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PREDICTION OF THERMAL CONDUCTIVITY OF AQUEOUS SOLUTION AT HIGH PRESSURES BY USING ARTIFICIAL NEURAL NETWORK

Article Highlights

- Thermal conductivity of aqueous solution is predicted with artificial neural network
- A feed forward artificial neural network with three neurons in its hidden layer is recommended
- Three inputs were used for this network: temperature, pressure and concentration

Abstract

The objective of this study is to predict thermal conductivity of aqueous solution with artificial neural network (ANN) model with three inputs (pressure, temperature and concentration). A feed forward artificial neural network with three neurons in its hidden layer is recommended to predict thermal conductivity. The accuracy of this method evaluated by regression analysis between the predicted and experimental value shows desired results.

Keywords: neural network, aqueous solution, thermal conductivity.

Thermal conductivity data are required for calculating design parameters, developments and utilization of geothermal and ocean thermal energy, efficient operation of high-temperature energy-generating systems, geology and mineralogy, for hydrothermal synthesis, biological processes of living organisms, and in prediction of heat and mass transfer coefficients under both laminar and turbulent regimes [1,2].

Thermal conductivity data for aqueous solutions are also so important in engineering. They are needed in many industrial and scientific applications, such as calculation of flow and heat and mass transfer rates in various pieces of industrial equipment.

Using the artificial neural network (ANN) model to predict thermal conductivity of aqueous solution is a new concept in order to achieve desired results. Many researchers use ANN model in various fields of chemical engineering.

Loueyan *et al.* used the artificial neural network for the prediction of thermal conductivity of pure gases at atmospheric pressure and a wide range of

temperature based on their critical properties and molecular weight [3]. Kurt *et al.* investigated the thermal conductivity of ethylene glycol-water solution by ANN model with good results [4]. Sablani *et al.* suggested an ANN model for the prediction of thermal conductivity of bakery product based on their temperature and apparent density [5]. Singh *et al.* estimated the thermal conductivity of moist porous materials with ANN approach [6]. Hu *et al.* derived a model for the thermal conductivity of unconsolidated porous medium based on a capillary pressure saturation relation [7]. Zhou *et al.* calculated the electrical conductivity of recombined milk by artificial neural network, aiming to establish a nonlinear relationship that accounts for the effect of milk constituents and temperature on the electrical conductivity of recombined milk [8].

The aim of this study is to use a neural network model to predict the thermal conductivity of aqueous solutions based on experimental values at different temperature, pressure and concentration. Three inputs were used for this network: temperature, pressure and concentration and has three layers: input layer with three inputs, hidden layer with three neurons and output layer with one output that is thermal conductivity and the coefficient of determination (R^2), was used as a measure to evaluate how the trained

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network estimation is compatible to the experimental data.

Artificial neural network

An artificial neural network (ANN) is an information processing paradigm that is inspired by the way biological nervous system, such as the brain and process information. The key element of this paradigm is the novel structure of the information processing system. It is composed of a large number of highly interconnected processing elements that called (neurons) working in unison to solve specific problems. An ANN has the ability to recognize nonlinear and complex relationships.

The commonest type of artificial neural network consists of three groups, or layers, of units: a layer of "input" units is connected to a layer of "hidden" units, which is connected to a layer of "output" units [9].

- The activity of the input units represents the raw information that is fed into the network.
- The activity of each hidden unit is determined by the activities of the input units and the weights on the connections between the input and the hidden units.
- The behavior of the output units depends on the activity of the hidden units and the weights between the hidden and output units.

The basic structure of the artificial neuron model is as follows:

There are $m+1$ inputs with signals x_0 through x_m and weights w_0 through w_m . Usually, the x_0 input is assigned the value +1, which makes it a *bias* input with $w_{k0} = b_k$. This leaves only m actual inputs to the neuron: from x_1 to x_m . The output of the k^{th} neuron is:

$$y_k = \phi \left(\sum_{j=0}^m w_{kj} x_j \right) \quad (1)$$

where ϕ is the transfer function.

There are several types of ANNs, such as feed forward network, radial basis function network, ART network, auto associative network and recurrent neural network [10].

Feed forward neural networks are the most commonly used for the function approximation, that we have used this type in our work. Feed forward

ANNs allow signals to travel one way only, from input to output, there is no feedback (loops), the output of any layer does not affect that same layer. Feed forward ANNs tend to be straightforward networks that associate input with output.

