

Study of an Improved Quantum Particle Swarm Optimization-Based Framework for Neural Network Optimization in Modelling of Polymer Data

Kakali Das^{1,*}, Amrita Mitra¹, Sagardeep Ghosh¹, Suchismita Maiti², Soumyabrata Saha³, Pushpita Roy⁴, Anubrata Mondal⁵, Pijush Dutta¹

Abstract

The accurate forecasting of polymer viscosity at various physicochemical conditions has been quite critical due to the nonlinear interactions and interrelations between the variables. This paper suggests a better hybrid modelling framework, which involves the use of Artificial Neural Networks (ANN) and more advanced versions of Quantum Particle Swarm Optimization (QPSO) to better predict polymer viscosity. The input parameters taken are, namely, log (shear rate), polymer concentration, NaCl concentration, Ca 2+ concentration, and temperature, and the output response is log(viscosity). The proposed framework systematically compares classical Particle Swarm Optimization (PSO), QPSO, Differential QPSO (DQPSO), and Gaussian QPSO (GQPSO) to optimize ANN weights and bias parameters. Of these, GQPSO uses a mechanism of Gaussian mutation to enhance population diversity, preventing premature convergence. Mean squared error (MSE), root mean square error (RMSE), relative error, and fitness value are used to assess the performance of each model on testing and cross-validation data. The findings show that predictive accuracy is definitely improved with the change of the optimization strategy towards GQPSO. The ANN-GQPSO model has the lowest values of RMSE and the greatest values of fitness, indicating better convergence and strength. Further analysis of the comparative study reveals that the Gaussian mutation improves the global search ability, which allows the model to break out of local minima and more accurately represent intricate nonlinear correlations in the data set. Besides the performance indicators, the study provides evidence of the significance of optimization schemes in modeling polymer systems with

the help of neural networks. The model proposed, ANN-GQPSO, is a fixed and computationally valuable system to forecast the viscosity of polymers that does not have to make use of high-scale tests.

Keywords: Quantum particle swarm optimization (QPSO), gaussian mutation, artificial neural network (ANN), polymer rheology, hybrid optimization framework

*Author for Correspondence

Kakali Das

E-mail: kakalidas300@gmail.com

¹Assistant Professor, Department of Computer Science & Engineering, Greater Kolkata College of Engineering and Management, West Bengal, India

²Associate Professor, Department of Information Technology, Narula Institute of Technology, West Bengal, India

³Associate Professor, Department of Information Technology, JIS College of Engineering, West Bengal, India

⁴Assistant Professor, Department of Information Technology, Narula Institute of Technology, West Bengal, India

⁵Assistant Professor, Department of Electrical Engineering, Greater Kolkata College of Engineering and Management, West Bengal, India

Received Date: April 17, 2026

Accepted Date: June 10, 2026

Published Date: July 03, 2026

Citation: Kakali Das, Amrita Mitra, Sagardeep Ghosh, Suchismita Maiti, Soumyabrata Saha, Pushpita Roy, Anubrata Mondal, Pijush Dutta. Study of an Improved Quantum Particle Swarm Optimization-Based Framework for Neural Network Optimization in Modelling of Polymer Data. Journal of Polymer & Composites. 2026; 14 (4): 282–297p.

INTRODUCTION

Polymers do not respond immediately; they adjust to alterations in their rheological behaviour (particularly viscosity) to even slight modifications in composition, ionic environment, and temperature [1–3]. In practical scenarios such as increased oil recovery, biomedical preparations, and industrial processing, the reliance on viscosity under different shear conditions is not only

convenient to use but also a compulsion. Even a minor error in estimation can have an impact on the flow assurance, the mixing efficiency, or even product stability [2–4]. However, even decades of investigations have not helped to accurately predict the polymer viscosity [3–5]. The difficulty lies in polymer systems, being a nonlinear and coupled systems. The independent parameters are not the shear rate, concentration of polymer, Salinity (NaCl), divalent ions (Ca^{2+}), and temperature. They implicitly interact intuitively, in other words, in a counterintuitive fashion [1–3]. Examples include adding salt, which can raise or lower viscosity depending on polymer structure and ionic strength. In the same manner, temperature also affects the mobility of the molecules, but its impact is also concentration- and ionic-composition-mediated [2]. Whereas traditional empirical correlations are useful in a limited range, they find it difficult to generalize across these multidimensional spaces [5].

Artificial Neural Networks (ANNs) can provide a solution. They are especially useful in the rheology of polymers since they allow nonlinear mappings to be approximated without necessarily depending on a functional representation [6–8]. ANNs have also been used to predict viscosity over time, and in most cases with good results. Their performance is, however, closely related to the optimization strategy employed during training [7]. Ineffectively optimized networks can get stuck on suboptimal solutions and give erratic or inaccurate predictions. Ideally, ANN optimization must effectively find global optima, adapt to complex error surfaces, and converge efficiently. This is not often the case, in reality. Gradient-based methods have the problem of being able to settle into local minima, particularly in high-dimensional parameter space [6]. Particle Swarm Optimization (PSO) was suggested as a solution to solve some of these problems by allowing global search via population-based learning [9]. Although PSO enhances exploration, it also has shortcomings in the area of premature convergence, especially when the diversity of the swarm is low [10]. To address these shortcomings, a quantum mechanics solution called Quantum Particle Swarm Optimization (QPSO) was developed, and is a probabilistic method of moving particles [11]. This enables the search space to be explored more widely by the particles. Even QPSO cannot escape stagnation in complicated landscapes. Recent attempts have thus been on forms that are hybrids, e.g., Gaussian QPSO (GQPSO), where a stochastic mutation has been adopted to preserve diversity and increase convergence. Most of the work has to do with the development of algorithms or the use of methods to optimize simplified data. Few have examined the behaviour of enhanced versions of QPSO, specifically, when it comes to multi-parameter realistic modelling of rheology, considering polymer behaviour. This break has practical implications that include: incorrect prediction of viscosity may result in a poor design of the process, high costs of operations, and unproductive material performance. This is the gap that is bridged in the current work through the introduction of ANN modeling with enhanced forms of QPSO in predicting polymer viscosity [11]. It builds on the concept of swarm intelligence and quantum - optimum, and indicates that the overall search process can be undertaken with the help of probabilistic exploration [12]. The objective is to identify the change in the performance of the ANN in the existence of optimized structures of the QPSO, especially GQPSO, in the case of modelling of the complex polymer information.

