Review Article

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Review of modeling schemes and machine learning algorithms for fluid rheological behavior analysis

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Abstract: Machine learning's prowess in extracting insights from data has significantly advanced fluid rheological behavior prediction. This machine-learning-based approach, adaptable and precise, is effective when the strategy is appropriately selected. However, a comprehensive review of machine learning applications for predicting fluid rheology across various fields is rare. This article aims to identify and overview effective machine learning strategies for analyzing and predicting fluid rheology. Covering flow curve identification, yield stress characterization, and viscosity prediction, it compares machine learning techniques in these areas. The study finds common objectives across fluid models: flow curve correlation, rheological behavior dependency on variables, soft sensor applications, and spatial–temporal analysis. It is noted that models for one type can often adapt to similar behaviors in other fluids, especially in the first two categories. Simpler algorithms, such as feedforward neural networks and support vector regression, are usually sufficient for cases with narrow range variability and small datasets. Advanced methods, like hybrid approaches combining metaheuristic optimization with machine learning, are suitable for complex scenarios with multiple variables and large datasets. The article also proposes a reproducibility checklist, ensuring consistent research outcomes. This review serves as a guide for future exploration in machine learning for fluid rheology prediction.

Keywords: machine learning, rheology, viscosity

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Abbreviation

AI	artificial intelligence
ANFIS	adaptive neuro-fuzzy inference system
ANN	artificial neural networks
BP	backpropagation
ELM	extreme learning machine
FFNN	feedforward neural network
GA	genetic algorithm
GC	group contribution
GMDH	group method of data handling
LM	Levenberg–Marquardt
MLP	multilayer perceptron
MSE	mean squared error
PNN	polynomial neural network
PSO	particle swarm optimization
RBFNN	radial basis function neural network
SVR	support vector regression

Symbol

τ	shear stress
τ_{yield}	yield stress
η	viscosity/apparent viscosity

$\eta_{plastic}$	plastic viscosity
$\dot{\gamma}$	shear rate
k	consistency index
n_p	power law exponent
k_T	thermal conductivity
P	pressure
T	temperature
ρ	density
w_{fluid}	weight percentage

1 Introduction

Investigating the rheological parameters of fluids can be challenging, especially when considering their dependence on specific variables. Understanding these rheological parameters is critical for a wide range of real-world applications, as fluid behavior significantly impacts various industries. For example, the viscosity and rheological properties of drilling fluids are critical for efficient drilling operations. Failure to predict these parameters accurately can lead to costly drilling problems, including wellbore instability and equipment damage [1]. Industries that use polymers rely on accurate rheological data for extrusion, molding, and forming processes. Inadequate predictions can result in defects, waste, and production delays [2]. The rheological properties of concrete and cement mixtures influence their workability and curing behavior. Poor predictions can result in construction defects and reduced durability of structures [3]. In addition, fluid rheology is crucial in the design and performance of smart materials, including shape memory alloys and responsive fluids, as it ensures the desired response to external stimuli. Accurate control of rheological parameters is essential for these materials to function as intended and meet the specific requirements of various applications [4].

The nonlinear behavior of materials, such as shear thickening or thinning [5,6], can be influenced by various factors. The factor can be the fabrication techniques and compositions [7]. Furthermore, external stimuli such as magnetic fields and temperature can also affect the materials [8,9]. Due to the effort to understand and predict these complex behaviors, various classical models have been developed to characterize fluid behavior. Among them, the power law and Bingham plastic models are well-known for describing the behavior of non-Newtonian fluids [10,11]. Both models are utilized to predict viscosity and shear stress as a function of shear rate. Meanwhile, several extended models have also been formulated to accommodate the effects of other variables, such as temperature [12,13] and magnetic fields [9,14]. It is important to note that conventional models often have limited applicability or a restricted range of independent variables [15,16]. With the advance of computational technology and data availability in various databases, machine learning approaches have become more popular to overcome the limitations of conventional models for predicting rheological parameters.

Machine learning models, including artificial neural networks (ANN), are applied to predict the rheological properties of fluids. For example, the methods can be used in pattern prediction of viscosity [17] and yield stress [9,14] as a function of various variables. The models have been proven to provide a reliable prediction for rheological parameters, especially viscosity [15] and shear stress [18,19], as a function of composition structures, particle concentrations, and operating variables. The models are generated using universal methods for learning the experimental dataset using a set of equations and algorithms. Several other machine learning techniques can also be applied, such as extreme learning machine (ELM), group method of data handling (GMDH), polynomial neural networks (PNNs), support vector regression (SVR), adaptive neuro-fuzzy inference system (ANFIS), and radial basis function neural networks (RBFNN). The high number of previous works opens the possibility of selecting and employing the most effective artificial intelligence (AI) technique in a specific field of rheology [15].

Investigating, mapping, and discussing the current works are essential for considering the appropriate application or development of the machine learning model in a particular rheological behavior modeling case. A review article has discussed viscosity prediction using traditional empirical and machine learning models in automotive radiators [20]. However, the discussion is limited to nanofluids and covers only articles published up to 2016. In fact, after 2016, numerous articles have contributed to the more advanced application of various machine learning methods, such as in [21,22]. Although Hemmati-Sarapardeh *et al.* [15] have attempted to summarize the existing techniques up to 2018 while proposing a committee machine intelligence system, the discussion is not comprehensive enough and only limited to the nanofluids application. In oil and gas, a review article about the machine learning application for drilling fluid has shown the method's potential for tackling the computationally expensive nature of the traditional methods [23]. In food, the early review of the machine learning application is only limited to the methods of ANFIS and ANN [24]. Nnyigide and Hyun [25] also discussed the potential of the machine learning application for food rheology while highlighting that the method is still relatively new and needs more exploration.

