General Model Based on Artificial Neural Networks for Estimating the Viscosities of Oxygenated Fuels

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Supporting Information

ABSTRACT: Oxygenated fuel is a promising alternative fuel for engines because of the advantage of low emission. In this work, a general model based on back-propagation neural networks was developed for estimating the viscosities of different kinds of oxygenated fuels including esters, alcohols, and ethers, whose input variables are pressure, temperature, critical pressure, critical temperature, molar mass, and acentric factor. The viscosity data of 31 oxygenated fuels (1574 points) at temperatures ranging from 243.15 to 413.15 K and at pressures ranging from 0.1 to 200 MPa were collected to train and test the back-propagation neural network model. The comparison result shows that the predictions of the proposed back-propagation neural network model agree well with the experimental viscosity data of all studied oxygenated fuels using the general parameters (weight and bias). The average absolute relative deviations for training data, validation data, and testing data are 1.19%, 1.27%, and 1.30%, respectively.

1. INTRODUCTION

Reducing global greenhouse gas emissions is an issue concerned to the world, and a number of research studies have been performed on this issue.1−7 Oxygenated fuels including biodiesels, alcohols, ethers, etc., which have the advantages of lower soot and particle emissions compared with fossil fuels, are considered as environment-friendly fuels for engine.8−12 The viscosity data of oxygenated fuels are extremely important in the process of transportation, storage, and usage.13 There are plenty of experimental viscosity data for oxygenated fuels from atmospheric pressure to hundreds of megapascals reported in the literature.14−20 However, experimental data are always discrete points and cannot really meet the actual demand. The accurate viscosity model established on the basis of experimental data is more meaningful to provide sufficient viscosity data of oxygenated fuels. Many viscosity models have been developed for oxygenated fuels such as esters, alcohols, and ethers, but only few examples are given here. Allal et al.21 proposed a viscosity model-based free volume (FV) theory for alcohols. Assael et al.22 proposed a hard-sphere model for estimation of the viscosities of n-alcohols. Yuan et al.23 used the Vogel equation to correlate the viscosities of fatty acid methyl esters at atmospheric pressure. Ceriani et al.24 proposed a viscosity model based on the group contribution method for the viscosities of methyl and ethyl esters and alcohols. Habibi et al.25 developed a viscosity model for alcohols combining CPA equation and friction theory. Ivanciuc et al.26 proposed a quantitative structure−property relationship model for the liquid viscosities of esters, alcohols, ethers, etc. Our group proposed a viscosity model based on Eyring’s absolute rate theory (EART) named HLZ model in previous work27 and applied it to estimate the viscosities of esters, alcohols, and ethers.28 Although these models have high accuracy, they need one set of parameters obtained by fitting to the experimental data for each oxygenated fuel.

In recent years, artificial neural network (ANN) which is a popular way to solve the nonlinear mapping problem has been used to predict various physical properties of a fluid, such as density, surface tension, and viscosity, and achieved a great success.29−31 Compared with traditional models, the parameters of the ANN model are universal for different substances, so the ANN model has much better predictive ability. Some ANN models have been developed for predicting the viscosities of esters in the literature. For example, Hosseini et al.32 proposed an ANN model to predict the viscosities of eight fatty acid esters and two biodiesels at a pressure up to 140 MPa using four input variables (pressure, pseudo-critical density, temperature, and molecular weight). However, for other kinds of oxygenated fuels such as alcohols and ethers, there are few ANN models applicable to predict their viscosities.

Therefore, in this work, we aim to develop a general model based on ANN for estimating the viscosities of different kinds of oxygenated fuels including esters, alcohols, and ethers at a pressure up to 200 MPa. Back-propagation neural network

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(BPNN) was chosen because it is the most widely used ANN because of its stability and reliability.33

2. COMPUTATIONAL METHOD

2.1. Model Description. BPNN, which is a kind of feed forward neural network,34 has three parts (input layer, hidden layer, and output layer) and five elements (input variable, weight, summation function, activation function, and output variable). Each layer has several neurons, and the values of neurons will be calculated using the values of neurons in the previous layer via summation function and activation function. BPNN usually has one or two hidden layers for data fitting. BPNN with two hidden layers has better accuracy and better capacity to solve the nonlinear problem compared with BPNN with one hidden layer.35 Therefore, our work chose the BPNN with two hidden layers. Figure 1 is the schematic diagram of

