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# Prediction of the specific volume of polymeric systems using the artificial neural network-group contribution method

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ABSTRACT

In this work, the specific volumes of some polymeric systems have been estimated using a combined method that includes an artificial neural network (ANN) and a simple group contribution method (GCM). A total of 2865 data points of specific volume at several temperatures and pressures, corresponding to 25 different polymeric systems have been used to train, validate and test the model. This study shows that the ANN–GCM model represent an excellent alternative for the estimation of the specific volume of different polymeric systems with a good accuracy. The average relative deviations for train, validation, and test sets are 0.0403, 0.0439, and 0.0482, respectively. A wide comparison between our results and those of obtained from some previous methods show that this work can provide a simple procedure for prediction the specific volume of different polymeric systems in a better accord with experimental data up to high temperature, high pressure (HTHP) conditions



## 1. Introduction

Polymeric systems almost affect on all aspects of our life. These systems are widely used for industrial and academic purposes. For example, Poly ethylene glycols (PEGs), are frequently used in the pharmaceutical and cosmetic fields as solvents, carriers, humectants, lubricants, binders, bases, and coupling agents and also for extraction, separation, and purification of biological materials [1]. In recent years, great interest has been focused on the measurement, correlation, and prediction of thermodynamic properties of polymers. Thermodynamic properties of polymeric systems play an important role in the polymer industry and are often a key factor in polymer production, processing, and material development, especially for the design of advanced polymeric materials [2–8].

During the past decades, some attempts have been made to predict the specific volume and other thermodynamic properties of polymeric systems [2–14]. Different authors used different equations and methods to predict and reproduce the thermodynamic properties of polymer systems. Most of these attempts are restricted to the limited systems and little systematic work has been devoted to test the ability of these equations to predict the thermodynamic properties of these systems.

An artificial neural network (ANN) can be a suitable alternative to model the different thermodynamic properties. Neural networks generally consist of a number of interconnected processing elements or neurons. How the inter-neuron connections are arranged and the nature of the connections determines the structure of a network. How the strengths of the connections are adjusted or trained to achieve a desired overall behavior of the network is governed by its learning algorithm [15]. In other words, ANN is an especially efficient algorithm to approximate any function with a finite number of discontinuities by learning the relationships between the input and output vectors [16]. Thus, an ANN is an appropriate technique to model the nonlinear behavior of chemical properties. Recently, neural networks have been used to estimate the different thermodynamic properties such as density, melting point, vapor pressure, etc. for different classes of materials [17–27]. In the last years, some limited attempts have been made to develop ANN models to predict the specific volume of polymeric systems [13,14,28]. Yousefi and Karimi [13,14] developed the ANN models for prediction the specific volume of limited polymeric systems. They used the genetic algorithm to train the neural networks in an unsupervised manner. Zhang and Friedrich [28] reviewed the application of artificial neural networks to polymer composites.

This study was undertaken to investigate the specific volumes of 25 different polymeric systems at different temperatures and pressures using a combined method that includes an artificial neural network (ANN) and a simple group contribution method (GCM) up to the extremely HTHP conditions.

