ACTUAL SHEAR RATE PREDICTION ASSOCIATED WITH WALL SLIP PHENOMENON USING RADIAL BASIS FUNCTION NETWORK

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ABSTRACT

Wall slip can be defined as a phenomenon where the particles in a suspension move away from the wall boundary, leaving a thin liquid-rich layer adjacent to the boundary. Such a phenomenon may induce a significant impact on rheological measurements, particularly on viscosity, shear stress, and shear rate. Suspension has wide applications such as food processing, personal care products, pharmaceuticals, paints, medicine, and agrochemicals. The traditional technique for the actual shear rate prediction is challenging yet difficult and non-favourable from the perspective of time and cost-effectiveness. Therefore, the development of a mathematical computational model that can perform the prediction task with an acceptable level of accuracy is highly needed. Since radial basis function network (RBFN) can perform input-output mapping in a highly accurate manner, both approaches are employed to generate the actual shear rate prediction model. Through the model evaluation using a series of statistical analyses, it was found that RBFN model V is the best model as it shows the highest coefficient of determination (0.9998), lowest mean squared error (0.001058) and root mean squared error (0.001447), most negative Akaike information criterion (-18426.5) and Bayesian information criterion (-18415.5), and the smallest percentage error. The developed model can serve as an alternative tool to predict the actual shear rate of a suspension under an experimental-less condition.

Keywords: Actual Shear Rate, Radial Basis Function Network, Rheology, Suspension, Wall slip

1.0 INTRODUCTION

Rheology can be defined as a branch of physics that deals with the flow of matter. There are several interesting rheology-related phenomena such as shear-induced migration, pattern formation, and wall slip. Among all, wall slip is the main focus of this research study.

Wall slip is a scenario that occurs in a two-phase or multiphase flow system where the suspended particles in the suspension migrate away from the solid wall boundaries, leaving a thin liquid-rich layer adjacent to the wall. Such a low-viscous layer induces a lubricant effect which enables fluid particles to flow over the boundaries easily (Alshahrani *et al.*, 2022; Barnes, 1995; Hatzikiriakos, 2015; Ponalagusamy, 2017). Under such circumstances, the rheological measurements, i.e. viscosity, shear rate, and shear stress, can be significantly affected. There may be several reasons behind the occurrence of wall slip, such as chemical, gravitational, steric, hydrodynamic, and viscoelastic forces (Ahuja and Singh, 2009; Barnes, 1995; Gudala, *et al.*, 2021).

As reported by Martin *et al*. (2008), slip as well as an apparent slip of suspension near solid surfaces is quite common in food products. In addition, the wall slip effect may be significant until dominating the perceived behaviour of a product. Under this condition, it becomes a challenging task to perform certain operations for industrial purposes, especially in manufacturing, transportation and designing of materials (Barnes, 2004; Raja *et al.*, 2021; Singh *et al.*, 2023; Wu *et al.*, 2022). For example, the operation of the pumping process for slippery materials cannot be optimised because the wall slip cannot be simply neglected in the selection of a suitable pump. Hence, it is essential to have a study on wall slip and develop an appropriate approach to ease the user while dealing with wall slip issues.

A series of laboratory experiments have been conducted to investigate the factors affecting wall slip. First of all, a range of previous research has proposed that the wall slip is appreciably affected by the size of suspended particles in suspension. As reported by Gulmus and Yilmazer (2005), wall slip velocity increases when the particle size increases due to the steric hindrance effect. The observation is in agreement with the comparison of findings between Jana *et al*. (1995) and Ahuja and Singh (2009). Concentration is another factor that influences wall slip. Several groups of researchers have carried out the research studies based on their preferences. Chen *et al*. (2008) claimed that in slurry flow, wall slip velocity shows an increasing trend with the decreases of volumetric concentration. A similar finding was also found in Chin *et al*. (2018a).

In addition, temperature has been identified as the third key element, playing a significant role in wall slip analysis. Wall slip can be originated from the thermal effects near the wall boundary (Barnes, 1995; Malkin *et al.,* 1993; Valdez *et al.,* 1995). Such a phenomenon can be explained by the Kinetic Theory. The fact was further supported by Soltani and Yilmazer (1998) who reported that the increasing temperature will lead to the increase of wall slip velocity values.

