STM JOURNALS

Journal of
Polymer & Composites

ISSN: 2321-2810 (Online)
ISSN: 2321-8525 (Print)
Volume 14, Issue 5, 2026
September-October
DOI (Journal): 10.37591/JoPC

https://journals.stmjournals.com/jopc

Research JoPC

Hybrid Quantum–Machine Learning Framework for Nonlinear Rheological Modeling of Polymer and Composite Materials

Pijush Dutta[1,7,*], Pradip Deb[2], Pooja Nagpal[3], Shantanu Naskar[4], Anubrata Mondal[4], Tan Yi Fei[5], Chua Fang Fang[6],

Abstract

In polymer and composite materials, a major challenge lies in predicting their nonlinear rheological response, owing to complex multiscale interactions that are not captured by traditional constitutive laws or conventional machine learning approaches. In this study, a hybrid Quantum–Machine Learning (QML) model comprising Quantum Support Vector Machine (QSVM) and Quantum Neural Network (QNN) architectures is proposed for viscosity prediction without requiring any specific rheological equation. To train and test the proposed model, 420 samples, including shear rate, temperature, and composition-related parameters, were employed. Statistical metrics – like MSE, RMSE, MAE, and R^2 – were used to evaluate predictive performance. The results show that both quantum models outperform the classical machine learning approaches, where the QNN has the highest prediction accuracy (R^2 = 0.970) with RMSE = 0.0435 and MAE = 0.0324 for the testing set, and also has a very good generalization capacity. Moreover, a comparative study was also performed on this model for validation purposes. A sensitivity analysis indicated Polymer concentration and temperature as the key parameters determining the viscosity behavior. The results prove the potential of hybrid quantum–classical frameworks as powerful and data-rich tools for rheological modeling, the intelligent optimization of manufacturing processes, and future developments in materials informatics in Industry 5.0.

***Author for Correspondence**
Pijush Dutta
E-mail id: pijushdutta009@gmail.com

[1]Assistant Professor, Department of Computer Science & Engineering, Greater Kolkata College of Engineering and Management, Kolkata, West Bengal, India
[2]Assistant Professor, Department of Bachelor of Computer Application, Global College of Science and Technology, Krishnagar, West Bengal, India
[3]Associate Professor, Faculty of Management, CMS Business School, Jain (Deemed to Be University), Bangalore, Karnataka, India
[4]Assistant Professor, Department of Electrical Engineering, Greater Kolkata College of Engineering and Management, Kolkata, West Bengal, India
[5]Associate Professor, Centre for Smart Systems and Automation, COE for Robotics and Sensing Technologies, Faculty of Artificial Intelligence and Engineering, Multimedia University, Persiaran Multimedia, 63100 Cyberjaya, Selangor, Malaysia
[6]Associate Professor, Centre for Advanced Analytics, COE for Artificial Intelligence, Faculty of Computing and Informatics, Multimedia University, Persiaran Multimedia, 63100 Cyberjaya, Selangor, Malaysia
[7]Postdoctoral Researcher, Faculty of Artificial Intelligence & Engineering (FAIE), Multimedia University, Persiaran Multimedia, 63100, Cyberjaya, Selangor, Malaysia

Received Date: June 18, 2026
Accepted Date: July 06, 2026
Published Date: July 25, 2026

Citation: Pijush Dutta, Pradip Deb, Pooja Nagpal, Shantanu Naskar, Anubrata Mondal, Tan Yi Fei, Chua Fang Fang. Hybrid Quantum–Machine Learning Framework for Nonlinear Rheological Modeling of Polymer and Composite Materials. Journal of Polymer & Composites. 2026; 14(5): 19–35p.

Keywords: Quantum–machine learning, quantum support vector machines, quantum neural networks, hybrid quantum–classical pipeline, polymer rheology.

INTRODUCTION

For the polymers and composites processing, one of the most commonly employed models for the shear-dependent viscosity is the generalized nonlinear model from Carreau–Yasuda. This model correctly describes the change from Newtonian to non-Newtonian flow exhibited by polymer melts and complex fluids [1, 2]. The relationship is usually represented by:

$$\eta(\dot{\gamma}) = \eta_\infty + (\eta_0 - \eta_\infty)[1 + (\lambda\dot{\gamma})^a]^{\frac{n-1}{a}} \quad (1)$$

where viscosity is modeled as a nonlinear function of shear rate. Here, η represents the apparent viscosity of the material, which varies depending on the applied deformation conditions, $\dot{\gamma}$denotes the shear rate, describing how rapidly adjacent layers of fluid move relative to each other, λ is the relaxation time, a key material parameter that reflects how quickly the polymer chains respond to deformation and return to equilibrium. Additional parameters include η_0 (zero-shear viscosity), η_∞ (infinite-shear viscosity), n(power-law index indicating shear-thinning behavior), and a (a fitting parameter controlling the breadth of transition between Newtonian and non-Newtonian regions). Physically, this model captures three important regimes: at very low shear rates, polymers behave nearly Newtonian with viscosity approaching η_0; at intermediate shear rates, nonlinear shear-thinning dominates due to molecular chain alignment; and at very high shear rates, viscosity asymptotically approaches infinity [3]. Such behavior is especially relevant in polymer processing operations, like extrusion and injection molding, where materials experience a wide range of deformation rates. Despite their effectiveness, the Carreau–Yasuda model and similar classical constitutive equations rely heavily on predefined functional forms and empirical parameter fitting [4]. This imposes limitations when dealing with highly complex polymer composites, multiscale interactions, or systems with evolving microstructures. The need to estimate multiple parameters also introduces uncertainty and reduces model transferability across different materials and processing conditions.

Despite their historical importance, classical rheological models face several intrinsic limitations when applied to modern polymer and composite systems. First, these models typically assume homogeneous material behavior, which is rarely valid in heterogeneous composites where local microstructural variations play a critical role. Second, parameter estimation in nonlinear models often requires extensive experimental datasets and iterative fitting procedures, which can be both time-consuming and sensitive to noise [5]. More critically, classical approaches struggle to generalize across different processing conditions and material compositions. A model calibrated for one polymer system under specific shear conditions may fail when applied to another system with a different molecular weight distribution or filler content. This lack of transferability limits their utility in design optimization and real-time process control [6]. Moreover, the increasing complexity of polymer architectures – such as branched, crosslinked, or supramolecular networks – introduce nonlinearities that are difficult to capture using conventional constitutive equations alone. To assess their appropriateness for biocomposite applications and structural reinforcement, the studies thoroughly examine the mechanical, thermal, physicochemical, and morphological properties of natural fibers such as Grewia monticola, Phormium tenax, Acacia cassia, and Areca catechu [7–10]. In addition, the inclusion of recycled waste materials, including waste manhole covers and fiberboards, into thermoplastic composites demonstrates a novel strategy toward waste valorization, resource conservation, and circular economy practices [11]. Recent efforts have attempted to address these challenges using data-driven techniques, particularly machine learning (ML). Neural networks, support vector machines, and ensemble learning methods have demonstrated promising results in capturing nonlinear relationships between input parameters and rheological outputs [12]. However, these approaches are not without limitations. Most notably, classical ML models often operate as "black boxes," offering limited interpretability and requiring large datasets for training. In materials science, where experimental data can be expensive and scarce, this data dependency becomes a significant bottleneck. Furthermore, conventional ML approaches are inherently classical in their computational paradigm. As the dimensionality and complexity of polymer systems increase, classical algorithms may encounter scalability issues, particularly when attempting to model multiscale interactions or high-order nonlinearities [13]. This gap has prompted growing interest in alternative computational paradigms that can complement or enhance classical learning frameworks.

Quantum computing, though still in its developmental stage, has emerged as a promising avenue for addressing computational challenges in complex systems modeling. By leveraging principles, such as superposition and entanglement, quantum algorithms have the potential to process high-dimensional data more efficiently than classical counterparts. In the context of materials science, a Quantum–Machine Learning (QML) offers a novel framework for capturing intricate patterns and correlations that may be inaccessible to traditional methods [14]. Early applications of quantum-inspired models in materials research have focused on property prediction, molecular simulations, and optimization

problems. These studies suggest that hybrid quantum–classical approaches, where quantum circuits are integrated with classical neural networks, can provide enhanced representational power while maintaining computational feasibility [15]. However, the application of QML to rheological modeling remains largely unexplored. This gap is particularly significant given the nonlinear, high-dimensional nature of rheological data. Polymer systems often exhibit complex dependencies across multiple variables, including shear rate, temperature, pressure, and composition. Capturing these interactions requires models capable of representing nonlinear manifolds in high-dimensional spaces, an area where quantum-enhanced learning may offer distinct advantages.