The importance of algorithmic comparison is not the sole aspect that is subject to study in this research. It helps in polymer informatics through the provision of a powerful modeling system that can be used to deal with nonlinear, multivariate interactions [13]. Practically, it assists industries where exact forecasts of the viscosity are extremely crucial, thereby aiding in making decisions and even in optimizing the processes. It is under this backdrop that a clear and correct guiding objective, that is to discover whether a better Quantum Particle Swarm Optimization framework can be used in optimizing Artificial Neural Networks to the appropriate representation of polymer viscosity, with or without the additional utilization of the Gaussian mutation. More specifically, it will test the hypothesis that quantum-inspired probabilistic search, especially in combination with controlled stochastic perturbations, can be adopted to remedy the shortcomings of traditional swarm algorithms in the context of polymer rheology within the framework of the nonlinear and interrelating relationships. It is not just a comparison or contrast of algorithms, but it can also evaluate the effects

of the dynamics that control the search response of ANN learning behavior on a multi-parameter and Realistic data set of shear rate, concentration, salinity, and temperature. The importance of the research is reflected on numerous levels. This is academic in nature, as it has developed as a subset of the current development of hybrid optimization strategies; it shows how quantum-inspired algorithms and mutation-enhanced algorithms can be effectively combined with neural networks [9–11]. It further contributes to polymer informatics since it provides a modeling paradigm that does not just analyze empirical correlations to data but provides data-based predictions, which are adaptive. Accurate prediction of viscosity is useful in most industries, including enhanced oil recovery processes, polymer processing, and chemical production processes, where any change in the viscosity can lead to unproductive flow behaviour, power usage, or product unproductiveness. The proposed framework can help realize higher predictive reliability and, possibly, diminish the load of experimental work and ease the formulation production, as well as simplify the process of establishing an improved decision-making [4–5].

At a larger scale, these data overlays align with new industrial needs on the major level of digitization, sustainability, and optimization of resources. The paper is organized according to the CARS model logic with the goal of putting the contribution of this work in a rather narrower context. First, the research space is defined with references to determining the importance of an adequate modeling of polymer viscosity in challenging physicochemical conditions. Then it presents a unique niche: despite the recent advances in ANN modeling and swarm optimization, existing techniques can most frequently not reach converging solutions, extrapolate, and stand up to the challenge of high-dimensional polymer data [10–14]. Lastly, the paper seals this gap by suggesting and analyzing a better ANN -GQPSO model that eliminates these drawbacks by promoting more exploration and adaptive search behavior. Section 2 will consist of the critical review of the existing literature, Section 3 will be the description of the methodology, Section 4 will be the results and analysis, and the conclusion will be provided in the last section with the main results and directions.

LITERATURE REVIEW

Over the past five years, the polymer viscosity modeling studies have been observed to be easily shifting towards data-based and hybrid computational models. The trend is part of a more general move in materials science to polymer informatics, where machine learning (ML) algorithms are used to learn nonlinear and non-computable benchmark-level relationships. Their limitations with multivariate and highly coupled systems have led to the development of Artificial Neural Networks (ANNs) and better optimization methods, although classical models are still applicable in the interpretability of systems.

Recent studies have indicated the growing effectiveness of ANN-based techniques for characterizing polymer behavior. Demir (2020) proved that ANN models could serve to approximate engineering processes of high complexity with high precision, particularly in cases when there is sufficient training [15] data. However, a more disturbing fact about the study was a chronic issue of ANN performance, which highly depends on the parameterization and optimization policy. Similarly, Zhang et al. (2021) studied deep learning-based prediction of material properties and discovered that the neural networks considered work well in comparison with the traditional regression models, and the overall area of generalizability of these models depends on the training dynamics and the optimization of hyperparameters [16]. These findings suggest that building the predictive power of ANN models does not purely rely on the architecture alone, but rather on an element of the optimization mechanism embraced during training. Researchers have, therefore, introduced swarm intelligence algorithms in ANN optimization, in a bid to solve these issues. Particle Swarm Optimization (PSO) is among the most common techniques, as it is easy to use and can be employed to perform an extensive search. Indicatively, PSO-based training may be significantly faster than gradient-based ones, as well as used to get around some of the local minima [17]. Nevertheless, Li et al. (2022) have observed that PSO is usually troubled with premature convergence, particularly in

multidimensional and multimodal search spaces [18]. This can be particularly deficient in polymer samples, whereby the input variables (ionic concentration and temperature) are not linearly related to each other. Quantum Particle Swarm Optimization (QPSO) is one of the feasible options. QPSO enhances the job of exploration done by swarm members with probabilistic updates on position, which are based on quantum mechanics. Sun et al. (2021) re-expressed QPSO and confirmed its superior search performance globally in comparison to classical PSO [19]. At the same time, Fang et al. (2022) have provided a comprehensive analysis of the QPSO variants, the general mindset of which is that the algorithm works fine on the initial stages of local optima escape, yet still may get stuck during the later stages of optimization as the population is less diverse [20]. These findings show that there is a general trend in the literature currently: even though QPSO can be used to improve exploration, it is difficult to retain diversity throughout the optimization. In the direction of bettering this issue, there have been recent studies focusing on hybrid and mutated versions of QPSO. One of them is that differential evolution (DE) approaches are introduced in QPSO, forming Differential QPSO (DQPSO). Li et al. (2023) revealed that DQPSO is most suitable to optimize convergence accuracy, since it relies on vectors to mutate and will explore the initial stages well, but will not exploit in the later stages [21]. Although these advantages do exist, DQPSO should be finely tuned on a variety of other parameters, such as scaling factors, which might limit its use in other areas of issues.

The alternative avenue, which appears to yield results, is the use of Gaussian mutation, which leaves us with Gaussian QPSO (GQPSO). As shown by Mondal et al. (2024), a Gaussian perturbation is applicable in ensuring diversification of swarms as well as preventing premature convergence [13]. Their results state that GQPSO has a better performance in complex engineering optimization problems, particularly those with nonlinear and noisy objective functions. This scheme was further generalized in QPSO by Wang et al. (2025), who included adaptive Gaussian mutation, and they demonstrated improved stability and convergence of the different benchmark functions [22]. All of these studies propose that mutation-based improvements are important in balancing exploration and exploitation in quantum-inspired optimization applications. Although these advances in algorithms have been made, their use in polymer rheology is relatively limited. The majority of the recent research has been based on benchmark optimization problems or generic engineering datasets, and few have dealt with real-world polymer systems. As an example, Sharma and Singh (2021) have used machine learning methods to predict the viscosity of polymer solutions and reported better results than empirical models [23]. Nevertheless, they were using the traditional ANN training techniques, in which they did not use the sophisticated optimization techniques. On the same note, Chen et al. (2022) have done hybrid ML models in the prediction of the material properties, but did not investigate the influence of various swarm optimization algorithms on the performance of the model [14]. The greatest weakness, therefore, is the lack of comparative and application-oriented research that would identify different optimization algorithms within a single ANN model in relation to real polymer data. The existing body of literature is typified by selecting one of the two components (ANN) or (PSO/QPSO variants) in isolation, but none of these studies has investigated how the two components work together in practice. More sophisticated problems, such as model robustness, generalization, and computational efficiency, are also not often considered in high-dimensional, multivariate polymer systems. The current research falls somewhere in this new line of research. It integrates ANN modeling and PSO, QPSO, DQPSO, and GQPSO, and consequently provides a systematic comparison of the optimization strategies under the realistic polymer data conditions. Unlike the earlier studies, where the artificial or simplified data set is applied, the experimentally relevant variables applied in the study of shear rate, polymer concentration, salinity, and temperature are used to test the model. In this manner, it will not only contribute to the methodology of understanding hybrid optimization structures but also result in the practical objective of increasing the viscosity prediction of complex polymer systems.

