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Viscosity of ionic liquids using the concept of mass connectivity and artificial neural networks

José Omar Valderrama*,,†, Jéssica Makarena Muñoz**,***, and Roberto Erasmo Rojas*****

*Dept. of Mech. Eng., Faculty of Engineering, University of La Serena, Casilla 554, La Serena, Chile
**Centro de Información Tecnológica, Mons. Subercaseaux 667, La Serena, Chile
***Dept. of Chemistry, Faculty of Sciences, University of La Serena, Casilla 554, La Serena, Chile
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Abstract−Artificial neural networks (ANN) and the concept of mass connectivity index are used to correlate and predict the viscosity of ionic liquids. Different topologies of a multilayer feed forward artificial neural network were studied and the optimum architecture was determined. Viscosity data at several temperatures taken from the literature for 58 ionic liquids with 327 data points were used for training the network. To discriminate among the different substances, the molecular mass of the anion and of the cation, the mass connectivity index and the density at 298 K were considered as the independent variables. The capabilities of the designed network were tested by predicting viscosities for situations not considered during the training process (31 viscosity data for 26 ionic liquids). The results demonstrate that the chosen network and the variables considered allow estimating the viscosity of ionic liquids with acceptable accuracy for engineering calculations. The program codes and the necessary input files to calculate the viscosity for other ionic liquids are provided.

Key words: Ionic Liquids, Viscosity, Neural Networks, Molecular Structure

INTRODUCTION

Ionic liquids have gained special attention due to their special potential uses as green solvents and possible replacements for traditional volatile organic solvents [1]. Ionic liquids have some unique characteristics such as high chemical stability, wide liquid temperature range, good solvents for many compounds, and low vapor-pressure, among other special characteristics. During recent years, researchers of different areas of chemistry, physics, and chemical engineering have presented several studies on different aspects of ionic liquids, mainly experimental data [2,3]. For the selection of the most suited ionic liquid for a given application, some physical, chemical and thermodynamic properties are needed, and some of them have been experimentally determined. Despite this progress, there is still ample space for research, in particular in the area of property measurement, correlation and prediction.

Viscosity is a transport property that is of special interest when dealing with ionic liquids (ILs). If an IL is to be used as a solvent, a low viscosity is desirable, so pumping costs are reduced and mass transfer rates are increased. If the IL is to be used as a lubricant, lubricant additive or in membrane processes, a high viscosity is desirable. The viscosity is strongly dependent on temperature and in the case of ionic liquids is also highly dependent on the type of cation and anion [4]. The viscosities of ILs are commonly higher than those of common fluids and organic solvents. For instance, for 1-butylnitrile-3-methylimidazolium chloride the viscosity at 293 K is 5,222 cP [5] and can be as high as 257,000 cP for 1-butyl-3-[3-(2-hydroxybenzylamino)propyl]-3H-imidazolium hexafluorophosfate as reported by Ouadi et al. [6]. These are relatively high values when they are compared with 1.0 cP for water or 900 cP for glycerol, at the same temperature [7].

A reasonable amount of viscosity data has been published in the literature and efforts to compile these data have been done. The database of the National Institute of Standards and Technology, NIST [8] includes 1524 data points for 68 ionic liquids, while Zhang et al. [9] report 593 data points for 432 ionic liquids. However the quality of the data has not been thoroughly evaluated and high differences are found between viscosity values reported by different authors. Fig. 1(a) shows values of viscosity from different authors, as reported by Zhang et al. [9], for [bmim][BF4] and Fig. 1(b) shows data reported in the NIST database [8] for [bmim][PF6]. As observed in the figures, high differences of viscosity values are found and not much explanation is found in the original sources about this type of discrepancy. It is clear then that better quality data on viscosity of ionic liquids is necessary for practical applications or for the development of viscosity models for ionic liquids. Due to these highly different values of viscosity, appropriate analysis and selection of data is necessary before attempting any modeling procedure. Part of the data selected for the study presented here were used for training the artificial neural networks (ANN), and part of the data were used for testing the trained network by predicting the viscosity of other ionic liquids not used during the training process. Also, it is necessary to determine the main independent variables, besides the temperature, that affect viscosity.

