

Physics-informed Neural Network-based Prediction of Multi-factor Coupled Thermal-oxidative Aging Behavior in Polyamide66-Glass Fiber Composites

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Abstract Accelerated aging tests are widely used to rapidly evaluate the durability of materials, of which thermal-oxidative aging is the most common approach. To quantitatively predict the effects of multiple coupled factors, this study takes polyamide66 reinforced with glass fiber (PA66-GF) as a model system and proposed a high-precision paradigm for coupled thermal-oxidative aging. By integrating Arrhenius-type reaction kinetics with oxygen diffusion, a predictive formula that holistically captures the nonlinear synergistic effects of multiple factors was developed, thereby overcoming the limitations of traditional single-variable models. A systematic evaluation of the stepwise improved formulas through nonlinear fitting showed that the coefficient of determination (R^2) increased from 0.223 to 0.803, elucidating the fundamental reason why conventional approaches fail in quantitative prediction. These formulae were further embedded as physical constraints into a physics-informed neural network (PINN), which further enhanced the predictive performance, with the proposed formula achieving a peak R^2 of 0.946. The results highlight that robust data fitting alone is insufficient; the decisive factor for the success of PINN lies in whether the embedded formula faithfully reflects the underlying physical mechanisms. When applied to polyamide 6 reinforced with glass fiber (PA6-GF), the Formula-constrained PINN maintained a high level of accuracy ($R^2=0.916$), demonstrating its strong cross-system generalizability. In summary, this work establishes a robust hybrid physics-machine learning framework that combines high accuracy with transferability for predicting the thermal-oxidative aging behavior of composite material systems.

Keywords PA66-GF composites; Accelerated aging; Modified Arrhenius model; Dimensionless; Physics-informed neural network (PINN)

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INTRODUCTION

Fiber-reinforced composites are widely used in the automotive, aerospace, electrical, and electronic industries, where their long-term service reliability is crucial to the safety and stability of engineering systems.^[1–5] To accelerate the development and performance evaluation of new materials, accelerated aging tests are commonly employed to complete material screening and iterative optimization within a shortened timeframe^[6] among which thermal-oxidative aging is the most widely adopted method. Under prolonged exposure to high temperatures and oxygen-rich environments, the polymer matrix undergoes free-radical oxidation reactions, chain scission, and cross-linking,^[7–9] while Fiber-matrix interfacial degradation also occurs, collectively leading to a pronounced decline in the mechanical prop-

erties of the composite.^[10] This degradation process is accompanied by multi-scale structural evolution, making it extremely challenging to predict the resulting performance behavior. More critically, there is often a substantial gap between the conditions of accelerated aging tests and actual service environments, leading to long-standing concerns regarding extrapolation accuracy and scientific reliability of test data for engineering applications.^[11] Therefore, it is imperative to develop a predictive model capable of accurately capturing the evolution of mechanical properties, thereby enabling the rapid and reliable transformation of accelerated aging data into realistic service performance behavior.^[12]

At present, most studies on aging adopt a controlled-variable experimental design. For example, Richaud *et al.*^[13] investigated the effect of pressure on the thermal-oxidative aging of polypropylene by comparing high-pressure and atmospheric conditions. Similarly, Courvoisier *et al.*^[14,15] examined the influence of sample thickness on the oxygen permeability of polyethylenimine (PEI) and polyetheretherketone (PEEK), whereas Faulkner *et al.*^[16] highlighted the dominant role of thickness in regulating aging behavior under high-pressure

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oxygen environments. Although these studies have revealed the effects of individual factors^[17], their applicability under complex service conditions involving multifactor coupling is highly limited. Consequently, such approaches often remain at the level of qualitative analysis^[18] and fail to achieve accurate quantitative predictions of thermal-oxidative aging processes under actual operating conditions.^[19,20]

To achieve quantitative prediction, researchers have proposed various mechanism-driven modeling approaches^[21,22], such as numerical models based on diffusion–reaction governing equations^[23] solved using finite element^[24–27] or finite difference methods, as well as molecular dynamics (MD) simulations^[28] and chemical kinetic models. These approaches incorporate physical processes, such as oxygen diffusion and chemical reaction kinetics, thereby providing theoretical support for understanding thermal-oxidative aging behavior.^[29–33] However, the key parameters of these models are highly dependent on the specific characteristics of the material, including its chemical structure, crystallinity, filler content, and cross-linking degree.^[34] As a result, when a new material is introduced, extensive experimental measurements and parameter fitting must be performed.^[2] In addition, Wang *et al.*^[35,36] separately established third-order polynomial nonlinear models using tensile strength and oxidation induction time as indicators. Although such empirically based extrapolation methods can, to some extent, provide predictive insights under realistic service conditions^[37,38], they remain at the level of mathematical fitting and fail to capture the underlying physical mechanisms beyond the assumed conditions. Consequently, their extrapolation capability in unseen operating scenarios is inherently limited.^[17,39,40] Overall, mechanistic models are theoretically generalizable but lack parameter universality, while empirical models offer flexibility in prediction but lack mechanistic support^[17]; thus, neither approach can fully meet the practical demands of engineering applications.

Unlike traditional analytical or numerical simulation methods, machine learning (ML) provides a novel approach for addressing the aforementioned challenges.^[2,41] ML can automatically learn complex nonlinear relationships among variables from limited, high-dimensional experimental data without relying on a complete mechanistic model.^[42–44] Previous studies^[45] have demonstrated that ML performs well in various applications,^[46] such as predicting concrete aging factor,^[47] analyzing material aging behavior using spectroscopic methods,^[48,49] and inferring natural lifetimes from accelerated aging data.^[50] By bypassing the need for complicated physical mechanism derivations, ML models can significantly reduce modeling complexity while improving the prediction accuracy. However, purely data-driven ML models often overlook the underlying physical mechanisms, which may lead to biased predictions and lack interpretability,^[17] thereby limiting their acceptance in engineering applications. Consequently, integrating ML with physical mechanisms has emerged as a key strategy to enhance both the reliability and interpretability of predictive models.^[2,17,51,52]

