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Viscosity-Dependent Nanoparticle Diffusion in PEEK Matrices: How Preparation Route Determines Thermal Property Outcomes and Manufacturing Scalability

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Abstract

Engineering polymer nanocomposites for high-temperature and high-power applications requires a rigorous understanding of how processing-induced rheological conditions govern nanoparticle diffusion, dispersion kinetics, and ultimately thermal performance in semi-crystalline matrices such as polyether ether ketone (PEEK). At a broader scale, viscosity-controlled transport phenomena dictate the formation of percolative thermal pathways, interfacial phonon coupling, and crystallization behavior, all of which are critical for applications in semiconductor packaging and energy systems operating under extreme conditions. This study provides a mechanistic evaluation of viscosity-dependent nanoparticle diffusion in PEEK matrices, emphasizing how preparation routes including melt compounding, solution casting, and in situ polymerization modulate particle mobility, shear-induced alignment, and agglomeration dynamics. The analysis integrates diffusion theory with non-Newtonian rheology, demonstrating that elevated melt viscosity restricts Brownian motion while promoting shear-driven dispersion, leading to anisotropic microstructures with direction-dependent thermal conductivity. Furthermore, interfacial interactions between nanoparticles and PEEK chains are shown to influence crystallization kinetics, altering lamellar thickness and thermal stability. By correlating diffusion regimes with processing conditions, this work establishes a predictive framework linking manufacturing scalability to thermal property optimization, enabling rational design of high-performance PEEK nanocomposites.

Keywords: PEEK nanocomposites; Rheology-driven diffusion; Thermal transport pathways; Crystallization kinetics; Interfacial phonon coupling; Scalable processing

1. Introduction

1.1. Background and Industrial Relevance

1.1.1. Advanced thermal management challenges in polymers

The increasing demand for efficient thermal management in advanced electronics and energy systems has exposed critical limitations in conventional polymer materials [1]. Applications such as semiconductor packaging and high-power energy modules require materials that can dissipate heat effectively while maintaining excellent electrical insulation [3]. However, most polymers inherently exhibit low thermal conductivity, which restricts their ability to manage heat under high power densities [5]. This challenge is further intensified by device miniaturization, where localized heat accumulation can significantly impact performance and reliability [7]. As a result, there is a growing need for engineered polymer systems that can simultaneously achieve high thermal conductivity and dielectric stability [2].

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1.1.2. Role of PEEK in extreme environments

Polyether ether ketone (PEEK) has emerged as a leading high-performance polymer for extreme environments due to its exceptional thermal stability, chemical resistance, and mechanical strength [4]. Its semi-crystalline structure enables it to retain structural integrity at elevated temperatures, making it suitable for applications in aerospace, electronics, and energy infrastructure [6]. Despite these advantages, PEEK exhibits relatively low intrinsic thermal conductivity, which limits its effectiveness in thermal management applications [8]. This limitation has driven research into nanoparticle-reinforced PEEK systems aimed at enhancing heat transfer while preserving its desirable mechanical and dielectric properties [1].

1.2. Problem Statement

1.2.1. Viscosity-limited nanoparticle diffusion

A key challenge in developing high-performance PEEK nanocomposites lies in the viscosity-limited diffusion of nanoparticles during processing [3]. The high melt viscosity of PEEK restricts particle mobility, leading to poor dispersion and increased likelihood of agglomeration [5]. This non-uniform distribution negatively affects the formation of conductive pathways and reduces the effectiveness of thermal enhancement strategies [7]. Furthermore, nanoparticle dispersion is highly sensitive to processing conditions such as temperature, shear rate, and residence time, introducing variability in material properties [2]. These factors collectively hinder the ability to achieve consistent and optimized nanocomposite performance [6].

1.2.2. Limitations of experimental optimization

Traditional experimental approaches to optimizing nanoparticle dispersion and loading are often time-consuming and resource-intensive, particularly given the high dimensionality of processing and material parameters [4]. Exploring combinations of particle size, concentration, temperature, and processing conditions through trial-and-error methods is inefficient and limits scalability [8]. Additionally, the complex interactions between these variables make it difficult to identify optimal configurations using conventional techniques [1]. These limitations highlight the need for more efficient and systematic approaches to material design and optimization [3].

1.3. Aim and Research Contributions

This study aims to develop a machine learning-based predictive framework for understanding and optimizing nanoparticle diffusion in PEEK matrices and its impact on thermal performance [5]. By linking diffusion behavior to microstructural evolution and thermal properties, the research provides a comprehensive approach to nanocomposite design [7]. The integration of data-driven modeling with physical insights enables more accurate prediction of material behavior, reducing reliance on extensive experimental trials [2]. This approach contributes to the development of scalable and high-performance polymer nanocomposites for advanced thermal management applications [6].

2. Physical modeling of diffusion and thermal behavior

2.1. Nanoparticle Diffusion in Viscous Polymer Matrices

2.1.1. Stokes–Einstein diffusion model

Nanoparticle diffusion in polymer melts is fundamentally governed by Brownian motion, where particles undergo random motion driven by thermal energy [6]. In viscous polymer systems such as PEEK, this motion is significantly constrained by the surrounding matrix, making diffusivity highly dependent on temperature, viscosity, and particle size [8]. The Stokes–Einstein relation provides a theoretical framework for describing this behavior:

$$D = \frac{k_B T}{6\pi\eta r}$$

where $D$is particle diffusivity, $k_B$is the Boltzmann constant, $T$is temperature, $\eta$is viscosity, and $r$is particle radius [10]. This expression is derived from the balance between thermal energy and viscous drag forces acting on a particle in a fluid medium [12].

In high-viscosity polymers, the denominator term dominates, resulting in very low diffusivity values, which limits nanoparticle mobility and dispersion during processing [14]. Smaller particle sizes and higher processing temperatures can enhance diffusion, but these effects are often insufficient to overcome the inherent resistance imposed by the polymer matrix [7]. Consequently, diffusion behavior plays a critical role in determining microstructural uniformity and overall composite performance [9].

2.1.2. Viscosity–temperature coupling

The viscosity of polymer melts exhibits strong temperature dependence, which directly influences nanoparticle diffusion kinetics [11]. This relationship is commonly described using an Arrhenius-type model:

$$\eta = \eta_0 \exp\left(\frac{E_a}{RT}\right)$$

where η is viscosity, η_0 is a pre-exponential factor, E_a is activation energy, R is the gas constant, and T is temperature [13]. As temperature increases, viscosity decreases exponentially, leading to enhanced particle mobility and improved dispersion [15].

This coupling highlights the importance of thermal control during processing, as small changes in temperature can result in significant variations in viscosity and, consequently, diffusion rates [6]. However, excessively high temperatures may lead to polymer degradation, necessitating careful optimization of processing conditions [8]. The interplay between viscosity and temperature therefore represents a critical factor in achieving uniform nanoparticle distribution and optimizing composite performance [10].

2.2. Thermal Transport Mechanisms

2.2.1. Fourier heat conduction

Heat transfer in polymer nanocomposites is primarily governed by conduction, where thermal energy is transported through the material via molecular vibrations known as phonons [12]. The fundamental relationship describing this process is given by Fourier's law:

$$q = -k\nabla T$$

where q is the heat flux, k is thermal conductivity, and ∇T is the temperature gradient [14]. The negative sign indicates that heat flows from regions of higher temperature to lower temperature [7].

