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REVIEW ARTICLE

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Integration of response surface methodology (RSM), machine learning (ML), and artificial intelligence (AI) for enhancing properties of polymeric nanocomposites-A review

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Abstract

This review elucidates the amalgamation of machine learning (ML), artificial intelligence (AI), and response surface methodology (RSM) for the optimization of fabrication and the enhancement of the properties of polymeric nanocomposites. It analyzes recent accomplishments, methodologies, and future possibilities in this interdisciplinary field. Polymers and their nanocomposites are garnering attention because of their cost-effectiveness, biodegradability, and non-toxicity. Polymeric nanocomposites have been employed in several technical applications; nevertheless, their restricted mechanical, electrical, and thermal properties have impeded their extensive use. Numerous additives, including clay, fiber, and two-dimensional materials such as graphene or MoS_2, were extensively employed as nanofillers to enhance their qualities. The effects of filler concentration are thoroughly examined by conventional approaches; however, optimization via statistical techniques may be more

Abbreviations: ANN, Artificial neural network; AFM, Atomic force microscopy; AV, Actual value; BA, Boric acid; BB, Box–Behnken; BN, Boron nitride; CCD, Central composite design; CCRD, Central composite rotatable design; CNT, Carbon nanotube; COF, Coefficient of friction; $CaCO_3$, Calcium carbonate; DF, Desirability function; DOE, design of experiment; EDX, Energy dispersive X-rays; EGNPs, Exfoliated graphite nanoplatelets; EPDM, Ethylene-propylene diene monomer; EMI, Electromagnetic interface; FC, Fuel cell; FM, Flexural modulus; FS, Flexural strength; FTIR, Fourier-transform infrared spectroscopy; HVAC, Heat ventilation and Air conditioning; LDPE, Low-density polyethylene; LLDPE, Linear low-density polyethylene; MAPP, Maleic anhydride polypropylene; MC, Methyl cellulose; MPa, Mega Pascal; MoS_2, Molybdenum disulfide; MWCTs, Multiwalled carbon nanotubes; ML, Machine Learning; NPs, Nano particles; OA, Orthogonal array; PAN, Polyacrylonitrile; PE, Polyethylene; PLA, Polylactic acid; PLGA, Polylactic acid co glycolic acid; PP, Polypropylene; PS, Polystyrene; PSF, Polysulfone; PTFE, Polytetrafluoroethylene; PV, Predicted value; PVA, Polyvinyl alcohol; PVDF, Polyvinylidene fluoride; RSM, Response surface methodology; SC, Super capacitor; SEM, Scanning electron microscopy; SEBS, Styrene ethylene butylene styrene; SF, Sisal fiber; SIBS, Styrene-isobutylene-styrene; SiO_2, Silicon dioxide; SEBS, Styrene-ethylene-butylene-styrene; SRT, Scrap rubber tire; T_g, Glass transition temperature; TM, Taguchi Method; TMDs, Tri metal dichalcogenides; UTS, Ultimate tensile strength; UTM, Universal testing machine; XGnPs, Exfoliated Graphene Nano platelets; XRD, X-ray diffraction; AI, Artificial intelligence.

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suitable. The optimization method produces accurate results with a reduced number of tests. Diverse statistical techniques, including Taguchi and RSM, alongside ML algorithms, can be employed to ascertain the optimal filler concentration, type, fabrication method, characterization, and process parameters to enhance the properties, manufacturing, or efficiency of polymers or polymer-based nanocomposites. The response surface methodology (RSM) produces superior results compared to Taguchi and conventional methods. Nonetheless, ML/AI can also be utilized to attain additional improvements in the requisite mechanical, thermal, electrical, and electrochemical properties. Recent advancements in the optimization of polymeric nanocomposites are emphasized, and the use of machine learning and artificial intelligence techniques is proposed for future progress.

Highlights

- Summarized techniques to enhance polymeric nanocomposites properties.
- Presented process, production, and additive optimization of various polymers.
- Summarized statistical techniques and ML-based nanocomposites efficiency.
- Future directions: ML and AI to improve polymeric nanocomposite properties.

KEYWORDS

artificial intelligence (AI), engineering applications, machine learning (ML), optimization, polymeric nanocomposites, response surface methodology (RSM)

1 | INTRODUCTION

Polymers are recognized for widespread engineering applications including flexible solar cell,[1] packing,[2] electromagnetic interface (EMI) shielding, fuel cell (FC), super capacitors (SC),[3] bio-photonic devices,[4] aerospace components,[5,6] pharmaceutical and medical apparatus,[7] construction materials[8] and automotive industries.[9,10] They are grasping attention because of their low cost, light weight, degradability, and nontoxicity.[11–13] To make them viable for diverse functionalities, tremendous efforts have been recorded to enhance their properties (mechanical, structural, electrochemical) by introducing various additives (e.g., sisal fiber, clay, Graphene),[14] Molybdenum disulfide (MoS_2),[15] boron nitride (BN),[16] multiwalled carbon nanotubes (MWCNTs)[17] and metal dichalcogenides (TMDs) at nano scale level.[18] For instance, initially, the concentration effect (10% ~ 20%) of sisal fiber (SF) and benzoylated sisal fiber (BSF) was investigated on the mechanical properties. Polystyrene (PS) was chosen as the base polymer for comparison.[19] The prepared nanocomposite material with PS@wt.20% of SF significantly increased >10% of the tensile strength compared to pristine PS polymer matrix. Likewise, clay is also effectively incorporated into PS chains to boost their ultimate tensile strength (UTS). After incorporating ~5 wt% nanofiller, the promising increase in mechanical (tensile) strength (>20%) was evident.[20] These studies opened a new window to enhance the mechanochemical features of base polymers with the inclusion of nanofiller materials. Although it could be seen that nanofillers have a positive impact on the properties of base polymers the impact of the concentration of 2D materials has been examined by trial-and-error approaches up to this point. Hit-and-trial methods are typically used randomly for improvement and may not be suitable for systematically enhancing the properties or performance of polymeric nanocomposites. In contrast, optimization through statistical techniques will be suitable for this purpose. Typically, the design of experiments (DOE) technique is a statistical methodology in which independent variables are intentionally varied over many runs in an experimental set scheme to investigate the relationship between independent parameters and responses/output. That includes Taguchi Method (TM), Response Surface Methodology (RSM) and Artificial Neural Network (ANN) which have been used for collecting and analyzing data to give valid conclusions[21–25] and predicting the possible trend of increase of properties of polymers in advance. Such a prediction is extremely useful for making cost-effective decisions regarding the production of polymeric products without sacrificing performance. Although there are numerous optimization techniques available, there is a dearth of literature providing a summary of systematic optimization of polymer-based nanocomposites. Therefore, this review integrates the Taguchi Method (TM), Response Surface Method (RSM) and Machine Learning (ML) and Artificial Intelligence (AI) techniques to optimize the parameter-dependent properties of polymeric nanocomposites. Initially, the basic concepts, definitions, adaptation, and their effective utilization with examples of TM and RSM have been highlighted. Effects of various fillers on polymeric nanocomposites have been investigated using an optimization technique. Then, a systematic discussion about optimizing the process parameters for optimal production of nanocomposites and enhanced properties was provided. These applied statistical methods will be discussed in detail in the following sections. At the end, the incorporations of ML/AI algorithms (autoencoder, support vector machine (SVM)) and their application to optimize the desired properties of polymeric nanocomposites using various inputs have been discussed in brief. Limitations and advantages of these optimization techniques have been discussed. This review paves the way for designing nanocomposites for engineering with improved electromechanical, thermal, and structural properties. The importance of this review article lies in its comprehensive integration of RSM, ML, and AI for optimizing polymeric nanocomposites. This approach has not been explored in previous studies. Similar articles deal with individual aspects such as statistical optimization or modeling, but in this comprehensive review, a holistic perspective is provided by comparing and integrating these methodologies to highlight their combined potential. It provides the current challenges, gaps, and future directions, which make this, review a valuable resource for researchers aiming to leverage cutting-edge computational tools for enhanced material performance. In addition, this article will provide a better understanding of the role of RSM, ML, and AI in improving polymeric nanocomposites and highlighting potential industrial applications. The number of studies published on employing RSM, ML, and AI for improving the properties of polymeric nanocomposites has increased considerably since 2000, with a peak in 2022 (Figure 1). The study includes prediction and optimization of properties of polymeric nanocomposites, modeling of mechanical properties of nanocomposites, and AI-enabled polymer processing technology. In 2023, a study was published in which a novel method combining RSM with AI was developed and compared with traditional methods to optimize electrospun nanofiber production conditions, demonstrating improved mechanical properties. This trend shows that advanced computational methods are increasingly being used to optimize material properties and processing parameters.

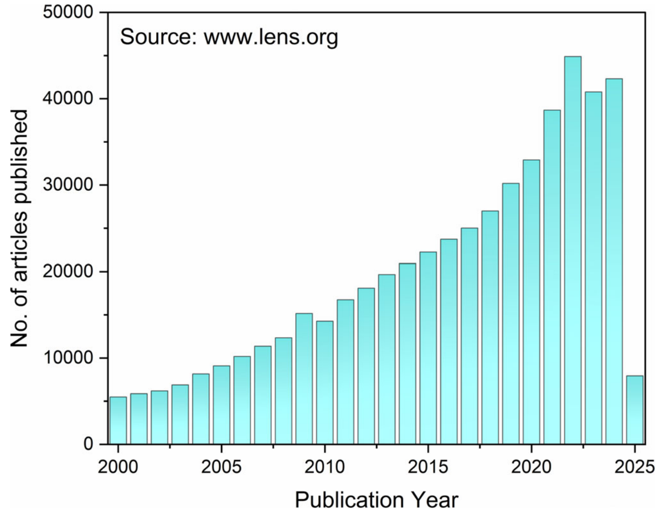


FIGURE 1 Scholarly works published since 2000 in polymer composites (*Source*: www.lens.orG).

2 | PROCEDURES

Optimizing features is an intricate and multidimensional process that requires adjusting multiple parameters to attain certain performance characteristics. In this study, a systematic approach was followed to explore the integration of RSM, ML, and AI for optimizing the properties, production, performance parameters, and additive selection of polymeric nanocomposites. Initially, a literature review was conducted to collect relevant studies on the optimization of polymeric nanocomposites using various techniques. The collected data were classified based on the type of base polymers and optimization criteria. The integration of ML and AI was studied to identify key advancements and challenges. Furthermore, various ML algorithms employed for improving nanocomposite properties were reviewed. An assessment of the utilization of polymeric nanocomposites in various applications was also carried out.

2.1 | Optimization of properties of polymeric nanocomposites

Polymeric nanocomposites consist of polymers strengthened with nanoscale fillers, showcasing many qualities such as mechanical strength, electrical conductivity, thermal stability, and barrier properties.[26] However, fully achieving these features necessitates meticulous consideration of certain essential aspects. Choosing suitable polymers with precise chemical and physical characteristics, adjusting nanofiller amount and distribution, controlling processing variables including temperature (T), pressure (P), and curing time, and adding compatibilizers and coupling agents are all essential for the optimization process.[27,28] Most importantly, the interfacial contact, dispersion, and orientation of nanofillers within the polymer matrix, along with the overall microstructure of the nanocomposite, are crucial factors in determining its specific characteristics.[29,30] Advanced optimization techniques such as RSM and TM offer structured methods to investigate parameter space, create effective experiments, gather data, and construct mathematical models that depict the intricate connections between input variables and desired outcomes. By employing these optimization methods, researchers can discover the best combination of parameters that result in nanocomposites with customized properties, greater performance, and increased applicability for various applications.[31–34] Enhancing characteristics in polymeric nanocomposites with RSM and/or Taguchi not only pushes forward materials research but also has significant promise for technical advancements in industries including automotive, aerospace, electronics, energy, and healthcare.

TM is a potent optimization approach commonly applied in engineering and manufacturing. It provides a structured method to enhance product or process design by analyzing the impact of different elements and their interactions on performance attributes. The primary objective of the Taguchi Method is to provide stability and reduce the influence of fluctuations in input factors, such as material characteristics, process settings, and environmental factors, on the final outcome.[35] This method utilizes orthogonal arrays and signal-to-noise ratios to effectively design experiments and evaluate data, allowing researchers to pinpoint the most significant components and ideal parameter configurations. The Taguchi Method is advantageous for optimizing complicated systems with limited resources due to its cost-effectiveness and time efficiency. Engineers and scientists can enhance product quality, minimize variability, improve performance, and provide more reliable and robust solutions to fulfill client needs by using this strategy. For instance, Zheng and co-workers reported the systematic investigation on optimizing the composition for enhanced mechanical properties of polypropylene (PP) (20 ~ 60 wt%), talc (5 ~ 20 wt%) and maleic anhydride grafted polypropylene (MAPP; 0 ~ 5 wt%) composites using Taguchi technique. The SEM image (Figure 2A) illustrates the uniform dispersion of talc in the typical formulated composite materials (PP 20 wt%, talc 5 wt%, and MAPP 0 wt%). For the optimization purpose, Taguchi L9 (3^3) orthogonal array (OA) with full factorial design is employed and nine (09) experiments were conducted to optimize the ultimate tensile strength (UTS), tensile modulus (E), flexural modulus (FM), and flexural strength (FS). The results indicate that the optimum conditions are ~60 wt% Polypropylene, 5 wt% of MAPP and 20 wt% of talc for optimal increase in the aforementioned properties.[36] Similarly, Fittipaldi and co-workers studied the optimization effect of melt temperature (218 ~ 274 °C), mold temperature (50 ~ 120 °C) with injection rate of (45 ~ 120 $mm^3\ s^{-1}$) and packing time (2 ~ 10 s) on Poly(styrene-block-isobutylene-block-styrene) (SIBS) employing Taguchi method. Taguchi L9 (3^3) orthogonal array (OA) was used with three (03) levels and nine (09) experiments were conducted to optimize the ultimate tensile strength (UTS). The predicted value (PV) and actual value (AV) of UTS via Taguchi technique was ~17.96 and ~ 17.25 MPa, respectively.[37] The result indicates that the predicted value has ~3.9% error compared to experimental results, which are relatively low, and in the acceptable range in decision point of view. In parallel, RSM was also applied to compare the results at corresponding testing conditions. The obtained optimal value of melt temperature, injection rate and packing time was 245 °C, 45 $mm^3\ s^{-1}$ and 10 s, respectively. At these optimum conditions, the predicted (RSM) and actual value (experimental results) of UTS was ~17.9 and ~ 17.7 MPa, respectively. SEM images of failure mechanisms and adopted artificial neural network (ANN) structure are shown in Figure 2B,C. The experimentally achieved UTS is ~40% superior to output without optimized parameters. It is also concluded that without compromising the biocompatibility of fiber and reinforcement agent, the closeness between the values (actual vs. predicted) obtained employing RSM is a better optimizing technique than Taguchi method.[37] Furthermore, the optimized input parameters have also a positive impact on the investigation of the failure mechanism. Figure 2D shows that uniform morphology and narrow section failure mechanism at slow (optimized) injection could be achieved subjective to mechanical testing. It is obvious that the righteous choice of applied optimization technique has great influence on the generated outcomes regardless of the input parameters. The Taguchi technique could only be used only when the range of independent factors are definite.[35,37] It could be considered as the limitation of Taguchi optimization. In other words, Taguchi method might not be straight forward approach with continuous factors. In contrast, RSM is another efficient statistical technique commonly used in experimental design and optimization.[38] It provides a systematic and efficient approach to representing and examining the complex relationships between input variables and output results. RSM involves the construction of mathematical models to represent the behavior of a system or process, sometimes employing polynomial regression. By utilizing these models, scientists can