To meet this integration demand, a physics-informed neural network (PINN) has emerged and demonstrated unique advantages and broad application prospects.^[53] PINN incor-

porate physical laws directly into the loss function of neural networks, enabling deep integration of data-driven learning with physical constraints and theoretically achieving both high predictive accuracy and mechanistic interpretability.^[54–57] Aref *et al.*^[55] employed a physics-constrained multi-agent neural network driven by strain energy and thermodynamic hard constraints to successfully predict the evolution of the mechanical behavior of crosslinked elastomers under thermal-oxidative and hydrolytic aging conditions. Liu *et al.*^[58] predicted the fatigue life of natural rubber (NR) at different environmental temperatures by integrating a crack-initiation-based physical model with a physics-informed neural network. However, the development of PINN faces two major challenges. First, the lack of systematic and comprehensive experimental data under complex service conditions limits the model training and validation.^[2,51,59,60] Secondly, the embedded physical Formulas in most existing studies are largely based on empirical fitting or additive variable assumptions, relying on local dimensionality reduction approximations^[61] that fail to fully capture the nonlinear coupling mechanisms among multiple factors such as temperature, oxygen partial pressure, and thickness.^[62–64] For instance, Ciutacu *et al.*^[65] proposed a lifetime prediction model that couples the oxygen partial pressure and temperature. Therefore, it is evident that although the traditional PINN framework can maintain physical consistency with limited labeled data, its training paradigm based on local equations and separate loss terms is inadequate for achieving holistic modeling in highly coupled multi-factor scenarios. Treating each governing equation as an independent loss component not only fragments the interactions among variables but also confines the model to fitting local patterns and lacks a systematic representation of the overall synergistic mechanisms. Therefore, it is essential to develop a novel predictive formula that holistically reflects the nonlinear synergistic interactions among multiple factors and embeds it as a soft physical constraint within the PINN framework, thereby enabling the rapid, high-accuracy fitting of accelerated aging data and reliable extrapolation to real service conditions.

Therefore, this study focuses on polyamide66 glass fiber-reinforced composites (PA66-GF), with the aim of constructing an engineering-oriented predictive framework that directly captures the evolution of mechanical properties without relying on intermediate chemical indicators. By leveraging a self-developed dynamic and adjustable accelerated aging platform, high-fidelity mechanical aging data were systematically collected under various temperature, oxygen partial pressure, and specimen thickness conditions. From a modeling perspective, a dimensionless^[66,67] predictive formula was proposed based on diffusion and Arrhenius reaction kinetics (as shown in Fig. 1). Methodologically, we first evaluated the fitting performance of the progressively refined formulas within a nonlinear regression framework. The final formula was then embedded as a soft constraint into the loss function of the PINN. By jointly minimizing the data error and physical residual, the PINN enabled automatic optimization of the physical parameters. Furthermore, to examine its generalizability, the proposed formula was transferred to polyamide6 glass fiber-reinforced composites (PA6-GF) within the PINN

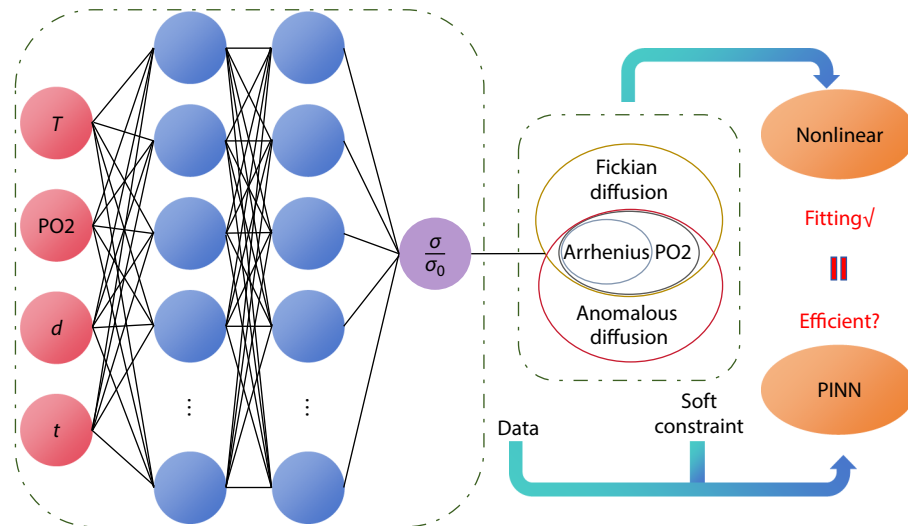


Fig. 1 Summary of the article.

framework for validation. This framework can serve as a rapid and reliable approach for predicting mechanical properties under complex engineering conditions.

EXPERIMENTAL

Dataset Collection

In this study, a self-developed thermal-oxidative aging device with multifactor coupling control (as shown in Fig. 2) was employed to collect high-fidelity mechanical aging data under various conditions of temperature, oxygen partial pressure, and specimen thickness, resulting in a dataset comprising 178 samples (as shown in Fig. 3). The accelerated aging test conditions for the samples are listed in Table 1. The dataset covers a continuous gradient of operating states, ranging from oxygen-deficient environments to medium- and high-oxygen pressure conditions, providing a reliable foundation for subsequent modeling and analysis.

Material Preparation

This study focused on PA66 composites reinforced with 25 wt% glass fiber (PA66-GF) supplied by Chongqing Sanlei Fiberglass Co., Ltd. ISO527-21BA tensile specimens were prepared via in-



Fig. 2 Dynamic high heat oxygen partial pressure accelerated aging device.

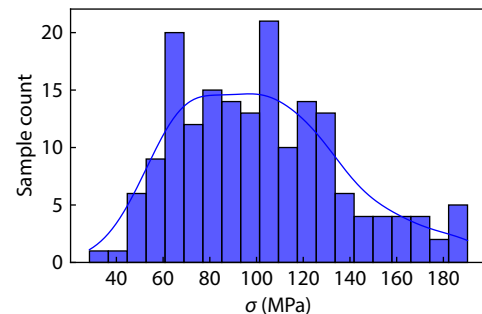


Fig. 3 Distribution of tensile strength for PA66 composites with different thickness under a set of heat oxygen aging.

Table 1 Thermal-oxidative aging test conditions.

Aging temperature T (°C)	Oxygen partial pressure PO ₂ (MPa)
160, 170, 180, 190	0, 0.0036, 0.0090, 0.0209, 0.0600, 0.0627, 0.1254, 0.1672, 0.1881, 0.2100, 0.3150

jection molding using a standard injection molding machine. The specimens had a length of 60.00 mm, a width of 5.00 mm, and thicknesses of 3.00, 1.50, and 0.75 mm, respectively.

