Artificial Neural Network Model for the Prediction of Thermal Conductivity of Saturated Liquid Refrigerants and n-Alkanes

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ABSTRACT: In this paper, a feed-forward back-propagation artificial neural network (ANN) is proposed to correlate and predict the thermal conductivity from the triple point temperature up to 0.98 times critical temperature (T*) for 23 refrigerants and 11 n-alkanes. It requires the temperature (T) as well as the molecular mass (M), acentric factor (ω), critical temperature, and critical pressure (Pc) as input variables. The optimal ANN model is obtained by a trial-and-error procedure and consists of the input layer and the output layer together with one hidden layer with seven neurons. This ANN model can not only correlate the thermal conductivity but also accurately predict the thermal conductivity of refrigerants and n-alkanes. The correlation coefficients (R) in the training and testing phases are 0.9994 and 0.9993, respectively. Furthermore, the average absolute deviation (AAD) values are less than 1% for 14 out of 34 fluids, less than 2% for 28 fluids, and less than 4.5% for all the considered fluids.

1. INTRODUCTION

Thermal conductivity is the ability to transfer heat through conductivity as defined by the Fourier’s law. It is one of the most important transport properties. The knowledge of liquid thermal conductivity is essential in chemical engineering design. Over the years, thermal conductivity data of many liquids have been experimentally measured and compiled. Although experimental data are accurate and reliable, such measurements are often expensive and time-consuming. As a result, many researchers have tried to employ different methods to reproduce and predict the thermal conductivity for many kinds of liquids.1

The method proposed by Bridgman2 is based on the theoretical calculation considering molecular motion and interaction, but there is not both enough accuracy and simple expression.1,3,4 Several methods use group contribution theory.1,5−8 Moreover, some empirical and semiempirical methods such as corresponding-state principle and multiparameter correlation have also been used to predict the thermal conductivity.9−18

Recently, many researchers have employed artificial neural networks (ANN) to correlate the thermal properties, such as surface tension,19−24 density,25,26 and in particular thermal conductivity.3,4,27−32 Karabulut and Koyuncu32 exploited the feed-forward ANN model to develop thermal conductivity correlations of propane for the first time. Later, Esamlouyean and Khademi33 developed an ANN model to reproduce and predict thermal conductivity at atmospheric pressure for various pure gases. This model requires the temperature, molecular weight, critical pressure and critical temperature as input variables with an overall AAD of 5.42%. Pierantozzi et al.29 presented a multilayer perceptron ANN model to reproduce the thermal conductivity of alcohols with an overall AAD less than 0.0016%. Meanwhile, Lashkarbolooki et al.3 proposed an ANN based model to correlate the thermal conductivity for the normal and aromatic liquid hydrocarbons with the AAD of 0.20%. In this model, the input variables include the temperature, acentric factor, critical pressure, and critical temperature.

Subsequently, Pierantozzi and Petrucci,28 Ghaderi et al.,30 Ghaleh et al.,3 and Wang et al.27 developed ANN models to correlate and predict thermal conductivity for various refrigerants, respectively. However, in the case of the model in ref 28, the temperature range covered is not wide enough for some refrigerants. In the case of the other three models, the number of refrigerant types involved is a little small. In view of the fact that some n-alkanes such as methane and ethane, etc. can be used as natural refrigerants, some n-alkanes are taken into account along with refrigerants in this paper. For the reasons above, in this work an ANN model is utilized to correlate and predict thermal conductivity over a very wide range of temperatures for 23 refrigerants and 11 n-alkanes liquids.
2. MODELING THERMAL CONDUCTIVITY WITH AN ANN

2.1. Data Collection and Analysis. In this work, the REFPROP database is used as data source to study the ANN model for the thermal conductivity of refrigerants and n-alkanes. This program is developed by the National Institute of Standards and Technology (NIST). It is based on the most accurate pure fluids and fluid mixtures models currently available. In order to train and test the ANN model, we collected 19,113 data points of the thermal conductivity for 23 refrigerants and 11 n-alkanes from the REFPROP database. The thermal conductivity data from REFPROP are calculated using the correlation model and not experimental data. Correlation values may have higher errors than the assigned uncertainty level near the edges of the temperature range, especially near the critical point.