Table 1 shows several existing literature reviews related to rheological parameter predictions and machine learning-

Table 1: Literature review of machine learning and rheological properties

Ref	Modeling objects	Reviewed machine learning	Predicted rheology parameters	Focus on machine learning	Focus on rheological properties	Remarks
[26]	Biodiesel production studies	ANN	Viscosity, kinematic viscosity	Yes	No	
[27]	Biofuel's life cycle	ANN	Apparent viscosity, kinematic viscosity, and plastic viscosity	Yes	No	
[28]	Food process modeling	RNNs, deep neural networks with restricted Boltzmann machine algorithm, genetic algorithm-ANN, and ANFIS	Viscosity, loss modulus, storage modulus, and stress relaxation	Yes	No	Only focus on neural networks
[25]	Food rheology	ANFIS and ANN	Apparent viscosity	Yes	Yes	Covered only ANFIS and ANN
[24]	Honey Rheology	ANFIS and ANN	Apparent viscosity and complex viscosity	No	Yes	
[29]	Ionic Liquids	Least square SVM, ELM, and MLP	Viscosity	Yes	No	
[30]	Magnetorheological (MR) fluids	ANN ELM RBF	Yield stress	No	Yes	
[31]	Nanofluid modeling using ANN	ANN	Dynamic viscosity	Yes	No	ANN
[32]	Nanofluids using machine learning	ANN	Dynamic viscosity	Yes	No	Focus on nanofluids
[33]	Nanofluids in general	BP-ANN, GMDH, GA BP-ANN, and self-organizing maps	Dynamic viscosity	No	No	
[34]	Statistics of the ANN study for nanofluids	BP-ANN, GMDH, GA BP-ANN, and self-organizing maps	Dynamic viscosity	Yes	No	
[35]	Mud models	ANN	Plastic viscosity	No	Yes	

based models. It includes studies on biodiesel production, biofuel's life cycle, and food process modeling, predominantly using models like ANN, recurrent neural network (RNN), and ANFIS. Most studies focus either on machine learning or rheological properties, not both, leading to a less detailed discussion. The exception is Nnyigide and Hyun's work [25], which covers both aspects but is limited to food applications and specific models like ANFIS and ANN. Overall, there appears to be a lack of in-depth reviews on the application of ANN in fluid rheology, suggesting an area ripe for further exploration and analysis.

Although there are numerous reviews of machine learning applications on fluids, the existing reviews only cover a specific field without summarizing the generalization of the applicability of methods and reproducibility. The summary and classification of the current methods will be beneficial to the application of different machine learning methods to various fields or open the integration of the existing techniques with other methods in other fields.

Therefore, this study aims to identify the most effective machine learning algorithms for predicting fluid rheology behaviors by discussing and mapping the input and outputs of various schemes in various fields. The comparisons consider the existing applied machine learning model methods for building a fluid rheological model. The content of this article consists of five parts. First, the methodology for conducting the literature review is discussed. The following parts are the fields applying machine learning, the modeling purposes, the input and output schemes determination, data preparation and preprocessing, and several issues related to the machine learning algorithm, including the training methods and model topologies. The final part is about the conclusion and the possible future research directions.

2 Methodology

This section presents the methodology for surveying the article and an overview of the historical development of the research. The search was conducted using Scopus, Google Scholar, and Web of Science. First, the Scopus search is performed using a combination of words related to machine learning methods in keywords, which are "neural networks," "machine learning," "ANN," "GMDH," "artificial intelligence," "ANFIS," "neuro-fuzzy," "SVR," "support vector," "multilayer perceptron," "random forest," and "ELM." The keywords involving rheological properties of fluids, which are "viscosity," "shear stress," "rheology," "rheological," and "Bingham," were also used. Books and chapters are excluded. The conference proceedings were selected only from peer-reviewed articles. A search using Google Scholar and Web of Science was also conducted using the same keywords to capture works with reliable sources and a high number of citations. The references and the cited articles in the selected documents are carefully examined to check for potentially missed articles.

The number of articles published up to 2024 is shown in Figure 1. The figure is obtained from data based on Scopus with the mentioned keywords and criteria, with articles numbered 2,849 before further filtering. Based on the figure, the application of machine learning methods

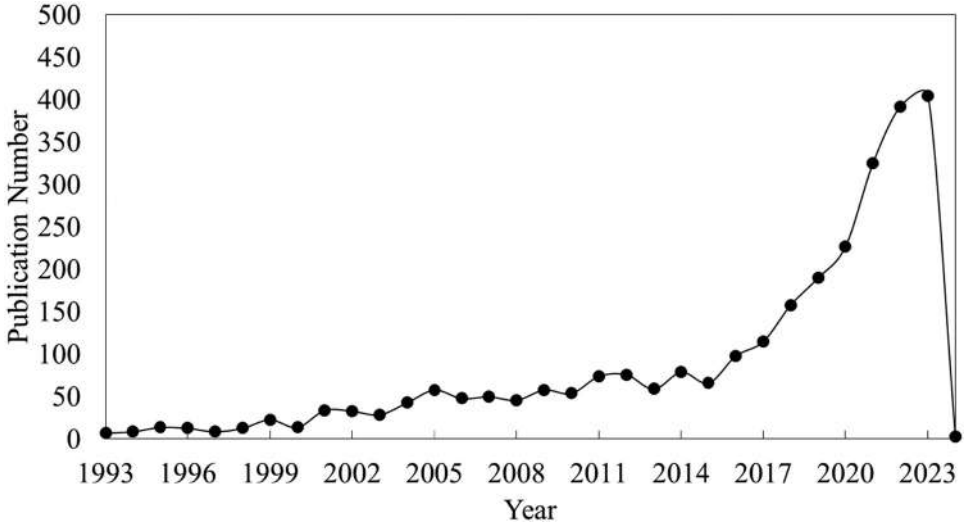

Figure 1: The published article related to machine learning methods, fluid viscosity, and fluid shear stress between 1993 and 2022.

has gained attention in the last two decades, reaching up to about 400 by 2023. The probable reason for the increasing trend is the advances in computational tools and machine learning methods. Those data are then filtered to fit the scope of this study. The exclusion ensures that the review process considers only studies with rheological parameters or variables as the output. The content of the articles was thoroughly inspected to ensure that the article satisfyingly fulfills the criteria, which are machine learning applications in predicting fluid rheological behavior consisting of viscosities, shear stress, and yield stress. After the article is filtered, 113 main articles are selected, which become the main foundation of the survey article. Material with a semi-solid state is also included as long as it satisfies the mentioned criteria. Based on a quick look at the published articles, various applications of diverse machine learning methods across multiple domains and the integration of existing methodologies with approaches from different fields are identified.

Figure 2 shows the general timeline of each major field. The ANN application for predicting petroleum viscosity is the oldest, marked by the application of multilayer perceptron (MLP) for several crude oil data [36], with the latest being the application in drilling fluids by Davoodi *et al.* [37]. The ANN application in food is the second oldest, with sucrose modeling by Bouchard and Granjean [38], followed by smart materials [39] and Mooney viscosity [40] prediction. The applications in nanofluids [41] and ionic liquids [42] can be considered the youngest in 2011. Several other fields that have applied machine learning but only have a few numbers are refrigerants, cement, asphalt, and others.

