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Toward artificial intelligence-based modeling of vapor liquid equilibria of carbon dioxide and refrigerant binary systems

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Abstract: The objective of this study is to design and validate a highly accurate approach based on an artificial neural network (ANN) to predict both bubble and dew point pressures of various CO_2–refrigerant binary systems in the temperature range of 263.15–367.30 K and pressure of 0.18–9.09 MPa. 503 Experimental vapour–liquid equilibria (VLE) data of nine different CO_2-refrigerant binary mixtures were used for preparation, validation and testing of ANN model. The developed ANN model correlates bubble and dew point pressure to reduced temperature, critical pressure, acentric factor of refrigerant, and distibution of CO_2 between the vapour and liquid phases. Trial and error procedure reveals that a three-layer neural network with fourteen neurons in the hidden layer is able to predict the pressure with mean square error (*MSE*), average absolute relative deviation (*AARD*), root mean square error (*RMSE*), and correlation coefficient (R^2) of 0.0133, 2.79 %, 0.1153 and 0.99836, respectively. The results confirmed that the ANN model can accurately apply for predicting the VLE data of different binary CO_2–refrigerant systems.

Keywords: artificial neural networks; refrigerant; phase equilibria; bubble pressure; dew pressure.

INTRODUCTION

Vapour–liquid equilibria (VLE) play a crucial role in designing, modelling, and control of process equipment.[1–5] Mixtures containing refrigerant are very interesting from both thermodynamics and phase diagrams point of views. Binary system including refrigerant generate different shapes of phase diagrams. On the other hand, in the previous decades, the supercritical fluid technology has become popular due to its advantages over conventional processes. High degree of mass transfer, favourable selectivity, low operating temperature and high effi-

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ciency are among these advantages. Carbon dioxide is widely used in the supercritical fluid applications because it is inexpensive, non-flammable, non-toxic, readily available, and moreover it has moderate critical conditions (T_c = 304.25 K, p_c = 7.38 MPa).[6] Therefore, the estimation of VLE for binary system of carbon dioxide and refrigerant is important issue.

The experimental measurement of VLE data is very expensive and needs very high tech instruments.[7] The cubic, non-cubic and hard-sphere equations of state (EoS) can be applied for estimating the VLE data and thermophysical properties.[8–10] Although these semi empirical equations were derived based on reliable physical principles and often show acceptable preciseness for predicting the phase behaviour of pure and mixtures, they have rare application in the process design software, because of their complex terms and many adjustable parameters that are required in mixing rules.[11–13] Adjustment of these parameters through iterative method is tedious, and moreover there exists no guaranty for finding the best set of parameters.[2,12]

On the other hand, the ANN-based models which often able to represent and accurately predict refrigerant properties within the experimental uncertainties, provide promising alternative to compensate the weakness of EoS.[12] In addition, prediction of VLE data using ANN will be easier than using complex analytic equations.[14] The utmost advantage of an ANN-based model is eliminating the complex equations, and replacing them with some matrices and transfer functions.[15]

The ANN-based model is already highly accepted as a practical technology offering an alternative way to tackle complex and vague problems.[16–24] The ANN-based models have recently found extensive application for the estimation of different properties of refrigerants.[25–33] Chouai *et al*. modelled vapour–liquid phase behaviour of some refrigerant fluids namely: R134a, R32, and R143a using neural network in a wide range of temperatures and pressures.[12] Laugier and Richon, used an ANN model to represent pressure, temperature, volume data of some refrigerants in wide ranges of operating conditions.[34]

Mohebbi *et al.* predicted the liquid density of nineteen pure components and six mixtures of refrigerants by the artificial neural network approach.[35] A back propagation ANN model for simultaneous estimation of the VLE of four binary systems was proposed by Karimi and Yousefi.[36] Performance of a multi-layer perceptron (MLP) neural network model for the estimation of dimethyl ether densities and vapour pressures was investigated by Moghadassi *et al.*[37] Potential application of the ANNs in determination of the specific volume and enthalpy and entropy changes of alternative refrigerants R404a, R407c and R508b for both saturated liquid–vapour (wet vapour) and superheated vapour regions have been investigated.[7,38–39] Arcaklioglu *et al.* investigated the performance of a vapour compression heat pump with different ratios of R12/R22 refrigerant mixtures