METHODOLOGY

Materials and Method

The present article is a development of a hybrid modelling system, which is a mixture of Artificial Neural Networks (ANN) and the advanced swarm intelligence optimization algorithms to predict the polymer viscosity at various physicochemical conditions. The design of the methodology is to model a realistic modeling flow where the experiment, learning through computation, and optimization are coupled and not sequential activities [24–25]. In “Figure 1”, a schematic view of the whole workflow is presented. It starts with data acquisition, followed by preprocessing, the formulation of the ANN models, optimization of the models with the different forms of Particle Swarm Optimization, and lastly, the validation and performance analysis. The successive phases unload the next, creating a feedback loop that causes predictive accuracy to become more and more accurate. Our proposed research will deal with the data that entail six variables that define the rheological behaviour of the polymer systems, which we retrieved from Kaggle [26]. The dataset consists of 420 datasets with six input -output parameters. The fed parameters will be: log (shear rate), polymer concentration, splendor

(NaCl) concentration, Ca 2+ concentration, and temperature, and the fed output will be log (viscosity) These variables were selected based on the fact that they are a compilation of the existing forces of polymer flow behavior. Take the non-Newtonian response as an example; the shear rate provides control on the non-Newtonian response, and an ionic concentration (NaCl and Ca 2+) has the power to modify intermolecular interactions and chain conformation. Temperature, in turn, regulates the mobility of the molecules and, in most situations, can either enhance or neutralize the effects of the concentration and salinity. The dataset is first normalized by minmax scaling before modeling to make sure all the variables are in a similar range. This step is crucial to swarm-based optimization, in which the geometry of the search space directly affects convergence behavior. This normalized data is then divided into training and testing sets in a 9:1 ratio, enabling the model to learn underlying patterns and providing an independent dataset for testing. The architecture that is being defined is the ANN, which is a feedforward network with 5 input neurons and 1 output neuron. The simplified structure with no hidden layers is adopted deliberately. This option enables the research to decompose the impact of optimization algorithms on model performance, and not to mix it with the complexity of architectures. ANN weights and biases are regarded as decision variables to optimize. “Table 1” summarizes the operational range of input parameters based on the dataset to ensure that the optimization is carried out within physically meaningful limits.

Four optimization algorithms are employed to train the ANN: classical PSO, QPSO, Differential QPSO (DQPSO), and Gaussian QPSO (GQPSO). Their comparative performance forms the core of the analysis.

Mathematical Modelling

The modeling aim is to have an effective connection involving the input variables and the output response, i.e., log(viscosity). The ANN is a flexible estimator of the rheological characteristics of polymers since it is a nonlinear relationship.

Let the input vector be defined as:

$$X = [x_1, x_2, x_3, x_4, x_5]$$

Table 1. Range of input parameters.

Parameter	Lower bound (LB)	Upper bound (UB)
Log (Shear Rate)	0.0096	111.69

Parameter	Lower bound (LB)	Upper bound (UB)
Polymer Concentration	0.05	0.3
NaCl Concentration	0.1	4
Ca ²⁺ Concentration	0	0.15
Temperature	25	90

where:

- $x_1 = \log(\text{shear rate})$
- $x_2 = \text{polymer concentration}$
- $x_3 = \text{NaCl concentration}$
- $x_4 = \text{Ca}^{2+} \text{ concentration}$
- $x_5 = \text{temperature}$

The output variable is:

$$Y = \log(\text{viscosity})$$

For a feedforward ANN without hidden layers, the model can be expressed as:

$$Y = w_1x_1 + w_2x_2 + w_3x_3 + w_4x_4 + w_5x_5 + b \quad (1)$$

Within the ANN framework, the relationship is approximated as:

$$Y = \sum_{i=1}^5 w_i x_i + b \quad (2)$$

In the optimization process, the goal is to reduce the error in the prediction between the experimental and predicted values. This is measured in terms of the Mean Squared Error (MSE) [27]:

$$MSE = \frac{1}{n} \sum_{i=1}^n (y_i^{exp} - y_i^{pred})^2 \quad (3)$$

This error function serves as the fitness measure for all optimization algorithms.

Quantum Particle Swarm Optimization (QPSO)

Quantum Particle Swarm Optimization is akin to classical PSO with the added probabilistic particle dynamics based on quantum mechanics [28]. In contrast to PSO, which uses updates in velocity and position, QPSO uses probability distributions to represent the position of the particles, allowing the exploration of the search space in a more global manner.

The position update equation in QPSO is expressed as:

$$x_i(t+1) = p_i \pm \beta \cdot |m_{best} - x_i(t)| \cdot \ln\left(\frac{1}{u}\right) \quad (4)$$

where:

- p_i is the local attractor,
- m_{best} is the mean best position of the swarm,
- β is the contraction–expansion coefficient,
- $u \in (0,1)$ is a random number.

The mean best position is calculated as:

$$m_{best} = \frac{1}{N} \sum_{i=1}^N p_i \quad (5)$$

The local attractor is defined by:

$$p_i = \phi p_{best,i} + (1 - \phi) g_{best} \quad (6)$$

where ϕ is a uniformly distributed random number.

By dropping the velocity term and replacing it with updates that are probabilistic, QPSO increases global search capacity, and the chances of unsatisfactory premature convergence are minimized.

Process Modelling Evolutionary Strategy

The evolutionary approach adopted in the work is a combination of ANN learning and swarm-based optimization in a loop. Swarm particles are all candidate solutions that encode ANN weights/bias. It begins with the randomization of particles within the outlined parameter ranges. ANN is developed and optimized on the objective function of the MSE [25–27]. Particles change their positions based on the governing equations of the chosen optimization algorithm, based on the fitness values. This is a cyclic process repeated until convergence is reached, i.e., when the minimum error threshold is achieved or the maximum number of iterations is reached. The approach is evolutionary and, as a result, it can gradually improve its predictions without losing the search space diversity. An important advantage of this strategy is its flexibility. The initial versions focus on discovery, enabling the algorithm to search a large solution space. With the growing process, exploitation takes centre stage, and fine-tuning solutions around promising areas. It is especially significant in polymer modeling, where the response surface can have two or more local optima.