Tensile Testing

The tensile properties of the materials were tested using an Instron 3365 electronic universal testing machine in accordance with ISO527-2:2012. The test environment was maintained at a constant temperature and humidity of (23 ± 2) °C and $50\% \pm 5\%$ RH. Each group of tests had at least 3 valid repeated samples, and the final results were averaged for analysis. The formula for calculating the tensile strength retention rate is as follows:

$$\text{Retention} = \frac{\sigma}{\sigma_0} \times 100\% \quad (1)$$

where σ_0 is the initial tensile strength and σ is the tensile strength after aging.

METHODS

To achieve a high predictive accuracy, physical interpretability,

and rapid response for engineering applications in modeling the aging behavior of composite materials, it is essential to develop a framework that efficiently integrates physical mechanisms with data-driven approaches. The core of this methodology lies in constructing a predictive formula capable of accurately characterizing multifactor coupling effects. This formula not only establishes the theoretical foundation of the model, but also plays a decisive role in ensuring the predictive accuracy of the subsequent PINN and enabling rapid and reliable predictions in practical engineering applications. Table 2 provides a complete list of the symbols and abbreviations used in this study along with their definitions and corresponding units for easy reference.

Traditional Arrhenius Formula

Ciutacu *et al.*^[65] proposed an empirical kinetic formula for glass-fiber-reinforced epoxy systems, in which temperature, oxygen partial pressure, and time are combined in an Arrhenius-type form, with a power-law term for oxygen partial pressure introduced to predict the degradation of flexural strength. This approach validated the universality of using a closed-form response formula to link environmental factors with the deterioration of the mechanical properties.

In this section, maintaining the original framework of the

empirical formula proposed by Ciutacu *et al.*,^[65] the model parameters were recalibrated based on the service characteristics of PA66-GF during the thermal-oxidative aging process, thereby enabling the adaptation and extension of the formula to this new material system.

Similarly, assuming that the degradation of the material properties during the thermal-oxidative aging process follows first-order kinetics, its evolution can be expressed as:

$$-\frac{d\sigma}{dt} = k\sigma^a \quad (2)$$

where k is the rate constant, t is the aging time and a is the total degradation reaction order. Here, let $a=1$, and the reaction follows first-order kinetics.

During the initial stage of thermal-oxidative aging, materials may undergo structural changes, such as increased crystallinity, molecular chain rearrangement, enhanced interfacial bonding, residual stress release, and limited crosslinking, resulting in a transient strengthening effect. Jia *et al.*^[68] reported that during aging at 121 °C, short glass fiber reinforced polyamides exhibited an increase in static tensile strength due to structural changes, including an increase in crystallinity and crystalline perfection. To further describe this phenomenon, a material constant, denoted as a , was intro-

Table 2 Definition of parameters used in the kinetic model.

Parameter	Description	Unit
σ	The tensile strength after aging	MPa
σ_0	The initial tensile strength	MPa
t	Aging time	s
k	The rate constant of the thermal-oxidative aging reaction, which follows the Arrhenius temperature dependence.	s^{-1}
a		–
a	Structural adjustment constant	–
σ'	The effective initial tensile strength of the material during the early stage of thermal aging	MPa
A		s^{-1}
E_a	The activation energy	$\text{kJ}\cdot\text{mol}^{-1}$
R	The gas constant	$\text{J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$
T	The thermal aging temperature	K
A_0	The reaction intensity factor under the reference state	$s^{-1}\cdot\text{MPa}^{-n}$
n	The oxygen partial pressure correction coefficient	–
PO_2	Standard atmospheric pressure	MPa
$\langle r^2(\tau_d) \rangle$	The diffusion mean square displacement	m^2
τ_d	The characteristic timescale required for oxygen molecules to complete diffusion across the entire sample with different thickness	s
K_β	The generalized diffusion coefficient	$\text{m}^2\cdot\text{s}^{-\beta}$
β		–
τ	The characteristic diffusion time	s
D	The diffusion coefficient	$\text{m}^2\cdot\text{s}^{-1}$
d	Thickness	m
D_0	Pre-exponential factor	$\text{m}^2\cdot\text{s}^{-1}$
E_{D0}	The activation energy for oxygen diffusion under the ideal Fickian assumption	$\text{kJ}\cdot\text{mol}^{-1}$
c		–
A_0'	The intensity coefficient of the comprehensive effects of multiple factors	–
$E_{\text{eff},0}$	The effective activation energy that comprehensively accounts for both the reaction and Fickian diffusion processes	$\text{kJ}\cdot\text{mol}^{-1}$
τ_z		s
z	The thickness exponent	–
D_z	The effective diffusion coefficient	$\text{m}^2\cdot\text{s}^{-1}$
m	The thickness response exponent	–
D_{Z0}	The pre-exponential factor for anomalous diffusion	$\text{m}^2\cdot\text{s}^{-1}$
E_{Dz}	The generalized effective diffusion activation energy	$\text{kJ}\cdot\text{mol}^{-1}$
$E_{\text{eff},1}$	The effective activation energy that comprehensively accounts for both the reaction and anomalous diffusion processes	$\text{kJ}\cdot\text{mol}^{-1}$

duced into the model as a structural adjustment factor, enabling a more accurate characterization of the evolution of the material from initial structural reorganization to subsequent matrix degradation.

$$\sigma' = a\sigma_0 \quad (3)$$

where σ' represents the effective initial tensile strength of the material during the early stage of thermal aging and a is a structural adjustment constant determined through data analysis.

Based on the Arrhenius formula, the relationship between the reaction rate constant k and temperature T can be expressed as:

$$k = A \times \exp\left(-\frac{E_a}{RT}\right) \quad (4)$$

where A is the exponential factor, E_a is the activation energy, R is the gas constant ($8.314 \text{ J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$), and T is the thermal aging temperature (K). The rate constant k follows the Arrhenius formula.

By substituting the rate formula into the performance attenuation formula and combining it with the correction term a , the expression for the evolution of the performance retention rate over time can be obtained as follows:

$$\text{Retention} = a \exp\left[-A \exp\left(-\frac{E_a}{RT}\right)\right] \quad (5)$$

Furthermore, considering the effect of oxygen partial pressure on the reaction rate, this study introduces the oxygen partial pressure correction coefficient PO_2^n as follows:

$$A = A_0 \text{PO}_2^n \quad (6)$$

where A_0 is the reaction intensity factor under the reference state and n is the oxygen partial pressure correction coefficient.

