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Prediction of tribological behavior of solid lubricants using artificial neural network

Jijo Jose [1], Abhijeet Shivaji Suryawanshi [2], NIranjana Behera [3*]

[1] Department of Mechanical Engineering, Amal Jyothi College of Engineering, Erumely Road, 686518 Koovappally, Kerala, INDIA.
[2] Department of Mechanical Engineering, Marathwada Mitramandal's College of Engineering, Karvel Nagar, 411052 Karvenagar, Pune, INDIA.
[3] School of Mechanical Engineering, VIT University Vellore, 109 CDMM Block, 632014 Vellore, Tamilnadu, INDIA.
*Corresponding author: beheranira@rediffmail.com

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Bayesian regularization

ABSTRACT

Under high vacuum and high temperature conditions, liquid lubricants cannot deliver their usual performance of lubrication. In such situations, solid lubricants are highly recommended. Present study investigates the tribological behavior of metal lubricated with powders such as cupric oxide, zirconium dioxide and molybdenum disulfide. The tests were performed under various conditions of load and temperature in a reciprocating wear test apparatus. Subsequently artificial neural network models have been developed for prediction of wear and coefficient of friction. ANN models were developed using three different training methods: Bayesian regularization, Scaled conjugate gradient and Levenberg Marquardt. Bayesian regularization training method shows better performance with lowest mean square error value of 2.50E-7 and highest coefficient of determination of 0.99.

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1.0 INTRODUCTION

Solid lubricants are applied in various industries because of their unique properties and versatile applications. These lubricants, in powdered form, offer significant advantages, particularly in situations where traditional liquid lubricants may be impractical or pose challenges. They efficiently lower wear and friction between moving surfaces by creating a protective coating, which increases equipment longevity, efficiency, and energy efficiency. In addition to outperforming conventional liquid lubricants in high-temperature applications they help keep surfaces cleaner and avoid contamination. Furthermore, powder lubrication is a desirable alternative for economical and environmentally friendly operations due to its many applications, low maintenance requirements, and environmental advantages. The relevance of solid lubricants lies in their adaptability to diverse operating conditions, including high temperatures and extreme pressures, making them suitable for applications where liquid lubricants may fail. In order to maximize the benefits of the solid lubricants, proper selection of lubricants according to the necessary application is quite necessary.

1.1 Relevance of Solid Lubricants

In extreme conditions for tribological applications, solid lubrication is considered the primary method to manage friction and wear (Donnet et al., 2004). At low temperatures in aerospace/space applications it is impractical to use liquid lubricant as it becomes too viscous or solidified (Roberts, 1990). Liquid lubricants used in hydrodynamic bearings operating at high temperatures experience thermal instability, leading to deterioration and degradation of the lubricant (Stachowiak et al., 1993). According to Arrhenius law, the rate of chemical reactions in liquid lubricants doubles with every 10°C increase in temperature, impacting the lubricating capability. Molybdenum disulfide exhibits frictional characteristics comparable to a hydrodynamic lubricating film (Heshmat and Brewe, 1995; Heshmat and Brewe, 1996). Similar pressure development mechanism was also observed for liquid lubricants in slider bearings and dampers (Heshmat, 1992; Heshmat, 2000; Heshmat and Heshmat, 1999). A numerical solution was presented for powder-lubricated journal bearings with elliptical-bore (Rahmani et al., 2016). A numerical analysis of powder-lubricated bearings having three lobes was conducted indicating that larger particles offer enhanced load-carrying capacity and stability (Jose et al., 2021). An experimental investigation was performed to evaluate the effectiveness of solid lubricants (Jose et al., 2020a). A review of the selection of solid lubricants, load values and temperature conditions for experimental evaluations was presented (Li et al., 2001).

1.2 Selection of Load, Temperature and Type of Powder

Researchers have clearly demonstrated the ability of powders to act as lubricants between two surfaces, successfully reducing wear and friction (Godet et al., 1991). However, there is not much of research on wear and friction analysis when using dry powder as a lubricant with pure metal. Zinc oxide powder was found to improve the friction resistance of M50 steel alloy in a pin-on-disc tribometer with varying load (3-12 N) and temperature (150-450 °C) conditions (Elsheikh et al., 2020). Wear tests were conducted for sliding between a ball specimen and a flat specimen under the loads 30 N, 40 N and 50 N. Although the subjected load is point load in the test but the magnitude of loads was calculated based on the pressure developed in a journal bearing and the area of journal surface (Patil et al., 2019). Thermal analysis of journal bearings unveiled that the operating temperatures can vary from 50 °C to 120 °C while the journal speed range is 400-2000 rpm (Torgal and Saini, 2015). This shows a reason of selecting the temperatures 50 °C, 100 °C and 150 °C for the tests.

