# Prediction of the Liquid Vapor Pressure Using the Artificial Neural Network-Group Contribution Method

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**ABSTRACT:** *In this paper, vapor pressure for pure compounds is estimated using the Artificial Neural Networks and a simple Group Contribution Method (ANN–GCM). For model comprehensiveness, materials were chosen from various families. Most of materials are from 12 families. Vapor pressure data of 100 compounds is used to train, validate and test the ANN-GCM model. Vapor pressure data were taken from literature for wide ranges of temperature (68.55-559.15 K). Based on results, the best structure for feed-forward back propagation neural network is Levenberg-Marquardt back propagation training algorithm, logsig transfer function for hidden layer and linear transfer function for output layer. The multiplayer network model consists of temperature, acentric factor, critical temperature, critical pressure and the structure of molecules as inputs, 10 neurons in the hidden layer and one neuron in the output layer corresponding to vapor pressure. The weights are optimized to minimize error between experimental and calculated data. Results show that optimum neural network architecture is able to predict vapor pressure data with an acceptable level. The trained network predicts the vapor pressure data with average relative deviation percent of 1.18%.*


**KEY WORDS:** *Artificial neural network, Group contribution method, Liquid vapor pressure, Equation of state.*

## INTRODUCTION

Thermodynamic properties of pure fluids such as vapor pressure, density, heat capacity and thermal conductivity are very important in design of different chemical processes. Vapor pressure is one of the most important properties in chemical processes. The vapor pressure curve is unique for each substance, but the general shape of curve is similar for all of them [1]. For a limited number of substances vapor pressure has been reported in many points. The number of points is limited for most substances, so obtaining the equations for estimation and interpolation points is very important.

The vapor pressure can be obtained from equation of state. Two parameters equations of state such as *Peng-Robinson* [2], *Soave-Redlich-Kwong* [3] and *Patel Teja* [4] were widely used in predicting vapor pressure of compounds.

For predicting thermodynamic properties including vapor pressure, it can be used of Group Contribution Method (GCM). *Chein* [5] predicted the vapor pressure using of GCM. He predicted the vapor pressure by average absolute percentage deviation of 5%. *Avaullee et al.* [6] presented a group contribution method

for estimating the critical properties and acentric factors of paraffins, naphtenes and aromatics with emphasis on extrapolating to very heavy compounds. They predicted the properties with average deviation between 0.6 and 6.5%. *Marrero et al.* [7] predicted critical properties by using GCM. They showed the new method making significant improvements both in accuracy and applicability. *Coutsikos et al.* [8] presented a group-contribution model for the prediction of vapor pressures of organic solids. The obtained predictions by them are not very accurate. *Moller et al.* [9] presented a new group contribution method for the prediction of liquid vapor pressures for non-electrolyte organic compounds. They found the relative error of 5% in pressure. *Nannoolal et al.* [10] proposed a group contribution method for the estimation of the normal boiling point of nonelectrolyte organic compounds. *Ceriani et al.* [11] proposed a group contribution method for the estimation of vapor pressure and heat of vaporization of organic liquids. This method improved the prediction of normal boiling point.

The artificial neural networks can be a suitable alternative to model the different thermodynamic properties. An Artificial Neural Network (ANN) is an information processing method inspired from the human brain functioning rules [12]. ANN models are composed of computational points called neurons which are able to store experimental knowledge. ANNs are an especially efficient algorithm to approximate any function with a finite number of discontinuities by learning the relationships between the input and output vectors [13]. Thus, ANNs are appropriate techniques to model the nonlinear behavior of chemical properties.

Today, use of neural networks to predict thermodynamic properties such as vapor pressure is increasing. *Potukuchi et al.* [14] predicted vapor pressure of volatile inorganic compounds by using an artificial neural network. *Kuhne et al.* [15] investigated vapor pressure for hydrocarbons and halogenated hydrocarbons from chemical structure by using a Neural Network. *Potukuchi et al.* [14] predicted vapor pressure of volatile organic compounds including nitric acid, hydrochloric acid and ammonia. *Gandhidasan et al.* [16] predicted vapor pressures of

aqueous desiccants for cooling applications by using an artificial neural network. Aqueous desiccants investigated by them included calcium chloride, lithium chloride, and lithium bromide. *Lazzus* [17,18] estimated solid vapor pressure for inorganic and inorganic compounds by a neural network. He investigated solid vapor pressure for 250 compounds. He also predicted vapor pressure and density of ionic liquids by using a neural network [19]. *Rohani et al.* [20] compared artificial neural network systems and SAFT equation to obtain vapor pressure and liquid density of pure alcohols.

In this paper, liquid vapor pressure is predicted by using a combined method that includes the Artificial Neural Networks and a simple Group Contribution Method (ANN–GCM). 100 substances have been investigated. To assess the accuracy of this model, calculated vapor pressure from ANN–GCM model and predicted by some EOSs, namely, Peng–Robinson, Soave–Redlich–Kwong and Patel Teja have been compared.

## ARTIFICIAL NEURAL NETWORK

Artificial neural networks are used in a wide range of applications such as prediction of thermodynamic properties. Neural networks generally consist of a number of interconnected neurons that are organized in one or more layers. Usually, artificial neural networks are comprised of one input layer, one hidden layer and an output layer [21]. Output of each neuron is calculated by using transfer function (Eq. (1)).

$$y_j = F(S_j) \tag{1}$$

Where $S_j$, $y_j$ and $F$ are input of jth neuron before applying transfer function, output of jth neuron and transfer function. Input of each neuron is calculated from outputs of previous layers (Eq. (2)):

$$S_j = \sum_i w_{ij} y_i + b_j \tag{2}$$

Where $w_{ij}$ and $b_j$ are weights connecting ith neuron (from previous layer) and bias of jth neuron.