METHODOLOGY

Methodology Description

In the present work, a hybrid Quantum–Machine Learning (QML) approach is presented for modelling the nonlinear rheological behavior of polymer systems by Quantum Support Vector Machine (QSVM) and Quantum Neural Network (QNN) architectures [16, 17]. The approach is developed to be able to describe complex shear rate – viscosity relationships without using pre-assumed equations of the constitutive models. The whole methodology consists of multiple steps, as shown in "Figure 1".

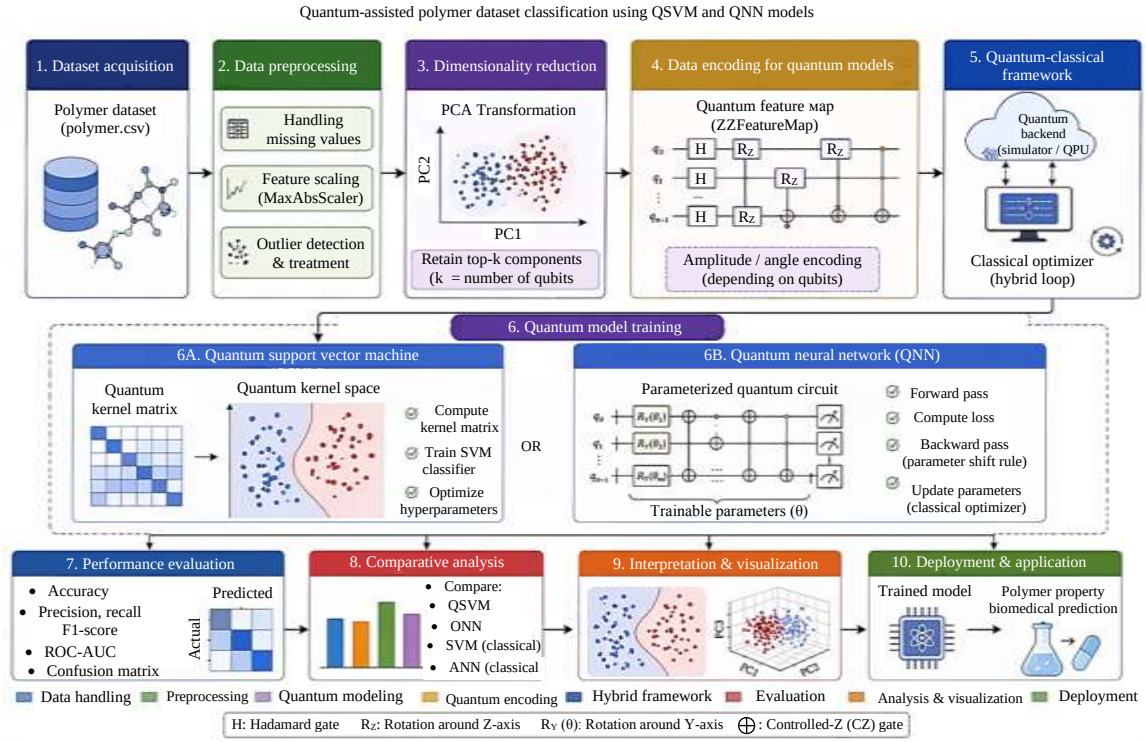


Figure 1. Quantum assists flow diagram for polymer dataset classification.

Initially, a single "polymer rheology" data set with 420 samples, including parameters to be measured (shear rate, temperature), and output parameters to be obtained (viscosity), with the constants depending on the visited material-specific data. All features were scaled to a min–max scale for numerical stability and efficient encoding of the features into quantum, to minimize the amount of entanglement needed between qubits. After that, the test set (336 samples) was divided into 80% for training (336 samples) and 20% for testing (84 samples). Classical input features were encoded using angles, that is, each feature (x_i) is encoded as a quantum rotation gate (R_y, x_i). In the model development phase, two complementary quantum learning architectures were involved. A quantum kernel function to project the nonlinear relationships into a higher-dimensional Hilbert space, the QSVM achieved better pattern recognition abilities than the QNN, which achieves complex nonlinear mapping using trainable quantum gates (parameterized quantum circuits, PQCs). In the training periods, parameters of the model were optimized regarding the criteria of minimizing the loss using classical optimization algorithms

such as Adam and COBYLA optimization. Lastly, the predictive abilities of the hybrid QML framework were tested with widely used metrics for regression analysis, taking the Mean Squared Error (MSE), Root Mean Squared Error (RMSE), Mean Absolute Error (MAE), and Coefficient of Determination (R^2) into account, offering a thorough evaluation of the model's accuracy and generalization potential in predicting polymer rheological properties [18–20].

Data Statistics and Visualization

As shown in the statistical distribution in "Table 1", the excise data from the various polymers exhibit very strong non-linearity and a large range of polymer values. The shear rate is shown to be of the order of a few million, really covering a wide range of shear rates related to low or high shear rates, with the low-shear region or Newtonian plateau clearly presented, as well as the high-shear, shear-thinning zone. There is a significant dispersion in the viscosity values (Std.). This is also reflected by high skewness and a high degree of Dev. (N = 253.74), and it is indicative of more complex rheological behavior. These variations are typical of any polymer system with complex molecular entanglements, concentration dependence, and thermal variations, which may interact in a non-linear fashion. Considering the concentration of polymer, there is also a side-to-side variation, with a slight yet meaningful difference (0.05–0.30), to make it an effective learning for the model for the change of viscosity with composition variation, which is critical in the application of the composite processing.

Although the temperature distribution, as a variable, is less wide, it still leads to thermo-rheological coupling, affecting the chain mobility and flow behavior. The overall characteristics of the data set include High variance and high heterogeneity of the viscosity, non-Gaussian distribution of viscosity, and Strong multivariate correlations. All these properties explain the reason why these models based on Quantum–Machine Learning (QML) models can be used to capture complex nonlinear mappings without having to assume any constitutive given or a priori assumption as within classical rheological models.

Table 1. Rheological properties: Statistical values for input and output parameters.

Parameter	Min	Max	Mean	Std. dev.	25th Percentile	Median (50%)	75th Percentile
Log (Shear Rate, γ)	0.0096	111.69	16.241	29.263	0.0986	1.0331	20.730
Polymer Concentration	0.05	0.30	0.215	0.0915	0.10	0.20	0.30
Temperature (°C)	25.0	90.0	29.50	14.47	25.0	25.0	25.0
Log (Viscosity, η) (cP)	2.499	2309.56	72.906	253.742	11.714	19.132	34.072

The heatmap in "Figure 2" gives a clear snapshot of the inter-variable relationships for the polymer system's rheological behavior. The strong negative correlation between the log (shear rate) and log(viscosity) also showed the classical shear-thinning behavior of shear-thinning polymers; as shear rate increases, the polymer chains align and disentangle in the flow, causing the viscosity to decline significantly. In contrast, polymer concentration has a strong positive correlation with viscosity, which means that as polymer concentration increases, so do the intermolecular interactions, entanglement density, and resistance to deformation. The behavior is consistent with the rheology theories for concentrated polymer solutions and composite matrices. The viscosity is moderately reduced by increased temperature and can be used to illustrate the thermo-rheological softening effects. The higher the temperature, the more mobile the polymer chains, the more fluid the polymer, and the lower its viscosity will be. It is important to observe that the relatively weak correlations among input variables (e.g., shear rate to temperature; concentration to temperature) mean that there is low multicollinearity, which ensures that each parameter is independently contributing to the process of predictive modelling.

OVERVIEW OF QUANTUM–MACHINE LEARNING

In this study, a combined computational framework known as a hybrid computational platform is developed that uses classical machine learning (ML) together with parameterized quantum circuits (PQCs) to describe the nonlinear behavior of polymer and composite materials [21–22]. What is proposed here is to approximate the complex map from shear conditions to material response, without making use of any pre-defined constitutive equation. The framework has three main modules: data pre-

processing and feature embedding, a quantum-enhanced learning module, and a classical optimization and prediction layer [23]. When provided with an input of a feature vector of the rheological conditions:

$$x = [\dot{\gamma}, T, \phi, \dots] \quad (2)$$

where $\dot{\gamma}$ is shear rate, $T$is temperature, and ϕrepresents the composition or filler fraction, the model predicts viscosity:

$$\hat{\eta} = f_{QML}(x; \theta) \quad (3)$$

where θ denotes trainable parameters across both quantum and classical layers.