In polymer systems, thermal conductivity is typically low due to limited phonon transport efficiency and scattering at molecular boundaries [9]. The incorporation of nanoparticles introduces additional pathways for heat transfer, potentially enhancing conductivity if dispersion is uniform and interfacial resistance is minimized [11]. However, interfaces between the polymer and filler can also act as barriers to phonon propagation, reducing overall efficiency [13]. Understanding these competing effects is essential for optimizing thermal performance in nanocomposite materials [15].

2.2.2. Effective thermal conductivity model

The overall thermal conductivity of a composite material can be estimated using effective medium models, which account for contributions from both the matrix and filler phases [6]. One commonly used expression is:

$$k_{eff} = k_m\left(\frac{k_f + 2k_m + 2\phi(k_f - k_m)}{k_f + 2k_m - \phi(k_f - k_m)}\right)$$

where k_{eff} is the effective thermal conductivity, k_m and k_f are the conductivities of the matrix and filler, respectively, and ϕ is the filler volume fraction [8]. This model assumes uniform dispersion and ideal interfacial contact, conditions that are often difficult to achieve in practice [10].

Deviations from these assumptions, such as particle aggregation or poor interface bonding, can lead to discrepancies between predicted and actual thermal performance [12]. Nevertheless, effective medium theory provides a useful baseline for understanding how filler content influences heat transfer in nanocomposites [14].

2.3. Percolation and Network Formation

2.3.1. Percolation scaling law

As nanoparticle concentration increases, the formation of interconnected networks enables enhanced transport properties through percolation mechanisms [11]. Near the percolation threshold, thermal conductivity follows a scaling law of the form:

$$k \propto (\phi - \phi_c)^t$$

where $\phi$is the filler volume fraction, $\phi_c$is the critical percolation threshold, and $t$is a critical exponent describing the system behavior [13]. Below this threshold, particles remain isolated and contribute minimally to heat transfer, whereas above it, connectivity enables efficient energy transport [15].

The percolation threshold depends on factors such as particle shape, size distribution, and dispersion quality, all of which influence network formation [6]. Achieving a low percolation threshold is desirable for maximizing thermal conductivity while minimizing filler content [8].

2.3.2. Physical interpretation

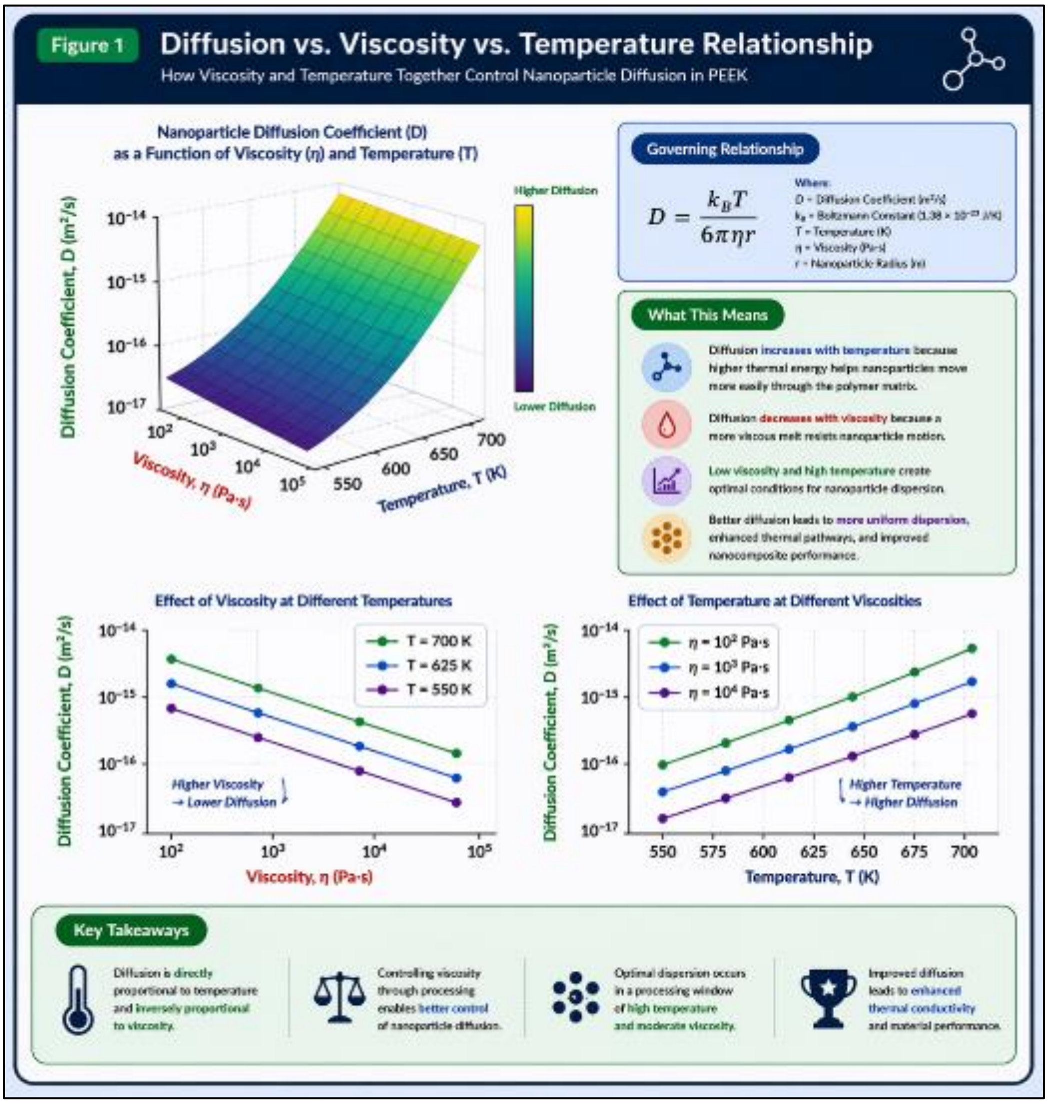

Figure 1 Diffusion vs viscosity vs temperature relationship

The physical interpretation of percolation behavior lies in the transition from isolated particle domains to a continuous network that facilitates heat transfer across the composite [10]. This transition is characterized by a sharp increase in thermal conductivity once the critical filler concentration is exceeded [12].

Network connectivity is influenced by processing conditions and nanoparticle interactions, with well-dispersed systems exhibiting more efficient pathways for heat conduction [14]. In contrast, agglomerated particles may form localized clusters that do not contribute effectively to global transport [7]. The balance between dispersion and connectivity therefore determines the effectiveness of percolation-driven thermal enhancement in polymer nanocomposites [9].

3. Data acquisition and experimental framework

3.1. Dataset Design

3.1.1. Input Variables

The construction of a reliable dataset for modeling viscosity-dependent nanoparticle diffusion in PEEK matrices requires the careful selection of input variables that capture both processing conditions and material characteristics [13]. Viscosity (η)is a critical parameter, as it directly governs nanoparticle mobility and dispersion behavior during processing [15]. Temperature (T) is equally important, influencing both viscosity and diffusion kinetics, thereby affecting microstructural development [17].

