Tribology International 44 (2011) 603–609

Contents lists available at ScienceDirect

Tribology International

journal homepage: www.elsevier.com/locate/triboint

Artificial neural networks for predicting sliding friction and wear properties of polyphenylene sulfide composites

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ARTICLE INFO

Article history:
Received 9 July 2010
Received in revised form
21 December 2010
Accepted 23 December 2010
Available online 11 January 2011

Keywords:
Polymer composite
Friction
Wear
Artificial neural network

ABSTRACT

In this paper the potential of using artificial neural networks (ANNs) for the prediction of sliding friction and wear properties of polymer composites was explored using a newly measured dataset of 124 independent pin-on-disk sliding wear tests of polyphenylene sulfide (PPS) matrix composites. The ANN prediction profiles for the characteristic tribological properties exhibited very good agreement with the measured results demonstrating that a well trained network had been created. The data from an independent validation test series indicated that the trained neural network possessed enough generalization capability to predict input data that were different from the original training dataset.

1. Introduction

To develop and test a new composite material for tribological application is a complex process. It is necessary to select the right material composition (matrix, fillers, reinforcing phase, lubricants, etc.), the suitable manufacturing process, and to consider the operating parameters and environmental effects under which the material will function. In addition, the study and understanding of the sliding friction and wear process of polymer composites is a time-consuming, complicated task and involves high costs. One feasible solution can be the development of a predictive design tool that can operate with a comparatively small experimental database and be able to draw conclusions about non-linear relationships, even from noisy and complex data. Moreover, this tool should show good conformation between predicted and measured results (i.e. give reasonable accuracy). ANN modeling exhibits unique qualities such as non-linearity, adaptive learning, generalization, and model independence, i.e. no prior specification of the relationship or form of relationship between variables is required [1–3]. Therefore, it fully matches the imposed requirements.

Until now, the application of ANN to polymers and polymer composites, especially for dealing with their tribological properties, is still at a basic level of research [4–7]. Therefore, the exploration of the performance potential and the enhancement of the prognostic qualities are still matters of further research.

2. Artificial neural network approach

An ANN is a biologically inspired mathematical model. Similar to the brain, a neural network is a massively parallel collection of small and simple processing units [1,2,8–10]. An ANN collects its knowledge by detecting the patterns and relationships in data and learns through experience, not from programming [11,12]. Thus, while it may interpolate between data with some confidence, it cannot accurately extrapolate, and any trials at such predictions should be viewed with great care [12]. Based on the fact that an ANN learns by example, it is not necessary for it to know the theory behind a phenomenon. The modeling process is opaque similar to a "black-box" operation, therefore it is difficult to ascertain any physical relationships within the dataset using an ANN [12–14]. The main advantage of the neural network approach over conventional regression analysis is that the network constructs a solution without the need to specify the relationships or the form of relationships between variables. This feature is very helpful for modeling problems where the relationships between inputs and outputs are not clear enough or the solutions are not easily formulated in a short time [3,4,11,12,15].

The structure of an ANN (Fig. 1a) is organized in layers of units (called neurons), namely the input layer, hidden layer(s), and output layer. The numbers of units (neurons) in the input and output layer are fixed to be equal to that of input and output

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doi:10.1016/j.triboint.2010.12.011

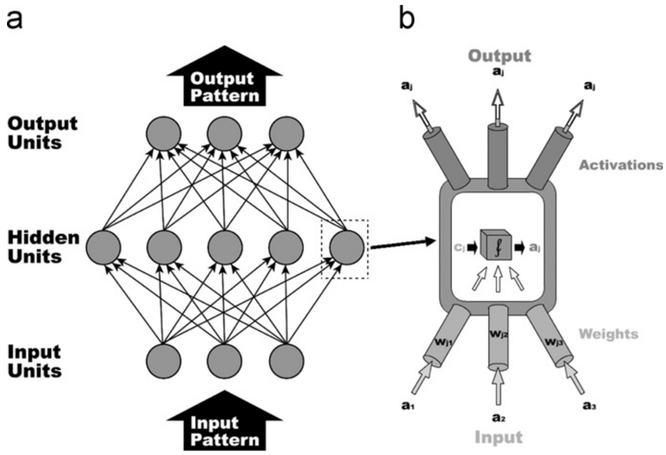

Fig. 1. Schematic representation of (a) artificial neural network, (b) artificial neuron.

variables. The hidden layer can contain more than one layer, and in each layer the number of units (neurons) is flexible [1–3,11,16].