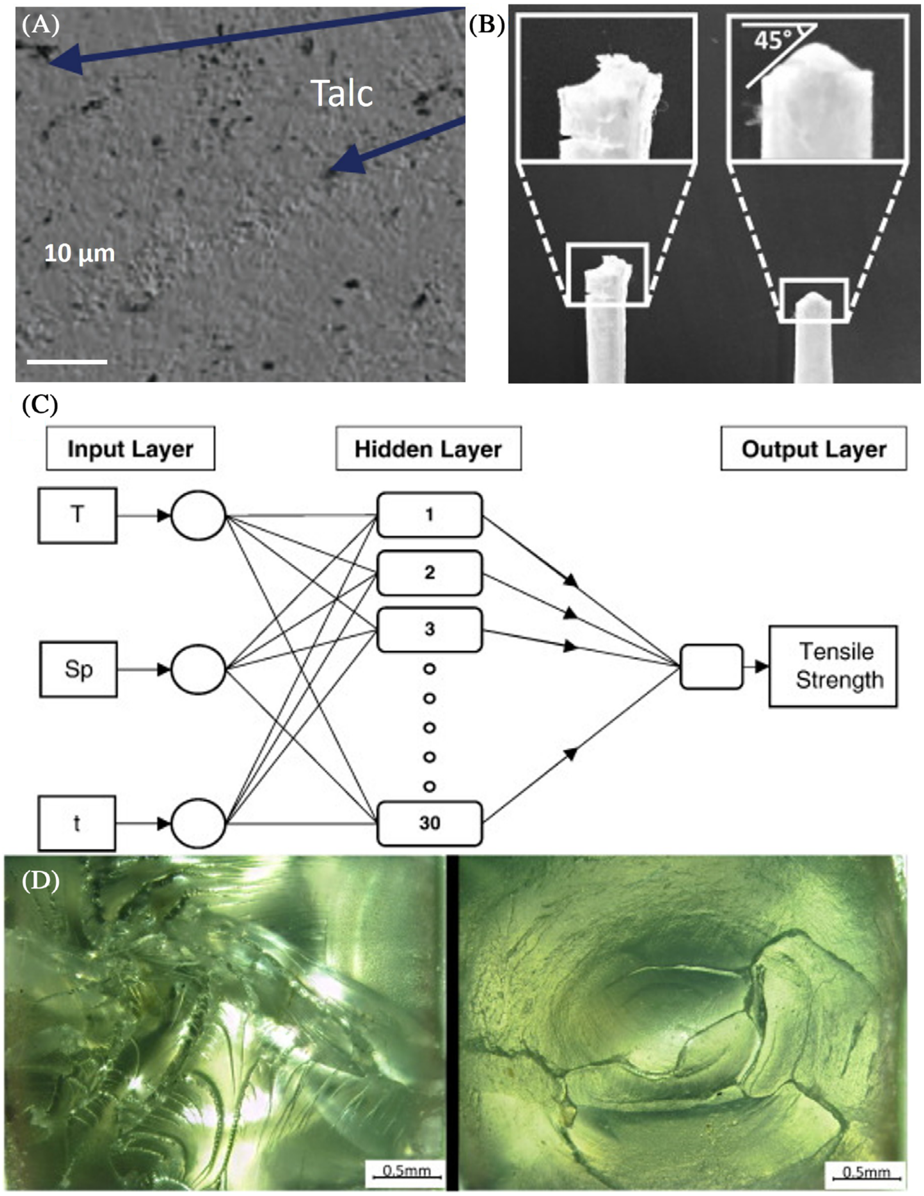


FIGURE 2 (A) Uniform dispersion of talc nanoparticles,[36] (B) Different failure mechanisms at optimized parameters,[37] (C) Adopted ANN structure,[37] (D) Morphological changes after failure.[37]

analyze the response surface and ascertain the optimal input variable combination that produces the intended output response. RSM optimizes resource allocation through the reduction of required experiments while preserving accurate predictions and comprehension of the analyzed system. It is extraordinarily beneficial for understanding the interplay of variables and identifying critical elements that significantly impact the result. It has the potential to be applied in various fields such as manufacturing, engineering, chemistry, and process optimization to improve the quality, efficacy, and performance of products.[39] The desire function (DF) that is provided by RSM is another feature that assists in effectively reaching the ideal level. RSM is able to make more specific predictions regarding square terms and interactions between parameters, whereas Taguchi is only able to make predictions regarding linear interactions. There is the possibility that RSM may generate three-dimensional surfaces of independent variables in order to highlight the influence that independent parameters have on the response that is expected. Comparatively, RSM provides results that are superior or more exact than Taguchi technique.[37,40–43]

As discussed in the previously, an efficient and powerful optimization method using mathematical and statistical methods for empirical modeling is RSM. Use it to optimize input parameters for maximum output. RSM analyses independent variable interactions, unlike other experimental designs. RSM optimization yields accurate data with fewer experiments. Engineers can use RSM in textile, polymer, optical, industrial, and automotive industries.[44] Typically, in RSM three different design

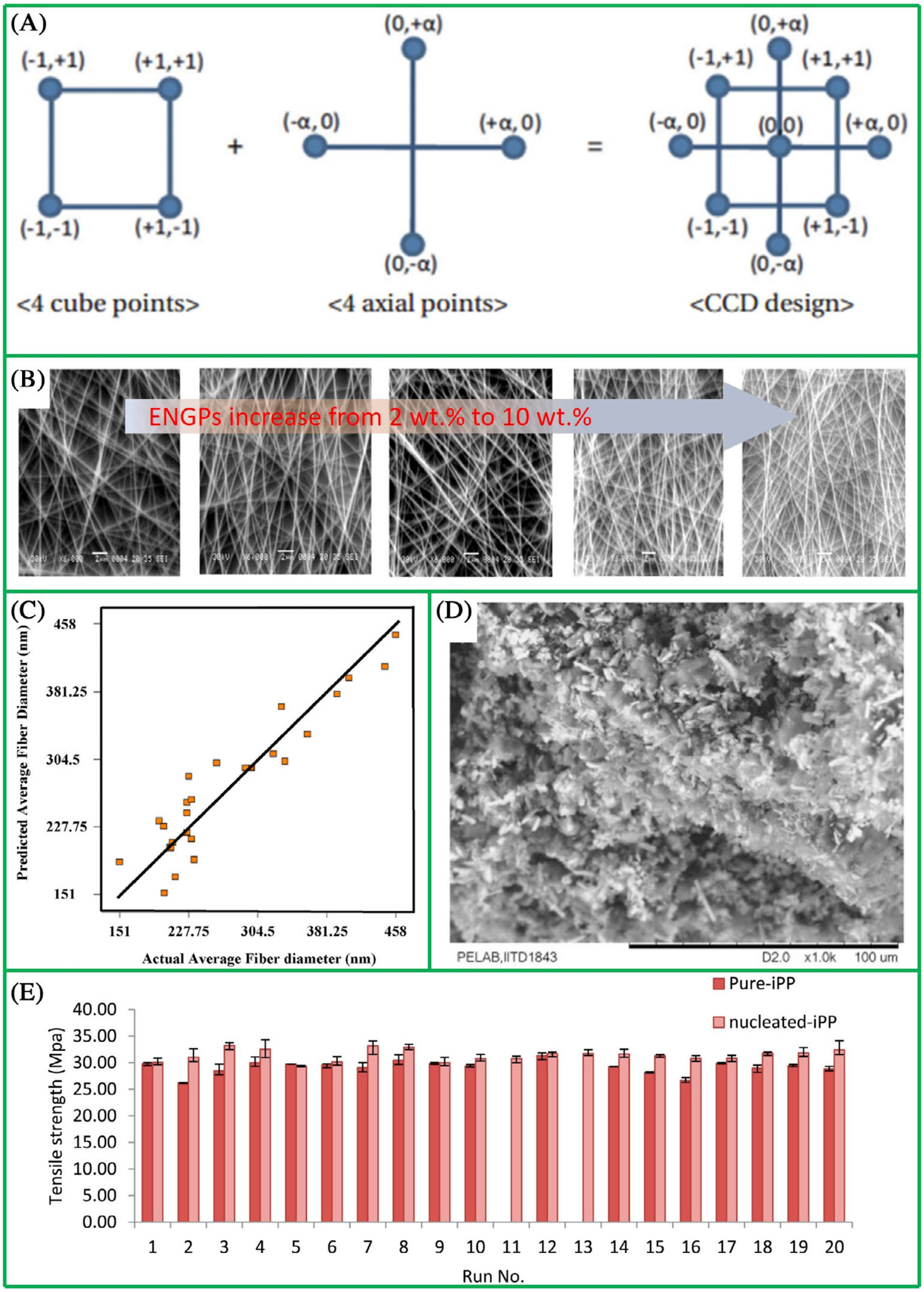


FIGURE 3 (A) Central composite design (CCD),[45] (B) Morphology evolution at 2 wt% ~ 10 wt% of ENGPs,[47] (C) Fitting between the RSM predicted fiber diameter and actual average obtained diameter values,[47] (D) Incorporated α-nucleating agent HPN 20E into nanocomposite,[50] (E) Comparison graph of tensile strength with pure-iPP and nucleated iPP nanocomposites.[50]

points could be analyzed (i) factorial point (−1, 1), (ii) axial point ($-\propto$, $+\propto$) and (iii) center point (0, 0) as shown in the Figure 3A.[45,46] The factorial points are the low and high level of independent variables. Axial or star points are extreme design levels that fall outside the minimum and maximum level of the independent parameters. Center points are midpoint cells that have all their independent variables at their zero level. Center point replica could be used for evaluation of experimental error (age %). The RSM has different design approaches in which Box Behnken (BB)[47] and Central Composite design (CCD)[48–51] are the most used design approaches. In this section of the review we will only focus on the RSM that was applied to different polymeric nanocomposites utilizing polyacrylonitrile (PAN), polystyrene (PS), polyethylene (PE) and polypropylene (PP), polysulfone, and others as a base polymers to optimize the process factors, properties, and production yield of polymers.[52–61] Zoalfakar and coworkers, for instance, computed the average fiber diameter of electrospun polyacrylonitrile (PAN) nanofibers utilizing RSM and the Box-Benkhen (BB) technique. After optimizing electrospinning parameters (19 kV applied voltage, Berry's number of 10, 25° spinning angle, and 16 cm deposition distance), the average PAN fiber diameter was found to be ∼208 nm with a standard deviation of ∼37 nm. The study also investigated the impact of dispersing exfoliated graphite nanoplatelets (EGNPs) on the composite diameter. Figure 3B shows the morphological evolution with the incorporation of EGNPs. At ∼10 wt% EGNPs, a minimum fibril composite diameter of ∼182 nm was obtained. The closeness of actual and predicted values is represented in Figure 3C. These findings provide valuable insights for optimizing fabrication processes and understanding the effect of nanoparticle dispersion on fiber characteristics.

In addition, Rizvi and co-workers employed a design of experiment (DoE) methodology, more precisely response surface methodology (RSM) with a central composite design (CCD), to assess the tensile properties in relation to mold temperature (T_{mold}), melt temperature (T_{melt}), and injection rate. The α-nucleating agent (HPN-20E) was introduced into iPP (polymer matrix) at a weight concentration of ∼1.0 wt% by means of a co-rotating twin-screw extruder operating at laboratory scale. The SEM image (Figure 3D) confirms HPN-20E in the nanocomposite material was successfully incorporated. Following the drying process, the compounded granules were shaped into tensile samples utilizing a micro-injection molding machine. The responses obtained were Young's modulus (E, N. mm), tensile strength (UTS, MPa), and work to break (%age, N. mm) as determined by a universal testing machine (UTM). The findings from the analysis of variance (ANOVA) experiments demonstrated the presence of significant interactions between mold and melt temperatures (T_{mold} vs. T_{melt}), which suggests that their impact on the tensile properties is multifaceted (Figure 3E). Conventional methodologies that manipulate a single parameter sequentially have demonstrated diminished efficacy in establishing a correlation between injection molding variables and tensile properties.[50]

In CCD, the number of experiments is greater compared to BB design (CCD > BB experiments). The second order polynomial equation for obtaining response is given in Equation 1:

$$y=\beta_0+\sum_{i=1}^{k}\beta_i x_i+\sum_{i=1}^{k}\beta_{ii}\overset{2}{\underset{i}{x}}+\sum_{\substack{i=1\\ i<j}}^{k-1}\ \sum_{j=2}^{k}\beta_{ij}x_i x_j+\in \tag{1}$$

Here y is the response, $x_i\, and\, x_j$ are the coded values for ith and jth variables respectively and β_0 is a constant and $\in$ is the error.[62] Various tests such as ANOVA, lack of fit, regression analysis and sum of square could be obtained and conducted to validate the competence of chosen model. Independent parameters could be assessed or identified by conducting these tests. Significance of the polynomial equations can be evaluated by using ANOVA. Regression would be significant and lack of fit would be non-significant for a well fitted model. Various terms of the model will be significant depends on probability value termed as p-value. The $p < 0.05$ indicates significance and $p < 0.001$ will be considered as highly significant. To estimate significance of model, Fischer's test termed as F-test could be conducted. Significance of every term of the model can be tested by the F-test value and p-value. To measure quality of well fitted model, value of coefficient of determination (RS) and adjusted coefficient of determination (adj-RS) could be determined.[63–66] A model will be well fitted for actual data if the RS value is close to value 1 and value of RS should be <0.80 for a well fitted model. High RS (typically >0.80) value demonstrate reasonable closeness between the predicted and observed results and shows the adequacy of the model. From previous studies it is observed that value of RS greater than 0.75 is acceptable. Closeness between RS and adj-RS value shows that non-significant terms have omitted from the model and demonstrate adequate accuracy of the model.[67–73] This commentary represented the RSM working and acceptable level of parameters with various tests. Thus the next section will focused on the optimization of performance parameters of various base polymers employing RSM.

2.2 | Optimization of performance parameters

It is essential to optimize the performance parameters of polymeric nanocomposites to improve their properties and facilitate different applications. Important parameters such as filler content, dispersion, interfacial interactions, and processing conditions must be thoroughly evaluated. Optimizing filler loading helps achieve a balance between reinforcing and filler agglomeration. Even distribution of fillers in the polymer matrix improves mechanical characteristics and decreases chances of failure. Enhanced interfacial bonding enhances load distribution, while adjusting manufacturing conditions enables manipulation of the material's microstructure. Specific features can be attained by taking into account the needs of the application and the surrounding conditions. Enhancing performance parameters allows for the creation of sophisticated materials with enhanced characteristics. Polylactide co-glycolide (PLGA) nanoparticles are a versatile and promising foundation polymer for developing nanocomposites. PLGA, known for its ability to degrade naturally and compatibility with living tissues, is highly suitable for many medicinal uses [74,75]. Nanocomposites may be customized to display distinct features and functions by integrating nanoparticles into the PLGA matrix. Nanoparticles consist of various components such as metals, metal oxides, and organic compounds, allowing for a wide range of functions to be combined. Nanoparticles improve the mechanical strength, thermal stability, and barrier qualities of PLGA.[76] They also provide unique features including antibacterial activity, drug transport capability, and imaging contrast. Additionally, the regulated release of enclosed medications from PLGA nanocomposites enables precise and prolonged drug administration, showing great potential for cutting-edge biomedical uses [75]. PLGA nanoparticles are a promising basis polymer in nanocomposites for several applications including tissue engineering, drug delivery systems, and diagnostic imaging, leading to new and creative solutions.[75,77] The effects of weight ratio (wt%) of Polylactide co-glycolide (PLGA) to insulin (6 ~ 34 wt: wt) and volume ratio (vol: vol) of poly vinyl alcohol/acetone (5:30 vol.: vol.) on Polylactide co-glycolide nanoparticles were investigated to optimize the insulin entrapment efficiency. Ten (10) experiments were performed which were suggested by central composite design (CCD) to predict the response.