Common transfer functions are logarithmic function (logsig), hyperbolic tangent function (tansig) and linear

*Table 1: Structural groups used in the proposed ANN+GCM method.*

| No. | Group | No. | Group |
|---|---|---|---|
| 1 | >C< | 14 | >N< |
| 2 | >CH- | 15 | -F |
| 3 | -CH$_2$- | 16 | -Cl |
| 4 | -CH$_3$ | 17 | -I |
| 5 | =CH$_2$ | 18 | -S-(Ring) |
| 6 | =CH- | 19 | –CH$_2$–(Ring) |
| 7 | ≡CH | 20 | >CH–(Ring) |
| 8 | -O- | 21 | =CH–(Ring) |
| 9 | -OH | 22 | >C<(Ring) |
| 10 | >C=O | 23 | –O–(Ring) |
| 11 | =O | 24 | -NO |
| 12 | –NH$_2$ | 25 | >N<(ring) |
| 13 | ≡N | 26 | -H |

function (purelin) that are defined in Eqs. (3) - (5), respectively:

$$y_j = \frac{1}{1 + e^{-S_j}} \tag{3}$$

$$y_j = \frac{e^{S_j} - e^{-S_j}}{e^{S_j} + e^{-S_j}} \tag{4}$$

$$y_j = S_j \tag{5}$$

Number of inputs in the input layers depends on number of independent variables input and is defined by the nature of problem.

To evaluate the accuracy of proposed ANN model for prediction of liquid vapor pressure data at different temperatures, some statistical parameters, including Average Relative Deviation Percent (*ARD%*), the average deviation percent (*Bias%*), correlation coefficient (*R²*) and the Root Mean Square Error (*RMS*) were utilized which are defined in Eqs. (6) - (9) [22,23]:

$$ARD\% = \frac{1}{N} \sum_{i=1}^{N} 100 \times \left| \frac{P_i^{exp} - P_i^{cal}}{P_i^{exp}} \right| \tag{6}$$

$$Bias\% = \frac{1}{N} \sum_{i=1}^{N} 100 \times \left( \frac{P_i^{exp} - P_i^{cal}}{P_i^{exp}} \right) \tag{7}$$

$$RMS = \sqrt{\frac{1}{N} \sum_{i=1}^{N} \left( P_i^{exp} - P_i^{cal} \right)^2} \tag{8}$$

$$R^2 = \frac{\sum_{i=1}^{N} \left( P_i^{exp} - \bar{P} \right)^2 - \sum_{i=1}^{N} \left( P_i^{exp} - P_i^{cal} \right)^2}{\sum_{i=1}^{N} \left( P_i^{exp} - \bar{P} \right)^2} \tag{9}$$

Where N is the number of liquid vapor pressure data points; $P_i^{exp}$ is the ith experimental vapor pressure; $P_i^{cal}$ is the predicted vapor pressure with ANN model and $\bar{P}$ is the average value of experimental vapor pressure data.

100 substances including 2044 points are investigated. Data are extracted from various articles [24-72]. These data were taken from paper that the experimental error reported less than ±1%. For train and testing the ANN model, 70% of the data are used to train the neural network and 20% for validating and 10% for testing. In this paper, liquid vapor pressure is estimated as a function of critical temperature, critical pressure acentric factor and temperature. [73-75]

In addition to these properties, the structure of molecules is considered as variables [6]. Table 1 shows 26 groups used as entrance variables. When the group does not appear in the substance, the value associated with the structural group is defined as 0. Some examples of the structure of molecules are shown in Table 2.

The chosen neural network is Feed-forward back propagation with Levenberg-marquardt back propagation training function. In this paper, one hidden layer is selected. To choose the best transfer functions for hidden and output layers different combinations of transfer

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*Table 2: Some examples of the structure of molecules.*

| Component | Formula | structural group | | | | |
|---|---|---|---|---|---|---|
| **R-134a** | $C_2H_2F_4$ | >C< | -CH$_2$- | -F | | |
| | | 1 | 1 | 4 | | |
| **Ethyl butanoate** | $C_6H_{12}O_2$ | -CH$_3$ | -CH$_2$- | -O- | >C=O | |
| | | 2 | 3 | 1 | 1 | |
| **Trifluoroiodomethane** | $CF_3I$ | >C< | -F | -I | | |
| | | 1 | 3 | 1 | | |
| **Naphthalene** | $C_{10}H_8$ | =CH-(Ring) | >C< (Ring) | | | |
| | | 8 | 2 | | | |
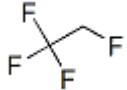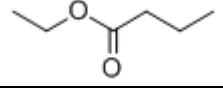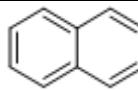
*Table 3: The values of ARD% of different transfer functions with the optimal number of neurons in each case.*

| Transfer function | | No. of neuron | | ARD% |
|---|---|---|---|---|
| Logsig | Purelin | 11 | Train | 1.4381 |
| | | | Test | 1.5853 |
| Logsig | Tansig | 12 | Train | 1.7574 |
| | | | Test | 1.9366 |
| Logsig | Logsig | 13 | Train | 3.0382 |
| | | | Test | 4.3307 |
| Tansig | Purelin | 10 | Train | 1.1743 |
| | | | Test | 1.2138 |
| Tansig | Tansig | 12 | Train | 1.6049 |
| | | | Test | 1.8401 |
| Tansig | Logsig | 10 | Train | 2.6401 |
| | | | Test | 3.1277 |

functions have been tested. Since no information about the optimal number of neurons has been reported for the calculation of liquid vapor pressure of substances, trial and error is the best way to determination the optimal number of neurons. The optimal number of neurons in the hidden layer was determined based on the minimum *ARD%*.