1. ANN in Property Estimation

Good descriptions of ANN are given in the literature [10,11]. A complete list of properties that have been analyzed in the literature using different approaches of ANN was reported by Taskinen and Yliruusi [12]. Properties such as boiling point, critical temperature,

†To whom correspondence should be addressed.
E-mail: jvalderr@userena.cl

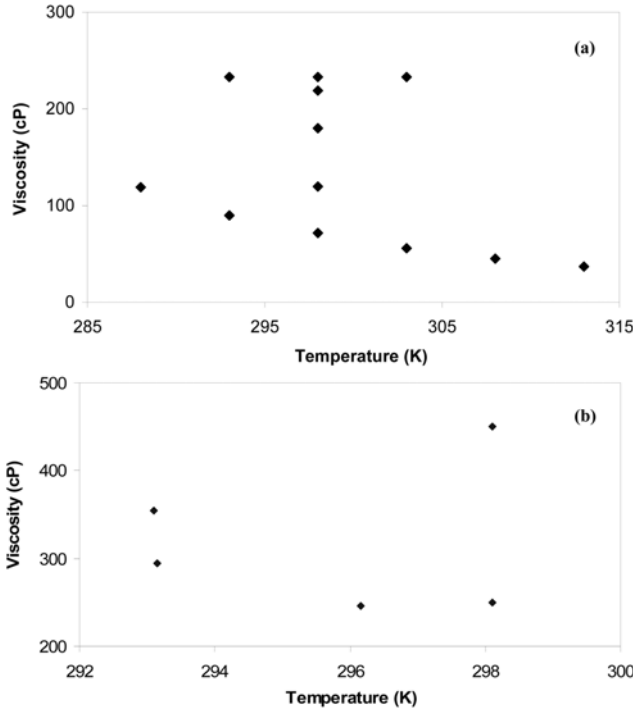

Fig. 1. Viscosity data from different sources: (a) data from Zhang et al. [9], for 1-butyl-3-methylimidazolium tetrafluoroborate [bmim][BF4]; and (b) data from NIST [8] for 1-butyl-3-methylimidazolium hexafluorophosphate [bmim][PF6].

critical pressure, vapor pressure, heat capacity, enthalpy of sublimation, heat of vaporization, density, surface tension, viscosity, thermal conductivity, and acentric factor, among others, were thoroughly reviewed.

Several applications of ANN to correlate and predict the viscosity of ionic liquids have been presented in the literature. Suzuki et al. [13] developed a back propagation neural network model for correlating and predicting the viscosity-temperature behavior of a large variety of organic liquids. The reliability of the proposed model was assessed by comparing the results against calculated viscosities by two existing group-contribution approaches. Konno et al. [14] evaluated the viscosity of lubricants employing molecular dynamics simulation and prediction based on artificial neural network. The proposed ANN method relates basic properties including melting temperature, boiling temperature, molecular weight, and density with viscosity. Murata et al. [15] proposed a simple method for predicting liquid viscosities of pure components and mixtures from chemical structures only. For pure components the constants of an Andrade type equation were predicted using an ANN. For mixtures the viscosity was predicted using the ASOG-VISCO group contribution method. Padmavathi et al. [16] developed models to predict the viscosity of polybutadiene rubber using ANN. The authors related the viscosity to process variables.

Although some works on application of ANN to correlate viscosity of ionic liquids have been presented [4,17], the use of the mass connectivity index, a concept that encodes structure information, as an independent variable has not been tested. Besides that, most papers available in the open literature describing the use of neural networks for predicting fluid properties do not give a detailed description that allows other researchers to reproduce the results and to make appropriate use of the ANN model. This is done in this paper by providing, as supplementary material, the ANN model, consisting of the program codes to train the network and to predict viscosities, and also the files containing the data used for training and prediction. All this will allow any reader to reproduce the results and to predict viscosities of other ionic liquids.

2. Defining the Independent Variables

Considering that properties commonly available for organic fluids such as critical properties, normal boiling temperature, or acentric factor are not readily available for ionic liquids, the variables chosen for training the network were limited to those more readily available or that could be easily estimated. The independent variables considered are the temperature, the density, the mass of the cation, the mass of the anion, and the mass connectivity index, as explained in what follows.