The artificial neuron (Fig. 1b) is basically a simple calculator that works in the following way: inputs of the neuron (a_1, a_2, a_3) are multiplied by the corresponding weights assigned to them (w_{j1}, w_{j2}, w_{j3}). The weights represent the model fitting parameters. The products are then summed together to form the combined input c_j, where $c_j = a_1 w_{j1} + a_2 w_{j2} + a_3 w_{j3}$. To ensure that the output, a_j, of a neuron does not exceed its maximum or minimum activation values, a neuron's combined input must be put through an activation function (commonly a sigmoid function) that "squashes" it into the required activation value range (between 0 and 1). The output a_j is then transferred to the neurons in the layer above to which this neuron is connected. Consequently, an artificial neuron is a non-linear function of its inputs and an ANN can be viewed as a superposition of simple non-linear functions [1,2,17,18]. The problem is then to find the values of the coefficients (or weights) that give the best fit between the output of the neural network and the known experimentally measured data. The process of evaluating these coefficients is known as training [19]. When the ANN produces the desired output, which means it is trained to a satisfactory level, the weighted links between the processing units are saved. These weights are then used as an analytical tool to predict results from a new set of input data on which it was not trained before.

3. Experimental: materials, processing, and testing

In order to build a well balanced model, it is important to collect a suitable dataset. Likewise, it is significant when training a neural network to collect data, which cover the entire operating range of the system at a sampling rate sufficient to capture its generalizable behavior [20]. Following these rules, a new measurement series was performed with thermoplastic matrix composites. The matrix material used was polyphenylene sulfide (Fortron grade 0214, Ticona GmbH, Germany). Diverse traditional reinforcing agents and additives as well as sub-micro particles were chosen to enhance the matrix property profile: pitch-based short carbon fiber (Kureha M-2007S, Kureha Chemicals GmbH), graphite (Superior 9039, Superior Graphite Europe Ltd.), PTFE (Dyneon 9207, Dyneon), sub-micro TiO_2 (Kronos 2310, Kronos Titan GmbH). The matrix was mixed with the fillers in a twin-screw extruder (ZE25Ax44D, Berstorff GmbH, Germany). Finally, the materials were injection molded into rectangular plates ($80 \times 80 \times 4$ mm^3) using an injection molding machine (Allrounder, Arburg GmbH) at a barrel temperature of 310–335 °C depending on the corresponding filler loading fraction. The mold temperature was set to 150 °C. In total, 29 different material combinations were manufactured. The microstructure of one such material is shown in Fig. 2.

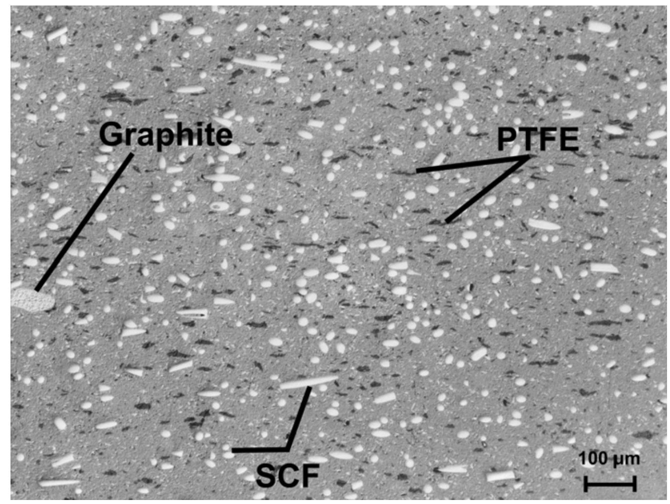

Fig. 2. Light micrograph of a PPS-based composite material containing 10 vol% SCF, 5 vol% TiO_2 (300 nm), 10 vol% Gr, 5 vol% PTFE.