## RESULTS AND DISCUSSION

Table 3 shows *ARD%* of different transfer functions with the optimal neurons number in each case. According to Table 3, neural network with tansig-purelin transfer functions with 10 neurons in hidden layer has the least *ARD%*. Fig. 1 shows the values of *ARD%* in contrast with different neurons number in hidden layer with tansig-purelin transfer function. Table 4 shows the *ARD%*, $RD_{max}$, *Bias%*, $R^2$ and *RMS* for all data sets using the proposed neural network.
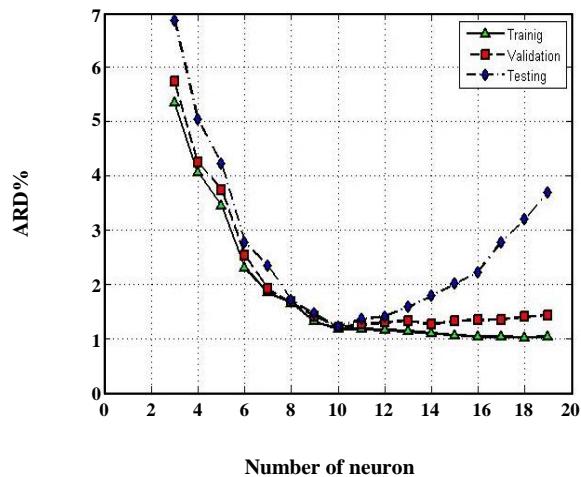


*Fig. 1: Average absolute deviation (ARD%) as a function of the number of neurons in the hidden layer*

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*Table 4: Statistical parameters for data sets.*

|                | ARD%   | $RD_{max}$ | Bias%   | RMS    | $R^2$    |
|----------------|--------|------------|---------|--------|----------|
| **Training set**   | 1.1743 | 14.0604    | -0.0414 | 0.0210 | 0.999994 |
| **Validation set** | 1.1983 | 17.1748    | -0.2848 | 0.0217 | 0.999997 |
| **Testing set**    | 1.2138 | 10.5827    | -0.0726 | 0.0214 | 0.999997 |
| **Total set**      | 1.1830 | 17.1748    | -0.0932 | 0.0212 | 0.999995 |
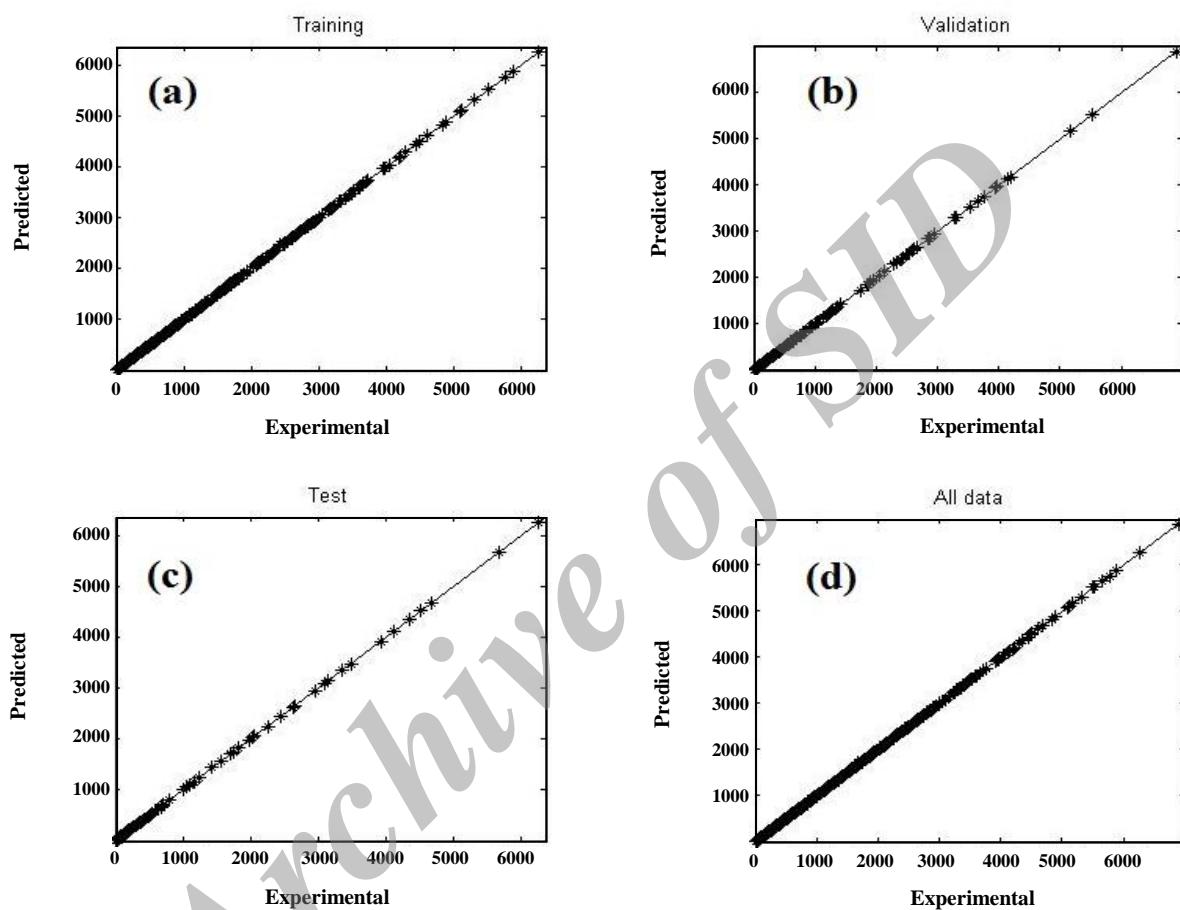


*Fig. 2: Comparison between predicted and experimental data for training (a), validation (b), test (c) and total data (d) sets*

The results show that the artificial neural network can be accurately trained and that can estimate the liquid vapor pressure with acceptable accuracy. In this estimating, the root mean square error is 0.021, 0.022 and 0.21 respectively for the training, validation and test data.

Comparisons between experimental and calculated values for all data sets are shown in Fig. 2. The optimum weights and biases for the neural network are shown in Table 5. The weights and biases in Table 5 are able to recalculate the obtained results in this paper.

To assess the accuracy of the this model in prediction of liquid vapor pressure, the ARD% values between experimental and calculated vapor pressure from ANN–GCM model and predicted by some other methods, namely, Peng–Robinson, Soave–Redlich–Kwong and Patel Teja have been compared. The three equations of state were used for prediction of phase behavior of all substances.

