques were utilized for automated microscopic image analysis to quantify particle distribution and morphology. The proposed framework provides an efficient computational tool for optimizing sonochemical synthesis parameters and supporting the development of high-performance multifunctional composite materials.

2. Methodology

2.1. Experimental preparation

TiO₂–cotton composites were synthesized using a sonochemical deposition process. Commercial 100% cotton fabrics with different fabric weights (110–238 g m⁻²) were used as the substrate, while titanium tetraisopropoxide (TTIP) served as the TiO₂ precursor. Before synthesis, the cotton samples were ultrasonically cleaned in a deionized water–ethanol solution (1:1 v/v) for 15 min to remove surface contaminants and improve nanoparticle adhesion.

The cleaned fabrics were immersed in the precursor solution and treated using an ultrasonic probe operating at 20 kHz. Six processing parameters were systematically varied during synthesis: fabric GSM, horn power (10–50%), sonication time (15–45 min), sonication cycles (1–5), precursor concentration (0.5–5 ml), and processing temperature (30–75 °C). These parameters were selected to investigate their influence on nanoparticle formation and coating quality. The overall workflow of the proposed framework is illustrated in Figure 1.

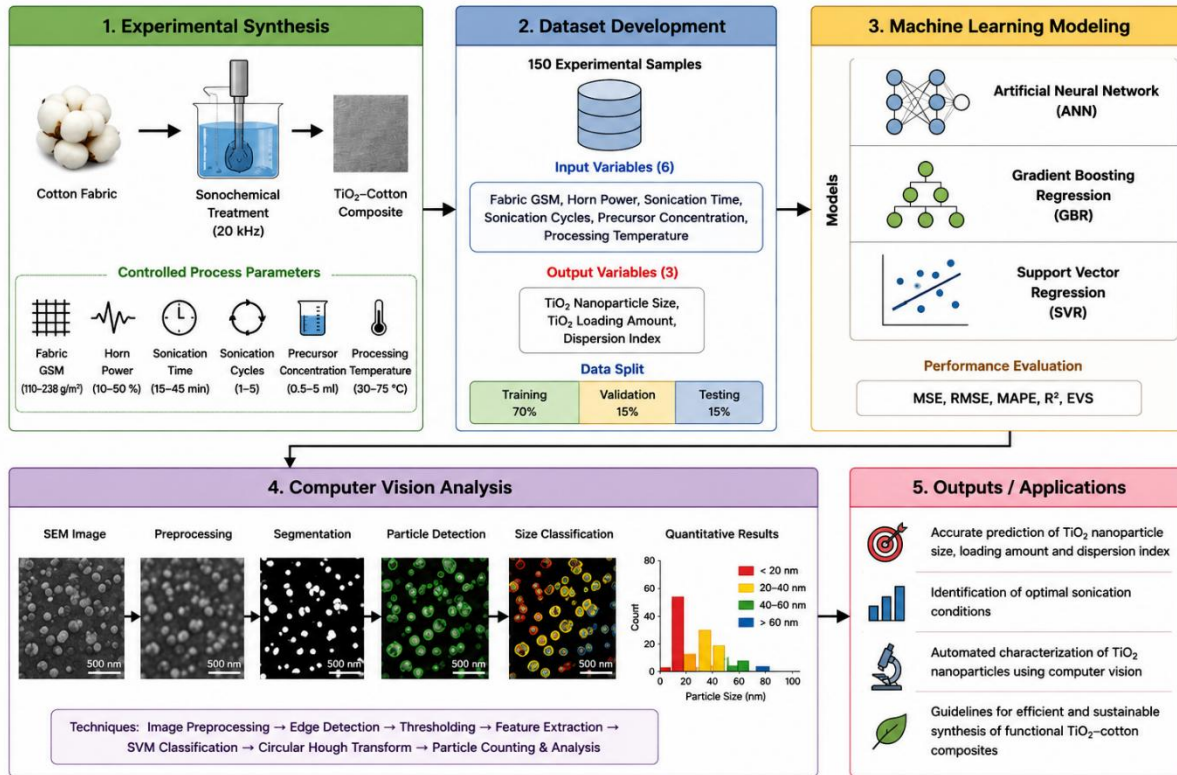


Figure 1. Overall workflow of the proposed AI-driven process–structure modeling framework.