Viscosity is the majority of predicted parameters, followed by shear stress. Meanwhile, a yield stress variable was first predicted in 2005 for the smart materials applied in dampers [43]. The long history of machine learning applications in various fluids is a baseline for future advancement. For example, besides using ANN, SVR, and RBFNN, a deep neural network is also applied to predicting food rheological properties [44]. The well-known methods in other fields have also been integrated with the existing machine learning methods. An example is the ionic liquids in chemistry for combining the group contribution (GC) method with ANN [45].

3 Simulation schemes

Machine learning's role in predicting rheological behavior relies on setting clear goals for the models and choosing the right input and output variables. Before selecting a machine learning algorithm and configuring the model, it is essential to decide the model's purpose. Crucial to this process is the selection of appropriate inputs and outputs, as incorrect choices can lead to wrong correlations and unnecessarily extended training times. Identifying the usual modeling purpose can be obtained by reviewing

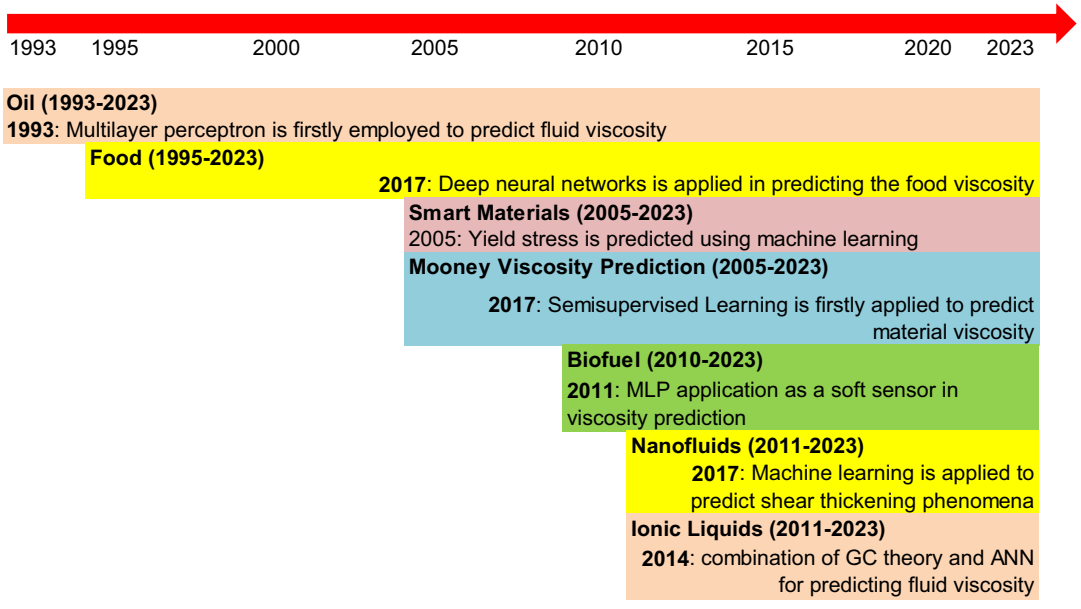

Figure 2: Timeline of the published articles for each field related to rheological properties prediction using machine learning methods.

the input-output schemes of existing works and observing their similarities and differences. Table 2 lists these variables and their predicted outcomes, supported by relevant research. While all output variables are related to rheology, the inputs vary and can include shear rate, temperature, and composition, among others.

Several other works proposed alternatives by providing inverse models. The models treat the required rheological parameters as the inputs, with the composition as the output. This kind of input–output scheme can be considered an inverse modeling scheme. Inverse modeling to predict the material composition based on certain material parameters is still rare, such as in magnetorheological fluids [98], NiMnGa [99], and salts [100].

The usual simulation purposes, based on the observation of Table 2, can be classified into three groups. The first group deals with the efforts to replicate the rheological behavior through the flow curve trend. The shear stress can be utilized to check whether the fluid is Newtonian by plotting shear stress and viscosity η as a function of shear rate. The second group involves the effects of changes in the different operating conditions and compositions of the behaviors. The first and second groups can be considered similar if the shear rate is included as an input. If the shear rate is excluded, the model is classified in the second group. The third group is the viscosity prediction in soft sensor platforms. Meanwhile, the last group is about the rheological parameter distribution prediction as a function of geometrical features.

3.1 Predicting the flow curve correlation with various variables

Predicting the flow curve of a material can be beneficial in identifying the fluid's behavior over a specific shear rate range. Flow curves need at least one shear rate variable as input. The apparent viscosity *vs* shear rate correlation is often used to check whether the fluids have a shear thinning or thickening pattern. Shear thinning shows decreasing viscosity with the increase in shear rate. On the other hand, shear thickening shows an increasing trend, although it will usually reach a peak and then decrease after reaching a specific shear rate value. Most models of non-Newtonian fluids show shear-thinning trends, such as cement slurries [80,81], foods [54], drilling fluids [93], and magnetorheological fluids [18,82]. The work of the ANN application for predicting shear thickening can only be found in the works of Arora *et al.* [86].

Further study about the machine learning application for predicting shear thickening behavior should be explored rather than using phenomenological models [101]. In terms of predicted variables, it is not recommended to predict both shear stress and apparent viscosity using a single model like the study conducted by Dumitriu *et al.* [55] because the predictions would be redundant if the shear rate is involved. The shear stress can be calculated from the apparent viscosity as long as the shear rate is known, and *vice versa*.

From the flow curve, the rheological parameters can be calculated using rheological equations. Figure 3 is

Table 2: Mapping of the predicted rheological parameter or related variables and several functions of machine learning applications

No.	Predicted variables	Machine learning inputs	Selected reviewed studies
1	Viscosity		
	(1) Apparent, relative, and dynamic viscosity in a flow curve	Shear rate and other variables	[21,22,46–62]
	(2) Viscosity-composition correlation	Composition and other variables	[21,22,51–60,38,61–70,39,71,72,41,46–50]
	(3) Soft sensor	Signals from measurement devices and others	[40,73–79]
2	Shear stress		
	(1) Shear stress flow curve	Shear rate and other variables	[12,18,55,80–86]
	(2) Shear stress-composition correlation	Composition and other variables	[55,80,81,84,87]
	(3) Shear stress distribution-geometrical features correlation	Geometry/size and other variables	[19,88–92]
4	Rheological model parameters		
	(1) Yield stress		
	(i) Direct prediction	Compositions, temperature, or other variables	[43,93]
	(ii) Extended calculation	Shear rate and other variables	[80–82,84]
	(2) Plastic viscosity	Compositions or other variables	[43,93,94]
	(3) Power law parameters	Compositions or other variables	[50,70,75,95–97]