An extensive literature study is needed for the selection of right solid lubricant. To improve tribological properties, many dry granular powders have been used in earlier research in combination with materials such metals, polymers, ceramics, sintered metals, and composites. Wear rate and coefficient of friction significantly reduced when molybdenum disulphide was added to iron-copper-tin composite materials (Mushtaq et al., 2019). Using MoS2 as additive in SAE 20W40 lubricant in wear test (loads range 75-125 N) of an alloy steel the wear loss was reduced by 60% (Charoo et al., 2017).

At higher temperatures, zirconium oxide exhibits superior strength, superior resistance to wear, high hardness, and increased fracture toughness in comparison to steel. Wear rates were found to decrease when different amounts of zirconium oxide are included into polymethyl methacrylate composites (Akinci et al., 2014). Zirconium oxide was used as additives in polyalphaolefin oil in the reciprocating wear test of two sliding steel specimens, which showed a significant reduction in the coefficient of friction as compared to that by using only base oil (Shah et al., 2015).

Granular powdered copper oxide has demonstrated improved anti-wear and anti-friction properties. Research on the tribological properties of zirconia composites containing copper oxide revealed enhanced resistance to wear and friction at higher temperatures (Kong et al., 2014). When copper oxide nanoparticles were added to multi-grade engine oil, their effects under 40 N and 60 N loads at different concentrations were investigated. This ultimately improved the effective friction coefficient because the particles help in converting the existing friction of sliding into a rolling friction (Jatti and Singh., 2015).

An extensive study of the literature led to the choice of solid lubricants for the reciprocating wear test on the steel sample. Because of their excellent tribological properties, CuO, MoS_2 and ZrO_2 were chosen as powder lubricants for the experimental analysis. Although there is a significant amount of research on the performance of solid lubricants in bearings, none of it attempts to explore how temperature and load variations affect the lubricating efficiency of powder lubricants. Therefore, present study evaluates the performance of powder lubricants in reciprocating wear test apparatus under load and temperature conditions similar to those in journal bearings. The tribological properties of steel specimens under the lubrication of three powders (CuO, MoS2 and ZrO2) were evaluated at three different loads (30 N, 50 N and 70 N) and different temperatures (50 °C, 100 °C and 150 °C) similar to those found in journal bearings.

1.3 Artificial Neural Network in Tribology

In recent times, ANNs have become a robust technique for data-driven modeling in various engineering domains, including mechanical and structural engineering as well as in tribology and machine tool treatment (Hayajneh et al., 2009; Myshkin et al., 1997; Warde et al., 1999). Notably, several investigations applied neural networks to analyze wear tests (Pierce et al., 2008; Schooling et al., 1999). Artificial neural network is fundamentally designed based on the architecture of natural brains (Bell, 2015; Sarkar et al., 2018).

ANN was applied to evaluate the effects of roughness and non-circulation the load and friction (Pradhan et al., 2022). Wear of composites occurring in friction stir processing technique was predicted using artificial neural network (Dinaharan et al., 2022). ANN was applied to predict elasto-hydrodynamic lubrication central film thickness and boundary friction in gears and rolling element bearings (Walker et al., 2023). ANN was applied to investigate the wearing-in period and the true wear coefficient (Argatov et al., 2021). A study explored the potential of ANN in predicting the sliding friction and wear properties of polymer composites (Gyurova et al., 2011). Taguchi experimental design of experiments with ANN is applied for predicting the tribological behavior of epoxy composites (Padhi et al., 2013). Friction coefficient was predicted for fiber-reinforced polyester composites was predicted (Nirmal, 2010). ANN is applied to predict the friction and wear properties composite materials (polyether ether ketone) by varying the content of carbon fiber (Zhao, 2023). Adaptive neuro fuzzy interface system (ANFIS) was used for the prediction of wear of PTFE material under different parameters such as speed, load and sliding distance (Dhande, et al., 2023). The use of ANN has transformed the investigation of friction and wear characteristics materials. Most of the ANN models are developed for predicting wear and coefficient of friction in components of different materials. Although ANN technique has been applied successfully in various fields, few researchers have applied this technique in predicting the tribological properties in solid lubricants. This data-centric approach would empower the researchers and engineers to customize solid lubricants, optimize operational regimes, and devise innovative strategies to mitigate friction and wear, ultimately enhancing efficiency, reliability, and sustainability across various industrial applications. Hence in this study ANN technique has been applied to predict the coefficient of friction and the wear rate based on the experimental investigation. The accuracy of the models is assessed by comparing it to the experimental data (Jose et al., 2020b).