The sliding friction and wear tests to generate the experimental data were performed on a Wazau pin-on-disk (P-o-D) test rig. During testing a rotating polymer pin is pressed against a stationary steel disk (Fig. 3a). For the purpose of testing, samples were cut into pins with a contact surface of 4×4 mm^2. In order to ensure identical flow conditions during injection molding (i.e. to have equal fiber orientation) only the middle section of the plates was chosen for machining the samples. All the samples were cut so that the loading applied was in the mold filling (melt flow) direction (Fig. 3b).

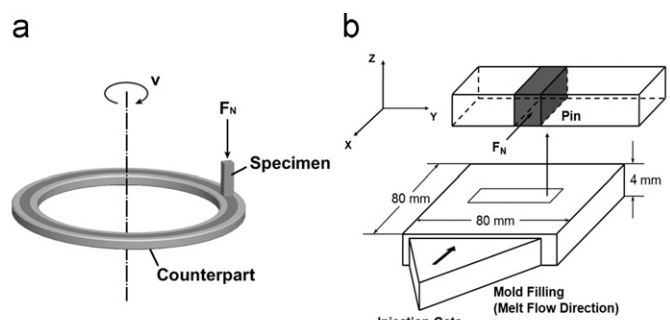

Fig. 3. Schematic representation of (a) pin-on-disk sliding test configuration, (b) sample selection for P-o-D testing.

The sliding friction and wear tests were carried out under dry testing conditions and at room temperature. The testing parameters were varied as follows: applied pressure (p) in the range from 1 to 4 MPa, using an increment of 1 MPa; sliding speed (v) of 1 and 3 m/s. At least three pins were tested per testing condition, and the average values were taken. The counterface was a 100 Cr6 (German standard DIN 616) steel disk (LS 2542, INA-Schaeffler KG), where the average surface roughness at the beginning of the test was about $R_a = 0.19$ µm, and the hardness amounted to around 63 HRC. Prior to executing the tests, the contact surface of the pin was polished by abrasion against fine silicon carbide paper (grit number P 400, Buehler, Germany) for a very short time to render the same level of surface finish for all the test specimens. Subsequently, the polymer pin and steel counterface were cleaned with isopropanol and acetone, respectively, followed by drying. The testing time was fixed to 20 h, allowing the system to reach steady-state tribological conditions. For some of the materials, e.g. pristine PPS, the test was stopped after 1 h due to excessive wear. In the course of the experiments both the normal load (F_N) and friction force (F_F) were recorded simultaneously to determine the coefficient of friction

$$\mu = \frac{F_F}{F_N} \tag{1}$$

The surface temperature was recorded by an embedded subsurface thermocouple fixed into the non-contacting surface, namely at the rear side of the stationary steel counterface. The specific wear rate, w_s, was calculated from the mass loss of the specimen after the test over the total test duration (Eq. (2)). This includes some small inaccuracy, due to the averaging over the running-in and steady state phases, but makes the evaluation procedure easier [21].

$$w_s = \frac{\Delta m}{\rho v t F_N} \,[\mathrm{mm^3/Nm}] \tag{2}$$

in which the individual quantities have the following meanings: F_N is the normal force applied to the specimen during sliding, Δm is the mass loss, ρ is the density of the material being tested, v is the sliding speed, and t is the testing time.

4. Collected datasets, ANN architecture, and learning algorithm

Five training datasets were collected or expanded throughout a period of three years (Fig. 4). All datasets used for training and prediction include the material compositions and testing conditions as input parameters, respectively. The output parameters were the tribological properties (Table 1). 80–90% of the data in each dataset was used for training; the remaining 10–20% of the dataset was utilized for testing the ANN prediction quality. The data for the specific wear rate was initially normalized (logarithmically compressed) and scaled to the range $[-1, 1]$ in order to improve the learning speed as these values fall in the region of the sigmoid transfer function. After training, the normalized output values were converted to real values. The transfer functions used were the *tansig* function for the hidden layer and *purelin* function for the output layer. The training and testing processes were repeated 200 times. The maximum number of iterations (epochs) in the training process was set to 1000. The training process stopped when either the value of end iteration was reached or the mean relative error (MRE) minimum was attained.

$$\mathrm{MRE} = \frac{1}{n}\sum_{i=1}^{n} \frac{|d_i - o_i|}{d_i} \tag{3}$$

in which d_i is the desired value, o_i is the predicted output value, and n is the number of data (total number of entries).