Considering the combined effects of oxygen partial pressure and aging time, the following empirical formula was constructed to describe the evolution of material performance with respect to environmental factors:

$$\text{Retention}(\text{PO}_2, T, t) = a \exp\left[-A_0 \text{PO}_2^n \exp\left(-\frac{E_a}{RT}\right)\right] \quad (7)$$

Fickian Diffusion Predictive Formula

In Section **Traditional Arrhenius Formula**, we find that the empirical model proposed by Ciutacu *et al.*^[65] treats each influencing factor in a separate and independent manner. This approach inevitably weakens or even neglects the coupling effects among multiple variables, making it difficult to accurately characterize aging behavior under complex service conditions. To address this limitation, the present study aimed to develop a predictive formula that can holistically capture the nonlinear synergistic interactions among multiple factors, thereby preserving their intrinsic interrelationships to the greatest extent possible. Based on the coupled effects of key variables, such as oxygen partial pressure, thickness, and temperature, we propose a total rate constant K to comprehensively describe their combined influence.

$$K = k(\text{PO}_2, T, d) \quad (8)$$

where $k(\text{PO}_2, T, d)$ represents the combined effects of oxygen partial pressure, temperature, and thickness on the aging reaction rate. The influence of the temperature on the aging rate is described by Eq. (4).^[69] To eliminate the impact of pressure units on the model parameters, a reference oxygen partial pressure of

$\text{PO}_2=0.101325 \text{ MPa}$ was introduced for nondimensionalization such that the oxygen partial pressure term was expressed in a dimensionless form. By substituting this relationship into Eq. (6), the model can maintain consistency across different pressure units.

The effect of thickness on the aging rate arises from the modulation of oxygen diffusion. The characteristic diffusion time τ represents the time required for oxygen molecules to diffuse across the material thickness d . Because the macroscopic aging rate varies significantly with the sample thickness and oxygen permeability, it is difficult to directly compare or analyze the results under a common baseline. To overcome this issue, the normalized time t/τ was introduced, which reflects the progress of the aging process relative to the diffusion process. This normalization eliminates the incomparability among samples with different thicknesses or permeabilities, allowing experimental data to be compared and interpreted within a unified physical framework. When the diffusion of oxygen molecules in the sample follows a power-law relationship,^[70] it can be expressed as:

$$\langle r^2(\tau_d) \rangle = K_\beta \tau^\beta \quad (9)$$

where $\langle r^2(\tau_d) \rangle$ is the diffusion mean square displacement, τ_d is the characteristic timescale required for oxygen molecules to complete diffusion across the entire sample thickness, K_β is the generalized diffusion coefficient, and β is the diffusion exponent.

Assuming that the diffusion behavior of the material follows the classical Fick's law ($\beta=1$), Eq. (9) can be simplified as

$$\tau = \frac{d^2}{D} \quad (10)$$

where D is the diffusion coefficient, and τ is the characteristic diffusion time.

The diffusion process is a thermally activated migration behavior, and its rate exhibits an exponential dependence on temperature, similar to that of the reaction rate. Therefore, D also follows the Arrhenius relationship:

$$D = D_0 \times \exp\left(-\frac{E_{D0}}{RT}\right) \quad (11)$$

where E_{D0} is the activation energy for oxygen diffusion under the ideal Fickian assumption.

As pointed out by Raji *et al.*^[4], when establishing the time dependence of a parameter, the power-law form is usually the first expression to be attempted, and its mathematical representation is given by

$$f(t) = t^c \quad (12)$$

where c is the time exponent.

Finally, the retention expression can be further generalized as:

$$\text{Retention} = a \exp\left[-A_0' \left(\frac{\text{PO}_2}{\text{PO}_{20}}\right)^n (tD_0)^c d^{-2c} \exp\left(-\frac{E_{\text{eff},0}}{RT}\right)\right] \quad (13)$$

Let

$$E_{\text{eff},0} = E_a + cE_{D0} \quad (14)$$

where A_0' represents the intensity coefficient of the comprehensive effects of multiple factors and $E_{\text{eff},0}$ is the effective activation energy that comprehensively accounts for both the reaction and Fickian diffusion processes.

Anomalous Diffusion Predictive Formula

However, in actual complex service environments, the microstructure of PA66-GF, such as the distribution of crystalline regions, degree of crosslinking, and interfacial architecture, can significantly influence the effective migration pathways of oxygen molecules, causing the oxygen diffusion behavior to deviate from the ideal Fickian diffusion assumption and exhibiting anomalous diffusion characteristics ($\beta \neq 1$). To capture this reaction-diffusion nonequilibrium behavior within the model more comprehensively, a generalized diffusion-controlled time scale is introduced in this study:

$$\tau_z = \frac{d^z}{D_z} \quad (15)$$

Let

$$z = \frac{2}{\beta} \quad (16)$$

$$D_z = K^{1/\beta} \quad (17)$$

$$m = cz \quad (18)$$

where τ_z is the generalized diffusion-controlled time, z is the thickness exponent, D_z is the effective diffusion coefficient, and m is the thickness response exponent.

The generalized diffusion coefficient D_z also obeys an Arrhenius formula:

$$D_z = D_{z0} \times \exp\left(-\frac{E_{Dz}}{RT}\right) \quad (19)$$

where D_{z0} is the pre-exponential factor for anomalous diffusion and E_{Dz} is the generalized effective diffusion activation energy.

Finally, the retention expression can be further generalized as:

$$\text{Retention} = a \exp\left[-A'_0 \left(\frac{\text{PO}_2}{\text{PO}_{2,0}}\right)^n (tD_0)^c d^{-m} \exp\left(-\frac{E_{\text{eff},1}}{RT}\right)\right] \quad (20)$$

Let

$$E_{\text{eff},1} = E_a + cE_{Dz} \quad (21)$$

where $E_{\text{eff},1}$ is the effective activation energy that comprehensively accounts for both the reaction and anomalous diffusion processes.

Physics-Informed Neural Network (PINN)

To systematically investigate how the quality of the response formula influences the predictive performance and mechanistic consistency of the model, we first performed nonlinear fitting of Eqs. (5), (7), (13), and (20) using experimental data to evaluate their fitting capability and applicability under purely data-driven conditions. Subsequently, these four formulas were individually embedded as soft constraints into the PINN framework, with each model trained separately to enable a comparative analysis of the effects of different formula constraints on the accuracy and interpretability of the PINN. Specifically, the model training simultaneously minimized two types of loss: (i) the fitting error based on macroscopic retention observations and (ii) the mechanistic residuals derived from the embedded formulas. To ensure robustness, a 10-fold cross-validation strategy was employed, and a shallow neural network architecture (2–3 hidden layers) was adopted to maintain a balance between the model complexity and data scale.