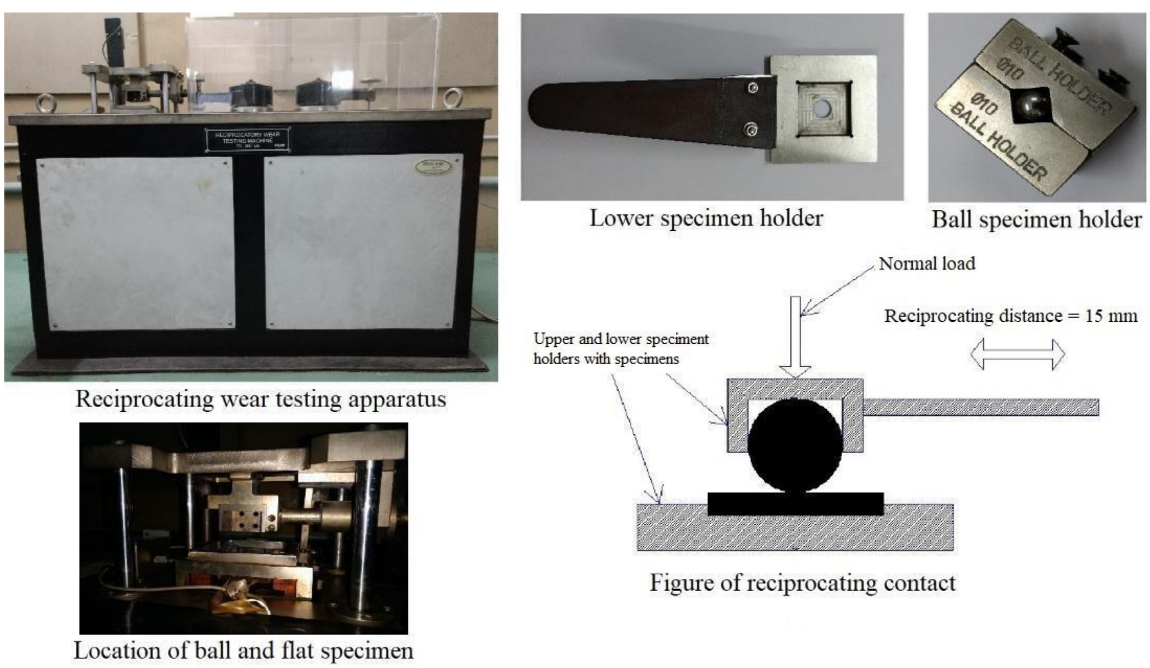


Figure 1: Reciprocating wear test

2.0 EXPERIMENTAL PROCEDURE

2.1 Test Sample Preparation

A flat specimen of AISI 52100 steel underwent a heat treatment process to achieve the desired hardness. This process involved heating the specimen to approximately 850 °C and holding it at that temperature for 45 minutes, followed by oil quenching. Subsequently, the specimen was tempered at 150 °C. The heat-treated specimen was then machined to dimensions of 30 × 30 × 10 mm. Prior to testing, each specimen was thoroughly cleaned using methyl alcohol and acetone. The upper specimen in the tribological test was a 10 mm diameter ball, also composed of AISI 52100 steel. The chemical composition of the material is detailed in Table 1. The surface roughness of the prepared specimens was measured to be approximately 0.431 μm.

The hardness of the lower flat specimens was determined using a micro-Vickers hardness tester. A load of 5 N was applied at three randomly selected points on each specimen, with a dwell time of 10 seconds per measurement. The average hardness of the flat specimen was found to be 800 kg/mm^2, while the ball specimen exhibited a hardness of 677 kg/mm^2.

2.2 Wear Test

Wear test was performed in a reciprocating wear test rig (Ducom TR-285-M9) following ASTM G181-11 standard, Figure 1. To generate necessary pressure, a small ball was made to reciprocate with as speed of 0.3 m/s within a stroke length of 15 mm in the setup. In order to enhance the lubrication process, solid lubricants (Zirconium dioxide, molybdenum disulfide and cupric oxide), was introduced within the gap between ball and specimen across three distinct load and temperature combinations: 50 °C, 100 °C and 150 °C, and at 30 N, 50 N and 70 N loads. The test specimens were subjected to loading using calibrated dead weights. A built-in heater within the experimental setup was employed to maintain the desired test temperature. Key parameters, including friction force and coefficient of friction, were continuously monitored and recorded at regular intervals throughout the test duration. Each experimental run was conducted for a fixed duration of 5 minutes. The experimental parameters utilized are summarized in Table 1. A total of fifteen tests were performed involving various parameters, Table 1.