using an ANN-based model.[26] Zhang developed an ANN-based generalized correlation approach for the estimation of refrigerant mass flow rate through adiabatic capillary tubes.[28] Balcilar *et al.* used an ANN model to estimate the measured convective heat transfer coefficient and the pressure drop of R134a flowing downward inside a vertical smooth copper tube.[32] Sencan *et al.* proposed an ANN model to determine the heat conduction coefficient, dynamic viscosity, kinematic viscosity, thermal diffusivity, density, specific heat capacity of some refrigerants.[33] Arcaklioglu *et al.* show the possibility of the use of neural networks for the calculation of the performance of a vapour-compression refrigeration system using refrigerant mixtures.[27] Coquelet *et al.* reported that an ANN can be used to calculate thermodynamics properties.[29]

To the best of our knowledge there is no study relating to the application of the ANN approach for the prediction of bubble and dew point pressure of binary mixture containing CO_2 and refrigerant compounds in literature. Therefore, instead of complex rules and mathematical routines, the ANN model was considered to determine both bubble and dew point pressures of binary mixtures containing CO_2 and refrigerants compounds as numerical equations.

METHODS

Artificial neural networks

Artificial neural networks, *i.e.*, nonlinear learning paradigms originated from the working procedure of biological nervous systems.[40] These artificial intelligence models, that are also known as learnable processing paradigms, constitute of some layers with given number of neuron. Among various types of ANN approaches, the multi-layer perceptron (MLP) networks have found high popularity for function approximation.[41,42] MLP neural network have proved itself through approximation of any unknown nonlinear function without prior knowledge of the distribution of the input data.[43,44] In the present work, the MLP neural network, with strictly feed-forward flow of signals, as shown in Fig. 1, has been applied for the considered task. The network has two processing layers in which each layer consists of some processing units namely neurons. Each layer directly receives their input from a previous layer and sends their outputs to a subsequent layer. The entry signals (independent variables) are fed into the first layer of neurons, while the last layer is responsible for the calculation of the independent variable(s).

It can be found, from Fig. 1, that a single hidden layer neural network model has been used to predict both bubble point (BP) and dew point (DP) pressure (dependent variable) as a function of reduced temperature, (T_r), critical pressure (P_c), acentric factor of refrigerant (ω), and composition of CO_2 in the vapor (y_{CO_2}) and liquid (x_{CO_2}) phases.

Input layer of the developed MLP model has five independent variables. Mole fractions of CO_2 in liquid and vapour phase are two of these independent variables. It is obvious that y_{CO_2} and x_{CO_2} should be given for DP and BP calculation, respectively. On the other hand, y_{CO_2} in BP calculation, and x_{CO_2} in DP calculation should not be used. Hence, in these circumstances they have been inactivated by setting their values equal to zero. It does not mean that these variables are zero, in fact it was done to provide a situation for the estimation of DP and BP by a single ANN model. Therefore, for the estimation of DP and BP with a single MLP model, y_{CO_2} and x_{CO_2} has to be zero, respectively.

Contrary to the analytical correlations neural networks models do not need an explicit formulation of the mathematical or physical relationships of the handled problem.[14,20,45–49]

During the preparation of an ANN model, the strength of each connection, *i.e.*, weights, should be adjusted by applying the appropriate learning algorithm.

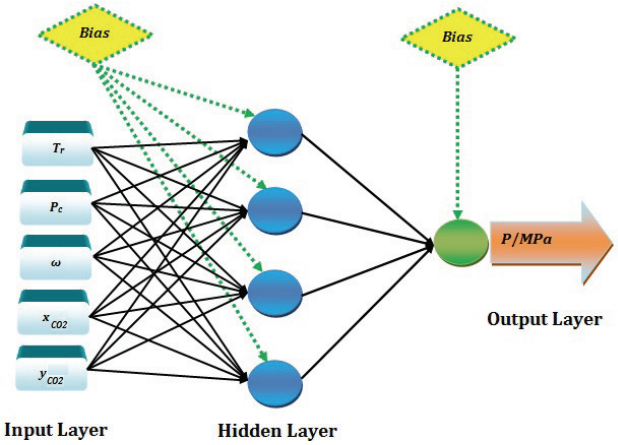

Fig. 1. Schematic of the proposed MLP network for estimating VLE data for CO_2–refrigrant binary systems.