The results for each substance are illustrated in Table 6. Four last columns in the table show these average relative

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*Table 5: The weight and bias values of the optimal architecture.*

| Neuron | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
|---|---|---|---|---|---|---|---|---|---|---|
| T | 3.1790 | 0.0389 | 0.0657 | 3.0672 | 2.5814 | 2.9727 | 0.0121 | 3.5517 | -2.6035 | -2.3839 |
| $T_c$ | -1.4526 | -1.5128 | 1.8472 | -0.9421 | -3.0187 | -4.4137 | 0.0023 | 1.2904 | 3.0202 | 3.0399 |
| $P_c$ | 0.0873 | 0.7597 | -1.1891 | 0.7637 | 1.1003 | 0.8235 | -0.0218 | -2.3599 | -1.0282 | -1.1226 |
| ω | -1.5685 | -0.3218 | 0.4540 | -1.3973 | -0.6499 | -0.1957 | -0.0094 | 3.1082 | 1.3910 | 0.5295 |
| >C< | -0.5018 | 0.1512 | -0.1129 | -0.5765 | -0.0056 | -0.2755 | -0.0239 | -1.3963 | 1.3994 | -0.0182 |
| >CH- | -0.2717 | 0.3157 | -0.3519 | -0.3414 | 0.0418 | -0.0058 | -0.0121 | -0.2721 | -0.0772 | -0.0636 |
| -CH2- | -0.8591 | 0.2035 | -0.1595 | -0.6318 | -0.5141 | -0.3609 | -0.0032 | 0.7454 | 1.9981 | 0.5384 |
| -CH3 | -0.0949 | -1.0044 | 0.7774 | -0.7547 | -0.0578 | 0.4666 | 0.0451 | 1.3914 | -1.4271 | 0.1194 |
| =CH2 | 0.9999 | 0.1803 | 0.1364 | 0.3652 | 0.1123 | -0.3379 | -0.5894 | -2.1147 | 0.8298 | -0.1378 |
| =CH- | -0.3575 | -0.3952 | 0.0730 | 0.1725 | -0.2121 | -0.2495 | 0.0069 | -0.6650 | -0.2586 | 0.23066 |
| ≡CH | 0.2799 | 0.0328 | -0.4086 | 0.5553 | -0.1781 | -0.2455 | 0.5861 | -0.4507 | 0.02183 | 0.1840 |
| -O- | -0.8481 | -0.6060 | 1.4125 | -0.7676 | -0.1553 | -0.2706 | -0.0029 | 2.1250 | 0.6684 | 0.1945 |
| -OH | 0.1854 | -0.0402 | -0.0862 | -0.2753 | 0.0306 | 0.51007 | 0.0146 | -0.3961 | -1.5567 | -0.0042 |
| >C=O | 0.1088 | -0.1617 | 0.0668 | -0.0200 | -0.0187 | 0.1809 | 0.0098 | 0.5123 | 0.2643 | 0.0119 |
| =O | -1.5366 | -0.1316 | -0.1018 | -0.4519 | 0.0456 | -0.0031 | 0.0331 | -0.7124 | 1.1358 | -0.0333 |
| –NH2 | 0.4097 | -0.5378 | 0.4475 | -0.4758 | -0.229 | 0.3351 | 0.0380 | -0.7249 | 0.5088 | 0.2408 |
| ≡N | 1.3794 | -0.4204 | -1.1464 | 1.4089 | -0.2805 | 0.3370 | 0.7334 | -0.6440 | 0.2434 | 0.0144 |
| -F | 1.0016 | 0.0841 | -0.2830 | 0.8677 | -0.1121 | 0.4453 | 0.0228 | 0.0033 | -0.1356 | 0.2160 |
| -Cl | 0.6871 | 0.4427 | -0.8256 | 0.6723 | -0.2666 | -0.0346 | 0.4349 | -1.7958 | -1.6765 | 0.3438 |
| -I | 0.6862 | 0.2578 | -0.3742 | 0.7180 | -0.0041 | 0.0302 | 0.0589 | 1.1860 | -1.5286 | -0.0889 |
| -S-(ring) | 1.5980 | -0.0030 | 0.6069 | 0.2394 | 0.0392 | 0.5324 | -0.0307 | 0.0256 | -0.1789 | -0.2143 |
| –CH2–(ring) | 0.1571 | -0.1370 | 0.0527 | -0.0681 | -0.0284 | -0.1840 | 0.0150 | 1.2048 | -0.2807 | 0.0482 |
| >CH–(ring) | -2.9784 | -0.0606 | 0.2764 | -3.2277 | -0.1731 | -0.6134 | -0.0345 | 0.5368 | 0.5306 | 0.2110 |
| =CH–(ring) | -0.0121 | -0.5558 | 0.3832 | -0.2617 | -0.0222 | 0.0910 | 0.0229 | 0.8595 | -0.5632 | 0.0335 |
| >C<(ring) | -0.9727 | 0.2892 | 0.0741 | -1.1641 | -0.0856 | -0.2715 | -0.0208 | -0.3217 | -0.2257 | 0.1309 |
| –O–(ring) | 0.6645 | 0.2271 | -0.2448 | 0.5166 | 0.4389 | 0.2720 | -0.0669 | 0.0272 | -0.4474 | -0.4259 |
| -NO | 0.9408 | 0.4756 | -0.8520 | 1.5007 | 0.5499 | 0.5373 | 0.0876 | 0.5385 | -0.3447 | -0.4109 |
| >N<(ring) | -1.0456 | 0.2473 | -0.6771 | 0.3668 | 0.1098 | 0.4167 | 0.2709 | 0.3552 | -1.6013 | -0.0364 |
| -H | 1.4655 | 0.3270 | -0.6212 | 0.5894 | -0.3884 | 0.4989 | 0.1489 | 0.3211 | -0.7827 | 0.2096 |
| >N< | 0.8210 | 0.1107 | -0.0424 | 1.0511 | 0.3609 | 0.2161 | -0.0248 | -0.3774 | -0.1669 | -0.3767 |
| Bias | -1.4948 | -2.0845 | -1.1197 | -2.5030 | -1.8673 | -1.1423 | 0.0521 | 0.9029 | 1.0902 | 1.6648 |
| Output layer weights | -2.7942 | -2.3020 | -0.9860 | 3.4034 | 2.7796 | 6.9701 | -1.2553 | 0.0378 | 2.9561 | 2.7800 |
| Bias | | | | | | | | | | 1.1119 |