2.2 Dataset development

A dataset comprising 150 experimental samples was established under different sonication conditions to investigate the influence of processing parameters on the structural characteristics of TiO₂-cotton composites. Each experimental sample consisted of six input variables, namely fabric GSM, horn power, sonication time, sonication cycles, precursor concentration, and processing temperature. The corresponding output responses included TiO₂ nanoparticle size, TiO₂ loading amount on the cotton surface, and nanoparticle dispersion index, which were experimentally measured following the synthesis process. Prior to machine learning model development, Pearson correlation analysis was performed to examine the relationships among the input variables. The results indicated relatively low correlations between the selected features, confirming their suitability for predictive modeling and minimizing the risk of multicollinearity. Subsequently, the complete dataset was randomly partitioned into training, validation, and testing subsets using a ratio of 70%, 15%, and 15%, respectively, to ensure reliable model training, parameter optimization, and unbiased performance evaluation.

2.3 Machine learning modelling

Three machine learning algorithms employed to predict the structural characteristics of the TiO₂-cotton composites are ANN, GBR, and SVR. The ANN model was developed to capture the nonlinear relationship between synthesis parameters and composite characteristics. The network consisted of six input neurons, one hidden layer, and one output neuron for each predicted response. Sigmoid activation functions were adopted in the hidden layer, while a linear activation function was used in the output layer. The network was trained using the Levenberg–Marquardt optimization algorithm together with the Adam optimizer to minimize prediction error. GBR was employed as an ensemble learning algorithm that sequentially constructs decision trees, where each new tree corrects the prediction errors of the previous one. This approach enables accurate modeling of complex nonlinear relationships and is particularly effective for relatively small experimental datasets. SVR was implemented as a nonlinear

regression model capable of mapping input variables into a higher-dimensional feature space through kernel functions. This allows the algorithm to model nonlinear dependencies between processing parameters and composite properties while maintaining good generalization performance. The predictive capability of the three algorithms was compared using identical training, validation, and testing datasets.

2.4 Computer vision-based image analysis

Computer vision techniques were utilized to quantitatively characterize the synthesized TiO₂ nanoparticles from scanning electron microscopy (SEM) images. **SEM image processing and particle characterization followed the procedure described in our previous study [18].** The image analysis pipeline consisted of image acquisition, preprocessing, grayscale conversion, Gaussian noise filtering, edge detection, threshold segmentation, feature extraction, particle classification, and particle counting. SVM-based image classification was employed to distinguish nanoparticles according to their particle size, while the Circular Hough Transform was used to identify individual particles and estimate particle density on the cotton surface. This automated procedure significantly reduces manual measurements and provides repeatable quantitative characterization of nanoparticle morphology and dispersion.

2.5 Performance evaluation

The predictive performance of ANN, GBR, and SVR was evaluated using five statistical performance indicators: Mean Squared Error (MSE), Root Mean Squared Error (RMSE), Mean Absolute Percentage Error (MAPE), Explained Variance Score (EVS), and the coefficient of determination (R^2). Lower values of MSE, RMSE, and MAPE indicate better prediction accuracy, whereas higher EVS and R^2 values demonstrate stronger agreement between predicted and experimental results.

These evaluation metrics were employed to compare the three machine learning models and identify the most suitable algorithm for predicting nanoparticle size, surface loading, and dispersion characteristics of sonochemically synthesized TiO₂-cotton composites.

3. Results and discussion

The predictive performance of the developed machine learning models was evaluated using the experimental dataset consisting of 150 samples. Three nonlinear regression algorithms, are ANN, GBR, and SVR, were employed to predict TiO₂ nanoparticle size, surface loading amount, and nanoparticle dispersion index under different sonication conditions. The prediction accuracy was assessed using MSE, RMSE, MAPE, and R^2 .

Figure 2 presents the prediction performance of the ANN model for the three output variables. The predicted values closely follow the experimental measurements, demonstrating that the network successfully captured the nonlinear relationship between the sonication parameters and composite characteristics. The regression results showed high agreement between predicted and experimental values, indicating that ANN effectively modeled the complex interactions among horn power, sonication time, precursor concentration, temperature, and sonication cycles. These results confirm the capability of ANN for predicting material behavior using relatively small experimental datasets.