illustrated based on the described method in the previous studies, showing the graphical illustration for predicting rheological parameters. The calculation consists of three steps: (a) training the model, (b) the prediction process, and (c) calculating the derived parameters based on rheological equations. For the training process, the data should include the input and the target that will be deployed in the training algorithm and machine learning model. For flow curve prediction, one of the inputs should be the shear rate and the output should be either apparent viscosity or shear stress. In the training process, the user needs to determine the hyperparameters first and choose a suitable machine learning method, which will be discussed further in Section 5.1. The optimization algorithm will tune the parameters within the model. The trained model is then tested to determine its performance when facing unseen data. If the performance is acceptable, it can be deployed in the prediction platform. The shear rate ranges together, and other inputs can then be inputted into the model to predict the apparent viscosity or shear stress range. Based on the obtained flow curve, the derived parameters can be calculated. If the modeled fluid is a non-Newtonian fluid with a yield stress, the Bingham plastic equation can be used [102], formulated as $\tau = \tau_{\text{yield}} + \eta_{\text{plastic}}\dot{\gamma}$, where τ, τ_{yield}, η_{plastic}, and $\dot{\gamma}$ are, respectively, shear stress, yield stress, plastic viscosity, and shear rate. Another possible equation is the power law model [103], formulated as $\tau = k\dot{\gamma}^n$ or $\eta = k\dot{\gamma}^{(n-1)}$, where k and n_p are consistency index and power law exponent, respectively. Other rheological equations can also be employed, such as Herschel Bulkley, biplastic Bingham, and Papanastasiou [104–106]. For the fitting process of the rheological equations to the flow curve, several studies proposed automatic rheological parameter estimation methods using metaheuristic methods, such as particle swarm optimization (PSO) and genetic algorithm (GA) [84,107,108].

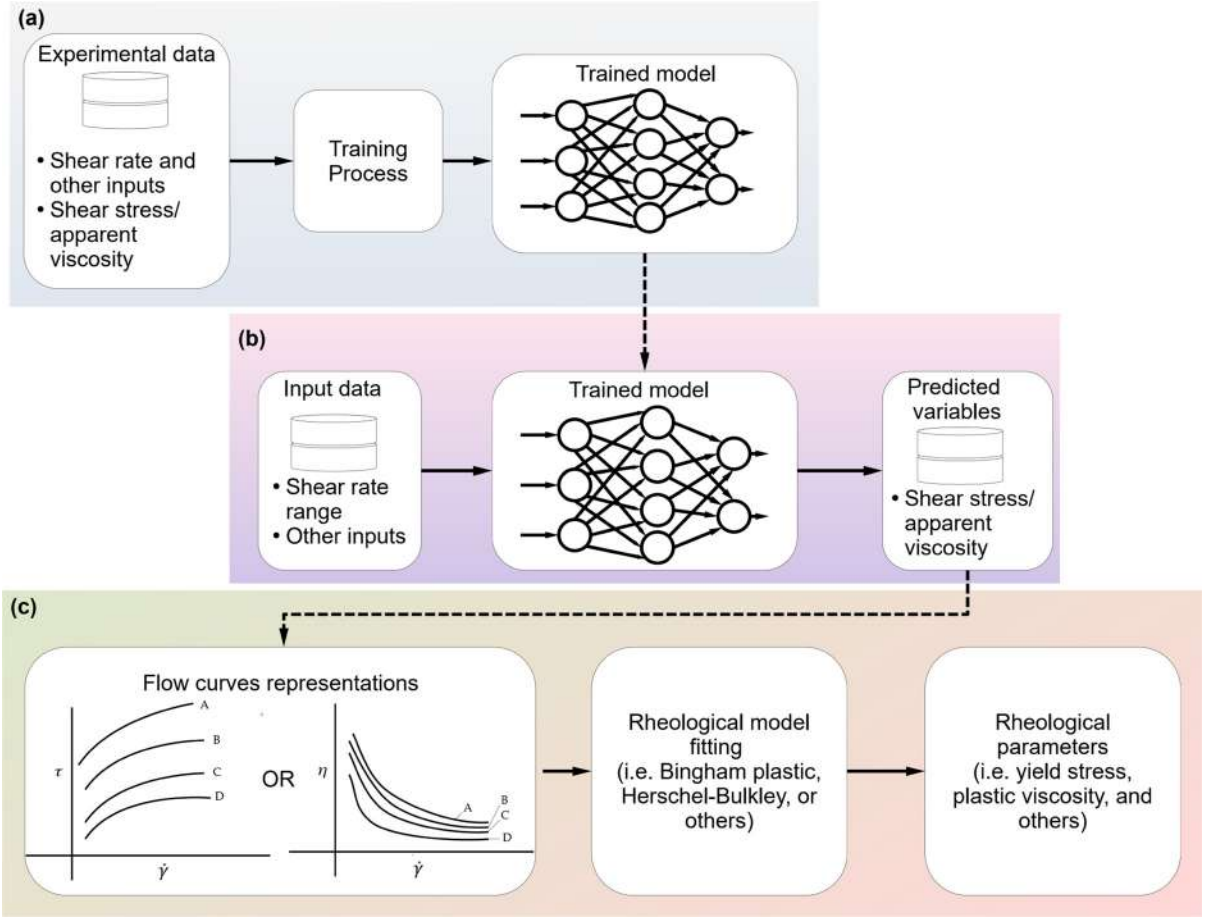

Figure 3: Illustration of an extended calculation of rheological parameter based on the flow curve as the machine learning output.

3.2 Prediction of rheological parameters with various variables and composition

This group considers the fluids' compositions and other variables to represent the material's rheological behavior. This kind of modeling scheme can support the material fabrication or characterization process. If the correlation between inputs and outputs can be identified using machine learning, the post-processing activity will be easier to perform. The input sensitivity analysis can be applied to determine which variable has the most impact on the rheological behavior of materials, such as in Torkar *et al.* [95] and Fayazi *et al.* [109]. Nanofluids can be considered the most advanced field for the application of machine learning in rheology in the form of dynamic viscosity predictions. Thermal conductivity is also predicted along the dynamic viscosity [110–113]. Composition optimization to search for the best combination for a particular application can also be one of the possible utilizations. Because of the variety of probable materials, the challenges of this group's developments vary, such as the vast possibility of the inputs and output configurations, the data training–testing division methods, and others. Another challenge is that the predicted variables are associated with other variables, such as the thermal properties [111,113,114]. Table 2 shows that the studies included in this group are the most commonly used in simulation schemes.