The optimum values of PLGA input parameter to insulin weight ratio and poly vinyl alcohol/acetone volume ratio are 20:30 (wt%: wt%) and 10:15 (vol.: vol.), respectively. The results clearly exhibit that at these optimum conditions the predicted value (PV) of entrapment efficiency was 85% ~ 90%.[78] Likewise, Song and co-workers investigated the effect of the volume ratio (vol: vol.) of organic solvent and aqueous phase (0.1: 0.8 vol.: vol.) with 1 ~ 10 min of duration of homogenization and 2 ~ 6 krpm of agitation speed on Polylactide co-glycolide nanoparticles to optimize the particle size and entrapment efficiency (%). Twenty (20) experimental runs were suggested by RSM to predict response (i.e., entrapment efficiency). The optimum value of the volume ratio of organic solvent and aqueous phase, homogenization duration, and agitation speed were 0.6 vol.: vol., ~4 min and ~ 3.5 krpm, respectively. The obtained results showcase that the optimum condition leads toward the predicted value of particle size and efficiency of ~252.7 nm and 54.52%, respectively.[79]

Polyvinyl alcohol (PVA) and polylactic acid (PLA) are commonly used as primary polymers in polymeric nanocomposites.[80] PVA is a water-soluble artificial polymer known for its exceptional ability to create films, high tensile strength, and flexibility.[81] It has a high level of hydroxyl functionality, making it compatible with different nanofillers and improving the adhesion between the polymer matrix and the filler.[82] These remarkable characteristics make it an outstanding choice for creating nanocomposites with enhanced mechanical, barrier, and thermal properties. Coles and co-workers successfully prepared the nanocomposites of PVA via electro-spinning method. They investigated the effect of electrostatic potential (5 ~ 15 KV) with 5 ~ 15 cm of collection distance, concentration of polyvinyl alcohol and polylactic acid solution (6 ~ 13.4 wt%) and conductivity (salt or no salt) on base polymer through 30 experiments by design of experiment to optimize the several responses. Their results revealed that the deposition rate, current and fiber diameter were the most response parameters, and their optimized values ensure highest output. It was found to be that rate of deposition and fiber diameter increasing with concentration (6% ~ 10.6%) and potential difference (10 ~ 15 KV).[83] These findings could provide insights on the PVA based nanocomposites at low and high concentrations for RSM based optimized performance of nanocomposites. On the other hand, PLA is a biodegradable polymer made from renewable sources like corn starch or sugarcane.[84] In recent years, it has garnered considerable attention because of its environmental advantages and biocompatibility. PLA has excellent mechanical strength and thermal stability, making it a great option for a variety of engineering applications.[85] When utilized as the foundational polymer in nanocomposites, PLA provides the benefit of effortless integration with various nanoparticles, resulting in improved characteristics including heightened tensile strength, enhanced thermal stability, and decreased gas permeability. The synergistic effects arise from combining PVA and PLA as basic polymers in polymeric nanocomposites.[86] PVA offers superior film-forming characteristics and increased interfacial adhesion, while PLA offers biodegradability and higher mechanical qualities. The nanocomposites show improved tensile strength, excellent gas and moisture barrier characteristics, and higher thermal stability. The combination of these polymers enables the creation of sustainable nanocomposites with a minimized environmental footprint. Another high-performance engineering polymer Polysulfone, is being widely studied as a basis material for creating nanocomposites because of its outstanding thermal stability with glass transition temperature (T_g) ranging from 185 ~ 190 °C, impressive mechanical strength, and remarkable chemical resistance. This polymer has a distinctive set of features that make it well-suited for a variety of applications, such as membrane technology, biomedical devices, aerospace components, and electronic packaging. Researchers are seeking to improve the features of polysulfone matrices and customize their performance for specific uses by integrating nanoparticles into them. Integrating nanoparticles provides the chance to enhance mechanical properties, thermal stability, gas separation efficiency, and electrical conductivity, along with other desired traits. Moreover, the ability of polysulfone to be compatible with a variety of nanoparticles makes it an ideal platform for investigating the combined effects and potential synergies between the polymer and nanofillers. It is essential to recognize the significance of polysulfone as a fundamental polymer for nanocomposites in order to progress the creation of functional materials with improved performance and expand their practical uses. For instance, Ng and co-workers studied the effect of silicon dioxide ($0 \sim 12$ wt %) and polyvinyl alcohol ($0 \sim 2$ wt%) on polysulfone membrane utilizing RSM as an optimization technique. The RSM generated surface plots (Figure 4A,B) represents the optimized parametric condition. The successful formation of nanocomposites (PSF + SiO_2 and PSF + PVA) is confirmed with FTIR as the stretching of C═C in the benzene ring (PSF + SiO_2) and overlapping of C═C, C—H stretch (PSF + PVA) could be observed from Figure 4C. The Central Composite design (CCD) with 5 levels was used and 13 experiments runs were performed to optimize the permeability and salt rejection of polysulfone membrane. The predicted value of permeability and salt rejection was 40.4274 $Lm^{-2}h^{-1}bar^{-1}$ and 82.1253% respectively, at 10.24 wt% of silica nanoparticles and 1.71 wt% of polyvinyl alcohol. At these optimum conditions, the predicted value of permeability and salt rejection was 61.9260 $Lm^{-2}h^{-1}bar^{-1}$ and 97.5850%, respectively.[87] Agglomeration in materials can negatively impact their mechanical characteristics, leading to decreased strength, reduced toughness, increased brittleness, altered elastic properties, changing fracture behavior, and reduced fatigue life. To reduce these impacts, it is important to use procedures that decrease agglomeration, including appropriate dispersion techniques, surface modification, and monitoring processing parameters. Figure 4D is a schematic illustration of better dispersion to agglomeration of nano particles in nanocomposite materials. Whereas the scanning electron microscopy (SEM) and energy dispersive X-rays (EdX) display the cross-sectional view and well dispersed Si nanoparticles in the fabricated materials with PVA and without PVA incorporation (Figure 4E). Furthermore, minimizing agglomeration can reduce negative effects and enhance the mechanical characteristics of composite materials. In parallel, Jamalludin and co-workers reported the effects of polyethylene glycol ($7 \sim 14$ wt%), triaminopyrimidine (0.5 wt%) and $0 \sim 2.5$ wt% of Graphene oxide on polysulfone membrane using RSM. They also employed CCD to optimize permeability and rejection of polysulfone membrane. Their results revealed that the predicted value of permeability and rejection was 293.678 $Lm^{-2}h^{-1}$ and 92.0001%, respectively at 8.74 wt% of polyethylene glycol, 0.50 wt% of triaminopyrimidine and 2.50 wt% of Graphene oxide. The actual experimental values of permeability and rejection at these optimum levels were 301.562 $Lm^{-2}h^{-1}$ and 91.562%, respectively. These results elucidate the error between predicted and actual values of permeability and rejection were 7.884% and 0.4381% respectively[88] with in the acceptable range. Apart from polysulfone, polyethylene is also a widely used thermoplastic polymer, consisting of repeating ethylene units. While lacking the sulfone group found in polysulfone, polyethylene boasts flexibility, low density, and good impact resistance and inferior thermal stability (T_g; $-100 \sim -130\,°C$). Generally, it also exhibits lower mechanical strength compared to polysulfone and the usage into engineering applications necessitates the enhancement in the thermophysical and mechanical properties. Similar to other nanomaterials Nano zinc/polyethylene (Zn-PE) composites were studied using RSM to determine the influence of talc particles and glass fiber on polyethylene base polymer. In a BB design with three levels, the independent parameters were the applied load ($9.81 \sim 29.43$ kg), the sliding distance ($125.64 \sim 376.92$ m), and the sliding velocity ($0.2904 \sim 0.6282$ m s^{-1}). The wear performance of hybrid nanocomposites was optimized through 15 trials. Disc testers with pins were used for mechanical testing. For polyethylene hybrid composites, the anticipated minimum volume loss and coefficient of friction (COF) were $\sim$9.81 N of applied load, 0.2094 m s^{-1} of sliding velocity, and 222.10 m of sliding distance. When working with glass fiber, the ideal values for applied stress ($\sim$9.81 N), sliding velocity (0.4251 m s^{-1}), and sliding distance (376.92 m) were found.[89] Figure 4F showcases the comparison of volume loss (%) at optimized with RSM and unoptimized conditions. Likewise, SEM image depicting the failure initiated by fractures and grooves within nanocomposite at loading condition (Figure 4G).

Another unique thermoplastic polymer is polystyrene with substantial distinctions in its characteristics. Polystyrene is stiffer and harder than polyethylene, having a glass transition temperature (T_g) of around 100 °C, making it around 2–3 times stiffer than polyethylene. Polystyrene melts at 240–260 °C, whereas low-density polyethylene (LDPE) melts at 120–140 °C and high-density polyethylene (HDPE) melts at 130–140 °C.[90] Polystyrene usually has a melt viscosity of approximately 10^2 to 10^3 Pa·s, and it impacts the flow characteristics during processing. Polystyrene with lack of biodegradability and tendency to become litter are environmental problems, along with inferior tensile and fatigue properties.[91] Owolabi and co-workers employed RSM to obtain the optimal properties of polystyrene-based nanocomposites. They studied the effects of reaction temperature ($60 \sim 120$ °C),

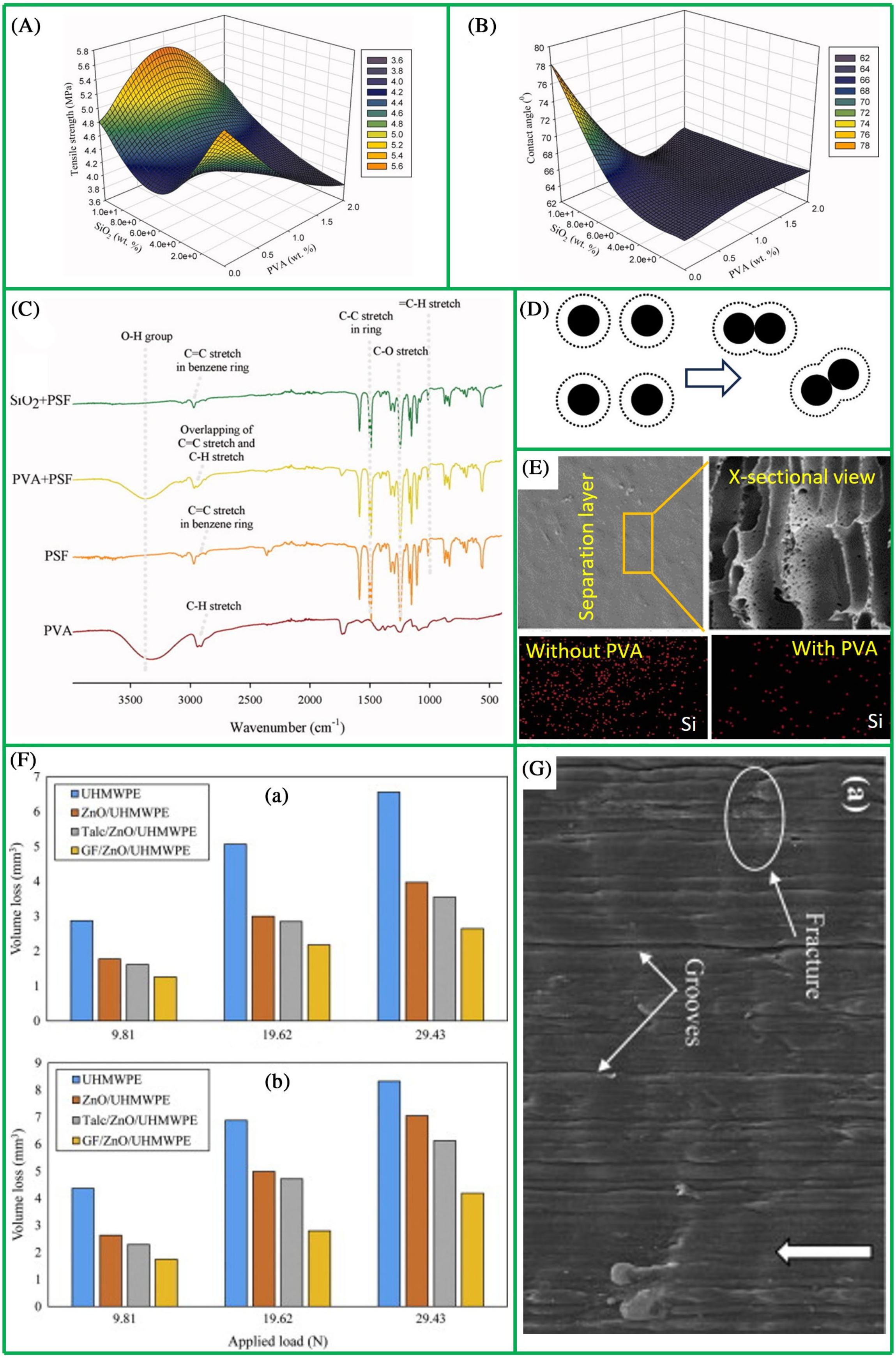


FIGURE 4 Legend on next page.

initiator concentration ($0.0515 \sim 0.1135\ \mathrm{mol\ L^{-1}}$) and reaction time ($30 \sim 70$ min) on solution polymerization of styrene. Their experimental design consisted of a CCD method with 5 levels and 20 combinations to optimize the monomer conversion. The optimized value of reaction temperature, initiator concentration, and reaction time was 120 °C, $0.1135\ \mathrm{mol\ L^{-1}}$, and 30 min, respectively. At these optimum conditions, the predicted and actual experimental values of monomer conversion were 76.82% and 70.86%, respectively.[92]

The impact of nanoflake dispersion and filler loading on the mechanical property of polymeric nanocomposites is also crucial. The distribution of nanoflakes in the polymer matrix significantly affects the material's overall performance. Nanoflakes that are well-dispersed create a strong link with the polymer, allowing for effective transmission of load and leading to notable enhancements in mechanical strength, stiffness, and toughness. Poor dispersion can cause agglomeration, which can restrict the reinforcing potential and decrease the mechanical qualities of the material. The filler loading, which refers to the concentration of nanoflakes in the polymer matrix, is also significant. Higher filler loading typically improves mechanical characteristics by increasing reinforcement with a greater concentration of nanoflakes. There is an ideal loading range, but exceeding it might cause a decrease in mechanical characteristics due to greater agglomeration and less contact between the polymer and filler. It is crucial to find the right balance between dispersing nanoflakes and loading fillers to create polymeric nanocomposites with customized mechanical properties for particular uses. Figure 5A schematically represents the high and low filler loading conditions in the polymeric nanocomposite, while dispersion of the flakes is clearly witnessed with the SEM images (Figure 5B). Furthermore, it is underscored that the distribution and concentration of nanoflakes have a significant influence on the mechanical and electrical characteristics of polymeric nanocomposites. For instance, Arshad and coworkers conducted a thorough assessment of the effect of the concentration and distribution of nanoflakes on the characteristics of polystyrene-MoS_2 nanocomposites. Nanocomposites were fabricated using different amounts of MoS_2 nanofiller, namely 0.1, 0.3, 0.5, and 0.7 wt%. They found a clear relationship between the weight percentage of MoS_2 nanofiller and mechanical, electrical, and dielectric properties. The stress–strain behavior, ultimate tensile strength (UTS), and elongation percentage showed a direct correlation with the content of MoS_2 filler (Figure 5C). In addition, the electrical conductivity (measured in $\mathrm{S\ m^{-1}}$) and dielectric loss showed a direct relationship with the weight percentage of MoS_2, as depicted in Figure 5D–F. Furthermore, Raza and co-workers utilized RSM to optimize the input parameters for the enhanced mechanical performance of nanocomposites by considering Graphene wt%, sonication time, and reaction temperature as input factors. Results showed that at ∼0.60 wt% of Graphene, ∼10 min sonication, and a temperature of ∼25 °C, nanocomposites showcased a significant increase in UTS, elongation, and modulus of elasticity (E) by 97.36%, 82.70%, and 174.08%, respectively (Figure 5G). All these findings elucidate that RSM optimization could be beneficial for the optimization of the mechanical, electrical, and dielectric performance of various polymeric nanocomposites. All these findings clearly highlight the effective utilization of RSM in the optimization of performance parameters.