One way of determining the variables that affect viscosity is by analyzing empirical and semi-empirical models available for correlating and predicting viscosity. Such models are usually based on the use of adjustable parameters for each fluid (correlations), on the corresponding state principle (semi-empirical and predictive), and on group contribution methods (semi-empirical and predictive). Table 1 presents a selection of models proposed in the literature for correlating and predicting the viscosity of liquids [7,20]. However, these generalized correlations and models were not developed for ionic liquids and have not been thoroughly tested for appropriateness and accuracy with these special fluids. As seen in Table 1, besides the temperature, the density is commonly used in several correlations, so the density at 298 K is one of the input variables for training the network. The mass of the anion and cation are also used to consider the important influence of the type of anion and cation as suggested in the literature [4]. The structure is also an important factor for determining the properties of an ionic liquid [3]; and in this work this factor is considered by including the mass connectivity index, a molecular parameter recently defined by the authors [21]. In summary, the proposed ANN method uses as independent variables the temperature, the density, the mass of the cation, the mass of the anion, and the mass connectivity index (T, ρ, M^+, M^-, λ). The viscosity data were taken from the NIST Database [8].

Table 1. Selected predictive and correlating models for the viscosity, as given Reid et al. [7] and Bretsznajder [20]

Method	Calculated property	Variables included
Andrade	Log (μ)	ρ, 1/T, specific constants
Bachinskii	$1/\mu$	ρ, specific constants
Cornelissen-Waterman	Log (μ/ρ)	1/T, specific constants
Guzmán	Log (μ)	T, specific constants
Orrick y Erbar	Log (μ)	T, M, ρ
Przezdziecki y Sridhar	μ	T, Tc, Pc, Vc, Tf, Vmf
Reynolds	Log (μ)	1/T, specific constants
Souders	Log (μ)	T, M, ρ
Thomas	Log ($\mu/\rho^{1/2}$)	T, Tc, specific constants
Thorpe y Rodger	μ	T, specific constants
Van Velzen et al.	Log (μ)	T, specific constants
Vogel	Log (μ)	T

To develop an accurate model to predict the viscosity of ionic liquids in the form developed in this work, the following files were written:

i) An excel file containing the independent variables: temperature, density, mass of the cation, mass of the anion, and mass connectivity index (T, ρ, M^+, M^-, λ)

ii) An excel file containing the dependent variable: the viscosity (μ) or the logarithm of the viscosity Log(μ)

iii) A Matlab code for the ANN that consists of two parts: i) a training section and ii) a prediction section.

In the training section the program reads the input data (the two excel files), defines the architecture, trains the defined network, generates the weight and bias matrixes, and stores such data for prediction. In the prediction section the program reads the weight and bias matrixes and the excel file containing the variables for which the viscosity is to be predicted, and store the results in an output file.

Table 2 describes all files involved in the proposed method and Fig. 2 presents a flow diagram of the ANN program developed in this work, showing the connections between the program codes and the excel files containing the required information for training and prediction. The flow diagram is useful for better understanding the codes used and provided as supplementary material. In this way any reader or researcher can make use of them for predicting the viscosity of other ionic liquids.

The most basic architecture normally used for this type of application involves a back propagation feed-forward neural network containing three layers: the array input layer, one hidden layer and the output layer [10]. In the application described in this work this simple architecture did not provide good results, especially during

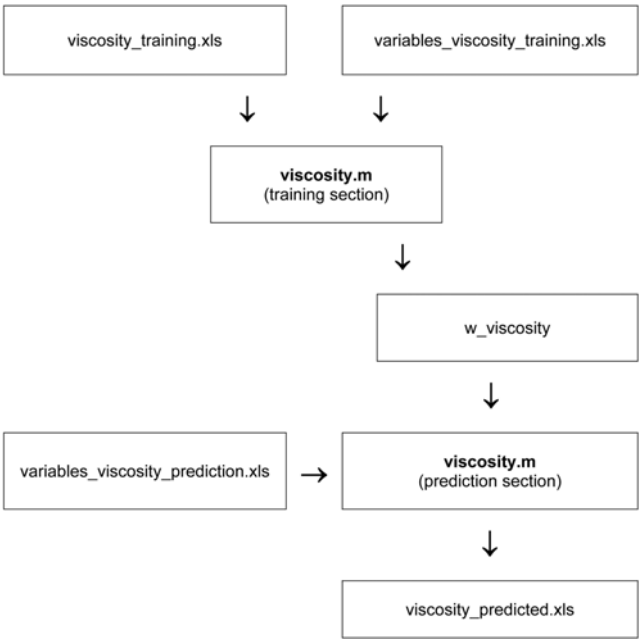

Fig. 2. Flow diagram showing the connections between the different files and program used in this work for training and prediction.