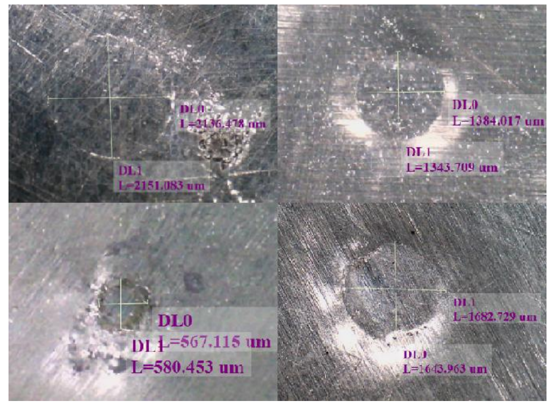
Table 1: Parameters considered in the experiment.

Levels	**-1**	**0**	**1**
Load (N)	30	50	70
Solid lubricant	Zirconium oxide	Copper oxide	Molybdenum disulfide
Temperature(°C)	50	100	150

Table 2: Elements present in AISI 52100 steel.

Components	**Weight percentage (%)**
Iron	97.116
Chromium	1.09
Carbon	0.96
Manganese	0.57
Silicon	0.21
Sulphor	0.023

a) Wear track on tested specimen.



b) Wear scar images on aluminium foil.

Figure 2: Micrograph images of test specimens.

At the conclusion of each sliding wear test, the mass loss of the specimen due to wear was recorded to calculate the wear rate. The wear track generated on the lower flat specimens is illustrated in Figure 2(a). Subsequently, the wear scar from the upper ball specimen was transferred onto an aluminum foil with a thickness of 20 microns. Representative images of the wear scars obtained from three different tests are presented in Figure 2(b). The diameter of the wear scar imprints was measured using a Dynalite microscope.

Before conducting the test, acetone and methyl alcohol were used to clean each specimen. A 10mm diameter AISI 52100 steel ball of definite compositions served as the upper specimen for the test, Table 2. The resultant wear track produced on the lower flat specimens during the sliding wear test, Figure 2 (b). Following each test, the imprint of wear scar from the upper ball specimen was imprinted onto 20-micron-thick aluminum foil. Wear scars occur on the ball specimen, Figure 2 (c).

3.0 ARTIFICIAL NEURAL NETWORK (ANN)

3.1 ANN Model

ANN comprises of several neurons connected through weighted linkages along which signals pass. The input signals with connections weights are received by each neuron from the other neurons and these neurons deliver this signal as an output signal (Meyveci et al., 2012; Li et al., 2001). In the same manner, the outputs can be the endmost result for a network, or it can be input to different neuron. Each network comprises of an input layer, an output layer and one or more hidden layers. The iterative procedures used to execute all of the training data in a network are called epochs. The training algorithm plays the role of changing the value of weights in an ANN. In the literature, various training algorithms were introduced (Askarzadeh et al., 2013; Chandwani et al., 2015; Sarangi et al., 2014).

An ANN model is developed for prediction of wear of material lubricated with solid lubricants. The model consisted of a feed-forward back-propagation with three layers. The input layer is introduced with three variables, namely load, solid lubricant and temperature. Fifteen sets of experimental data are applied to design the ANN model. Coefficient of friction and wear were the two variables which were assigned to the output layer. For training the network, three types of algorithms (Scaled Conjugate Gradient, Levenberg Marquardt, and Bayesian regularization) were applied. The data was split into 70% for training, 15% for testing and 15% for validation. Numbers of neurons are varied from 1 to 20 during each training process to find the optimum number of neurons. Number of input neurons and output neurons of the network architecture were 3 and 2 respectively. Number of neurons in the hidden layer and output layer were 9 and 1 respectively.