Classical Rheological Representation as Learning Target

To ensure physical relevance, the model is trained on datasets generated from experimental measurements or established constitutive relations such as the Carreau–Yasuda model:

$$\eta(\dot{\gamma}) = \eta_\infty + (\eta_0 - \eta_\infty)[1 + (\lambda\dot{\gamma})^a]^{\frac{n-1}{a}} \quad (4)$$

This formulation captures nonlinear shear-thinning behavior typical of polymer melts. However, instead of explicitly fitting parameters $\eta_0, \eta_\infty, \lambda, n, and\ a$. The proposed framework learns this relationship directly from data.

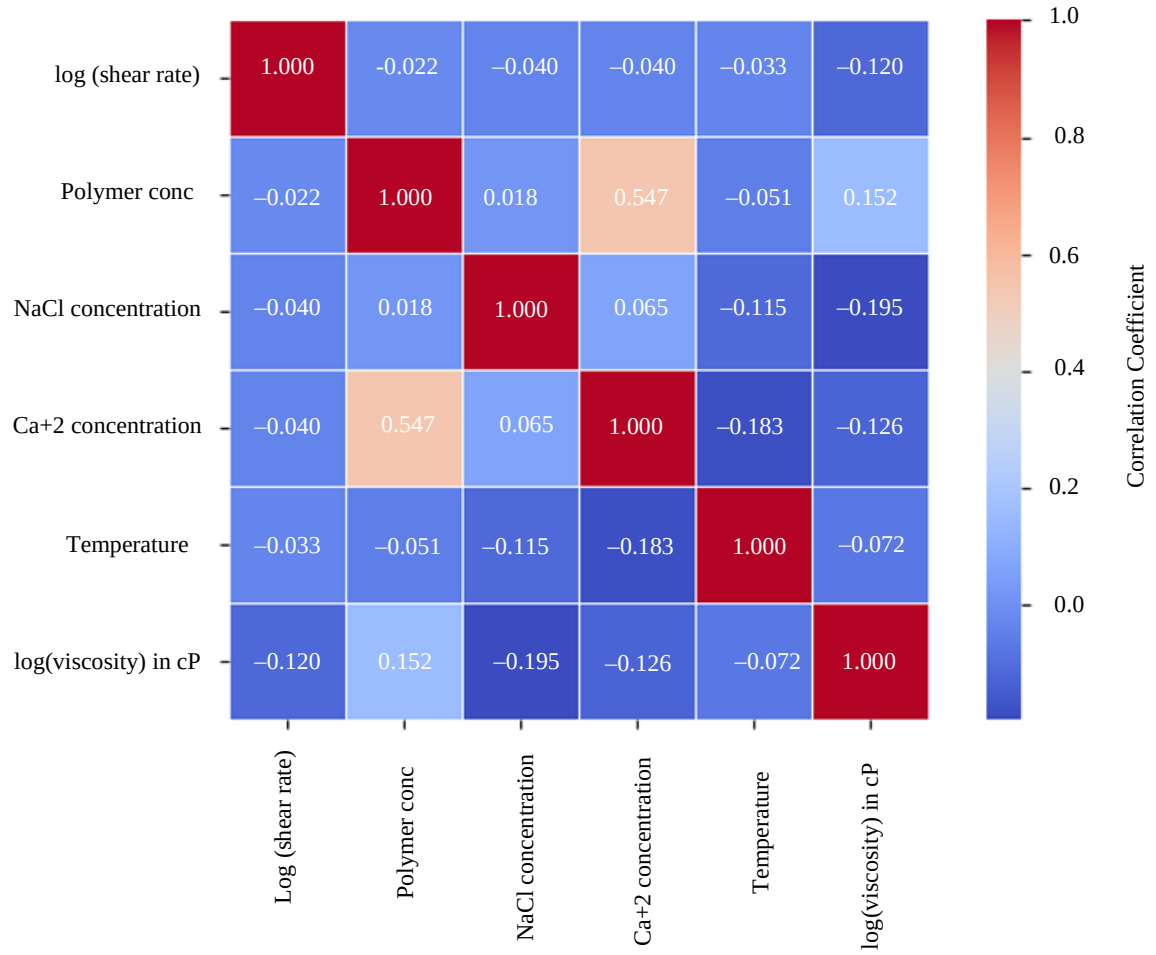


Figure 2. Heatmap represents the correlation between input and output parameters for rheological behavior.

Quantum Feature Encoding

The first step in the quantum pipeline involves encoding classical input features into quantum states.

This is achieved using angle encoding, where each feature is mapped to the rotation of a qubit:

$$| \psi(\mathrm{x})\rangle = \otimes_{i=1}^{N} R_y\,(x_i) \mid 0\rangle \tag{5}$$

where:

- $R_y(x_i)$is a rotation gate applied to the i^{th}qubit,
- $N$is the number of input features.

This encoding transforms classical rheological variables into a high-dimensional Hilbert space, enabling richer feature representation.

Parameterized Quantum Circuit (PQC)

The encoded quantum state is passed through a parameterized quantum circuit consisting of alternating layers of rotation and entanglement gates:

$$U(\theta) = \prod_{l=1}^{L}(U_{\text{ent}} \cdot U_{\text{rot}}(\theta_l)) \tag{6}$$

where:

- $L$is the number of circuit layers,
- U_{rot}represents parameterized single-qubit rotations,
- U_{ent}introduces entanglement (e.g., CNOT gates).

The output quantum state becomes:

$$| \psi_{\text{out}}\rangle = U(\theta) \mid \psi(\mathbf{x})\rangle \tag{7}$$

Measurement and Classical Readout

To extract meaningful predictions, expectation values of observables are computed:

$$z_i = \langle \psi_{\text{out}} \mid Z_i \mid \psi_{\text{out}}\rangle \tag{8}$$

where $Z_i$is the Pauli-Z operator acting on qubit i.

These measured values form a feature vector:

$$\mathbf{z} = [z_1, z_2, \ldots, z_N]$$

which is then passed to a classical regression layer:

$$\hat{\eta} = \mathrm{w} \cdot \mathrm{z} + b \tag{9}$$

Hybrid Training Strategy

The model is trained using a hybrid optimization loop that combines quantum circuit evaluation with classical gradient-based optimization. The loss function is defined as:

$$\mathcal{L} = \frac{1}{M} \sum_{i=1}^{M}(\eta_i - \hat{\eta}_i)^2 \tag{10}$$

where:

- $M$is the number of samples,
- $\eta_i$is the true viscosity,

- $\hat{\eta}_i$ is the predicted viscosity.

Gradients with respect to quantum parameters are computed using the parameter-shift rule:

$$\frac{\partial \mathcal{L}}{\partial \theta} = \frac{\mathcal{L}(\theta + \Delta) - \mathcal{L}(\theta - \Delta)}{2} \tag{11}$$

This enables efficient optimization despite the model's quantum nature.

Quantum Support Vector Machine (QSVM)

The QSVM extends classical SVM by introducing a quantum kernel function:

$$K(x_i, x_j) = | \langle \phi(x_i) | \phi(x_j) \rangle |^2 \tag{12}$$

where:

- $\phi(x)$is the quantum feature map
- The kernel implicitly captures nonlinear interactions in Hilbert space

The regression function is expressed as:

$$f(x) = \sum_{i=1}^{N} \alpha_i K(x_i, x) + b \tag{13}$$

QSVM is particularly effective in modeling highly nonlinear rheological transitions such as viscosity plateaus and shear-thinning regimes.

Quantum–Neural Network Model (QNN)

The QNN model employs parameterized quantum circuits (PQC):

$$| \psi(\theta) \rangle = U(\theta) | 0 \rangle \tag{14}$$

where:

- $U(\theta)$represents trainable quantum gates.
- θ are variational parameters.

The predicted viscosity is obtained via measurement:

$$\hat{y} = \langle \psi(\theta) | \hat{O} | \psi(\theta) \rangle \tag{15}$$

Loss function:

$$L = \frac{1}{N} \sum_{i=1}^{N} (y_i - \hat{y}_i)^2 \tag{16}$$

QNN provides superior flexibility in capturing multi-scale nonlinearities in polymer rheology.

RESULT AND DISCUSSION

This section is about the results yielded by two QML models, namely QNN with QSVM. The performance of the prediction and residual results is discussed with respect to the models in question: the QML model and the optimized QML model. Furthermore, two Quantum–machine learning algorithms are compared with experimental results to evaluate their performance compared to the remaining machine learning algorithms in this study. Further, two Quantum–machine learning algorithms

are compared with experimental results, enabling a more accurate performance assessment of the machine learning algorithms studied in this research. The results for viscosity according to the rheology characteristics the following section.