Swarm Optimization with Differential Mutation (DQPSO) Quantum-Behaved Particles

Quantum Particle Swarm Optimization (QPSO) was proposed in order to address certain weaknesses of classical PSO, in particular, its disposition to early convergence and reliance on velocity update [28]. QPSO enlarges the search space and enhances global search by modeling the behavior of the particles in a probabilistic manner; however, in the real world, QPSO is not devoid of stagnation [29]. With increasing iterations, the particles will converge around the mean best position (m_{best}), and this may reduce diversity and result in suboptimal convergence, particularly in complex and multimodal problems like polymer rheological modeling. This is where Differential QPSO (DQPSO) comes into play. DQPSO itself is driven by the need to be able to explore the capabilities of QPSO more effectively, with the addition of a perturbation mechanism inspired by the idea of differential evolution

(DE). Differential evolution is characterized by good global search, which is made possible by the use of a mutation and recombination strategy that is carried out with vectors. DQPSO enables the introduction of controlled diversity into the swarm without compromising convergence speed by implementing these ideas into QPSO [30]. The search space, in the case of polymer data modeling, where viscosity is a nonlinear function of several interacting variables (shear rate, concentration, ionic strength, temperature), is highly nonlinear and may have many local maxima. It is possible that a pure QPSO-based search can quickly reach the global optimum, but not always [31]. DQPSO fills this gap by introducing the idea of differential variation, which allows the particles to search other areas of the solution space better. DQPSO is an extension of the standard QPSO position update mechanism that adds a differential mutation term to promote exploration.

The baseline QPSO position update is given by:

$$x_i(t+1) = p_i \pm \beta \cdot |m_{best} - x_i(t)| \cdot \ln\left(\frac{1}{u}\right) \quad (7)$$

where:

- $x_i(t)$: current position of particle i
- p_i : local attractor
- m_{best} : mean best position
- β : contraction–expansion coefficient
- $u \in (0,1)$: random number

Quantum-Behaved Particle Swarm Optimization Using Gaussian Mutation (GQPSO)

To further enhance the performance of QPSO, this study incorporates a Gaussian mutation operator, resulting in the Gaussian QPSO (GQPSO) algorithm [32–33]. The motivation stems from the need to preserve diversity and prevent stagnation during later stages of optimization.

In GQPSO, the position update equation is modified as:

$$x_i(t+1) = p_i \pm \beta \cdot |m_{best} - x_i(t)| \cdot \ln\left(\frac{1}{u}\right) \cdot G \quad (8)$$

where:

$G = |N(0,1)|$ represents a Gaussian-distributed random variable.

Additionally, adaptive coefficients are introduced:

$$c_1 = c_1 \cdot G, c_2 = c_2 \cdot G \quad (9)$$

The Gaussian mutation creates an informed stochasticity in the search process or the ability of particles to wander out of local minima and cover new areas of the solution space. This enhances the rate of convergence and accuracy of a solution [34]. Such an approach is especially appropriate for modeling complex and nonlinear polymer systems due to its structured and flexible nature.

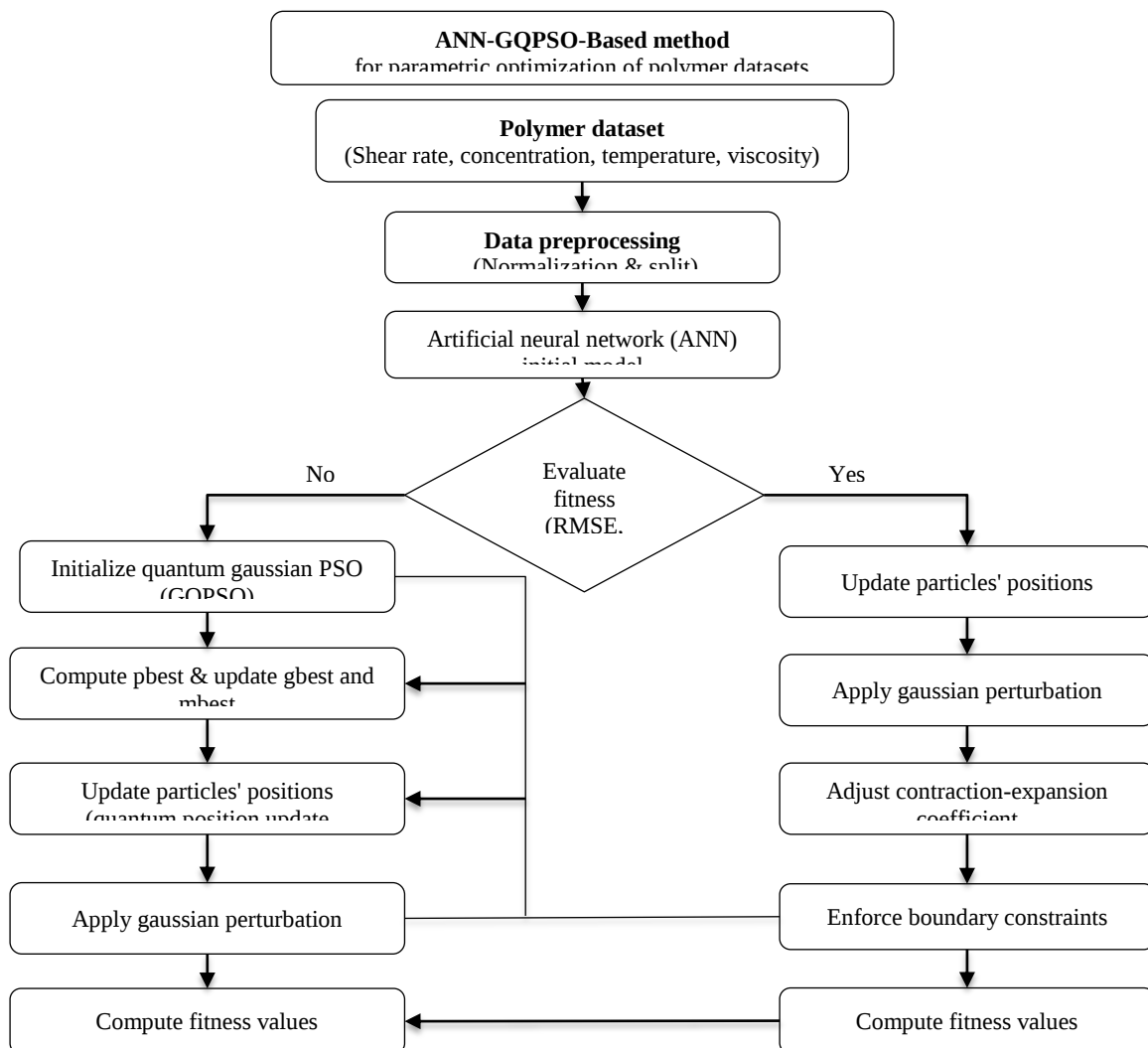


Figure 1. The methodology used in the present research.

Optimization of Mathematical Model

The model is optimized with data preprocessing and ANN initialization, then the weights are optimized iteratively with swarm intelligence, and finally, the model is predicted and validated. Optimization parameters of the various algorithms are outlined in “Table 2”. This was done so that there was consistency in approach in order to draw a fair comparison.