3.3 Supporting measurement and manufacturing system (soft sensor)

This group was intended to deploy machine learning methods as soft sensors to predict fluid rheological properties. Practical applications usually involve measurement signals as inputs. The signal can originate from the devices or measurement systems where the fluid is applied or processed. One of the objectives is to determine variables that are not easy to measure or variables that need additional instrumentation to measure. For example, in predicting the viscosity of a device, it is not always simple to measure the fluid's temperature, pressure, and various operating conditions. Therefore, the viscosity needs to be predicted based on the device's working condition or the previous calibration or observation results. For example, Alabi and Williamson [76] indicate the viscosity of the kraft black liquor in a centrifugal pump using the pump torque, flow rate, shaft speed, and the pump's mechanical status. Padmavati *et al.* [40] used device and sensor signals of agitators and reactors to predict the processed fluid viscosity. This method can also be a solution to overcome the difficulty in estimating the Mooney viscosity in rubber processing, as discussed by Zheng *et al.* [77,78] and Jin *et al.* [79].

This method can also be employed to calibrate a measurement device [115]. For example, in biofuel, the neural network model was applied to predict the kinematic viscosity based on the various spectral values of the near-infrared spectroscopy [73]. Ahadian *et al.* [74] also used the capillary rise time of liquids to estimate their surface tension and viscosity.

3.4 Prediction of rheological parameter distribution

The estimation of shear stress and viscosity distribution in a flow channel or tunnel can be a challenging process. Although computational fluid dynamics can be a solution, the simulations require considerable computing time, especially when various geometries are involved. If multiple sensors are available, making predictions using machine learning can be one of the alternatives. The geometrical features, topological features, or parameter sizes are the main inputs, followed by other fluid movement variables, such as Reynold numbers [19].

4 Data preparation and preprocessing

Data preparation for machine learning in rheological modeling involves ensuring the reliability of measurements and includes activities such as data cleaning, removing outliers, averaging repeated measurements, and normalizing data. The choice between logarithmic or linear scale normalization depends on the shear rate range, and the division of data into training and testing sets is crucial to validate model performance, with options like 70-15-15 or ten-fold cross-validation techniques for improved results.

The data should be reliable in terms of the measurement system, uncertainties, materials manufacturer, and preprocessing. Table 3 shows the common activities related to data preparation, including removing outliers, normalizing methods, and dividing training and testing data. Several works eliminate the outlier first before further processing the data [40,116]. If training data consist of several measurement points in the same configuration in a

controlled environment (such as a rheometer), the data should be averaged first [67,73,117]. Data normalization is also an essential step to ensure the generalization of the produced models. Normalization can be carried out for input and output to standardize input ranges. The minimum and maximum normalized data range (a and b, respectively) can be any number, such as [0,1] or [−1,1], or [−0.9,0.9] or others. This normalization process can ensure the data to be simple and standardized. Most studies employ linear normalization. Therefore, if the input has a logarithmic relationship with the output, then normalization is employed for the logarithmic value of the raw data [118,119], which affects the trained model performance [118]. Other normalization methods include the regularization, standardization, or z-score normalization by considering the raw data mean (x_{mean}) and standard deviation (x_{std}). The advantage of this method is that the outlier can be handled properly and is well-suited for data with Gaussian or normal distribution. However, this method is unable to ensure the data to be within an exact range. Based on the available normalization method, because the character of each input is diverse, each input must be treated differently. For example, the shear rate range can be normalized using a logarithmic scale, while other inputs are normalized using a linear scale, as discussed in the work by Bahiuddin *et al.* [18].

The shear rate for predicting flow curves can be normalized using a logarithmic or linear scale based on the shear rate range of the training data, as shown in Table 3. Figure 4 shows an illustration of logarithmic or linear scale normalization for shear rate and viscosity-based flow curves. If the shear rate range as input is wide, covering the region with a gradually changing gradient, the logarithmic scale normalization can be a suitable choice. Meanwhile, linear scale normalization can be used when the shear rate range covers a relatively steady gradient or possesses a relatively constant Bingham model based on plastic viscosity. The logarithmic scale normalization is suitable not only for shear rate inputs but also for normalizing the viscosity as output [120].

The testing and training data selection is another important step in validating a model's performance. The common method to determine the training and testing is to split or randomly split the data based on the predetermined varying percentages, as shown in Table 3. On several platforms, the data are divided into training, validation, and testing data, especially in the backpropagation (BP)-based training algorithm. Training and validation data are input for the training process. Hence, the arrangement can be 70% for training, 15% for validation, and 15% for testing (also denoted as 70-15-15), or, in Table 3, mentioned as 85%:15%. If the model shows high accuracy for the training case but low accuracy for the testing case, the condition will yield the so-called overfitting phenomenon. Hence, the model needs to be reevaluated. Another unusual scenario is when the model has better accuracy in the testing data compared to the training data. This scenario is uncommon because the

Table 3: Data preparation and preprocessing activities

Activity	Remarks	Selected related studies
Preparation	Removing outliers	[40,78,79,116]
	The training data are the average values of the repeated measurement data	[67,73,117]
	Pearson correlation approach for selecting the independent variables	[63]
Normalization	Linear normalization/min–max normalization between:	
	– 0.01 and 0.9	[63]
	– −1 and 1	[121–123]
	– 0.05 and 0.95	[95]
	– 0 and 1	[58,60]
	Logarithmic scale/normalization for shear rate and linear normalization for other inputs, suitable for predicting flow curve	[12,18,84,119,120]
	Regularization/standardization/z-score normalization, suitable for data with Gaussian distribution	[76]
Division of data	Percentage of training and testing data;training data are inputted into training algorithms that can be used for the training and validation process	
	80%:20% or (randomly split)	[63,124]
	60%:40% (Randomly split)	[116]
	70%:30% (Randomly split)	[124,125]
	75%:25% (Randomly split)	[47,126]
	85%:15% (Randomly split)	[82,127]
	90%:10% (Randomly split)	[128]
	Test data are manually determined	[18,60,86,119]