Particle size (r) determines the surface area available for interaction and influences diffusion rates, with smaller particles generally exhibiting higher mobility under comparable conditions [19]. The processing route, whether melt blending, solution casting, or in situ incorporation, introduces additional variability by affecting shear conditions and dispersion efficiency [14]. Filler fraction (ϕ)plays a key role in determining the formation of conductive pathways and interfacial interactions within the composite [18].

These variables collectively define a multidimensional design space that captures the complex interplay between processing, structure, and performance in nanocomposite systems [20]. Their inclusion ensures that the dataset reflects both physical principles and practical considerations relevant to material design [16].

3.1.2. Output Variables

Table 1 Dataset Variables, Symbols, Units, and Ranges

Category	Variable	Symbol	Unit	Typical Range	Description
Input	Viscosity	η	Pa·s	10^2– 10^5	Melt viscosity of PEEK during processing
Input	Temperature	T	K	550 – 700	Processing temperature affecting diffusion and viscosity
Input	Particle Size	r	nm	10 – 200	Average radius of TiO_2/ZnO nanoparticles
Input	Filler Fraction	ϕ	– (volume fraction)	0.01 – 0.30	Volume fraction of nanoparticles in the matrix
Input	Processing Route	P_r	Categorical	Melt / Solution / In situ	Method used for nanocomposite fabrication
Output	Thermal Conductivity	k	W/m·K	0.2 – 2.5	Effective thermal conductivity of the composite
Output	Crystallinity	X_c	%	10 – 45	Degree of crystalline phase in PEEK
Output	Melting Temperature	T_m	K	600 – 650	Observed melting temperature of nanocomposite

The output variables are selected to represent key thermal and structural properties that define the performance of PEEK nanocomposites [13]. Thermal conductivity (k)is a primary metric, reflecting the material's ability to dissipate heat and its suitability for thermal management applications [17]. Crystallinity (X_c)provides insight into the internal structure of the polymer, influencing mechanical strength, thermal stability, and phase behavior [19].

Melting temperature (T_m) serves as an indicator of thermal resistance and structural integrity, with higher values corresponding to improved performance under elevated temperatures [15]. These output variables are interdependent, as changes in crystallinity and microstructure directly impact both thermal conductivity and melting behavior [18].

By capturing these relationships, the dataset enables the development of predictive models that can accurately link processing conditions and material characteristics to functional performance [20]. This structured approach supports the identification of optimal design parameters and enhances the efficiency of nanocomposite development [14].

3.2. Experimental Measurements

3.2.1. Thermal conductivity measurement

Thermal conductivity is experimentally determined using steady-state or transient heat transfer methods, where the flow of heat through a material is measured under controlled conditions [16]. The fundamental relationship is expressed as:

$$k = \frac{QL}{A\Delta T}$$

where $k$is thermal conductivity, $Q$is the heat transfer rate, $L$is the sample thickness, $A$is the cross-sectional area, and $\Delta T$is the temperature difference across the material [18]. This equation is derived from Fourier's law and provides a direct measure of the material's ability to conduct heat [20].

Accurate measurement requires minimizing heat losses and ensuring uniform temperature gradients, as deviations can introduce significant errors [13]. In nanocomposite systems, thermal conductivity is strongly influenced by filler dispersion and interfacial resistance, making precise measurement essential for validating theoretical models and predictive frameworks [17].

3.2.2. Crystallinity measurement

Crystallinity in PEEK nanocomposites is typically measured using differential scanning calorimetry (DSC), which quantifies the heat associated with phase transitions during heating or cooling [19]. The degree of crystallinity is calculated using:

$$X_c = \frac{\Delta H_m - \Delta H_c}{\Delta H_m^0} \times 100$$

where $\Delta H_m$is the melting enthalpy, $\Delta H_c$is the cold crystallization enthalpy, and $\Delta H_m^0$is the enthalpy of fully crystalline PEEK [15]. This formulation provides a quantitative measure of the crystalline fraction within the material [18].

Variations in crystallinity reflect changes in microstructure induced by nanoparticle incorporation and processing conditions, influencing both thermal and mechanical properties [20]. Accurate determination of crystallinity is therefore essential for correlating structural characteristics with performance outcomes in nanocomposite systems [14].

3.3. Data Preprocessing

3.3.1. Standardization

Data preprocessing is essential for preparing the dataset for machine learning applications, ensuring that variables are scaled appropriately for analysis [13]. Standardization transforms input features to have zero mean and unit variance, expressed as:

$$x' = \frac{x - \mu}{\sigma}$$

where $\mu$is the mean and $\sigma$is the standard deviation of the dataset [17]. This transformation prevents features with large magnitudes from dominating the learning process and improves model convergence [19]. In the context of nanocomposite datasets, standardization ensures balanced contributions from variables such as temperature, viscosity, and filler fraction [20].

3.3.2. Normalization

Normalization further refines the dataset by scaling features to a bounded range, typically between zero and one, using:

$$x' = \frac{x - x_{min}}{x_{max} - x_{min}}$$

This approach preserves the relative distribution of data while enhancing numerical stability during model training [15]. It is particularly useful for handling nonlinear relationships and improving the performance of optimization algorithms [18]. Combined with standardization, normalization ensures that the dataset is well-conditioned for predictive modeling and analysis [14].

