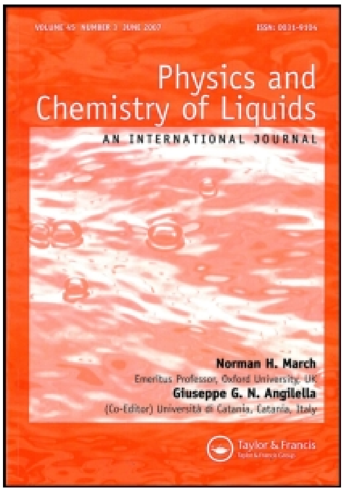

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Analysis of ultrasonic velocity in refrigerants using artificial neural network

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Several researchers have reported numerous measurements on ultrasonic velocity as a function of temperature and pressure using various experimental techniques. A large amount of experimental data is required in order to obtain accurate results for the chemical substances used. The present article explores the evaluation of ultrasonic velocity as a function of molecular weight, temperature and pressure using an artificial neural network (ANN) in six refrigerants. The network so developed predicts the ultrasonic velocity successfully. Statistical analysis of the results was performed using standard deviation (%) and relative average deviation. The correlation coefficient in our analysis was found to be 0.9999. The trained weights, obtained from ANN, are further employed to form equations to predict ultrasonic velocity at other temperatures and pressures.

Keywords: Ultrasonic velocity; Pressure dependence; Refrigerants; Artificial neural network; Leverberg–Marquardt algorithm; Feed forward network

1. Introduction

Many researchers [1,2] have studied the effect of pressure on the ultrasonic velocity. The effect has been explored by Smith and Lawson [3] and by Litovitz and Carnevale [4]. It is observed that pressure and temperature have a strong effect on the ultrasonic velocity, which is associated with the thermodynamic behavior of the fluid [5], and shares a very complex relationship. According to Erol Arcaklioğlu [6], refrigeration is one of the most important industrial applications, and it is usually based on chlorofluorocarbon (CFC) compounds. Moreover, the number of chemical substances to replace CFCs is very high and considerable experimental work as well as new models are required. Keeping all these points in mind, in the present study, we have formed the neural network having three inputs and one output. Data of six refrigerants namely trichlorofluoromethane (CCl_3F), 1,1-dichloro-2,2,2-trifluoroethane ($C_2HCl_2F_3$), monochlorodifluoromethane ($CHClF_2$), monochloropentafluoroethane ($CClF_2$-CF_3),

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dichlorotetrafluoroethane ($C_2Cl_2F_4$) and bromotrifluoromethane ($CBrF_3$), determined on sing around technique at 2 MHz have been collected from the literature [7–10].

2. Theory

Motivated by the functioning of neurons, scientists have applied the concept of artificial neural network (ANN) to complex problems which are difficult to solve using traditional methods [11–13]. The artificial neuron accepts any number of inputs simultaneously. Using weights, these inputs are connected to processing element, where the summation of these weighted inputs is taken. With the help of transfer functions these are processed and converted into the output.

3. Training procedure

The learning procedure of the ANN is completely a trial and error method [14]. The training of ANN requires large training data set. The ANN model has presented the known values of input/output vector pairs, which are as shown in table 1.

Table 1. Training data.