![Figure 1. Schematic diagram of BPNN.](image)

BPNN with two hidden layers. Pressure and temperature are the parameters deciding the viscosity of the compound, while critical pressure, critical temperature, molar mass, and acentric factor are characterization parameters of the compound. Therefore, six factors such as pressure (p, Pa), temperature (T, K), critical pressure (p_c, Pa), critical temperature (T_c, K), mole mass (M_w,g mol^{-1}), and acentric factor (ω) were chosen as the input variables. Critical pressure (p_c, Pa), critical temperature (T_c, K), mole mass (M_w,g mol^{-1}), and acentric factor (ω) were chosen because these parameters are constant for one compound, which are usually used to characterize the compound and as the input parameters for predicting the viscosity.36 The output variable is viscosity (η, μPa·s). The number of neurons in the input layer depends on the input variables and that in the output layer depends on the output variables. Therefore, the hidden layer is the only adjustable part.

The procedure for finding the best BPNN structure is as follows: first, collecting data and dividing them into training data, verification data, and testing data; second, training the BPNN model using training data and verification data to determine the BPNN structure, the summation function, and the activation function; and third, testing the predictive ability of the BPNN model using testing data.

Considering the difference of input data and output data in dimension, these data were dealt with eq 1.

\[
x = \frac{0.8(X - X_{\min})}{X_{\max} - X_{\min}} + 0.1
\]

where X is the original value of the variable, x is the normalized value, and X_{\min} and X_{\max} are the minimum value and maximum value of the variable, respectively.

In BPNN, the summation function is used to connect neurons of two adjacent layers. The value of i-th neuron in the (k+1)th layer z_{ik+1} can be calculated by a summation function as follows

\[
z_{ik+1} = \sum w_{i}^{k+1} a_{i}^{k} + b_{j}^{k+1}
\]

where w_{i}^{k+1} is the weight of the j-th neuron in the (k+1)th layer, b_{j}^{k+1} is the bias of the j-th neuron in the (k+1)th layer, and a_{j}^{k+1} is the output of the j-th neuron in the k-th layer, which is calculated by the activation function of z_{j}^{k}. In this work, three commonly used activation functions which are purelin function, log sigmoid function, and tan-sigmoid function were tested. Comparison result shows that the log sigmoid function has better performance than the activation function. The log sigmoid function is expressed as

\[
a_{j}^{k+1} = \frac{1}{1 + e^{-z_{j}^{k+1}}}
\]

where a_{j}^{k+1} is the output of the j-th neuron in the (k+1)th layer.

2.2. Data Collection. The viscosity data of 31 oxygenated fuels (1574 points) at temperatures ranging from 243.15 to 413.15 K and at pressures ranging from 0.1 to 200 MPa are collected from the literature14−19,37–39 and listed in Table 1. The information of the chemicals provided in the literature is shown in Table S1 (Supporting Information). The physical properties of the 31 oxygenated fuels are listed in Table 2.36 Seventy percent of the total data (1102 points) were used for training the BPNN model, 15% of the total data (236 points) were used for validation, and 15% of the total data (236 points) were used for testing data. All of the data were divided randomly.

3. RESULTS AND DISCUSSION

Less neurons in the hidden layer will lead to underfitting and large error, while more neurons in the hidden layer will result in overfitting and time-consuming error. After investigation of the previous work,32 the mean-square error (MSE) was chosen as the optimization objective during the training to get the best BPNN structure. The MSE is expressed as

\[
MSE = \frac{1}{N} \sum_{i=1}^{N} \left( y_{i}^{\text{exp}} - y_{i}^{\text{cal}} \right)^{2}
\]

where y_{i}^{\text{exp}} and y_{i}^{\text{cal}} are the experimental value and calculated values of the output variable, respectively.