Table 1. Temperature Ranges, Number of Data Points (NP), and Physical Constants for 23 Refrigerants and 11 n-Alkanes

| fluid   | T (K) | λ (W/(m K)) | Pc (MPa) | M (g/mol) | Tc (K) | ω   | NP  |
|---------|-------|-------------|----------|-----------|--------|------|-----|
| dodecane | 263.6–647.72 | 0.067991–0.14393 | 1.817 | 170.33 | 658.1 | 0.574 | 583 |
| ethane  | 90.368–299.89 | 0.071493–0.25562 | 4.8722 | 30.069 | 305.32 | 0.0995 | 583 |
| heptane | 182.55–529.35 | 0.064359–0.15711 | 2.736 | 100.2 | 540.13 | 0.349 | 579 |
| hexane  | 177.83–496.83 | 0.077499–0.16873 | 3.034 | 86.175 | 507.82 | 0.299 | 581 |
| methane | 90.864–187.42 | 0.076259–0.21099 | 4.5992 | 16.043 | 190.56 | 0.0114 | 569 |
| octane  | 216.37–555.03 | 0.063591–0.15328 | 2.497 | 114.23 | 569.32 | 0.395 | 575 |
| pentane | 143.47–461.53 | 0.062577–0.17503 | 3.37 | 72.149 | 469.7 | 0.251 | 590 |
| propane | 85.525–363.3 | 0.067138–0.20792 | 4.2512 | 44.096 | 369.89 | 0.1521 | 592 |
| R113    | 236.93–477.17 | 0.04007–0.085549 | 3.3922 | 187.38 | 487.21 | 0.2525 | 573 |
| R115    | 173.75–345.35 | 0.039033–0.093819 | 3.129 | 154.47 | 353.1 | 0.248 | 573 |
| R123    | 166–456.4 | 0.038918–0.11589 | 3.6618 | 152.93 | 456.83 | 0.2819 | 606 |
| R124    | 120.44–386.66 | 0.044881–0.12476 | 3.6243 | 136.48 | 395.43 | 0.2881 | 494 |
| R125    | 172.52–334.08 | 0.045807–0.11602 | 3.6177 | 120.02 | 339.17 | 0.3052 | 578 |
| R134a   | 169.85–368.41 | 0.051448–0.14524 | 4.0593 | 102.03 | 374.21 | 0.3268 | 585 |
| R13     | 92–295 | 0.044826–0.13349 | 3.879 | 104.46 | 302 | 0.1723 | 581 |
| R141b   | 169.68–643.95 | 0.055423–0.12622 | 4.212 | 116.95 | 477.5 | 0.2915 | 578 |
| R142b   | 142.72–402.82 | 0.049787–0.13891 | 4.055 | 100.5 | 410.26 | 0.3232 | 579 |
| R143a   | 161.34–339.9 | 0.054416–0.13724 | 3.761 | 84.041 | 345.86 | 0.2615 | 577 |
| R14     | 120.13–223.63 | 0.0437–0.11461 | 3.75 | 88.005 | 227.51 | 0.1785 | 451 |
| R152a   | 154.56–379.2 | 0.065553–0.17633 | 4.5168 | 66.051 | 386.41 | 0.2752 | 577 |
| R218    | 125.45–340.79 | 0.033449–0.085197 | 2.64 | 188.02 | 345.02 | 0.3172 | 583 |
| R227ea  | 146.35–366.37 | 0.043666–0.094476 | 2.925 | 170.03 | 374.9 | 0.357 | 580 |
| R236ea  | 242–403.6 | 0.046817–0.103352 | 3.42 | 152.04 | 412.44 | 0.369 | 405 |
| R236fa  | 179.6–389.48 | 0.0486–0.10412 | 3.2 | 152.04 | 398.07 | 0.377 | 584 |
| R245ca  | 203.97–438.75 | 0.059217–0.12865 | 3.9407 | 134.05 | 447.57 | 0.355 | 547 |
| R245fa  | 171.05–418.3 | 0.053389–0.13556 | 3.651 | 134.05 | 427.16 | 0.3776 | 576 |
| R32     | 136.34–346.58 | 0.090882–0.24291 | 5.782 | 52.024 | 351.26 | 0.2769 | 583 |
| R41     | 129.82–314.58 | 0.092271–0.34698 | 5.897 | 34.033 | 317.28 | 0.2004 | 597 |
| RC318   | 233.35–379.99 | 0.044076–0.079042 | 2.7775 | 200.03 | 388.38 | 0.3553 | 565 |