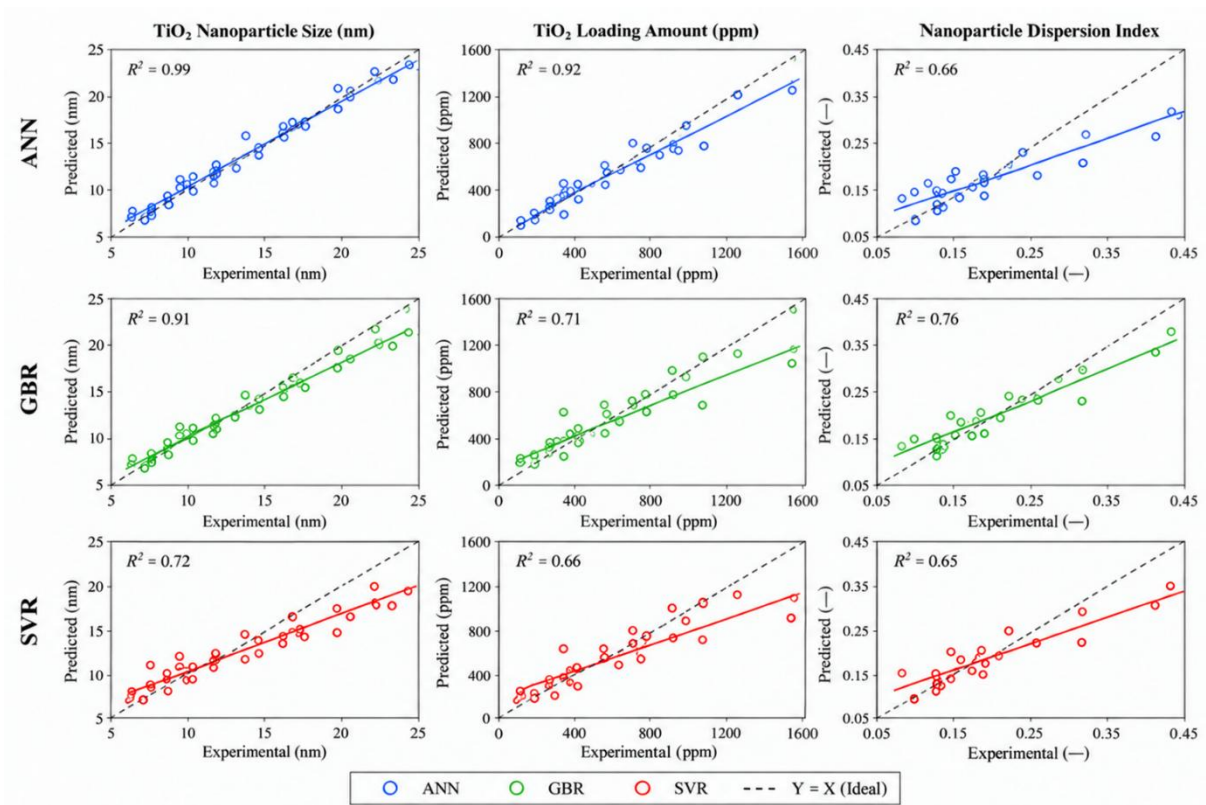


Figure 2. Prediction performance of ANN, GBR, and SVR models for TiO₂ nanoparticle size, TiO₂ loading amount, and nanoparticle dispersion index.

Figure 3 compares the predictive performance of ANN, GBR and SVR using RMSE, MAPE, R^2 and EVS. For nanoparticle size, ANN achieved the highest R^2 (0.990), compared with GBR (0.912) and SVR (0.716), and the lowest RMSE (1.03 nm), compared with 1.38 nm and 2.48 nm, respectively. However, GBR achieved the lowest particle-size MAPE (3.12%), compared with ANN (4.21%) and SVR (6.85%), indicating that model rankings depend on the evaluation metric. For dispersion index, GBR achieved the highest R^2 (0.759) and the lowest RMSE (0.025), compared with R^2 values of 0.663 and 0.649 and RMSE values of 0.038 and 0.027 for ANN and SVR, respectively. These results support output-specific model selection rather than identifying a single model as superior across all predicted characteristics.