Application of ANN on the experimental data

In this work, we developed an ANN model to predict thermal conductivity of three aqueous solution (BaCl_2 , SrCl_2 and $\text{Sr}(\text{NO}_3)_2$). A set of data at different concentration, temperature and pressure for three aqueous solutions were collected from open literature [1,2]. Table 1 shows the characterization of collected data, *i.e.*, concentration, temperature and pressure range for these species where the thermal conductivities were given in the literature. Different fractions of each data set were used for training and testing of the neural model for each solution. In general, each neural model was trained with 80% of total data and the remaining was used for testing of model. Details of the selected data set are given in Table 1.

After collecting data (which were normalized using a simple normalization method in the (0-1) range), temperature, pressure and concentration were used as the inputs of ANN model and thermal conductivity as a output that can be described as a function of temperature pressure and concentration as follows:

$$k = f(T, P, C) \quad (2)$$

We have three neurons in the input layer equal to the number of input parameters and one neuron in output. After trying different networks we decided that the optimum number of neurons in hidden layer was three. Therefore, the developed ANN architecture has a configuration of 3-3-1 neurons (Figure 1).

RESULT AND DISCUSSION

Figure 2 shows the correlation between the predicted and experimental thermal conductivity test data of BaCl_2 aqueous solution. Figure 3 also shows this comparison for SrCl_2 solution and Figure 4 features the comparison for $\text{Sr}(\text{NO}_3)_2$ with a high degree of accuracy.

Table 1. Characterization of collected data and different fractions of each data set for training and test of neural model; pressure range: 0.1-100 MPa; temperature range: 293-473 K

Species	Total data	Training data	Testing data	Concentration, %
BaCl_2	300	240	60	2.5-20
SrCl_2	240	192	48	2.5-15
$\text{Sr}(\text{NO}_3)_2$	240	192	48	2.5-15

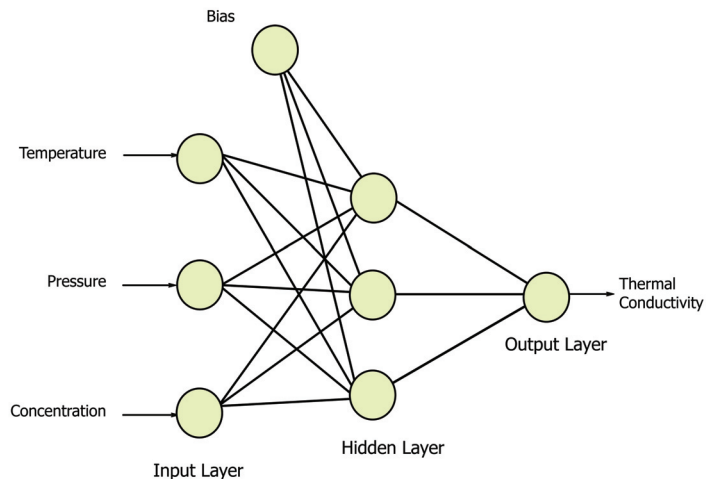


Figure 1. General structure of the neural network.

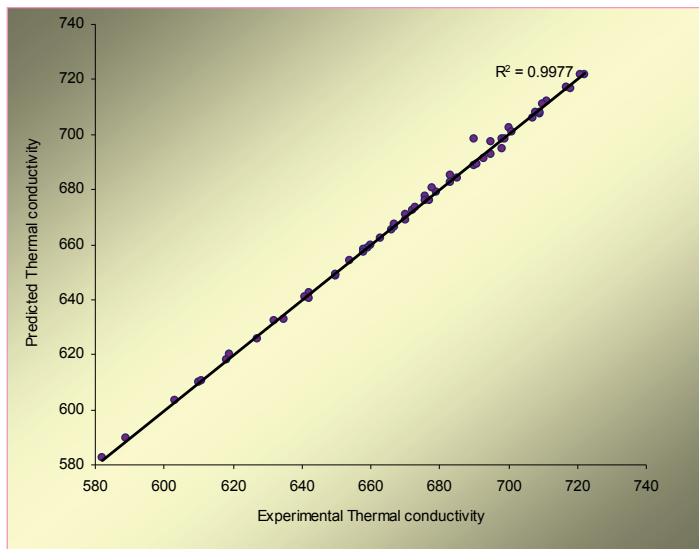


Figure 2. Correlation of experimental data vs. neural network predictions for testing data set for BaI₂.