3.2 Algorithm Functions

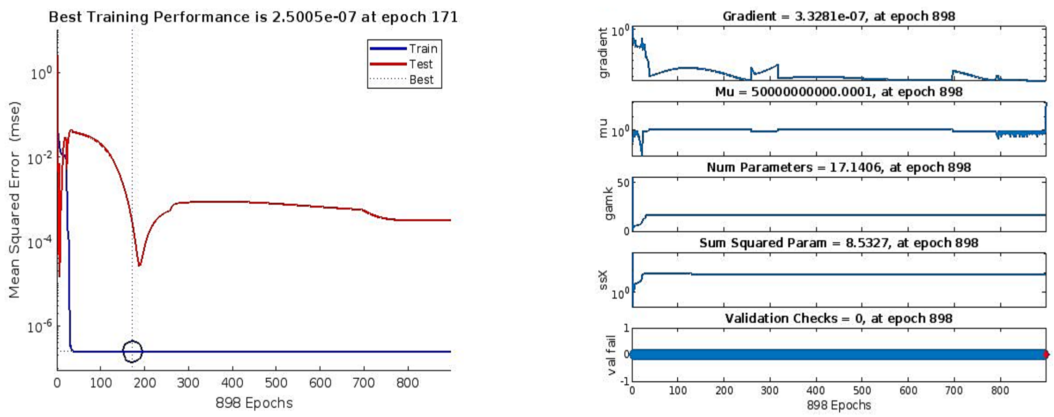
Wear and coefficient of friction of materials were predicted using three categories of algorithm functions namely, Scaled Conjugate Gradient (SCG), Levenberg Marquardt (LM) and Bayesian regularization (BR). The LM algorithm takes less time but needs a lot more memory. Although BR algorithm takes more time, but it gives better outcomes for a noisy and limited dataset. In this, the training stops when the adaptive weight reaches to minimum value. Scaled Conjugate method occupies less memory space. In this case, when training is stopped due to a lack of generalization progress, there is an increase in mean square error in the validation samples.

3.3 Prediction Accuracy of Algorithms

Prediction accuracy of a training algorithm depends upon factors such as error functions, learning rate and number of iterations. Difference between the predicted and test data represents the error function in the network. Weights are updated for minimizing the error functions. Performance of a network is assessed by implementing various quality parameters, such as coefficient of determination (R^2) and mean square error (MSE). For optimum results the value of MSE should tend to zero and the coefficient of determination value should tend to one. Coefficient of determination indicates the strength of correlation between the experimental and predicted data.

3.3 Neuron Independence Check

In a hidden layer, the number of neurons was altered from 1 to 20. The optimum value of number of neurons can be decided based on value of MSE and R2 value (Jones et al., 1997; Pati et al., 2015; Wiciak-Pikuła et al., 2020). The values of mean square error and network control parameters were stable after 171 training epochs, showing that the training was accurate, Figure 3a. The parameters (gradient, momentum constant (mu), gamk, sum squared parameter (ssX), and val fall) vary with number of epochs, Figure 3b. The parameter "gradient" represents the performance gradient of back propagation of the network. The governing parameter Mu, or momentum, is nearly identical to the inversion of Hessian matrix. The parameter "gamk" represents the number of coefficients used. The parameter "Vail fails" shows the number of times the validation failed in a learning process. Bayesian regularization network with one hidden layer having 9 neurons yields optimum results, Table 3.



(a) (b)

Figure 3: Variation in (a) Mean square error (MSE) and (b) control parameters during training.

Table 3: Neuron independence check (using BR algorithm).

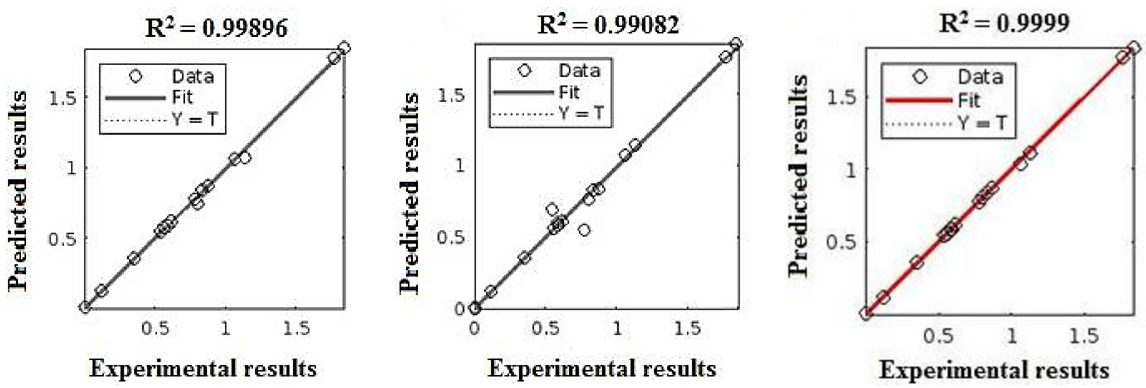
No. of neurons	**Coefficient of regression (R^2)**	**Mean square error (MSE)**
1	0.95840	0.011479
2	0.97599	0.00015702
3	0.99794	7.58E-06
4	0.99944	0.0001499
5	0.99714	2.80×10^{-7}
6	0.99794	3.48×10^{-9}
7	0.99834	2.66×10^{-7}
8	0.99870	4.45×10^{-9}
9	0.99990	2.50×10^{-7}
10	0.99447	2.41×10^{-7}
11	0.98923	2.65×10^{-7}
12	0.99874	2.63×10^{-7}
13	0.99626	2.52×10^{-7}
14	0.99596	2.44×10^{-7}
15	0.99900	1.35×10^{-7}
16	0.99852	2.65×10^{-7}
17	0.99088	7.68×10^{-7}
18	0.99944	6.46×10^{-7}
19	0.99956	2.57×10^{-7}
20	0.99353	2.51×10^{-7}

Table 4: MSE and R^2 values using different training algorithms.