Currently, it is a challenging task to determine the actual shear rate for suspension that experienced wall slip as it requires several laboratory datasets. In terms of time and cost, it is non-effective. Therefore, a mathematical model which can mimic the rheological actual shear rate under wall slip condition with an acceptable level of accuracy is essential. In this digital era, the application of artificial intelligence (AI) has become the main trend in various fields and industries. Radial basis function network (RBFN) is one of the popular AI approaches that have been widely applied for problem-solving purposes (Du *et al.,* 2006; González-Camacho *et al.,* 2012; Hannan *et al.,* 2010; Khamis *et al.,* 2018; Venkatesan and Anitha, 2006). Since the approach has shown a relatively outstanding result while applied in different fields of study, it motivates the authors to develop the actual shear rate prediction model using the RBFN approach.

In this research study, the main target is to propose a computational mathematical model that can serve as an alternative to the rheological actual shear rate prediction. A series of RBFN models are developed and trained using all of the critical elements that affect the wall slip (Chin *et al.,* 2018a). The developed models are then evaluated and compared in terms of their appropriateness through statistical analyses. The novelty of the research study is the introduction of AI approaches into the rheological application which allows the users to predict the actual shear rate of a suspension under an experimental-less condition. The basic concept of this research study is shown in Figure 1.

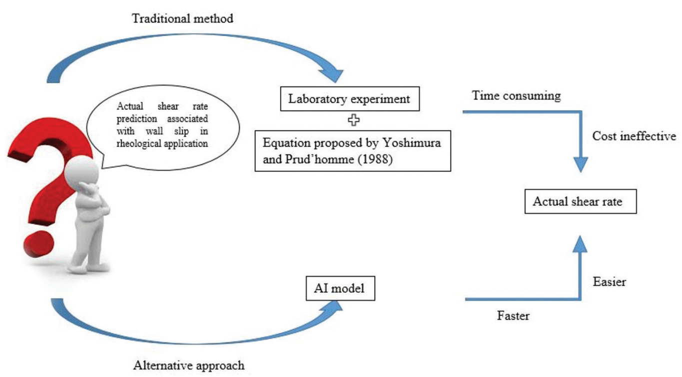

Figure 1: Overall Concept of the Research Study

2.0 MATERIALS AND METHODS

2.1 Data Collection

Laboratory rheological tests were carried out to collect a series of raw data as a preliminary preparation for the AI model development. The tested samples were mixed using poly (methyl) methacrylate (PMMA) and glycerine.

To ensure the credibility of the experiment data, the standard procedures were strictly followed (Ahuja and Singh, 2009; Chin *et al.,* 2018a; Yoshimura and Prud'homme, 1988). First of all, the density of both PMMA particles and glycerine was 1300 kg/m^3 (Chin *et al.,* 2018a; Shaliza *et al.,* 2015). The rationale behind this was to yield a neutrally buoyant suspension. In addition, the density differences might lead to a creaming effect, inducing an adverse impact on the result accuracy. Next, Ahuja and Singh (2009) and Buscall *et al.* (1993) stated that the impact on the viscosity might be significant even if there was only a small mismatch of particle fraction in suspension. Thus, it was important to ensure that the suspensions were mixed with an exact ratio according to the desired volumetric concentration.

The rheological tests were conducted using rheometer equipped with a parallel plate of diameter size 50 mm under two different gap heights of 0.75 mm and 1.0 mm respectively. Several experiment conditions were set, where the tests were run under six different volumetric concentrations (40%, 45%, 48%, 50%, 52%, and 55%), five different temperatures (15°C, 25°C, 35°C, 45°C and 55°C) and three different particle sizes (18 μm, 75.3 μm and 195.5 μm).

2.2 Radial Basis Function Network (RBFN)

A radial basis function network (RBFN) is a variant of the three-layer feedforward neural network. It consists of input layer, hidden layer and output layer where each layer has its role. The input layer, which corresponds to the inputs, is used to link the network to its environment, the hidden layer contains several RBF activation nodes which apply a nonlinear transformation to the input variables, while the output layer is mainly for the presentation of the final output.

