Article **ECORFAN Journal Democratic Republic of Congo**
December 2022, Vol.8 No.15 1-10

Development of an artificial neural network for the prediction of the thermodynamic property enthalpy in the NH_3-H_2O mixture

Implementación de una red neuronal artificial para la predicción de la propiedad termodinámica entalpia en la mezcla NH_3-H_2O

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DOI: 10.35429/EJDRC.2022.15.8.1.10 Received July 10, 2022; Accepted December 30, 2022

Abstract

There are many different methodologies for calculating the enthalpy thermodynamic property in the ammonia-water mixture, which is mainly used in the analysis of absorption refrigeration systems and power, so its prediction becomes essential not only for theoretical evaluations, also for the design of industrial equipment. In this work an alternative methodology, an artificial neural network (ARN) is approached. Two neural networks were designed: ARN A and ARN B. ARN A has three main input variables: Pressure (P), Temperature (T) and Ammonia Concentration in the mixture (x), to obtain the output variable: enthalpy. ARN B has as a particular case that the variable Temperature (T) is replaced by the phase in which the mixture is found (q); both networks were compared with experimental data reported in open literature and with the EES™ software. The two networks are capable of predicting the enthalpy of the Ammonia-Water mixture, ARN A with an acceptable prediction range between 100 kPa and 11,000 kPa, and ARN B from 5,000 kPa to 10,000 kPa.

Ammonia-water, Artificial neural network, Enthalpy

Resumen

Existen diferentes metodologías para el cálculo de la propiedad termodinámica Entalpia en la mezcla amoniaco-agua, la cual es principalmente empleada en el análisis de sistemas de refrigeración por absorción y de potencia, por lo que su predicción se vuelve indispensable no solo para las evaluaciones teóricas sino también para el diseño de equipos industriales. En este trabajo se aborda una metodología alternativa, una red neuronal artificial (RNA). Se diseñaron dos redes neuronales: Red A y Red B. La Red A cuenta con tres variables principales de entrada: Presión (P), Temperatura (T) y Concentración de Amoniaco en la mezcla (x), para obtener la variable de salida: Entalpia. La Red B, tiene como caso particular que se sustituye la variable Temperatura (T) por la fase en la que se encuentra la mezcla (q); ambas redes fueron comparadas con datos experimentales reportados en literatura abierta y con el software EES™. Las dos redes son capaces de predecir la entalpia de la mezcla Amoniaco-Agua, la Red A con un rango de predicción aceptable entre 100 kPa y 11,000 kPa, y la Red B de 5,000 kPa a 10,000 kPa.

Amoniaco-agua, Red neuronal artificial, Entalpia

Citation: VERA-ROMERO, Iván, PEREZ-AVIÑA, L. Fernando, MÉNDEZ-ÁBREGO, V. Manuel and MARTÍNEZ-REYES, José. Development of an artificial neural network for the prediction of the thermodynamic property enthalpy in the NH3-H2O mixture. ECORFAN Journal-Democratic Republic of Congo. 2022. 8-15:1-10.

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Introduction

The thermodynamic properties of the ammonia-water mixture are widely used in the design and simulation of absorption refrigeration equipment, flow extraction, power equipment, among others (Kalina, 1983; Stecco & Desideri, 1989). Mainly, the enthalpy property is used to perform energy balances (Tillner-Roth & Friend, 1998b), it is for this reason that having a reliable methodology is of utmost importance for obtaining this property (Thorin, 2001; Thorin et al., 1998).

There are different solution methodologies for the calculation of thermodynamic properties for the ammonia-water mixture (Tillner-Roth & Friend, 1998a), which can be mainly divided into 7 groups, which are (Thorin, 2000): cubic equation of state, Gibbs energy of Excess, law of corresponding states, group contribution method, polynomial functions and viral equation of state, therefore the possibility of an eighth methodology is detected which corresponds to that of constructing an artificial neural network (ANN) and which so far has not been widely explored as a prediction possibility (Vera-Romero & Heard-Wade, 2017b).

Some mathematical models have been programmed in software such as the Engineering Equation Solver (EES™) and the REFPROP™ of the National Institute of Standards and Technology (NIST) because of their certainty and range of application; however, these softwares are commercial. The latter work with different methodologies, EES uses the methodology of (Ibrahim, 1993), while REFPROP NIST uses the methodology developed by (Tillner-Roth & Friend, 1998a).