Training algorithms	**Number of hidden layers**	**Optimum number of neurons**	**Optimum numbers of epoch**	**Mean square error (MSE)**	**Coefficient of determination (R^2)**
LM	1	11	14	9.77×10^{-5}	0.9989
SCG	1	8	21	0.00584	0.9908
BR	1	9	171	2.50×10^{-5}	0.9999

4.0 RESULTS AND DISCUSSIONS

In this study, three types of training algorithms were applied to conduct the regression analysis. The ANN model was formed using the transfer function TANSIG available in Matlab ANN toolbox. The network is trained using 11 of the 15 data sets as input variables, validated using 2, and tested using the remaining 2. MSE and R2 values are calculated which are presented in Table 4. Lowest MSE and highest R2 value were found using the BR algorithm. Figure 4 shows plot of experimental and predicted results. The network using Bayesian regularization algorithm yielded optimum results when numbers of the epoch, numbers of neurons and numbers of hidden layers equal to 171, 9 and 1 respectively. The overall regression coefficients found using LM, SCG and BR algorithms are 0.9989, 0.9909 and 0.9999 respectively. It seems that there is hardly much difference in the values of regression coefficient. The calculated mean square error values using LM, SCG and BR algorithms are 9.77×10^{-5}, 0.00584 and 2.50×10^{-7}.



(a) (b) (c)

Figure 4: Parity plot using (a) Levenberg marquardt, (b) Scaled conjugate gradient and (c) Bayesian regularization.

Wear can be predicted using ANN technique because the model shows high accuracy and hence it is a better option than the traditional methods. ANN also predicts the parameters in a shorter duration of training, which shows that it is simple and affordable (Arefi-Oskoui et al., 2017). The majority of related papers describe how the parameters can be predicted with little error by using the trained ANN model (Bulut et al., 2021).

The experiment considered load, temperature, and solid lubricant as variables affecting the coefficient of friction. The main effects plot presented in Figure 5 illustrates the influence of load, temperature, and solid lubricant on the coefficient of friction. Furthermore, the surface plot of the coefficient of friction is specifically focussed on the three different solid lubricant used in the experiment, Figure 6.

The investigation revealed that molybdenum disulfide and zirconium dioxide exhibited the lowest and highest mean friction coefficient respectively. Under a load increase of 130% (from 30 N to 70 N), the friction coefficient exhibited a reduction from 1.15 to 0.55, representing a 52% decrease. In instances of lower loads, an elevated mean coefficient of friction was identified, and as the load increased, a corresponding reduction in the mean coefficient of friction was observed. Comparable fluctuations in the coefficient of friction for molybdenum disulfide associated with varying loads were similarly documented in the studies (Boyd et al., 1945; Hyde, 1957).

Likewise, with a temperature rise of 200% (from 50 °C to 150°C), the mean friction coefficient decreased by 64% (from 1.25 to 0.45). With an elevation in temperature, there is a decrease in coefficient of friction, reaching its minimum value at 150 °C. Similar variation in the coefficient of friction for molybdenum disulfide with change in temperature has been found in literature (Peterson et al., 1954).

Similarly, the highest friction coefficient was noted under the conditions of the lowest temperature (50 °C) and the least applied load (30 N), whereas the lowest friction coefficient was found at the highest temperature (150 °C) and the greatest applied load (70 N).

Each of the input parameters or features has different importance or significance for a given model. The importance or significance can be assigned as a score to the input parameter. A higher score means that the specific parameter will have a bigger effect on the model used to predict a given variable. In this study, Random Forest Regressor algorithm is used to determine the feature importance as shown in Figure 7. Among the three parameters (powder, load and temperature), temperature is the most influential parameter. Second, load is also a significant parameter. The difference between the scores of loads and temperature is very low.

4.1 Limitations of the Model

Following are the limitations of this model:-

Restricted Operating Conditions: The ANN was trained using data from a limited set of load and temperature combinations (30–70 N, 50–150 °C). The model's performance under conditions outside this range remains unknown.

Material Specificity: The model is based solely on tests involving three solid lubricants (Cupric oxide, zirconium dioxide and molybdenum disulfide) applied to AISI 52100 steel specimens. This restricts its applicability to other materials or composite systems with different tribological behaviors.