The feature that distinguishes the RBFN from the traditional neural networks is its activation function. In RBFN, the activation function in the hidden layer is conventionally implemented as a Gaussian function (Eq. 1).

$$radbas(n) = e^{-n^2} \tag{1}$$

The raw experimental data were grouped into training and testing sets with a ratio of 80% to 20%. The RBFN models were constructed and trained by applying shear stress, volumetric concentration, temperature and particle size as inputs while the actual shear rate was kept as the output. The activation function was set as the Gaussian function. One of the challenges in constructing the architecture of RBFN is the determination of spread constant value. Therefore, a series of RBFN was developed using a wide range of spread constant from 0.0001 to 50 using the trial-and-error method. The performance of each model was then evaluated. The architecture design of RBFN is shown in Figure 2.

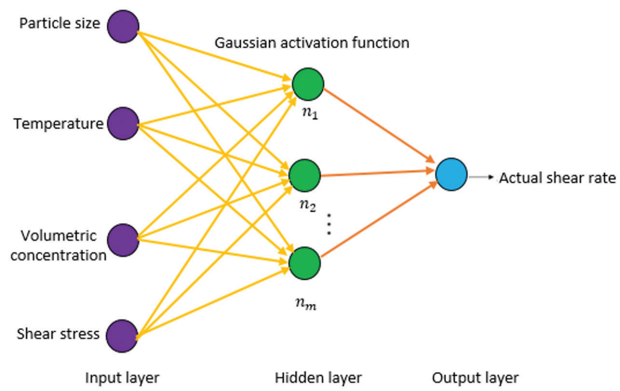

Figure 2: Architecture of RBFN

2.3 Statistical Analyses

The performance of all the developed AI models was examined using a series of statistical analyses, i.e. coefficient of determination (R^2), mean absolute error (MAE), root mean squared error (RMSE), percentage error (% error), Akaike information criterion (AIC) and Bayesian information criterion (BIC), to determine their appropriateness in predicting the actual shear rate for suspension under wall slip condition (Chin *et al.,* 2019).

$$R^2 = \left(\frac{n\sum x_i y_i - \sum x_i \sum y_i}{\sqrt{n\sum x_i^2 - (\sum x_i)^2}\sqrt{n\sum y_i^2 - (\sum y_i)^2}}\right)^2 \quad (2)$$

$$\text{MAE} = \frac{\sum|y_i - x_i|}{n} \quad (3)$$

$$\text{RMSE} = \sqrt{\frac{1}{n}\sum(y_i - x_i)^2} \quad (4)$$

$$\text{Percentage error} = \frac{|True\ value - Predicted\ value|}{True\ value} \times 100\% \quad (5)$$

$$\text{AIC} = -2\log L + 2\text{K} \quad (6)$$

$$-2\log L = n(\log 2\pi + 1 + \log\frac{RSS}{n}) \quad (7)$$

$$\text{BIC} = -2\log L + \text{K}\log n \quad (8)$$

where n is the number of data pairs, x is the observed variable, y is the predicted variable, K is the number of model parameters (the number of variables in the model plus the intercept), L is maximised likelihood, and RSS is residual sum of squares.

3.0 RESULTS AND DISCUSSION

When designing the architecture of RBFN, a wide range of spread constant was applied. Due to the large number of developed models for each AI approach, only the selected models were presented and discussed in this section.

3.1 RBFN Models Evaluation

A total number of 9000 datasets were collected from rheological tests. Among the datasets, 7200 datasets (equivalent to 80% of total datasets) were used to train the RBFN model while the rest 1800 datasets were reserved for testing purposes. There is no concrete rule for data splitting, however, it is important to ensure the AI models were trained with a sufficient amount of data to enhance their reliability. As reported in previous studies, the most common percentage for training data is between 60% to 80% while for testing data the value should be 40% to 20% (Akter and Desai, 2018; Alimissis *et al.,* 2018; Zhang *et al.,* 2018). In this case, the upper limit was chosen to allow the models to learn the most possible input-output pattern.

The performance of each RBFN model was evaluated and tabulated in Table 1. Firstly, from the perspective of the coefficient of determination, the R^2 value for all of the examined models is considerably high (approximately 1) which indicates there is a strong correlation between the predicted and actual values. Secondly, in terms of error analyses, a low error value is always an indicator of good performance. In this case, from Table 1, it can be seen that both MAE and RMSE values show a fluctuating trend and generally perform better when the spread constant is an odd number.