Sample	Molecular weight (g)	Temperature (K)	Pressure (MPa)	Ultrasonic velocity ($m\,s^{-1}$)	Total sets
(1) CCl_3F	137.37	298.15	0.1056–74.77	743.5–1029.1	55
		333.15	0.3111–74.41	627.5–954.6	
		353.15	0.5192–73.86	557.4–914.1	
(2) $C_2HCl_2F_3$	152.93	283.15	0.0506–75.50	745.7–1044	93
		293.15	0.0756–74.01	711–1015.1	
		298.15	0.0913–74.44	693.7–1006.2	
		303.15	0.1094–75.59	676.4–999.1	
		373.15	0.7871–75.40	440.9–864.4	
(3) $CHClF_2$	86.48	288.15	0.680–49.90	599–889	115
		293.15	0.910–50.71	574.5–880.2	
		298.15	1.049–50.90	550–866.8	
		303.15	1.196–51.05	525.1–851.7	
		323.15	1.941–50.02	424.5–793.9	
(4) $CClF_2$-CF_3	154.48	293.15	0.801–49.04	373.1–711	121
		298.15	0.911–49.65	352–703	
		303.15	1.039–49.16	329.9–690.5	
		308.15	1.176–49.66	309.2–682.6	
		313.15	1.333–50.88	291.2–677.7	
		323.15	1.676–50.09	255.2–654.9	
(5) $C_2Cl_2F_4$	170.92	283.15	0.128–50.20	601.6–853.2	96
		293.15	0.181–49.46	571.8–830.7	
		298.15	0.214–50.66	550.8–820.1	
		313.15	0.338–50.60	501.9–791.3	
		323.15	0.447–51.17	467.3–772.4	
(6) $CBrF_3$	148.914	293.15	1.428–52.07	326.1–649.9	75
		298.15	1.612–51.03	309.1–635.8	
		313.15	2.273–52.44	258.5–614.5	
		323.15	2.915–50.69	223.5–589.7	

Neural network learns through the patterns of the data presented to it. The three-layered feedforward network is selected with supervised learning, i.e. network with bias values. The three layers are input layer, hidden layer and output layer. The training data is presented through the input layer. Here, we have taken molecular weight (g), temperature (K) and pressure (MPa) as input parameters and ultrasonic velocity ($\mathrm{m\,s^{-1}}$) as the output parameter. The input and output parameters are stored in a file as a column vector. The hidden layer of feedforward network consists of 10 logsig transfer functions. It is a continuous and differentiable transfer function. The range of logsig is $(0, +\infty)$. It takes the form,

$$f(Z) = \frac{1}{1 + \exp(-Z)} \tag{1}$$

where Z is the weighted sum of the inputs.

The output layer consists of one purelin transfer function whose range is $(-\infty, +\infty)$. The model is trained using the Leverberg–Marquardt learning algorithm [15]. The network has calculated the output vector for each input vector. An error term is evaluated by comparing the calculated output vector and the actual output vector called target. The performance function selected is the sum squared error. Using the error term, the weights and biases are updated to decrease the error. This procedure is repeated until the error goal of 1×10^{-4} and 2000 epochs is reached. The performance of the network is 0.00343387. The program script is written and executed in MATLAB 6.5.

4. Results and discussions

After training ANN, we have tested the network by giving data, which the network has not received earlier. During testing, to study the behavior of ultrasonic velocity as a function of pressure and temperature, we have used the trained weights and biases saved in the file (table 2).

In order to calculate ultrasonic velocity at various temperatures and pressures of the six refrigerants, mathematical equations are derived from the trained weights and the activation functions used in the ANN. As from statistical analysis, the results obtained from testing and training are extremely good, hence the above equations thus obtained

Table 2. Trained weights obtained through Leverberg–Marquardt algorithm. $Z_i = W1_i \times M + W2_i \times T + W3_i \times P + B1_i$.

S. No.	$W1_i$	$W2_i$	$W3_i$	$B1_i$
1	−18.44345	0.3965664	−0.3583145	9.241836
2	−2.547895	−3.455291	0.5432987	0.7701218
3	−5.872633	46.59074	−5.146459	−11.89008
4	−6.930737	113.5282	7.917632	−42.98610
5	−10.80257	0.06526527	−0.05090918	2.882611
6	−6.908178	43.65352	1.736176	−10.98907
7	40.73891	−0.2563958	0.1221067	−8.871200
8	3.026567	120.3034	6.670119	−34.57744
9	−0.1561430	24.01910	−9.124814	−8.440030
10	6.875672	15.97496	3.985813	−8.197750

are accurate. In the above formulation, 10 pairs of equations are required as ANN has 10 hidden neurons. In the output neuron, only one summation function is used as there is only one neuron which corresponds to the ultrasonic velocity. Molecular weights are normalized to get the data within the range of $(-1, 1)$.