The model was trained using the Adam optimizer. Its total

loss function incorporates both data fitting and physical consistency, and is defined as follows^[71,72]:

$$L = L_{\text{data}} + \lambda_{\text{phys}} L_{\text{phys}} \quad (22)$$

$$L_{\text{data}} = \frac{1}{N} \sum_{i=1}^N (\ln_{\text{nn}} R_i - \ln_{\text{true}} R_i)^2 \quad (23)$$

$$L_{\text{phys}} = \frac{1}{N} \sum_{i=1}^N (\ln_{\text{nn}} R_i - \ln_{\text{phys}} R_i)^2 \quad (24)$$

where $\ln_{\text{nn}} R_i$, $\ln_{\text{true}} R_i$ and $\ln_{\text{phys}} R_i$ are the neural network prediction, the experimental true value, and the logarithmic retention rate calculated from Eqs. (5), (7), (13), and (20), respectively.

RESULTS AND DISCUSSION

Nonlinear Curve Fitting

Evaluation of the predictive accuracy of the traditional formula

To evaluate the applicability of conventional empirical formulas in modeling thermal-oxidative aging, we first performed a nonlinear regression using Eqs. (5) and (7) to predict the tensile strength retention of the material. The results show that the R^2 values of the test set were 0.223 and 0.617, respectively. Although the introduction of the oxygen partial pressure in Eq. (7) led to a modest improvement in the fitting accuracy, the overall predictive performance remained unsatisfactory. Further analysis revealed that these empirical models did not explicitly account for the critical influence of the specimen thickness on the aging process. In particular, the thickness determines the effective penetration depth of oxygen, thereby governing the spatial distribution of the performance degradation. The omission of this key variable prevents the model from capturing the diffusion-constrained nature of aging, fundamentally limiting its predictive accuracy.

Reconstruction analysis under Fickian diffusion dominated control

As shown in Fig. 4, coupled Eq. (13) achieved a coefficient of determination (R^2) of 0.429 for the test set. Although Eq. (13) partially captures the synergistic effects among diffusion, temperature, and thickness, its overall goodness-of-fit remains relatively low, indicating that the model fails to fully represent the intrinsic characteristics of the actual oxygen diffusion process.

This suggests that the aging behavior of the material may deviate from the ideal Fickian diffusion pathway. In particular, under high temperature, elevated oxygen partial pressure, and large thickness conditions, oxygen molecules often cannot penetrate the material continuously and uniformly. As a result, the oxygen concentration exhibits a pronounced nonlinear gradient along the thickness direction, leading to a non-steady-state behavior and spatial heterogeneity of diffusion. These phenomena are the primary reasons for the limited predictive accuracy of the proposed model.

Reconstruction analysis under anomalous diffusion dominated control

To verify whether the diffusion control mechanism in the current system deviated from the ideal Fickian diffusion model, Eq. (20) was further fitted. The results show that this model achieved a higher $R^2=0.803$ on the test set, which is significantly better than that of the original model based on the Fickian as-

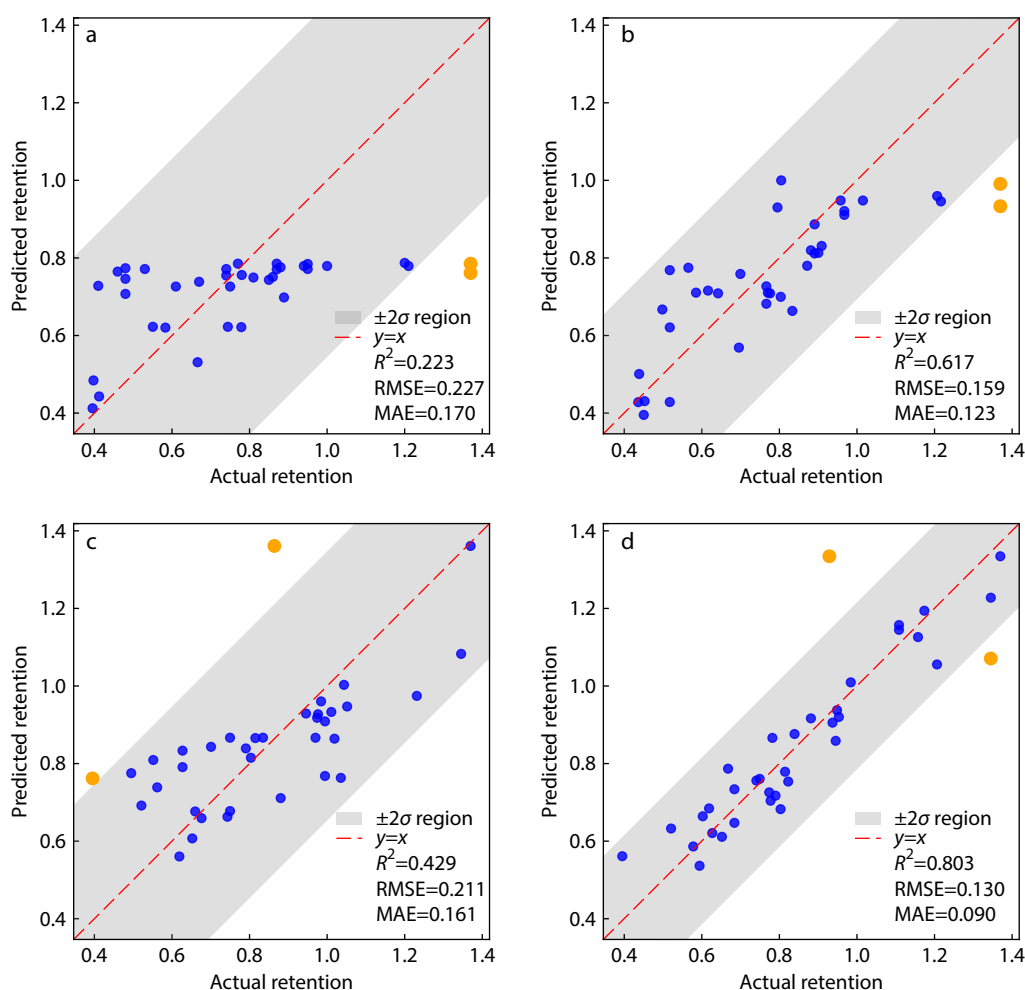


Fig. 4 Nonlinear fitting results of (a) Eq. (5), (b) Eq. (7), (c) Eq. (13), and (d) Eq. (20).

sumption, strongly demonstrating that the oxygen diffusion behavior in the system deviates from the ideal steady-state pathway. As illustrated in Fig. 4, with the model evolving from Eq. (5) to Eq. (20), the $\pm 2\sigma$ gray band representing the statistical range of prediction deviations (σ being the standard deviation of residuals) gradually narrows, reflecting significant improvements in the predictive accuracy and overall stability across different aging conditions. With only a few exceptions, most samples fell within this deviation band, and the limited outliers were mainly associated with high-temperature conditions, thickness values located at the boundaries of the sample distribution (0.75 mm or 3 mm), or aging times near the limits of the experimental design. In these regions, sparse sample coverage, more pronounced oxygen concentration gradients, and inherent measurement uncertainties make these points more susceptible to deviations from model predictions.