*Table 6: More detailed results about the correlated values.*

| | Name | Formula | T (K) | P (kPa) | ARD% | | | |
|---|---|---|---|---|---|---|---|---|
| | | | | | PR | SRK | PT | ANN |
| 1 | Methane | $CH_4$ | 96.48-122.03 | 23.52-220.08 | 0.53 | 4.39 | 28.91 | 0.67 |
| 2 | Ethane | $C_2H_6$ | 165-300 | 30.67-4353.5 | 0.48 | 1.34 | 12.90 | 0.48 |
| 3 | n-Butane | $C_4H_{10}$ | 280-424 | 133-3716.9 | 0.44 | 4.20 | 1.11 | 0.41 |
| 4 | Isobutene | $C_4H_8$ | 310-407 | 488.4-3584.3 | 0.27 | 5.14 | 0.75 | 0.03 |
| 5 | n-Pentane | $C_5H_{12}$ | 297.04-322.04 | 66.53-153.75 | 0.48 | 5.34 | 1.48 | 0.45 |
| 6 | n-Hexane | $C_6H_{14}$ | 294.26-372 | 17-237.74 | 0.76 | 1.45 | 1.41 | 0.89 |
| 7 | n-Octane | $C_8H_{18}$ | 338.71-399.82 | 12.57-103.63 | 4.20 | 2.71 | 12.43 | 1.35 |
| 8 | n-Decane | $C_{10}H_{22}$ | 371.21-392.79 | 8.82-19.92 | 1.28 | 1.88 | 21.23 | 1.77 |
| 9 | Hexadecane | $C_{16}H_{34}$ | 495.45-559.15 | 20.00-101.33 | 2.12 | 2.14 | 26.99 | 2.10 |
| 10 | Acetylene | $C_2H_2$ | 193.15-213.15 | 133.48-354.18 | 0.58 | 9.5 | 0.59 | 0.02 |
| 11 | Butadiene | $C_4H_6$ | 233.75-343.85 | 20.45-939.2 | 1.53 | 6.70 | 1.93 | 1.31 |
| 12 | Butylene | $C_4H_8$ | 255.37-291.48 | 34.76-140.52 | 3.70 | 7.64 | 24.51 | 1.11 |
| 13 | 1-Hexene | $C_6H_{12}$ | 389.32-499.76 | 456-5.3003 | 2.31 | 2.26 | 2.45 | 0.36 |
| 14 | Benzene | $C_6H_6$ | 283.25-373.45 | 5.74-182.65 | 4.50 | 1.75 | 8.20 | 1.03 |
| 15 | Cyclohexane | $C_6H_{12}$ | 283.85-551.23 | 6.97-3951.41 | 3.41 | 1.05 | 7.74 | 0.77 |
| 16 | Toluene | $C_7H_8$ | 324.06-402.21 | 12.136-166.04 | 3.66 | 1.28 | 3.18 | 0.86 |
| 17 | m-Xylene | $C_8H_{10}$ | 333.15-399.82 | 6.09-71,78 | 2.67 | 2.53 | 29.51 | 2.52 |
| 18 | p-Xylene | $C_8H_{10}$ | 333.15-399.82 | 6.58-73.57 | 2.28 | 4.61 | 1.58 | 1.06 |
| 19 | Naphthalene | $C_{10}H_8$ | 358.85-491.79 | 1.29-102.95 | 2.46 | 2.92 | 1.64 | 2.38 |
| 20 | n-Butylbenzene | $C_{10}H_{14}$ | 353.45-418.04 | 2.82-37.03 | 4.38 | 4.66 | 11.49 | 2.75 |
| 21 | 5-Ter-butyl-m-xylene | $C_{12}H_{18}$ | 383.06-442.9 | 4.4-37.78 | 6.11 | 7.53 | 8.58 | 2.69 |
| 22 | n-Hexylbenzene | $C_{12}H_{18}$ | 422.76-462.97 | 11.83-40.69 | 1.83 | 1.84 | 17.07 | 1.76 |
| 23 | Ethylbenzene | $C_8H_{10}$ | 366.48-466.48 | 21.25-311.87 | 1.91 | 3.20 | 3.25 | 1.15 |
| 24 | Acetic acid | $C_2H_4O_2$ | 349.82-422.04 | 24.24-239.87 | 3.16 | 4.34 | 11.21 | 1.40 |
| 25 | Acetic acid butyl ester | $C_6H_{12}O_2$ | 319.45-397.75 | 9.17-147.39 | 6.27 | 7.65 | 2.98 | 2.94 |
| 26 | Oleic acid | $C_{18}H_{34}O_2$ | 513.10-524.70 | 2.66-9.33 | 10.49 | 7.09 | 7.17 | 4.29 |
| 27 | Acetone | $C_3H_6O$ | 268.95-338.95 | 7.44-136.63 | 2.23 | 1.65 | 1.18 | 0.94 |
| 28 | 2-Butanone | $C_4H_8O$ | 305.22-388.55 | 17.99-282.20 | 1.13 | 2.03 | 1.67 | 1.23 |
| 29 | 2-Hexanone | $C_6H_{12}O$ | 294.11-399.66 | 1.80-100.32 | 8.43 | 11.56 | 3.71 | 2.26 |
| 30 | n-Hexanal | $C_6H_{12}O$ | 343.15-363.15 | 15.10-32.14 | 5.39 | 7.97 | 7.45 | 2.99 |
| 31 | Diethyl ether | $C_4H_{10}O$ | 301-396 | 79.28-1080.15 | 1.49 | 1.60 | 2.91 | 1.30 |
| 32 | Ethyl butanoate | $C_6H_{12}O_2$ | 305.22-427.44 | 2.70-245.03 | 3.13 | 4.85 | 11.27 | 2.60 |