$$G = \frac{2 \times (M - M_{\min})}{M_{\max} - M_{\min}} - 1 \tag{2}$$

In our application, the maximum value for molecular weight is 170.92 and the minimum value is 86.48. Temperature values are normalized as $t = T/1000$, whereas pressure values are normalized as $p = P/100$.

$$Z_1 = -18.44345G + 0.3965664t - 0.3583145p + 9.241836 \tag{3}$$

$$S_1 = \frac{1}{1 + e_1^{-Z}} \tag{4}$$

$$Z_2 = -2.547895G - 3.455291t + 0.5432987p + 0.7701218 \tag{5}$$

$$S_2 = \frac{1}{1 + e_2^{-Z}} \tag{6}$$

$$Z_3 = -5.872633G + 46.59074t - 5.146459p - 11.89008 \tag{7}$$

$$S_3 = \frac{1}{1 + e_3^{-Z}} \tag{8}$$

$$Z_4 = -6.930737G + 13.5282t + 7.917632p - 42.98610 \tag{9}$$

$$S_4 = \frac{1}{1 + e_4^{-Z}} \tag{10}$$

$$Z_5 = -10.80257G + 0.06526527t - 0.05090918p + 2.882611 \tag{11}$$

$$S_5 = \frac{1}{1 + e_5^{-Z}} \tag{12}$$

$$Z_6 = -6.908178G + 43.65352t + 1.736176p - 10.98907 \tag{13}$$

$$S_6 = \frac{1}{1 + e_6^{-Z}} \tag{14}$$

$$Z_7 = 40.73891G - 0.2563958t + 0.1221067p - 8.871200 \tag{15}$$

$$S_7 = \frac{1}{1 + e_7^{-Z}} \tag{16}$$

$$Z_8 = 3.026567G + 120.3034t + 6.670119p - 34.57744 \tag{17}$$

$$S_8 = \frac{1}{1 + e_8^{-Z}} \tag{18}$$

$$Z_9 = -0.1561430G + 24.01910t - 9.124814p - 8.440030 \tag{19}$$

$$S_9 = \frac{1}{1 + e_9^{-Z}} \tag{20}$$

$$Z_{10} = 6.875672G + 15.97496t + 3.985813p - 8.197750 \tag{21}$$

$$S_{10} = \frac{1}{1 + e_{10}^{-Z}} \tag{22}$$

The terms S_1–S_{10} and Z_1–Z_{10} represent the summation and activation functions of each neuron of the hidden layer respectively.

$$\begin{aligned} Z_{11} = {} & 9.768024S_1 + 5.525538S_2 - 0.09376878S_3 + 0.04508393S_4 \\ & - 73.69815S_5 + 0.1542588S_6 - 59.32642S_7 - 0.04497778S_8 \\ & - 0.1876630S_9 + 0.2297970S_{10} + 59.17101 \end{aligned} \tag{23}$$

$$\text{Ultrasonic velocity} = Z_{11} \times 2000 \tag{24}$$

Using the above equations, we get the ultrasonic velocities of the six refrigerants under study. For statistical analysis which is necessary as it indicates predictive capability of the network, we have evaluated standard deviation (%) [8], relative average deviation as follows:

$$\text{Standard deviation (\%)} = 100 \times \left\{ \frac{1}{n} \sum \left(\frac{(U_{(\text{Expt.})} - U_{(\text{ANN})})}{U_{(\text{ANN})}} \right)^2 \right\}^{1/2} \tag{25}$$

$$\text{Relative average deviation} = \frac{1}{n} \sum \left(\left| \frac{U_{(\text{Expt.})}}{U_{(\text{ANN})}} - 1 \right| \right) \tag{26}$$

where n is the number of data points used.