The initial weights and biases of the network were generated automatically by the written program. Based on a former methodology study the initially selected learning method with dataset I (Fig. 4) was the Powell–Beale conjugate gradient algorithm CGB (traincgb). However, it has been established within later research activities using an expanded version of dataset I (in total 84 independent data measurement points with PPS matrix composites) that the variable learning rate algorithm GDX (traingdx) performs superiorly over CGB both in terms of replicating the training data (higher accuracy) and rapid convergence. Thus, the GDX algorithm has been used in the further training of the ANN. The initially selected learning rate was 0.02. The computer used for performing the training and prediction was a Pentium (R) 4 CPU at 2.00 to 3.20 GHz.

The optimum network architectures for the coefficient of friction and specific wear rate were $7\text{-}[3\text{-}1]_2\text{-}1$ and $7\text{-}[9\text{-}3]_2\text{-}1$, respectively (Fig. 4). These two network architectures were experimentally found in a train-test procedure with the expanded version of dataset I (in total 84 independent data measurement points with PPS matrix composites). Over 400 different network configurations were evaluated by systematically varying both the number of hidden layers (between 1 and 2) and the number of neurons in the hidden layer (between 1 and 20). Each network was trained with 80–90% of the data and then tested by 10–20% of the data. This procedure was repeated 200 times. The performance of each network was assessed in terms of the mean relative error, defined by Eq. (3). The networks that yielded the lowest mean relative error were chosen subsequently for modeling the sliding friction and wear properties of the PPS composites as shown in Fig. 4.

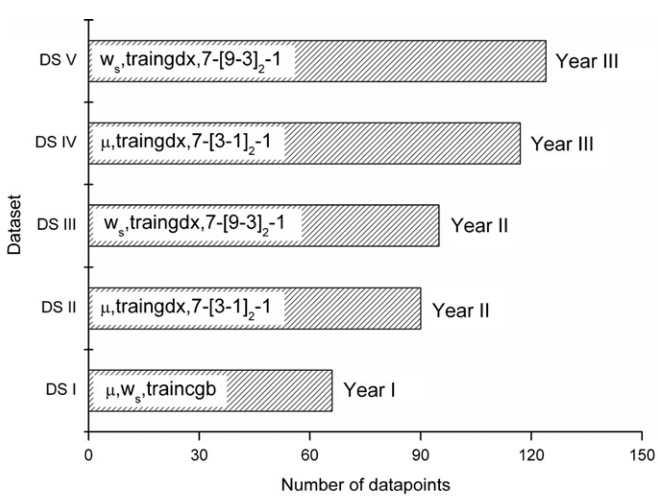

Fig. 4. Datasets, learning algorithm, and architecture of the ANN for sliding friction and wear prediction with PPS matrix composites.

5. Development of a graphical user interface (GUI) for training and prediction

A user-friendly graphical interface was developed at the Institute for Composite Materials (IVW GmbH) based on the

Table 1
Measured parameters and values used for input and output of the ANN.

Input				
Material compositions	PPS matrix (65–100 vol%)	Short carbon fiber (0–20 vol%)	TiO_2 (0–7 vol%)	PTFE (0, 5, 10 vol%) Graphite (0, 5, 10 vol%)
Testing conditions	Sliding speed (1, 3 m/s)	Applied pressure (1, 2, 3, 4 MPa)		
Output				
Tribological characteristics	Coefficient of friction	Specific wear rate		

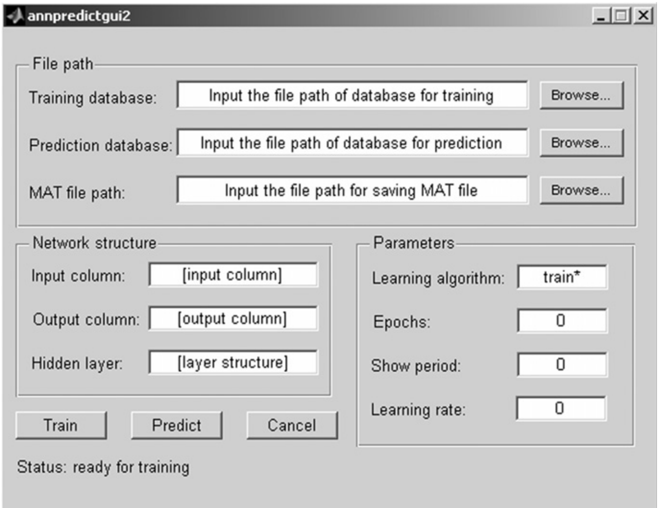

Fig. 5. GUI developed for ANN training and prediction.