Artificial neural networks (ANNs) are a branch of artificial intelligence, based on brain behavior, more explicitly on biological neurons (Díez et al., 2001). Currently they are widely used in different fields of knowledge, ANNs are also defined as well-specified mathematical systems designed to capture the highest class of intelligence found in the brain, i.e. to capture the functional capacity of the system (Takeyas, 2007).

Therefore, in this work, we intend to apply a methodology based on an ANN for obtaining the thermodynamic property enthalpy of the ammonia-water mixture, in order to evaluate energy balances in industrial processes (Vera-Romero & Heard-Wade, 2017a, 2018).

Methodology

For this work, we used the BackPropagation Network type (Maximiliano, 2019), which consists of learning a predefined set of input-output pairs given as an example (Bowen et al.; Dolling & Varas, 2002). First an input pattern is applied as a stimulus for the first layer of neurons in the network, it is propagated through all the upper layers until an output is generated, the result in the output neurons is compared with the desired output and an error value is calculated for each output neuron and to reduce this error it is validated through other methodologies. Two multilayer neural networks will be trained, Network A and Network B, which will have three input variables, Network A will have as input variables: Pressure (P), Temperature (T) and Ammonia Concentration (x), Network B will have as input variables: Pressure (P), mixture phase (q) and Ammonia Concentration (x), the networks will have two hidden layers for the connection of these variables and an output variable which is Enthalpy (h) as can be seen in Figure 1, showing the general network proposed for this work.

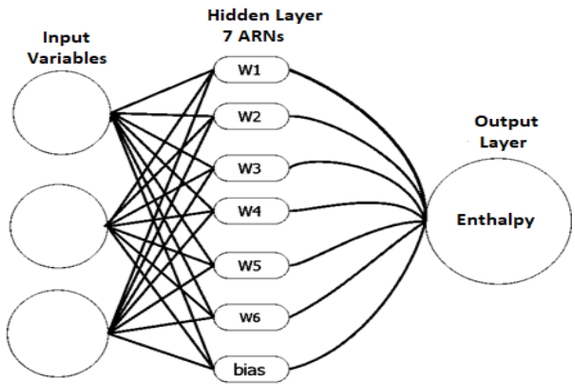

Figure 1 Proposed overall artificial neural network
Source: Own elaboration

The process for the realization of Network A and Network B can be basically divided into 5 main stages which are: data collection, data normalization, network programming, network training and validation of the results (fig 2).

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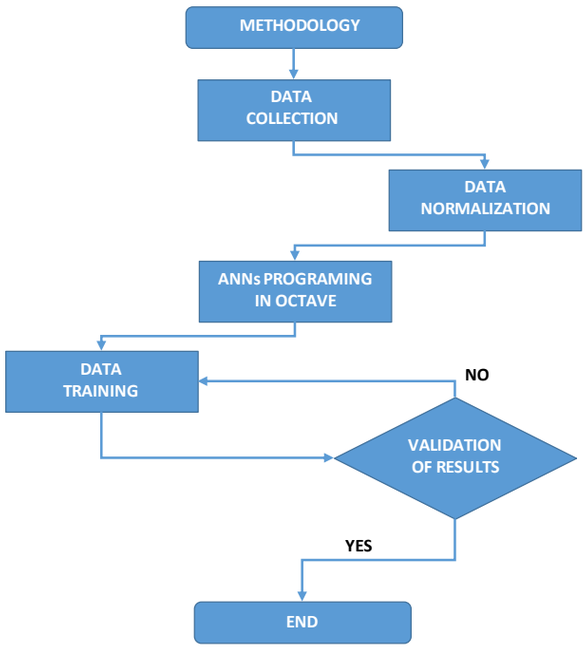

Figure 2 Diagram of the methodology used
Source: Own elaboration

Stage 1, data collection

Experimental data reported in literature (Gillespie et al., 1985; Macriss, 1964; Park & Sonntag, 1990) were obtained to train the networks. The two ANNs have three input variables and one output variable, the networks share two input variables which are Pressure (P) and Ammonia concentration in the mixture (x), and have a different input variable, Network A has the variable Temperature (T) and Network B has the mixture phase variable (q).