In our study, the results are satisfactory as relative average deviation is approaching zero and standard deviation is in between 0.35 and 2.71%. Statistical analysis of the results is presented in table 3.

The network generalizes well in case of $C_2HCl_2F_3$, as the training range for the temperature is 288.15–323.15 K, the network predicted ultrasonic velocities well at 283.15 K. Also in case of $CClF_2$–CF_3, the network extrapolated ultrasonic velocities at 283.15 K, 288.15 K with good accuracy as seen from the table 3. In all the six refrigerants, it is observed that, the velocities predicted on tested temperatures follow the trend as a function of temperature and pressure; it increases with increase in pressure but decreases with increase in temperature. Moreover, near the saturated pressure, the results are not very satisfactory in case of all the refrigerants under study. This may be due to unsteady state behavior of the refrigerants near the saturated vapor pressure as the temperatures taken for comparison as well as study are approaching the critical temperatures of the refrigerants respectively. This is reflected in the standard deviation (%) and relative average deviation in table 3. At temperatures 310.15, 325.15 and 360.15 K, the experimental values of ultrasonic velocities with varying pressures are not available. With the help of trained weights and biases, the respective values are predicted. In case of

Table 3. Statistical analysis of 10 neurons in the hidden layer.

Sample	Temperature (K)	Correlation coefficient	Standard deviation (%)	Relative average deviation
(1) CCl_3F	313.15	0.999972	0.658	0.005054
(2) $C_2HCl_2F_3$	313.15	0.999984	1.544	0.003196
	323.15	0.999845	2.235	0.012258
	333.15	0.999845	2.168	0.011537
	343.15	0.999845	2.235	0.012258
	353.15	0.999741	2.271	0.017086
	363.15	0.999886	1.483	0.011500
(3) $CHClF_2$	283.15	0.999989	0.366	0.003456
	308.15	0.999998	0.427	0.002051
	313.15	0.999998	0.745	0.001220
	318.15	0.999992	0.627	0.003825
(4) $CClF_2$-CF_3	283.15	0.999936	1.415	0.008506
	288.15	0.999992	1.078	0.002554
	318.15	0.999998	1.148	0.001316
(5) $C_2Cl_2F_4$	303.15	0.999998	0.355	0.001583
(6) $CBrF_3$	283.15	0.999794	2.718	0.018127
	303.15	0.999999	1.043	0.001522

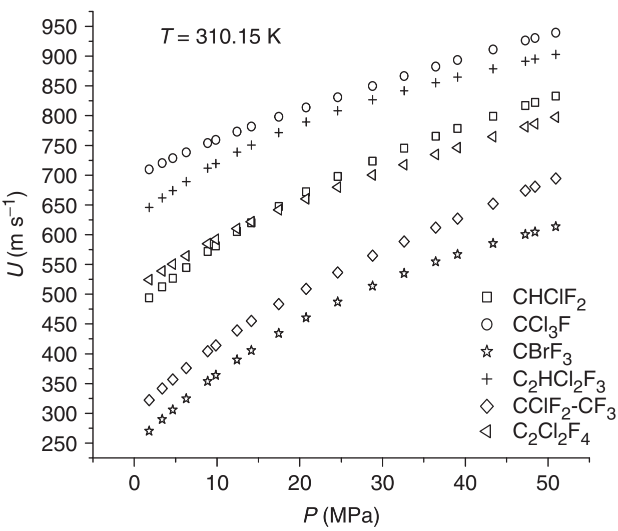

Figure 1. Plot of ultrasonic velocity, U *vs*. pressure, P, in CCl_3F, $C_2HCl_2F_3$, $CHClF_2$, $CClF_2$-CF_3, $C_2Cl_2F_4$ and $CBrF_3$ at 310.15 K.

$CHClF_2$ and $C_2Cl_2F_4$, it is observed that though $C_2Cl_2F_4$ has higher molecular weight than $CHClF_2$, but at pressure 14.15 MPa their ultrasonic velocities are similar. Moreover, the ultrasonic values of $C_2Cl_2F_4$ above the pressure 14.15 MPa decreases as compared with the velocity values of $CHClF_2$ with increasing pressure (see figures 1–3).

