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A Comparative Study on Various ANN Optimization Algorithms for Magnetorheological Elastomer Carbonyl Iron Particle Concentration Estimation

Kasma Diana Saharuddin[1], Mohd Hatta Mohammed Ariff[1,*], Irfan Bahiuddin[2], Nurhazimah Nazmi[1], Mohd Azizi Abdul Rahman[1], Mohd Ibrahim Shapiai[1], Fauzan Ahmad[1], Sarah 'Atifah Saruchi[3]

[1] Malaysia–Japan International Institute of Technology (MJIIT), Universiti Teknologi Malaysia, Jalan Sultan Yahya Petra, Kuala Lumpur, Malaysia
[2] Department of Mechanical Engineering, Vocational College Universitas Gadjah Mada, Yogyakarta, Indonesia
[3] Faculty of Manufacturing and Mechatronics Engineering Technology, Universiti Malaysia Pahang, 26600 Pekan, Pahang, Malaysia

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ABSTRACT

Estimation particle composition such as particle shape, size, and concentration are crucial prior to the fabrication process of magnetorheological elastomer (MRE) to avoid process repetition due to inaccurate formulation. Currently, most of MRE prediction model were purposely used to predict the rheological properties such as shear stress and dynamic modulus, known as forward model. Nonetheless, very few studies have been reported to be capable able of predicting particle composition particularly in MR materials, which known as inverse model. Therefore, this paper proposed a carbonyl iron particle (CIP) concentration based MRE prediction model using neural network algorithm. Neural network-based machine learning model is more approachable compared to conventional mathematical modelling approach due to easily identify trends and pattern while handling multi-variety data. Various optimization algorithms have been employed such as *Adam*, *RMSprop*, *SGD*, *AdaGrad*, and *Nadam* throughout the modelling process. As the results, given shear strain amplitude, magnetic flux density, storage modulus, and loss factor as model input, *SGD* gave the maximum prediction accuracy with 0.95 and 3.038 MPa of R^2 and RMSE, respectively. Hence, this model can be the basis to the MRE material and devices development particularly as the tool to reduce costing and time consuming.

1. Introduction

Magnetorheological elastomer (MRE) is a smart material that response to external magnetic fields, allowing it to alter the rheological behaviour such as dynamic viscoelastic properties, stiffness, and damping [1,2]. It is made up two primaries: a matrix based medium and magnetic particles. Various studies have been conducted to improve the MRE properties performance such as

* *Corresponding author.*
E-mail address: mohdhatta.kl@utm.my

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introduced additives [3], improved particle alignment in the presence of a magnetic field [4,5], and the production of varied particle compositions [6,7].

Studies of magnetic particle composition has focused on particle shape such as spherical and plate-like [8], particle size [9], and also particle concentration [10]. Different particle concentration yield to wide range of results, especially in MR effects, which widely known as changes in the property with the presence of magnetic field intensity [11]. Wu *et al.,* [10] in their studied introduced five different mass concentration of carbonyl iron particle (CIP) which were 20%, 30%, 40%, 50%, and 60%. It was reported that the MR effect increased as the ratio increased, except on 50% due to suddenly decreased where the debate on that topic was not further addressed.

Meanwhile, study from Yunus and co-authors [7] found that increasing of CIP concentration from 10 to 70 wt% would increase the magnetic forces since the distance between CIPs became shorter due to agglomeration. In addition, shear storage modulus was reported slightly increase from 10 to 30 wt% but remarkable increase from 50 to 70 wt%. Moreover, Johari and collaged [12] reported that the initial storage modulus increased as increased the CIP concentration from 50 to 80 wt% due to addition of particle in the MRE component but decreased the linear viscoelastic region limit indicates brittle behaviour and less elasticity.

Hence, it should be emphasized that the selection of particle concentrations is crucial in order to fulfil the necessary attributes, weather for material properties study or for device application. Nonetheless, fabrication procedure is considered to be time consuming and costly due to repeating process required to gain a consistent outcome [13,14]. Hence, modelling and simulation model is needed to accurately anticipate particle composition under certain conditions. Prediction model for estimating viscoelastic properties (forward model) such as stress relaxation and creep behaviour [15] or particle composition such as particle concentration and size [16] (inverse model) involved with mathematical derivation-based model [17,18] and also machine learning based model [19-21].