***Table 6: More detailed results about the correlated values. (Continued)***

| 33 | Tetrahydrofuran | $C_4H_8O$ | 288.15-339.05 | 15.20-101.33 | 3.74 | 2.17 | 6.57 | 1.53 |
|---|---|---|---|---|---|---|---|---|
| 34 | Ethyl acetate | $C_4H_8O_2$ | 350.19-373.15 | 3.14-10.72 | 20.16 | 24.13 | 31.67 | 4.47 |
| 35 | Acetaldehyde | $C2H4O$ | 260.93-324.82 | 24.59-320.16 | 10.82 | 5.86 | 12.96 | 0.95 |
| 36 | Acrolein | $C3H4O$ | 299.82-372.03 | 49.99-486.74 | 13.63 | 14.54 | 13.33 | 3.85 |
| 37 | Chloroform | $CHCl_3$ | 293.15-334.35 | 21.09-101.33 | 2.11 | 5.28 | 11.83 | 1.98 |
| 38 | HFC-227ea | $C_3HF_7$ | 249.03-373.80 | 54.05-2859.22 | 0.68 | 0.85 | 3.91 | 0.46 |
| 39 | HFC-236fa | $C_3H_2F_6$ | 239.024-397.97 | 20.71-3174.16 | 23.43 | 23.37 | 20.74 | 0.63 |
| 40 | HFC-245fa | $C3H3F5$ | 261.47-424.32 | 30.38-3479.18 | 0.67 | 0.36 | 3.84 | 0.32 |
| 41 | HFC-32 | $CH_2F_2$ | 233.15-351.15 | 177-5767.9 | 0.60 | 1.36 | 1.07 | 0.10 |
| 42 | HFC-161 | $C_2H_5F$ | 253.15-323.15 | 216.2-17003.9 | 1.20 | 1.43 | 5.36 | 0.46 |
| 43 | R-12 | $CCl_2F_2$ | 203.15-383.15 | 12.3-3978.5 | 0.94 | 0.87 | 7.32 | 0.90 |
| 44 | R-22 | $CHClF_2$ | 203.15-368.15 | 20.5-4883.5 | 1.63 | 1.17 | 4.62 | 0.92 |
| 45 | R-134a | $C_2H_2F_4$ | 233.15-373.15 | 51.8-3973.2 | 0.31 | 1.10 | 0.95 | 0.25 |
| 46 | R123 | $C_2HCl_2F_3$ | 271.55-308.06 | 29.9-129.9 | 15.19 | 13.21 | 7.10 | 1.08 |
| 47 | R141b | $C_2H_3Cl_2F$ | 270.92-312.31 | 25.41-129.11 | 1.55 | 1.29 | 7.78 | 0.07 |
| 48 | Trifluoroiodomethane | $CF_3I$ | 243.15-325.15 | 71.7-982.6 | 0.89 | 0.75 | 8.52 | 0.05 |
| 49 | Sulfolane | $C_4H_8O_2S$ | 421.89-516.333 | 1.95-39.34 | 1.51 | 5.43 | 7.10 | 1.00 |
| 50 | Methanol | $CH_4O$ | 292.56-337.65 | 12.01-101.25 | 2.79 | 6.10 | 23.39 | 1.19 |
| 51 | Ethanol | $C_2H_6O$ | 273.15-351.7 | 1.59-102.22 | 1.13 | 3.15 | 39.22 | 2.01 |
| 52 | 1,2-Ethanediol | $C_2H_6O_2$ | 389.12-495.44 | 4.70-201.40 | 3.32 | 3.99 | 29.23 | 2.02 |
| 53 | 2-Propanol | $C_3H_8O$ | 310.93-372.04 | 12.42-191.65 | 4.09 | 3.06 | 39.28 | 2.05 |
| 54 | Isopropyl alcohol | $C_3H_8O$ | 305.372-372.04 | 9.69-191.61 | 3.34 | 2.33 | 39.59 | 1.32 |
| 55 | 1-Butanol | $C_4H_{10}O$ | 333.15-341.48 | 9.28-13.75 | 5.18 | 3.87 | 44.71 | 4.19 |
| 56 | 1-Hexanol | $C_6H_{14}O$ | 366.67-432.33 | 8.32-106.98 | 7.35 | 6.06 | 34.09 | 2.90 |
| 57 | 1-Heptanol | $C_7H_{16}O$ | 382.30-452.97 | 8.32-111.28 | 7.34 | 6.17 | 32.53 | 2.34 |
| 58 | 1-Octanol | $C_8H_{18}O$ | 397.32-465.29 | 8.35-93.54 | 6.63 | 5.39 | 34.35 | 1.12 |
| 59 | 1-Nonanol | $C_9H_{20}O$ | 422.04-516.48 | 12.99-205.88 | 2.90 | 2.66 | 25.95 | 2.64 |
| 60 | 1-Tetradecanol | $C_{14}H_{30}O$ | 479.42-519.183 | 8.32-29.35 | 1.65 | 1.34 | 47.05 | 1.31 |
| 61 | 1-Methylmorpholine | $C_5H_{11}NO$ | 273.18-353.08 | 6.9-332.76 | 99.80 | 99.82 | 99.74 | 1.83 |
| 62 | 2-Methoxyethanol | $C_3H_8O_2$ | 346.6-416.6 | 15-176.5 | 6.98 | 7.75 | 36.48 | 1.11 |
| 63 | 1-Methoxy-2-propanol | $C_4H_{10}O_2$ | 342.3-411.8 | 15-176.5 | 29.42 | 29.44 | 4.07 | 1.19 |
| 64 | 2-Methyl-1-propanol | $C_4H_{10}O$ | 351.2-392.2 | 30-150 | 3.68 | 3.26 | 27.67 | 2.30 |
| 65 | Acetonitrile | $C_2H_3N$ | 293.14-379.13 | 9.42-205.90 | 3.26 | 5.46 | 9.21 | 0.92 |
| 66 | Ethanolamine | $C_2H_7NO$ | 372.04-442.04 | 5.48-55.08 | 20.64 | 19.35 | 10.05 | 3.44 |
| 67 | Aniline | $C_6H_7N$ | 355.37-372.04 | 2.83-6.47 | 7.16 | 14.37 | 5.36 | 4.34 |