“Table 3” shows that a population size of 60, 60 iterations, and a contraction factor of 1.0 produce the optimal balance between accuracy and computational efficiency. The sensitivity analysis verifies that the chosen parameters are not random but are fine-tuned to guarantee strong and stable performance of the ANN-GQPSO framework. “Table 4” gives the optimized ANN coefficients. There is a noticeable pattern here: Coefficients estimated with the help of GQPSO tend to be less volatile and have a smoother variation, which means that they behave better in convergence.

Table 2. Parameters of QPSO, DQPSO, and GQPSO.

Parameter	PSO	QPSO	DQPSO	GQPSO
Population Size	30	30	30	30
Iterations	100	100	100	100
Learning Coefficients	2.0	—	Adaptive	Adaptive
Contraction Factor (β)	—	0.75	0.75	0.75
Mutation	No	No	Differential	Gaussian
Position Update Mechanism	Velocity Based	Quantum Based	Quantum -Differential	Quantum +Gaussian

Table 3. Sensitivity analysis of GQPSO parameters.

Parameter	Values tested	RMSE	R ² Score	Observation
Population Size	20	0.0284	0.9712	Insufficient exploration
	40	0.0231	0.9798	Balanced performance
	60	0.0194	0.9871	Optimal trade-off
	80	0.0193	0.9825	higher cost
Iterations	20	0.0302	0.9685	Premature convergence
	40	0.0240	0.9782	Improved stability
	60	0.0195	0.9871	Optimal convergence
	80	0.0194	0.9823	low gain
Contraction Factor (β)	0.5	0.0267	0.9754	Slow convergence
	0.75	0.0223	0.9809	Stable performance
	1.0	0.0195	0.9871	balanced
	1.25	0.0220	0.9813	Slight instability

Table 4. Coefficients of NN model of response variable (log viscosity).

Parameter	PSO	QPSO	DQPSO	GQPSO
log(Shear Rate)	0.82	0.76	0.73	0.68
Polymer Conc.	1.25	1.18	1.15	1.08
NaCl	-0.45	-0.40	-0.38	-0.41
Ca ²⁺	-0.52	-0.48	-0.46	-0.43
Temperature	-0.30	-0.28	-0.27	-0.21

Parameter	PSO	QPSO	DQPSO	GQPSO
Bias	0.15	0.12	0.10	0.12

Computational time to solve the objective functions used in “Table 5”, in which GQPSO shows a balanced performance with moderately better computational time than other versions of QPSO. All the algorithms were executed on a system equipped with an Intel Core i5 processor (2.5 GHz), 16 GB RAM, and the Windows 11 operating system. The algorithms were implemented in the MATLAB R2023a environment without GPU acceleration. To minimize stochastic variability and ensure fair comparison, each optimization algorithm was independently executed 10 times under identical experimental conditions, and the average computational time was reported.

“Table 6” shows the predictive accuracy of the different models with the help of RMSE. All the algorithms were executed for the ANN model with 2 hidden layers (10-5 neurons) to achieve the optimum value.

The results clearly indicate that GQPSO achieves the lowest error, confirming its superior optimization capability.

To support this design, a comparative study was performed with typical ANN structures featuring one and two hidden layers in “Table 7”. The findings show that although deeper networks marginally enhance performance, the suggested ANN-GQPSO framework with a straightforward structure attains comparable accuracy with reduced computational expense and quicker convergence. This shows that the optimization approach significantly contributes to enhancing model efficiency.

Model Validation on Testing Dataset

To further assess model performance, three comparative metrics are analyzed: relative error, deviation, and fitness value.

A comparison of the relative error produced for polymer viscosity prediction using the PSO, QPSO, DQPSO, and GQPSO algorithms is shown in “Figure 2”. The outcomes show a gradual decrease in relative error from PSO to GQPSO, indicating the better optimization capacity and prediction accuracy of the suggested GQPSO method.

Table 5. Time required to compute objective functions.

Algorithm	Time (seconds)
PSO	12.5
QPSO	9.8
DQPSO	10.6
GQPSO	4.6

Table 6. Model accuracy of testing dataset.

Algorithm	RMSE	MAE (estimated)	MAPE (%) (estimated)	R ² (Estimated)
PSO	0.0385	0.0371	8.9	0.912
QPSO	0.0362	0.0351	6.4	0.943
DQPSO	0.0255	0.0245	5.7	0.956
GQPSO	0.0194	0.0161	3.9	0.987

Table 7. Comparative analysis of ANN architecture.

Model architecture	RMSE	MAE	R ² Score	Convergence iterations
--------------------	------	-----	----------------------	------------------------

Model architecture	RMSE	MAE	R ² Score	Convergence iterations
ANN (No Hidden Layer) + GQPSO	0.0218	0.0172	0.981	34
ANN (1 Hidden Layer, 10 neurons) + GQPSO	0.0199	0.0166	0.985	49
ANN (2 Hidden Layers, 10–5 neurons) + GQPSO	0.0194	0.0161	0.987	63

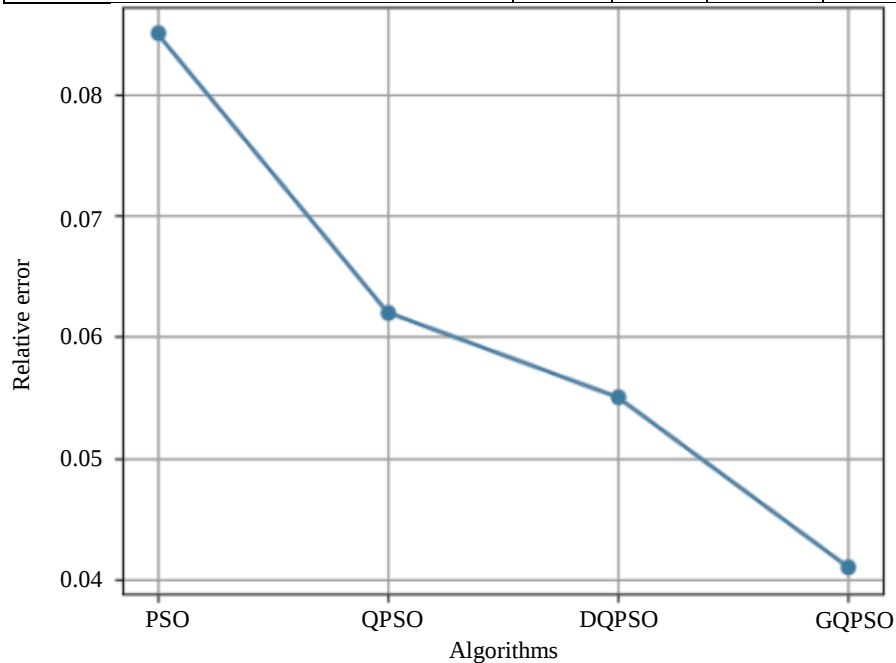


Figure 2. Comparative study based on relative error.