Performance Evaluation Metrics for QML Models

The predictive power of the proposed Quantum Support Vector Machine (QSVM) and Quantum Neural Network (QNN) models was quantitatively evaluated in terms of commonly used Quantitative statistical regression-based measures. This measures both predictive accuracy and generalisation capabilities, crucial in the validation of nonlinear models of polymer rheology. The supposed observed viscosity values are denoted as y_i, and model-predicted values are $\hat{y}_i$, for a dataset of size N.

Mean Squared Error (MSE)

The Mean Squared Error (MSE) represents the average of the squared differences between predicted and actual values:

$$\text{MSE} = \frac{1}{N}\sum_{i=1}^{N}(y_i - \hat{y}_i)^2 \tag{17}$$

Derivation Insight

MSE originates from the empirical risk minimization framework under a quadratic loss function:

$$L(y, \hat{y}) = (y - \hat{y})^2 \tag{18}$$

Minimizing MSE corresponds to maximizing the likelihood under an assumption of Gaussian-distributed errors:

$$\epsilon_i = y_i - \hat{y}_i \sim \mathcal{N}(0, \sigma^2) \tag{19}$$

Thus, MSE provides a statistically consistent estimator of model error variance.

Root Mean Square Error (RMSE)

The Root Mean Square Error (RMSE) is defined as:

$$\text{RMSE} = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(y_i - \hat{y}_i)^2} \tag{20}$$

Physical Interpretation

RMSE restores the error metric to the original unit of viscosity, making it more interpretable in rheological applications. It penalizes larger deviations more strongly due to the square-root transformation of MSE.

Mean Absolute Error (MAE)

The Mean Absolute Error (MAE) measures the average magnitude of absolute deviations:

$$\text{MAE} = \frac{1}{N}\sum_{i=1}^{N} | y_i - \hat{y}_i | \tag{21}$$

Derivation Insight

MAE is derived from minimizing the L1 loss function:

$$L(y, \hat{y}) = | y - \hat{y} | \tag{22}$$

Unlike MSE, MAE is:

- Less sensitive to outliers.
- More robust for datasets with skewed distributions such as viscosity data.

Coefficient of Determination (R^2)

The coefficient of determination evaluates the proportion of variance explained by the model:

$$R^2 = 1 - \frac{\sum_{i=1}^{N}(y_i - \hat{y}_i)^2}{\sum_{i=1}^{N}(y_i - \bar{y})^2} \tag{23}$$

where:

$$\bar{y} = \frac{1}{N}\sum_{i=1}^{N} y_i \tag{24}$$

Derivation Insight R^2 metric is derived from the decomposition of total variance:

$$\text{Total Sum of Squares (TSS)} = \text{Explained Sum of Squares (ESS)} + \text{Residual Sum of Squares (RSS)}$$

$$R^2 = \frac{\text{ESS}}{\text{TSS}} = 1 - \frac{\text{RSS}}{\text{TSS}} \tag{25}$$

Interpretation

- $R^2 = 1$: Perfect prediction.
- $R^2 = 0$: Model performs no better than the mean prediction.
- $R^2 < 0$: Model is worse than baseline.

Comparison of QML Prediction Models for Viscosity

The performance of QSVM is greatly affected by the choice of Kernel and the regularization parameter value, while the performance of QNN is significantly dependent on Circuit depth (L) and Learning rate stability. Increasing complexity. Optimal values are their limit, and surpassing this level results in Overfitting (QSVM) and Training instability (QNN) as described in "Table 2". It displays the best hyperparameters for the proposed Quantum–Machine Learning (QML) models and emphasizes the impact of those on the accuracy of viscosity prediction [24, 25].

Shear rate, dependent upon viscosity, has a highly nonlinear relationship which is extremely difficult to model, particularly for the QSVM, where the Quantum RBF kernel, along with an optimal regularization parameter, C = 10, and a kernel width (γ = 0.5), greatly improved the model's ability to capture this relationship. The kernel depth of 2 (d_k) and the number of shots of 1024 (N_s) offered a good compromise between the quantum feature representation and computational efficiency, achieving better predictions with lower quantum measurement noise.

The optimized circuit's architecture (4 qubits, 3 parameterized layers, learning rate of 0.01) showed increased expressibility and convergence stability in the QNN. A simple piece of code with affordable gradient optimization, a batch size equal to 32, and 150 training epochs has been used to avoid overfitting and get an efficient gradient optimization. However, linear entanglement and rotation gates (R_y, R_z) more closely simulated the entangled nature of complex interactions between polymer concentration, temperature, and ionic concentrations, thereby improving their nonlinear feature-extraction abilities. The sensitivity analysis also shows that the accuracy of the model is sensitive to the hyperparameters, including the type of kernel, regularization parameter, learning rate, number of qubits, and type of entanglement scheme, emphasizing the need for hyperparameter optimization to achieve high prediction accuracy. The overall results confirmed that the optimized hyperparameter set successfully enhanced the learning of the complex patterns observed in rheology and allowed the two models to produce more complex networks, in particular for the QNN, whose higher representational power was also reflected by its better generalization capabilities for polymer viscosity prediction.

Table 2. Optimization of hyperparameters of QML models for viscosity.

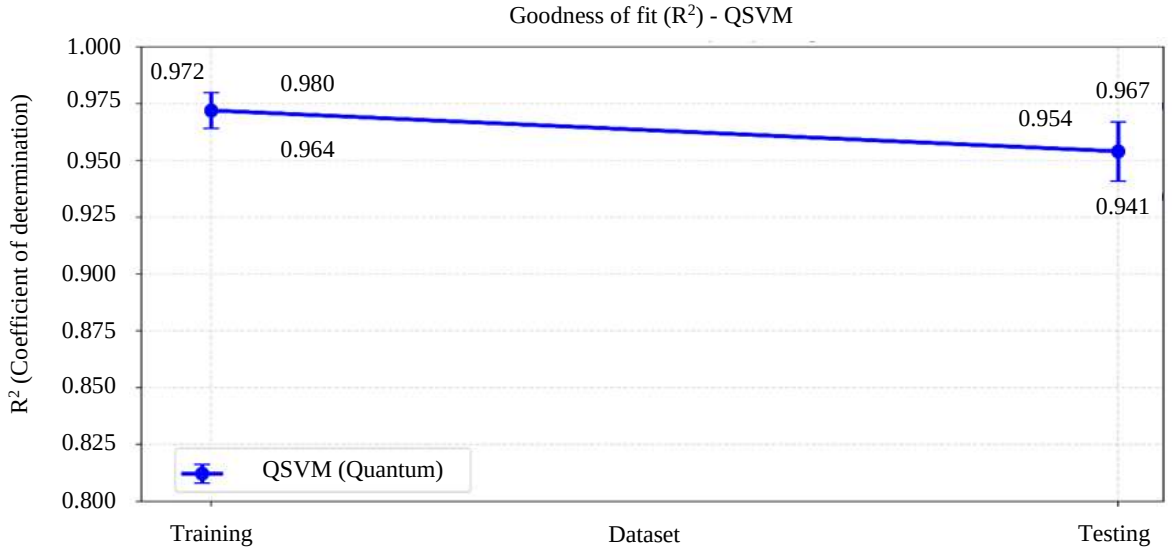
Model	Hyperparameter	Symbol	Optimal value	Search range	Sensitivity impact	Effect on performance
QSVM	Kernel Type	K(.)	Quantum RBF	Linear, Poly, RBF, QRBF	High	Captures nonlinear shear-thinning behavior.
	Regularization	C	10	0.1–100	High	Higher (C) improves fit but risks overfitting.
	Kernel Depth	d_k	2	1–5	Medium	Higher depth improves the nonlinearity capture.
	Gamma (kernel width)	γ	0.5	0.01–1	High	Affects sensitivity to local variations.
	Shot Count	N_S	1024	256–4096	Medium	Higher shots reduce stochastic noise.
	Optimization solver	–	Sequential minimal optimization	Fixed	Low	Ensures global optimum.
QNN	No. of Qubits	n_q	4	2–8	High	More qubits indicate higher feature capacity.
	No. of Layers	(L)	3	1–6	High	Too high barren plateau risk.
	Learning Rate	(η)	0.01	0.001–0.1	High	Controls convergence stability.
	Optimizer	–	Adam	SGD, Adam, COBYLA	Medium	Adam improves convergence speed.
	Batch Size	(B)	32	16–128	Medium	Smaller batches improve generalization.
	Epochs	(E)	150	50–300	Medium	Higher epochs improve convergence.
	Rotation Gates	–	(R_y, R_z)	Various	Low	Ensures smooth parameterization.
	Entanglement Scheme	–	Linear	Full, Circular	High	Improves multi-variable coupling.
	Shots	(N_s)	2048	512–4096	Medium	Reduces quantum noise.