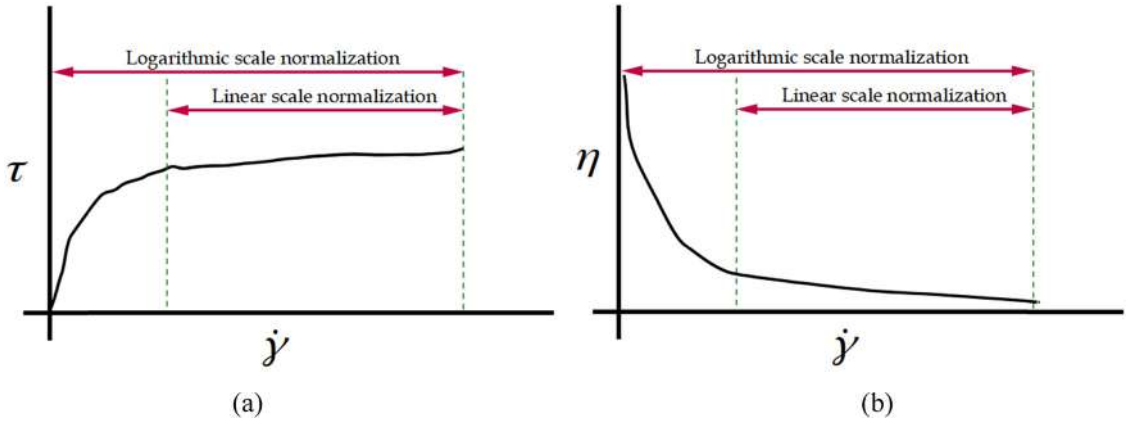

Figure 4: The alternative normalization methods based on the training data shear rate range for the flow curve based on (a) shear stress and (b) apparent viscosity.

testing data is usually less accurate than the training data. Although it could show a good model performance, it may also indicate that the testing data is not well determined. In other words, the testing data fails to identify how well the model performs on the new datasets [121]. Therefore, to solve this problem, different datasets can be selected manually [18,60,119]. The ten-fold cross-validation technique can also be an alternative to improve the model's performance further [73]. The amount of training and testing data is also a critical factor in developing the models. The amount of training data should be enough to represent the behavior of the fluids. If the modeled rheological behavior contains a few variations and a simple relationship, fewer data can be sufficient.

5 Machine learning methods selection

Choosing machine learning methods for fluid rheology involves decisions on model topology, training algorithms, and optimization techniques. Common models include feed-forward neural networks (FFNNs) with backpropagation (BP-ANN) or ELM. BP-ANN is a baseline, while ELM offers faster training. Other methods, such as ANFIS, RBFNN, SVR, and PNN, are also considered. Section 5 provides a concise overview of these models, comparing their strengths and weaknesses in predicting fluid rheology parameters. It also briefly touches on the potential of semi-supervised learning and the necessity of metaheuristic optimization for model topology. It also emphasizes the importance of reproducibility in machine learning research through a proposed checklist and the creation of a comprehensive database.

5.1 Model topologies and training algorithms

Various aspects need to be considered when selecting machine learning methods, such as the model topology or structure, training algorithm, and platform. Table 4 shows the hyperparameters, advantages, and disadvantages of the common methods for predicting variables and parameters related to fluids rheology. FFNN is the commonly employed model topology. FFNN can be trained using a BP algorithm known as BP-ANN or MLP. BP-ANN, as the classic and popular machine learning algorithm, is usually employed as the main proposed program and benchmarking method. The training algorithm can be selected from various methods. The most well-known approach is the Levenberg–Marquardt (LM) because it often shows the most accurate and rapid training time [48]. However, LM tends to have a high possibility of being trapped at a local solution. The hyperparameters include the layer number and the hidden neuron number in each layer. The layer can also be selected from one or two hidden layers, depending on whether one hidden layer has acceptable accuracy [48,63].

In terms of structure complexity, FFNN can be built from single or multiple hidden layers. A more complex topology can lead to a longer training time. Therefore, the less-hidden layer is preferable, considering that almost all fluid rheology cases can be solved using FFNN with one hidden layer. The hidden neuron number is usually set at fewer than 20, such as 12 [75], 15 [63], 6 [129], and 9 [130], to achieve acceptable accuracy in a simple case. In terms of the activation functions, the best function can be different from one case to another, depending on the datasets. FFNN can also be trained using ELM, which has the advantage of a faster training time and better generalization [18,83,84,90,119,120].

Table 4: Various common supervised learning algorithms are applied for predicting related parameters and variables in fluids rheology

Model topology	Training algorithm	Hyperparameters	Remarks (pros [+] and cons [−])	Selected related studies
FFNN (the topology can be a single or multi-hidden layer)	Backpropagation (also called BP-ANN or MLP) and LM	Number of hidden layers, number of neurons in each hidden layer, and activation functions	(+) The most popular method. Various platforms have accommodated the method (+) If the hyperparameters are carefully tuned, the model can accommodate various fluid rheological behaviors with relatively low complexity (−) The accuracy tends to be trapped in local solutions	[48,63,68,141]
	ELM		(+) Faster training time and more generalized solutions than BP-ANN (−) Unclear justification for the random assignment of the weighting inputs	[90,119,120]
ANFIS		Number of membership functions and type of membership functions	(+) In several cases, it has faster training time and higher accuracy than BP-ANN (+) Fewer adjustable parameters than FFNN and a well-structured knowledge presentation (−) If one of the training algorithms is BP training, there is a probable local solution	[60,68]
RBFNN		Number, center, width type of RBF	(+) Simple training algorithms have fewer adjustable parameters than FFNN and ANFIS (+) Adopting BP-ANN's ability to recognize the pattern within a data (−) It needs a relatively large hidden node number to fulfill the targeted accuracy (−) The possibility of the local solution after reaching a certain value of the hidden node number (−) In several cases, the accuracy is not better than ANFIS and FFNN	[60,63,131,142]
SVR and LS-SVR		Kernel type and parameters, regularization parameter, and epsilon	(+) Fast training time and best for localization results (−) Not suitable for large datasets	[63,82,120]
GMDH PNN		Degree of polynomial	(+) Several works claimed that PNN is less complex than the FFNN structures (+) The model equation is quite similar to the classic polynomial method (−) After comparing with other machine learning, the PNN performance is less accurate (−) Possibility of low generalization capability	[143,144]
FFNN with BP-ANN or FFNN with ELM or RBFNN or PNN combined with metaheuristic methods	GA or PSO for searching for the optimum model topology	Hyperparameters from the original model added with the optimization algorithm parameters	To search for the best-hidden node numbers in FFNN, the best-hidden node numbers, and spread values for RBFNN (+) The hyperparameters can be tuned automatically	[67,83,125]

(Continued)

Table 4: *Continued*

Model topology	Training algorithm	Hyperparameters	Remarks (pros [+] and cons [–])	Selected related studies
Combination of several machine learning algorithms, committee machine learning, and ensemble machine learning			(+) Avoid trial and error determination of the hyperparameters (+) Can have better accuracy than other algorithms, such as GA-PNN is better than ANFIS, and GA-RBFNN is better than SVR gene expression programming (–) Additional duration of the training process (+) High accuracy for fluid rheology cases (–) Contains multiple machine learning-based models that can be relatively too complex and have a longer training duration	[15,78,145]

Other alternative machine learning methods are ANFIS, SVR, PNN, and RBFNN. ANFIS is another well-known algorithm with comparable accuracy and faster training time than BP-ANN. This method is also known for its more interpretable nature compared to other black box models. In several comparative works [54,89,125], the prediction performance is better than that of BP-ANN. For kernel-based methods, SVR and RBFNN have the potential to capture nonlinear patterns in data. SVR has shown its accuracy in several works with BP-ANN [82]. However, SVR is less popular because it is quite challenging to tune the hyperparameters and can be hard to interpret while employing nonlinear kernels.