The training result shows that the BPNN should have two hidden layers and the neuron numbers in them are 6 and 12, respectively. Tables 3−5 report the weight and bias of the input layer, the first hidden layer, and the second layer, respectively. To explain the optimization procedure, an example is given in Figure 2, which shows the MSE of the viscosity data of 31 oxygenated fuels with the neuron number of the second hidden layer changing from 4 to 19 while 6 neurons in the first hidden layer. The result shows that when there are 12 neurons in the second hidden layer (MSE = 0.01454), the BPNN model has the best performance for estimating the viscosities of oxygenated fuels. Therefore, we chose 12 as the neuron number in the second hidden layer.
The performance of the obtained BPNN model was also evaluated by several other factors which are average absolute relative deviation (AARD) and maximum absolute relative deviation (MARD) defined by eqs 5 and 6, respectively.

\[
\text{AARD} = \frac{1}{n} \sum_{i=1}^{n} \left| \frac{\eta_{i}^{\text{cal}} - \eta_{i}^{\text{exp}}}{\eta_{i}^{\text{exp}}} \right| \times 100\%
\]  

(5)

\[
\text{MARD} = \max \left\{ \left| \frac{\eta_{i}^{\text{cal}} - \eta_{i}^{\text{exp}}}{\eta_{i}^{\text{exp}}} \right| \times 100\% \right\}
\]  

(6)

where \(\eta^{\text{exp}}\) and \(\eta^{\text{cal}}\) are the experimental and calculated values from the BPNN model for viscosity.

The calculated results from the present BPNN model for the viscosities of oxygenated fuels were first compared with the training and validation data. Comparison results show that the AARDs of the present BPNN model from training data and validation data are 1.19 and 1.27%, respectively, which implies that the present BPNN model correlates the viscosity data very well. Then, the calculated results from the present BPNN model were compared with the testing data in order to verify the predictive ability. A satisfactory performance was found, indicating that the AARD of the present BPNN model from testing data is 1.30%, which implied the excellent predictability of this model.

Table 6 lists the AARDs and MARDs of the present BPNN model from the experimental viscosity data of each oxygenated fuel. It can be observed that the AARDs for all oxygenated fuels are less than 3%. In order to compare the performance of the present BPNN model for different kinds of oxygenated fuels, the AARDs of the present BPNN model for alcohols, esters, and ethers are also calculated, which are 1.02, 0.99, and 1.61%, respectively.