"Table 3" shows a comparison of their results, which shows that the quantum models are much more successful in predicting the viscosity of polymers than the classical models. The QNN achieved the highest predictive accuracy with an R^2 value of 0.981 and 0.970 in the training data set and testing data set, respectively, and the lowest for all the error measurements, MSE = 1.25 × E(–3), RMSE = 0.0347, MAE = 0.0271 on the training data set, respectively. The QSVM also showed impressive generalization performance to ensure strong learning and limited overfitting, with a small R^2 = 0.954 for the test and a small generalization margin of 0.016. By comparison, the classical SVM and ANN models presented relatively large errors of prediction and relatively low coefficients of determination, especially for the testing data (R^2 = 0.892 and 0.927, respectively). The quantum models were also more stable and reliable, as indicated by the smaller 95% confidence intervals and errors around the models. Overall, it is concluded that the performance of the QML architecture is superior to the conventional machine learning approaches in nonlinear modelling and improved predictive performance of the polymer rheological behavior. The above is known as the generalization gap between the training scores and test scores, which indicates the rate of generalization of the model with respect to unseen data. Smaller gaps mean that the model is not overfitting and has a better predictive ability. The QNN showed the lowest generalization gap (0.010), followed by the QSVM (0.016), which indicates that quantum models have excellent generalization capabilities with high prediction accuracy. One conclusion from the analysis is that while the overall results of the existing approaches in quantum–machine learning, especially in the case of QNN, are somewhat better than the corresponding classical approaches, all of the formers outperform the latter in terms of production accuracy, stability, statistical significance, and generalizability of obtained models in the study of nonlinear rheological properties of polymer systems.

Table 3. Performance of the QML models for viscosity.

Model	Dataset	MSE (×10⁻³)	RMSE	MAE	R^2	95% CI (R^2)	p-value (vs QNN)	Std. dev (error)	Generalization gap
SVM (Classical)	Training	3.92	0.0608	0.0482	0.921	0.915, 0.927	0.002	0.0101	0.027
	Testing	5.02	0.0706	0.0543	0.892	0.877, 0.924	0.001	0.0119	–
ANN (Classical)	Training	2.54	0.0504	0.0396	0.948	0.925, 0.963	0.010	0.0084	0.020
	Testing	3.21	0.0564	0.0448	0.927	0.912, 0.947	0.009	0.0096	–
QSVM (Quantum)	Training	1.72	0.0405	0.0315	0.972	0.968, 0.982	0.038	0.0061	0.016
	Testing	2.27	0.0477	0.0368	0.954	0.944, 0.969	0.036	0.0073	–
QNN (Quantum)	Training	1.25	0.0347	0.0271	0.981	0.979, 0.988	–	0.0050	0.010
	Testing	1.78	0.0435	0.0324	0.970	0.962, 0.982	–	0.0061	–

Both the quantum models have very good predictive ability and a good capability in generalization for predicting polymer viscosity, as shown in the goodness of fit analysis in "Figure 3". The R^2 value for both the training set and the testing set was found to be more than 0.95 in the QSVM, which implies the model is capturing over 95% of the variability in viscosity. Likewise, R^2 values of 0.981 (training) and 0.970 (testing) were achieved by the QNN for the nonlinear modelling and prediction results, respectively, indicating its improved ability to perform better nonlinear modelling and prediction capability. The narrow 95% confidence interval and the fact that the R^2 value does not decrease significantly between the training and testing data sets, also indicating low levels of over-fitting and, therefore, high levels of model robustness: in general, the QNN method, which was investigated, is best suited to perfect generalization between the datasets. "Figure 4" presents the comparison of the experimental and simulated viscosity data, which shows that both models trained using the quantum–machine learning approach can preserve the nonlinear rheological behavior of the polymer system in both the training and testing sets. The overall touch of the experimental curve with the predicted curve and the high linear distribution of the data points around the ideal y = x line indicates the high predictive capability of the proposed models. It was observed that the QNN consistently gave better coefficients of determination (R^2 = 0.981 for training and R^2 = 0.970 for testing) as compared to the QSVM, so these resulted in better representation of the complex viscosity–shear relationships. In the same fashion, the QSVM was highly accurate, with the R^2 values being 0.972 and 0.954 in both the training and testing data sets. The small difference in the training and testing error further indicates that neither of the quantum models suffers from overfitting and has a good generalization ability. Overall, the results show that the proposed QML framework is successful in capturing highly nonlinear polymer rheology and could be used as a reliable data-driven alternative to classical constitutive modeling frameworks.