Lastly, AIC and BIC measure how well the data fits into the model. Similar to the MAE and RMSE, lower AIC and BIC values are always favourable. As shown in Table 1, model V with a spread constant of 21 has the most negative AIC and BIC value which means that it achieves the best performance in terms of AIC and BIC.

All the statistical analysis outcomes in Table 1 point that model V emerges as the model with the best performance. The appropriateness of model V is further verified through the percentage error analysis. In this study, the percentage error range was fixed in between ± 15%. From Figure 3, around 96% of the total datasets in model V fall within the threshold error range, meaning that the prediction model has shown great potential to achieve at least 85% accuracy. Moreover, as shown in Figure 4, the maximum percentage error of model V is also the lowest among all the investigated models.

Overall, model V appears as the best-performed RBFN model where it produced the highest coefficient of determination (0.9998), lowest mean squared error (0.001058) and root mean squared error (0.001447), most negative Akaike information criterion (-18426.5) and Bayesian information criterion (-18415.5), and the smallest percentage error.

3.2 Models Comparison

The application of AI technique in rheological wall slip is still at the beginning stage. In the previous study, a multilayer perceptron neural network (MLP-NN) model was developed for the actual shear rate prediction (Chin *et al.* 2018b), however, there is still room for improvement to achieve a higher level of prediction accuracy.

Table 1: Statistical Performance for Each RBFN Model

Models	Spread Constant	R^2	MAE	RMSE	AIC	BIC
I	17	0.9998	0.001095	0.001461	-18391.8	-18380.8
II	18	0.9995	0.001346	0.002058	-17156.8	-17145.8
III	19	0.9996	0.001290	0.001962	-17329.4	-17318.4
IV	20	0.9985	0.002302	0.003692	-15053.2	-15042.2
V	21	0.9998	0.001058	0.001447	-18426.5	-18415.5
VI	22	0.9997	0.001207	0.001644	-17965.6	-17954.6
VII	23	0.9994	0.001727	0.002430	-16559.3	-16548.3
VIII	24	0.9994	0.001641	0.002337	-16698.9	-16687.9

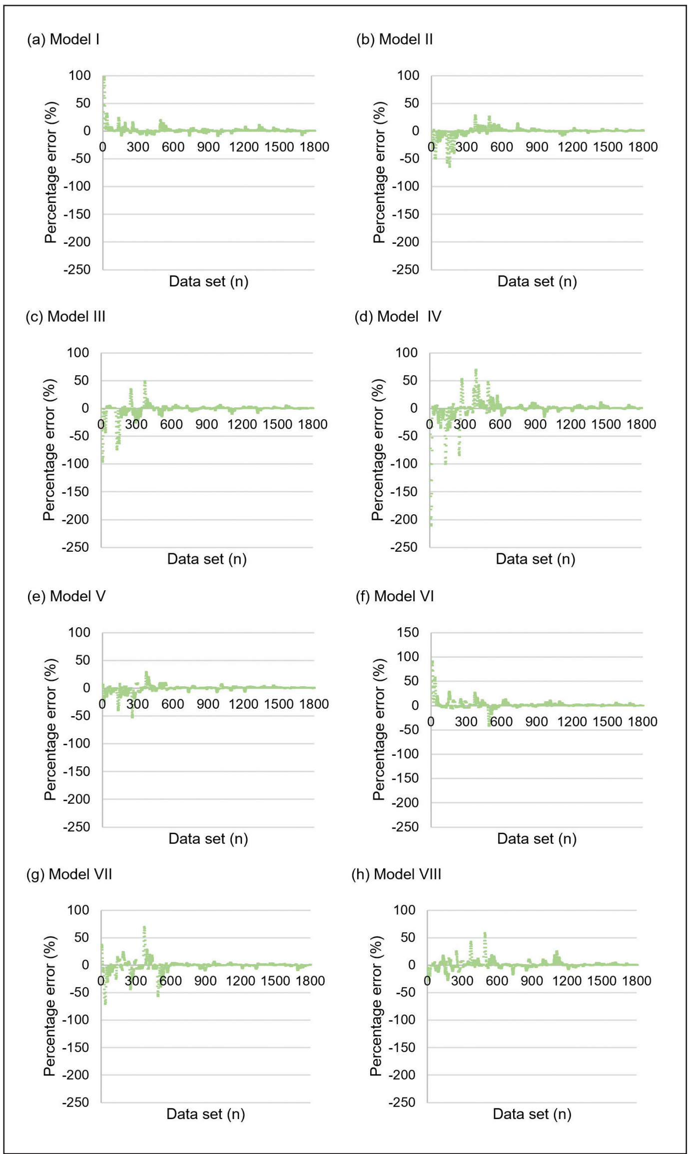

Figure 3: Percentage Error of the Respective Dataset Corresponding to Each RBFN Model

