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On The Estimation Of Phase Behavior Of CO2-Based Binary Systems Using ANFIS Optimized By GA Algorithm

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Summary

Since the world average temperature is on the rise, severe measurements should be considered due to decrease the concentration of greenhouse gases which are the main reason of global warming. Geological sequestration of the CO2 speculated as one of the most efficient method for mitigate the problem. As the injected CO2 stream is not always a pure one, a more accurate assessment of the impurities effects on various part of the sequestration process would be desired. As equations of state are not able to completely support the thermodynamic attributes of impure CO2 injected stream, developed computational modeling would be more appropriate. In this study, due to obtain a way of predicting vapor liquid equilibrium of CO2 binary mixtures, not fully depending on the experimental data, a novel and accurate computational method is presented. This alternative, uses Adaptive Neuro-Fuzzy Interference System (ANFIS) together with Genetic Algorithm as an optimization tool. As a result, the developed model shows a great i

Introduction

Significant climate changes due to global warming has known as a severe problem in this industrial era. To mitigate this issue, greenhouse gases (GHG) controlling policy should be considered. Since CO_2 is recognized as the main GHG, reduction measurements of its emission would promote the environmental problems brought about by the growth of worldwide average temperature [1]. Among all solutions, Carbon Capture and Storage (CCS) is argued as the most efficient procedure.

Implementing CO_2 sequestration projects requires an accurate assessment of effective parameters which are contribute in different stages of CCS process. One of the major important challenges to analysis, would be the effects of captured CO_2 impurities on surface and subsurface CCS phases. These impurities mainly include N_2, O_2, Ar, H_2O, CO, H_2, CH_4, H_2S, SO_x, NO_x, HCN, COS, NH_3 and CH_3OH [2]. Excessive amount of these components would considerably changes thermodynamic properties of injected fluid especially in reaction with reservoir rock and fluid. Hence, to accurately estimate thermodynamic attributes of impure CO_2 injected stream, developed computational modeling would be more appropriate. Regarding great differences between distinct experimental data and large uncertainties, in this study vapor liquid equilibrium (VLE) and phase behavior of binary mixtures of CO_2-N_2/O_2/Ar are used from literature to present a novel and accurate computational method. Therefore, in current work Adaptive Neuro-Fuzzy Interference System (ANFIS) is used and optimized by Genetic Algorithm (GA) to predict CO_2 VLE data. Conducting a comparison of the developed model with the experimental data shows that the model would be completely reliable. In addition to this, regarding to high accuracy and also great generalization capability, this model might be a good alternative to the conventional equations in simulators while modelling CCS projects.

Adaptive Neuro-Fuzzy Interference System (ANFIS)

ANFIS strategy is a method which have the ability to solve problems that comprise cognitive uncertainties. To meet that, ANFIS uses Fuzzy Logic (FL) in conjunction with neural network traits; hence, this provide solutions in a way more alike humans.

The ANFIS structure constitutes of 5 layers which are shown in Figure 1. As regards Fig. 1, the network includes two inputs (x,y) and one output (f). According to Sugeno rules [3] it is assumed that:

$$IF\ \ x = A_i\ \ , y = B_i\ \Longrightarrow\ f_i = p_i x_i + q_i y_i + r_i \tag{1}$$

In which (i) is the membership grade of a fuzzy set (A_1, A_2, B_1, B_2) and p_i, q_i and r_i are coefficients that should be optimized while conducting training process.

Each layer in ANFIS framework has a duty which is briefly explained in below [4]:

Layer 1: In this layer the linguistic terms are produced when Membership Functions (MF) (Eq.2) accept distinct input data. There are n nodes to relate input information to linguistic terms. Membership functions could be different however, they are usually based on Gaussian MF (Eq. 3) expressed in below:

$$O_i^1 = \mu_{A_i}(x) \qquad O_i^1 = \mu_{B_{i-2}}(y) \tag{2}$$

$$O_i^1 = \mu_{A_i}(x) = exp^{\left(-\frac{1}{2}\frac{(x-Z)^2}{\sigma_i^2}\right)} \qquad O_i^1 = \mu_{B_{i-2}}(y) = exp^{\left(-\frac{1}{2}\frac{(y-Z)^2}{\sigma_i^2}\right)} \tag{3}$$

Where Z, O and σ indicate Gaussian MF center, output and the variance in turn. Indeed, these parameters should be optimized during the training process of ANFIS.