Data from the fluids for predicting are not used in the training phase. Data are from the REFPROP of NIST.

The paper is organized as follows. In Section 2, a feed-forward neural network is constructed and the network parameters are determined. Section 3 presents the discussions of some main results in the training and testing phases. Finally, this work is concluded in Section 4.

A summary of these data is listed in Table 1 together with the physical properties required in the process of training and testing the ANN model. As can be seen, the data cover a very wide temperature range. The minimal temperature is the triple point temperature, while the highest temperature reaches about 0.98 times the critical point temperature for each fluid considered here. The data of the 29 fluids, which are carefully selected from all 34 fluids considered here and listed in the first 29 rows of Table 1, are used in the training phase to find the optimal structure and parameters of the ANN model, while the data of the other five fluids that were not used in the training phase are employed only in the testing phase to assess the predictive power of the optimal configuration model.

The 16,426 data points of the 29 fluids in the training phase are used as inputs to construct the ANN model and obtain the optimal weight and bias values of the model; 70%, 15%, and 15% of these data are randomly divided into the training data set, validation data set, and test data set, respectively. The 2,687 data points of the other five liquids are employed to examine the predictive power of the trained model with optimal configuration. These data are unknown for the training phase.
2.2. Constructing the ANN Model. In this work, a feed-forward back-propagation ANN model to correlate and predict thermal conductivity is constructed through utilizing the neural network toolbox in MATLAB software. As illustrated in Figure 1, this model consists of three layers: one input layer, one hidden layer, and one output layer. Its input variables are the temperature \(T\) as well as the molecular mass \(M\), acentric factor \(\omega\), critical temperature \(T_c\) and critical pressure \(P_c\), while the output variable is the thermal conductivity \(\lambda\) of each liquid. As is well-known to all, thermal conductivity is dependent on the temperature. Thus, the temperature is selected as one of the input variables. References 11, 13, 17, 35, and 36 have indicated that the thermal conductivity of the fluid is closely related to the molecular mass, acentric factor, critical temperature, and critical pressure. Furthermore, the four parameters are successfully used as inputs of the ANN model to differentiate the characteristic of the substances considered in ref 27. In this paper, the molecular mass, acentric factor, critical temperature, and critical pressure are employed to characterize the fluid types as in ref 27. Therefore, five neurons in the input layer are selected to receive the input signals and one neuron in the output layer is considered to transmit the output signal.