Neural Network Toolbox in Matlab 7.0.4 (The Math Works Inc.) environment [22] for performing network training and prediction with the ANN (Fig. 5). The developed software interface enables the user to load the acquired training and/or prediction databases in Excel format, which are then used for ANN training and/or prediction. The GUI permits the user to select the network architecture (input column, output column, and hidden layer), the training (learning) algorithm as well as some extra parameters such as learning rate, number of epochs and show period (the interval at which the training status is displayed). Once all the information has been entered and the network has been trained, the user activates the prediction. The output is returned to the GUI and saved in Excel format along with the MRE and the consumed time. The model will work with sufficient accuracy within the range of the dataset used in the training. If the user defines input conditions outside this range the software will still generate an output but it may not be correct. The user can also use the GUI to simulate results for new input parameters. No in-depth knowledge of Matlab or computer programming is necessary for successful navigation of the designed GUI.

6. Results and discussion

6.1. Effect of the size of training dataset

A comparison of the MRE generated after training of the ANN with the different training datasets (Table 2) shows that the predicting performance improves significantly with the enlarged datasets reaching a value of about 0.10 for the coefficient of friction and 0.55 for the specific wear rate. But what does a MRE of 0.55 really mean? It means that the average predicted value will be within 55% of the average measured value for the specific wear rate. Even if a predicted value is outside the measured range, the MRE can still be less than 1 provided that the average difference between the predicted values and measured values does not exceed 100% of the average measured value. A MRE greater than 1 implies that the average predicted value is outside the range of the measured values. This indicates that the number of data points is insufficient for the network prediction. It can be seen that the value of the MRE for sliding friction is much lower than for the specific wear rate. This outcome for the MRE is in agreement with previously published results from the authors [23,24] as well as by others [25]. Likewise, for the specific wear rate the measured values scatter in a very wide range (in some

Table 2
MRE evaluation of output data with the different training datasets.

Dataset	Number of data points	Property	MRE
DS I [23]	66	Coefficient of friction	>0.11
DS I [23]	66	Specific wear rate	>1.0
DS II [24]	90	Coefficient of friction	0.11
DS III [24]	95	Specific wear rate	0.72
DS IV	117	Coefficient of friction	≤ 0.10
DS V	124	Specific wear rate	≤ 0.55

cases up to more than 50%). For the coefficient of friction the values scatter was much smaller. Therefore, it is more difficult with the specific wear rate to adjust the weights to perfectly match all the values in the output layer.

6.2. Neural network training and model validation

There exist two stages in the development of proper artificial neural network models for dealing with a given problem. During the first stage, the so-called training stage, the network is trained by presenting a balanced set of training examples to it that effectively represents the environment of interest (i.e. system's operating range). The number of training examples depends to a great extent on the physical complexity of the considered problem. Therefore, for complex and noisy data the training dataset must be sampled at a scale, which is sufficiently fine to capture the underlying relationship. Training (learning) then allows the network to adjust and optimize its weights for modeling the assigned problem. In the process of training the designed neural network, one part of the training data should be used for training ($\approx 80\%$) and the rest ($\approx 20\%$) for testing the network performance in terms of the mean relative error. In the usual case the computer program should be written in a way to permit random partitioning of the whole training database in training subset and testing subset each time when it was run in order to optimize the training process. The aim during this stage is to obtain a network that will be able to generalize. In the second validation stage, the generalization abilities of the designed network are tested, i.e. the ability of the network to respond accurately to data never used in creating or training it. The validation test data should be drawn from the same data domain used to generate the training data. If the verification of the network is successful then the network can be used for practical cases.