The networks have the following characteristics

Each ANN has three sets of data for training and each set has two characteristics: each set has an isobar Pressure (P) and an ammonia Concentration (x) from 0 to 0.9999 where the only thing that varies is the Temperature (T) for Network A and the phase of the mixture (q) for Network B; and in each set of data the Concentration cycles again, this because the first part of the Concentration corresponds to the liquid state of the mixture and the second part corresponds to the gaseous state of the mixture.

For the two ANNs the Pressure (P) is isobar and in each network there are three different Pressures, i.e. a Pressure is set to find the results corresponding to each of the other two variables.

Subsequently, when the Pressure is fixed, the Concentration (x) is fixed and it is the third variable, either the Temperature (T) or the phase of the mixture (q), which ends up varying as well as the corresponding response variable (enthalpy). For the ammonia concentration (x) is taken from 0 to 0.9999 with intervals of 0.1. For the third set of data there is less data so the range of the concentration varies by 0.2.

For Network A, the Temperature corresponds to the Pressure and Ammonia Concentration of the experimental data used. The training pressures used were; 100 kPa, 200 kPa, 300 kPa, 5,000 kPa, 10,000 kPa and 11,000 kPa. For Network B, the third input variable used was the phase of the mixture (q), where it is defined as 1 if it is in liquid phase and 1 if it is in vapor phase, and the variable responds to the Pressure (P) and Concentration of the mixture (x). The training pressures used were; 5,000 kPa, 10,000 kPa and 11,000 kPa.

Stage 2, Data normalization

It is convenient to normalize the data before training a neural network. The normalization procedure consists of transforming the data so that they have a mean of 0 and a variance of 1 (eq. 1). Once the training is finished, denormalization should be used to return to the original domain of the data.

$$y = \frac{(X - X_{min})(d_2 - d_1)}{X_{max} - X_{min}} + d_1 \quad (1)$$

Where:

X is the value to be normalized

$(X_{max} - X_{min})$ is the range of the value X

$(d_2 - d_1)$ is the range to which the value of X

y is the normalized value

Stage 3, programming of the RNA

The programming of the ANN was carried out through GNU Octave™, which is a free software and programming language for mathematical development, which can replace Matlab™ for free; and therefore the programming of the neural networks could be carried out in it.

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At this stage, two programmings were made, one for the training and calculation of the weights and the other for the prediction of the enthalpy variable (h) for both networks.

Stage 4, ANN training

The training was handled in two parts: Weights and Error. The weights make the network learn which variable affects the result the most and what percentage of that variable will be used to arrive at the result.

A result variable is fed to compare with the result of the network, when comparing these results, an error is calculated and if the error is high, the weights are recalculated and rearranged, this process is repeated until a minimum error of 0.009 is obtained.

When the result of the network is the same or almost identical to that of the test variable, the network is considered to be trained (eq. 2-4).

$$E\% = \frac{EA}{DE} * 100 \quad (2)$$

$$EA = VR - VP \quad (3)$$

$$\sum EPP = \frac{\sum EA}{No.\ VR} * 100 \quad (4)$$

Where:

$E\%$ = Percentage error

EA = Absolute error

DE = Exact data

$No.VR$ = Number of actual values

VR = Actual value

VP = Predicted value

$\sum EPP$ = Average percentage error

Stage 5, ANN Validation

Once the ANNs are trained, the enthalpy variable (h) is predicted for each network where the results must be validated for accuracy. Validation of the results is carried out against the EES software.

If there is no large discrepancy between results the ANNs will be taken as successfully trained and otherwise the networks must be retrained.

Results and discussion

Two artificial neural networks were created, Network A and Network B, both were multilayer Back Propagation type networks, each network has three independent input variables and a dependent output variable, which is the thermodynamic property of interest known as enthalpy (h). The results obtained from the training and their comparisons with the results obtained by the methodology of (Ibrahim, 1993) programmed in the EES are shown for each of the trained networks, as well as the prediction error for both networks.

NETWORK A

The first network corresponds to a Back Propagation network of multilayer architecture as shown in Figure 3, the network is composed of three independent input variables: Pressure (P), Temperature (T) and Ammonia concentration (x) and a dependent output variable which is the enthalpy (h).