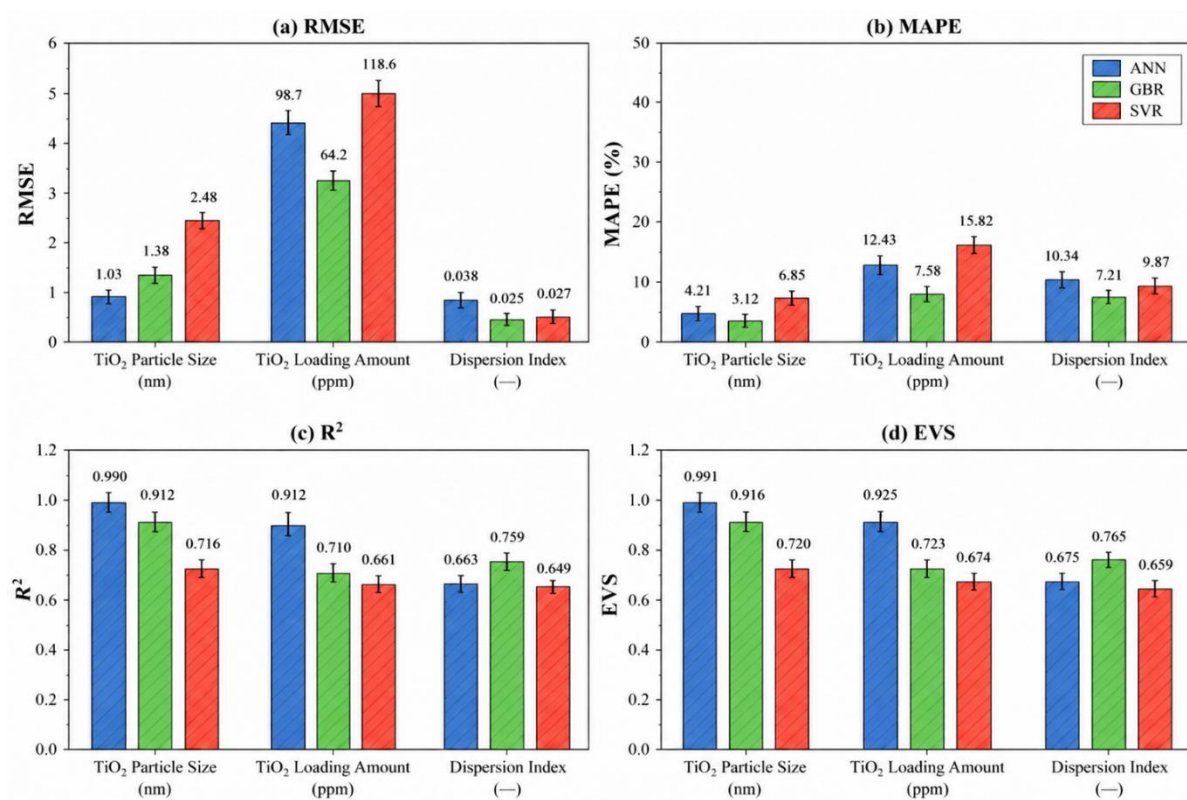


Figure 3. Comparison of prediction performance metrics for ANN, GBR, and SVR models.

Figure 4 presents the relative prediction errors of ANN, GBR and SVR for nanoparticle size, TiO₂ loading and dispersion index. The dashed horizontal lines indicate zero prediction error, while positive and negative values indicate overprediction and underprediction, respectively. These plots complement the aggregate performance metrics in Figure 3 by showing the distribution of prediction errors across the experimental values.