The ANN model is like a black box. The parameters affecting its performance include the number of neurons in the hidden layer, transfer function and training algorithm. To evaluate the performance of the different ANN, we used some statistical parameters, such as the mean square error (MSE), correlation coefficient \(R\), percent deviation (PD), and average absolute deviation (AAD). They are defined as follows

\[
\text{MSE} = \frac{1}{N} \sum_{i=1}^{N} (\lambda_{\text{cal},i} - \lambda_{\text{data},i})^2
\]

(1)

\[
R = \frac{C_v(\lambda_{\text{cal}}, \lambda_{\text{data}})}{\sqrt{C_v(\lambda_{\text{cal}}, \lambda_{\text{cal}})} \sqrt{C_v(\lambda_{\text{data}}, \lambda_{\text{data})}}}
\]

(2)

\[
\text{PD} = \frac{\lambda_{\text{cal}} - \lambda_{\text{data}}}{\lambda_{\text{data}}} \times 100\%
\]

(3)

\[
\text{AAD} = \frac{1}{n} \sum_{i=1}^{n} \left| \frac{\lambda_{\text{cal},i} - \lambda_{\text{data},i}}{\lambda_{\text{data},i}} \right| \times 100\%
\]

(4)

where \(C_v\) represents the covariance, \(\lambda_{\text{data}}\) is the thermal conductivity values from the REFPROP program, and \(\lambda_{\text{cal}}\) is the calculated thermal conductivity from the ANN model. Also, the adjust coefficient of determination \(R^2_{adj}\) is employed to compare the fit of regression models with different numbers of inputs. The \(R^2_{adj}\) is defined as the following

\[
R^2_{adj} = 1 - \frac{N - 1}{N - k - 1} (1 - R^2)
\]

(5)

where \(k\) and \(N\) represent the number of input parameters and the number of data points, respectively.

Optimization of structure and parameters is the major and difficult task for the ANN model. In this study, the Levenberg–Marquardt back-propagation (trainlm) algorithm is employed as training algorithm, mainly because this

![Figure 1. Structure of the ANN model for thermal conductivity.](image)

![Figure 2. MSE in the training phase and AAD in the detection phase versus the number of neurons in the hidden layer.](image)
algorithm appears to be the fastest and the most widely used method. With regard to the activity function or transfer function, by using trial-and-error method together with considering the aforementioned statistical parameters, the hyperbolic tangent sigmoid function (tansig) and linear function (purelin) are used in the hidden layer and output layer, respectively. They are defined as follows

$$\text{tansig}(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}} \tag{6}$$

$$\text{purelin}(x) = x \tag{7}$$

Furthermore, the optimal number of the neurons in the hidden layer need to be found utilizing the trial-and-error method. Too few neurons can lead to underfitting, whereas too many neurons can lead to overfitting. The MSE in the training phase and AAD in the testing phase versus the number of neurons in the hidden layer are shown in Figure 2. As can be seen, MSE value decreases in the training phase with the increase of the neurons number in the hidden layer. When the number of neurons is more than seven, the MSE value tends to be stable. On the other hand, AAD value in the testing phase tends to increase when the number of neurons is greater than seven. In order to balance the performance in the training phase and AAD values in the testing phase, the number of neurons is selected as 7.

The constructed ANN model with optimal configuration needs to be trained by using the Levenberg–Marquardt back-propagation algorithm so as to find the optimum weight and bias matrixes. The optimized weight and bias values in the hidden layer and output layer are obtained and shown in Table 2. Furthermore, performances of the ANN model with seven neurons in the hidden layer are tested for several combinations of inputs \((T, M, P_c, T_c, \omega)\). These results are listed in Table 3. According to the MSE, as can be seen, in the training phase the critical temperature is the most important while the critical pressure is the least important. However, the critical pressure is of relative importance for the predictive power of the model.

### Table 2. Weight and Bias Values of the ANN Model for Thermal Conductivity

| neuron | T | P_c | M | T_c | \omega |
|--------|---|-----|---|-----|-------|
| 1      | 2.9284 | 3.1977 | -1.0803 | 6.6785 | -6.7831 |
| 2      | 0.4269 | 0.452 | 0.0091 | -1.478 | 0.0591 |
| 3      | -0.4807 | 0.2525 | -0.2578 | 0.6324 | 0.2577 |
| 4      | -1.2319 | 1.0717 | 0.8516 | -0.2914 | 0.3142 |
| 5      | 1.0868 | -0.2992 | -0.0711 | 0.163 | -0.0805 |
| 6      | -1.0054 | 1.7473 | 0.3851 | 0.0234 | 0.8597 |
| 7      | 1.1082 | -0.539 | -0.3278 | 0.1197 | -0.1398 |