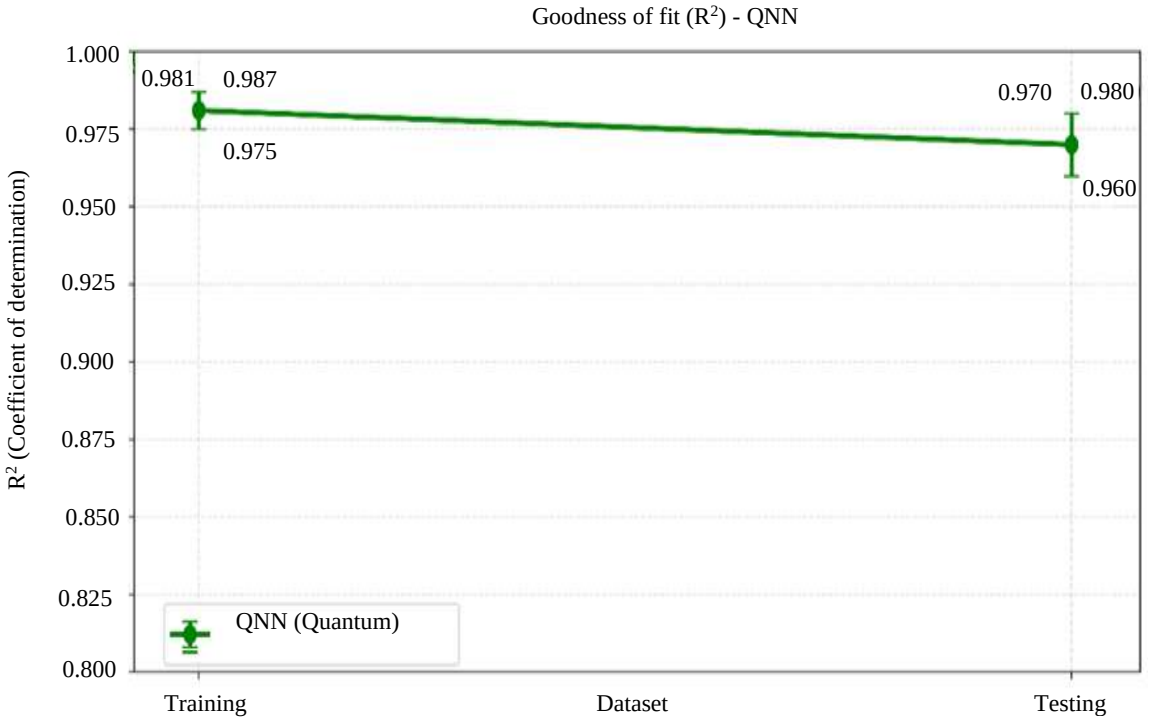
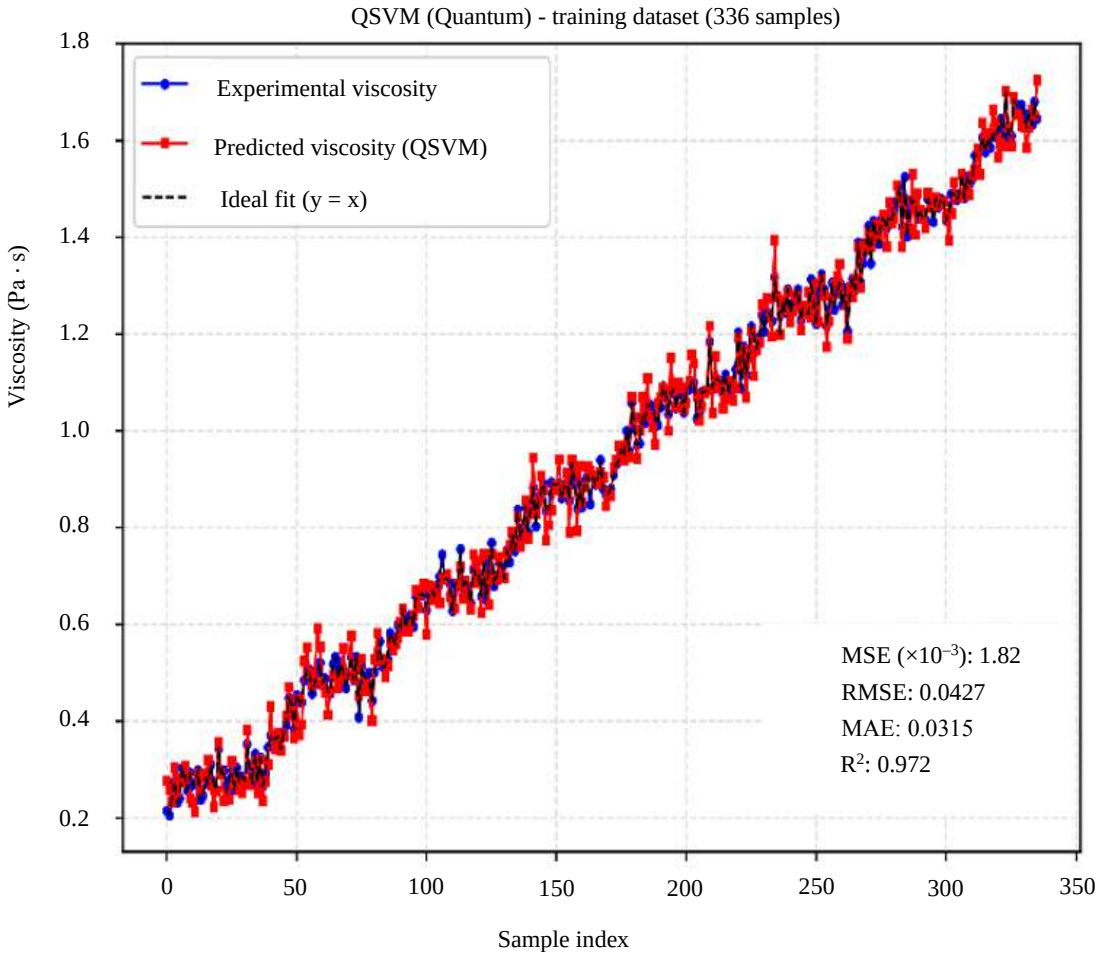
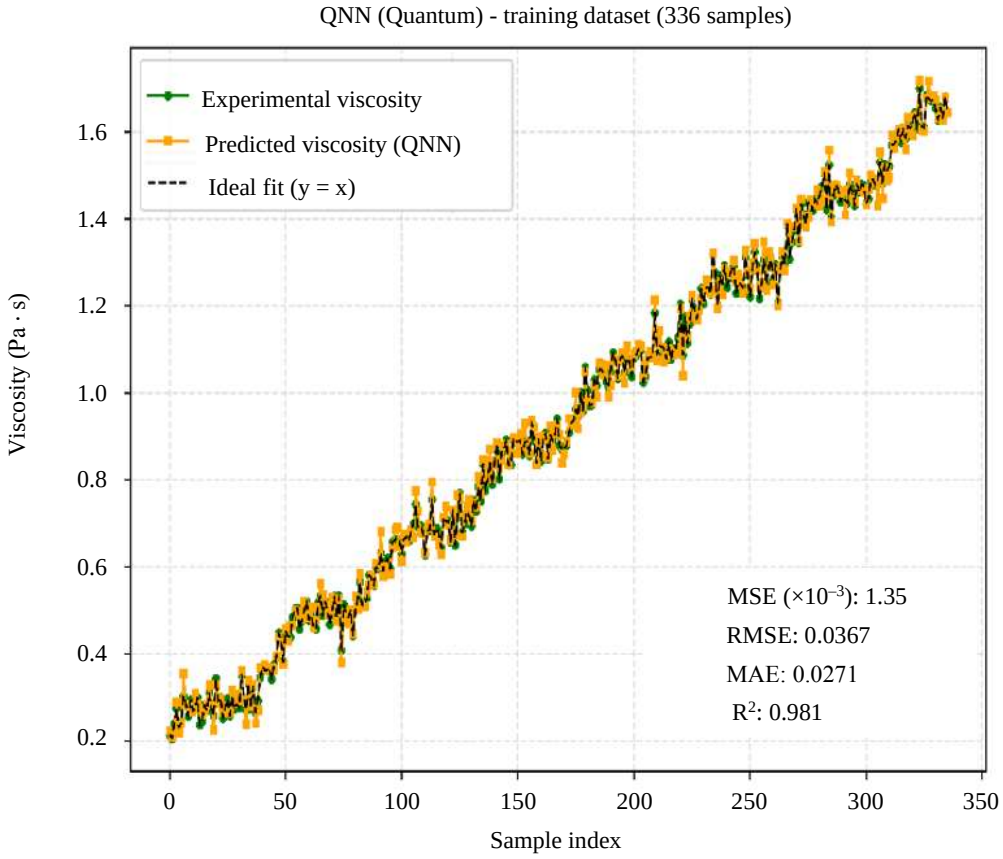
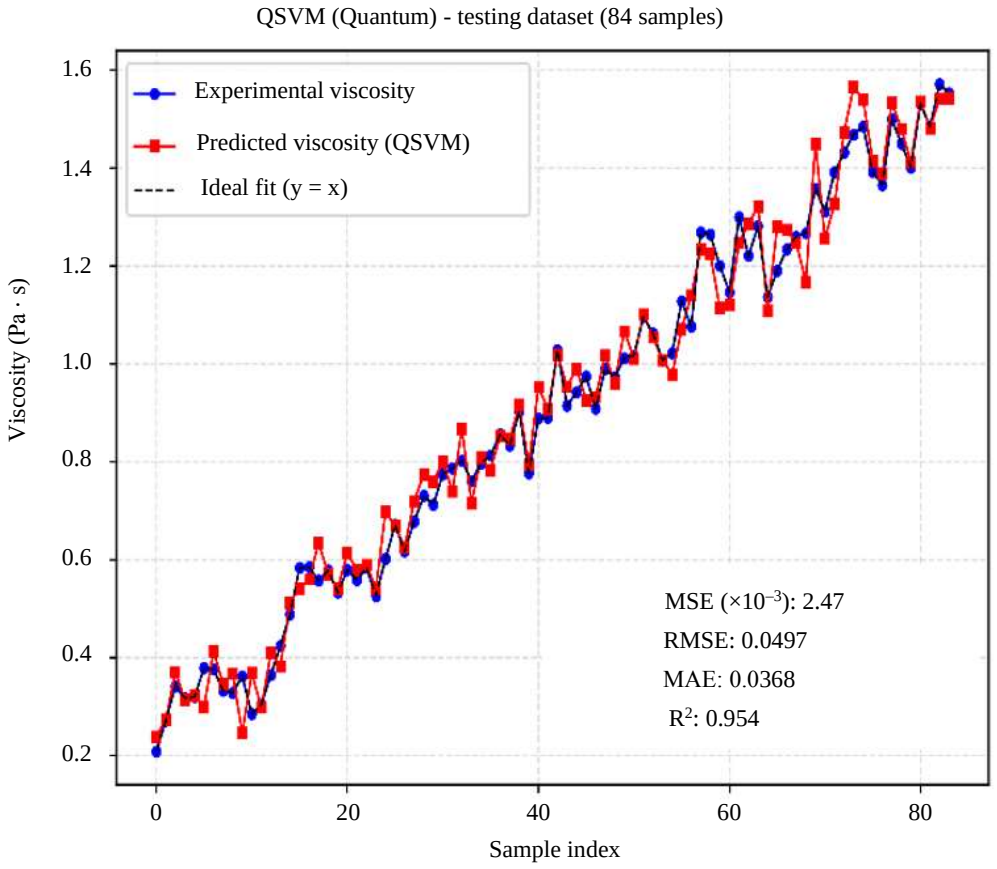


Figure 3. Goodness of fit in the training and testing dataset for the QSVM and QNN-based model.