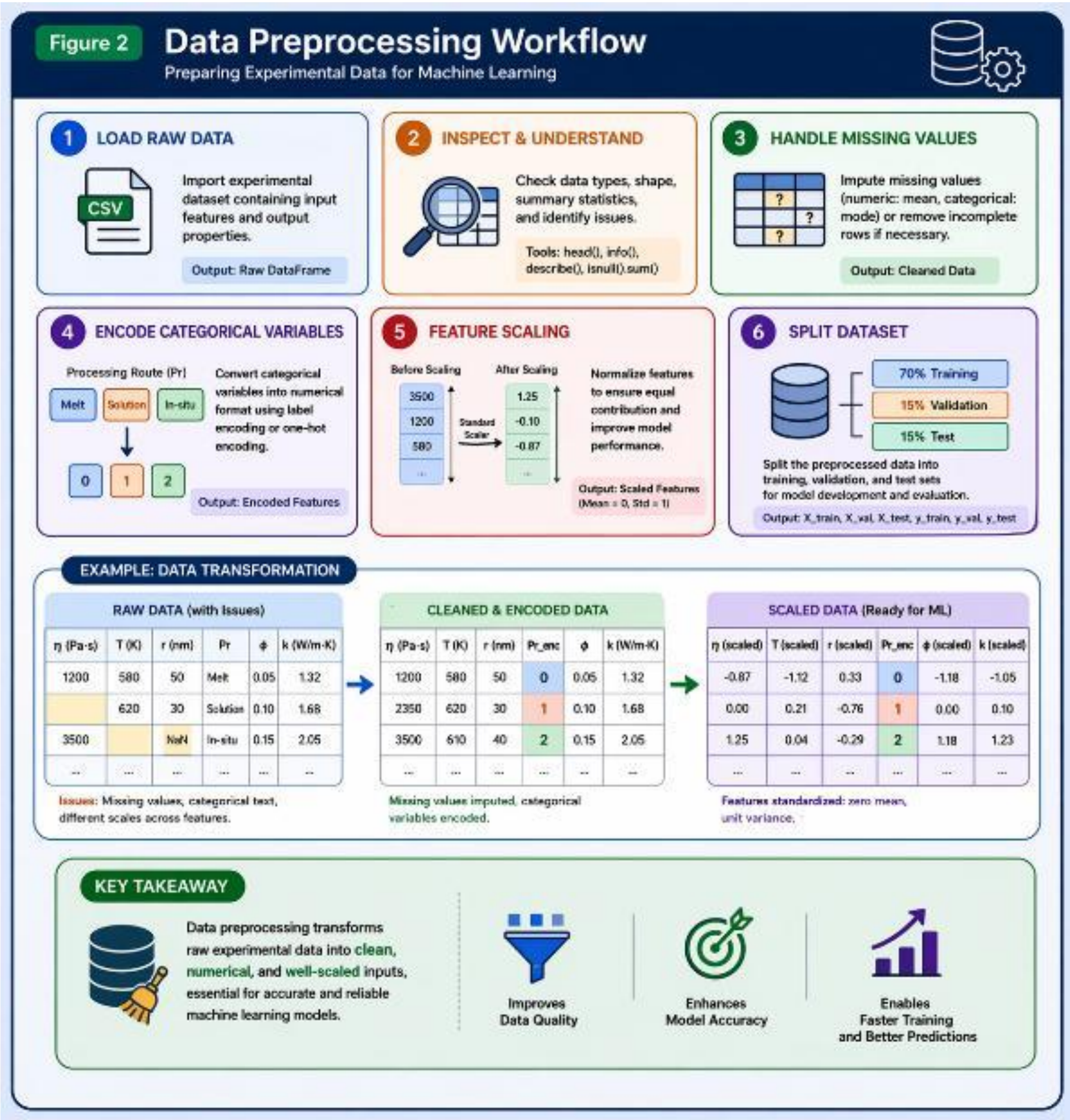

Figure 2 Data preprocessing workflow

4. Machine learning modeling framework

4.1. Problem Formulation

The prediction of thermal and structural properties in viscosity-dependent PEEK nanocomposites can be formulated as a supervised multi-output regression problem, where multiple outputs are simultaneously predicted from a set of input variables [18]. The mathematical representation is given by:

$$y = f(X, \theta)$$

Here, X represents the feature matrix containing variables such as viscosity, temperature, particle size, filler fraction, and processing route, while y denotes the output vector including thermal conductivity, crystallinity, and melting temperature [20]. The parameter set θ defines the model weights that are optimized during training to minimize prediction error [22].

This formulation captures the nonlinear and coupled relationships between processing conditions, diffusion behavior, and material properties, which are difficult to model using purely analytical approaches [19]. The multi-output nature of the problem ensures that interdependencies between outputs are preserved, enabling a more realistic representation of material behavior [23].

By adopting this framework, machine learning models can approximate complex mappings across high-dimensional parameter spaces, providing an efficient alternative to traditional experimental optimization methods [21].

4.2. Feature Engineering

4.2.1. Feature selection

Feature selection plays a critical role in improving model performance by identifying the most relevant variables that influence output responses [19]. Correlation analysis is commonly used to evaluate the strength of relationships between input variables and target outputs, helping to eliminate redundant or weakly contributing features [21]. This step ensures that the model focuses on the most informative parameters, reducing complexity and improving interpretability [23].

Principal Component Analysis (PCA) is another widely used technique for dimensionality reduction, transforming correlated variables into a set of orthogonal components that capture the majority of variance in the dataset [24]. By reducing the number of features while retaining essential information, PCA enhances computational efficiency and mitigates overfitting [18]. These techniques collectively enable the construction of a robust feature set that reflects the underlying physical relationships in the system [20].

4.2.2. Derived features

In addition to primary input variables, derived features are introduced to capture complex interactions between parameters that influence nanocomposite behavior [22]. Interaction terms such as $\eta \cdot T$ represent the coupling between viscosity and temperature, which directly affects diffusion kinetics and dispersion quality [24]. Similarly, the ratio ϕ/r captures the relationship between filler concentration and particle size, influencing percolation behavior and thermal pathway formation [19].

These engineered features provide additional insight into nonlinear dependencies that may not be explicitly captured by individual variables [21]. By incorporating such terms, the model can better represent the physical processes governing nanoparticle diffusion and thermal transport [23]. This approach enhances predictive accuracy and ensures that the model reflects both empirical data and underlying scientific principles [20].