On the other hand, despite the RBFNN potential because of the fewer adjustable parameters compared to BP-ANN, several comparative works show its performance lags behind or, at most, is comparable with other machine learning algorithms [15,60,63,116,131]. PNN is another form of neural network with polynomial equations as the activation functions. While this method shows its acceptable performance in several works [67], the polynomial has several potential problems, such as interpretability and overfitting. An automatic feature selection algorithm called GMDH was also proposed to tune PNN in several works [124,132]. To overcome the overfitting possibility, more optimization algorithms, such as GAs, need to be added to achieve acceptable accuracy [21]. If the computational cost is not a priority and the parameters cannot be tuned properly, GMDH PNN can be an alternative for predicting the fluid rheological behavior.

The common parameters to be evaluated for measuring the performances of various algorithms are the accuracy of the training case, testing cases, training time, and testing time. While the training time represents the complexity of the training algorithm and model structure, the testing time represents the complexity of the model structure. Compared with the experimental data, the accuracy and error represent the model's performance. While the accuracy of the training is utilized in the training process, the testing accuracy is crucial to determine the model performance for unlearned cases. Some articles have shown a very small error for the training but not for the testing, such as in the work by Al-Marhoun *et al.* [116]. The statistical parameters can be in the form of either mean squared error (MSE), mean absolute percentage error (MAPE), or coefficient of determination (R^2).

Several selected works are provided in Table 5, containing various examples of machine learning methods. From those cases, the complexity of a case can be described based on the data number, the number of input variables, and the model nonlinearity. For example, RBFNN is usually not superior when compared with other methods because it does not match the data in a work that has a high R^2

Table 5: Selected work and its statistical parameters for measuring the model performances

Authors	Fluids	Methods	Inputs	Outputs	Data number	Training	Testing
Hemmat Esfe *et al.* [22]	Multi-walled carbon nanotubes-ZnO/5W50 nanolubricant	BP-ANN	Temperature (T), particle diameter, particle volume concentration	k_{T}, η	N/A	R^2: 0.9998057	N/A
Razi *et al.* [62]	Water-based drilling fluids	BP-ANN	Shear rate ($\dot{\gamma}$), T, weight percentage	η_{plastic}	468	R^2: 0.976 MSE: 0.012	MSE: 0.014
Dargahi-Zarandi *et al.* [143]	Gas/vapor of hydrocarbon fluids	Hybrid GMDH ANN	Molecular weight, reduced pressure, reduced temperature, and density (ρ)	η	3,819	R^2: 0.997 MAPE: 3.44%	MAPE: 3.45%
Tatar *et al.* [133]	Heavy oil	RBFNN	T, weight percentage (w_{kerosene})	η	80	R^2: 0.999935	R^2: 0.999893
Aminian and ZareNezhad [125]	Biodiesels and blends	ANFIS	T, weight percentage($w_{biodiesel}$), the average number of carbon atoms	η	527	R^2: 0.9980	R^2: 0.9932
Specht *et al.* [146]	Asphalt–rubber	BP-ANN	The rubber content, rubber particle size, mixing duration, and temperature	η	1,792	R^2: 1.000	N/A
Ramzi *et al.* [54]	Iranian honey	ANFIS	Water content, T, and $\dot{\gamma}$	η	N/A	R^2: 0.999	R^2: 0.999
Kang *et al.* [120]	Ionic liquids	ELM	Molecular descriptors (Sσ-profile) $S_{c1\text{-}5}$ and $S_{A\ 1\text{-}6}$, T, pressure(P)	η	1,502	R^2: 0.985	R^2: 0.928
Bahiuddin *et al.* [119]	MR greases	ELM	$\dot{\gamma}$, magnetic field density (B), carbonyl-iron powder weight percentage (w_{CIP})	τ	900	R^2: 1.000	R^2: 0.999
Zhi *et al.* [131]	Six pure refrigerants	ANFIS	P, T, ρ	η	1,089	R^2: 0.9998 MAPE: 2.96%	R^2: 0.9995 MAPE: 4.15
Arora *et al.* [86]	Shear thickening fluids	BP-ANN	T, $\dot{\gamma}$	τ	N/A	R^2: 0.976	R^2: 0.974

value [133]. After careful review, the work only consists of 80 data, which is a relatively low number of data.

More advanced models can be employed to predict the rheological properties. The examples can be deep learning algorithms, such as convolutional neural networks (CNN) [134], extreme gradient boosting and random forest based on the gated recurrent unit [135,136], and recurrent neural networks [137,138]. The CNN has been applied to predict the creep modulus of cement paste [139]. Cement paste, especially in the context of its viscoelastic properties and time-dependent behavior, can exhibit some fluid-like characteristics, but it is not a traditional fluid. Extreme gradient boosting and random forest were employed to predict soft clays [140]. Soft, sensitive clay may exhibit solid-like properties. However, if the clay is subjected to stress or disturbance, it can undergo significant changes in its strength and behavior, resembling a fluid. This phenomenon is often referred to as quick clay behavior.

5.2 Metaheuristic methods for model topology optimization

Each model topology requires its own parameters to be tuned. The parameters that need to be predetermined by the user are called hyperparameters. The hyperparameters include the layers, the hidden node number, the activation function, and others, depending on the selected topology in the machine learning method employed. Metaheuristic optimization methods can be applied to search for the best-hidden node number automatically, such as PSO or GA. The GA is also applicable for RBFNN to tune the spread value [147] and GMDH to search for the best configuration [132]. The metaheuristic method has shown its capability to improve the model performance by finding the best configuration of the hidden node number in the network [60]. The usual drawback of metaheuristic method applications is the longer training time. Several examples of topology optimization are shown in Table 6.