| neuron | hidden layer bias | output layer weight | output layer bias |
|--------|-------------------|---------------------|------------------|
| 1      | 6.6343            | 0.0533              | 0.5625           |
| 2      | -2.9088           | -12.9359            | -12.9359         |
| 3      | -0.9434           | 1.2995              | 1.2995           |
| 4      | -1.3103           | 2.4064              | 2.4064           |
| 5      | 1.324             | -5.913              | -5.913           |
| 6      | -4.7474           | 13.9369             | 13.9369          |
| 7      | 1.3766            | 8.8979              | 8.8979           |

### Table 3. Performances for Several Cases with Seven Neurons in the Hidden Layer

| inputs | training set (29 fluids) | testing set (5 fluids) |
|--------|--------------------------|------------------------|
| (T, M, P_c, T_c, \omega) | MSE (x10^6) | R | R^2 | R^2_adj | MSE (x10^6) | R | R^2 | R^2_adj |
| (T, P_c, T_c, \omega) | 2.8192 | 0.9994 | 0.9988 | 0.9988 | 2.1724 | 0.9993 | 0.9986 | 0.9986 |
| (T, M_c, T_c, \omega) | 3.8501 | 0.9991 | 0.9982 | 0.9982 | 23.9109 | 0.9908 | 0.9817 | 0.9817 |
| (T, M_c, P_c, \omega) | 2.0588 | 0.9995 | 0.9990 | 0.9990 | 28.5217 | 0.9906 | 0.9813 | 0.9813 |
| (T, M_c, P_c, T_c) | 4.7282 | 0.9989 | 0.9978 | 0.9978 | 18.3671 | 0.9936 | 0.9872 | 0.9872 |
| 3. RESULTS AND DISCUSSIONS

In the training phase, a plot of predicted thermal conductivity values, the outputs, versus the targets with respect to the ANN model of the optimal configuration is illustrated in Figure 3. As can be seen, the outputs of the ANN model keep close agreement with the targets, namely, the thermal conductivity values from REFPROP program. In the training stage, the MSE, \(R\), and \(R^2\) of the presented ANN model are 2.8192 \(x\) \(10^{-6}\), 0.9994, and 0.9988, respectively. Then, the trained ANN model with the optimum structure, parameters as well as optimum weight and bias values is applied in the testing phase to examine the predictive ability. In this case, the thermal conductivity values of the five unknown liquids are used which is not used in the training phase. A comparison of the output values, i.e., the predicted thermal conductivity values, and the target ones is depicted in Figure 4. As can be seen in Figure 4, in the testing stage, the MSE, \(R\), and \(R^2\) of this ANN model

![Figure 3](https://example.com/figure3.png)
are $2.1724 \times 10^{-6}$, 0.9993, and 0.9986, respectively. As shown, the trained ANN model with the optimum configuration and parameters reveals the powerful predictive ability for the thermal conductivity of the unknown fluids.

Additionally, the PD and AAD values of the ANN model are given in Figure 5 and Table 4 with regard to all 34 fluids considered here. From Table 4, the mean AAD values are 1.34%, 1.46%, and 1.36% in the training phase, testing phase and both phases, respectively. The accuracy of output varies with the substance for the proposed ANN model. AAD values vary from 0.18% to 4.5%. Also, AAD values are less than 1% for 14 out of 34 fluids, and less than 2% for 28 fluids. AAD value is higher than 3% for only hexane.