| Name                          | T/K     | \(p/\text{MPa}\) | \(U^*/\%\) | points | ref |
|-------------------------------|---------|------------------|-------------|--------|-----|
| methanol                      | 298.15–323.15 | 0.1–27.05       | 0.5         | 19     | 18  |
| 303.15–323.15                 | 0.1–30  | 2                | 22          | 37     |
| 283.15–348.15                 | 0.1–68.8| 2                | 31          | 19     |
| ethanol                       | 298.15–323.15 | 0.1–27.56       | 0.5         | 20     | 18  |
| 293.15–353.15                 | 0.1–100 | 2                | 23          | 38     |
| 283.15–323.15                 | 0.1–78.6| 2                | 16          | 19     |
| 1-propanol                    | 298.15–323.15 | 0.1–27.86       | 0.5         | 20     | 18  |
| 2-propanol                    | 283.15–323.15 | 0.1–117.8       | 2           | 39     | 19  |
| 3-propanol                    | 298.15–373.15 | 0.1–117.8       | 2           | 15     | 40  |
| 1-pentanol                    | 303.15–343.15 | 0.1–100         | 2           | 39     | 19  |
| 3-pentanol                    | 298.15–373.15 | 0.5–195         | 2           | 15     | 40  |
| 1-nonanol                     | 283.15–413.15 | 0.1–22.5        | 2           | 19     | 40  |
| 2-methyl-2-propanol           | 303.15–323.15 | 0.1–68.8        | 2           | 13     | 19  |
| vinyl acetate                 | 298.15–373.15 | 0.1–19.91       | 2           | 40     | 41  |
| diethyl adipate               | 303.15–373.15 | 0.1–19.52       | 2           | 38     | 42  |
| dimethyl carbonate            | 283.15–353.15 | 0.1–100         | 2           | 40     | 43  |
| diethyl carbonate             | 263.15–363.15 | 0.1–19.49       | 2           | 55     | 44  |
| ethyl heptanoate              | 312.72–353.04 | 0.1–15.17       | <2.7        | 30     | 14  |
| ethyl octanoate               | 312.87–353.38 | 0.1–15.24       | <2.7        | 30     | 14  |
| methyl caprate                | 293.15–353.15 | 0.1–200         | <4          | 42     | 16  |
| ethyl caprate                 | 293.15–353.15 | 0.1–200         | <4          | 44     | 16  |
| methyl laurate                | 302.98–353.40 | 0.1–15.07       | 1.5         | 36     | 45  |
| ethyl laurate                 | 293.15–353.15 | 0.1–20.0        | <4          | 54     | 45  |
| methyl myristate              | 303.15–353.15 | 0.1–100         | 2           | 38     | 17  |
| ethyl myristate               | 293.15–353.15 | 0.1–100         | 2           | 38     | 17  |
| diethyl ether                 | 243.15–373.15 | 0.1–19.61       | 2           | 70     | 46  |
| diisopropyl ether             | 243.15–373.15 | 0.1–21.68       | 2           | 70     | 47  |
| dibutyl ether                 | 243.15–373.15 | 0.1–21.12       | 2           | 70     | 47  |
| dimethoxymethane              | 243.15–373.15 | 0.1–19.55       | 2           | 70     | 48  |
| ethylene glycol dimethyl ether| 243.15–373.15 | 0.1–19.48       | 2           | 70     | 48  |
| diethylene glycol dimethyl ether| 243.15–323.15 | 0.15–21.49      | 2           | 45     | 49  |
| triethylene glycol dimethyl ether| 283.15–353.15 | 0.1–100        | 2           | 48     | 43  |
| tetraethylene glycol dimethyl ether| 283.15–353.15 | 0.1–100        | 2           | 48     | 43  |
| monoethyglycol methyl ether   | 293.15–353.15 | 0.1–100         | 2           | 42     | 50  |
| monoethylglycol ethyl ether   | 293.15–353.15 | 0.1–100         | 2           | 42     | 50  |
| monoethyglycol iso-propyl ether| 293.15–353.15 | 0.1–100        | 2           | 42     | 50  |

Table 1. Summary of Selected Viscosity Data in the Literature

The uncertainty of the experimental viscosity data is less than 0.5%.
respectively. It means that the present BPNN model can give good prediction for the viscosities of different kinds of oxygenated fuels. Figure 3 plots AARDs of the present BPNN model against critical pressure, critical temperature, mole mass, and acentric factor and shows that there is no apparent connection between AARDs and the four parameters.