To complement our studies [26,27], within this work the previously designed neural networks were trained using expanded versions of already collected datasets for modeling both the coefficient of friction and specific wear rate. In addition, the generalization abilities of the two optimized networks were checked for unseen cases. Such network verification had not been done before. Only testing subsets were operated to examine the prediction ability of the designed networks, using data that has already been used in training the networks.

6.2.1. Coefficient of friction

Fig. 6a shows the prediction profile generated after training the ANN for predicting the coefficient of friction based on the largest collected training dataset in this study consisting of 117 independent data points (DS IV, Fig. 4). It is clearly seen that the predicted results (depicted as mesh data) are either close or identical to the corresponding experimentally measured values (depicted as black dots with error bars). These results infer that the network was able to respond correctly to the input patterns that were used for its training.

The validation of the network model is shown in Fig. 6b using an independent validation dataset within the range of the examined experimental conditions but never used in the network

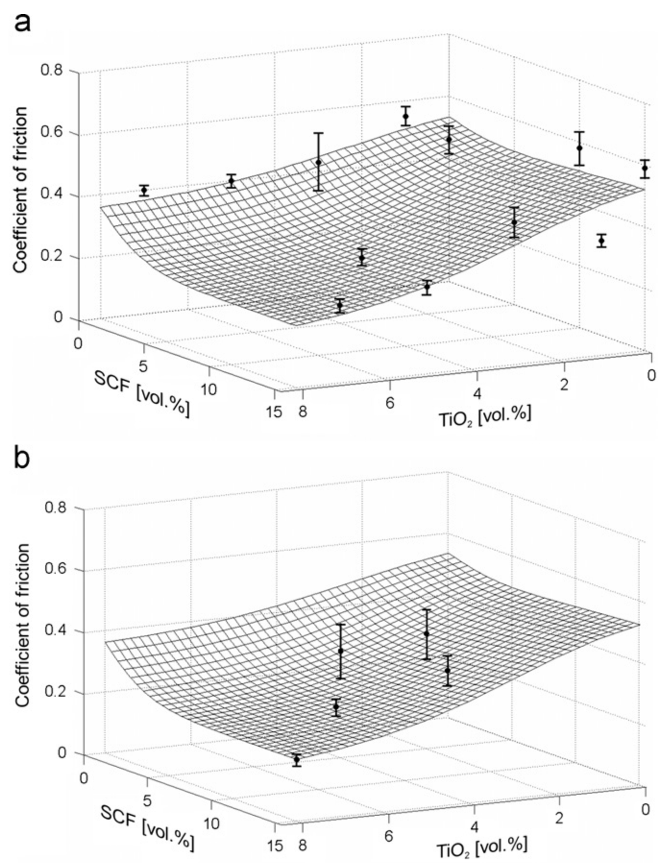

Fig. 6. Experimental (black points with error bars) vs. predicted (3D mesh) values of the coefficient of friction (average value in steady state) as a function of SCF- and sub-micro TiO_2-volume content: (a) training dataset, (b) validation dataset. The testing conditions were: $p=1$ MPa, $v=1$ m/s.