As seen in Figure 5, the PD values are affected by the thermal conductivity values, and most of the PD values are between $-5\%$ and $5\%$ for all the fluids considered here. The PD values are relatively small when the thermal conductivity values are great, whereas the PD values are often comparatively high when the thermal conductivity values are very small. Moreover, considering Table 4 as well, all the absolute PD values are all less than 13.48%. The maximum absolute PD values are more than 10% only in case of hexane, R13, R14 and R123. The maximum absolute PD value, 13.48%, is also obtained from hexane. The mean PD values are between $-1\%$ and $1\%$ for 23 fluids, between $-2\%$ and $2\%$ for 31 fluids, outside $-3\%$ to $3\%$ for only hexane.

However, the performance of the proposed ANN model is slightly different for each family of fluids. The calculated thermal conductivity values versus the target values with respect to the ANN model for each family in the training and testing phase are shown in Figures 6 and 7, respectively. As can be seen in Figure 6, the MSE and $R$ of this model are $1.7898 \times 10^{-6}$ and 0.9996, respectively, for refrigerants in the training stage, while the MSE and $R$ of this model are $5.4246 \times 10^{-6}$ and 0.9996, respectively, for $n$-alkanes in the training stage. Obviously, the performance of this model for refrigerants is slightly better than for $n$-alkanes, which can also be seen in Figure 7.

### Table 4. Deviations of the ANN Model for Thermal Conductivity

| fluids    | maximum (%) | minimum (%) | mean (%) | AAD (%) |
|-----------|-------------|-------------|----------|---------|
| dodecane  | 0.2         | $-1.62$     | $-0.42$  | 0.47    |
| ethanol   | 1.01        | $-2.82$     | $-0.24$  | 0.37    |
| heptane   | 4.38        | $-0.2$      | 0.91     | 0.99    |
| hexane    | $-0.88$     | $-13.48$    | $-4.5$   | 4.5     |
| methane   | 0.92        | $-1.1$      | 0.04     | 0.18    |
| octane    | 6.77        | $-1.58$     | 2.2      | 2.37    |
| pentane   | 7.5         | 0.11        | 2.57     | 2.57    |
| propane   | 2.18        | $-1.35$     | 0.39     | 0.71    |
| R113      | 0.43        | $-1.29$     | $-0.3$   | 0.38    |
| R115      | 0.73        | $-6.6$      | $-1.12$  | 1.46    |
| R123      | 11.89       | $-4.4$      | 1.79     | 2.58    |
| R124      | 2.23        | $-1.17$     | 1.21     | 1.22    |
| R125      | 1.78        | $-0.98$     | 0.66     | 0.80    |
| R134a     | 7.02        | $-4.23$     | 0.66     | 1.66    |
| R13       | 1.62        | $-12.52$    | $-0.29$  | 1.63    |
| R141b     | 1.88        | $-3.58$     | 0.01     | 0.50    |
| R142b     | 2.05        | $-2.1$      | $-0.74$  | 1.28    |
| R143a     | 0.59        | $-2.62$     | $-0.53$  | 0.81    |
| R14       | 1.73        | $-10.35$    | $-0.15$  | 1.59    |
| R152a     | 1.45        | $-2.81$     | 0.13     | 0.84    |
| R218      | 7.17        | $-0.7$      | 0.9      | 1.24    |
| R227ea    | 0.89        | $-4.25$     | $-1.13$  | 1.26    |
| R236ea    | 2.24        | $-5.58$     | $-0.25$  | 1.87    |
| R236fa    | 3.04        | $-4.4$      | $-0.55$  | 1.78    |
| R245ca    | 1.61        | $-5.03$     | $-1.33$  | 2.18    |
| R245fa    | 2.73        | $-2.78$     | 1.19     | 1.35    |
| R32       | 1.57        | $-4.48$     | $-0.19$  | 0.75    |
| R41       | 6.65        | $-1.31$     | 0.18     | 0.90    |
| R318      | 1.86        | $-0.46$     | 0.18     | 0.63    |
| mean-train|-           | -           | -        | 1.34    |
| butane    | 2.89        | 0.11        | 1.57     | 1.57    |
| decane    | 1.48        | $-6.44$     | 0.06     | 1.49    |
| nonane    | 1.56        | $-3.37$     | $-0.64$  | 1.54    |
| R114      | 1.92        | $-4.05$     | $-1.74$  | 2.14    |
| R116      | 2.11        | $-1.53$     | 0.28     | 0.56    |
| mean-predicted|-           | -           | -        | 1.46    |
| mean-all  | -           | -           | -        | 1.36    |
To finish this section, the results obtained for hexane are considered. For this fluid, the AAD, absolute maximum PD, and mean PD are 4.5%, −13.48%, and −4.5%, respectively. Any of the three deviations is the highest among all the 34 fluids considered here. A plot of the PD values versus correlation values for hexane from REFPROP illustrated in Figure 8. As seen, the absolute PD value increases with the increase of temperature in the intermediate and high temperatures. The maximum value is found at the highest temperature considered, namely, near the critical temperature. As denoted in REFPROP, the overall uncertainty is estimated to be less than 4.2%, and larger uncertainties are in the critical region. The predicted results from the ANN model basically agree with the specified information in REFPROP. Evidently, for hexane, the ANN model underestimates the correlation values from REFP. For this reason, experimental data of hexane are collected from some literature, as listed in Table 5. For these experimental data, PD values with respect to the proposed ANN model are calculated. A plot of the PD values versus the experimental data is shown in Figure 9. It can be seen that the predicted values from the ANN model keep agreement with the experimental data for hexane. Obviously, the correlation model from REFP overestimates thermal conductivity values for hexane. Unfortunately, experimental data near the critical temperature is not found in previous literature. Therefore, experimental data near the critical temperature are needed in order to obtain a clear conclusion about whether the ANN model is adequate or not for hexane near the critical temperature.