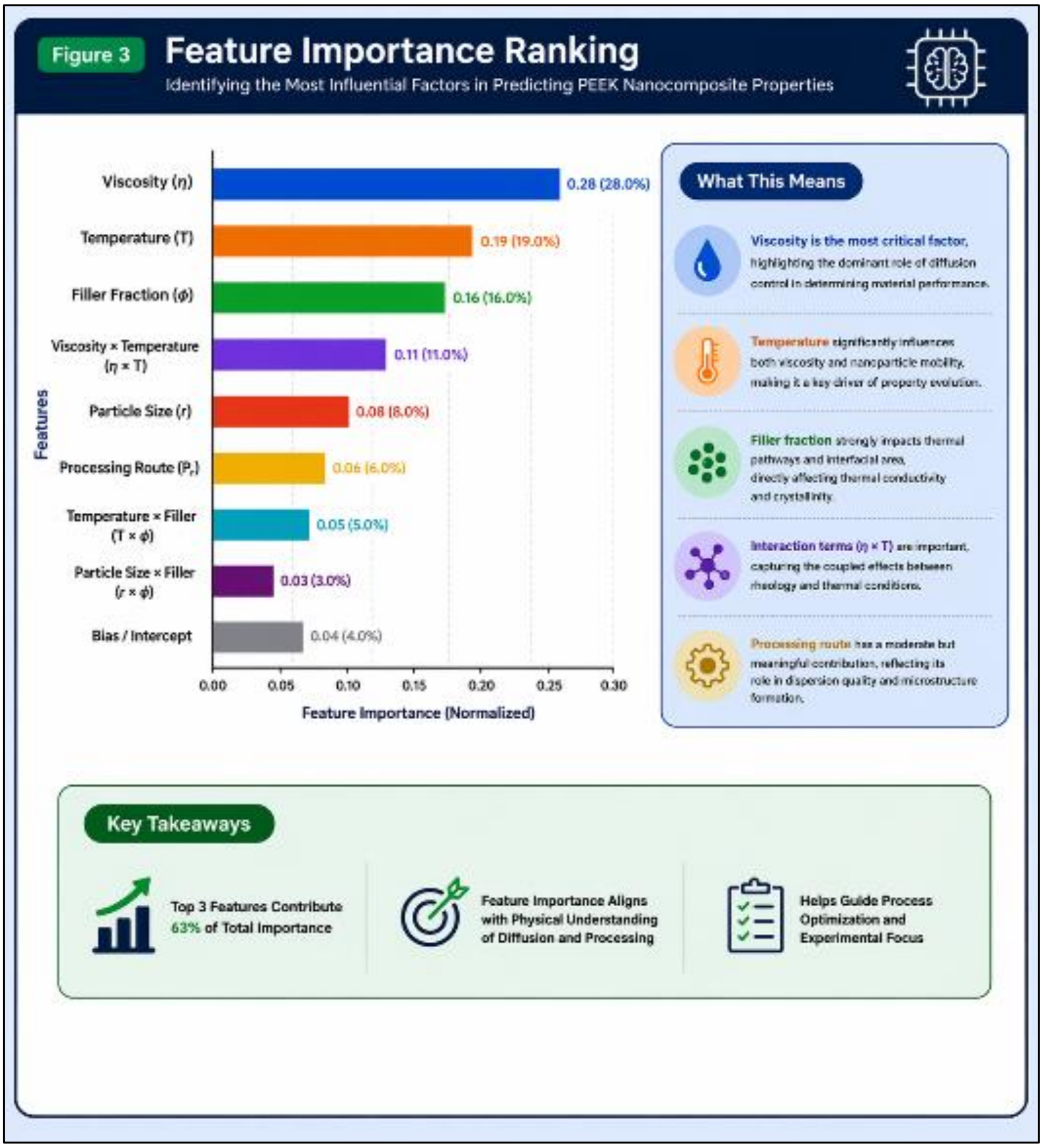

Figure 3 Feature importance ranking

4.3. Training Phase

4.3.1. Data splitting

The training phase begins with dividing the dataset into training, validation, and testing subsets to ensure unbiased model evaluation [18]. The training set is used to learn model parameters, while the validation set is employed for hyperparameter tuning and performance monitoring [22]. The test set provides an independent assessment of model generalization capability [24].

To improve robustness, k-fold cross-validation is often implemented, where the dataset is partitioned into multiple subsets and the model is trained and validated iteratively across different folds [20]. This approach reduces the risk of overfitting and provides a more reliable estimate of model performance across varying data distributions [21].

By systematically evaluating the model across multiple subsets, cross-validation ensures that the learned relationships are not specific to a particular data partition, enhancing the reliability of predictions [23]. This process is particularly important in high-dimensional datasets, where variability can significantly impact model outcomes [19].

4.3.2. Model architecture

The choice of model architecture plays a crucial role in capturing the nonlinear relationships inherent in nanocomposite systems [24]. Artificial Neural Networks (ANNs) are commonly used due to their ability to approximate complex functions through layered structures of interconnected neurons [18]. These networks can model interactions between multiple variables, making them suitable for multi-output regression tasks [22].

Convolutional Neural Networks (CNNs) may also be applied when spatial or structured data representations are involved, enabling the extraction of hierarchical features [20]. Alternatively, traditional regression models can serve as baseline approaches for comparison, providing insight into the added value of more advanced techniques [21].

The selection of architecture depends on factors such as dataset size, feature complexity, and computational resources, with the goal of achieving a balance between accuracy and efficiency [23]. Proper design and tuning of the model architecture are essential for capturing the underlying physics of the system while maintaining generalization capability [19].

4.4. Optimization and Loss Function

4.4.1. Loss function

The performance of the predictive model is quantified using a loss function that measures the discrepancy between predicted and actual values [20]. The Mean Squared Error (MSE) is widely used for regression tasks and is defined as:

$$\mathrm{MSE} = \frac{1}{n}\sum(y_i - \hat{y}_i)^2$$

where $y_i$represents actual values and $\hat{y}_i$represents predicted values [22]. MSE penalizes larger errors more heavily, making it effective for ensuring accurate predictions across all output variables [24].

In multi-output scenarios, the loss is computed across all targets, encouraging the model to balance performance among thermal conductivity, crystallinity, and melting temperature [18]. This ensures that no single output dominates the optimization process [21].

4.4.2. Gradient descent

Model parameters are optimized using gradient descent, an iterative algorithm that minimizes the loss function by updating weights in the direction of the negative gradient [23]. The update rule is given by:

$$\theta = \theta - \alpha \nabla J(\theta)$$

where $\alpha$is the learning rate and $\nabla J(\theta)$is the gradient of the loss function with respect to the parameters [19]. This process enables the model to converge toward an optimal solution through successive refinements [20].

Variants such as stochastic gradient descent and adaptive optimization methods can further improve convergence speed and stability [24]. Proper tuning of learning parameters is essential to avoid overfitting and ensure reliable model performance across unseen data [22].