Principle of the back-propagation

The learning stage tries to adjust the parameters of MLP model over the training dataset. Learning process using back propagation training algorithm involves two phases. During the first phase, the input variables are introduced and propagated through the network to compute the output values of an ANN model. This output is compared with its corresponding target values, resulting in an error signal, related to the input information. The second phase involves a backward pass of errors through the network, during which the parameters of the network would adjust so that the output approaches the observed data. The training continues until the calculated targets meet desired preciseness. Thereafter, the trained network will be tested by means of some input data that have not seen by the ANN model during the training stage. The most frequently used error function is the *MSE*:

$$\mathrm{MSE}=\frac{1}{\mathrm{N}}\sum_{\mathrm{i=1}}^{\mathrm{N}}\left(P_{\mathrm{i}}^{\mathrm{exp.}}-P_{\mathrm{i}}^{\mathrm{cal.}}\right)^{2} \quad (1)$$

where N is the total number of available training vectors, $P_{\mathrm{i}}^{\mathrm{exp.}}$ is the i^{th} desired target, and $P_{\mathrm{i}}^{\mathrm{cal.}}$ is the i^{th} calculated value by the ANN model.

According to the gradient descent, the back propagation changes the network parameters (weights and biases) with respect to the negative gradient of the error function toward the specific parameters of interest.

Selection the optimum configuration of MLP model

It is well known that the MLP feed-forward neural networks can approximate any spatially finite function, given a set of hidden nodes.[43,50–53] On the other hand, small number of neuron is not powerful enough to reach to the desired accuracy and often lead to under-fitting.

An optimum configuration of a MLP neural network is often determined by trial and error process. It has been proven that a MLP feed-forward network with the only single hidden layer can accurately correlate any multivariable function.[43,50–53] So, a single hidden layer MLP network is employed in this research for predicting the bubble and dew point pressure of binary system containing CO_2 and different refrigerants.

Number of hidden neurons is determined through a trial and error procedure which minimizes some error indices. In the present study, the number of hidden neurons has been determined through minimizing the *MSE*, *RMSE* and *AARD*, and maximizing R^2 values of training and validation datasetsas defined by Eqs. (2)–(4), respectively:

$$AARD = \frac{100}{N}\sum_{i=1}^{N} 100\left(\left|\frac{P_i^{\text{exp.}} - P_i^{\text{cal.}}}{P_i^{\text{exp.}}}\right|\right) \tag{2}$$

$$R^2 = \frac{\sum_{i=1}^{N}\left(P_i^{\text{exp.}} - \overline{\Delta P}\right)^2 - \sum_{i=1}^{N}\left(P_i^{\text{exp}} - P_i^{\text{cal.}}\right)^2}{\sum_{i=1}^{N}\left(P_i^{\text{exp.}} - \overline{\Delta P}\right)^2} \tag{3}$$

$$RMSE = \left\{\frac{1}{N}\sum_{i=1}^{N}\left(P_i^{\text{exp.}} - P_i^{\text{cal.}}\right)^2\right\}^{0.5} \tag{4}$$

The function defined by Eq. (5) is utilized as the transfer functions in both hidden and output layers:

$$f(x) = \frac{1}{1+\exp(-x)} \tag{5}$$

The correlation indicated by Eq. (5) is usually called logarithm sigmoid transfer function.

In the present study the Levenberg–Marquardt algorithm has been used as a training algorithm for updating the network parameters, *i.e.*, weights and biases. It has been reported that this optimization technique is more powerful than the conventional gradient descent techniques.[54–56]

RESULT AND DISCUSSION

In this study, 503 experimental VLE data points of different CO_2–refrigerant systems were collected from literature.[57–61] This databank includes bubble and dew point pressures for five and four binary CO_2 + refrigerant mixtures, respectively.[57–61] The refrigerant compounds are dichloromethane (R30), difluoromethane (R32), decafluorobutane (R610), 1,1,1,2,3,3,3,-heptafluoropropane (R227ea) and 1,1,1,2-tetrafluoroethane (HFC-134a). Table I shows the physical properties of pure components for all the substances involved in this study.[57–61] In the Table I, T_c is the critical temperature, P_c presents the critical pressure, and ω is the acentric factor.