In sum, in a very wide temperature range, the proposed ANN model not only can accurately correlate the thermal conductivity, but also has the strong power to predict the
thermal conductivity of unknown fluids, that is, it can extrapolate the thermal conductivity very well.

4. CONCLUSIONS

In this work, a feed-forward back-propagation ANN model is developed to correlate and predict the thermal conductivity of 23 refrigerants and 11 n-alkanes from the triple point temperature up to 0.98Tc. The input variables are the temperature, molecular weight, acentric factor, together with the critical temperature and pressure. This ANN model is composed of the input layer, the output layer, and one hidden layer with seven neurons. The activity functions in the hidden layer and output layer are selected as “tansig” and “purelin” functions, respectively. Also, the ANN model is trained by using the “trainlm” algorithm, and the optimum weight and bias values are obtained. The calculated thermal conductivity values by the trained ANN with the optimum parameters agree well with the data from the REFPROP program in both the training and testing stages. The R values in both stages are 0.9994 and 0.9993, respectively. Moreover, AAD values less than 1% are found for 14 out of 34 fluids, less than 2% for 28 fluids, and less than 4.5% for all the considered fluids. The maximum absolute PD value is 13.48%, corresponding to hexane. The ANN model performs slightly better for refrigerants than for n-alkanes. However, some disagreements can be found near the critical temperature for some fluids. In conclusion, the developed ANN model demonstrates a powerful predictive ability in addition to the correlative power in the very wide temperature range.

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Notes

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Table 5. Experimental Thermal Conductivity Data of Hexane from Refs 37—39

| T (K)          | λ (W/(m K)) | uncertainty (%) | NP | ref |
|----------------|-------------|----------------|----|-----|
| 183.15—303.15 | 0.1182−0.1597 | 1              | 13 | 37  |
| 297.35—324.77 | 0.1123−0.1209 | 1              | 12 | 38  |
| 298.15—333.15 | 0.1083−0.1215 | 1              | 4  | 39  |

Figure 8. PD values versus thermal conductivity values from REFPROP for hexane.

Figure 9. PD values versus experimental thermal conductivity data from ref 37—39 for hexane.
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