Unlike earlier formulations that compressed different operating conditions into a single equivalent variable, Eq. (20) explicitly captures the nonlinear interactions among temperature, oxygen pressure, thickness, and aging time, enabling the model to maintain stronger stability and physical consistency across a broader operating domain.

Analysis of PINN

To systematically investigate the applicability and stability of the

response prediction formulas in the PINN framework, this study kept the data loss weight at $\lambda_{\text{data}}=1$, embedded Eqs. (5), (7), (13), and (20) as soft physical constraints in the neural network, and performed a comparative analysis of their nonlinear fitting performance and physical loss weight λ_{phys} . Table 3 presents the results.

Eq. (5) is the classic Arrhenius model, accounting solely for temperature-driven reaction kinetics. Its standalone nonlinear fitting performance was poor ($R^2=0.223$), but improved to $R^2=0.788$ when embedded in the PINN. However, its physical-loss weight is extremely low ($\lambda_{\text{phys}}=1.00\times 10^{-4}$), indicating that the network relies almost entirely on data fitting and barely “sees” the physical constraint. This finding demonstrates that an oversimplified physical form lacking essential mechanistic

Table 3 Physical-loss weight (λ_{phy}) and test-set R^2 for different PINN formulas.

Eq.	λ_{phys}	Test- R^2	
		Nonlinear	PINN
5	1.00×10^{-4}	0.223	0.788
7	1.00×10^{-5}	0.617	0.712
13	0.60	0.429	0.893
20	0.65	0.803	0.946

components contributes little to network optimization, even when formally incorporated. Building on Eq. (5), Eq. (7) introduces an empirical term for oxygen partial pressure. Although the PINN's predictive accuracy with Eq. (7) exceeds that of pure data fitting, its physical loss weight remains negligible ($\lambda_{\text{phys}}=1.00\times 10^{-5}$), indicating that the physical term is effectively inactive during training and that optimization still relies predominantly on data loss. While the partial-pressure term provides local compensation in fitting, its empirical nature means that it does not incorporate genuine diffusion physics, and thus fails to establish a true data-physics synergy.

In contrast, Eq. (13) ($R^2=0.429$), while exhibiting slightly inferior standalone regression performance compared to Eq. (7), delivers a dramatic improvement when used as a PINN soft constraint ($R^2=0.893$), with its physical loss weight rising to $\lambda_{\text{phys}}=0.6$. This indicates that incorporating the Fickian diffusion mechanism substantially enhances the physical fidelity of the model, rendering the physics constraint a key factor in the optimization process. Although the ideal-diffusion assumption introduces systematic bias under certain non-steady-state conditions, the overall consistency of the mechanism enables PINN to actively recognize and leverage it. These findings clearly demonstrate that enhancing the physi-

cal completeness of the formula, even at the cost of a slight reduction in the pure data-fitting accuracy, can lead to superior generalization capability and more reliable predictions through effective physics-data coupling. By introducing an anomalous control exponent, the limitation of the ideal diffusion model in capturing non-steady-state behavior can be effectively addressed, significantly enhancing its capacity to represent complex processes. Eq. (20) achieves the highest standalone nonlinear fit ($R^2=0.803$) and further improves to $R^2=0.946$ when embedded in the PINN framework while maintaining stable convergence even at a physical-loss weight of $\lambda_{\text{phys}}=0.65$.

Compared with Figs. 4 and 5, both the standalone nonlinear regression models and their PINN-embedded versions exhibit a clear improvement trend: the $\pm 2\sigma$ gray bands in all subplots shrink substantially, and the prediction points become more tightly clustered along the diagonal, indicating a marked reduction in the prediction dispersion and a significant enhancement in the overall stability. This demonstrates that the introduction of physical constraints effectively strengthens model convergence and robustness, enabling the PINN to move beyond reliance solely on the statistical distribution of the data and converge toward a prediction behavior that better reflects the underlying physical mecha-

