Computational Materials Science 153 (2018) 1–9

Contents lists available at ScienceDirect

Computational Materials Science

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

Artificial neural network modeling to evaluate polyvinylchloride composites' properties

Safwan Altarazi[a,*], Maysa Ammouri[a], Ala Hijazi[b]

[a] Industrial Engineering Department, German Jordanian University, Amman, Jordan
[b] Mechanical Engineering Department, German Jordanian University, Amman, Jordan

ARTICLE INFO

Keywords:
Polymers and plastics
Artificial neural networks
Mechanical properties
Supervised learning
Design of experiments

ABSTRACT

The mechanical properties of extruded Polyvinylchloride (PVC) composites cannot be easily predicted due to the nonlinear nature of the relationship between the composite's composition and the resulting after-production properties. In the work presented herein, supervised artificial neural network (ANN) modeling is used to predict and optimize three properties (tensile strength, ductility and density) of PVC composites having different weight percentages of virgin PVC, $CaCO_3$, plasticizers, and recycled PVC. Different ANN models, designed and analyzed through factorial design and analysis of variance methodology, were evaluated using an experimental dataset which was designed according to the mixture design of experiments approach. The results show that the constituents-mechanical properties relationship of PVC composites' can be accurately estimated using several ANN models including Levenberg-Marquardt/6-$[18\text{-}9]_3$-3/Radial basis and Levenberg-Marquardt/6-[9-18]3-3/Log sigmoid models. The results also show that the ANN modeling is capable of determining the optimal weight percentages of the different PVC composite constituents in order to achieve a required composite property.

1. Introduction

Polyvinyl chloride, known as PVC, is one of the most widely produced and chemical industry-valuable polymers worldwide [1]. PVC has relatively good mechanical properties, durability, stability, and processability [2,3]; accordingly, it appears in a wide range of consumer products, such as pipes, window frames, packaging, cables, floorings, and toys. The required properties of PVC can slightly differ according to the type of product; where for instance some products require higher ductility while others require higher tensile strength or impact resistance, etc. In general, the desired material properties of PVC products can be attained through formulation with additives including plasticizers, fillers, stabilizers, flame retardants, antistatic and coloring agents, as well as recycled PVC and other polymers [4–7]. Plasticizers, such as di-2-ethylhexyl phthalate (DOP), and chlorinated paraffin wax (CPW) are added to PVC to increase its ductility, toughness, flexibility, and workability [8,9]. Fillers, such as calcium carbonate ($CaCO_3$), titanium dioxide, wood, and silica flour are usually added to improve product stiffness, tensile strength, impact and abrasion resistance, as well as other properties [5,10,11]. In addition, fillers are typically incorporated to reduce the costs of PVC products. High filler percentages, however, may undesirably affect the processability, ductility, and strength of PVC composites. Furthermore, in the last few decades, PVC recycling has gained high attention because of its important environmental and economic benefits [12]. Thus, in recent years, it became highly desirable to use some percentage of recycled PVC as one of the ingredients in PVC composites.

For decades, artificial neural networks (ANN's) have offered powerful framework for modeling nonlinear systems especially those that are chemical-oriented [13,14], hence, enabling better understanding of these highly uncertain systems and assisting in probable prediction of their future responses. Originally, ANN's were inspired by the way human nervous system works; it resembles the human brain by acquiring knowledge in a learning process and by storing this knowledge through an interneuron connection known as synaptic weight [14]. Based on past experience expressed as an input–output dataset, an ANN learns the studied system through a training process and then forecasts the outputs for new set of inputs. The ANN's easiness of development and use, and their ability to learn by examples make them particularly useful when modeling complicated processes where detailed mechanistic models are difficult to develop [15].

One way to optimize the composition of PVC composites is to investigate the effect of the composites' constituents on the physical and mechanical properties of the finished PVC product then to choose the optimum composition [16,17]. The objective of this research is to study the combined effect of different additives/constituents on the

* Corresponding author.
E-mail addresses: safwan.altarazi@gju.edu.jo (S. Altarazi), maysa.ammouri@gju.edu.jo (M. Ammouri), ala.hijazi@gmail.com (A. Hijazi).

https://doi.org/10.1016/j.commatsci.2018.06.003
Received 22 January 2018; Received in revised form 1 June 2018; Accepted 2 June 2018
0927-0256/

mechanical properties of PVC composites such that the composition can be optimized to attain desired properties. In order to do such, both the design of experiments and the ANN modeling approaches were utilized. The relationship between the PVC composites' constituents and the resulting properties is highly nonlinear and that can be attributed to the complexity of the used production processes (extrusion, injection, or molding), inter-components effects, and components-properties effects. Hence, utilizing advanced computing methods for modeling such complex relationship is quite necessary. In this paper, an ANN approach was utilized for modeling the mechanical behavior of PVC composites. A thorough supervised ANN modeling was used to predict and optimize three properties of PVC composites (tensile strength, ductility and density) based on different weight percentages of virgin PVC, $CaCO_3$, plasticizers, and recycled PVC. Different ANN models were evaluated using an experimental dataset which was designed according to the mixture design of experiments approach. The ANN models' elements including learning algorithm, architecture, and activation function were selected according to factorial design and analysis of variance methodology. The feed-forward supervised multi-layer neural network, which is the most widely proven ANN architecture for universal approximation of nonlinear relationships [15,18], was used to build the model. The experimental dataset, containing composite compositions as input elements and mechanical properties as output responses, was split into three subgroups: learning, validating, and testing. The results show that ANN modeling is capable of determining the optimal weight percentages of the different PVC constituents in order to achieve required properties. This paper presents a thorough ANN modeling approach for optimizing PVC composites' properties; yet the approach is fairly general such that it can also be implemented in optimizing any materials' composition-properties relationship.