Powder Characteristics Not Varied: Factors such as particle size, morphology, and distribution of the solid lubricant powders were not varied or included in the ANN model, though these may significantly influence friction and wear characteristics.

4.2 Statistical Analysis

To substantiate the performance differences among the three training algorithms - Levenberg-Marquardt (LM), Scaled Conjugate Gradient (SCG) and Bayesian Regularization (BR) - a statistical analysis was conducted alongside the evaluation based on mean square error (MSE) and coefficient of determination (R^2). A one-way Analysis of Variance (ANOVA) was performed using MSE values generated from simulated repeated trials for each algorithm. The ANOVA results demonstrated a highly significant difference among the groups, with an F-statistic of 56637.60 and a corresponding p-value of 1.23×10^{-49}, confirming the presence of statistically meaningful variations in performance.

Further, Tukey's pairwise comparison tests were conducted to examine differences between individual algorithm pairs. The pairwise t-test results yielded p-values of approximately 7.20×10^{-33} for LM vs SCG, 7.03×10^{-20} for LM vs BR, and 4.81×10^{-33} for SCG vs BR, all indicating highly significant differences. Among the three methods, the Bayesian Regularization algorithm consistently achieved the lowest MSE and highest R^2 values, with statistical evidence supporting its superior predictive accuracy over the LM and SCG algorithms. This rigorous statistical validation strengthens the conclusion that Bayesian Regularization offers the most reliable and accurate performance in the prediction of tribological behaviour in the present study.

(a)
(b)
(c)

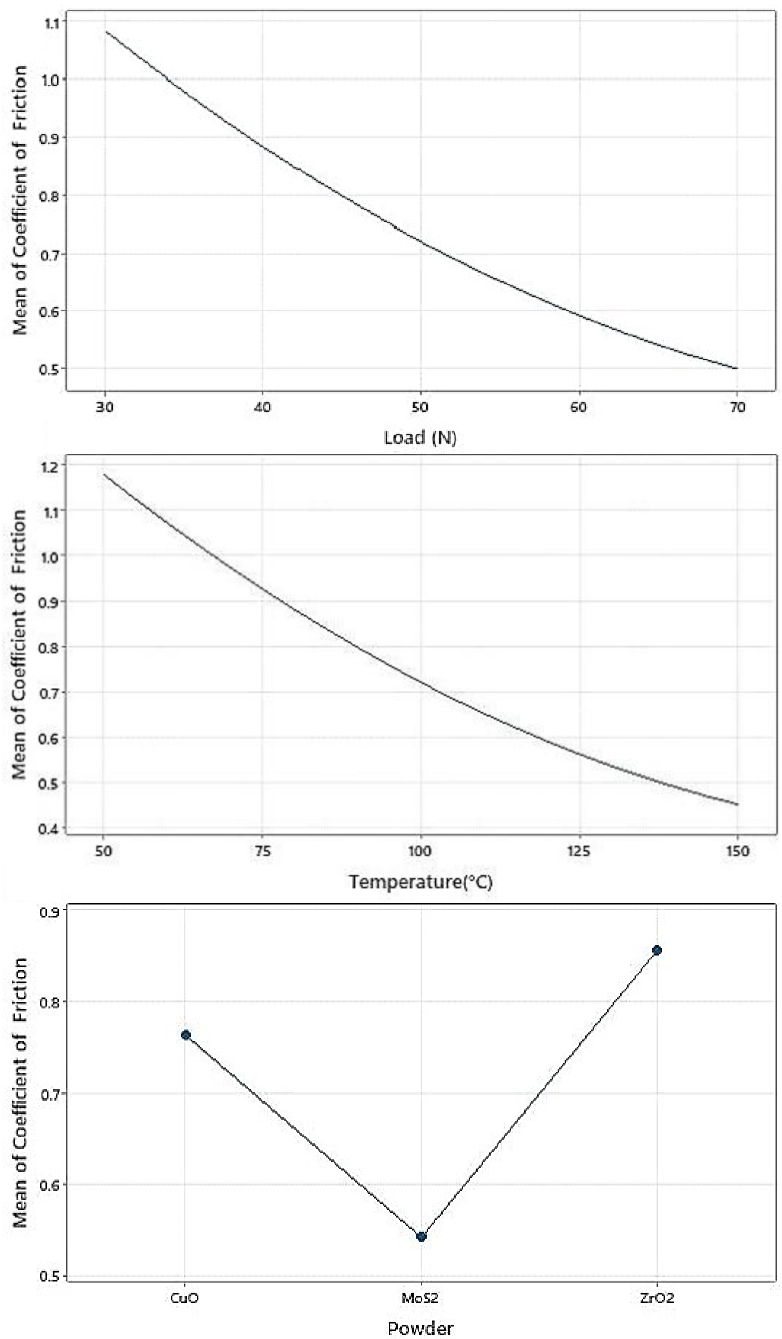
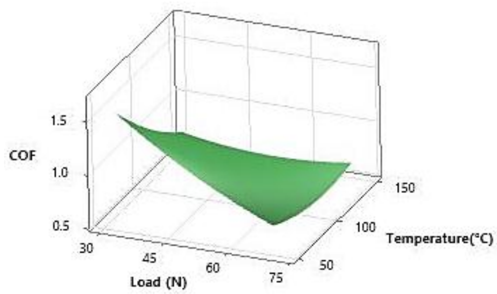
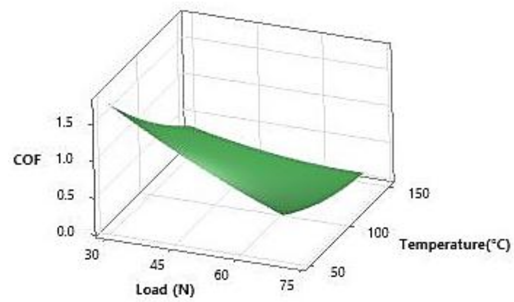