It should be mentioned that for increasing the convergence rate during the training stage, and avoiding of saturation of the parameters of ANN model, all of the experimental data are mapped into interval of [0.01 0.99] using Eq. (6):

$$V_{\text{normal}} = 0.01 + \frac{V - V_{\min}}{V_{\max} - V_{\min}} (0.99 - 0.01) \quad (6)$$

here, V can be any independent or dependent variable, $V_{\max}$ and $V_{\min}$ represent the maximum and minimum values of each variable, and V_{normal} indicates the normalized value.

Table I. Physical properties of the pure components

Component	T_c / K	P_c / MPa	ω
Carbon dioxide (solvent)[57]	304.2	7.37	0.225
R30[57]	510	6.08	0.199
R32[58]	351.55	5.831	0.271
HFC-134a[59]	374.3	4.065	0.3268
R227ea[60]	375.95	2.98	0.3632
R610[61]	385.84	2.289	0.372

The experimental databank containing 264 bubble point pressures and 239 dew point pressures were divided into three different groups, *i.e.*, training, validation and testing datasets. Seventy percent of the VLE data were used as training dataset to adjust the ANN and find its optimum architecture. Twenty percent was used for the validation of performance of the trained MLP model. And remaining ten percent of the experimental data which was not seen by the model were considered as a testing dataset to examine the real performance of the final neural network model. Table II reports the *MSE*, *RSME*, *AARD* and R^2 calculated for different MLP configurations, differing with respect to the number of hidden neurons for both training and validation datasets. It is obvious that the initial values of the network parameters, *i.e.*, weight and bias coefficients, affect the final values. Therefore, in order to reduce the effects of the initial guess on the final result, each network has been trained several times by applying different randomly generated initial values of the network parameters and only the best results have been reported. The values presented in Table II are the best obtained results during fifteen tries per each topology.

The network with the smallest error (*i.e.*, *MSE*, *RSME* and *AARD*), and suitable R^2, has to be chosen as the best configuration of MLP network. It is obvious that the MLP model with one hidden layer consisting of fourteen hidden neurons (bold rows) is the optimum structure.

The best MLP model (5-14-1 structure) provides *AARD* = 3.08 %, *MSE* = = 0.0178 and R^2 = 0.99735 for the remaining testing datasets which were not seen by the model at all. This model predicts the overall dataset (training + validation + testing) with *AARD* 2.79 %, *MSE* 0.0133, *RMSE* 0.1153 and R^2 = 0.99836.

As it was justified in the preceding sections, the three-layer perception neural network with fourteen hidden neurons was selected as the best model for

the estimation of bubble point and dew point pressure of various CO_2–refrigrant systems. The weights and biases of this developed MLP model are presented in Table III. This information is required for using the developed MLP approach and reproducing the reported results.

TABLE II. Trial and error procedure to find the optimum topology of ANN model

Hidden neuron[a]	Database	Statistical accuracy analysis			
		AARD	*MSE*	R^2	*RMSE*
5	Training	8.39	0.0639	0.99212	0.2527
	Validation	8.81	0.0762	0.99104	0.2760
6	Training	7.71	0.0533	0.99313	0.2310
	Validation	7.77	0.0700	0.99217	0.2646
7	Training	5.24	0.0320	0.99588	0.1790
	Validation	5.95	0.0799	0.99072	0.2827
8	Training	4.04	0.0287	0.99644	0.1695
	Validation	6.86	0.1128	0.98515	0.3359
9	Training	3.78	0.0183	0.99772	0.1354
	Validation	4.53	0.0449	0.99470	0.2119
10	Training	3.46	0.0275	0.99659	0.1659
	Validation	4.43	0.0422	0.99521	0.2055
11	Training	3.44	0.0122	0.99852	0.1103
	Validation	4.04	0.0223	0.99715	0.1492
12	Training	3.03	0.0127	0.99844	0.1127
	Validation	3.99	0.0225	0.99725	0.1499
13	Training	3.29	0.0127	0.99847	0.1127
	Validation	3.66	0.0207	0.99750	0.1438
14	**Training**	**2.54**	**0.0076**	**0.99909**	**0.0869**
	Validation	**3.52**	**0.0311**	**0.99612**	**0.1764**
15	Training	2.35	0.0090	0.99883	0.0951
	Validation	3.55	0.0104	0.99895	0.1019
16	Training	2.12	0.0092	0.99883	0.0958
	Validation	4.77	0.0177	0.99801	0.1330
17	Training	2.09	0.0069	0.99914	0.0831
	Validation	4.97	0.0254	0.99717	0.1594
18	Training	1.55	0.0065	0.99919	0.0809
	Validation	5.34	0.0264	0.99692	0.1624