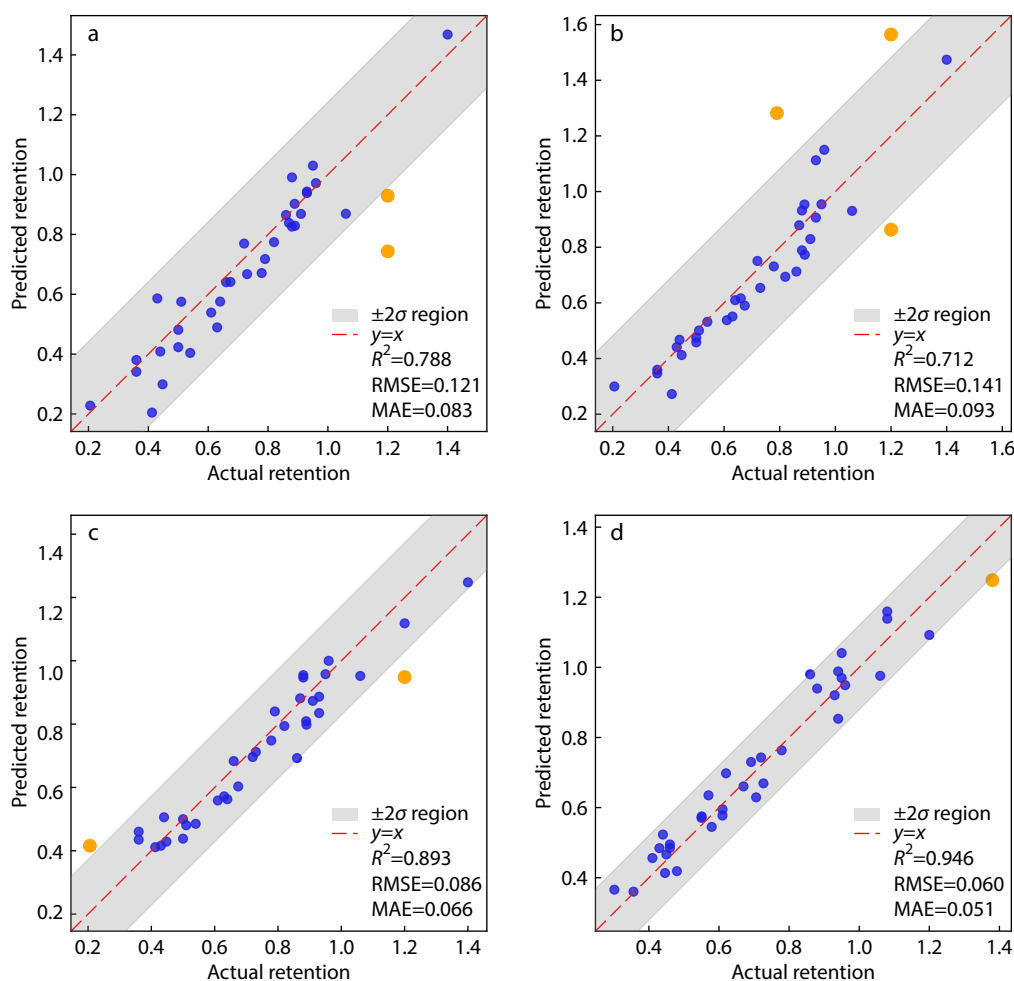


Fig. 5 PINN prediction results of (a) Eq. (5), (b) Eq. (7), (c) Eq. (13), and (d) Eq. (20).

nisms. Notably, even when the physical loss weights assigned to Eqs. (5) and (7) are close to zero within the PINN framework, their deviation bands in Fig. 5 still show a clear contraction. This suggests that the incorporation of physical formulations, even in a very weak form, provides a structured guiding direction for the optimization process, implicitly constraining the training dynamics through the underlying diffusion kinetics rather than allowing the model to fit only empirical data patterns. Consequently, consistent improvements were observed once the PINN framework was applied, highlighting the essential role of physical priors in enhancing model stability and generalization across different aging conditions.

These findings demonstrate that when the model accurately captures the dynamic coupling between reaction kinetics and diffusion, the physical constraint not only preserves the network's expressive power, but also strengthens its generalization and stability. In conclusion, the physical soundness of a formula's structure is a prerequisite for effective physics-data synergy. The more complete the embedded physics, the more instructive the physical loss term during training, enabling the neural network to reduce its reliance on large datasets and maintain robust extrapolation in sparse or unseen regimes. Conversely, empirical formulas lacking a solid physical foundation, even if they fit existing data well, tend to fail under physical constraints. This underscores the fundamental value of physic-informed neural networks, not merely to achieve high fidelity on available data, but also to enhance the model's ability to capture true physical laws and to extrapolate reliably under complex operating conditions.

Interpretation of the Formula-Constrained PINN

Table 4 presents the parameter values obtained from the PINN fitting for all formulas. As shown in Table 4, the fitted values of parameter a in Eqs. (5) and (7) were significantly overestimated, far exceeding the physically acceptable range. This suggests that these two formulas either suffer from overfitting or lack sufficient mechanistic representation, rendering them incapable of accurately capturing the actual reaction-diffusion process. As the model complexity increases, the parameter " a " obtained from Eqs. (13) and (20) gradually falls within a reasonable range, better representing actual physical behavior.

For the parameters obtained from the soft-constrained training of Eq. (20), the analysis shows that the temporal exponent $c < 1$, indicating that the degradation of mechanical performance over time does not follow strict first-order exponential kinetics, but rather exhibits a nonlinear pattern. This behavior arises from multi-scale synergistic effects during the aging process: heterogeneous regions such as crystalline domains, amorphous phases, and fiber-matrix interfaces exhibit different reaction rates, while the local oxygen partial pres-

sure dynamically evolves during the coupled diffusion-reaction process. The combined influence of these factors ultimately shapes the observed nonlinear power law decay behavior.

In addition, the thickness exponent is given by Eq. (18), where c describes the power-law variation with time, and z determines the dependence of the diffusion-controlled timescale on the thickness. Therefore, m reflects the combined effect of thickness on performance degradation. Referring back to Eq. (9), the fitted result shows that $\beta > 1$, indicating a super-diffusive characteristic.^[73,74] This phenomenon can be primarily attributed to two factors. First, the unique structure of the composite allows the glass fiber-matrix interfacial regions and porosity to serve as fast channels for oxygen migration. Meanwhile, the rapid consumption of oxygen at the surface generates a steep concentration gradient, resulting in a "suction pump" effect that accelerates oxygen penetration in thick-walled specimens. Second, the predictive formula used in this study simplifies the complex aging process into a limited number of parameters, making it difficult to fully capture multi-scale diffusion-reaction mechanisms. Thus, the obtained result should be interpreted as an effective representation under the modeling framework rather than as a direct intrinsic property of the material. Although this formula has certain limitations in mechanistic interpretation, it provides a concise, rapid, and practical predictive tool that can be directly integrated with performance design in engineering applications.

Cross-system Generalization Validation

To validate the universality of the proposed diffusion-reaction closed-form model, Eq. (20) was further applied to the PA6-GF system, where PA6-GF refers to polyamide6 composites reinforced with 30 wt% glass fiber, supplied by Chongqing Sanlei Fiberglass Co., Ltd. In total, 190 aging data points were collected for this system, and the corresponding post-aging tensile strengths are presented in Fig. 6(a). After retraining and parameter optimization with $\lambda_{\text{phys}}=0.5$, the model achieved a prediction accuracy of $R^2=0.916$ for the test set. More importantly, the overall distribution of the prediction points remained consistent with that of the PA66-GF model: most data fell near the $\pm 2\sigma$ reference band defined by PA66-GF and exhibited a tightly clustered alignment along the diagonal (as shown in Fig. 6b). This indicates that although the two materials differ in their specific parameter values, they share a similar diffusion-reaction-dominated degradation framework during thermal-oxidative aging, allowing the same set of physical constraints to achieve stable convergence across different material systems. Consequently, the proposed PINN structure is applicable not only to PA66-GF, but also maintains high predictive accuracy when the material system changes, demonstrating strong model applicability and

Table 4 Parameter fitting results of different Formulas within the PINN framework.