Layer 2: this layer (called firing strength layer) has the duty of checking qualification's efficiency and accuracy control. The related equation is illustrated in below:

$$O_i^2 = W_i = \mu_{Ai}(x).\mu_{B_{i-2}}(y) \tag{4}$$

Layer 3: Having normalized the second layer, third layer output is then provided as follow:

$$O_i^3 = \overline{W_i} = \frac{W_i}{\sum_{k=1}^{j} W_k} \tag{5}$$

Layer 4: Fourth layer is a multiple term of layer 3 and stipulated parameters of the Sugeno rule to create a new one as below:

$$O_i^4 = \overline{W_i} f_i = \overline{W_i}(p_i x + q_i x + r_i) \tag{6}$$

As mentioned before, p_i, q_i and r_i should be optimized to reduce the difference between experimental data and estimated results.

Layer 5: This layer would sum the average weighted to provide a qualitative rule:

$$O_i^5 = f = \sum_i \overline{W_i} f_i = \overline{W_1} f_1 + \overline{W_2} f_2 = \frac{\sum W_i f_i}{\sum W_i} \tag{7}$$

It should be noted that in the present study, Genetic Algorithm is applied to optimize ANFIS parameters.

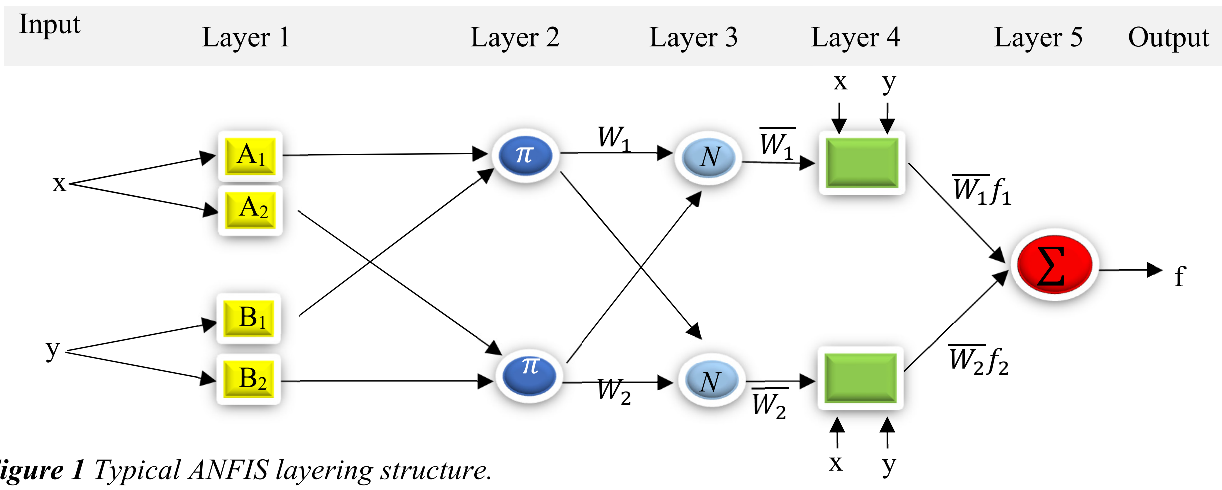

***Figure 1** Typical ANFIS layering structure.*

Genetic Algorithm (GA)

Genetic algorithm is an optimization method that imitate the process of natural selection in biological evolution. In this algorithm, the number of chromosomes are defined as the initial population and they have the duty of encoding candidate solutions (individuals) of an optimization case to acquire better solution. The term evolution represents generating individuals randomly in a string of consecutive generations in which the fitness of individuals would be evaluated. Consequently, some individuals are chosen stochastically according to their fitness. Being selected, individuals are then modified to create a novel population which is then employed in further iteration of the GA algorithm. Finally, reaching to an upper limit of generation or an eligible fitness value of the population, the algorithm performance would be terminated. The level of the fitness could be organized to consider multiple parameters to be optimized in order to its significance.

Model Development

Since accuracy is the key point of the model development process, utilization of authentic experimental data would be necessary. Hence, in this study 191 VLE experimental data of binary mixture of CO_2 and N_2/ O_2/Ar are gathered from literature. 58 data points for CO_2- N_2, 67 data points for CO_2- O_2 and 66 data points for CO_2-Ar system [5]. These information are includes pressure and temperature of the binary mixtures and their critical points. In order that 70% and the rest of the data are used as the training and testing processes in turn. As an output, CO_2 mole fraction in both liquid and vapor phases (X, Y) are estimated.

Conclusion

The current work presented a novel approach for estimating vapor-liquid equilibrium of CO_2 in binary mixtures with O_2, N_2 and Ar. To reach this aim a robust ANFIS model coupled with genetic algorithm.