[a]The best result obtained among 15 different trained MLP networks

Fig. 2 shows the correlation between the predicted and experimental data for training, validation as well as testing subsets. The perfect fit (prediction equal to experimental data) is shown by the solid line (equality line). Fig. 2 justifies a good agreement between the predicted values by ANN model and the experimental data points. In other words, the obtained results show the suitable feasibility of the used ANN model to predict well the VLE information of various refrigerants.

TABLE III. Parameters of the developed MLP model with 4-14-1 structure

Hidden layer						Output layer	
Weights (W_{ij}) and biases						Weights (W_{ij}) and biases	
T_r	p_c / MPa	ω	x_{CO_2}	y_{CO_2}	Bias	weights	Bias
2.4726	2.1039	7.1184	–1.3465	2.8227	–10.9128	–11.729	–12.8078
–16.7803	3.8958	3.2455	–17.4859	–9.7552	34.2786	–4.3338	
2.7566	13.5189	0.67771	6.1312	–3.3594	–16.7601	29.7553	
12.5283	–15.3762	–16.6662	–13.0899	30.1056	–2.9477	1.6626	
–3.3876	1.6712	5.1947	0.098545	–6.187	3.3551	–9.82	
–8.5193	5.7551	–1.1644	1.8966	3.0775	0.27062	–1.3	
–3.5299	15.5119	71.1323	3.5585	–4.3854	–69.9971	–10.7152	
–29.2003	37.5152	43.2983	24.6894	–44.486	–16.1718	0.7165	
50.2137	80.0686	–82.6355	0.664	5.2158	–27.9744	–48.4534	
–0.90984	–5.1262	–14.3265	0.040792	–2.3906	13.2472	–78.6005	
–1.6116	–7.2033	–16.4993	5.0896	–3.6278	12.909	31.1776	
–0.73499	47.3077	3.5594	–5.4488	–2.2725	–37.2833	62.2794	
–2.7058	–22.6202	–43.2347	0.35941	4.2717	35.8734	24.8758	
1.1797	4.51	3.0532	8.5072	–25.1228	24.3346	27.8949	

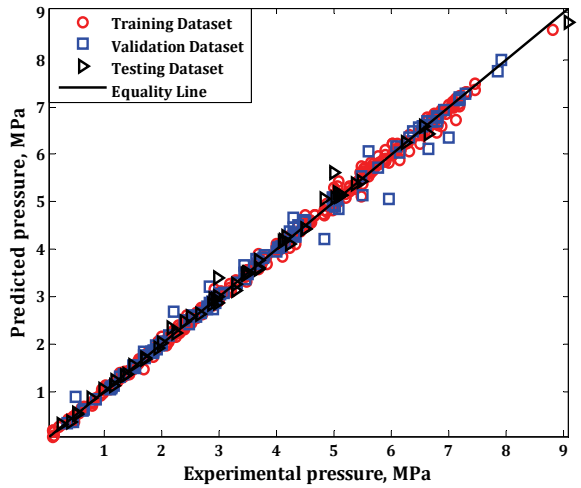

Fig. 2. Presentation of experimental versus predicted pressure for three different subsets.

Moreover, more details about the obtained results for both BP and DP of all binary systems were given in the Table IV. The obtained results show that the bubble point pressure of the considered binary mixtures are estimated with overall *MSE* 0.0033, *AARD* 2.08 % and R^2 0.99958. Furthermore, the developed MLP model predicted the dew point pressure data with the *MSE*, *AARD* and R^2 of 0.0261, 3.58 % and 0.99661, respectively.

Typically, both experimental[58] and calculated VLE data for the CO_2 + R32 binary system, as function of the distribution of CO_2 on different temperatures

were shown in Fig. 3. The presented results in Fig. 3 show not only the accuracy of the predicted VLE data using ANN model, but also confirm that the designed model is able to predict well the variation of the phase diagram of the binary mixtures respect to the composition and temperature. In other words, the obtained results show the capability of the proposed ANN model to use for estimating the bubble and dew point pressures of binary systems containing CO_2 and different refrigerant compounds.