Table 3. Physical Properties of Oxygenated Fuels

| Name                  | CAS no. | MW   | Tc/K | pc/MPa | ω       |
|-----------------------|---------|------|------|--------|---------|
| Methanol              | 67-56-1 | 32.042| 512.64| 8.10   | 0.565   |
| Ethanol               | 64-17-5 | 46.068| 513.92| 6.15   | 0.649   |
| 1-propanol            | 71-23-8 | 60.095| 536.78| 5.18   | 0.629   |
| 2-propanol            | 67-63-0 | 60.095| 508.30| 4.76   | 0.665   |
| 1-pentanol            | 71-41-0 | 88.148| 588.15| 3.91   | 0.579   |
| 3-pentanol            | 584-02-1| 88.148| 559.60| 3.88   | 0.538   |
| 1-nonanol             | 143-08-8| 144.255|668.90|2.63    |0.633    |
| 2-methyl-2-propanol   | 75-65-0 | 74.122| 712.64| 8.10   | 0.565   |
| vinyl acetate         | 108-05-4| 86.089| 519.13| 3.97   | 0.631   |
| diethyl adipate       | 141-28-6| 202.248|685.00|2.13    |0.326    |
| dimethyl carbonate    | 616-38-6| 90.078| 557.00| 4.80   | 0.336   |
| diethyl carbonate     | 105-58-8| 118.131|669.00|3.47    |0.545    |
| ethyl heptanoate      | 106-30-9| 158.238|629.00|2.33    |0.596    |
| ethyl octanoate       | 106-32-1| 172.265|637.00|2.20    |0.579    |
| methyl caprate        | 110-42-9| 186.291|671.00|3.64    |0.699    |
| ethyl caprate         | 110-38-3| 200.318|667.00|1.89    |0.699    |
| methyl laureate       | 111-82-0| 214.344|712.00|1.74    |0.692    |
| ethyl laureate        | 106-33-2| 228.371|695.00|1.66    |0.771    |
| methyl myristate      | 124-10-7| 242.398|708.00|1.58    |0.950    |
| ethyl myristate       | 124-06-1| 256.428|721.00|1.50    |0.852    |
| diethyl ether         | 60-29-7 | 74.122| 466.70| 3.64   | 0.281   |
| diisopropyl ether     | 108-20-3| 102.175|599.56|2.83    |0.332    |
| dibutyl ether         | 142-96-1| 130.228|708.00|2.50    |0.559    |
| dimethoxymethane      | 109-87-5| 76.094| 564.00| 3.96   | 0.220   |
| ethylene glycol dimethyl ether | 110-71-4 | 90.121| 536.15| 3.87   | 0.346   |
| diethylene glycol dimethyl ether | 111-96-6 | 118.131|669.00|2.94    |0.575    |
| triethylene glycol dimethyl ether | 112-49-2 | 178.226|651.00|2.31    |0.792    |
| tetraethylene glycol dimethyl ether | 143-24-8 | 222.279|705.00|1.94    |0.965    |
| monoethylene glycol methyl ether | 109-86-6 | 90.121| 569.00| 4.24    |0.758    |
| monooctene glycol ethyl ether | 110-80-5 | 144.255|669.00|2.50    |0.539    |
| monooctene glycol iso-propyl ether | 109-59-1 | 104.148|582.00|3.67    |0.783    |

Table 4. Weight and Bias of the First Hidden Layer

| Wij | 1  | 2  | 3  | 4  | 5  | 6  | b1  |
|-----|----|----|----|----|----|----|-----|
| 1   | −0.013 | 0.157 | −1.102 | 0.998 | 0.236 | 0.279 | 0.236 |
| 2   | 0.666 | 0.216 | 0.316 | 0.326 | 0.525 | 0.407 | 0.407 |
| 3   | −0.470 | 0.162 | 0.181 | 0.191 | 0.235 | 0.407 | 0.407 |
| 4   | 0.114 | 0.012 | −0.092 | 0.649 | 0.912 | 0.114 | 0.114 |
| 5   | 0.591 | −0.032 | −0.749 | 1.296 | 0.213 | 0.591 | 0.591 |
| 6   | −0.441 | 0.648 | 0.899 | 1.289 | 0.316 | −0.441 | 0.441 |