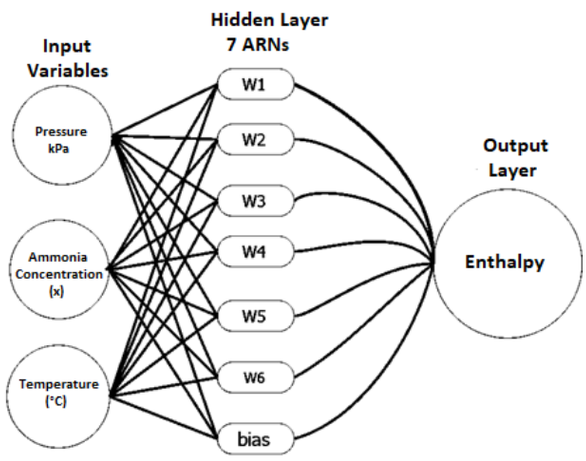

Figura 3 Red A Back multilayer propagation
Source: Own elaboration

For the training of this first network, the data were divided into three different groups, each with the corresponding values according to the output variable enthalpy (h), for each group corresponds a saturation pressure to which for each pressure corresponds a value of temperature (T) and a fraction of ammonia (x). The pressures used were 5,000 kPa, 10,000 kPa and 11,000 kPa.

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The input variable data including the output variable enthalpy (h) were obtained from experimental data (Park and Sonntag, 1991).

The network was trained until an acceptable error was found between the result of the output variable and the data entered for training. The percentage error for this case is acceptable, which means that network A was adequately trained. To reach this acceptable error, the network was trained four times changing the epochs and the number of values to be compared with those of the training, the minimum error was obtained by training the network A 200 epochs and 60% of checking results. The epochs are the times that the neural network repeats the training process of the network. After this, the prediction of the enthalpy property (h) was performed, where three sets of data were predicted, that is to say, in the same way as for the training, for each set of data there is a Pressure (P) to which corresponds a value of Ammonia Concentration (x) and Temperature (T). Four predictions were made corresponding to 3,000 kPa, 5,000 kPa, 10,000 kPa and 15,000 kPa, for each group of predictions a Pressure in kPa is taken, the Temperature entered varies from 120 °C to 320 °C using intervals of 20 °C, for the Ammonia Concentration (x) data was used from 0 to 0.9999 with intervals of 0.1.

The validation of these results was carried out with the EES software, entering the same values of the input variables to the network, where the results yielded by the EES and those yielded by the neural network, in this first training, were incongruent. It was possible to verify that the temperatures used by the EES software are very far from those entered in the ANN, another aspect that was detected and that influenced the neural network to yield erroneous results was that the input data base for the training was too poor to obtain acceptable results.

As mentioned in the fifth step of the methodology, in case the prediction results had a large discrepancy with the results of the EES software, the ANN would be retrained until having a congruence of results with those of the EES. Therefore, enthalpy was calculated in EES at low pressures; 100 kPa, 200 kPa and 300 kPa added to the above to increase the range of data for training and prediction.

In order to lower the discrepancy in the results and increase the training values, the two neural networks created, Network A and Network B, were merged, since they shared 3 input variables; Pressure (P), Temperature (T) and Ammonia Concentration (x) and the variable that each network had a difference was added, resulting in 4 input variables; Pressure (P), Ammonia Concentration (x), Temperature (T), and phase of the mixture (q) in order to increase the database and have better training and prediction results, resulting in the multilayer network architecture as shown in Figure 4.

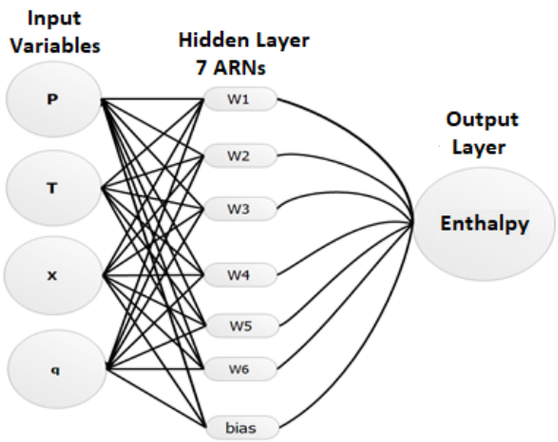

Figure 4 Modified multilayer network (Network A)
Source: Own elaboration

Network A was retrained with the new input variable called mixture phase (q) and by adding pressures of 100 kPa, 200 kPa, and 300 kPa to the training database. Network A prediction was again made using pressures of 150 kPa, 250 kPa, 350 kPa, 3,000 kPa, 7,000 kPa, and 8,000 kPa, for which corresponds a value of Saturation Temperature (T), an ammonia concentration (x) from 0 to 1 with intervals of 0. 1, and a value of the enthalpy phase variable of -1 (saturated liquid) and 1 (saturated vapor), to validate again this Network A, the enthalpy results were compared with those of the EES software. Figures 5 to 10 show the comparison of the results for each pressure in a Concentration (x) vs Enthalpy (h) graph.