Table IV. *MSE*, *AARD* and R^2 for the bubble and dew point pressure of CO_2–refrigerants binary systems

Component 2	*T* / K	*p* / MPa	Data	No. of data	Error analysis		
					MSE	*AARD*	R^2
R30[57]	311–327	4.11–9.09	BP	14	0.0114	1.78	0.99818
R32[58]	283–343	1.24–7.46	BP	47	0.0010	1.03	0.99985
R610[61]	263–353	0.18–6.86	BP	76	0.0043	2.88	0.99933
R227ea[60]	276–367	0.22–7.19	BP	92	0.0024	1.88	0.99970
HFC-134a[59]	323–343	1.69–7.12	BP	35	0.0035	2.41	0.99928
Overall BP	263–367	0.18–9.09	BP	264	0.0033	2.08	0.99958
R32[58]	283–343	1.24–7.46	DP	47	0.0038	1.95	0.99944
R610[61]	263–353	0.18–6.86	DP	66	0.0317	4.72	0.99529
R227ea[60]	276–367	0.22–7.19	DP	90	0.0183	2.96	0.99771
HFC-134a[59]	323–343	1.69–7.12	DP	36	0.0641	5.14	0.98719
Overall DP	263–367	0.18–7.46	DP	239	0.0261	3.58	0.99661

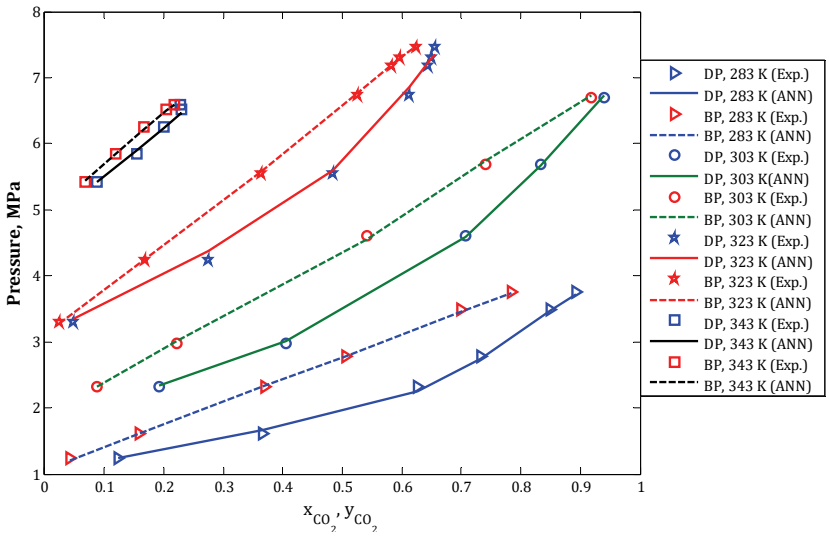

Fig. 3. Experimental *p*–*x*–*y* data for the CO_2 (1) + R32 (2) system,[58] and the associated predicted values by proposed ANN model for different temperatures.

The last part of the analysis is devoted to the investigation of the amount of association between independent and dependent variables. The correlation coef-

ficient analysis is the most well-known measure of this association.[62] This type of analysis is often of interest in data analysis and modelling research. In order to do it, three different correlation coefficient approaches, namely Spearman, Pearson and Kendall were employed.[62] The amplitude of these coefficients indicates the strength of relation and their signs represent the kind of relation, *i.e.*, direct or indirect between paired variables.[62] Values of coefficients of these approaches for the five possible pairs of independent-dependent variables is illustrated in Fig. 4. It is obvious that the reduced temperature shows the most reliable direct relation with the dependent variable, while acentric factor provides the most reliable indirect relationship.