2.3 | Optimization of production

Optimizing the production process of nanocomposites is crucial in the field of advanced materials and manufacturing. Nanocomposites are materials composed of a matrix strengthened by nanoparticles, exhibiting superior properties compared to conventional materials. Optimizing the production of these nanocomposites is crucial since it directly affects their performance, quality, and cost-efficiency. The fine tuning in fabrication parameters includes nanoparticle dispersion, mixing ratios, curing conditions, and processing by concentrating on the optimization process. This careful optimization with RSM allows for exact control and manipulation of the nanocomposites structure, morphology, and properties, resulting in increased mechanical strength, enhanced conductivity, superior thermal stability, and acceptable surface features. Optimizing production processes also leads to efficient resource use, less waste, and higher production output, promoting sustainable and economically feasible manufacturing methods. In this section, the optimization of the production of nanocomposites with respect to various base polymers has been focused. First of all, the effect of organoclay ($2\% \sim 6\%$) and polymerization time ($3 \sim 5$ h) on the

FIGURE 4 (A) Surface plot of tensile strength w.r.t. SiO_2 and PVA wt%,[87] (B) Surface plot of constant angle at optimal conditions of nanoparticles,[87] (C) FTIR spectra of base polymers and obtained nanocomposite materials,[87] (D) Agglomeration and uniform dispersion model within nanocomposite space,[87] (E) SEM micrograph and corresponding EDX elemental mapping of incorporated nanoparticles,[87] (F) Comparison of volume loss (%) at optimized and unoptimized conditions,[89] (G) Failure initiated by fractures and grooves within nanocomposite.[89]

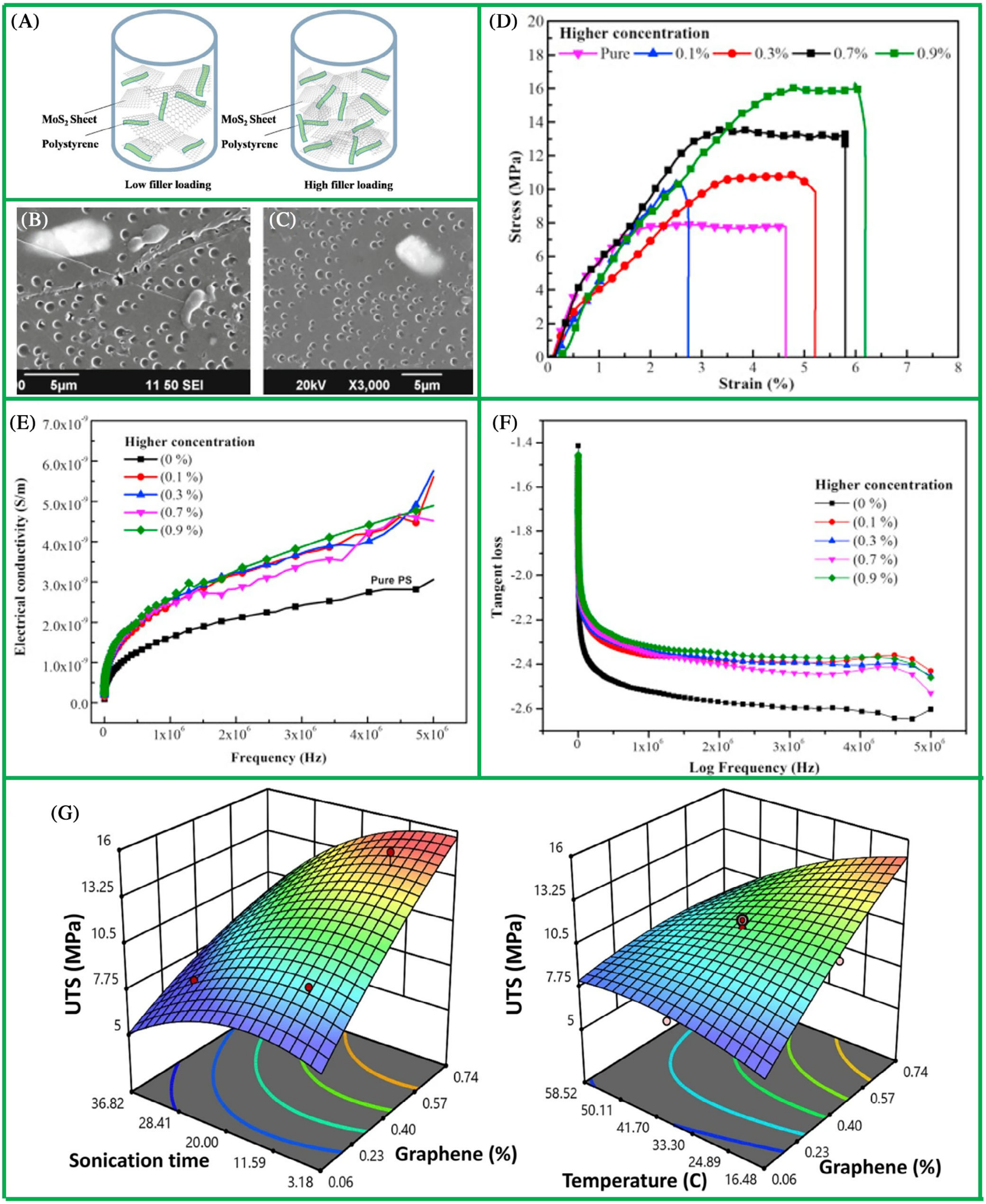


FIGURE 5 (A) Dispersion of nanosheets in the polymer composites,[95] (B, C) Incorporation of nanosheets,[11,18] (D–F) Stress–strain, electrical conductivity, and tangent loss measurement of nanocomposite material,[95] (G) Surface plot of UTS w.r.t. various input parameters.[96]

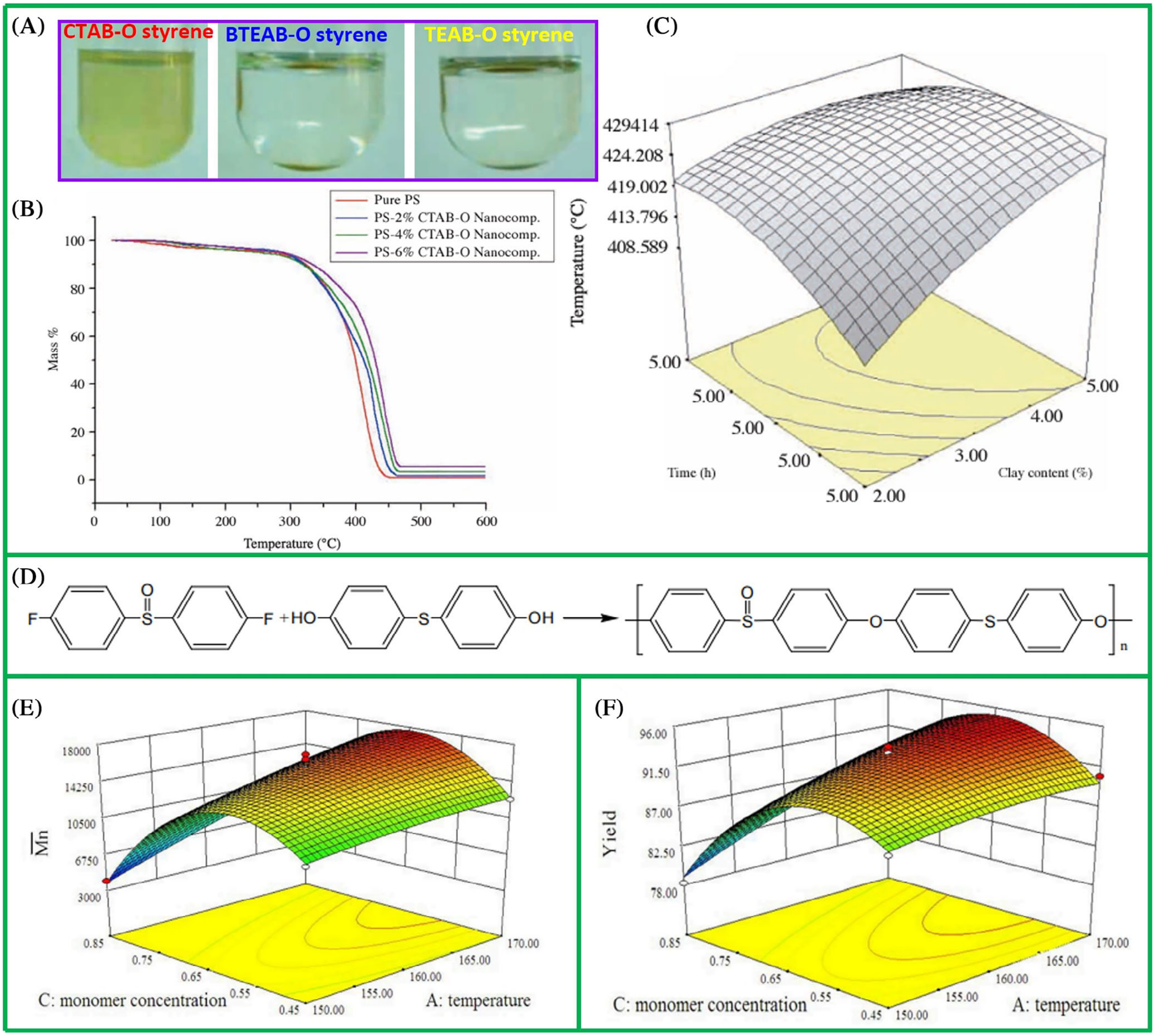


FIGURE 6 (A) Optical images of CTAB-o styrene, BTEAB-o styrene, and TEAB-o styrene mixtures,[93] (B) TGA curves elucidating the thermal stability of polymeric nanocomposites at various nanofillers,[93] (C) Surface plot of optimized temperature,[93] (D) Chemical illustration of PPSOESE synthesis,[97] (E, F) Surface plot of Mn and yield of PPSOESE with independent parameters.[97]

synthesis of Polystyrene/montmorillonite nanocomposites was investigated using RSM. The optical images showcase the variation in solution color of CTAB-O styrene, BTEAB-O styrene, and TEAB-O styrene (Figure 6A). Thermogravimetric analysis (TGA) curves illustrate the thermal stability of generated nanocomposite material. Among all the samples, PS-6% CTAB-O exhibited the highest thermal stability up to >400 °C (Figure 6B). The central composite design with five levels was used, and thirteen (13) experiments were conducted to optimize the mass loss temperature. The optimum value of wt% of organoclay and polymerization time was 6% and 3.8 h, respectively. At these optimum conditions, the highest predicted mass loss temperature was 429 °C (Figure 6C).[93] The effect of temperature (375 ~ 525 °C), heating rate (10 ~ 40 °C min^{-1}) and carrier flow gas rate (50 ~ 200 mL min^{-1}) on waste Polystyrene pyrolysis was investigated using RSM to enhance the styrene recovery. BB design with 03 levels was used, and 18 experiments were performed to optimize the styrene yield. The maximum value of recovered styrene (65.25%) was predicted at 470 ~ 505 °C temperature, 40 °C min^{-1} of heating rate, and 115 ~ 140 mL min^{-1} of carrier gas flow rate. At the optimum condition, the actual obtained value of recovered styrene was 64.52%.[94] Another high-performance thermoplastic polymer is poly(arylene ether-sulfone)s with outstanding mechanical properties, resistance to high temperatures, chemical corrosion, and ignition. These polymers contain arylenes linked with ether and sulfone groups, and some of them even have reactive end groups. Numerous obstacles necessitate thoughtful analysis and novel approaches to the fabrication of nanocomposites of poly(arylene ether-sulfone). To begin with, it is quite difficult to get the nanoparticles evenly distributed throughout the polymer matrix. Mechanical characteristics and performance of the nanocomposite are impaired due to nanoparticles' high surface energy and agglomeration tendency, which prevents their even distribution. Compatibility between nanoparticles and the poly(arylene ether-sulfone) matrix is a prerequisite for obtaining favorable characteristics in the nanocomposite.

The nanoparticles and polymer matrix can have poor interfacial adhesion due to variations in surface chemistry and thermal expansion coefficients, which can limit stress transmission and impede the improvement of mechanical characteristics. To address these challenges in producing Poly(arylene ether-sulfone)s nanocomposites, surface functionalization methods or the application of coupling agents are required to enhance compatibility and reinforce interfacial contacts. Novel strategies for altering surfaces and enhancing the dispersion of nanoparticles in polymers, as well as optimizing production settings, are necessary to address these challenges. For instance, Gu and co-workers studied the optimization of poly (phylene sulfoxide ether sulfide ether) (Figure 6D) nanocomposites fabrication by RSM. Their results revealed that the effect of reaction temperature ($150 \sim 170\ ^{\circ}C$), reaction time ($6 \sim 10$ h) and monomer concentration ($0.45 \sim 0.85$ mol mL^{-1}) on preparation of poly (phylene sulfoxide ether sulfide ether) has a positive impact. In their experimental scheme the BB design with 3 levels was used and 17 experiments were conducted to optimize molecular weight and yield of poly (phylene sulfoxide ether sulfide ether). The optimum value of reaction temperature, reaction time and monomer concentration were 170 °C, 9.13 h and 0.65 mol L^{-1} (Figure 6E,F). The predicted and actual experimental value of molecular weight and yield at optimum condition was 1.80×10^{-4}, 95.5%, 1.78×10^{-4} and 93.6%, respectively.[97]

2.4 | Optimization of mechanical properties

Numerous parameters, such as nanoparticle type, dispersion, interfacial interactions, and processing methods, affect the mechanical performance of polymeric nanocomposites. To attain the intended mechanical properties, including increased strength, stiffness, durability, and resistance to fatigue, an exhaustive comprehension of the fundamental mechanisms and the capability to manipulate the structure of the material with pinpoint accuracy at the nanoscale are essential. Through the optimization of the mechanical properties of polymeric nanocomposites utilizing various kinds of base polymers, the desired application could be realized (Table 1). In this section, we will discuss the effect of nanofillers on various base polymers.

Lin S-S and co-workers investigated the effect of the concentration of polytetrafluoroethylene ($0.04 \sim 0.12$ wt %), short glass fiber ($0.1 \sim 0.2$ wt%) and polycarbonate ($0.68 \sim 0.86$ wt%) on short glass fiber and polytetrafluoroethylene hybrid composites using RSM. The D-optimal design with two levels was used, and 19 experiments were conducted to optimize the tensile strength and flexural strength. Mechanical testing was performed on the 25 KN material testing system. The optimized values of tensile strength (101.38 MPa) and flexural strength (149.49 MPa) were predicted at 0.04% of polytetrafluoroethylene, 0.20% of short glass fiber, and 0.76% of polycarbonate. At these optimum conditions, the actual experimental values of tensile and flexural strength were 103.18 and 145.22 MPa, respectively.[98] Chieng B W and co-workers also used RSM to examine the effect of several process variables and the amount of Graphene on the tensile strength of polylactic acid/Graphene nanocomposites. Graphene loading ($0.1 \sim 0.5$ wt%), temperature ($160 \sim 180\ ^{\circ}C$), time ($10 \sim 20$ min) and speed ($25 \sim 75$ rpm) were used as independent variables in CCD with 3 levels and 30 experiments with 6 center points to optimize the tensile strength of polylactic acid/Graphene nanocomposites as presented. The optimal value of tensile strength ~61.61 MPa was found to be at 0.1 wt% Graphene loading, 160 °C of processing temperature, 10 min of blending, and a rotor speed of 25 rpm. The predicted results were verified by conducting experiments, and it was found that the obtained values were close as compared to the predicted values with some acceptable percentage error, as shown in Table 2.[99] Another study was conducted in which RSM was utilized to enhance the mechanical characteristics of polylactic acid/chitosan composite material containing silver nanoparticles (NPs). Polyethylene glycol with a concentration range of 5% to 25% and the percentage volume of polylactic acid/chitosan ranging from 20% to 80% were the independent variables in a Central Composite Design (CCD) with 5 levels and 12 experimental runs. The goal was to maximize mechanical characteristics, namely tensile strength and elongation at break. Tensile machines were used for mechanical testing. The highest values of tensile strength (about 8.32 MPa) and elongation at break (about 32.15%) were observed at around 7.93 wt% of polyethylene glycol, 28.79% volume of polylactic acid, and 71.21% chitosan. The error between the experimental and

TABLE 1 Summary of several studies utilizing optimization techniques.