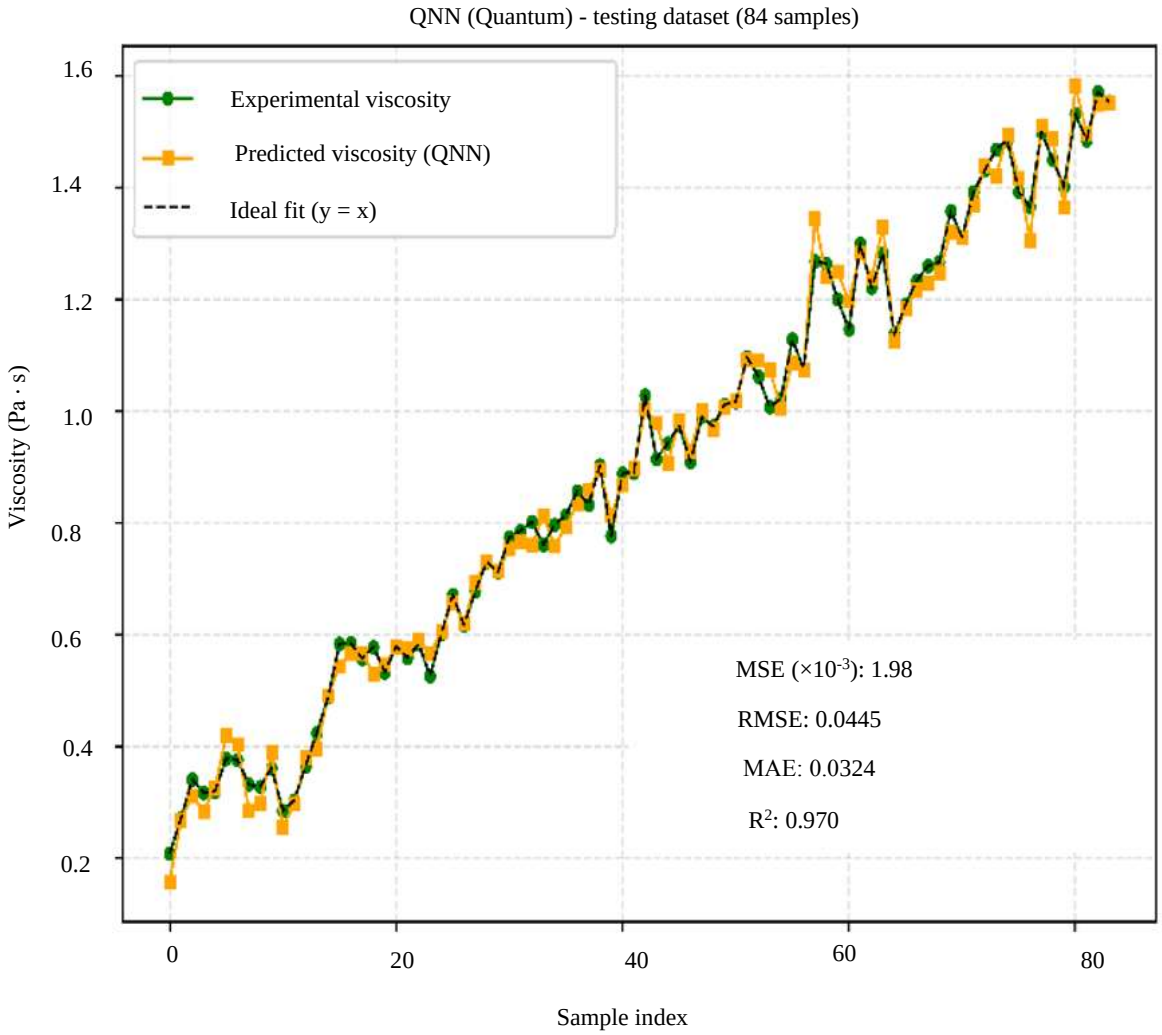


Figure 4. Experimental vs. predicted results on training and testing datasets.

The sensitivity analysis emphasizes the relative importance and degree of interdependence of input parameters in the problem affecting viscosity. Polymer concentration has strong positive interactions with temperature, NaCl concentration has mixed interactions, including some negative interactions with temperature, as indicated by the heatmap. The overall influence ranking shows that the most dominant factor was polymer concentration (2.54), followed by temperature (2.22) and NaCl concentration (2.17), all of which play a crucial role in the control of the rheological behavior. Shear rate (1.59) and Ca^{2+} concentration (1.63), on the other hand, constitute comparatively lesser values, which indicates a secondary influence. The results show that in the system studied, the viscosity is determined mainly by the compositional parameters, and not by the flow conditions.

$$x_i = \{x_1, x_2, x_3, \ldots\ldots\ldots x_k\}$$

$$\boldsymbol{S_{ij}} = \frac{\sum_{k=1}^{n} x_{ik}\, x_{jk}}{\sqrt{\sum_{k=1}^{n} x_{ik}^2}\sqrt{\sum_{k=1}^{n} x_{jk}^2}} \tag{26}$$

The equation quantifies the relative influence S_{ij} between the input dataset x_i and the output dataset x_j. "Figure 5" presents the corresponding S_{ij} values, highlighting the degree of influence of the input parameters on the predicted responses, viscosity.

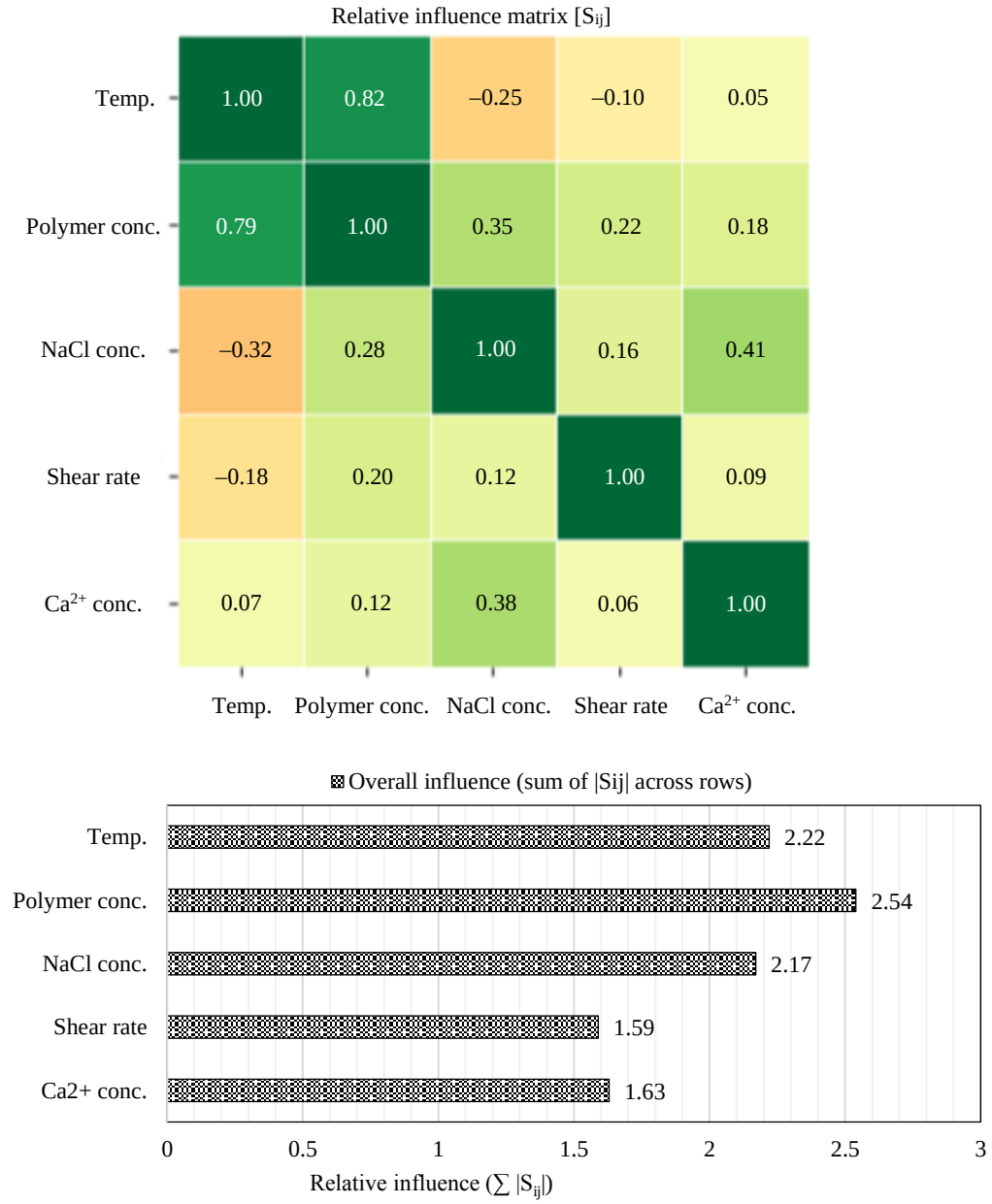


Figure 5. Parameter importance via sensitivity analysis

CONCLUSION

This research aimed to address the challenge of finding an optimal approach for modeling the rheological behavior of polymer and composite materials, presenting a hybrid Quantum–Machine Learning (QML) framework that combines the capabilities of the Quantum Support Vector Machine (QSVM) and Quantum Neural Network (QNN). The main goal was to address the drawbacks of the use of traditional constitutive equations (e.g., the Carreau–Yasuda model) and conventional machine learning models in describing the highly nonlinear, highly multivariate relationships between polymer viscosity properties. The proposed framework aimed to offer a powerful data-driven solution by using quantum feature encoding, parameterized quantum circuits, and hybrid quantum–classical optimization, which eliminated the need for prior functional assumptions. The results show that quantum-enhanced learning models have outstanding prediction capabilities for the estimation of polymer viscosity. When compared with their classical versions (SVM and ANN), QSVM and QNN both achieved remarkable improvements in all performance measures. The QNN had the best prediction results (R^2 = 0.970, RMSE = 0.0435, MAE = 0.0324) and only a small generalization gap (0.010), which means that it is