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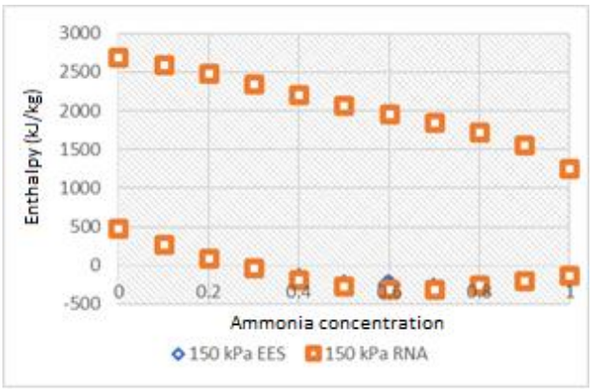

Figure 5 Network A vs EES at 150 kPa
Source: Own elaboration

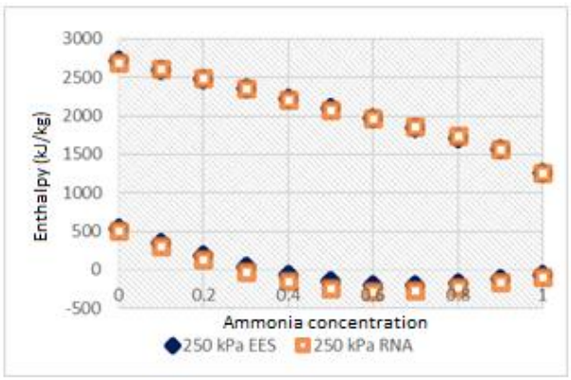

Figure 6 Network A vs EES at 250 kPa
Source: Own elaboration

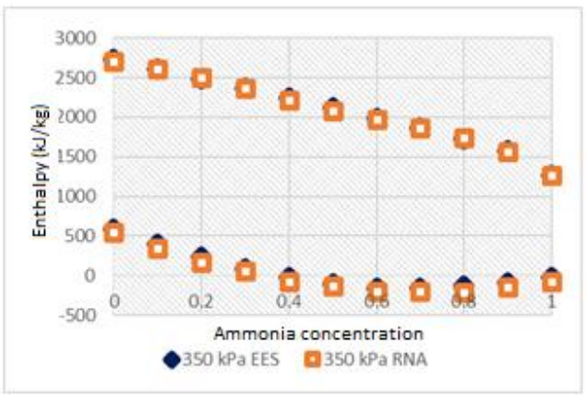

Figure 7 Network A vs EES at 350 kPa
Source: Own elaboration

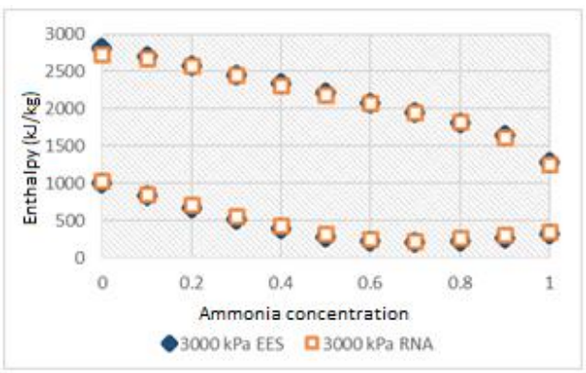

Figure 8 Network A vs EES at 3,000 kPa
Source: Own elaboration

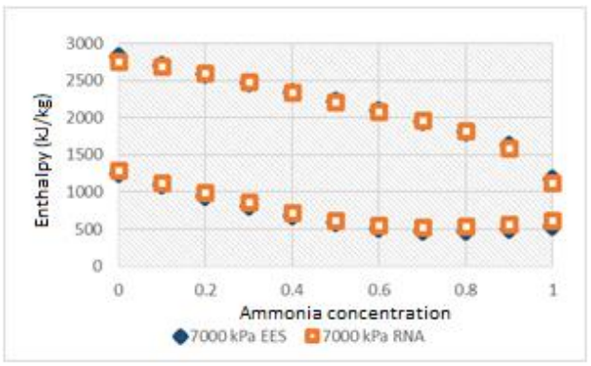

Figure 9 Network A vs EES at 7,000 kPa
Source: Own elaboration

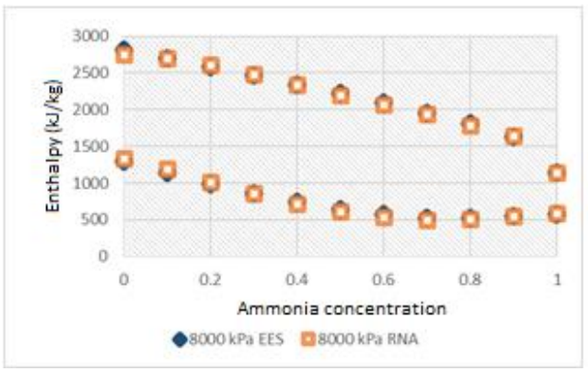

Figure 10 Network A vs EES at 8,000 kPa
Source: Own elaboration

The percentage error was plotted (Figure 11), where it is observed that the highest percentage of values are between the 0 error and the average percentage error resulting in 2.28%, which validates the ANN as trained and ready to make predictions that are between the range of 100 kPa and 10,000 kPa, the range may be higher or lower but within these values is where the highest prediction certainty is found.

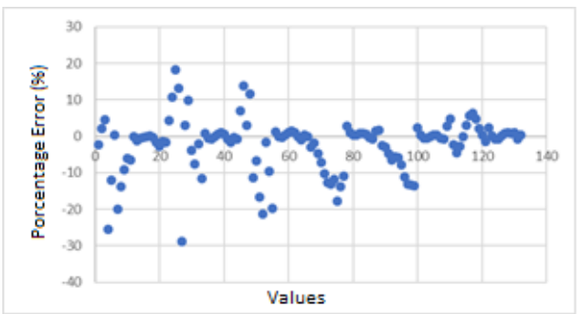

Figure 11 Percentage error of results Network A vs. EES
Source: Own elaboration

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After completing stage 5 of this work, which consisted of validating the ANN prediction with another methodology, in this case that of (Ibrahim, 1993), which is incorporated in the EES software, the general and specific objectives of this work were met, which consisted of creating an artificial neural network capable of predicting the thermodynamic property enthalpy in the binary mixture Ammonia-Water.

Discussion Red A