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***Table 6: More detailed results about the correlated values. (Continued)***

| 68 | Pyridine | $C_5H_5N$ | 316.48-442.03 | 7.06-280.18 | 6.82 | 7.59 | 11.554 | 2.49 |
|---|---|---|---|---|---|---|---|---|
| 69 | Ammonia | $NH_3$ | 223.15-387.15 | 40.9-6890.4 | 0.48 | 1.71 | 4.38 | 0.27 |
| 70 | Carbon dioxide | $CO_2$ | 235.78-296.88 | 1113.5-6255.61 | 1.87 | 1.03 | 4.70 | 0.02 |
| 71 | Nitrogen | $N_2$ | 68.55-91.89 | 28.38-453.81 | 4.57 | 3.33 | 21.88 | 1.79 |
| 72 | Water | $H_2O$ | 281.15-373.15 | 1.1-101.3 | 12.81 | 22.36 | 8.83 | 1.54 |
| 73 | Oxygen | $O_2$ | 92.59-99.82 | 126.59-250 | 2.01 | 0.55 | 22.67 | 0.52 |
| 74 | n-Butylcyclopentane | $C_9H_{18}$ | 343.15-402.26 | 5.53-47.51 | 2.45 | 1.59 | 8.72 | 1.90 |
| 75 | Cyclopentane | $C_5H_{10}$ | 273.3-343.21 | 14.34-191.64 | 2.16 | 1.39 | 10.35 | 1.29 |
| 76 | Methylcyclohexane | $C_7H_{14}$ | 284.62-392.24 | 3.13-163.7 | 2.57 | 1.48 | 6.25 | 1.84 |
| 77 | Ethylcyclohexane | $C_8H_{16}$ | 324.54-427.18 | 6.38-176.39 | 5.99 | 3.18 | 3.04 | 1.42 |
| 78 | n-Propylcyclohexane | $C_9H_{18}$ | 334.63-452.22 | 3.88-171.82 | 10.73 | 7.33 | 6.01 | 2.42 |
| 79 | Isopropylcyclohexane | $C_9H_{18}$ | 324.63-452.27 | 2.63-180.57 | 1.79 | 1.52 | 3.09 | 1.42 |
| 80 | n-Butylcyclohexane | $C_{10}H_{20}$ | 352.04-467.15 | 3.47-137.73 | 13.11 | 9.82 | 9.25 | 2.83 |
| 81 | n-Hexylcyclohexane | $C_{12}H_{24}$ | 422.22-467.26 | 12.2-47.38 | 2.03 | 1.05 | 21.35 | 0.94 |
| 82 | n-Heptylcyclohexane | $C_{13}H_{26}$ | 402.21-467.21 | 3.01-28.43 | 4.23 | 2.00 | 33.83 | 0.71 |
| 83 | n-Octylcyclohexane | $C_{14}H_{28}$ | 432.13-467.18 | 5.47-17.01 | 1.29 | 1.63 | 34.09 | 1.17 |
| 84 | Diethyl phthalate | $C_{12}H_{14}O_4$ | 479.25-520.32 | 8.32-29.35 | 2.85 | 2.66 | 54.42 | 1.37 |
| 85 | Cyclohexylbenzene | $C_{12}H_{16}$ | 383.01-462.66 | 1.78-29.7 | 2.48 | 2.54 | 10.54 | 1.95 |
| 86 | n-Octylbenzene | $C_{14}H_{22}$ | 432.94-462.87 | 5.14-14.26 | 3.60 | 2.99 | 35.33 | 2.33 |
| 87 | di-Butylsulfide | $C_8H_{18}S$ | 325.09-422.78 | 1.50-61.29 | 53.05 | 55.07 | 43.79 | 4.79 |
| 88 | di-Sec-butylsulfide | $C_8H_{18}S$ | 342.02-422.17 | 3.43-63.13 | 70.92 | 65.92 | 70.92 | 3.14 |
| 89 | 1,2–Bis(dimethylamino)ethane | $C_6H_{16}N_2$ | 294.75-364.97 | 1.77-40.04 | 6.22 | 16.08 | 1.56 | 1.26 |
| 90 | Ethyl methanoate | $C_3H_6O_2$ | 300-326.52 | 35.53-98.75 | 1.12 | 1.33 | 1.99 | 0.78 |
| 91 | Ethyl butanoate | $C_6H_{12}O_2$ | 341.38-393.55 | 16.16-99.4 | 1.09 | 1.06 | 8.65 | 1.08 |
| 92 | Propyl methanoate | $C_4H_8O_2$ | 309.09-352.95 | 18.52-99.07 | 2.16 | 1.24 | 1.85 | 1.08 |
| 93 | Propyl ethanoate | $C_5H_{10}O_2$ | 343.59-371.75 | 35.63-93.9 | 0.39 | 1.54 | 6.44 | 1.21 |
| 94 | Cumene | $C_9H_{12}$ | 346.69-392.87 | 15.14-39.87 | 2.39 | 0.97 | 3.38 | 0.56 |
| 95 | 3-Pentanone | $C_5H_{10}O$ | 347.05-364.75 | 40.01-73.35 | 2.04 | 1.45 | 4.75 | 1.35 |
| 96 | 3-Methylbutan-2-one | $C_5H_{10}O$ | 328.88-362.36 | 26.58-86.52 | 2.82 | 3.24 | 0.74 | 0.72 |
| 97 | 2-Hexanone | $C_6H_{12}O$ | 307.76-385.47 | 2.46-64.38 | 2.61 | 2.02 | 10.80 | 1.72 |
| 98 | 3-Hexanone | $C_6H_{12}O$ | 361.63-382.57 | 33.05-66.53 | 0.70 | 1.22 | 6.76 | 0.66 |
| 99 | 2-Heptanone | $C_7H_{14}O$ | 345.14-424.13 | 6.43-101.11 | 1.59 | 0.53 | 12.08 | 0.41 |
| 100 | 5-Nonanone | $C_9H_{18}O$ | 393.765-414.02 | 12.45-25.76 | 0.74 | 1.19 | 22.05 | 0.39 |
| | | | | | | | | |
| | Overall | | | | 5.55 | 5.68 | 12.91 | 1.18 |