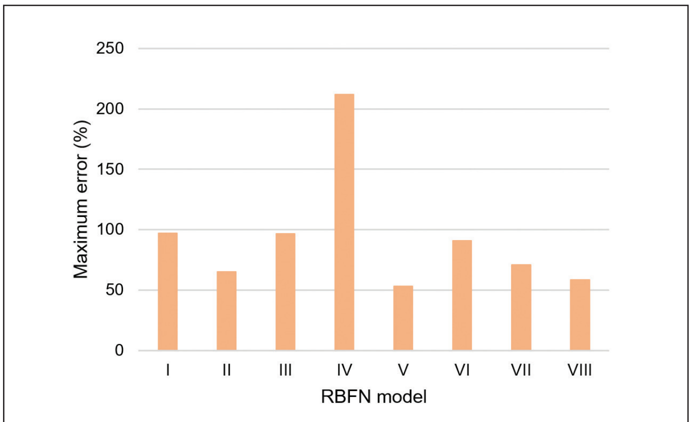

Figure 4: Maximum Percentage Error for Each RBFN Model

Under this section, the best-performed RBFN model will be compared with the MLP-NN model as developed by Chin *et al*. (2018b) using a series of statistical analyses, including coefficient of determination, mean absolute error, root mean squared error, Akaike information criterion, Bayesian information criterion and percentage error. As contained in Table 4, a significant improvement is clearly shown in terms of all the examined aspects while comparing the MLP-NN model to the RBFN model. At first, in the view of point of MAE and RMSE errors, the RBFN model produces a lower value than the MLP-NN model, meaning that the model RBFN model can produce more accurate output.

Next, a similar trend is also noticeable from the perspective of AIC and BIC. The most negative value is shown in the RBFN model, indicating that the predicted output fits better in the RBFN model than in the MLP-NN model.

Lastly, in terms of percentage error which is the most important indicator while developing an AI prediction model, the error is improved from the previously developed MLP-NN model (75%) to RBFN model (53%). In other words, the maximum percentage error has been greatly enhanced by the RBFN model.

Table 4: Comparison of the Best-Performed Model Corresponding to Each AI Technique

Model	MLP-NN (Chin *et al.* 2018)	RBFN
R^2	0.9967	0.9998
MAE	1.146804	0.001058
RMSE	1.652898	0.001447
AIC	-7657.3	-18426.5
BIC	-7646.4	-18415.5
Max. % Error	75	53

4.0 CONCLUSION

The main aim of this research study is to evaluate the appropriateness of the RBFN approach in generating the mathematical computational model which can perform a real-life output prediction within an acceptable level of accuracy.

During the development of RBFN, the determination of spread constant is a challenging task. Therefore, the trial-and-error method was applied to determine the best-suited parameters for the RBFN models which may lead to better prediction accuracy.

In this research study, several RBFN models were developed and their performance was evaluated under a series of statistical analyses. Based on the examined results, model V (with a spread constant of 21) emerges as the best-performed RBFN model where it has the highest R^2-value of 0.9998, lowest MAE and RMSE which recorded at 0.001058 and 0.001447 respectively, most negative AIC and BIC each with a value of -18426.5 and -18415.5, and the smallest maximum percentage error of 53%. Comparing the developed RBFN model with the MLP-NN model from previous literature, the improvement in terms of model performance is significantly noticed, where the maximum percentage error has been reduced from 75% to 53%, showing a significant enhancement.

This shows that the AI prediction model can be improved by implementing the other more advanced approaches where such approaches can make use of their special feature and enhance the overall performance.

5.0 ACKNOWLEDGMENT

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PROFILES

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