Table 2. Description of the files given as supplementary material to predict viscosities of other ionic liquids

Nº	File	Description	Details
1	viscosity.m	Matlab code for training the net with viscosity data (training section) and predicting viscosity (prediction section)	Reads the viscosity and the independent variables for training and the variables for prediction
2	viscosity_prediction.m	Matlab code to predict the viscosity of ionic liquids using the trained ANN	Reads the independent variables for predicting the viscosity for other ionic liquids (T, ρ, M^+, M^-, λ)
3	w_viscosity	Stores the ANN model with all the parameters obtained during training	Contains the weight matrix, the bias array and other files that define the ANN model
4	variables_viscosity_training.xls	Contains the independent variables for training the network (T, ρ, M^+, M^-, λ)	Has 327 rows for 58 ionic liquids including the independent variables used for training
5	viscosity_for_training.xls	Contains the values of viscosity to be used to train the network	Has 327 rows corresponding to the viscosity of 58 ionic liquids at different temperatures
6	viscosity_correlated.xls	Contains the values of viscosity determined by the network during training	The calculated viscosities are to be compared with the input values to check the accuracy of the trained network
7	variables_viscosity_prediction.xls	Contains the required information for predicting the viscosity for the IL (T, ρ, M^+, M^-, λ)	Similar to the file *variables_for_training.xls* but has 31 rows for 26 ILs including the independent variables
8	viscosity_predicted.xls	Stores the predicted data for further study and analysis, if desired.	The program *viscosity_prediction.m* automatically creates this file
9	viscosity_results	Optional file for calculating the deviations or any other analysis of the results that may be required.	The user transfer results from the files viscosity_correlated.xls and viscosity_predicted.xls for statistical analysis

Table 3. The Matlab code *viscosity.m* is used in this work to train the network and check its predictive capabilities

```
%viscosity.m
%
%THIS IS THE MATLAB CODE FOR TRAINING AN ANN WITH VISCOSITY DATA, USING AS INDEPENDENT
%VARIABLES THE TEMPERATURE, THE DENSITY, THE MASS OF THE CATION, THE MASS OF THE ANION, AND THE
%MASS CONNECTIVITY INDEX
%
%TRAINING SECTION
%Reading independent variables for training (temperature, cation mass, anion mass, and
%the groups forming each molecule
p=xlsread('variables_viscosity_training'); p=p';
% %Reading the dependent variable for training (density at the temperatures listed in the file variables_training');
t=xlsread('viscosity_for_training'); t=t';
% Normalization of all data (values between –1 y +1)
[pn,minp,maxp,tn,mint,maxt]=premnmx(p,t);
% Definition of ANN:( topology, activation functions, training algorithm)
net=newff(minmax(pn),[5,15,15,1],{'tansig','tansig','tansig','purelin'},'trainlm');
% Definition of frequency of visualization of errors during training
net.trainParam.show = 10;
% Definition of number of maximum iterations (epochs) and global error between iterations (goal)
net.trainParam.epochs = 1000; net.trainParam.goal = 1e-6;
%Network starts: reference random weights and gains
w1 = net.IW{1,1}; w2 = net.LW{2,1}; w3 = net.LW{3,2}; w4 = net.LW{4,3};
b1 = net.b{1}; b2 = net.b{2}; b3 = net.b{3}; b4 = net.b{4};
%First iteration with reference values and correlation coefficient
before_training = sim(net,pn);
corrbefore_training= corrcoef(before_training,tn);
%Training process and results
[net,tr]=train(net,pn,tn);
after_training = sim(net,pn);
% Back-Normalization of results, from values between –1 y +1 to real values
after_training = postmnmx(after_training,mint,maxt); after_training=after_training';
Res = sim(net,pn);
% Saving results, correlated densities in an excel file
dlmwrite('viscosity_correlated.xls',after_training,char(9));
%Saving the network (weights and other files)
save w_viscosity
%
%PREDICTING SECTION
%THIS IS THE MATLAB CODE FOR PREDICTING THE VISCOSITY OF ANY IONIC LIQUID USING THE
%TRAINED ANN DETERMINED ABOVE
%
%Reading weight and other characteristics of the trained ANN saved in the file W
load w_viscosity
% Reading of Excel file with new independent variables to predict densities
pnew = xlsread('variables_viscosity_prediction'); pnew=pnew';
% Normalization of all variable (values between -1 y +1)
pnewn = tramnmx(pnew,minp,maxp);
% Testing the ANN obtaining the properties for the variables provided by the file variables_viscosity_for_prediction
anewn = sim(net,pnewn);
% Transformation of the normalized exits (between -1 y +1) determined by the ANN to real values
anew = postmnmx(anewn,mint,maxt); anew=anew';
% Saving the predicted properties in en Excel file
dlmwrite('viscosity_predicted.xls',anew,char(9));
```