Sr. No	Polymer	Filler	Design	Independent Variable	Response	Testing	Remarks	Ref.
1	PLGA	Insulin, poly vinyl alcohol, acetone	CCD	wt. ratio, volume ratio	Entrapment efficiency (%)	N/A	Optimized efficiency	78
2	PLGA	N/A	CCRD	Volume, duration of homogenization and agitation speed	Mean particle size and entrapment efficiency	N/A	Prepared the PLGA NPs.	79
3	Polyvinyl alcohol	Polylactic acid	N/A	Electrostatic potential, collection distance, concentration of polyvinyl alcohol and conductivity	Deposition rate and fiber diameter	N/A	It was concluded that RSM successfully demonstrate the interaction effect between various independent variable.	83
4	Polysulfone	Silicon dioxide and polyvinyl alcohol	CCD	wt% of SiO_2 and polyvinyl alcohol	Permeability and salt rejection	N/A	It was concluded that error was present due to unavoidable parameters.	87
5	Polysulfone	Polyethylene glycol, triaminopyrimidine and Graphene oxide	CCD	wt% of Polyethylene glycol, triaminopyrimidine and Graphene oxide	Permeability and rejection of polysulfone membrane	N/A	It was concluded that predicted and real values are reasonably close to acceptable error. It was also found that the peak of Graphene was reported at 26.22°	88
6	Polyethylene	Fiber and nano ZnO	BB	Applied load, sliding distance and sliding velocity	Wear performance	Pin on disc tester	It was concluded from. the study that RSM successfully finds the most significant parameter	89
7	Polystyrene	N/A	CCD	Reaction temperature, initiator concentration and reaction time	Monomer conversion	N/A	It was concluded that RSM successfully predicted the response and the model suggested by RSM could be used for industrial purpose.	92
8	Polystyrene	Asphalt binder and soyabean oil	N/A	PS molecular weight, PS content and test temperature	Critical low and high temperature	N/A	It was concluded that models suggested by RSM were accurate.	163
9	Polystyrene	Montmorillonite	CCD	wt% of Organoclay polymerization time	Mass loss temperature	N/A	It was concluded that based on p-value, RSM can easily categorize independent variables.	93
10	Polystyrene	N/A	BB	Temperature, heating rate and carrier flow gas rate	Yield	N/A	RSM successfully increased the yield by 12% than the previously reported.	94
11	Poly(phylene-sulfoxide-ether-sulfide-ether)	N/A	BB	Reaction temperature, reaction time and monomer concentration	Average number molecular weight and yield	N/A	It was concluded that for significant model, p-value must be less than 0.05	97

(Continues)

TABLE 1 (Continued)

Sr. No	Polymer	Filler	Design	Independent Variable	Response	Testing	Remarks	Ref.
12	Polycarbonate	Polytetrafluoroethylene and short glass fiber	D-optimal	wt% of polytetrafluoroethylene, short glass fiber and polycarbonate	Tensile strength and Flexural strength	MTS	Less than 3% error was obtained, which demonstrate responses were well optimized.	98
13	Polylactic acid	Graphene	CCD	Graphene loading, temperature, time and speed	Tensile strength	UTM	It was concluded that RSM can predict the response with multiple independent variables, but experiments will increase with an increase of independent factors.	99
14	Polylactic acid	Silver nanoparticles, polyethylene glycol and chitosan	CCD	wt% of polyethylene glycol, % volume of polylactic acid/chitosan	Tensile strength and elongation	UTM	In case of tensile strength, 2.08% error is obtained and in case of elongation, 3.89% error is obtained.	101
15	Methyl cellulose	ZnO nanoparticle and pediocin	CCD	wt% of ZnO nanoparticles and pediocin	Tensile strength, elongation, and load at break	UTM	The optimum value of ZnO nanoparticle and pediocin was reported at 20% and 15% respectively.	102
16	Epoxy	Nano silica or Nano clay	CCD	wt% of Nano silica, nano clay and fiber orientation	Flexural strength	UTM	Predicted and real value of flexural strength was 17.7 MPa and 17.2 MPa, which shows response, is well optimized.	104
17	Epoxy	Nano silica or Nano clay	CCD	wt% of Nano silica, nano clay, and fiber orientation	Tensile and impact strength	UTM and Izod impact machine	RSM successfully increased the tensile strength by 6.4%. RSM also increases the impact strength by 203.5%.	103
18	Poly vinyl alcohol	Nano fiber	CCD	Solution concentration, voltage, and distance	Fiber diameter and tensile strength	UTM	It was concluded that concentration has the highest effect on fiber diameter.	105
19	Poly vinyl alcohol	glycerol, bacterial cellulose, and boric acid	CCRD	Wt % of glycerol, bacterial cellulose, and boric acid	UTS, elongation, elastic modulus, tensile toughness, puncture strength	UTM	Closeness between the predicted values and actual values demonstrates that RSM is a decent optimization technique.	106
20	Polyoxy-methylene	Glass fiber, polytetrafluoroethylene	CCD	PTFE content and PTFE etch time	Tensile strength, elastic modulus, toughness, and hardness	UTM	It was concluded that a factor or process will be well optimized if the value of DF is close to 1.	107
21	Polyethylene	N/A	BB	Temperature, rotational speed, and traverse speed	Flexural strength	Three point bent test using GT-7010 A2	It was concluded that flexural strength would increase at high rotational speed and low traverse speed.	108
22	Polypropylene	ethylene-propylene-diene monomer and Scrap rubber	mixture design	wt % of PP, EPDM and SRT	(i) tensile strength (ii) Impact strength	impact tester and UTM	It was concluded that RSM can easily predict the response with minimal experiments.	109

TABLE 1 (Continued)

Sr. No	Polymer	Filler	Design	Independent Variable	Response	Testing	Remarks	Ref.
23	Polypropylene	Nano clay and $CaCO_3$	BB	(I) Melt flow index of PP (II)wt % of Nano clay and $CaCO_3$	(i) Tensile Modulus (ii) Tensile strength (iii) Impact strength	Zwick machine and Notch charpy impact tester Rezilimpactor	RSM successfully increased the tensile modulus by 45%. RSM also increases the impact strength by 54%.	110
24	Polypropylene	clay/carbon nanotube	CCD	Multiwall CNT %, Mixing speed and Melting temperature	Tensile strength, Young modulus and Elongation	UTM	RSM successfully increased the tensile strength by 57%. RSM also increases the modulus by 63%.	113
25	Polypropylene	Low density polyethylene and titanium oxide	BB	wt% of LLDPE, SEBS and titanium dioxide nano-particles	Tensile strength and elongation at break	Zwick Roell series autograph UTM	It was concluded that all three independent variables have a considerable effect on responses.	111
26	Polypropylene	Silk fiber	BB	Temperature, time, and pressure	Tensile strength, impact strength and flexural	UTM	The closeness between the predicted values and actual values demonstrates that RSM is a decent optimization technique. Values are 98% close to each other.	114
27	Polypropylene	Talc and Graphene	BB	wt % of talc, MAPP, and Graphene	(i) tensile strength, tensile modulus, Impact strength	Zwick/Roell machine and Santam pendulum impact tester	It was concluded that predicted and real values are reasonably close to acceptable error. It was observed that RSM can easily demonstrate the positive or negative effect of independent variables on response with the help of 3D surface plot.	112
28	Polystyrene	Abaca fiber	BB	Wt % of abaca fiber and maleic anhydride	Impact and tensile strength, Tensile and flexural modulus	UTM and Toyoseiki pendulum impact machine	It was concluded from the study that for appropriate model, R-squared should be close to 1. It was also found that RSM can easily predict the large number of responses.	115
29	Polystyrene	Vinyl clay	CCD	Wt % of clay and polybutadiene rubber	Impact strength, flexural strength, and flexural modulus	UTM	Predicted and real values are very close to each other which demonstrate that RSM is a decent optimization technique	116
30	Polystyrene	Nano clay and nano ZnO	CCD	wt% of Nano clay and nano ZnO	UTS, strength at break, elastic modulus, Light index, yellowness index and whiteness index	UTM and (1) Zwick/Roell machine	It was concluded that for an appropriate model, lack of fit must be non-significant otherwise. Predicted and real value must be considerably close.	69

TABLE 2 Verification of experiments at optimum point.

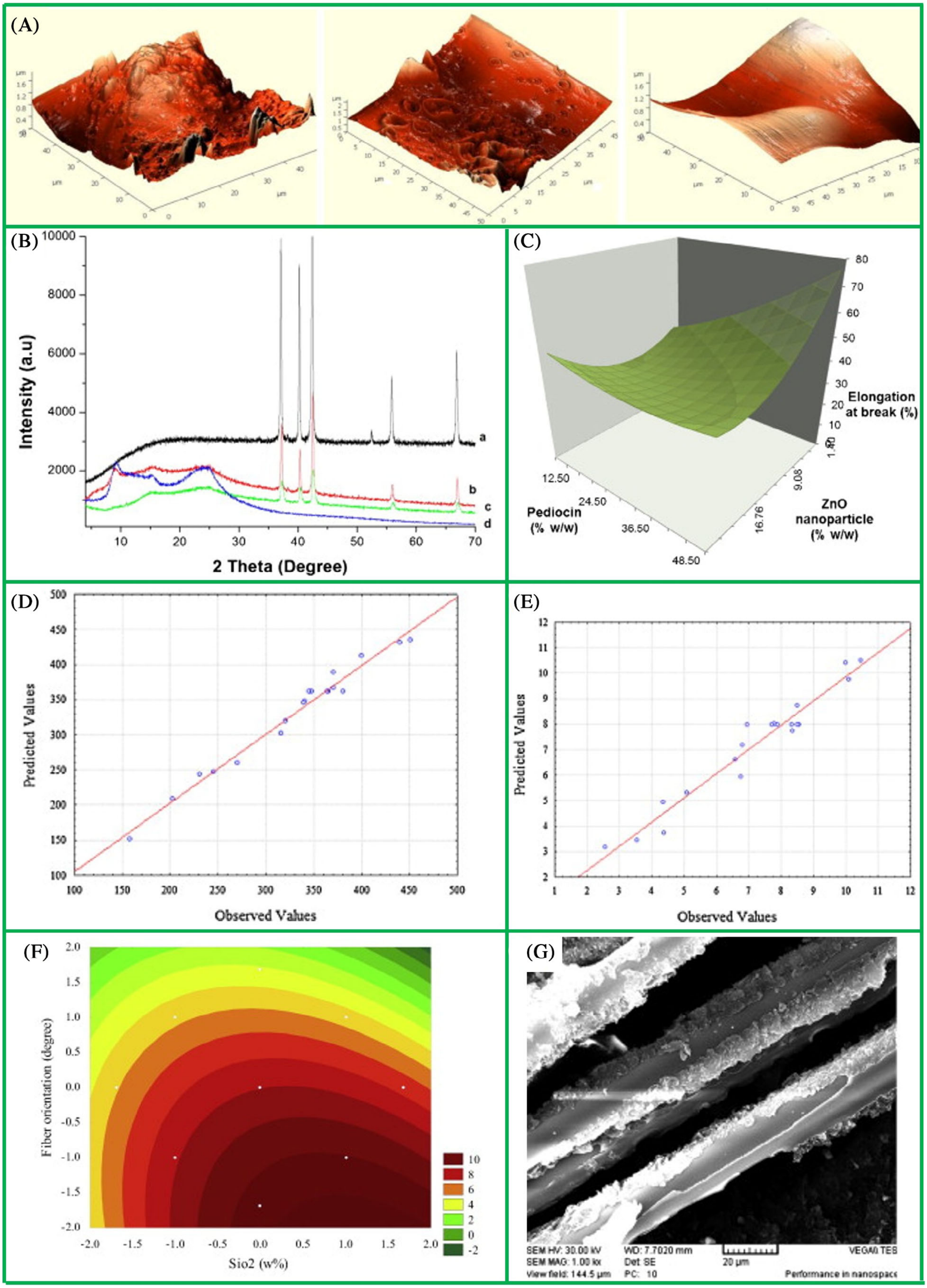
Sr. No	Response				Tensile Strength		
Run #	Graphene (wt%)	Temperature (C)	Time (min)	Speed (RPM)	Predicted Value	Experimental value	Error (%)
1	0.1	160	10	25	61.1662	61.4900	0.53
2	0.1	160	10	25	61.1662	61.8300	1.08
3	0.1	160	10	25	61.1662	62.2300	1.74

TABLE 3 Verification of experiments at optimum point.

Sr. No	Independent factor		Verification		
Response	Concentration of polyethylene glycol	Percentage volume of PLA/chitosan	Predicted Value	Experimental value	Error (%)
Tensile Strength	7.93	28.79	7.99	7.82	2.08
Elongation at break	7.93	28.79	32.6	31.41	3.89

projected values for the concentration of polyethylene glycol was 2.08%, and for the % volume of polylactic acid/chitosan, it was 3.89% as displayed in Table 3.[100,101]

Recently, Methyl cellulose (MC), a copolymer originating from cellulose, shows promise as a fundamental polymer for creating nanocomposites. MC possesses advantageous features including biocompatibility, biodegradability, non-toxicity, and exceptional film-forming capability, which render it a compelling option for many applications. MC, when utilized as the foundational polymer in nanocomposites, offers a secure structure for integrating nanoparticles, enabling the creation of sophisticated materials with superior properties. The hydroxyl groups in MC provide potential for functionalization, allowing for the incorporation of certain chemical functions and enhancing interactions with nanoparticles. Additionally, the rheological characteristics of MC can be adjusted to enhance the dispersion and orientation of nanoparticles, resulting in enhanced mechanical strength, thermal stability, and barrier properties of the nanocomposites produced. The utilization of methyl cellulose as a primary polymer in creating nanocomposites allows for the creation of environmentally friendly materials that may be applied in several industries including packaging, biomedical engineering, and electronics. Espitia and co-workers successfully fabricated nanocomposite films with pediocin and ZnO nanoparticles. The Atomic force microscopy (AFM) images show surface characteristics of nanocomposite material at various ZnO and PED wt%; that is, ZnO (19.5%, 11%, and 0%) and PED (33%, 50%, and 0%), respectively (Figure 7A). Likewise, XRD patterns illustrate the crystal structure variation with incorporation of nano particles (Figure 7B). In addition, the effect of ZnO particles (2.5 ~ 19.5% w: w) and pediocin (15 ~ 50% wt) on co-polymer methyl cellulose/ZnO nanoparticles were investigated by using RSM to optimize the Mechanical properties of methyl cellulose copolymer. Thirteen experiments were conducted which were suggested by CCD to optimize tensile strength, elongation, and load at break. The mechanical testing was performed on UTM and the optimum value of ZnO nanoparticle and pediocin was found to be 20% and 15% respectively (Figure 7C).[102] In another study, Rostamiyan and co-workers used RSM to optimize the mechanical properties of epoxy-based nanocomposites. Glass fiber, nano SiO_2 and nano clay were used as nanofiller. The effect of nano silica (1 ~ 5 wt%), nano clay (1 ~ 5 wt%) and fiber orientation (0° ~ 90°) were selected as independent variables in CCD with 5 levels and 20 experimental runs to optimize the several response that is, flexural strengths, tensile strength, and impact strength and to determine interaction influence between independent variables. Mechanical testing was conducted at UTM. It was found that flexural strength was mainly affected by nano silica while tensile strength was not affected by nano silica. A reverse effect is observed between nano clay and fiber orientation to maximize flexural strength while nonlinear effect of nano clay and interaction between nano silica and nano clay were not significant for impact strength. The closeness of predicted and observed tensile and izod impact strength of nanocomposite film is shown in Figure 7D,E. In the case of flexural strength, the optimum value of nano clay, nano silica and fiber orientation are 4 wt%, 3.5 wt% and 0°. At the RSM generated optimized values (Figure 7F), the maximum value of flexural strength (~17.77 MPa) was



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predicted. In case of tensile strength, the optimum value of nano clay, nano silica and fiber orientation are 1.1 wt %, 3.5 wt% and 9°. At these values, the maximum value of tensile strength (~488.53 MPa) was predicted. In case of impact strength, the optimum value of nano clay, nano silica and fiber orientation are 5 wt%, 4.03 wt% and 0°. At these values, maximum impact strength (11.35 KJ m^{-2}) was predicted. The predicted results were verified by conducting experiments and obtained experimental values of flexural strength, tensile strength and impact strength are ~17.2 MPa, ~480 MPa and (11.1 KJ m^{-2}), respectively.[103,104] In addition, they also observed the fracture mechanism of nanocomposites and SEM image representing the fracture surface morphology at the optimized tensile strength shown in Figure 7G. As discussed in the previous sections, PVA is a highly suitable foundation polymer for the construction of nanocomposites that possess exceptional mechanical properties. The addition of nanoparticles to PVA matrices results in the development of nanocomposite materials that exhibit improved overall strength, rigidity, and toughness. The versatility of these sophisticated materials across multiple sectors demonstrates the potential of nanocomposites based on PVA for the development of next-generation technologies. The Effect of solution concentration (10 ~ 14%), voltage (17 ~ 21 KV) and distance (10 ~ 20 cm) on polyvinyl alcohol nano fiber was investigated through RSM to optimize the mean fiber diameter and tensile strength. The SEM image showcases the morphology of incorporated nanofibers in polymeric composite (Figure 8A). In the optimization process, 20 experiments were conducted which were suggested by central composite design (CCD) to predict the response. The test was conducted at UTM. The optimal value of mean fiber diameter and tensile strength was 98 nm and 4.8 MPa, respectively at ~17.8 KV of voltage, 10.8% of concentration and 18 cm of distance. The actual experimental value of mean fiber diameter and tensile strength was ~95 nm and ~ 4.5 MPa which shows predicted values were reasonably close to experimental values.[105] For optimizing the mechanical characteristics of polyvinyl alcohol nanocomposites, the RSM software was utilized. In order to optimize the UTS, elongation, elastic modulus, toughness, puncture strength, puncture deformation, puncture elastic modulus, and puncture toughness, the effect of glycerol (0% to 50% weight-to-weight ratio), bacterial cellulose nano crystal (0% to 5% weight-to-weight ratio), and boric acid (0% to 15% weight-to-weight ratio) was found to be investigated using CCD with five levels and 20 experimental runs. Mechanical testing was done on a universal material testing machine. The optimum values of UTS, elongation, elastic modulus, tensile toughness, strength of puncture, deformation of puncture, puncture's elastic modulus and puncture's toughness are ~72.84 MPa, 293.43%, ~1867.10 MPa, 91.33 MJ m^{-3}, 4.64 MPa, 31.80%, ~243.63 MPa and ~ 930.16 KJ m^{-3} respectively which were obtained at 13.89% of glycerol, 5% of bacterial cellulose nano crystal and 1.96% of boric acid (BA). The predicted results were verified by conducting experiments and it was found that predicted values were reasonably close to experimental values with acceptable percentage error.[106] The Chain straingtheing mechanism for enhanced properties have also been discussed (Figure 8B). Kunnan Singh JS and co-workers also employed RSM to examine the effect of polytetrafluoroethylene (PTFE) on Mechanical properties of polyoxymethylene/glass fiber/ polytetrafluoroethylene composite. PTFE content (1.7 ~ 7.3 wt%) and PTFE etch time (2.9 ~ 17.1 min) were used as an independent variable in central composite design with two levels and 13 experiments with 5 center points to optimize the different responses that is, tensile strength, elastic modulus, toughness and hardness. The DF method was used to optimize the multiple responses. The target value of tensile strength, elastic modulus, toughness and hardness were set at ~108 MPa, ~8300 MPa, ~2000 KJ m^{-3} and ~ 115 HRR, respectively. It was found that at 6.5% of PTFE content and ~ 10 min of PTFE etching time, the optimal value was achieved. The predicted value of tensile strength, elastic modulus, toughness and hardness were set at ~108.4 MPa, ~8190.5 MPa, 1937.23 KJ m^{-3} and 115 HRR, respectively. Figure 8C,D clearly shows the corresponding SEM images represents the successful inclusion PTFE into polymeric composites film whose properties were optimized.[107] The research highlighted the potential of methyl cellulose (MC), polyvinyl alcohol (PVA), and epoxy-based nanocomposites, refined through statistical techniques (RSM/CCD), for attaining superior mechanical properties (e.g., Espitia's 20% ZnO/15% pediocin in MC films, Rostamiyan's epoxy composites with 3.5% SiO_2). Nonetheless, significant deficiencies persist: (1) **Restricted focus—** excessive emphasis on mechanical properties disregards thermal and electrical performance as well as long-term environmental stability; (2) **Unsubstantiated sustainability assertions—**claims of biodegradability and eco-friendliness are devoid of empirical lifecycle or toxicity