Even so, machine learning model is preferable due to easily identify trends and patterns, required no human intervention, and handling multi-variety data [22-24]. Several studies on material science research have been conducted in order to anticipate fabrication process related parameter such as particle size of polymeric nanoparticles [25] and nanoparticle size of arbitrary methacrylates [26]. Latest, a prediction on particle size, particle concentration and milling time of MR fluid have been done with more than 80% accuracy.

All of this research used the neural network approach, which is well renowned for its ability to deal with nonlinear behaviour and complex input-output relationship. Meanwhile, optimization algorithm in neural network is critical in determining model performances. Common optimizers such as Adam [27,28] and RMSprop [29,30] can be found specifically in the prediction of viscoelastic material properties. However, because model performance is strongly dependent on data set, there are no optimizers that explicitly offer for material property or fabrication process parameter prediction.

Therefore, this work aims to design the ANN model for predicting CIP concentration based MRE with specified input shear strain amplitude, magnetic flux density, dynamic storage modulus, and loss factor and CIP concentration in weight percentage as model output. In this study, the effect of various optimization technique consists of *Adam*, *RMSprop*, *SGD*, *AdaDelta*, *AdaGrad*, *Nadam*, and *AdaMax* will be thoroughly investigated as it may affect the modelling performance. This work includes a proposed modelling approach based on ANN method, the MRE material fabrication process and data collecting, the result and discussion and lastly, the conclusion.

2. Artificial Neural Network Model

In this work, back-propagation artificial neural network algorithm (BP-ANN) is used to predict the CIP concentration based on selected input data. In general, BP-ANN algorithm is a supervised learning where it will bring forward the information from input neuron and at the last layer, the error between targeted value and estimation value will be measured. The error will be backpropagated to improve the performance by updating the weight and bias until the error is acceptable. There are many trainings algorithm used in BP-ANN to update weight and bias as the optimizer. In *Keras* library, various optimizer can be found such as *Adam*, *RMSprop*, *SGD*, *AdaDelta*, *AdaGrad*, *AdaMax*, and *Nadam*. Further explanation on each *Keras* optimizer can be found as follow.

2.1 Optimization Techniques

i. Adaptive Moment Estimation (*Adam*)
Adam is the combination of RMSprop and *momentum* optimizer to provide an optimization algorithm that can handle sparse gradients on noisy problems. The update operation considers only smooth version of the gradient and include bias correction mechanism [31].

ii. Root Mean Square Propagation (*RMSprop*)
RMSprop changes the *AdaGrad* optimizer on how the gradient is accumulated. Instead of taking the cumulative sum of squared gradients, the gradients are accumulated into an exponentially weighted average [31]. Furthermore, RMSprop choose different learning rate for each parameter.

iii. Stochastic Gradient Descent (*SGD*)
SGD is considered as a good learning algorithm for large training data set to train the neural network where the new updated parameter involved with a single or a few parameters such as learning rate to reduce variance and lead to stable convergence [32].

iv. Adaptive Gradient (*AdaGrad*)
AdaGrad adapt all model parameters by scaling them inversely proportional to the square root of the sum of all the historical squared values of gradient [32]. In addition, a high gradient for the parameters will have a reduced learning rate and parameters with small gradient will have increase in learning rate [31]. On the other way, *AdaGrad* ignored the need to manually tune the learning rate [33].

v. Adaptive Learning Rate (*AdaDelta*)
AdaDelta is an extension of *AdaGrad* presenting the modification on learning rate decay by introducing some fixed window and tracks only available gradients within the window, instead of accumulating the gradients [31,33].

vi. Adaptive Movement Estimation Maximum (*AdaMax*)
AdaMax is an extension to the *Adam* optimization algorithm. Broadly, it is extension to the gradient descent optimization algorithm that generalizes the approach to the infinite norm (maximum) and may results in a more effective optimization on some problems.

vii. Nesterov-acceleration Adaptive Moment Estimation (*Nadam*)
Nadam is one of the extensions of *Adam* optimizer which modified with Nesterov's accelerated gradient (NAG) [33] which one of the improved types of momentum optimization algorithm. *Nadam* uses decaying step size and first moment hyperparameters that can improve performance.

2.2 Neural Network Hyperparameter Setting

Neural network hyperparameter can be tuned which lead to the changes of model parameter such as weight and bias. Thus, the selection of model hyperparameter is very crucial to get higher prediction model accuracy. After considering the model performances and effect on training time, related tuning hyperparameter is chosen as mentioned in Table 1.