prediction. Therefore, two hidden layers were required, as explained in the following section. Table 3 presents the program *viscosity.m* showing the Matlab code used for training and for testing the network. The program is formed by two parts: a training section in which the network is trained using the data stored in the files *viscosity_for_training.xls* and *variables_viscosity_training.xls*. The optimum network is that giving the lowest deviations in the prediction section. This guarantees that the ANN not only learned but also has the capability of predicting the viscosity for cases not considered during the training. Once the ANN has been trained and the parameters of the optimum network (weights and bias) have been determined, three files are automatically created by the program *viscosity.m:* i) a file *viscosity_correlated.xls* containing the values of *viscosity* that the network learned during training; and ii) a file *w_viscosity* containing all matrixes that define the ANN model; and iii) a file *viscosity_predicted.xls* containing the values viscosity determined by the trained network.

The Matlab program loads the ANN model stored in file *w_viscosity* (line 43 in Table 3), which contains the weight matrix defined during training. Then, the file *variables_ viscosity_prediction.xls* is automatically loaded. This file contains 31 rows with the values of the independent variables for those cases for which the viscosity needs to be estimated. Using the model stored in the file *w_viscosity*, the program determines the viscosity for the 31 cases considered in this study for testing the ANN model. The program automatically creates an excel file named *viscosity_predicted.xls* where the predicted viscosities are stored. The program *viscosity.m* presented in Table 3 should be used if another model needs to be obtained, but it should not be used to predict the viscosity for other ionic liquids or for the same ionic liquids at other temperatures.

To apply the trained network for estimating the viscosity of other ionic liquids at specified temperatures the program *viscosity_prediction.m* must de used. This is done as follows: i) create a file similar to *variables_viscosity_prediction.xls* (let's say *new_variables_viscosity.xls*) containing the variables (T, ρ, M^+, M^-, λ); ii) run the program *viscosity_prediction.m* (program that loads the ANN model stored in file *w_viscosity*; iii) open file new_viscosity_predicted.xls were the predicted values are stored. These predicted values can be transferred to other files for statistical analysis if desired.

RESULTS AND DISCUSSION

Since no additional information about the recommended number of layers and neurons has been found for the calculation of properties for any type of substances, the optimum number of layers and neurons was determined by trial and error. Simplicity of the architecture and accuracy of the results were the requirements imposed to find the optimum architecture. Fig. 3 shows the absolute and maximum deviation in correlating the viscosity as a function of the number of neurons in the inner layers, with five neurons in the input layer, a value that the authors have successfully used in other applications [22]. The independent variables in the calculations shown in Fig. 3 are T, ρ, M^+, M^- and λ and the accuracy of the

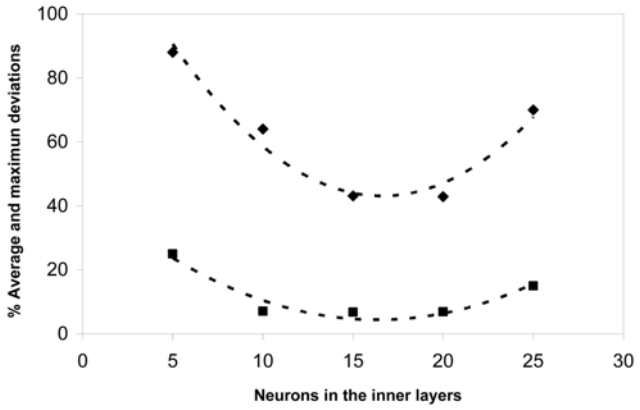

Fig. 3. Deviations in correlating viscosity data as a function of the number of inner neurons (n) for an ANN of architecture (5, n, n, 1). In the figure, ◆ are maximum deviations and ■ are average deviations.