FIGURE 7 (A) AFM images of nanocomposite material at various ZnO and PED wt%,[102] (B) XRD pattern at various ZnO and PED wt%,[102] (C) Surface plot of elongation at break (%) w. r. to ZnO and pediocin nanofillers,[102] (D, E) Closeness of predicted and observed tensile and izod impact strength of nanocomposite film,[103] (F) Contour plot of ultimate izod impact strength (UIS),[103] (G) Fracture surface morphology at the optimized tensile strength value of nanocomposite samples.[103]

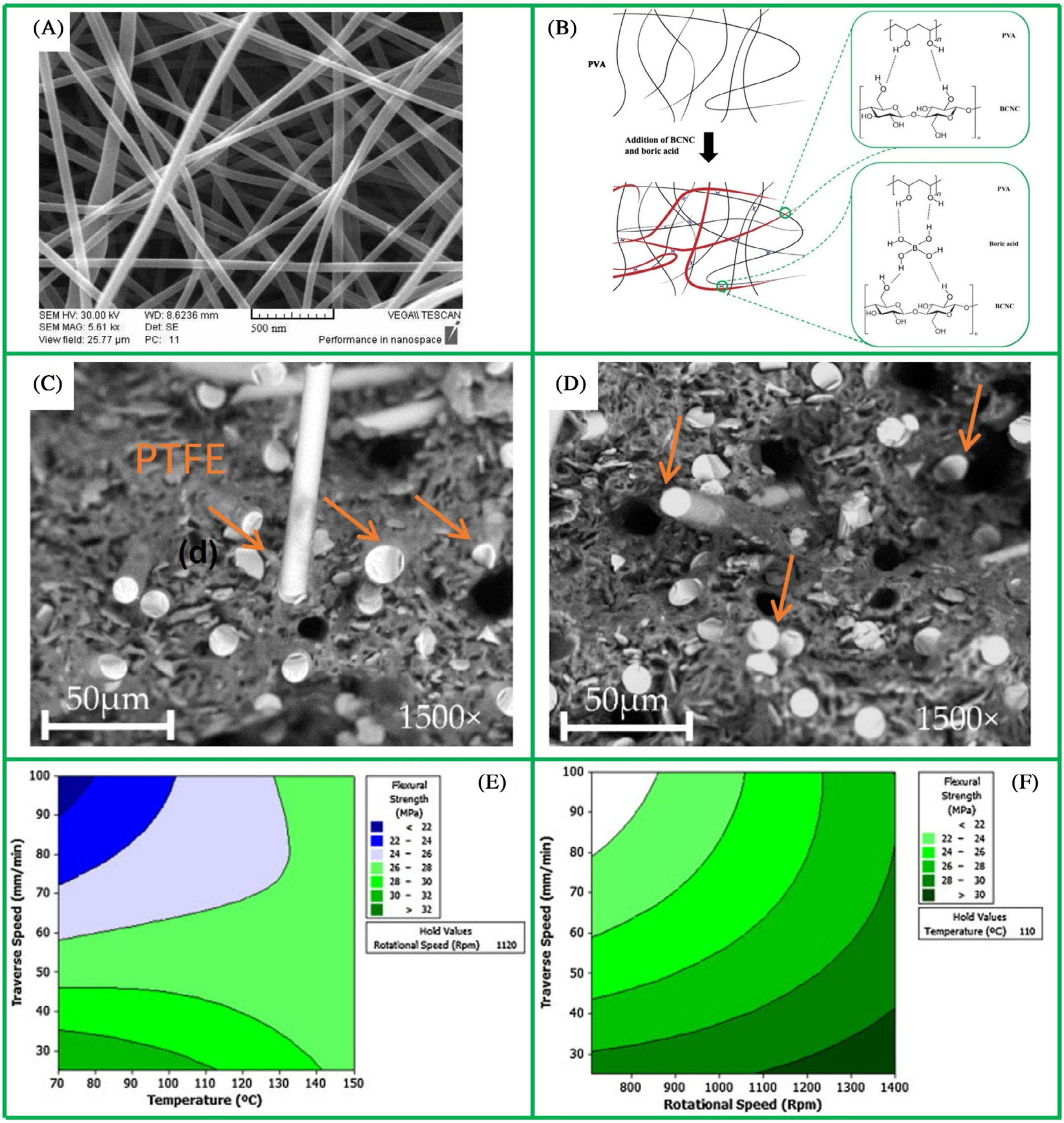

FIGURE 8 (A) Morphology of incorporated nanofibers in polymeric composite,[105] (B) Chain straightening mechanism of polymeric nanocomposites,[106] (C, D) SEM images of PTFE included at various concentrations,[107] (E, F) Contour plots of transverse speed versus temperature (°C) and rotational speed (rpm).[108]

evaluations; (3) **Scalability impediments**—absence of discourse regarding cost, industrial viability, or challenges related to nanoparticle dispersion at scale; (4) **Interaction neglect**—oversimplified assumptions regarding nanoparticle-polymer interactions (e.g., ZnO-pediocin dynamics) may overlook intricate interfacial behaviors. Future endeavors should emphasize multifunctional testing (e.g., thermal and electrical properties for electronics), empirical validation (humidity and UV resistance), environmental impact analyses (degradation kinetics and ecotoxicity), and scalability evaluations (process economics and reproducibility). Interdisciplinary collaboration between materials science, artificial intelligence and machine learning is crucial for transforming these laboratory-scale advances into viable, sustainable solutions.

Azarsa E and Mostafapour A. investigated the effect of different welding parameters that is, temperature ($70 \sim 150\,^{\circ}C$), rotational speed ($710 \sim 1400$ rpm) and traverse speed ($25 \sim 100$ mm min^{-1}) on polyethylene sheet using RSM. The BB design with 3 levels was used and 15 experiments were conducted to optimize the flexural strength of the polyethylene sheet. The flexural strength test was performed by a three-point bending unit using the GT-7010 A2 device. The optimum values of temperature, rotational speed, and traverse speed were $100\,^{\circ}C$, 1400 rpm, and 25 mm min^{-1}, respectively. At these optimum conditions, the maximum value of flexural strength (~33.9 MPa) was predicted which is shown by RSM-generated response of transverse speed versus temperature (°C) and rotational speed (rpm) (Figure 8E,F).[108]

2.5 | Optimization of additives

The attributes of polypropylene may be greatly enhanced by additives, which enable producers to tailor the material to meet certain needs. By integrating additives, it is feasible to improve important characteristics, such as thermal stability, UV resistance, flame retardancy, impact strength, and melt flow behavior. Various groups of additives, such as fillers, reinforcements, plasticizers, stabilizers, flame retardants, lubricants, and colorants, can have an impact on polypropylene. Fillers and reinforcements, such as glass fibers or mineral fillers, could greatly improve the mechanical characteristics of polypropylene, resulting in increased stiffness, strength, and durability. Plasticizers, on the other hand, can increase elongation and flexibility, making it better suited for uses that call for elasticity and impact resistance. Comprehending the impact of additives on polypropylene is of the utmost importance for engineers, researchers, and manufacturers seeking to optimize or develop novel products. Through meticulous selection and integration of appropriate additives and optimized parameters employing the best optimization technique, it is feasible to unleash a wide range of opportunities for polypropylene, customizing its characteristics for specific uses and broadening its potential in the constantly growing field of materials research. For instance, Da Costa and co-workers utilized the RSM technique to optimize the mechanical properties of a polypropylene (PP) ternary mixture in which EPDM and SRT were used as fillers to increase the properties of polypropylene (Figure 9A). The reported results revealed the impact of wt% of polypropylene ($0.5\% \sim 1\%$), EPDM ($0\% \sim 0.25\%$) and SRT ($0\% \sim 0.25\%$) as independent variables in mixture design. The design of experimentation indicates that 13 experimental runs were performed to optimize tensile strength (TS) and impact strength (IS). Testing was performed on the most widely adopted universal testing machine (UTM) and impact tester. The optimum values of polypropylene, EPDM, and scrap rubber tire were found to be ~50%, ~25%, and ~25%, respectively (Figure 9B).[109] The morphology of samples is also characterized to visualize the fracture mechanism as shown in Figure 9C. In addition, RSM was applied to examine the effect of nano-clay and calcium carbonate on the mechanical properties of Polypropylene/nano clay/calcium carbonate ($CaCo_3$) nanocomposites. The surface features of samples were supplemented by AFM (Figure 9D). Their results also revealed that the Melt flow index of polypropylene (4, 10, and 16) g/min^{-1}, content of Nano clay (2, 4, and 6) wt%, and calcium carbonate (8, 14, and 20) wt% were used as independent variables in BB design with 3 levels and 15 experiments to optimize the tensile modulus, tensile strength, and impact strength. Mechanical testing was done on a Z050 Zwick and impact tester. It was found that at a low melt flow index of polypropylene, tensile modulus and tensile strength show a positive effect. Tensile modulus and tensile strength increase with the addition of Nano clay. In the case of calcium carbonate, tensile modulus increases with increasing percentage of calcium carbonate, but tensile strength increases to a certain point and then decreases. Impact strength decreases with the addition of nano clay and calcium carbonate. The optimum Mechanical properties were obtained at g/min^{-1} of melt flow index of polypropylene, 2 wt% of nano clay, and 8 wt% of calcium carbonate, respectively.[110] RSM was applied to optimize process variables of polypropylene ternary nanocomposites to enhance mechanical properties. Clay and carbon nanotubes (CNTs) were used as nanofillers. Multiwall carbon nanotubes ($0.1\% \sim 1\%$), melting temperature ($170 \sim 250\,^{\circ}C$) and mixing speed ($50 \sim 200$ rpm) were used as independent variables in CCD.

Seventeen experiments were conducted to optimize ultimate tensile strength (UTS) and young's modulus (E). Mechanical testing was done on the universal testing machine (UTM). The predicted maximum value of tensile strength and young's modulus was ~ 51.98 and ~ 1757 MPa, respectively, at the optimum level of carbon nanotube loading (0.17%), melting temperature ($165.45\,^{\circ}C$) and mixing speed (119.11 rpm). The obtained experimental values of tensile strength and elastic modulus were ~ 52.30 and ~ 1759.32 MPa, respectively.[113] The effect of PE ($20 \sim 60$ wt %), titanium dioxide ($0 \sim 4$ wt%) and SEBS ($0 \sim 6$ wt%) on PP ternary nanocomposites was investigated by using RSM. Fifteen experiments were conducted, which were suggested by BB design to optimize several responses, that is, tensile strength and elongation. The test was performed at UTM.

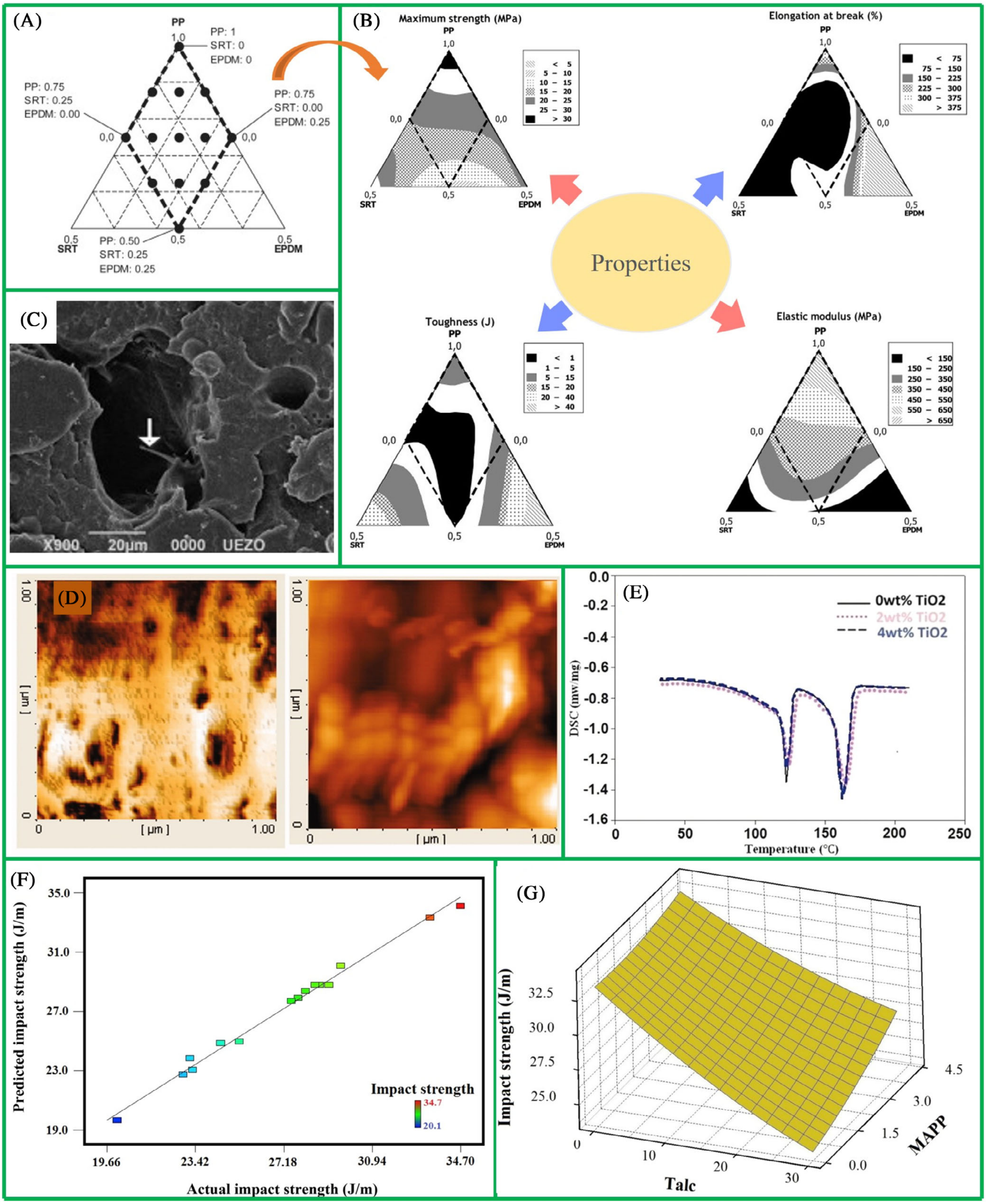

FIGURE 9 (A, B) Representation of three composite design vertices of PP, EPDM, and SRT and corresponding optimized properties,[109] (C) Fracture end of nanocomposite with various wt% of PP, EPDM, and SRT,[109] (D) AFM image of nanocomposite material,[110] (E) DSC graph of nanocomposite material,[111] (F) Closeness of RSM predicted impact strength and actual impact strength,[112] (G) Surface plot of impact strength with different parameters.[112]