As it can be seen in Figures 2,3, predicted X and Y have a huge similarity to the actual ones. The obtained results highlighted that the developed model can thoroughly estimate VLE values in such binary systems with adequate accuracy. Also as inserted in Table 1, the statistical indexes (including Coefficients of determination (R^2), Root mean squared errors (RMSE) and Standard deviations (STD) express great degree of accuracy in performance of this predictive tool. Therefore, it would be reliable to employ the approach, while implementing CCS simulations in case of huge impurities.

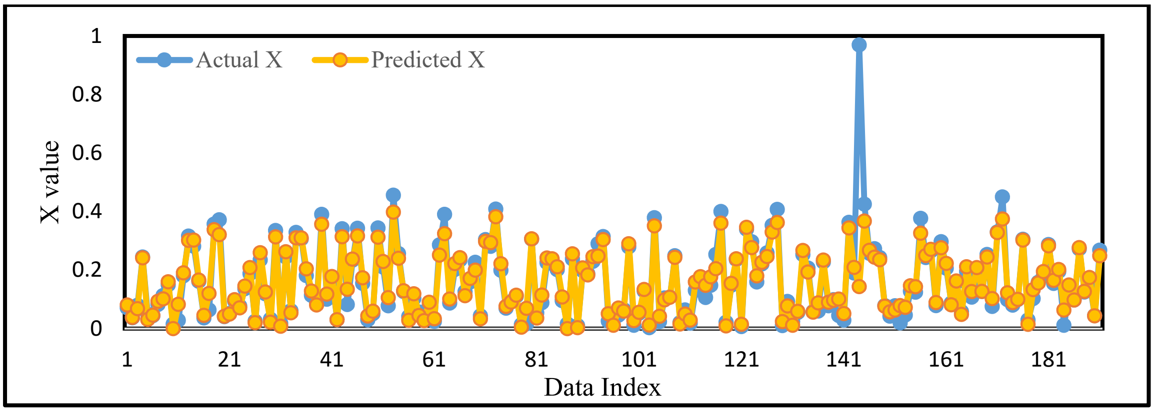

Figure 2 *The ANFIS and experimental values of liquid mole fraction of CO_2 against the number of data points.*

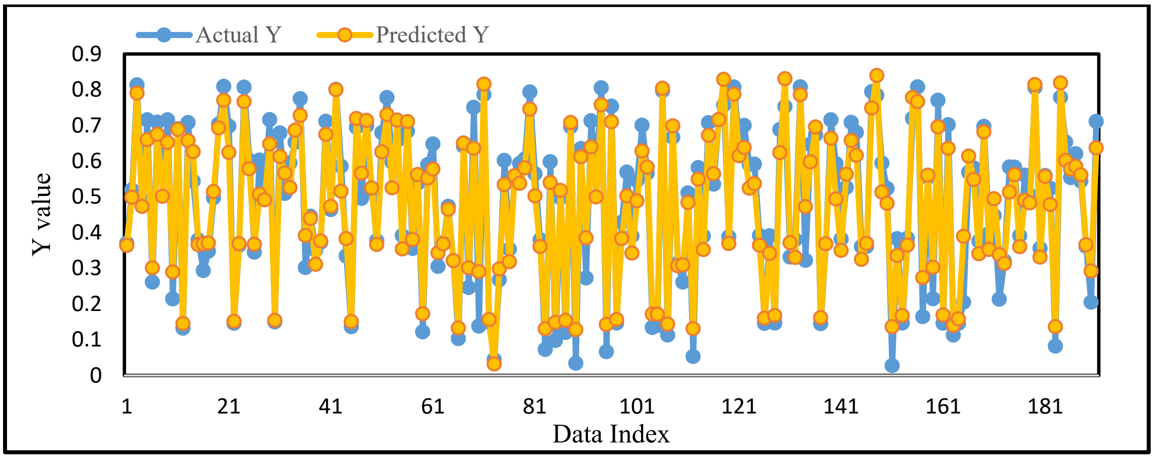

Figure 3 *The ANFIS and experimental values of vapor mole fraction of CO2 against the number of data points.*

Table 1 *The determined statistical parameters for prediction of liquid and vapor mole fractions of CO_2*

	Prediction of Y		**Prediction of X**	
	Training phase	Testing phase	Training phase	Testing Phase
R2	0.94851	0.92948	0.9963	0.89324
RMSE	0.05029	0.057117	0.0212	0.11189
STD	0.05024	0.05756	0.021292	0.11243

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