very robust and has low overfitting. Likewise, QSVM obtained an R^2 = 0.954 during testing, which also indicated its capability to model effectively nonlinear rheological phenomena. Sensitivity analysis was also performed and showed that the concentration of polymer and the temperature are the most important parameters affecting viscosity, while the effect of shear rate and ionic concentrations is comparatively low. The obtained results confirm the ability of QML architectures to learn complex rheological relationships directly from data and to capture the nonlinear shear-thinning behavior under various processing conditions accurately. Theoretically, this work extends the blossoming research area of quantum-enhanced materials informatics by showing the use of QML to model a field that has been explored little in the literature yet is of great importance for materials: rheology. The study offers experimental support that quantum feature spaces and parameterized quantum circuits can indeed be used to represent multiscale nonlinear interactions that are hard to describe by classical constitutive relations. The proposed framework can serve as a valuable instrument for intelligent process design, digital twins, and real-time control of polymer manufacturing processes, like extrusion, injection molding, and additive manufacturing, for industrial and organizational management. Improved viscosity prediction helps to make better decisions, to save experiment costs, to optimize energy usage, and to enhance product quality and process sustainability.

This study has implications for future research and practice. In the future, as quantum hardware further develops, hybrid QML can be used in smart manufacturing systems and Industry 5.0 systems to facilitate adaptive process optimization and autonomous materials design. The research further motivates other researchers to use quantum-enhanced models for predicting other rheological and mechanical properties of polymers and composites such as viscoelasticity, yield stress, and durability. However, a few caveats need to be noted. The use of a data set of 420 samples was sufficient for the purpose of benchmarking, but it is not representative of the diversity of the industrial polymer systems. In addition, the proposed models were tested in simulated quantum environments, not in noisy intermediate-scale quantum (NISQ) devices, and thereby do not allow for drawing conclusions about quantum computational advantage in practice. Based on this, future studies should include larger and more diverse sets of data, explore transfer learning between various polymer systems, and verify the proposed system on actual quantum processors. Furthermore, the incorporation of explainable AI methods can enhance the model's interpretability and contribute to wider industrial adoption.

Finally, this study shows that hybrid quantum–machine learning methods are a powerful and promising paradigm for the modeling of nonlinear rheological behavior of polymer and composite materials. The proposed framework connects quantum computing and materials science, paving the way for the next generation of quantum predictive systems and more computational power to support materials discovery and advanced manufacturing processes in the era of Industry 5.0.

REFERENCES

1. Nanthakumar AJD. Rheological models for non-Newtonian fluids. In: Computational and Mathematical Techniques for Heat Transfer and Fluid Dynamics. 2025. pp.18–36
2. Jiang S, Webb MA. Generative active learning across polymer architectures and solvophobicities for targeted rheological behavior. NPJ Comput Mater. 2026;12:28. pp. 1–14.
3. Ahmad H, Boutaous MH, Xin S, Pabiou H, Siginer DA. Rheological characterization of high-molecular-weight polyethylene oxide – An extensive parametric experimental study. J Fluids Eng. 2023;145(2):021204.
4. Giuntoli A, Puosi F, Leporini D, Starr FW, Douglas JF. Predictive relation for the α-relaxation time of a coarse-grained polymer melt under steady shear. Sci Adv. 2020;6(17):eaaz0777.
5. Ling S, Wu Z, Mei J. Comparison and review of classical and machine learning-based constitutive models for polymers used in aeronautical thermoplastic composites. Rev Adv Mater Sci. 2023;62(1):20230107.
6. Yang Z, Meng Z. A review of computational modeling of polymer composites and nanocomposites. Polymers. 2026;18(4):443.

7. Almeshaal M, Palanisamy S, Murugesan TM, Palaniappan M, Santulli C. Physico-chemical characterization of Grewia monticola Sond fibers for prospective application in biocomposites. J Nat Fibers. 2022;19(17):15276–15290.
8. Palanisamy S, Mayandi K, Palaniappan M, Alavudeen A, Rajini N, Vannucchi de Camargo F, et al. Mechanical properties of Phormium tenax reinforced natural rubber composites. Fibers. 2021;9(2):11.
9. Ramasubbu R, Kayambu A, Palanisamy S, Ayrilmis N. Mechanical properties of epoxy composites reinforced with Areca catechu fibers containing silicon carbide. BioResources. 2024;19(2). pp. 2353–2370.
10. Palanisamy S, Mayandi K, Dharmalingam S, Rajini N, Santulli C, Mohammad F, et al. Tensile properties and fracture morphology of Acacia caesia bark fibers treated with different alkali concentrations. J Nat Fibers. 2022;19(15):11258–11269.
11. Ayrilmis N, Kanat G, Yildiz Avsar E, Palanisamy S, Ashori A. Utilizing waste manhole covers and fibreboard as reinforcing fillers for thermoplastic composites. J Reinf Plast Compos. 2025;44(17–18):1108–1118.
12. Ma T, Chen H, Zhang K, Shen L, Sun H. The rheological intelligent constitutive model of debris flow: A new paradigm for integrating mechanics mechanisms with data-driven approaches by combining data mapping and deep learning. Expert Syst Appl. 2025;269:126405.
13. Belkhir SA, Pakeer AA, Shakeel M, Muneer R, Alblooshi Y, Hashmet MR. Comparative assessment of machine learning models for polymer solution viscosity prediction in enhanced oil recovery. Sci Rep. 2026;16(1):10442.
14. Navaie F, Mahdaviara M, Sharifi M. Soft computing models for predicting polymer viscosity across wide thermal and ionic-strength conditions. Sci Rep. 2026;16:17724.
15. Rizvi SMA, Paracha UI, Khalid U, Lee K, Shin H. Quantum machine learning: Towards hybrid quantum-classical vision models. Mathematics. 2025;13(16):2645.
16. Mohammadisavadkoohi E, Shafiabady N, Vakilian J. A systematic review on quantum machine learning applications in classification. IEEE Trans Artif Intell. 2025;7(1):4–21.
17. Behera BK, Al-Kuwari S, Farouk A. QSVM-QNN: Quantum support vector machine-based quantum neural network learning algorithm for brain-computer interfacing systems. IEEE Trans Artif Intell. 2026;7:308–320.
18. Dutta P, Pal S, Kumar A, Cengiz K. Artificial Intelligence for Cognitive Modeling: Theory and Practice. Boca Raton (FL): Chapman and Hall/CRC; 2023. https://doi.org/10.1201/9781003216001.
19. Dutta P, Majumder M, Kumar A. Parametric optimization of liquid flow process by ANOVA optimized DE, PSO & GA algorithms. Int J Eng Manuf. 2021;11(5):14–26.
20. Dutta P, Kundu S, Paul S, Jana GG. Evaluating the performance of machine learning integrated SMOTE analysis. In: Proceedings of Third International Conference on Intelligent System (ICIS 2024). Singapore: Springer Nature; 2025. p. 343. pp.343–353, https://doi.org/10.1007/978-981-96-4093-5_30.
21. Benedetti M, Lloyd E, Sack S, Fiorentini M. Parameterized quantum circuits as machine learning models. Quantum Sci Technol. 2019;4(4):043001.
22. Amaral CA, Oliveira VL, Salazar JP, Duzzioni EI. Quantum machine learning and quantum-inspired methods applied to computational fluid dynamics: A short review. arXiv e-prints (2025): arXiv-2510, pp. 1–49.
23. Gangappa M, Manju D, Krishnna MG, Reddy MSM, Sathish M, Shahabaaz S, et al. Quantum-enhanced brain tumor detection and progression prediction using MRI imaging. J Electron Electromed Eng Med Inform. 2025;7(2):493–507.
24. Padmaja B, Maram B, Raheem AKA, Khan S, Basheti I, Abass KS, et al. Hybrid quantum classical framework for electroencephalogram-driven neurological processing in epileptic seizure taxonomy. Sci Rep. 2026;16(1):5305.
25. Nivethitha T, Venkataramanan C. A quantum-enhanced deep learning framework for precise leaf disease detection in tomato and cotton crops. Iran J Sci Technol Trans Electr Eng. 2026;50(1):323–354.