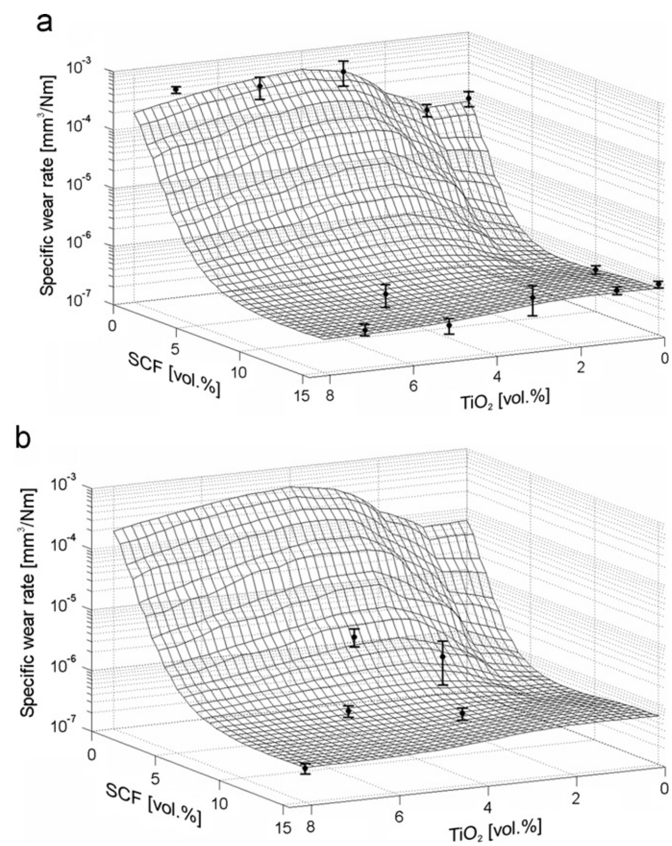

Fig. 7. Experimental (black points with error bars) vs. predicted (3D mesh) values of the specific wear rate as a function of SCF- and sub-micro TiO_2-volume content: (a) training dataset, (b) validation dataset. The testing conditions were: $p=1$ MPa, $v=1$ m/s.

development. Exact prediction is established for all validation points. The latter is an indicator that the designed model is able to interpolate accurately for input data different from the training data.

6.2.2. *Specific wear rate*

Fig. 7a displays a surface plot of the predicted values for the specific wear rate together with measured data that has been used in training the network based on the largest dataset collected in this work (124 independent data points, DS V, Fig. 4). In contrast to former predictions [26,27], in this case the prediction was done for the continuous range of carbon fiber loading fraction, namely 0–15 vol% using an increment value of 1 vol% prior to applying the "meshgrid" command in Matlab. Using a smaller increment of fiber volume fraction avoids the sudden drop in the predicted specific wear rate data since the wear rate decreases rapidly as SCF volume fraction increases. As for the concentration range of TiO_2 particles, for all the cases this was kept constant, namely 0–8 vol% with 1 vol% increment value. For the entire training test data the predicted results are either correct or very close to the actual measured values (Fig. 7a). At this stage it can be concluded that the training of the network is satisfactory, i.e. the network has learnt the complex relationship between the selected input and the corresponding output for the examples presented in the training dataset.

The developed and trained ANN model until now successfully mapped the relationship between various input parameters and the output specific wear rate values. Still, for its practical use it must be checked if it is also able to generalize this relationship. The validation of the network model for the specific wear rate is presented in Fig. 7b. All validation test points were predicted exactly (or within the error bands limits). These results indicate that the developed ANN model for predicting the specific wear rate is both reasonably correct and able to generalize well.

At this stage, it is possible to use the excellent generalization capability of the optimized ANN models to analyze the impact of the two fillers, namely SCF and sub-micro TiO_2, on the sliding friction and wear properties of PPS composites over a much broader range without performing exhaustive experimental work. It is obvious from Fig. 6 that the combination of the two fillers results in a lower coefficient of friction. Although the mechanisms of reduction in coefficient of friction contributed by each of the two fillers are different, it is clear that they can work together simultaneously. As shown already experimentally [7], short carbon fibers play a key role in improving the wear resistance of PPS, as a single or second reinforcing phase. It is predicted that the specific wear rate decreases with increasing volume fraction of SCF, however less steeply at larger volume fractions (≥ 7 vol%). With the incorporation of both short carbon fibers and TiO_2 sub-micro particles in PPS matrix, a hybrid reinforcement effect can be found. For higher SCF concentrations (≥ 8 vol%), the specific wear rate exhibited a drop-off tendency with the increase of TiO_2 content in the range 1–8 vol%. This type of relationship is in agreement with the experimental results of Zhang and Friedrich [28] for epoxy composites. Such favorable synergistic effects between carbon fibers and sub-micro TiO_2 have also been foreseen by ANNs in PTFE matrix composites [29]. According to both the experimental results and the ANN prediction, the composition of PPS with 15 vol% SCF and 8 vol% TiO_2 (300 nm) gives the best wear resistance (i.e. the lowest specific wear rate).