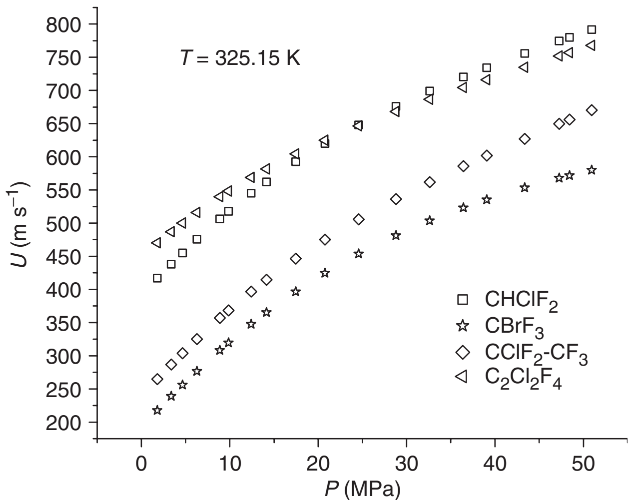

Figure 2. Plot of ultrasonic velocity, *U vs.* pressure, *P*, in $CHClF_2$, $CBrF_3$, $CClF_2$-CF_3 and $C_2Cl_2F_4$ at 325.15 K.

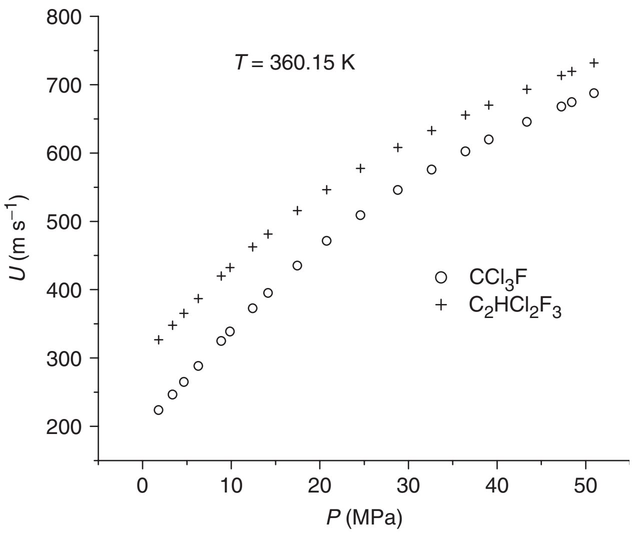

Figure 3. Plot of ultrasonic velocity, *U vs.* pressure, *P*, in CCl_3F and $C_2HCl_2F_3$ at 325.15 K.

5. Conclusions

The artificial neural network seems to be working as a powerful tool to predict ultrasonic velocity in refrigerants at different temperatures and pressures. In the present article, ultrasonic velocity as a function of pressure and temperature is studied. Equations obtained from ANN are incorporated to obtain ultrasonic velocity within the range taken up for training. The correlation coefficient 0.9999, reflects the higher accuracy of the present ANN, but fails to predict the exact value of the ultrasonic velocity in case of $CClF_2$-CF_3 at saturated vapor pressure as it is a mathematical tool having no sense of the physical system. The error in the experimental value could be one of the reasons.

Nomenclature

Symbols

ANN	artificial neural network
M	molecular weight
T	temperature in K
P	pressure in Mpa
t	normalized value of temperature
p	normalized value of pressure
$M_{\max}$	maximum value of molecular weight
$M_{\min}$	Minimum value of molecular weight
G	normalized variable of molecular weight
$U_{(\mathrm{Expt.})}$	experimental value of ultrasonic velocity
$U_{(\mathrm{ANN})}$	Predicted value of ultrasonic velocity
n	number of data used

Subscript

Expt.	experimental value

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