Eq.	a	A_0	n	m	c	D	E_a
5	2.890×10^4	4.470×10^4	—	—	—	—	74.61×10^3
7	6.291×10^4	5930.000	0.3183	—	—	—	72.76×10^3
13	1.297	1774.000	0.1744	—	0.225	1.000×10^{-10}	33.04×10^3
20	1.218	6.468×10^4	0.6280	0.27	0.655	8.717×10^{-4}	67.54×10^3

Note: the parameters listed in the table are unified for clarity. The corresponding symbols in the original formulas may differ.

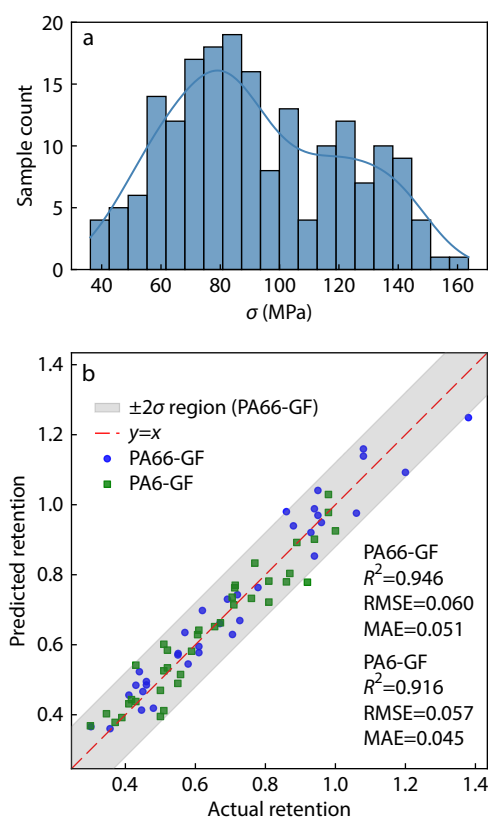


Fig. 6 (a) Distribution of tensile strength after aging for the PA6-GF samples; (b) PINN prediction results for PA6-GF.

material-level generality. These results provide compelling support for extending the framework to a broader class of polyamide composites.

$$\text{Retention} = 0.962 \times \exp \left[-1.066 \times 10^5 \times \left(\frac{\text{PO}_2}{0.101325} \right)^{0.684} \times \left(t \times 1.187 \times 10^{-3} \right)^{0.768} \times d^{-0.24} \times \exp \left(-\frac{73.4 \times 10^3}{RT} \right) \right] \quad (25)$$

CONCLUSIONS

This study utilized a self-developed controllable accelerated aging platform to generate high-fidelity datasets under coupled conditions of oxygen partial pressure, temperature, and film thickness, fundamentally alleviating the limitations of scarce multi-factor experimental data. The results reveal that the failure of traditional empirical formulas under multi-field coupling conditions stems from their excessive simplification of the aging mechanism, which emphasizes only chemical reaction kinetics while neglecting critical nonlinear coupling factors, such as oxygen diffusion and thickness effects. By integrating diffusion and Arrhenius-type reaction kinetics into a unified theoretical framework, we found that predictions based on the ideal Fickian diffusion assumption deviated significantly from the experimental data. To address this limitation, an anomalous diffusion mechanism was introduced, and a modified predictive formula was proposed to elucidate the synergistic control of material aging by the reaction rate and diffusion capacity. This for-

mula demonstrated superior predictive accuracy in both purely data-driven fitting and PINN-based modeling. The findings emphasize that strong data-fitting performance alone does not guarantee the effectiveness of physical constraints within a PINN model; rather, the decisive factor for PINN performance lies in whether the embedded formula faithfully represents the true underlying physical mechanisms. When transferred to the PA6-GF system for validation, the proposed formula maintained an excellent accuracy and cross-system generalization capability. When transferred to the PA6-GF system for PINN validation, the formula maintained excellent accuracy and cross-system generalization capability.

Future work will focus on mechanistic transfer and parameter recalibration for other composites, such as PBT- and PPE-based systems, to evaluate the applicability and scalability of the closed-form formula across a broader range of composite families. This study not only provides a novel technical paradigm for the rapid assessment of aging behavior in materials but also lays a solid theoretical foundation for mechanistic modeling and aging behavior prediction of composites under complex coupled service conditions, including humid heat, ultraviolet exposure, and salt spray.

Conflict of Interests

The authors declare no interest conflict.

Data Availability Statement

Data supporting the findings of this study are available from the corresponding author upon reasonable request.

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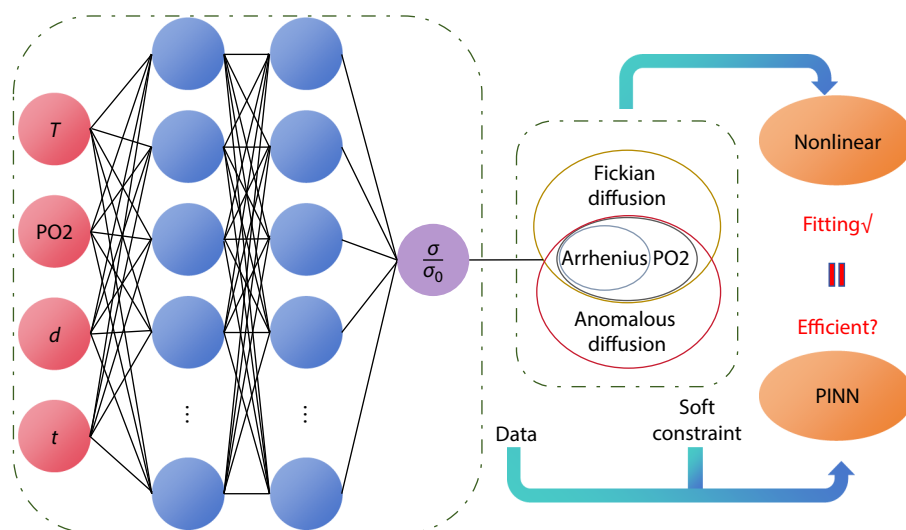
Graphical Abstract

Physics-informed Neural Network-based Prediction of Multi-factor Coupled Thermal-oxidative Aging Behavior in Polyamide66-Glass Fiber Composites

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This work presents a physics-informed neural network (PINN)-based method for predicting the thermal-oxidative aging of polyamide composites, in which a diffusion-reaction coupled formula is embedded as a soft constraint to ensure physical consistency under multifactor coupling and to enable cross-system generalization.



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