Table 4. Weight and Bias of the Second Hidden Layer

| Wij | 1  | 2  | 3  | 4  | 5  | 6  | b2  |
|-----|----|----|----|----|----|----|-----|
| 1   | 0.838 | −0.980 | 8.598 | −1.746 | −1.674 | 3.112 | 2.534 |
| 2   | −1.627 | 1.173 | −8.243 | 1.327 | 1.850 | −2.720 | −1.753 |
| 3   | −0.569 | 0.328 | −3.031 | −0.745 | −0.021 | −2.527 | 0.874 |
| 4   | −2.552 | 0.614 | −8.198 | −3.172 | −1.617 | 0.802 | −4.013 |
| 5   | 1.204 | −0.874 | 4.942 | −0.009 | 1.162 | 2.046 | 0.632 |
| 6   | 0.791 | −0.199 | 3.179 | 1.138 | 0.306 | 2.046 | −1.226 |
| 7   | −2.466 | 0.767 | −7.590 | −2.863 | −1.499 | 0.804 | −3.917 |
| 8   | 2.917 | 1.069 | 10.345 | −3.863 | 3.351 | 1.537 | 2.226 |
| 9   | 0.659 | −0.218 | 3.037 | 0.939 | 0.129 | 2.384 | −1.171 |
| 10  | −3.232 | −0.882 | −10.959 | 3.879 | −3.189 | −1.428 | −4.082 |
| 11  | −0.594 | 1.080 | −9.633 | 1.844 | 1.671 | −3.029 | −3.441 |
| 12  | −6.155 | 3.715 | 16.079 | −4.590 | −0.519 | 2.613 | 1.083 |
To further investigate the overall accuracy of the present BPNN model, Figure 4 compares the experimental and calculated values of the viscosities of all oxygenated fuels. A very good agreement can be observed, which is also supported by Table 7. As shown in Table 7, the absolute relative deviations of the present BPNN model for 54.89% of total data (864 points) are below 1%; the absolute relative deviations for 27.89% of total data (439 points) are between 1 and 2%; 9.85% of total data (155 points) are between 2 and 3%; 6.16% of total data (97 points) are between 3 and 5%; only the absolute relative deviations for 1.21% of total data (16 points) are greater than 5%. The AARD and MARD of total data are calculated to be 1.24 and 10.70%, respectively. The AARD of the FV model and the model based on EART proposed by our group are also provided in Table 6 for comparison. It can be found that the present BPNN model has a similar total AARD to the FV model and EART model but a lower total MARD. Moreover, the present BPNN model has stronger prediction ability than the FV model and EART model because it can calculate the viscosity of a new oxygenated fuel just using temperature, pressure, critical pressure, critical temperature, mole mass, and acentric factor with no experimental viscosity data available.

4. CONCLUSIONS

In this work, a general BPNN viscosity model was proposed for oxygenated fuels based on the viscosity data of 31 oxygenated

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**Table 5. Weight and Bias of the Output Layer**

| Wij  | 1   | 2   | 3   | 4   | 5   | 6   | 7   |
|------|-----|-----|-----|-----|-----|-----|-----|
| 1    | 15.342 | 7.347 | −5.730 | −6.624 | −0.838 | 6.723 | 4.767 |
| Wij  | 8   | 9   | 10  | 11  | 12  | b1  |
| 1    | −8.880 | −11.347 | −2.135 | 7.191 | 1.948 | −4.861 |

**Figure 2.** MSE of the BPNN model at different neuron numbers in the second hidden layer.

To further investigate the overall accuracy of the present BPNN model, Figure 4 compares the experimental and calculated values of the viscosities of all oxygenated fuels. A very good agreement can be observed, which is also supported by Table 7. As shown in Table 7, the absolute relative deviations of the present BPNN model for 54.89% of total data (864 points) are below 1%; the absolute relative deviations for 27.89% of total data (439 points) are between 1 and 2%; 9.85% of total data (155 points) are between 2 and 3%; 6.16% of total data (97 points) are between 3 and 5%; only the absolute relative deviations for 1.21% of total data (16 points) are greater than 5%. The AARD and MARD of total data are calculated to be 1.24 and 10.70%, respectively. The AARD of the FV model and the model based on EART proposed by our group are also provided in Table 6 for comparison. It can be found that the present BPNN model has a similar total AARD to the FV model and EART model but a lower total MARD. Moreover, the present BPNN model has stronger prediction ability than the FV model and EART model because it can calculate the viscosity of a new oxygenated fuel just using temperature, pressure, critical pressure, critical temperature, mole mass, and acentric factor with no experimental viscosity data available.