La Red A se entrenó a 100 kPa, 200 kPa, 300 kPa, 5,000 kPa, 10,000 kPa and 11,000 kPa and for each pressure corresponded a value of Temperature and Ammonia Concentration in the mixture, enthalpy property predictions were made at pressures of 150 kPa, 250 kPa, 350 kPa, 3,000 kPa, 7,000 kPa, and 8,000 kPa with their corresponding values of Temperature and Ammonia Concentration in the mixture. A total of 132 values corresponding to each input variable were predicted, these data were validated with the EES software with an average percentage error of 2.28%, where the highest percentage error value was 28.77 %. This is because the calculated enthalpy was at low pressures, e.g., at a pressure of 150 kPa, a temperature of 312.8 °C and an Ammonia concentration of 0.3, Network A predicted enthalpy of -23.91 kJ/kg while for EES it resulted in -19.06 kJ/kg, with an absolute error of the results of 4.85 kJ/kg and can be considered an acceptable variation for energy balances. However, the percentage error is 25.48 %, which is high, but justified by its equation which depends on the absolute error and the actual value, the lowest value of percentage error was 0.01425 %. The Red A is able to predict the enthalpy with results with a low range of acceptable error between 100 kPa and 10,000 kPa.

RED B

The second network corresponds to a Back Propagation network of multilayer architecture as shown in Figure 12, the network is made up of three independent variables and one dependent variable, the independent input variables are: pressure, enthalpy phase and ammonia concentration and the dependent output variable is the enthalpy.

Unlike Network A, in this network the independent variable Temperature is changed by the independent variable enthalpy phase (q); this variable is given two values which will depend on the phase in which the mixture is found, i.e. -1 for liquid phase and 1 for vapor phase.