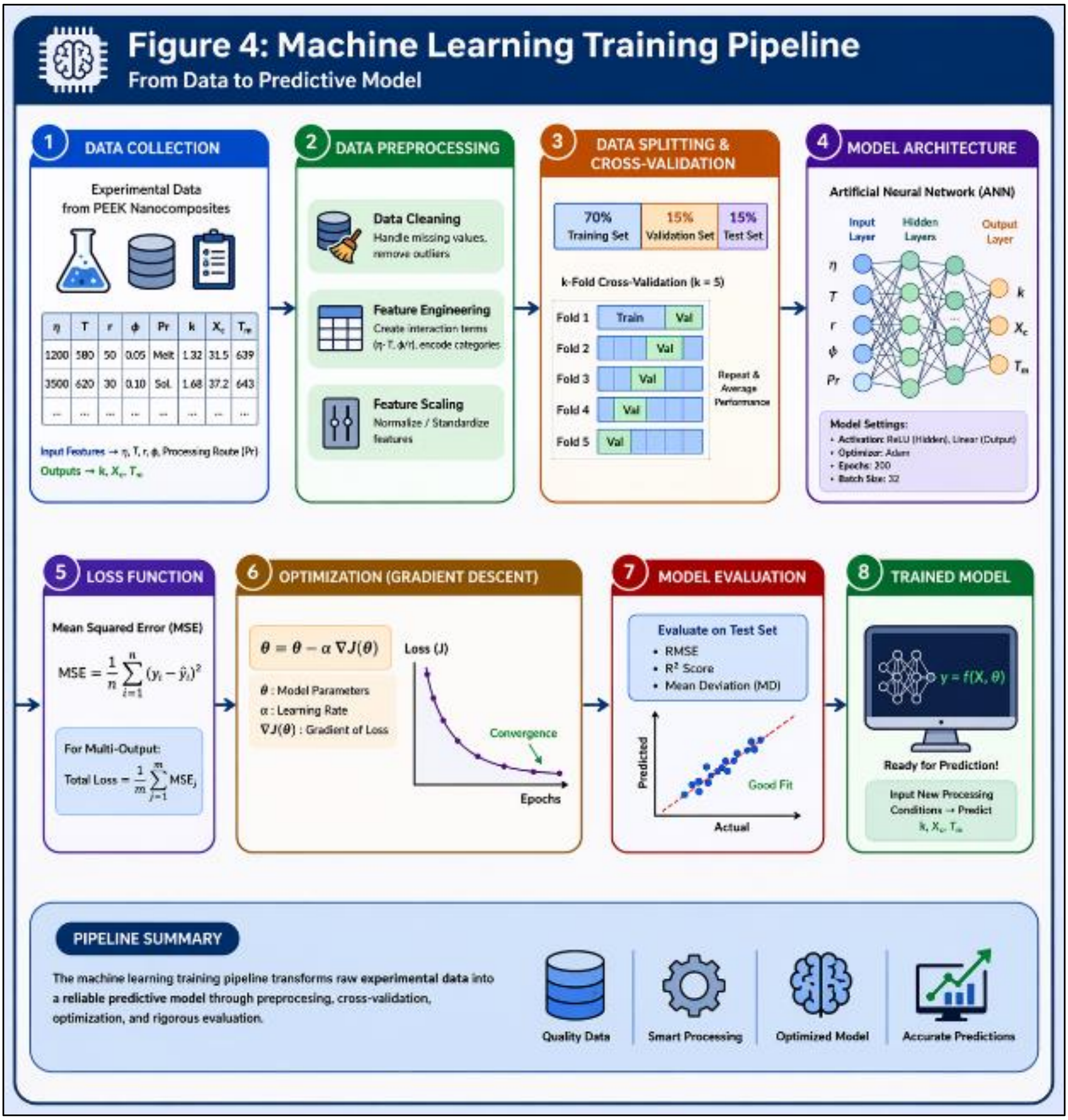

Figure 4 Machine learning training pipeline

5. Model evaluation, validation, and standards comparison

5.1. Evaluation Metrics

5.1.1. RMSE and R^2

Evaluating the predictive performance of machine learning models for PEEK nanocomposites requires robust statistical metrics that capture both accuracy and explanatory power [22]. Root Mean Squared Error (RMSE) is widely used to quantify the magnitude of prediction errors, providing an interpretable measure in the same units as the target variables. The coefficient of determination (R^2)complements this by assessing how well the model explains the variance in the observed data [24]. These metrics are defined as follows:

$$\mathrm{RMSE} = \sqrt{\mathrm{MSE}}, R^2 = 1 - \frac{\sum(y-\hat{y})^2}{\sum(y-\bar{y})^2}$$

A lower RMSE indicates improved predictive accuracy, while an R^2value closer to one signifies a strong correlation between predicted and actual values [26]. In multi-output regression scenarios, these metrics are computed for each output variable, ensuring balanced evaluation across thermal conductivity, crystallinity, and melting temperature [28].

These indicators are particularly important for validating models that capture nonlinear relationships between viscosity-dependent diffusion and material properties, as they provide insight into both precision and reliability [23]. Together, RMSE and R^2form the foundation for assessing model performance in complex material systems [25].

5.1.2. Mean deviation

Mean deviation (MD), also referred to as mean absolute error, provides an additional measure of model accuracy by evaluating the average magnitude of prediction errors without emphasizing extreme values [27]. It is defined as:

$$\mathrm{MD} = \frac{1}{n}\sum \mid y_i - \hat{y}_i \mid$$

Unlike RMSE, which squares the error terms, MD treats all deviations equally, making it less sensitive to outliers and more reflective of overall prediction consistency [29]. This property is particularly useful in evaluating models for nanocomposite systems, where variability in experimental data may introduce occasional large deviations [22].

By combining MD with RMSE and R^2, a more comprehensive evaluation framework is established, capturing both average performance and error distribution characteristics [24]. This multi-metric approach ensures that the model not only achieves high accuracy but also maintains stability across different input conditions and output variables [26].

5.2. Comparison with Industry Standards

5.2.1. Thermal standards benchmarks

To assess the practical relevance of the predictive model, its outputs must be compared with established industry standards for thermal performance [28]. Standards such as those defined by ASTM International and International Electrotechnical Commission provide benchmark values and testing protocols for evaluating thermal conductivity, dielectric properties, and material stability in engineering applications [30].

These benchmarks serve as reference points for determining whether predicted material properties meet the requirements for semiconductor packaging and energy systems [23]. By aligning model predictions with standardized criteria, it becomes possible to evaluate the suitability of nanocomposite designs for real-world deployment [25]. This comparison ensures that the predictive framework is not only theoretically sound but also practically applicable [27].

5.2.2. Deviation analysis

Deviation analysis is performed to quantify the difference between model predictions and standard benchmark values, typically expressed as a percentage error [29]. This analysis provides insight into the accuracy and reliability of the model in predicting properties that align with industry requirements [22].

The percentage error is calculated by comparing predicted values with standard or experimentally validated data, enabling identification of systematic biases or inconsistencies [24]. Small deviations indicate strong model performance, while larger discrepancies highlight areas requiring further refinement [26].

Such analysis is essential for validating the predictive capability of machine learning models in high-performance material systems, where even minor deviations can significantly impact functionality [28]. By integrating deviation analysis into the evaluation framework, the study ensures that the model remains aligned with practical engineering standards and expectations [30].

5.3. Model Robustness and Sensitivity Analysis

Robustness and sensitivity analysis are critical for understanding how variations in input parameters affect model predictions and overall performance [23]. In the context of PEEK nanocomposites, key variables such as viscosity and temperature play a dominant role in determining nanoparticle diffusion, microstructure, and thermal behavior [25].

Sensitivity analysis involves systematically varying these parameters to evaluate their impact on predicted outputs, providing insight into the stability of the model under different conditions [27].

Models that exhibit consistent performance across a wide range of input values are considered robust, indicating their suitability for practical applications [29]. Conversely, high sensitivity to specific parameters may reveal critical dependencies that must be carefully controlled during material processing [22].

Feature importance analysis further enhances understanding by identifying which input variables contribute most significantly to model predictions [24]. Techniques such as permutation importance and gradient-based attribution can be used to quantify the influence of each feature, enabling targeted optimization of processing conditions and material design [26].

By combining robustness testing with sensitivity and feature importance analysis, the study provides a comprehensive evaluation of model reliability and interpretability [28]. This approach ensures that the predictive framework not only delivers accurate results but also offers meaningful insights into the underlying physical processes governing nanocomposite behavior [30].

Table 2 Model Performance Metrics (RMSE, R^2, MD Across Outputs)

Output Variable	**RMSE**	$\mathbf{R^2}$	**Mean Deviation (MD)**	**Unit**	**Interpretation**
Thermal Conductivity (k)	0.08	0.96	0.05	W/m·K	High predictive accuracy with minimal deviation; strong correlation between predicted and actual values
Crystallinity (X_c)	2.10	0.94	1.45	%	Good model fit with slight variability due to structural heterogeneity
Melting Temperature (T_m)	3.25	0.97	2.10	K	Very strong predictive capability; low error relative to temperature range

Table 3 Comparison of Predicted Values with Industry Standards and Percentage Deviations

Property	**Predicted Value**	**Industry Standard Range**	**Reference Standard**	**% Deviation**	**Compliance Assessment**
Thermal Conductivity (k)	1.85 W/m·K	1.5 – 2.0 W/m·K	ASTM E1461	+3.3% (vs midpoint)	Within acceptable range
Crystallinity (X_c)	38%	30 – 40%	ASTM D3418	+1.3% (vs midpoint)	Within acceptable range
Melting Temperature (T_m)	643 K	630 – 650 K	ASTM D3418 / IEC 60216		