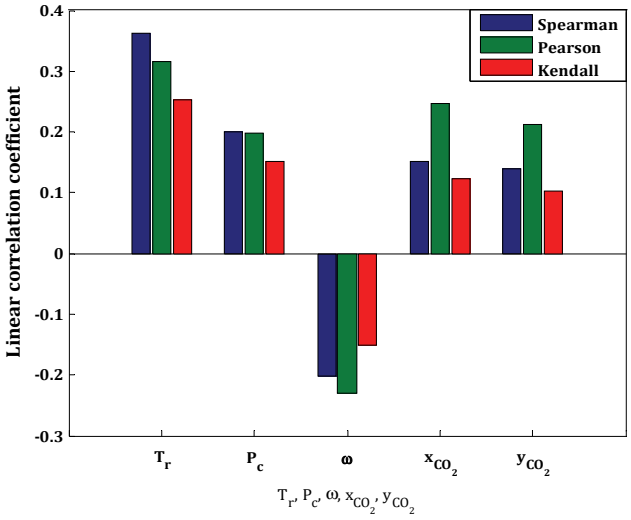

Fig. 4. Linear correlation coefficient between independent and dependent variables.

CONCLUSIONS

A MLP neural network with 5-14-1 structure was used to predict bubble and dew point pressure of five and four binary carbon dioxide + refrigerant systems, respectively. 503 experimental data points were used to design the proposed MLP network. Seventy percent of the experimental data were randomly chosen to train the network, and twenty percent of them were used during the validation process. The remaining ten percent of the databank are left to examine the real performance of the final neural network model. The optimum MLP model shows overall *AARD* = 2.79 %, *MSE* = 0.0133, *RMSE* = 0.1153, and R^2 = 0.99836 for the prediction of VLE information of the considered binary mixtures. Considering these statistical indices, the proposed MLP model can be reliably used to estimate the bubble and dew point pressures of the CO_2 + refrigerant systems, within the ranges of temperature and pressure considered in this study.

NOMENCLATURE

AARD	Absolute average relative deviation
ANN	Artificial neural network
BP	Bubble point
DP	Dew point
EoS	Equations of state
exp	Exponential function
HFC-134a	1,1,1,2-Tetrafluoroethane
MLP	Multi-layer perceptron
MSE	Mean square error
RMSE	Root mean square error
R^2	Correlation coefficient
R227ea	1,1,1,2,3,3,3-Heptafluoropropane
R30	Dichloromethane
R32	Difluoromethane
R610	Decafluorobutane
V	Variable
VLE	Vapor–liquid equilibria
f	Transfer function
N	Number of data points
p	Pressure
p_c	Critical pressure
Δp	Average value of experimental pressure data
T_c	Critical temperature
T_r	Reduced temperature
ω	Acentric factor
x_{CO_2}	Mole fraction of CO_2 in the liquid phase
y_{CO_2}	Mole fraction of CO_2 in the vapor phase

Superscript/subscript

c	Critical
cal	Calculated
exp	Experimental
max	Maximum value
min	Minimum value
normal	Normalized value
r	Reduced

И З В О Д

МОДЕЛОВАЊЕ РАВНОТЕЖЕ ПАРА–ТЕЧНОСТ БИНАРНИХ СМЕША УГЉЕН-ДИОКСИДА И РАСХЛАДНИХ ФЛУИДА ПРИМЕНОМ ВЕШТАЧКИХ НЕУРОНСКИХ МРЕЖА

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Циљ овог рада је анализа могућности примене вештачких неуронских мрежа (ANN) за предвиђање вредности притисака у тачки кључања и тачки росе бинарних

смеша расхладних флуида са CO_2, у опсегу температура 263,15–367,30 K и притисака 0,18–9,09 MPa. За припрему, валидацију и проверу модела на бази неуронских мрежа коришћено је девет различитих бинарних смеша CO_2 са расхладним флуидима, са укупно 503 експериментална података за равнотежу пара–течност (VLE). Развијени ANN модел се користи за корелисање притисака у тачки кључања и тачки росе у зависности од редуковане температуре, критичног притиска, фактора ацентричности расхладног флуида и удела CO_2 у обе фазе. Поступком пробе и грешке изабрана је трослојна неуронска мрежа са четрнаест неурона у скривеном слоју за предсказивање вредности притиска, уз следећа одступања: *MSE* грешка је 0,0133, *AARD* грешка је 2,79 %, *RMSE* грешка је 0,1153 и са вредношћу R^2 од 0,99836. Резултати су показали да се неуронска мрежа може користити за прецизно предсказивање равнотежних података пара-течност у смешама расхладних флуида и CO_2.

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