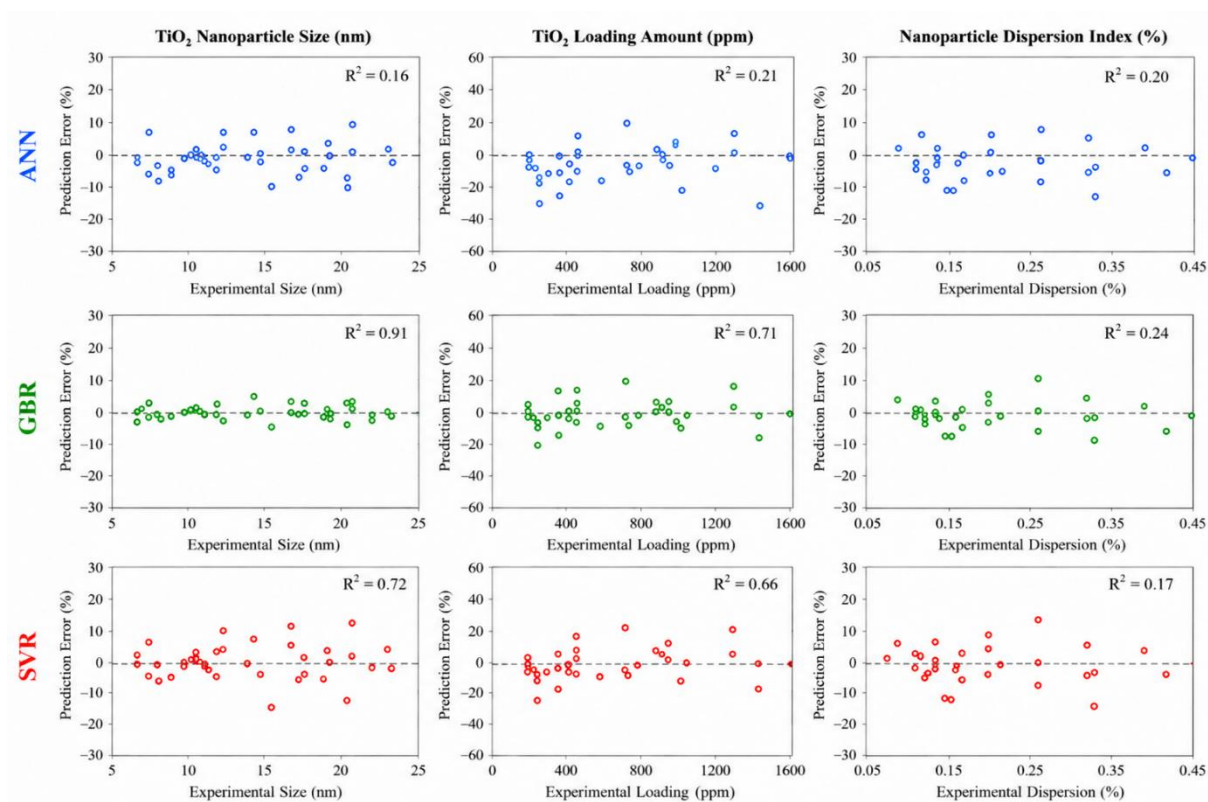


Figure 4. Residual error analysis of ANN, GBR, and SVR models for predicting TiO₂ nanoparticle size, TiO₂ loading amount, and nanoparticle dispersion index.

Computer vision analysis was employed to characterize TiO₂ nanoparticles from SEM images, as illustrated in Figure 5. The image-processing workflow included preprocessing, edge detection, segmentation, particle recognition and size classification. It was applied to detect particles and estimate their size distribution. However, its measurement accuracy was not independently quantified against manual annotations. Independent validation of particle-size estimates, counting performance and SVM classification therefore remains necessary. The workflow demonstrates the potential of computer vision to support automated characterization of nanoparticle-coated composites.