5.3 Semi-supervised and unsupervised learning necessity

The general training methods are supervised and unsupervised, with a difference in terms of the employed labeled or unlabeled data in the training process. Almost all of the discussed methods are supervised algorithms that consider the model output or labeled data. On the other hand, unlabeled data can be valuable in viscosity prediction cases, especially in the rubber mixing process [77,78,149]. Recently, in the manufacturing industry, various measurements originating from the control system have been stored on a centralized server as a historical database. It is challenging to manually identify which data are relevant to the changes in certain product viscosity. Furthermore, the data, such as temperature distributions, pictures, or videos taken from the manufacturing process, can be considered unstructured. Therefore, the data can be treated as unlabeled and input into machine learning together with labeled data to check various possibilities, such as clustering or other purposes. By considering both labeled and unlabeled data for the training process, the training algorithm can be regarded as semi-supervised machine learning.

Several studies conducted semi-supervised learning for the prediction of viscosity in the rubber mixing process [77]. Incorporating semi-supervised learning in the rubber mixing process allows for the effective use of both labeled and unlabeled data. This approach, particularly with clustering algorithms, can enhance the prediction of viscosity and help identify relevant patterns in the unlabeled data. Given the limited application of this method in rheological fluids, there is significant potential for further exploration and development. ELM and its variants have also been used because of the shorter training time characteristics [77]. For example, the just-in-time regularized ELM (JRELM) has about a 40-s difference with just-in-time SVR [77,79]. The use of algorithms like JRELM, which offers time efficiency, suggests that semi-supervised learning can be optimized for industrial applications where timely data processing is crucial. The broader adoption of this method could lead to more

Table 6: The applied topology optimization methods

No.	Topology	Optimization algorithm	Tuned parameters	Ref.
1	GMDH-type PNN	GA	Hidden layers and bias coefficients	[132]
2	FFNNs	GA	Hidden layer neuron number	[54]
3	RBFNN	GA	The maximum value of the number of neurons and spread	[15,133]
4	RBFNN	PSO	The maximum value of the number of neurons and spread	[15]
5	ANFIS	PSO	Gaussian membership function	[148]

accurate and efficient rheological analysis in various industrial contexts.

5.4 Explainable AI

Machine learning models, particularly in complex domains like fluid rheology, often face limitations in interpretability. Traditional machine learning models, while powerful in prediction, are commonly seen as "black boxes," providing little insight into the reasoning behind their outputs. This lack of transparency can be a significant barrier, especially in fields where understanding the underlying phenomena is as crucial as accurate predictions. Explainable AI (XAI) emerges as a potential solution to this challenge. By making AI models more interpretable, XAI allows users to understand the decision-making process of these models. For instance, the use of deep learning for predicting fluid viscosity, as seen in the PfAbNet-viscosity model, becomes more interpretable through feature attribution analysis [150]. This analysis reveals how specific biophysical properties influence the model's predictions.

Similarly, Shapley Additive Explanations (SHAP) calculations are being used to identify the impact of each input on the prediction of viscosity and surface tension in ionic liquids, aiming to elucidate the decision-making process of the trained machine learning model [151]. The potential of XAI is particularly important for predicting fluid viscosity and rheology, where understanding the physical principles underlying the predictions is crucial. Despite its importance, the application of XAI in this field is still relatively rare, indicating a significant opportunity for further exploration and development across various domains.

5.5 Reproducibility

Reproducibility is an important part of machine learning for future improvement and to ensure the validity of the proposed method [152]. This issue becomes more apparent, considering these studies involve at least two different fields, such as computer science and fluid rheology. Several works have not included important details to enable the reproduction of the applied machine learning methods. Meanwhile, although some works have tried to compare their proposed models with the previously proposed methods, the benchmarked models have not been described in detail, especially regarding the training settings and topology. Therefore, a checklist is presented in Table 7, showing the information an article needs to provide to ensure reproducibility.

A database of fluids for further usage of machine learning can support the future reproducibility of the proposed works. The database can be a collection of the training data or the models obtained in each case. Therefore, the models should be downloadable to enable further applications. A work in ionic liquids has started the collection of the dataset in various instances to perform a prediction when an unlearned composition is introduced [153].

Table 7: The suggested available information to maintain the reproducibility in a research article about rheological parameter prediction using machine learning

Steps	The suggested available information
Data acquisition	• Materials composition, manufacturer, preparation, and fabrication • Characterization procedures and instrument details • Citation is needed if the data is taken from other sources • The data range of the inputs and outputs • Data distribution (if relevant)
Data preprocessing	• Normalization method • Data selection from repeated experimental data • Outlier removal • Division methods of the training and testing data
Training process	• Simulation platforms, such as Matlab, Python, Weka, Julia, or R • Source of the code for the training algorithm and the modification details (if any) • Training time (if relevant)
Model topology	• Input and output description • Detailed setting of the obtained topology/structure (such as layer number, hidden neuron number, and activation function, depending on the selected network topology)
Post-processing	• Extended calculation of other derived parameters (if relevant) • Model performances or accuracies of the training and testing data

6 Conclusions and future research directions

This review explores the use of various machine learning methods in modeling fluid rheology. It covers a range of behaviors and predictive techniques, including flow curve modeling and different input–output schemes for fluid characterization. The maturity of these methods in several applications is highlighted, with a focus on flow curve modeling and alternative schemes for fluid characterization. The review indicates that the choice of the most effective machine learning model depends on factors like case complexity. Simple models like ANN, ELM, and SVR are adequate for scenarios with fewer variables and data points and are applicable in areas like nanofluids and smart materials. However, complex data or behaviors require more advanced hybrid algorithms. These are particularly useful in applications like ionic liquids, drilling fluid characterization, and polymerization.

The conclusion of the review emphasizes the significance of training time in machine learning applications, suggesting algorithms like ELM for situations where rapid processing is crucial. It specifically recommends time-dependent methods like recurrent neural networks and long short term memory for modeling complex behaviors in non-Newtonian fluids, where temporal dynamics are essential. Adaptive algorithms are highlighted as valuable for processes that undergo frequent changes. Moreover, the review points out the relevance of unsupervised algorithms in handling unlabeled data, which is particularly pertinent in industrial settings where data from material processing might not be precategorized.

The survey acknowledges the potential for further exploration in this field, particularly in developing models for linking microstructure to rheological properties using deep learning. The possibility of semi-supervised or unsupervised machine learning methods, especially in the polymer industry, and the concept of inverse modeling for predicting compositions are also highlighted. The review concludes with the possibility of employing explainable AI to make machine learning models more interpretable.

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