Table 4. The Matlab code *viscosity_prediction.m* is used in this work to predict the viscosity of other ionic liquids using the trained network

```
1  %viscosity_prediction.m
2  %
3  %THIS IS THE MATLAB CODE FOR PREDICTING THE VISCOSITY OF ANY IONIC LIQUID USING THE TRAINED ANN
4  %DETERMINED USING THE PROGRAM viscosity_training.m
5  %
6  %Reading weight and other characteristics of the trained ANN saved in the file W
7  load w_viscosity
8  % Reading of Excel file with new independent variables to predict densities
9  pnew = xlsread(' new_variables_viscosity.xls'); pnew=pnew';
10 % Normalization of all variable (values between –1 y +1)
11 pnewn = tramnmx(pnew,minp,maxp);
12 % Testing the ANN obtaining the properties for the variables provided by the file variables_viscosity_for_prediction
13 anewn = sim(net,pnewn);
14 % Transformation of the normalized exits (between –1 y +1) determined by the ANN to real values
15 anew = postmnmx(anewn,mint,maxt); anew=anew';
16 % Saving the predicted properties in en Excel file
17 dlmwrite('viscosity_predicted.xls',anew,char(9));
```

network was checked by determining the deviations between the calculated values of viscosity after training and data from the literature. As observed, the minimum average deviation and the minimum highest deviation occur when the inner layers contain 15 neurons. Thus, the architecture of the proposed ANN model has four layers: 5 neurons in the input array, 15 neurons in the each of the hidden layers, and 1 neuron in the output layer, (5,15,15,1).

The average relative percent deviation $\%\Delta\mu$ and average absolute percent deviation $\%|\Delta\mu|$ between the calculated value of viscosity (μ^{cal}) and the data from the literature (μ^{lit}) were calculated as:

$$\%\Delta\mu = \frac{100}{N}\sum_{1}^{N}\left[\frac{\mu^{lit}-\mu^{cal}}{\mu^{lit}}\right]_i \quad (1)$$

$$\%\Delta\mu = \frac{100}{N}\sum_{1}^{N}\left[\frac{|\mu^{lit}-\mu^{cal}|}{\mu^{lit}}\right]_i \quad (2)$$

During training, all absolute deviations between correlated and literature values of viscosity were below 7.2% and only 12 of the 327 points (3.7% of the points) showed deviations greater than 5%. The relative average deviation was 0.03% and the absolute average 0.92%. These values are considered to be accurate enough as to say that the ANN learned in an appropriate way.

Table 5. Average relative deviations for the viscosity predicted by the ANN model proposed in this work. The temperature is in Kelvin and the viscosity in cP

Cation	Anion	T	μ^{cal}	$\%\Delta\mu$
[N4444]	[doc]	323	1473.7	0.25
[emim]	[ESO4]	323	34.7	0.77
[hmim]	[bti]	303	55.1	0.12
[hdmim]	[bti]	313	63.4	0.71
[mmim]	[bti]	298	37.0	−2.74
[Empy]	[ESO4]	303	113.5	−0.41
[bmpy]	[bti]	313	34.0	−0.13
[b2nic]	[bti]	298	528.7	−0.44
[hdmpy]	[bti]	323	35.1	0.33
[bmpyr]	[bti]	303	58.6	−1.44
[hmim]	[BF4]	303	132.8	0.53
[hmim]	[BF4]	313	81.7	−0.03
[dmim]	[MSO4]	313	37.3	−4.90
[emim]	[TfO]	308	28.7	−0.92
[emim]	[TfO]	328	16.1	0.62
[bmim]	[MSO4]	303	160.8	−0.08
[bmim]	[MSO4]	323	62.5	0.48
[bmim]	[TfO]	298	88.3	4.65
[bmim]	[TfO]	323	29.5	−4.29
[bmim]	[C8S]	333	95.3	−2.50
[emim]	[bti]	298	31.7	−2.75
[emim]	[bti]	323	14.8	−4.22
[bmim]	[bti]	313	27.0	−1.70
[bmim]	[ta]	323	25.1	−3.50
[bmim]	[Ac]	303	310.7	0.54
[hpeepy]	[bti]	313	91.1	0.11
[hdmapy]	[bti]	303	85.1	−1.05
[hmdmapy]	[bti]	323	38.5	4.04
[emim]	[ESO4]	303	80.3	4.75
[bmim]	[MDEGSO4]	303	711.5	−2.66
[moim]	[BF4]	303	169.8	0.55
			Average	**−0.49**