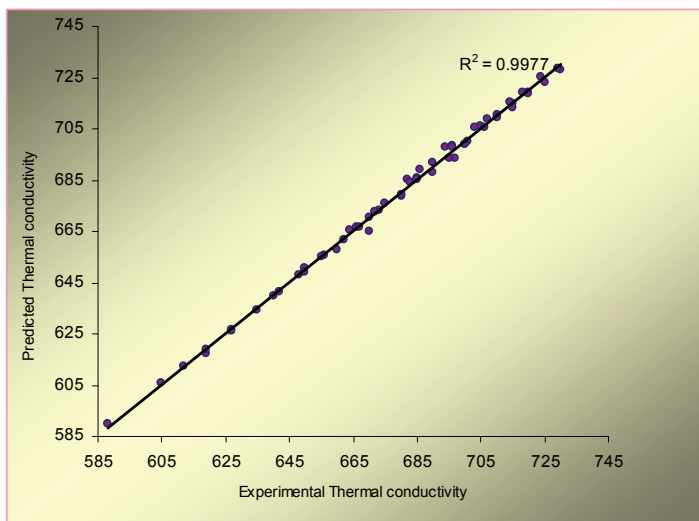


Figure 3. Correlation of experimental data vs. neural network predictions for testing data set for SrCl₂.

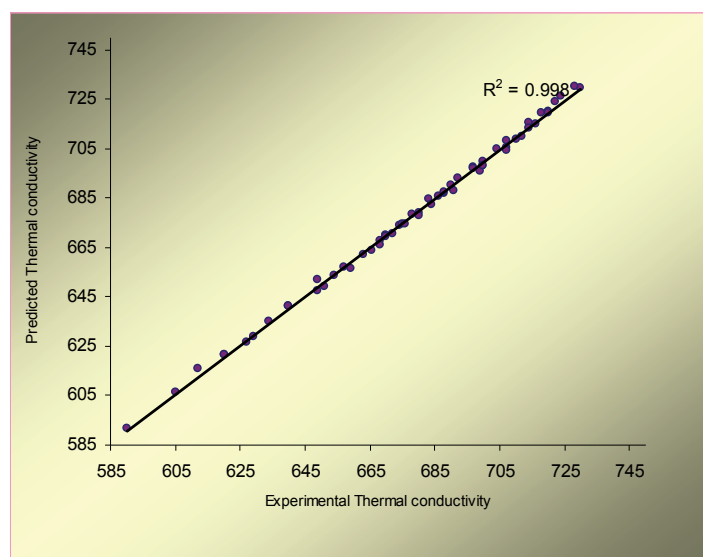


Figure 4. Correlation of experimental data vs. neural network predictions for testing data set for $\text{Sr}(\text{NO}_3)_2$.

Regression analysis between the predicted and experimental values used to evaluate accuracy of this prediction. The correlation coefficient (R^2 value) in this case was very close to 1, which was about 0.999. However it should be noted that only the randomly selected test data from experimental data set were used in comparison between predicted and experimental values. Also, different neural networks were compared using their mean square error (*MSE*) and mean relative error (*MRE*).

MSE values for the aqueous solution of BaI_2 , SrCl_2 and $\text{Sr}(\text{NO}_3)_2$ were 0.0015, 0.0018 and 0.0017, respectively, while the *MRE* values for these aqueous solutions were 2.6, 2.33 and 2.55, respectively.

CONCLUSION

In this paper we show that an artificial neural network model can predict the thermal conductivity of aqueous solution with high degree of accuracy. Input values that used in this model were temperature, pressure and concentration with a feed forward structure that has a hidden layer with three neurons (3-3-1

neuron configuration). The regression coefficient shows that the ANN model is a good method for predicting thermal conductivity of aqueous solutions.

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NAUČNI RAD

PREDVIĐANJE KOEFICIJENTA TOPLOTNE PROVODLJIVOSTI VODENOG RASTVORA NA VISOKIM PRITISCIMA POMOĆU VEŠTAČKE NEURONSKE MREŽE

Cilj ovog proučavanja je predviđanje koeficijenta toplotne provodljivosti vodenog rastvora pomoću modela veštačke neuronske mreže sa tri ulazne promenljive (pritisak, temperatura i koncentracija). Za predviđanje koeficijenta toplotne provodljivosti preporučuje se veštačka neuronska mreža sa povratnim rasprostiranjem signala unapred sa tri neurona. Tačnost ove metode je procenjena regresionom korelacijom između predviđenih i eksperimentalnih vrednosti. Pokazano je dobro slaganje između njih.

Ključne reči: neuronska mreža, vodeni rastvor, koeficijent toplotne provodljivosti.