6.3. Effect of internal lubricants in hybrid polymer systems

The created ANN models were also applied for studying the effect of loading fraction of Gr and PTFE in a hybrid reinforced PPS containing 10 vol% SCF and 5 vol% TiO_2 (Fig. 8). It is readily apparent that the predicted results exhibit good correlation with the measured values. Under these mild conditions the average coefficient of friction in steady state (Fig. 8a) is more or less insensitive to the addition of both lubricants. The specific wear rate shows a decreasing trend when the loading fraction of both fillers is increased up to a center level and then reduces only slightly. Optimum results can be attained with a Gr loading fraction of 3 vol% and PTFE loading fraction of 6–7 vol%. Likewise, it can be seen that a high loading fraction of Gr or PTFE (10 vol%) when acting as single lubricating phase is also beneficial in diminishing wear. The results for the specific wear rate conform well to former experimental results with a PEEK thermoplastic matrix [30].

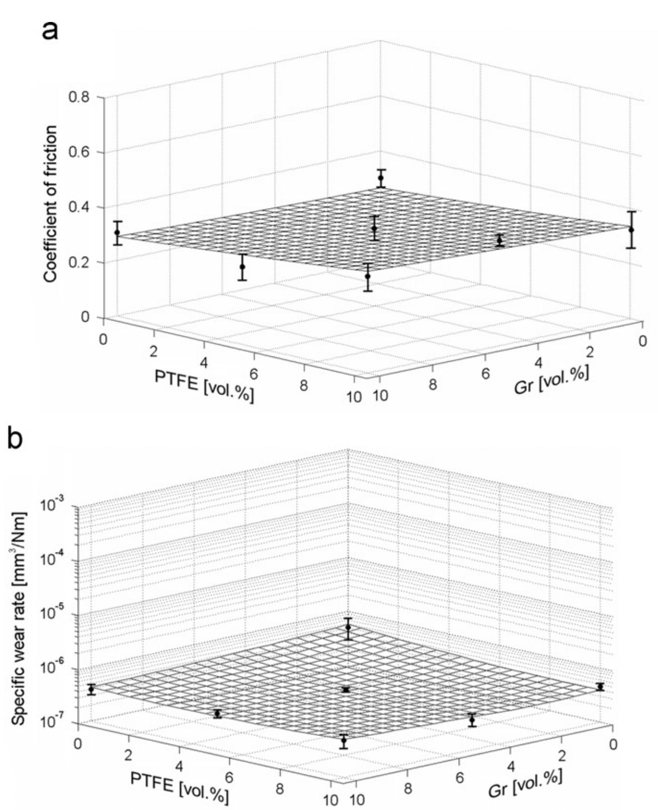

Fig. 8. ANN predicted 3D plots of (a) coefficient of friction (average value in steady state) and (b) specific wear rate of a hybrid reinforced PPS/SCF/TiO_2 system as function of Gr- and PTFE-volume content. The measured data are plotted as black points with error bars. The testing conditions were: $p=1$ MPa, $v=1$ m/s.

7. Summary

Through the application of the ANN technique to preexisting experimental datasets collected from pin-on-disk tests with PPS composites, it was demonstrated that it is possible to develop a neural network model that is able to learn from examples presented to it and construct proper fitting function that correctly reproduces not only the characteristic tribological properties for these examples but is also able to interpolate correctly for unseen cases from the same knowledge domain. The latter illustrated the power of the neural network approach to predict the evolution of characteristic tribological parameters as a function of material type, applied pressure and sliding speed without having to perform the total number of experimental combinations. The surface can also be used to evaluate cost-performance benefits.

According to both the experimental results and the ANN predictions, the composition of PPS with 15 vol% SCF and 8 vol% TiO_2 gives the best wear resistance (i.e. the lowest specific wear rate). Subsequently, the lubricating contributions of Gr and PTFE in such multi-component materials were studied via the designed ANNs. Under the selected mild conditions ($pv=1$ MPa m/s) there was only minor influence with the addition of Gr and PTFE. This might be related to the slow release and supply of the internal lubricants from the polymer matrix to the sliding interface under these operating conditions.

Acknowledgements

The authors sincerely acknowledge the German Research Foundation (DFG) for the financial support of this research work within DFG FR 675/45-1 and DFG SCHL 280/7-2. Equally, we would like to thank the companies Ensinger GmbH (Germany) and Ticona GmbH (Germany) for supplying some of the raw materials as well as the company FACT GmbH (Germany) for lending the tool for injection molding.

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