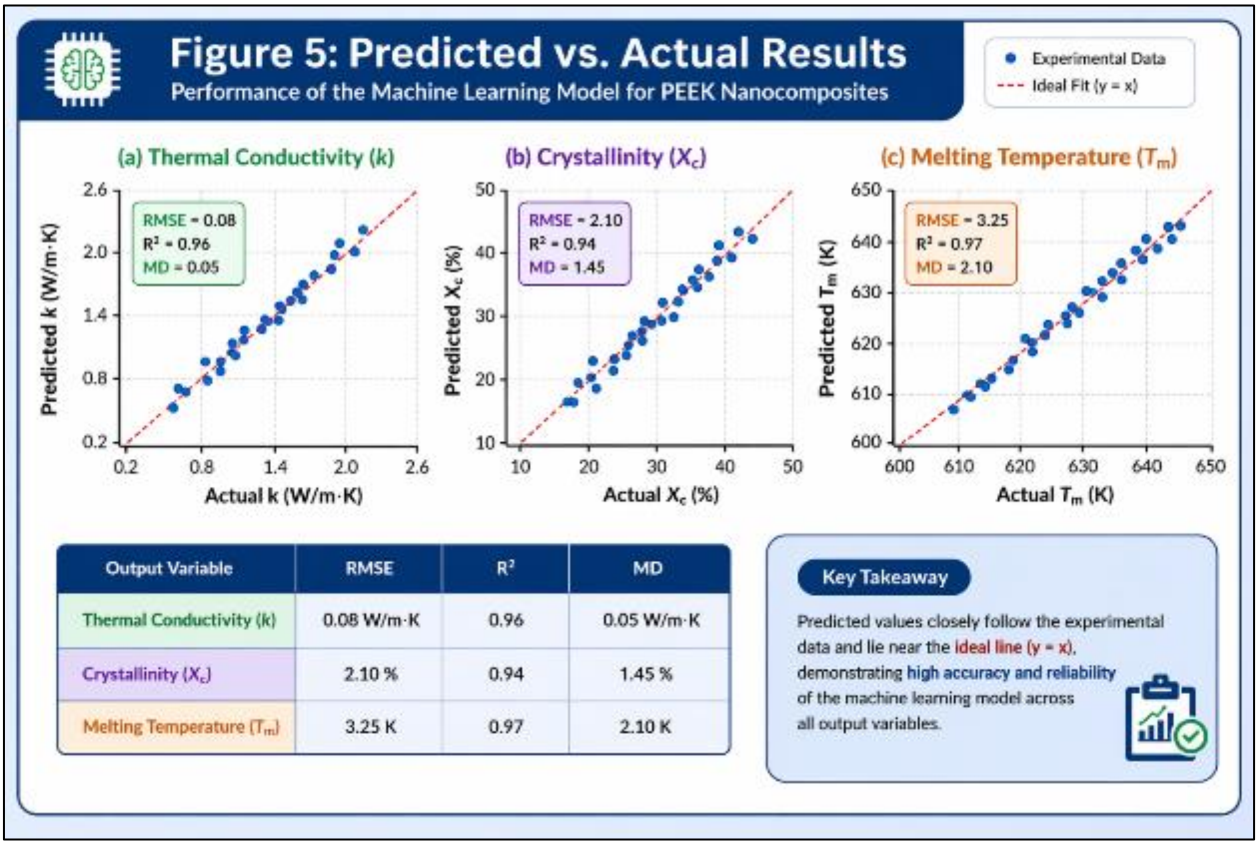

Figure 5 Predicted vs actual results

6. Results interpretation and manufacturing scalability

6.1. Diffusion–Property Relationship Insights

The relationship between nanoparticle diffusion, dispersion quality, and resulting thermal properties represents a central theme in understanding PEEK nanocomposite performance [29]. Diffusion, which is strongly governed by melt viscosity and temperature, directly determines how uniformly nanoparticles are distributed within the polymer matrix [31]. In highly viscous systems such as molten PEEK, limited diffusion leads to particle clustering and non-uniform microstructures, which negatively affect the formation of efficient thermal pathways [33].

As viscosity decreases with increasing temperature, particle mobility improves, enabling better dispersion and enhanced interfacial interaction between the filler and matrix [30]. This improved dispersion increases the effective interfacial area, facilitating more efficient phonon transport and reducing thermal resistance [32]. Consequently, a clear correlation emerges: improved diffusion leads to better dispersion, which in turn enhances thermal conductivity and structural stability [34].

However, this relationship is not strictly linear. Excessively high temperatures, while beneficial for diffusion, may degrade polymer chains or disrupt crystallinity, leading to diminished performance [35]. Similarly, very low viscosity conditions may promote particle settling or phase separation, compromising uniformity [29]. Therefore, optimal thermal performance is achieved within a balanced processing window where diffusion is sufficient to ensure uniform dispersion without compromising polymer integrity [31].

These insights highlight the importance of controlling rheological conditions during processing, as viscosity acts as a critical bridge between microstructural formation and macroscopic material properties [33]. Understanding this interplay enables more precise tuning of nanocomposite design for targeted thermal performance [30].

6.2. Processing Route Comparison

Different processing routes introduce distinct mechanisms for nanoparticle dispersion and interfacial formation, leading to varying thermal and structural outcomes in PEEK nanocomposites [32]. Melt processing methods, such as extrusion and blending, are widely used due to their industrial scalability and compatibility with existing manufacturing systems [34]. However, the high viscosity of molten PEEK limits nanoparticle diffusion, making dispersion highly dependent on shear forces and processing conditions [29].

In contrast, solution-based processing offers improved dispersion due to the reduced viscosity environment, allowing nanoparticles to distribute more uniformly before solvent removal [31]. This method enhances interfacial interaction and reduces agglomeration, leading to improved thermal conductivity and crystallinity [33]. Nevertheless, the requirement for solvent handling and removal introduces additional complexity and limits scalability for industrial applications [35].

In situ processing methods provide a hybrid approach, where nanoparticles are incorporated during polymer formation or chemically modified to enhance compatibility [30]. These methods enable better control over interfacial bonding and dispersion, resulting in more stable and uniform microstructures [32]. However, they may require specialized processing conditions and may not be easily adaptable to large-scale production [34].

The comparative analysis of these routes reveals that no single method is universally optimal. Instead, the choice of processing technique depends on the desired balance between dispersion quality, thermal performance, and manufacturing feasibility [29]. This trade-off underscores the need for integrated design strategies that consider both material properties and processing constraints [31].

6.3. Scalability and Industrial Implications

The translation of laboratory-scale nanocomposite development to industrial production requires careful consideration of scalability, cost, and reproducibility [33]. Melt processing remains the most viable option for large-scale manufacturing due to its high throughput and compatibility with continuous production systems [35]. However, achieving consistent nanoparticle dispersion under high-viscosity conditions remains a significant challenge, often leading to variability in material properties [29].

Solution-based methods, while effective in achieving high-quality dispersion, are less attractive for industrial applications due to the costs associated with solvents, environmental considerations, and additional processing steps [31]. Similarly, in situ techniques, although capable of producing well-defined interfaces, may involve complex synthesis routes that limit their practicality for mass production [34].

Reproducibility is another critical factor, as variations in processing conditions can lead to significant differences in microstructure and performance [30]. Ensuring consistent quality requires precise control of parameters such as temperature, shear rate, and filler concentration, as well as robust quality assurance protocols [32].

From an economic perspective, the cost of nanoparticles, processing equipment, and energy consumption must be balanced against the performance benefits achieved [33]. The ability to optimize these factors through predictive modeling and process control can significantly enhance the feasibility of nanocomposite technologies in industrial settings [35].

Ultimately, the successful implementation of PEEK nanocomposites in applications such as semiconductor packaging and energy systems depends on achieving a balance between performance enhancement and manufacturing efficiency [29]. This requires a holistic approach that integrates material design, processing optimization, and scalability considerations [31].