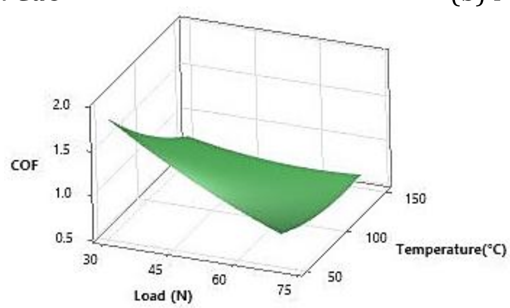
Figure 5: Main effect plots for coefficient of friction.



(a) Powder: CuO



(b) Powder: MoS_2



(c) Powder: ZrO_2

Figure 6: Surface plot of coefficient of friction COF vs. temperature (°C) and load (N).

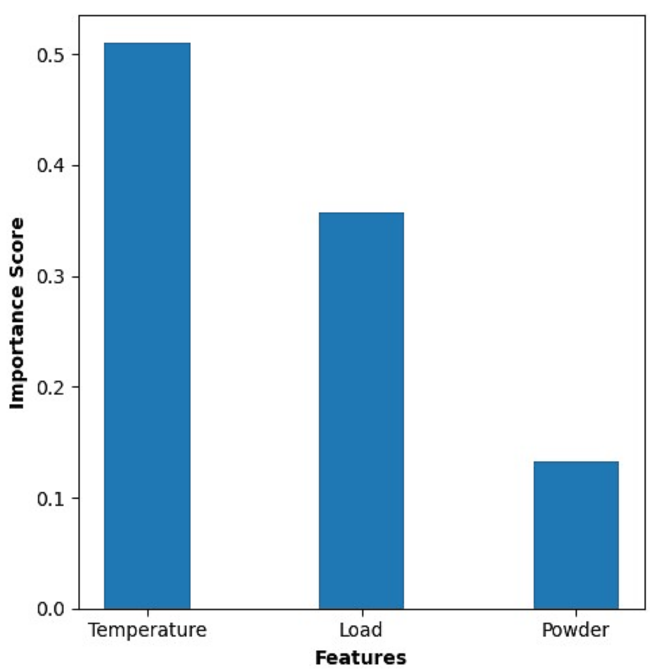


Figure 7: Feature importance plot.

5.0 CONCLUSION

In this study, the tribological parameters (such as wear and coefficient of friction) of dry sliding of metal lubricated with solid lubricant (Cupric oxide, zirconium dioxide and molybdenum disulfide) were calculated by performing reciprocating wear test. A back-propagation ANN model using three types of algorithms SCG, BR and LM) was formed for prediction of parameters. The network was trained for evaluating the performance of the network based on various quality measures such as MSE and R^2 value. The predicted data is found to be matching very well with experimental data with large ANN values. Bayesian regularization algorithm performs better than other two algorithms even if sample size is small and noisy. Scaled conjugate gradient performs poorly as compared to other algorithms.

LIST OF ABBREVIATIONS

ANN	Artificial neural network
BR	Bayesian regularization
CuO	Copper oxide
mu	Gradient, momentum constant
LM	Levenberg Marquardt
MoS_2	Molybdenum disulphide
MSE	Mean square error
R^2	Coefficient of determination
SCG	Scaled conjugate gradient
ssX	sum squared parameter
ZrO_2	Zirconium oxide

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