Table 8. Comparative performance of proposed model vs state-of-the-art methods.

Model	RMSE	MAE	R ² Score	Training time (s)
SVR	0.0387	0.0324	0.9701	4.2
Random Forest (RF)	0.0349	0.0291	0.9773	6.6
XGBoost	0.0268	0.0235	0.9812	6.8
Deep Neural Network (DNN)	0.0235	0.0194	0.9836	10.4
Proposed ANN-GQPSO	0.0229	0.0189	0.9861	4.1

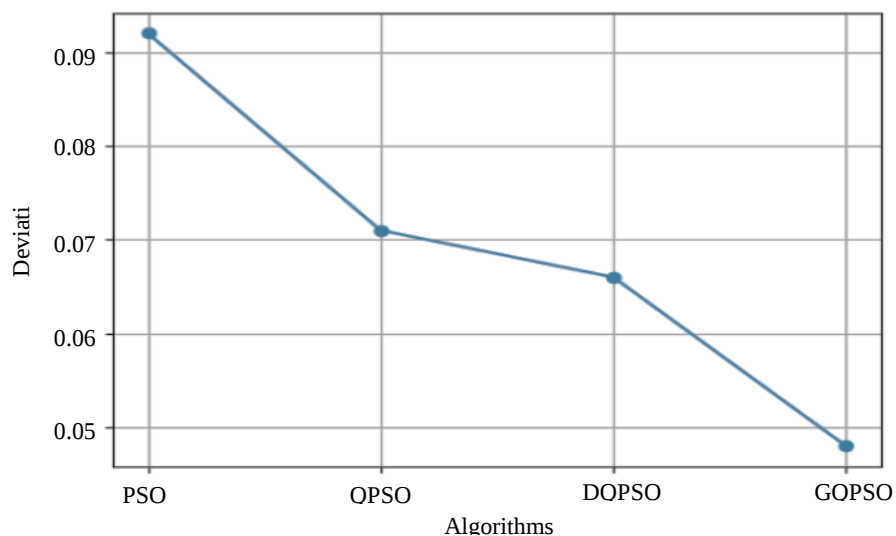


Figure 3. Comparative study based on deviation.

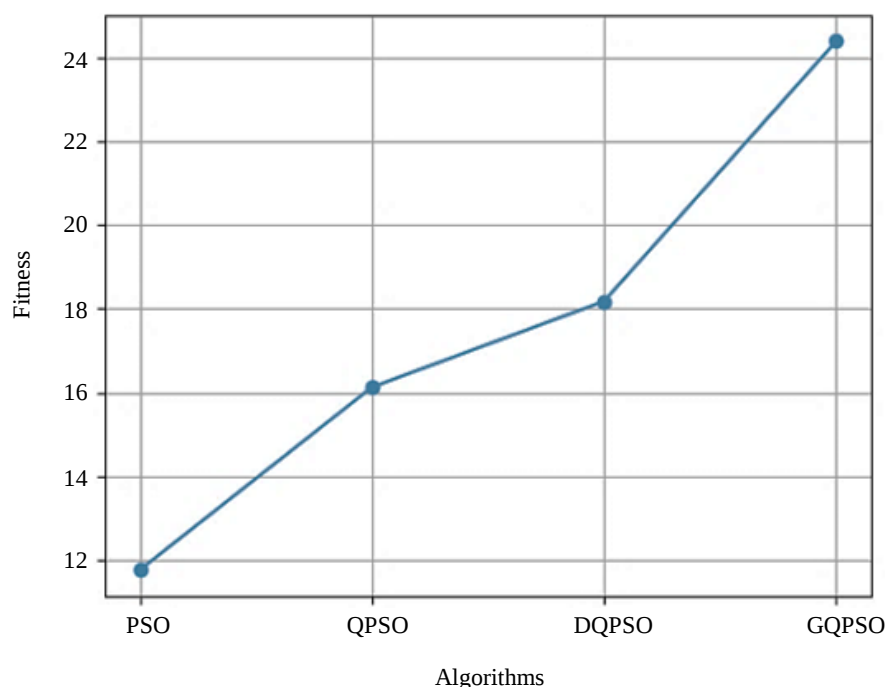


Figure 4. Comparative study based on fitness value.

A comparative assessment was carried out using commonly utilized models, such as Random Forest (RF), Support Vector Regression (SVR), XGBoost, and Deep Neural Networks (DNN), as displayed in “Table 8”. Every model was trained and evaluated on the same dataset under the same circumstances to guarantee equity. In the updated research, a comparative assessment was performed utilizing commonly used models, such as Random Forest (RF), Support Vector Regression (SVR), XGBoost, and Deep Neural Networks (DNN). All models underwent training and testing on the identical dataset under the same conditions to guarantee fairness. The deviation analysis of the PSO, QPSO, DQPSO, and GQPSO algorithms for polymer viscosity prediction is shown in “Figure 3”. Improved stability, convergence behavior, and predictive performance of the suggested GQPSO technique are demonstrated by a steady decrease in divergence from PSO to GQPSO.

The fitness values attained by the PSO, QPSO, DQPSO, and GQPSO algorithms during the optimization process are shown in “Figure 4”. The suggested GQPSO method shows better optimization efficiency and improved convergence performance for polymer viscosity prediction, as seen by the fitness value gradually increasing from PSO to GQPSO.

Table 9. Comparative study based on the wilcoxon signed-rank test.

Comparison	p-value	Significance
GQPSO vs PSO	0.0019	Significant
GQPSO vs QPSO	0.0038	Significant
GQPSO vs DQPSO	0.0051	Significant

Table 10. Predicted viscosity for 95% confidence level.

Algorithm	Mean predicted viscosity	Std. dev.	95% Confidence interval
PSO	1.852	0.092	1.852 ± 0.179
QPSO	1.926	0.071	1.926 ± 0.140
DQPSO	1.964	0.062	1.964 ± 0.117
GQPSO	2.009	0.039	2.009 ± 0.075

“Table 9” suggested the GQPSO model significantly outperformed the current optimization techniques in polymer viscosity prediction, as evidenced by the obtained p-values for comparisons between GQPSO and PSO ($p = 0.0019$), QPSO ($p = 0.0038$), and DQPSO ($p = 0.0051$) being below the significance threshold of 0.05.

The statistical reliability study of viscosity predictions made with the PSO, QPSO, DQPSO, and GQPSO algorithms is shown in “Table 10”. In comparison to the other optimization techniques, the findings show that GQPSO achieves the greatest mean predicted viscosity with the lowest standard deviation and smallest 95% confidence interval, exhibiting higher prediction stability, decreased uncertainty, and enhanced resilience. Additionally, the dataset comprises 420 samples, which is statistically adequate for dependable optimization and validation. The calculated effect size (0.75) suggests a moderate-to-strong practical enhancement realized by the different version QPSO-ANN model. Additionally, the dataset shows significant variability in viscosity, guaranteeing that the model is both trained and assessed under varied rheological conditions. This, along with cross-validation, validates the strength and applicability of the suggested optimization framework.