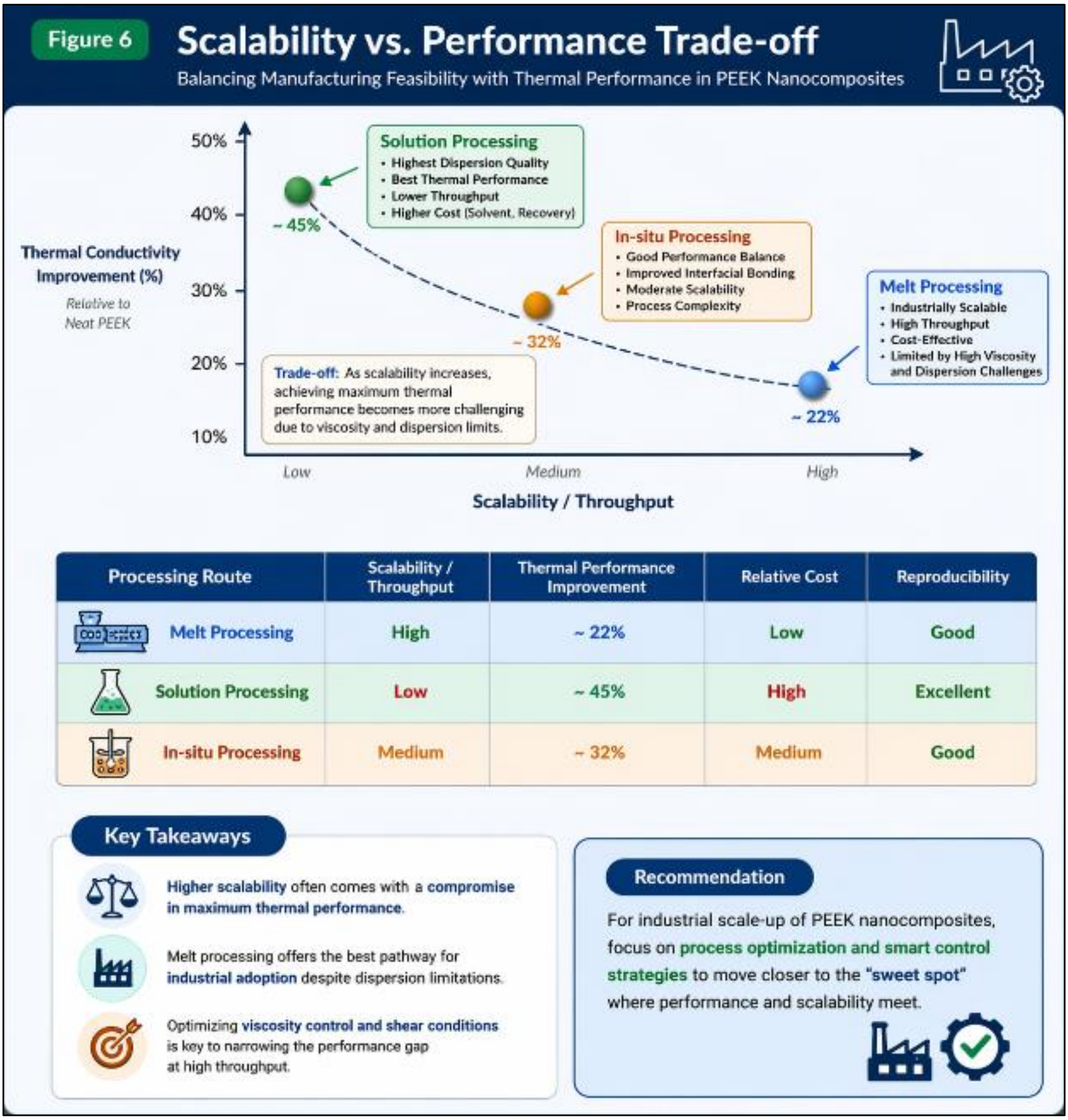

Figure 6 Scalability vs performance trade-off

7. Conclusions and future work

7.1. Key Findings

This study provides a comprehensive understanding of how viscosity-dependent nanoparticle diffusion governs the thermal performance of PEEK-based nanocomposites, particularly when integrated with machine learning-based predictive modeling frameworks. One of the central findings is that diffusion behavior, strongly influenced by viscosity and temperature, serves as a primary determinant of nanoparticle dispersion, which in turn directly impacts thermal conductivity, crystallinity, and melting temperature. Improved diffusion leads to more uniform filler distribution, enabling the formation of efficient thermal pathways and enhanced interfacial interactions.

The integration of machine learning models has revealed complex nonlinear relationships between processing parameters and material properties that are difficult to capture using traditional analytical approaches. Feature engineering techniques, including interaction terms such as viscosity–temperature coupling, have significantly improved predictive accuracy by embedding physical insights into the modeling process. The multi-output regression framework further demonstrated the importance of simultaneously predicting interdependent properties, ensuring consistency between thermal and structural responses.

Additionally, the study highlights that optimal thermal performance is achieved within a narrow processing window, where sufficient nanoparticle mobility ensures uniform dispersion without compromising polymer stability. The findings emphasize that diffusion is not an isolated parameter but part of a coupled system linking processing conditions, microstructure formation, and macroscopic performance. This diffusion–structure–property relationship provides a critical foundation for designing high-performance nanocomposites tailored for advanced thermal management applications.

7.2. Limitations

Despite the robustness of the proposed framework, several limitations must be acknowledged. First, the dataset used for model training may not fully capture the entire range of processing conditions and material variations encountered in industrial settings. The limited availability of high-quality experimental data, particularly at extreme temperatures or filler concentrations, can constrain the generalizability of the model.

Second, the modeling approach relies on certain assumptions regarding uniform dispersion, ideal interfacial interactions, and consistent material behavior, which may not always hold true in practical applications. Variations in nanoparticle morphology, surface chemistry, and processing inconsistencies can introduce deviations that are not fully accounted for in the model.

Furthermore, while machine learning models provide high predictive accuracy, they may lack complete interpretability, particularly in complex architectures such as deep neural networks. This can make it challenging to extract mechanistic insights directly from model outputs. Addressing these limitations requires the integration of more comprehensive datasets and the development of hybrid modeling approaches that combine data-driven techniques with fundamental physical principles.

7.3. Future Research Directions

Future research should focus on expanding the scope of nanocomposite design through the incorporation of hybrid nanofillers, where combinations of materials such as TiO_2, ZnO, and other conductive or functional nanoparticles are used to achieve synergistic effects. These systems have the potential to overcome the limitations of single-filler approaches by enhancing both thermal conductivity and structural stability simultaneously.

Another promising direction involves the integration of real-time machine learning control within processing systems. By coupling predictive models with in situ monitoring techniques, it becomes possible to dynamically adjust processing parameters such as temperature, shear rate, and residence time to achieve optimal nanoparticle dispersion and material performance. This approach could significantly improve reproducibility and scalability in industrial manufacturing.

Additionally, the development of more interpretable machine learning models, combined with advanced characterization techniques, will enhance the understanding of diffusion-driven microstructural evolution. Such efforts will enable the creation of more reliable and physically grounded predictive frameworks, ultimately advancing the design of next-generation polymer nanocomposites for high-performance thermal applications.

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