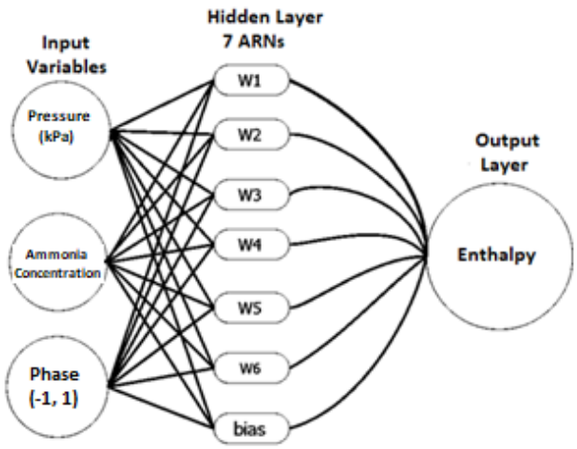

Figure 12 Network architecture B
Source: Own elaboration

In the same way that Network A was trained, in Network B the data were divided into three different groups, each set of data has the corresponding values according to the output variable enthalpy (h). For the first group of data the lowest pressure established in the literature of the experimental data of (Park & Sonntag, 1990) was taken, each group of data corresponds to a training pressure which are 5,000 kPa, 10,000 kPa and 11,000 kPa to each of them corresponded a value of ammonia concentration from 0 to 0.9 with intervals of 0.1 and a phase value of the mixture which is -1 if it is saturated liquid and 1 if it is saturated vapor.

Once the training of the network was finished, the resulting data were denormalized in order to have a better appreciation of them. With the denormalized data and once passed to a matrix in Excel^{TM}, the data entered for training were plotted against the training results of the network as shown in Figure 13; in which you can see the coincidence of the points and that they have the same behavior, which makes it clear that it was an acceptable training. Having the denormalized data, the percentage error was calculated as shown in Figure 14.

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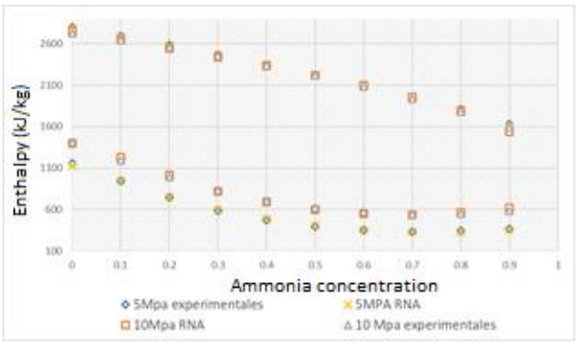

Figure 13 Experimental data (Park & Sonntag, 1990) vs Red B
Source: Own elaboration

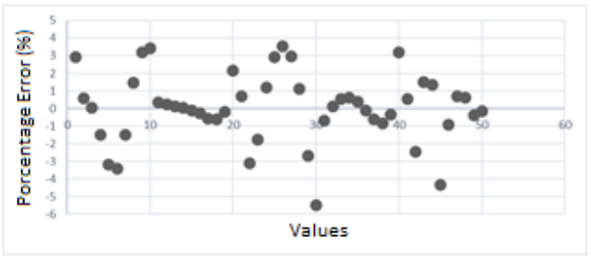

Figure 14 Percentage error of training Red B
Source: Own elaboration

Once verified that the training error is as close to zero as possible, the enthalpy prediction was made at two different pressures. The first prediction was made at a pressure of 6,000 kPa, the range of the ammonia concentration variable was from 0 to 0.9999 and for the mixture phase variable (q) it was in liquid and vapor phase (-1, 1).

The second prediction was made at a pressure of 7,000 kPa, the range for the variable ammonia concentration was from 0 to 0.9999 and for the variable mixture phase was liquid and vapor phase (-1, 1). The results of the prediction were plotted to see its behavior in a diagram Ammonia Concentration vs Enthalpy compared against the values obtained by the EES (Figures 15 and 16), which corresponds to a Pressure of 6,000 kPa and 7,000 kPa, where it can be observed that they have the same behavior shown in the Network A literature, so it can be concluded that the network performed a satisfactory prediction.