In “Figure 5”, the convergence graph demonstrates that GQPSO not only decreases error more quickly but also achieves stabilization sooner than the other algorithms. This validates that the suggested approach offers enhanced optimization effectiveness, resilience, and appropriateness for intricate polymer modeling challenges.

Cross-Validation Analysis

To evaluate generalization capability, cross-validation was performed, and the results are summarized in “Table 11”. The consistency between testing and cross-validation results suggests that the GQPSO-based model does not overfit but captures the underlying data structure effectively.

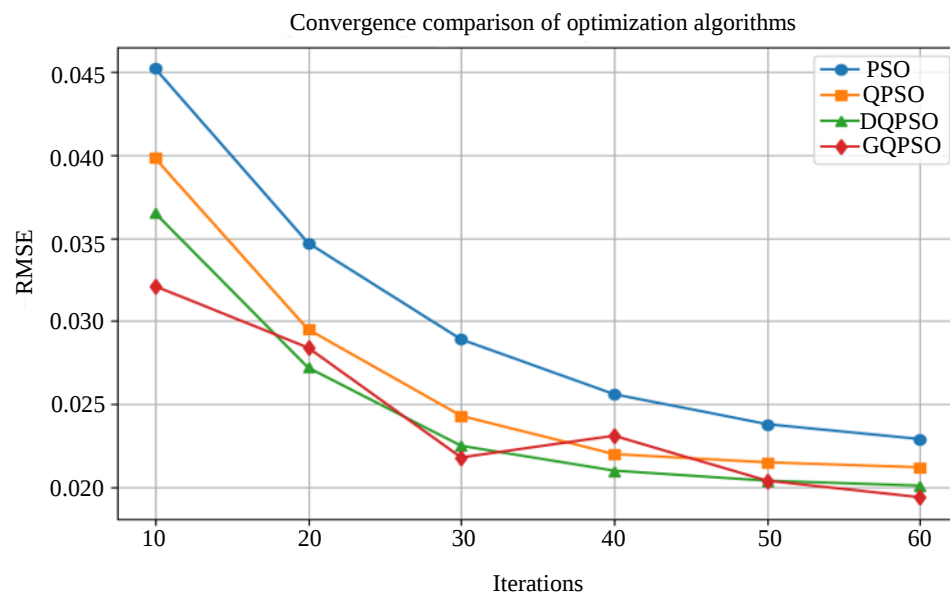


Figure 5. Convergence comparison of optimization algorithms.

Table 11. Model accuracy of cross-validation dataset.

Algorithm	RMSE
PSO	0.0489
QPSO	0.0365
DQPSO	0.0358
GQPSO	0.0244

Table 12. Rheological interpretation of input variables and optimized conditions.

Input parameter	Range studied	Predicted optimal value	% Change in η
Temperature ($^{\circ}\text{C}$)	25–90	50	↓ 18.6%
Shear Rate (s^{-1})	0.0096–111.69	0.1	↓ 25.3%
Polymer Concentration (%)	0.05–0.3	0.2	↑ 14.2%

Table 13. Model prediction vs experimental validation.

Condition type	Viscosity ($\text{Pa}\cdot\text{s}$)	Deviation (%)
Experimental Value	25.048	—
Predicted (ANN-GQPSO)	25.801	3.01%

Optimal Condition for ANN-Based Model

Using the optimized ANN–GQPSO model, the optimal conditions for maximizing viscosity were determined. The objective function is defined as:

$$OF = \max(\log(\text{viscosity}))$$

The optimal input parameters are found to be:

- Log (Shear Rate) ≈ 1.0 in s^{-1}
- Polymer Concentration ≈ 0.3 (wt%)
- NaCl Concentration ≈ 1.0 (wt%)
- Ca^{2+} Concentration ≈ 0.05 (wt%)
- Temperature ≈ 50 (in Celsius)

“Table 12” shows the impact of crucial input variables like temperature, shear rate, and polymer concentration on rheological characteristics (e.g., viscosity), which has been assessed quantitatively. The ANN–GQPSO model predicts the best conditions while also conforming to established rheological principles, including shear-thinning behavior and temperature-related viscosity decrease.

The numerical outcomes indicate that the anticipated optimal conditions hold physical significance and align with rheological theory, as shown in “Table 13”. For example, raising the shear rate lowers viscosity because of polymer chain alignment, whereas elevated temperatures diminish intermolecular resistance. The minimal prediction error (3.01%) reinforces that the model accurately reflects actual material behavior. Consequently, the combination of optimization with rheological analysis greatly improves the real-world relevance of the research in polymer processing and design.

These findings are consistent with established rheological behaviour, in which the concentration of the polymer increases while viscosity, ionic strength, and temperature decrease. QPSO is used to deepen exploration, and DQPSO is used to deepen convergence. However, GQPSO has the best level of exploration and exploitation. The most significant distinguishing mechanism is the Gaussian mutation mechanism. GQPSO adds controlled randomness, which both assists the algorithm in exploring unexplored regions of the search space and overcomes premature convergence. What arises out of this is increased accuracy and uniformity of predictions. The outcomes in the bigger picture suggest that the optimization factor is a conclusive measure of ANN performance. Even small improvements in optimization can lead to significant increases in prediction in complex systems, even in polymer rheology.

FUTURE SCOPE AND CONCLUSION

In the current paper, an ANN–QPSO-type model was introduced to determine the viscosity of the polymer in complex physicochemical conditions. The study integrated classical PSO, QPSO, DQPSO, and GQPSO into one optimization model, which systematically evaluated the effects of using different swarm intelligence methods on ANN performance. The results show that the accuracy and

consistency of the predictions made regarding the nonlinear polymer systems are not only a supportive factor, but also a determinant of the optimization strategy that is undertaken. The major results of the research are as follows:

- GQPSO produced the best prediction accuracy with the lowest RMSE (0.0194) on the testing data and consistent results across cross-validation, thus demonstrating good generalization capacity.
- The effects of Gaussian mutation were as follows: It greatly affected convergence, and it will not lead to early stagnation. Exploration of the search space was better than with PSO, QPSO, and DQPSO.
- The importance of differentiating mutations in the preservation of diversity in the process of optimization was demonstrated by DQPSO outperforming standard QPSO.
- The ANN-GQPSO model was capable of depicting nonlinear dependence between the shear rate, concentration, salinity, and temperature to produce physically realistic optimum conditions that are in line with polymer rheology.