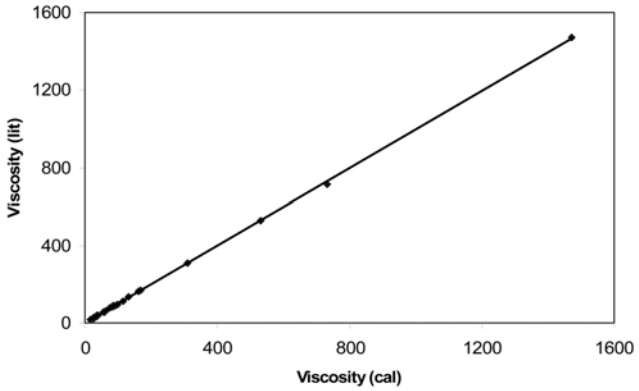

Fig. 4. Predicted and calculated viscosities for the 31 ionic liquids shown in Table 5.

Table 6. Some statistical results of the proposed ANN model

Deviations	Training set (327 points)	Prediction set (31 points)
$\%\Delta\mu_{max}$	7.19	4.75
$\%\Delta\mu$	0.03	−0.49
$\|\%\Delta\mu\|$	0.92	1.68
Points with $\|\%\Delta\mu\|>1$	82	14
Points with $\|\%\Delta\mu\|>2$	40	11
Points with $\|\%\Delta\mu\|>5$	12	0
Points with $\|\%\Delta\mu\|>10$	0	0

Once the training was successfully done and the optimum network architecture was determined, 31 input data (T, ρ, M^+, M^-, λ) for 26 ionic liquids not used in the training process were fed to the ANN predictive program *viscosity_prediction.m* and the viscosity was determined. The input data were provided in the file *variables_viscosity_prediction.xls*. The predicted 31 values of viscosities are shown in Table 5, while Fig. 4 shows a graphical picture of the good predictive capabilities of the trained network. In the prediction step, all values gave deviations below 5%, being the average −0.49% and the absolute average 1.68%. Table 6 summarizes some statistical values such as average, absolute and maximum deviations found between predicted and experimental viscosities.

To evaluate the viscosity of any ionic liquid the user must introduce a line with the information shown in the *variables_viscosity_prediction.xls* file and run the program *viscosity_prediction.m* using Matlab. An excel file *viscosity_predicted.xls* containing the predicted viscosity will be generated in the same workspace in which all files must be allocated. The file *viscosity_results.xls* is an optional file for calculating the deviations or any other analysis of the results that may be required.

CONCLUSIONS

Artificial neural networks and the concept of mass connectivity

index were used to successfully correlate and predict the viscosity of ionic liquids. The accuracy of the method was checked by comparing predicted and literature values of viscosity of ionic liquids not used during training of the network. The viscosity of other ionic liquids can be predicted with acceptable accuracy for engineering calculations. The files provided as supporting information allow readers to reproduce the results presented in this paper and to predict the viscosity of other ionic liquids.

SUPPORTING INFORMATION AVAILABLE

Additional Supporting Information includes nine files as described in Table 2: Matlab code for training and testing the ANN, Matlab code to predict the viscosity of ionic liquids using the trained network, the ANN model (weight matrix), a file containing the variables for training, a file containing the viscosity to be used to train the network, a file containing the variables for prediction, and a file where the predicted values are stored. If readers and researchers use these files for further work, this paper must be cited.

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NOMENCLATURE

Symbols

M^+ : molecular mass of the cation
M^- : molecular mass of the anion
T : temperature
R : ideal gas constant
T_c : critical temperature
P_c : critical pressure
V_c : critical volume
V_{mf} : molar volume at the normal melting point

Greek Letters

μ : liquid viscosity
ρ : liquid density at 298 K
l : mass connectivity index
%Δ : percent average relative deviation
%|Δ| : percent average absolute deviation

Sub/Superscripts

cal : calculated
lit : literature
max : maximum

Abbreviations

ILs : ionic liquids
ANN : Artificial Neural Networks
Log : base 10 Logatrihm

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