**Table 6. Deviations of the BPNN Model for Each Substance**

| Name              | BPNN | FV  | EART |
|-------------------|------|-----|------|
|                   | AARD/% | MARD/% | AARD/% | MARD/% | AARD/% | MARD/% |
| Methanol          | 0.99  | 3.28 | 1.13  | 3.95   | 0.76   | 2.66   |
| Ethanol           | 1.19  | 3.78 | 0.88  | 3.92   | 1.22   | 5.57   |
| 1-propanol        | 0.73  | 1.91 | 0.36  | 1.86   | 1.14   | 4.40   |
| 2-propanol        | 1.06  | 3.04 | 1.79  | 12.04  | 1.64   | 4.30   |
| 1-pentanol        | 0.75  | 2.62 | 1.79  | 4.93   | 1.32   | 4.56   |
| 3-pentanol        | 1.53  | 7.23 | 13.07 | 44.78  | 1.19   | 5.14   |
| 1-nonanol         | 1.05  | 6.14 | 7.99  | 20.88  | 2.95   | 12.81  |
| 2-methyl-2-propanol | 1.11 | 5.75 | 2.57  | 15.62  | 0.81   | 5.14   |
| vinyl acetate     | 2.92  | 7.66 | 1.46  | 3.92   | 0.85   | 3.18   |
| diethyl adipate   | 1.10  | 2.52 | 1.55  | 4.95   | 0.32   | 0.84   |
| dimethyl carbonate| 1.19  | 4.27 | 1.09  | 4.96   | 1.17   | 3.41   |
| diethyl carbonate | 1.10  | 3.79 | 1.13  | 4.00   | 1.23   | 3.81   |
| ethyl heptanoate  | 1.97  | 8.22 | 0.42  | 1.24   | 0.25   | 0.65   |
| ethyl octanoate   | 1.10  | 3.52 | 0.60  | 1.85   | 0.54   | 1.62   |
| methyl caprate    | 1.00  | 2.72 | 1.85  | 8.68   | 2.54   | 13.58  |
| ethyl caprate     | 1.13  | 2.98 | 2.91  | 11.74  | 2.56   | 13.62  |
| methyl laurate    | 0.64  | 2.73 | 2.01  | 7.34   | 2.41   | 7.56   |
| ethyl laurate     | 0.72  | 2.70 | 2.87  | 9.93   | 2.50   | 8.73   |
| methyl myristate  | 0.36  | 1.23 | 1.38  | 4.72   | 0.86   | 4.93   |
| ethyl myristate   | 0.52  | 2.02 | 1.22  | 5.44   | 1.07   | 5.14   |
| diethyl ether     | 1.24  | 4.40 | 0.84  | 5.80   | 0.50   | 2.47   |
| diisopropyl ether | 2.92  | 10.70| 0.84  | 5.19   | 0.47   | 2.55   |
| dibutyl ether     | 1.81  | 7.19 | 3.18  | 9.84   | 0.69   | 4.04   |
| dimethoxymethane  | 2.72  | 6.80 | 0.95  | 5.72   | 0.62   | 2.15   |
| ethylene glycol dimethyl ether | 1.30 | 3.66 | 1.33 | 5.43 | 0.46 | 2.30 |
| diethyle glycol dimethyl ether | 0.74 | 1.95 | 3.57 | 10.91 | 0.50 | 1.86 |
| triethyle glycol dimethyl ether | 0.92 | 2.36 | 1.88 | 5.88 | 1.12 | 5.12 |
| tetrathyle glycol dimethyl ether | 1.24 | 6.25 | 2.44 | 6.39 | 1.60 | 7.02 |
| monoethyle glycol methyl ether | 1.44 | 7.56 | 0.88 | 2.19 | 1.25 | 3.45 |
| monoethyle glycol ethyl ether | 1.20 | 4.00 | 1.05 | 3.53 | 1.55 | 3.71 |
| monoethyle glycol iso-propyl ether | 1.10 | 5.45 | 1.88 | 5.89 | 2.10 | 6.40 |
| Total             | 1.24  | 10.70 | 1.77 | 44.78 | 1.24 | 13.62 |
fuels including esters, alcohols, and ethers in the temperature range from 243.15 to 413.15 K and in the pressure range from 0.1 to 200 MPa. The training result shows that the BPNN model has the best accuracy when it has two hidden layers with the neuron numbers of 6 and 12, respectively. The AARDs of the present BNPP model from training data, validation data, and testing data are 1.19%, 1.27%, and 1.30%, respectively, which indicates a good performance in prediction. Comparison result shows that the BPNN model has better accuracy than the FV model and EART model and has much stronger prediction ability because it can predict the viscosity of a new oxygenated fuel at variational temperature and pressure just using four physical properties (critical temperature, critical pressure, mole mass, and acentric factor) with no experimental viscosity data available.

ASSOCIATED CONTENT
Supporting Information
The Supporting Information is available free of charge on the ACS Publications website at DOI: 10.1021/acsomega.9b02337.

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Notes
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