*Table 7: Compare the results from ANN-GCM with EOSs for each group.*

| Family | ARD% | | | |
|---|---|---|---|---|
| | PR | SRK | PT | ANN |
| **Hydrocarbon** | 1.436 | 4.206 | 10.514 | 0.842 |
| **Aromatic** | 3.847 | 3.067 | 14.283 | 1.676 |
| **ester** | 1.190 | 1.292 | 4.732 | 1.037 |
| **ether** | 7.130 | 8.187 | 13.105 | 2.475 |
| **Aldehyde** | 9.946 | 9.456 | 11.246 | 2.596 |
| **Amin** | 11.540 | 13.778 | 8.988 | 3.423 |
| **Alcohol** | 12.994 | 12.937 | 37.834 | 1.944 |
| **Refrigeration** | 3.418 | 3.065 | 6.048 | 0.545 |
| **Hydrofluorocarbon** | 5.316 | 5.474 | 6.984 | 0.394 |
| **ketone** | 2.476 | 2.765 | 7.082 | 1.075 |
| **Halogen** | 2.116 | 5.28 | 11.833 | 1.984 |
| **Acid** | 6.641 | 6.36 | 7.120 | 2.876 |
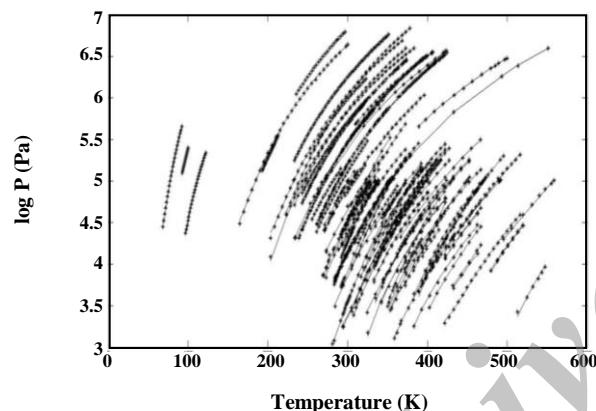


*Fig. 3: Comparison between ANN predicted (-) and experimental data.*



*Fig. 4: Comparison between Peng-Robinson predicted (-) and experimental data.*

deviation percents for various models. The predictions of ANN–GCM model are better than investigated EOSs. As observed in this table, for EOSs the average relative deviation percents have a wide range for substances but for neural network model the average relative deviation percents for these substances are within the same ranges. Comparisons between experimental and calculated values for ANN model and EOSs are shown in Figs. 3 to 6. The results from ANN-GCM with EOSs for each group are compared and shown in Table 7. For all of group, AAN model can predict the vapor pressure data better than EOSs.

**CONCLUSIONS**

In this work, artificial neural network model is developed to estimate the liquid vapor pressure of pure substances.

From 2044 existence points, 70% of them have applied for training, 20% for validating and 10% for testing. Based on obtained results, the best structure for neural network is Feed-forward back propagation network, Levenberg-marquardt back propagation training function, tangsig transfer function for hidden layer and purelin transfer function for output layer. Optimal number of neuron in hidden layer is 10 neurons. The weights are optimized to minimize the derivation between the calculated and experimental liquid vapor pressure data. The relative average error in estimating the vapor-liquid equilibrium was found to be quite low. The obtained results show that the optimum neural network architecture was able to predict vapor pressure data with an acceptable level of accuracy of *ARD %* of 1.183, *R*$^2$ of 0.999995, *Bias%* of -0.093 and RMS of 0.021.

*Table A.1: Number of structural group for Ethyl butanoate.*

| No. | Group | | No. | Group | |
|---|---|---|---|---|---|
| 1 | >C< | 0 | 14 | >N< | 0 |
| 2 | >CH- | 0 | 15 | -F | 0 |
| 3 | -CH$_2$- | 2 | 16 | -Cl | 0 |
| 4 | -CH$_3$ | 3 | 17 | -I | 0 |
| 5 | =CH$_2$ | 0 | 18 | -S-(Ring) | 0 |
| 6 | =CH- | 0 | 19 | –CH$_2$–(Ring) | 0 |
| 7 | ≡CH | 0 | 20 | >CH–(Ring) | 0 |
| 8 | -O- | 1 | 21 | =CH–(Ring) | 0 |
| 9 | -OH | 0 | 22 | >C<(Ring) | 0 |
| 10 | >C=O | 1 | 23 | –O–(Ring) | 0 |
| 11 | =O | 0 | 24 | -NO | 0 |
| 12 | –NH$_2$ | 0 | 25 | >N<(ring) | 0 |
| 13 | ≡N | 0 | 26 | -H | 0 |



*Fig. 5: Comparison between Patel-Teja predicted (-) and experimental data.*
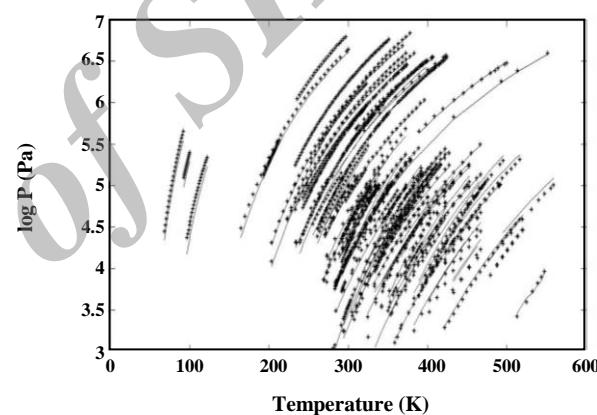


*Fig. 6: Comparison between SRK predicted (-) and experimental data.*

**Appendix A**

Instructions for running the program: The usage of the network is easy. Put the mat file ('ANN_GCM.mat') into the current folder of the MATLAB software (any version). Then, load the net to the workspace (using this command: _load ('ANN_GCM.mat'). To get the value of vapor pressure from the net, you must follow the following example step by step:

Assume that you want to predict the vapor pressure of Ethyl butanoate at 360.7778 K. The group contribution parameters should be defined from the structure of Ethyl butanoate. The number of each group has been given in Table A.1.

Then following commands should be entered in the MATLAB command window:

>> input = [360.7778;567;3060;0.460990012;0;0;2; 1;0;0;0;;1;0;1;0;1;0;0;0;0;0;0;0;0;0;0;0;0;0;0;0;0];

>> Preesure = sim(net,input)

Result is 39.4907, where its experimental value is equal to 33.4658 (ARD % is 0.0743).

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