The optimum values of LLDPE, titanium oxide, and SEBS were 24.85%, 3.02%, and 6%, respectively. At these optimum values, the maximum value of tensile strength (∼21.41 MPa) and elongation (∼184.47 mm) was predicted. The obtained experimental values of tensile strength and elongation at the optimum condition were 21.89 MPa and 187.73 mm, respectively, which shows the closeness between experimental and predicted values. Furthermore, heat flow through samples has also been investigated, and the DSC graph shows the changes in endothermic heat flow path with the inclusion of 2 and 4 wt% of TiO_2 into the polymeric matrix (Figure 9E).[111] The effect of different process parameters, that is, temperature (165 ∼ 180 °C), time (7 ∼ 15 min) and pressure (35 ∼ 45 bar) on silk fiber/polypropylene composite was investigated using RSM. BB design with 3 levels was used, and 17 experiments were conducted to optimize the tensile, impact, and flexural strength of silk fiber/PP composite. Mechanical testing was performed on UTM and impact strength tester. The optimum values of temperature, time, and pressure were 180 °C, 7 min, and 35 bar, respectively. At these optimum conditions, the predicted values of tensile, impact, and flexural strength were 36.98 MPa, 30.47 KJ m^{-2} and 37.13 MPa, respectively. The actual experimental values of tensile, impact, and flexural strength were 36.16 MPa, 29.03 KJ m^{-2} and 38.12 MPa, respectively, which shows the closeness of the predicted and experimental values.[114] RSM was applied to examine the effect of talc, MAPP, and exfoliated Graphene NPs on the mechanical properties of PP/talc/exfoliated Graphene NPs composite sheet. Talc (0 ∼ 30 wt%), xGnPs (0 ∼ 1.5 wt%) with 0 ∼ 4 wt% of MAPP were used as independent variables in BB design with three coded levels and 15 experimental runs to optimize several responses, that is, tensile modulus, tensile strength, and impact strength. Results showed that xGnPs have a major influence on tensile strength as compared to talc and MAPP, while Talc has a major influence on tensile modulus and impact strength as compared to xGnPs and MAPP, respectively. The optimized results were attained at 30 wt% talc, 4 wt% MAPP, and 0.69 wt% xGnPs with maximum tensile strength, tensile modulus, and impact strength (Figure 9F,G). Predicted values of tensile strength, tensile modulus, and impact strength were ∼ 42.8 MPa, ∼937.9 MPa and ∼ 27.9 J m^{-1}, respectively. Predicted results were verified by conducting experiments, and it was found that experimental values were close to predicted values with some acceptable percentage error (Table 4).[112]

TABLE 4 Results of confirmation experiment for optimal condition.

Response	Predicted value	Experimental value
Tensile strength (MPa)	42.8	43.0 ± 5.1
Tensile modulus (MPa)	937.9	911.7 ± 28.5
Impact strength (J m^{-1})	27.9	27.4 ± 4.9

Likewise, Polypropylene, another thermoplastic polymer that is, Polystyrene, is highly adaptable and has achieved great appeal in a variety of sectors. These benefits stem from its extraordinary clarity, lightweight nature, and superior insulating characteristics. However, to optimize its performance and broaden its scope of use, additives are frequently included into polystyrene matrices. These additives exert a significant impact on the characteristics of the underlying polymer, leading to a wide range of alterations and enhancements. Mechanical properties that is, impact and tensile strength, tensile modulus, flexural strength, and flexural modulus of abaca fiber reinforced high impact strength were optimized using RSM. The effects of abaca fiber (30 ∼ 50 wt%) with 1 ∼ 3 wt% of maleic anhydride and impact modifier (4 ∼ 6 wt%) were investigated for several responses that is, mechanical properties were investigated using box–behnken design with three levels. Mechanical testing was done on a Universal testing machine and toyoseiki pendulum impact machine. Predicted values of impact strength, tensile strength, tensile modulus, flexural strength, and flexural modulus were 59.10 J m^{-1}, ∼12.29 MPa, ∼1.31 GPa, ∼43.81 MPa and ∼ 4.17 GPa respectively at 36.76 wt% abaca fiber, 3 wt% of maleic anhydride, and 4 wt% of impact modifiers with a desirability of 77.37%.[115] The effect of clay (1 ∼ 4 wt%) and polybutadiene rubber (4 ∼ 9 wt%) on Polystyrene/vinyl clay nanocomposites was investigated by RSM to increase the Mechanical properties that is, impact strength, flexural modulus, and flexural strength of Polystyrene/vinyl clay nanocomposites. Thirteen experiments were conducted, which were suggested by central composite design to predict the response. Mechanical testing was done on universal testing machines and impact testing machines. It was found that the optimal value of clay and polybutadiene rubber was 2.69 and 6.54 wt%. At this optimal level, the predicted values of flexural strength, flexural modulus and impact strength were ∼ 47.5471 MPa, ∼2565.22 MPa and ∼ 38.7679 J m^{-1}, respectively.[116] RSM was applied to examine the effect of ZnO and organoclay on Mechanical and color properties of Polystyrene sheet. ZnO (0 ∼ 2 wt%) and organoclay (0 ∼ 7.01 wt%) were used as independent variables in CCD with 5 levels and 13 experimental runs with 5 center points to optimize the different responses that is, UTS, strain at break, elastic modulus, Light index, and whiteness index. The optimized results were attained at 0.81 wt% of ZnO and 0.57 wt% organoclay with the best Mechanical properties. The predicted results were verified by conducting

TABLE 5 Predicted and experimental data for responses at optimum point.

Response	Predicted value	Experimental value	Percentage error
UTS	38.0409	32.74 ± 2.29	13.93
Strain at Break	1.9445	1.89 ± 0.09	2.87
Young modulus	2299.61	2170.83 ± 151.96	5.60
Light Index	57.0479	53.99 ± 0.54	5.36

experiments, and it was found that obtained and predicted values were close to each other with some acceptable percentage error shown in Table 5.[69]

2.6 | Machine learning and artificial intelligence integration

Machine Learning (ML) and Artificial Intelligence (AI) provide robust instruments for the analysis of intricate datasets, pattern recognition, and predictive modeling. In the realm of polymeric nanocomposites, ML and AI tools can enhance nanofiller selection, elucidate structure–property correlations, and optimize processing parameters to accurately predict polymeric nanocomposite desired attributes (Figure 10). These computational techniques can process extensive datasets, derive significant insights, and assist researchers in formulating nanocomposites with customized attributes.

2.6.1 | Material selection

Machine learning (ML) algorithms can aid in the selection of suitable nanofillers and polymer matrices according to certain qualities including ultimate tensile strength (UTS), thermal conductivity (TC), modulus of elasticity, and other electrochemical and dielectric properties. Through the analysis of data regarding the characteristics of various nanofillers and polymers, machine learning algorithms can suggest appropriate pairings for applications.

2.6.2 | Structure–property relationships

There is the potential for artificial intelligence (AI) tools to create correlations between the structure of polymeric nanocomposites (such as filler dispersion and interfacial interactions) and the properties of these nanocomposites. In order to get insights into how different structural aspects influence material performance, researchers can train models using experimental data. This enables them to create nanocomposites with the qualities that they are looking for.

2.6.3 | Optimization of processing parameters

In order to improve the properties of polymeric nanocomposites, machine learning algorithms can be used to optimize processing factors such as curing temperature, mixing duration, and filler loading. The researchers are able to determine the optimal processing parameters by utilizing optimization algorithms. These parameters are designed to optimize the performance of the material while simultaneously decreasing expenses and energy usage.

2.6.4 | Predictive modeling

Predictions of the mechanical, thermal, and electrical properties of polymeric nanocomposites can be made using artificial intelligence models that have been trained on experimental data. Researchers are able to immediately evaluate the performance of new material compositions without having to do extensive experimental testing, thanks to these prediction models, which can function as virtual testing platforms. Machine learning and artificial intelligence both contribute to the efficient development of sophisticated nanocomposites by properly predicting the properties of the materials.

2.7 | ML Algorithms for optimization of nanocomposite properties

Polymeric nanocomposites have undergone ML to anticipate their material properties, optimize procedures, perform microstructural investigations, and quantify uncertainties that may emerge in the material and its properties due to complex production processes. Optimization represents a vital use of ML. The resource-intensive procedure of repeatedly training diverse models is involved, and it may become unmanageable for intricate simulations. The iterative execution of an optimization algorithm entails comparing multiple models to discern viable alternatives until a satisfying result is attained. An optimization problem comprises three essential components: (i) variables, which are the

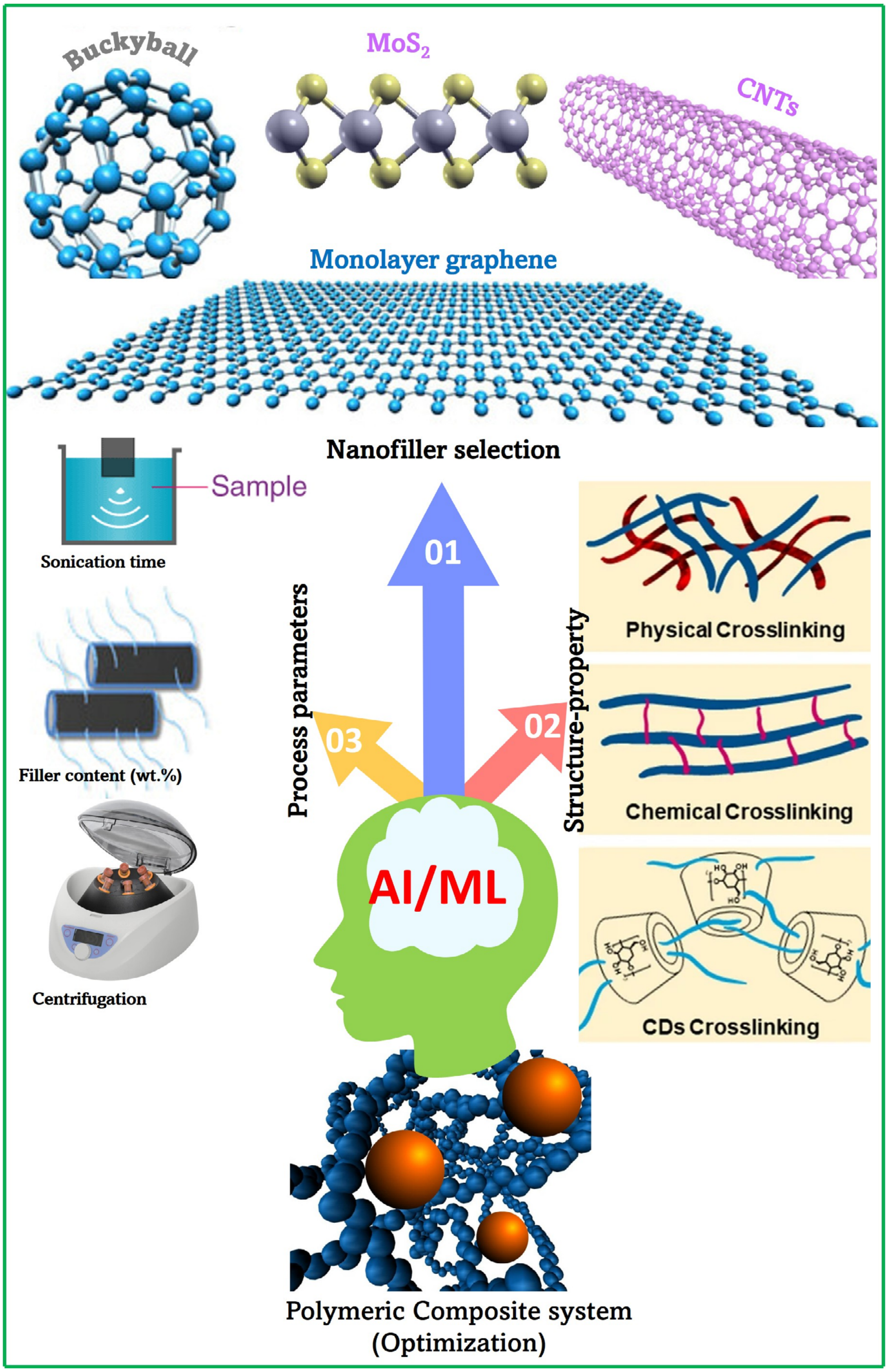

FIGURE 10 Machine learning (ML) and artificial intelligence integration into polymeric nanocomposites material selection, structure– property optimization, process control parameters.

parameters subject to adjustment by the algorithm; (ii) constraints, which delineate the boundaries for these parameters; and (ii) the objective function, which represents the goal the algorithm aims to accomplish. Optimization methods are categorized based on design factors, goal functions, and restrictions. Various ML algorithms (supervised/unsupervised) can be used to improve the performance of polymeric nanocomposites. In unsupervised learning, a machine acquires knowledge alone, without supervision. The machine is trained with a dataset (material selection, polymer matrix, methods and fabrication techniques) that is unlabeled, unclassified, or uncategorized, requiring the algorithm including isolation forest, autoencoder, clustering (K-means, PCA) and one class support vector machine (SVM) to operate on this data autonomously (Figure 11). K-means, in particular, organizes data into a predetermined number of clusters by minimizing the variance within each cluster, which is referred to as inertia. The formula (Equation 2) is employed to determine the inertia:

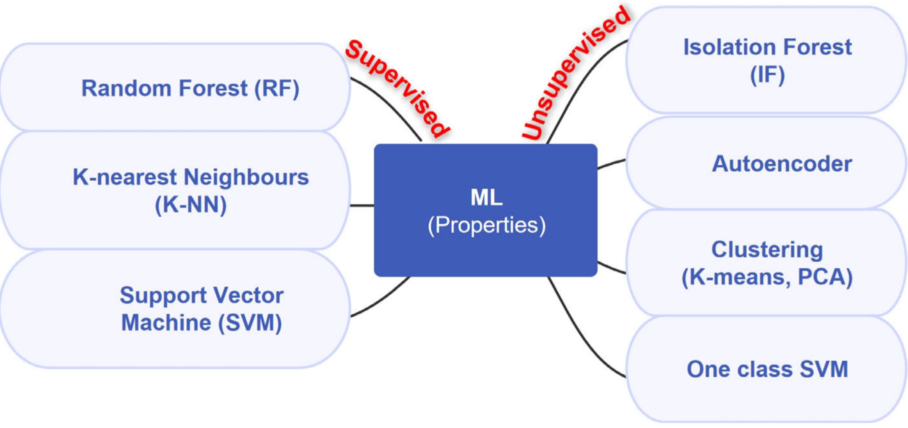

FIGURE 11 Schematically illustrated ML algorithms to optimize the properties of nanocomposites.

$$J(c) = \sum_{i=0}^{N} \min \left[x^{(i)} + \mu_j \right]^2 \quad (2)$$

Another prevalent deep-learning framework is the Autoencoder, which has been extensively utilized in the creation of polymeric nanocomposites and its properties optimization. The architecture consists of an encoder, latent space, and decoder, forming a deep learning model (Figure 12). The fundamental idea is to compress the input data (structural, fabrication parameters and simulation results) via the encoder layer and transform it into latent representations (latent space). The decoder layer is utilized to recreate the input data from the latent space. When anomalous data is communicated through the trained model, it will produce a substantial reconstruction error that is beyond a specified threshold, after a series of network updates and training on normative data. The divergence between the input data and the reconstructed data is referred to as the reconstruction error.

Conversely, "supervised learning" refers to the process whereby an algorithm such as random forest (RF), K-nearest neighbors (k-NN) and SVM acquires knowledge from a training dataset, analogous to a student learning under the guidance of an instructor (Figure 11). Learning ceases when the algorithm achieves an acceptable level of performance. In the nanocomposites setting, a dataset of polymers, types of filler, sonication time, temperature, and so forth with labeling can be used to train the machine for optimized mechanical properties. The schematic representation of SVM is depicted in Figure 13, and the algorithm can be articulated by the subsequent equations:

When integrating multiple data streams from various characterization techniques, fabrication methods, material selection, process control, properties, and modeling, the ability to handle high-dimensional and complex data is one of the key advantages of using ML algorithms for polymeric nanocomposites property optimization,

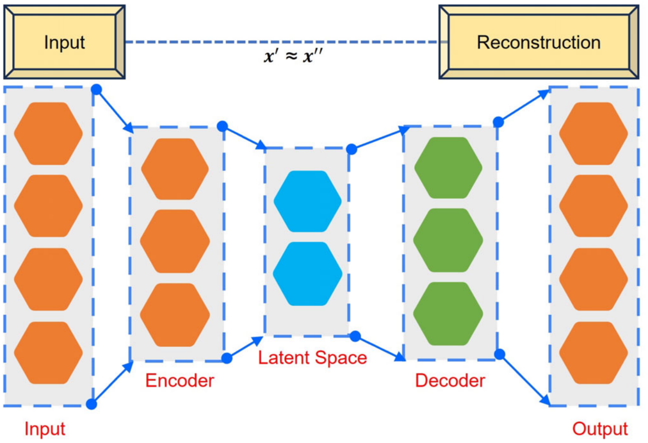

FIGURE 12 Autoencoder/decoder algorithm to optimize the properties of nanocomposites.

particularly deep learning models. One of the primary deep learning methods that is vast in extracting essential discriminative features from high-dimensional or unstructured data, such as images or text, is convolutional neural network (CNN). The development of a variety of embedding models, which can convert any input data (text, videos, audio, or images) into a vector representation, has been precipitated by the advent of large language models (LLM), particularly multi-model features. As shown in Figure 14, the arbitrary properties (1, 2, 3, 4, and 5) of polymeric nanocomposites have been optimized using a complex data set of various inputs. This input can be encoded and enable the model to extract the desired properties. The feature representations are input into convolutional neural network layers, succeeded by fully connected layers. The model's trainable layers are subsequently updated iteratively through a gradient descent technique to discern patterns in the data for either property optimization or process enhancement.