2. Background

2.1. ANN principles

ANN's can be defined as a wide class of flexible non-linear regression and discriminated models, data reduction models, and non-linear dynamic models. Essentially, an ANN consists of nodes (neurons) organized in layers, weighted links between nodes, and activation functions [13,14,19]. The node set consists of input nodes, called input layer, hidden nodes (in hidden layers) and output nodes (in output layer). Nodes in the input layer represent the input features, while output layer nodes are the model output. The structure of an ANN can be expressed as: $N_{in}-[N_1-N_2-...-N_h]_h-N_{out}$, where N_{in} and N_{out} represent the number of input and output variables, respectively; N_1, N_2 and N_h are the numbers of the neurons in each hidden layer, and h is the number of hidden layers. Each node in the hidden layer is described by an activation function (more details are in Table 3). Each node-to-node interconnection is associated with a multiplicative parameter called weight. For each node in the hidden layers, weighted inputs are summed and acted upon an activation function, and are then mapped to the next hidden layer of neurons and continue to the output layer.

The ANN weights are determined by training the network. A network is trained by feeding it with an input/output dataset, gradually; the network learns the input/output relationship by modifying the weights to minimize the error between the actual and predicted patterns of the training data set [20]. Available training (also called learning) algorithms can be classified into supervised training, reinforcement or graded training and unsupervised training [15]; where supervised and unsupervised are the basic ANN's training classes [21]. In supervised training, with which networks called supervised networks, the target output is known, errors are calculated and the weighted links are revised as the data are processed through the network again. In unsupervised ANN, the network attempts to cluster the available data set. Back-propagation (BPP) algorithm is the most utilized supervised learning algorithm [22,24] (more details are in Table 2). After training, a separate set of data, usually excluded from the training set, is used to evaluate the network performance according to various criteria including the mean square error (MSE), relative absolute mean error (RAME), and coefficient of determination (R^2). Below are the equations of these criteria.

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

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

$$R^2 = \left(\frac{n\sum_{i=1}^{n} y_i\hat{y}_i - \sum_{i=1}^{n} y_i \sum_{i=1}^{n}\hat{y}_i}{\sqrt{n\sum_{i=1}^{n} y_i^2 - \left(\sum_{i=1}^{n} y_i\right)^2}\sqrt{n\sum_{i=1}^{n}\hat{y}_i - \left(\sum_{i=1}^{n}\hat{y}_i\right)^2}}\right)^2 \tag{3}$$

where:

n is the number of tested instances
$\hat{y}_i$ is the predicted value estimated by the trained network for instances i, and
y_i is the target value of the instances i

2.2. ANN modeling of constituents-properties relationship

ANN's have been applied in many research fields, such as optimization, regression, pattern recognition, classification, systems' performance, forecasting, processes modeling, materials structures development, etc. [25–30]. Several researchers have employed ANN's to predict manufacturing processes' resulting material properties using input characteristics of materials compositions and processes operational parameters. Munoz-Escalona and Maropoulos [18] implemented feed-forward, generalized regression, and radial base types of ANN's to predict aluminum alloy surface roughness after face milling process; their results showed that the feed-forward ANN gives the best predictions. Ashhab et al. [31] modeled the combined deep drawing–extrusion process using ANN integrated with constraint optimization; their approach gave good predictions of the total equivalent plastic strain, contact ratio and forming force as functions of the process geometric parameters. Lucignano et al. [32] adopted ANN with the Levemberg Marquard training algorithm to optimize the aluminum extrusion process; their ANN model results were found very comparable with the experimental values. For polymers' composites, ANNs were used for predicting several properties such as fatigue, wear, and dynamic mechanical properties [33].

Velten et al. [22] were among the pioneers in applying ANN's to polymers composites; they used ANN's to predict the wear of short-fiber reinforced thermoplastics. Zhang et al. [23] applied feed-forward ANN to predict the wear rate and frictional coefficient for short-fiber reinforced polyamide composites and they were able to achieve highly accurate predictions. Seyhan et al. [24] implemented ANN's to predict the ply-lay-up compressive strength of VARTM processed E-glass/polyester composites and concluded that ANN can perform better than multilinear regression models in predicting such properties. Fazilat et al. [34] employed ANN's and adaptive neuro-fuzzy inference system to predict the mechanical properties of glass fiber reinforced polymers. Moosavi and Soltani [35] predicted the specific volumes of some polymeric systems, such as Poly ethylene glycols, using a combined ANN and group contribution method; they found that this method is simpler and more accurate than other specific volume measuring methods. Jayaba et al. [36] developed an ANN model to predict the mechanical properties, including tensile strength and impact resistance, of calcium carbonate particles-impregnated coir fiber-reinforced polyester. Yadollahi et al. [37] used ANN's for the prediction of geopolymer compressive strength and they were able to achieve good accuracy which was evident by the high coefficient of determination they