Table 1
The neural network model hyperparameters

Network parameter	Setting value
Epoch	100
Batch size	1
Kernel Weight Initializer	Xavier Uniform
Hidden nodes number	12
Activation function	Tangent Hyperbolic
Learning rate	0.001

There are several inputs have been chosen to predict the CIP concentration which is dynamic storage modulus (G'), loss factor ($\tan\delta$), shear strain amplitude (γ), and magnetic flux densities (B). Meanwhile, CIP concentration (W_p) as output model. The inputs model is normalized before being used to train so that the model may easily read the data. Hence, the neural network model architecture consists of input and output can be illustrated in Figure 1 showing the connection of the neuron between input layer, hidden layer, and output layer. In this work, *Keras* library was used as a Python interface to build the neural network model.

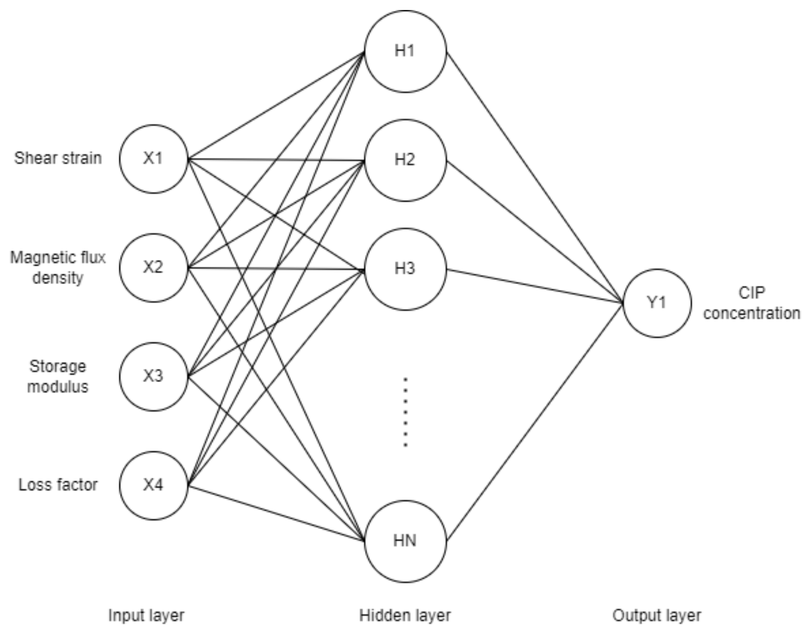

Fig. 1. The neural network model architecture

3. Material Fabrication and Data Set

3.1 MRE Fabrication Process

MRE fabrication process start by providing the raw material which are room temperature vulcanization silicon rubber (RTV-SR) as matrix and CIP as magnetic particle. MRE is fabricated on isotropic condition in which the particle embedded in the matrix is distribute homogenously. The RTV-SR and CIP were measured using a weighing balance before vigorously stirring with a mixer for about 10 minutes. The compound was cured for about 2 hours in a mould with a diameter of 40 cm and 1 mm thickness at room temperature without the presence of a magnetic field. The sample fabrication process involved five different CIP concentration which are 30, 40, 50, 60, and 70 wt.%. The samples were undergoing dynamic testing which is shear strain amplitude sweep testing using rotational MCR 302 rheometer from Anton Paar. During the testing, the frequency is kept constant on 1 Hz with temperature 28℃. Meanwhile, the magnetic field strength is varied by changing the magnetic flux densities which is 0 mT, 180 mT, 360 mT, 580 mT, 701 mT, and 850 mT.

3.2 Data Set and Performance Index

After completing the dynamic testing on all MRE samples, the data were collected and filtered before it can be used for modelling process. There were 900×4 of raw data set gained from the dynamic testing. From this total data set, the division for training and testing data set was done prior to the modelling process which done by randomly distributed. Table 2 present the respective input and output along with minimum and maximum range values.

Table 2
Respective data for modelling purpose

	Output		Input							
	CIP concentration		Shear strain		Magnetic flux density		Storage modulus		Loss factor	
Range	Min	Max	Min	Max	Min	Max	Min	Max	Min	Max
Value	30wt.%	70wt.%	0.0009%	25%	0mT	0.89479mT	0.0626MPa	0.538MPa	0.055	1.546

There were four performances index used in this work to analyse the prediction model results which is coefficient of determination (R^2), mean absolute error (MAE), mean square error (MSE), and root mean square error ($RMSE$). The R^2 present the correlation between prediction output and targeted value where the results towards 1 showing higher correlation while results towards zero showing low correlation. Furthermore, *MAE*, *MSE*, and *RMSE* present the measured error. The calculated index can be found as follow.