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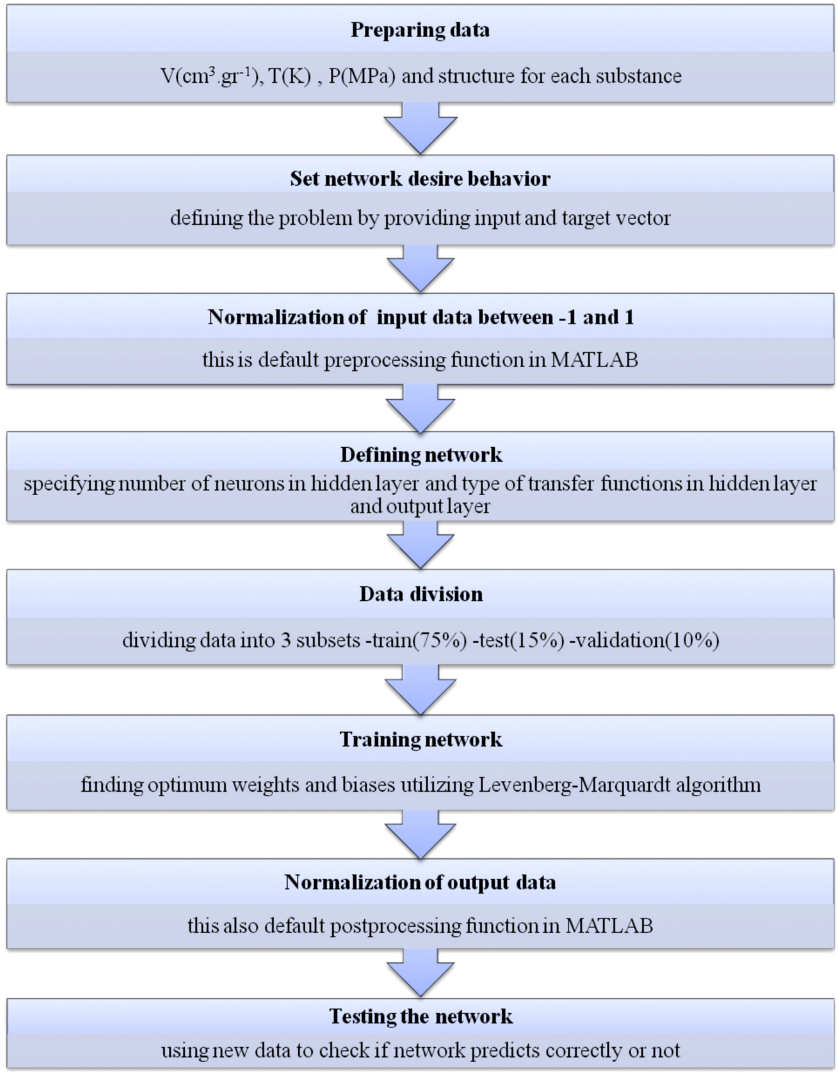


**Scheme 1.** The ANN–GCM model used in this work.

## 2. Methodology and modeling

Artificial neural networks (ANNs) are designed by simulation of human brain procedures and have been extensively used in various scientific and engineering areas such as estimations of physical and chemical properties [29]. These powerful tools can be usually applied to study the complicated systems especially at extreme conditions. The theoretical explanations about neural networks can be found in many references such as reference [30].

The database is divided into three subdata sets including the training, validation, and test sets. The training set is used to generate the ANN structure in which a neural network modifies the weights and biases in answer to initial information. The validation (optimization) set is applied for optimization of the model, and the test (prediction) set is used to investigate the prediction capability and validity of the obtained model. Testing stage has no effect on training and so provides an independent measure of network performance.

The process of division of database into three sub data sets is performed randomly. In this work, the total number of experimental data used to design the network is 2865, of which about 75%, 10%, and 15% of the main data set are randomly selected for training (about 2150 data points), validation (around 285 data points), and test (about 430 data points), respectively. The effect of the percent allocation of the three subdata sets from the database on the accuracy of the ANN model has been studied elsewhere [31]. Gharagheizi showed that the percent of test set allocated from the main dataset should be between 5 and 35%. If this percent is lower than 5% the accuracy of the model over the training set is greater than the test set. Also, if the percent is greater than 40% the obtained model cannot predict the test set as well as the training set. On the other hand, his work showed that the optimum percent of the test set is dependent to the nature of the problem. The optimum percent is the percent on which the accuracy of the model over the test set approaches the training set.

The experimental data points of the specific volumes at several temperatures and pressures, corresponding to 25 different polymeric systems have been used to train, validate and test the ANN–GCM model using the MATLAB software. Temperature ($T$), pressure ($P$), molecular mass ($M_w$), and the structural groups that form the molecules were given as input variables. The output parameter is specific volume. All data used in this work have been experimentally determined and the data obtained from theoretical models and also those data for which their accuracy is not guaranteed were not considered.