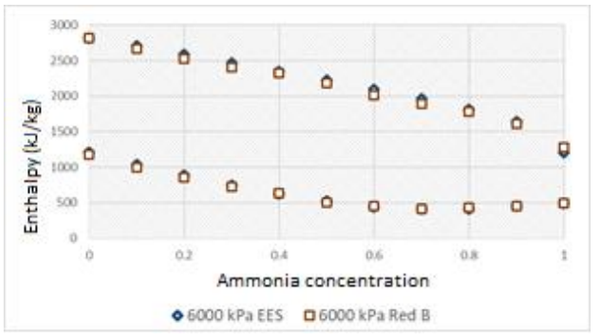

Figure 15 Results vs EES at 6,000 kPa, Network B
Source: Own elaboration

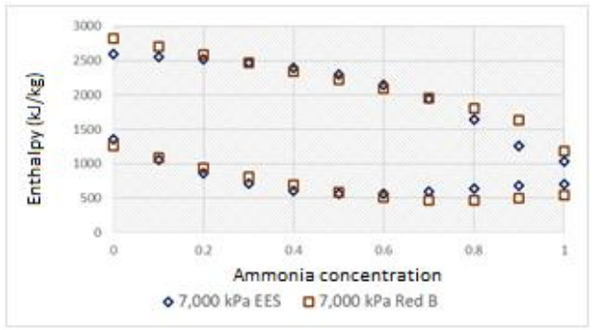

Figure 16 Results vs. EES at 7,000 kPa, Network B
Source: Own elaboration

Figure 17 shows the percentage error where it can be seen that most of the values are close to zero and the two most decentralized values were given when the ammonia concentration was one, this is because the EES takes the enthalpy of ammonia directly and the ANN takes the value calculated from the Network B training.

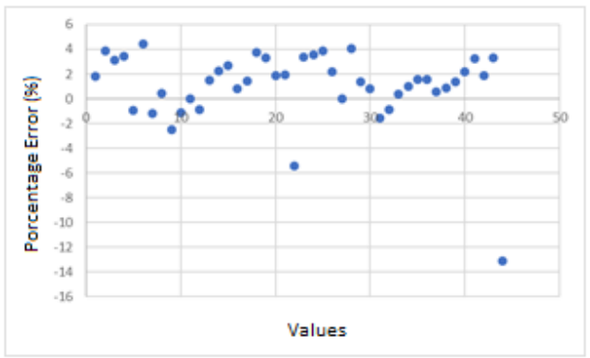

Figure 17 Percentage error in the validation between results vs. EES, Network B
Source: Own elaboration

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Discussion Red B

As with Network A, the results were validated with the EES software (Ibrahim, 1993); detecting that the objective is met, which is to create an artificial neural network capable of predicting the thermodynamic property enthalpy in the binary mixture Ammonia-Water, for the realization of energy balances in various thermodynamic processes.

Network B was trained at 5,000 kPa, 10,000 kPa and 11,000 kPa and for each pressure corresponded a phase value of enthalpy (q) and Ammonia concentration in the mixture (x), enthalpy property predictions were made at pressures of 6,000 kPa and 7,000 kPa, with a total of 44 prediction values and an average percentage error of 2. 30 %, where the highest error value was 13.13 %, this is due to the fact that the values given when the concentration of Ammonia is 1 the Network B continues calculating according to its training, while the EES gives the direct value of the Ammonia property and not of the mixture. While the lowest percentage error value was 0.0204 %. Red B is able to predict the enthalpy with results with a low range of acceptable error between 5,000 kPa and 10,000 kPa.

Conclusions

Both Network A and Network B are capable of predicting the enthalpy property of the binary mixture Ammonia-Water, for the predictions of each network there was a low margin of acceptable error when validating the results with the EES software, however, for these predictions to be under an acceptable range of percentage error (0.01425% and 0.0204 %) they have to be predicted within a training pressure range for each network. That is, for Network A between 100 kPa and 11,000 kPa and for Network B between 5,000 and 10,000 kPa should be used. Although the networks can predict with an indefinite range, they only predict effectively if the range of the input variables is within the training values, therefore, the prediction of the neural networks will depend on the range of training values; the more robust the neural network is, the more accurate values it can predict and the more variables it can predict.

The network can be trained with three variables and it could predict, not only the enthalpy, but also: entropy, phase of the mixture, ammonia concentration in the mixture, water concentration in the mixture, temperature and pressure. This shows that ANNs are an alternative that is still little explored, but with a great potential for applications, not only to predict thermodynamic properties of this mixture, but of any type of binary or multicomponent mixture, the only limitation is to have sufficient data in wide intervals, since the networks are limited to the extrapolation of their training values.

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