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

$$MAE = \frac{\sum_{i=1}^{n}|y_i - \hat{y}_i|}{n} \tag{2}$$

$$MSE = \frac{\sum_{i=1}^{n}(y_i - \hat{y}_i)}{n} \tag{3}$$

$$RMSE = \sqrt{\frac{\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}{n}} \tag{4}$$

Based on Eq. (1), Eq. (2), Eq. (3) and Eq. (4), variable $n, y, \hat{y}$ refer to number of observations in datasets, targeted output, and predicted output, respectively. Meanwhile, in Eq. (1), $\bar{y}_{output}$ refer to mean value of targeted output.

4. Results and Discussion

4.1 Effect of Various Optimizers on Performances Index

The model performances on training and testing data set at seven optimization algorithms have been observed and analyzed though four performances index which is R^2, MAE, MSE, and $RMSE$ where the results are tabulated in Table 3 and Table 4 for training and testing data set, respectively.

Table 3
Training data performance on various optimizer

Optimizer	*Adam*	*RMSprop*	*AdaDelta*	*AdaMax*	*Nadam*	*SGD*	*AdaGrad*
R^2	0.928	0.897	-5734	0.808	0.927	0.952	-6504
MAE	2.315	2.694	48.62	4.339	2.346	1.682	44.30
MSE	13.28	18.01	2566	30.73	13.75	9.229	2156
$RMSE$	3.645	4.244	50.65	5.543	3.708	3.038	46.43

Table 4
Testing data performance on various optimizer

Optimizer	*Adam*	*RMSprop*	*AdaDelta*	*AdaMax*	*Nadam*	*SGD*	*AdaGrad*
R^2	0.919	0.919	-4525	0.763	0.914	0.937	-8330
MAE	2.492	2.370	47.24	4.440	2.644	2.182	42.92
MSE	13.23	12.47	2411	28.73	14.43	11.51	2014
$RMSE$	3.637	3.532	49.10	5.360	3.799	3.393	44.88

Among all applied optimization algorithms, *AdaDelta* and *AdaGrad* optimizer produced lowest correlation accuracy with larger error on both training and testing data set showing that these two optimizers were not very suitable for particle concentrations estimation. Furthermore, *AdaMax* optimizer reached about 80% correlation accuracy on training set but lower than *RMSprop* especially on testing data set. Besides, it can be noticed that training accuracy exhibited by *RMSprop* optimizer is lower than testing accuracy. This might be due to data split on training and testing data set was not distributed well where data in testing set is less variance or less noise from training data set and thus, lead to the higher accuracy on testing set than training set.

A model will have good data splitting when having higher training accuracy and slightly lower on testing accuracy showing that data split was done evenly. Meanwhile, a model that have very higher training accuracy but very lower testing accuracy facing overfitting phenomenon where the model is not generalized well. Thus, data split should do properly to avoid biasness of data that might affect the performance of a model. On the other hand, *Adam* and *Nadam* optimizers produced similar model accuracy where *Adam* has slightly small error compared to *Nadam* optimizer on both training and testing data set. Meanwhile, *SGD* optimizer exhibits convincing model accuracy by having higher correlation and smallest error. *SGD* optimizer also showing smaller *MAE*, *MSE*, and *RMSE* value at testing data set showing the best optimizer among other optimization algorithms. Next, the comparison between targeted CIP concentrations and predicted CIP concentration is provided in graphical evaluation.

4.2 Carbonyl Iron Particle Concentration Prediction Performances

The comparison between targeted and predicted CIP concentrations have been done on three best optimization algorithms which is *Adam*, *Nadam*, and *SGD* to show each performance at given response such as magnetic field and storage modulus.

Based on Figure 2-4, it can observe that three optimizers simulation results may followed the targeted CIP concentrations. Nevertheless, all optimizers produced less prediction accuracy at 180 mT particularly on predicting 50 wt.% where *Nadam* optimizer exhibits about 6.12 wt.% error followed by *Adam* and *SGD* with 5.07 wt.% and 3.23 wt.% error, respectively. In addition, low prediction of CIP concentrations also occurred at 40 wt.% which happened at all magnetic flux densities. Hence, this showed that interpolation estimation particularly at 40 and 50 wt.% have slightly low performances compared to 30, 60, and 70 wt.%. However, the range of the error is acceptable especially from *SGD* optimizer that made *SGD* optimizer become the best optimization algorithm in predicting MRE CIP concentrations.