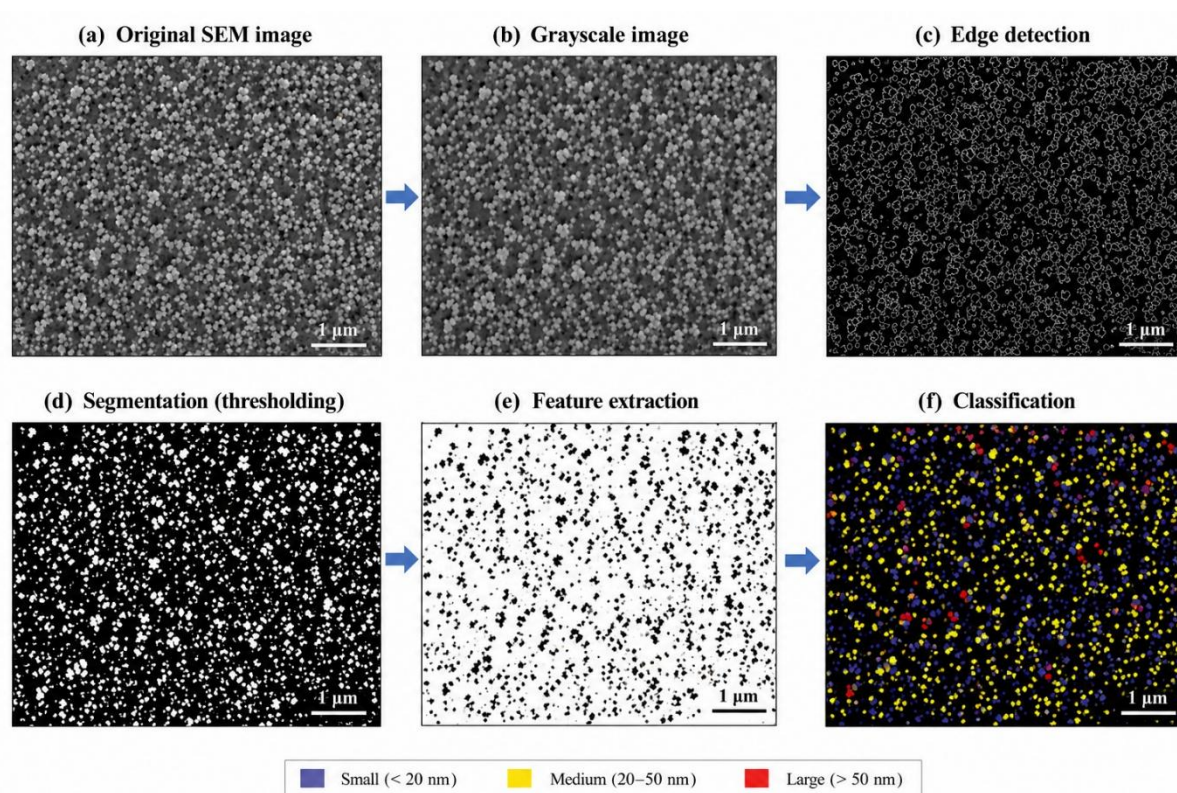


Figure 5. Computer vision workflow for TiO₂ nanoparticle analysis, including SEM image acquisition, grayscale conversion, edge detection, threshold segmentation, feature extraction, and particle classification.

Figures 2 and 3 summarize the predictive performance of the investigated models. ANN achieved the highest R^2 for nanoparticle size and TiO₂ loading, whereas GBR achieved the highest R^2 and lowest RMSE for dispersion index. The results support output-specific model selection. Together with the SEM image-analysis workflow shown in Figure 5, predictive modeling provides a framework for characterizing TiO₂–cotton composites and investigating relationships between synthesis conditions and structural characteristics.

4. Conclusion

This study presented an AI-driven framework for modeling the process–structure relationship of sonochemically synthesized TiO₂–cotton composites using machine learning and computer vision. ANN, GBR and SVR were evaluated for predicting nanoparticle size, TiO₂ loading and dispersion index from six processing variables. ANN achieved the highest R^2 for nanoparticle size (0.990) and TiO₂ loading (0.912), whereas GBR achieved the highest R^2 (0.759) and lowest RMSE (0.025) for dispersion index. The results indicate that model selection should consider the target characteristic and evaluation metric.

Furthermore, the computer vision framework successfully automated the analysis of SEM images through image preprocessing, segmentation, feature extraction, and particle classification, enabling rapid and quantitative characterization of nanoparticle morphology. The integration of machine learning and computer vision provides an efficient approach for optimizing sonochemical synthesis conditions while reducing experimental effort and analysis time. The proposed framework demonstrates the potential of AI-driven techniques for intelligent materials processing and offers a practical tool for the design and characterization of functional TiO₂–cotton composites.

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