Fast and accurate prediction of material properties can be provided by these ML models at a low computational cost. E. Champa-Bujaico and co-workers investigated the effect of various fillers on the mechanical properties of multiscale poly(3-hydroxybutyrate) (P3HB)-based nanocomposites. Different ML approaches were applied, including Random Forest (RF) and Recurrent Neural Network (RNN). The stiffness was improved by 132% with the addition of 1:2:2 wt% of sepiolite and multiwall carbon nanotube and WS_2 nanosheet, respectively. The models developed by ML are found to be a powerful tool for the optimization of the mechanical properties in multiscale hybrid polymer nanocomposites by saving resources and time in the experimentation.[117] Integration of ML will significantly enhance the properties and efficiency of material design. Furthermore, it will be helpful in reducing costs and experimental trials. The selection of the ML approach is based on various factors like the size of the dataset, computational constraints, and complexity of relationships, ensuring that the most suitable model is chosen for each specific case. The comparison between the various optimization methods with their advantages and limitations was shown in Table 6.

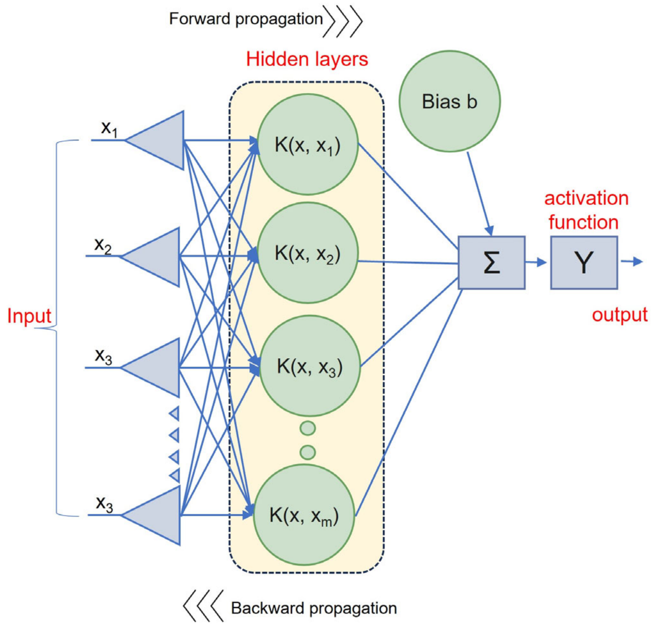

FIGURE 13 Schematically illustrated SVM to optimize the properties of nanocomposites.

2.8 | Utilization of optimized polymeric nanocomposites

The utilization of polymers and nanocomposites in engineering has significantly transformed multiple sectors by providing inventive resolutions to diverse obstacles. Polymers, due to their remarkable adaptability and customizable characteristics, are widely employed in several industries like aerospace, automotive, electronics, medical, and construction. Nanocomposites, however, merge the

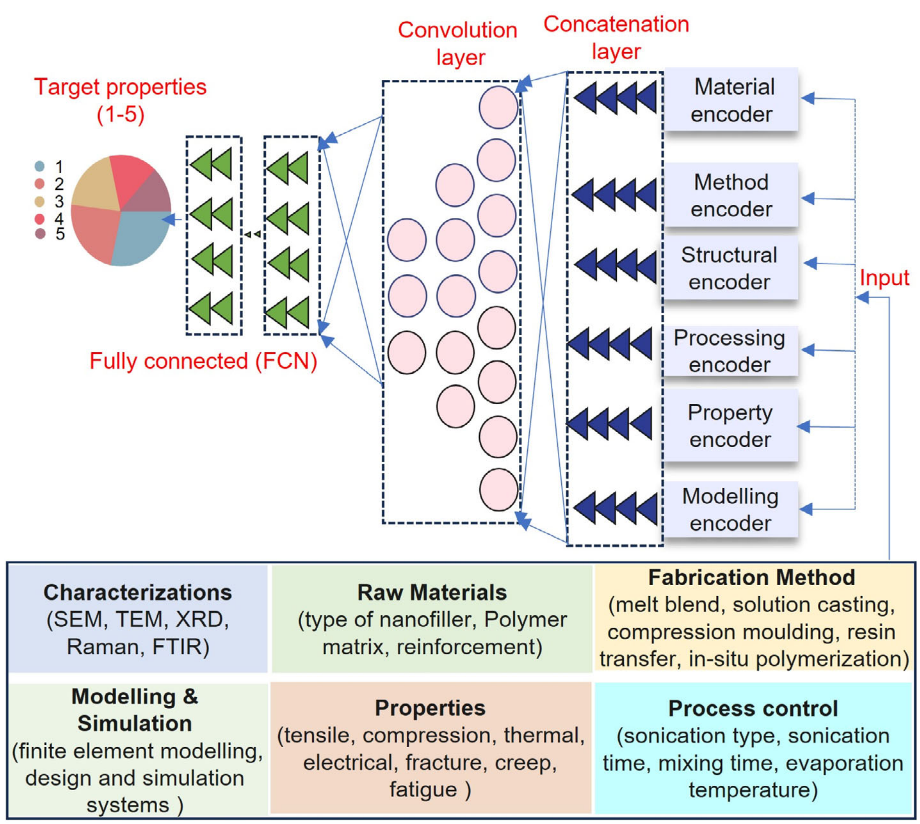

FIGURE 14 Integration of different types of inputs to ML for optimization of the properties.

TABLE 6 Comparison of various optimization techniques.

Technique	Advantages	Limitations	Best for	Ref.
RSM	Fewer experiments. Provides statistical insights.	Restricted to low-order polynomial relationships	Traditional optimization. Small datasets	118
Taguchi Method	Efficient experimental design, Reduces variability. Fewer experiments.	Assumes linear relationships. Less effective for highly nonlinear systems	Optimization of processing parameters with fewer experiments.	
Artificial Neural Networks (ANNs)	Able to represent complex nonlinear relationships. High accuracy	A large dataset is required. Risk of over fitting	Prediction of mechanical, thermal, and electrical property.	119
Random Forest (RF)	Handles small datasets well. Identifies important features	Less effective for high-dimensional data	Feature importance analysis. Optimization of properties.	120
Support Vector Machines (SVM)	Works well with small datasets, good for classification	Computationally expensive for large datasets	Classifying different polymeric composite types	121
Deep Learning (CNNs)	Extracts hierarchical features. Good for handling complex data.	Large training data is required. Needs high computational power.	Complex and multidimensional structure–property relationships	122
Autoencoders (AEs)	Extracts latent features. Lessens noise in data	Properties cannot be directly optimized.	Feature extraction. Reducing dimensionality	

advantages of polymers with the improved functionality of nanoparticles, hence expanding the horizons of material research. Engineers have utilized improved materials to achieve lightweight constructions, better mechanical strength, improved electrical conductivity, and provided customized capabilities. The engineering uses of polymers and nanocomposites are constantly pushing the limits of technological innovation, from creating high-performance composites for efficient transportation to developing bioresorbable implants for medicinal purposes.[123] Below are some examples of the uses of polymers. Polymer optical agents are extensively utilized in the field of cancer diagnostics.[124–127] They also exhibit an extensive variety of deployments in the medical field, that is, test tubes, petri dishes, medical cups, diagnostic components, and housings for medical devices because of their clarity and simplicity of sterilization. Nanocomposites with enhanced mechanical and electrical properties are successfully utilized in tissue engineering, bone disorder problems, drug delivery, infection therapy, and many more.[128–135] Given the energy conversion and storage need is of the need, pristine polymers and their nanocomposites, after optimized electrochemical and physical characteristics, were used in solar cell fabrication, fuel cells, and nano generators, as well as energy storage applications (Li-ion/sulfur batteries) due to their stability and adjustability.[136–142] As an example, polyvinylidene fluoride (PVDF) is the primary component for fabricating the electrodes for lithium-based energy storage systems[143] It is also used in photocatalytic devices.[144] Polymers are used in packing services because of their biodegradable nature and lightness. Polymer packaging services keep food insulated and keep food fresher longer. The cost of using polymer in a packaging service is less than other substitutes. Polymer boxes prevent the different food items from decomposition.[145,146] The mechanical and physical properties of polymer make it ideally suited for use in the construction industry. It can also be used to insulate ceilings, walls, and bath and shower units.[147,148] Polymer's better thermal properties make it suitable to use in HVAC systems, to minimize heat loss and increase the heat exchangers, water heaters, filters and motor's efficiency.[149,150] Polymers were also used in the automotive industry in the manufacturing of various car parts such as instrument panels, knobs, energy-absorbing door panels, headrests, side impact protection, roof liners, car air conditioning liners, and sound-reducing foam.[151–153] Polymers were used in the manufacturing of many electronic devices[154] such as televisions, LEDs, optoelectronic sensors, and actuators,[155–157] photovoltaic devices,[158] microwave ovens, transistors, vacuum cleaners, and computers.[159] They also serve the technology sector by protecting DVD cases and other devices. Polymers can be converted into different shapes and sizes; therefore, they are used in injection molding and extrusion. They are also used to make toys. Polymer is used in craft and art projects. It is also used for decorating purposes, such as candleholders. Polymers are also used in energy storage devices, that is, lithium-ion batteries and supercapacitors, due to their flexibility, safety performance, high electroactivity, and processability.[159–162]

3 | CONCLUSIONS

This study explored the application of optimization in polymeric nanocomposites. Based on the literature reports, the following conclusions may be made. (1) Mechanical characteristics, manufacturing, and process parameters of polymers or polymeric-based composites are well optimized using RSM as opposed to Taguchi since it delivers better results and fewer possible errors. (2) RSM can effectively illustrate the direct and/or inverse relationship between independent variables and responses through the creation of contour plots and 3D surface plots. (3) Response Surface Methodology (RSM) is a superior technique that yields precise results using a minimal number of tests in a shorter time frame compared to trial-and-error methods. (4) Optimization may save costs in process development and identify the critical factors that influence product performance. (5) The concentration of nanofiller significantly impacts the characteristics of polymer or polymer-based composites. (6) Optimizing process parameters, including concentration, temperature, speed, and duration, can enhance polymer yield. (7) Machine learning (ML) and artificial intelligence (AI) integration can further generate accurate predictions for enhanced properties, process control, and selection of filler materials.

3.1 | Outlook

With the ongoing advancement of nanomaterials, researchers can anticipate the emergence of novel and inventive nanofillers that possess improved characteristics. Subsequent research endeavors ought to be dedicated to investigating the potential of these unprecedented nanomaterials in conjunction with polymeric nanocomposites. Through the integration of these sophisticated additives and the application of Response Surface Methodology (RSM), the researchers can refine the concentration to attain unparalleled levels of efficacy with regard to desired attributes such as mechanical strength, thermal stability, and electrical conductivity. (i) Previously mechanical properties of polymers and polymers-based composites were investigated by trial-and-error methods whereas optimization through statistical techniques would be suitable for this purpose. Mechanical properties could be better optimized if optimization techniques were applied instead of conducting random experiments. (ii) Mechanical, electrical, and thermal properties of Graphene-polystyrene nanocomposites and MoS_2-polystyrene nanocomposites are investigated by classical methods. Thus, it still needs to be optimized by some statistical technique. (iii) 2D Graphene sheets are previously produced by traditional methods, such as Liquid exfoliation, dry exfoliation and mechanical exfoliation, which causes some restrictions such as low quality, poor dispersion and high cost. This may change if some optimization technique was applied on the synthesis of Graphene. The yield or quality of Graphene sheets may be optimized by varying centrifugation speed, centrifugation time and sonication time. (iv) The optimized weight percentage of nanofillers, sonication time after mixing and sonication temperature are a difficult or challenging task to obtain enhancement in Polymer properties. It could be done if some optimization technique was applied on synthesis of nanocomposites.

Further investigation into integrating multiple nanofillers with distinct functionalities is highly promising. To fashion multifunctional polymeric nanocomposites with customized performance characteristics by integrating additives possessing distinct properties, such as nano clays for barrier properties and nanoparticles for reinforcement, should be evaluated. By utilizing Response Surface Methodology, the concentration of individual fillers can be optimized, allowing for the precise modification of composite properties to align with the unique demands of a given application.

With the increasing focus on sustainability and environmental concerns, the future of polymeric nanocomposites lies in developing eco-friendly alternatives. To further explore the use of bio-based or recycled polymers as matrices and environmentally friendly nanofillers could be studied. The optimization of nanofiller concentration using Response Surface Methodology can aid in maximizing the performance of these sustainable nanocomposites while minimizing the use of non-renewable resources.

The incorporation of computational modeling methodologies, including finite element analysis and molecular dynamics simulations, into Response Surface Methodology has the potential to greatly augment comprehension and prognosis regarding the characteristics of polymeric nanocomposites. This area of research should also be emphasized.

While much of the current research on polymeric nanocomposites focuses on laboratory-scale studies, the future lies in scaling up the manufacturing processes and transitioning these materials to industrial applications. The optimization of nanofiller concentration using Response Surface Methodology should consider the challenges associated with large-scale production, such as processing limitations, cost-effectiveness, and reproducibility. Future studies should aim to bridge the gap between laboratory-scale research and industrial implementation, enabling the widespread application of polymeric nanocomposites.

It is essential to consider the health and safety consequences of polymeric nanocomposites as science advances. Future research should prioritize studying the possible toxicity and environmental consequences of nanofillers and their release during the lifespan of nanocomposites. By integrating health and safety factors into the optimization process, researchers may create guidelines and tactics to guarantee the secure and accountable utilization of polymeric nanocomposites in diverse applications.

It is possible that the field of polymeric nanocomposites could undergo a revolutionary change if machine learning and artificial intelligence were to be combined. Researchers can speed up the process of designing and developing high-performance materials by utilizing computational tools to perform data analysis, discover correlations, optimize parameters, and examine attributes. To further improve the capabilities of these technologies in the development of polymeric nanocomposites, future research efforts should concentrate on tackling difficulties such as the quality of the data, the interpretability of the models, and the integration of machine learning and artificial intelligence with simulations based on physics.

Overall, the future of improving characteristics in polymeric nanocomposites utilizing Response Surface Methodology (RSM), Machine learning (ML) and Artificial intelligence (AI) to optimize nanofiller concentration and performance is a promising and dynamic field. Progress in nanomaterials, sustainable nanocomposites, computer modeling integration, industrial scale-up, and health and safety issues will enhance this field. Researchers may fully utilize RSM as a strong tool to unleash the potential of polymeric nanocomposites and facilitate their wider implementation in many sectors.

AUTHOR CONTRIBUTIONS

Yasir Raza: Conceptualization, Collecting Literature, Visualization, Writing – original draft. Writing – review & editing. **Hassan Raza**: Conceptualization, Collecting Literature, Writing – review & editing. **Arslan Ahmed**: Project administration, Supervision, Writing – review & editing. **Moinuddin Mohammed Quazi**: Writing – review & editing. **Muhammad Jamshaid**: Writing – review & editing. **Muhammad Tuoqeer Anwar**: Supervision, Writing – review & editing. **Muhammad Nasir Bashir**: Writing – review & editing. **Talha Younas**: Writing – review & editing. **Ali Turab Jafry**: Supervision, Writing – review & editing. **Manzoore Elahi M. Soudagar**: Writing – review & editing.

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CONFLICT OF INTEREST STATEMENT

The authors declare no conflict of interest.

DATA AVAILABILITY STATEMENT

There is no new data generated in this manuscript.

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