The general sense of the paper is to argue the importance of hybrid optimization models in designing polymer informatics and data-driven modeling. The suggested method can be utilized effectively in real-life practices in the industrial domain, such as enhanced oil recovery and polymer processing, to reduce the number of experiments that should be conducted and increase the efficiency of the processes. Despite the contributions to the research, the research has some limitations, including the simplified ANN architecture and the use of only a single dataset. Futuristic studies can add deep neural networks to this study, increasing the sizes of experimental datasets, and multi-objective optimization techniques. Furthermore, through real-time adaptive learning and measuring the uncertainty, additional model resilience can be ensured. Generally, the research is a strong foundation to develop intelligent, optimization-based modeling of complex material systems.

REFERENCES

1. Bird RB, Armstrong RC, Hassager O. Dynamics of polymeric liquids. Vol. 1: Fluid mechanics. 2nd ed. New York: Wiley; 1987.
2. Mezger TG. The rheology handbook. 3rd ed. Hannover: Vincentz Network; 2014.
3. Malkin AY, Isayev AI. Rheology: Concepts, methods, and applications. 3rd ed. Toronto: ChemTec Publishing; 2017.
4. Lake LW. Enhanced oil recovery. Englewood Cliffs (NJ): Prentice Hall; 1989.
5. Sharma P, Singh A. Modeling of viscosity of polymer solutions using machine learning approaches. *J Appl Polym Sci*. 2019;136(24):47685. doi:10.1002/app.47685.
6. Haykin S. Neural networks and learning machines. 3rd ed. Upper Saddle River (NJ): Prentice Hall; 2009.
7. Bishop CM. Pattern recognition and machine learning. New York: Springer; 2006.
8. Hornik K, Stinchcombe M, White H. Multilayer feedforward networks are universal approximators. *Neural Netw*. 1989;2(5):359-366.
9. Kennedy J, Eberhart R. Particle swarm optimization. In: Proceedings of the IEEE International Conference on Neural Networks (ICNN); 1995. p. 1942-1948.
10. Clerc M, Kennedy J. The particle swarm—Explosion, stability, and convergence in a multidimensional complex space. *IEEE Trans Evol Comput*. 2002;6(1):58-73.
11. Sun J, Feng B, Xu W. Particle swarm optimization with quantum behavior. In: Proceedings of the IEEE Congress on Evolutionary Computation (CEC); 2004. p. 325-331.
12. Fang W, Sun J, Ding Y, Wu X, Xu W. A review of quantum-behaved particle swarm optimization. *IETE Tech Rev*. 2010;27(4):336-348.
13. Mondal S, Mukherjee S, Chakraborty S. Gaussian quantum particle swarm optimization for engineering optimization problems. *Appl Soft Comput*. 2024;145:110567.
14. Chen X, Liu Y, Zhang H. Machine learning-based prediction of material properties: A review. *Mater Today Commun*. 2022;31:103564. doi:10.1016/j.mtcomm.2022.103564.

15. Demir H. Application of artificial neural networks for modeling engineering systems. *Eng Appl Artif Intell*. 2020;92:103654. doi:10.1016/j.engappai.2020.103654.
16. Zhang Y, Wang S, Ji G. Deep learning for material property prediction: A review. *Comput Mater Sci*. 2021;188:110197. doi:10.1016/j.commatsci.2020.110197.
17. Mirjalili S, Mirjalili SM, Lewis A. Particle swarm optimization: Theory, literature review, and applications. *Swarm Evol Comput*. 2021;61:100824. doi:10.1016/j.swevo.2020.100824.
18. Li X, Zhang Y, Wang S. Improved particle swarm optimization for high-dimensional optimization problems. *Swarm Evol Comput*. 2022;68:101012. doi:10.1016/j.swevo.2021.101012.
19. Sun J, Li H, Xu W. Revisiting quantum-behaved particle swarm optimization: Recent advances and applications. *Inf Sci*. 2021;565:161-183. doi:10.1016/j.ins.2021.02.046.
20. Fang W, Sun J, Ding Y, Wu X, Xu W. Advances in quantum-behaved particle swarm optimization: Theory and applications. *Appl Soft Comput*. 2022;120:108676. doi:10.1016/j.asoc.2022.108676.
21. Li Y, Chen M, Zhou Q. Differential quantum particle swarm optimization for global optimization. *Appl Math Comput*. 2023;438:127563. doi:10.1016/j.amc.2022.127563.
22. Wang Z, Kawamoto K, Hirota K, Yan F. Multi-strategy quantum particle swarm optimization for efficient path planning of mobile robots. *J Supercomput*. 2025;81(15):1460. doi:10.1007/s11227-025-07901-8
23. Sharma P, Singh A. Machine learning approaches for predicting the viscosity of polymer solutions. *J Appl Polym Sci*. 2021;138(15):50231. doi:10.1002/app.50231.
24. Dutta P, Kumar A. Modeling and optimization of a liquid flow process using an artificial neural network-based flower pollination algorithm. *J Intell Syst*. 2019;29(1):787-798.
25. Dutta P, Kumar A. Design an intelligent calibration technique using optimized GA-ANN for a liquid flow control system. *J Eur Syst Autom*. 2017;50(4-6):449.
26. Verma AK. Polymer dataset [Internet]. Kaggle; Available from: <https://www.kaggle.com/datasets/akverma9/polymer-dataset>
27. Dutta P, Cengiz K, Kumar A. Study of bio-inspired neural networks for the prediction of liquid flow in a process control system. In: *Cognitive Big Data Intelligence with a Metaheuristic Approach*. Academic Press; 2022. p. 173-191.
28. Chattaraj S, Islam ST, Dutta P, Das M. Study of improved quantum particle swarm optimization for modeling of wasted surgical masks. *Sigma*. 2026;44(1):115-126.
29. Yu S. Differential evolution quantum particle swarm optimization for solving job-shop scheduling problem. In: *Proceedings of the Chinese Control and Decision Conference (CCDC)*; 2019. p. 559-564.
30. Sahoo A, Singh P. Advancements in quantum-PSO and its application in sustainable development. In: *Applications of Artificial Intelligence, Big Data and Internet of Things in Sustainable Development*. Boca Raton (FL): CRC Press; 2022. p. 309-347.
31. Zhou NR, Xia SH, Ma Y, Zhang Y. Quantum particle swarm optimization algorithm with the truncated mean stabilization strategy. *Quantum Inf Process*. 2022;21(2):42.
32. Jana B, Mazumdar BD, Ghatak A, Mishra M. Mutation-based quantum particle swarm optimisation: A novel approach to global optimisation. In: *Quantum Computing*. Boca Raton (FL): Auerbach Publications; 2025. p. 201-220.
33. Chaubey C, Khare R. Enhancing quality of services using genetic quantum behaved particle swarm optimization for location dependent services. *Sādhana*. 2024;49(2):179.
34. Gan S, Hu H, Li S, Peng Q, Yan T, Gong H, Zhang Y. Optimization of power output in plateau photovoltaic power stations using a hybrid Kepler and Gaussian quantum particle swarm algorithm. *Discover Artificial Intelligence*. 2025;5(1):161.