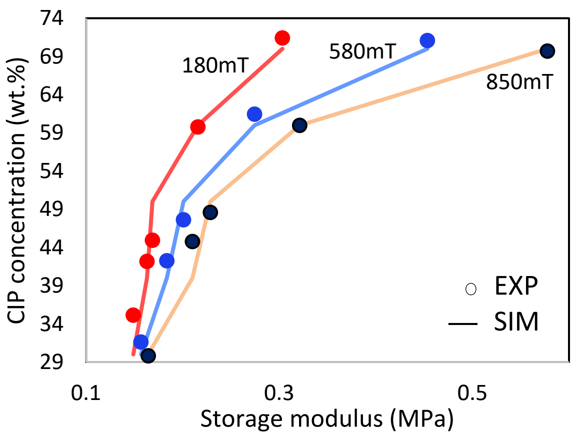

Fig. 2. *Adam* Optimizer

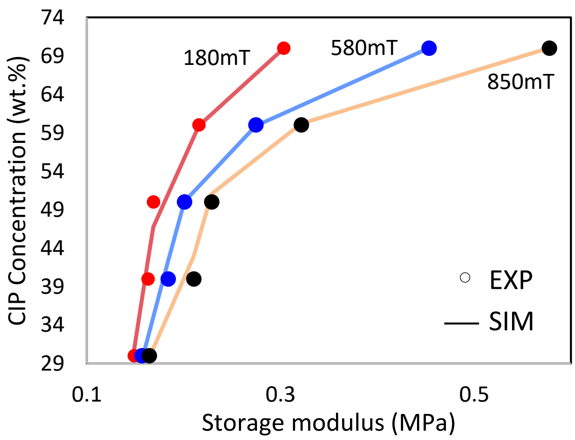

Fig. 3. *SGD* Optimizer

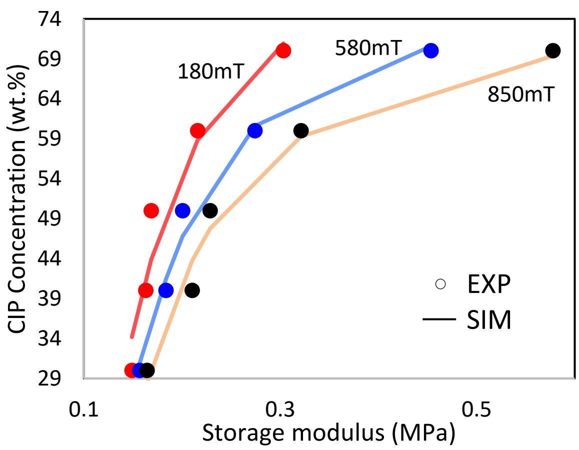

Fig. 4. *Nadam* Optimizer

5. Conclusions

As the conclusion, a neural network-based machine learning approach was used to construct a prediction model to forecast the CIP concentration of MRE. Seven models were developed based on different optimization algorithms which is *Adam*, *RMSprop*, *SGD*, *AdaDelta*, *AdaGrad*, *Nadam*, and

AdaMax. As the results, three optimizers showed favourable prediction performances which are *Nadam*, *Adam*, and *SGD.* It is truth that adaptive optimizers (*Adam* and *Nadam*) are faster in reaching the minimum cost function and compared to SGD during the training process. However, SGD is more generalized compared to adaptive optimizers. This is due to adaptive optimizers often converge to the sharp minima while SGD prefer to find flat minima or asymmetry valleys. In other words, adaptive optimizers have chances to stuck at local minima while SGD could better escape from sharp minima and converge to flatter minima which might be the best minima of the function. This can be proved from the performance index where SGD produced smallest *RMSE*, *MSE*, *MAE* and larger R^2 value to show that it is the best optimizers for CIP concentration estimation. Also, comparison between actual concentration and predicted concentration showing that SGD followed well the pattern on all concentrations. Thus, model with SGD optimizer can be the basis platform for MRE material and devices development. Furthermore, this work also can be a basis framework for MRE model development for predicting fabrication or manufacturing process related parameters such as particle sized and additives content in order to reduce costs and time consumption.

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