A Comparative Survey of Modeling Absorption Tower Using Mixed Amines

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Abstract

In natural gas treatment, the removal of CO_2 and H_2S in acid gases is a critical concern. There are various purification technologies that can be used for the removal of acid gas impurities. Absorption of acid gas into amines is one preferred method in gas industries. In the past, single amines was used, but recently in order to improve absorption performance, mixed amines with different solubility and reaction rates have been used.

In this study, artificial neural network ANN is used as a method to model the absorption tower when uses mixed amines. A specified model which is simple in calculation and good in accuracy was developed. In this model back propagation learning is used and the corresponding parameters have been optimized. Finally, the new method has been compared with conventional mass transfer and equilibrium methods. The obtained results confirmed the simplicity and accuracy of the developed method.

Keywords: Absorption tower, Mixed amines, Artificial neural network, Mass transfer method, Equilibrium method

Introduction

The gas purification for removing impurities, such as CO_2 and H_2S, is one of the main parts of natural gas (NG) treatment industry. For this process, the most important alkanolaminesused, are monoethanolamine (MEA), diethanolamine (DEA), di-isopropanolamine (DIPA) and N-methyldiethanolamine (MDEA) [1]. Since mid-80s of 20th century, mixed alkanolamines have been used. That was simply due to enhance absorption performance of alkanoamines. Mixed amines can provide any degree of selectivity and absorption rate [2].So modeling and simulation of amine absorption tower with amine mixtures as absorption solvent are very useful. It is many years now that the simulation and modeling of amine absorption tower in natural gas sweetening process has been studied [3].

With respect to the accuracy and fast calculations; two main methods namely; "equilibrium" and "mass transfer"; were developed. Basing on fundamental principles, either individual method has its own subdivisions.

Comparing to mass transfer method, low accuracy is the main disadvantage of the equilibrium method which is capable of faster calculation. On the other hand, hydraulic parameters of absorption tower and other details that are used in mass transfer method make the calculation more complicated and time consuming [3-4]. In order to overcome such disadvantages, another method should be developed. So, for modeling absorption tower, ANN methods applied, because of its ability to solve nonlinear complicated equations with higher speed and better accuracy.

Methods of modeling the amine absorption tower

Absorption of H_2S and CO_2 in a solvent is consisted of two successive mechanisms of mass transfer and reaction. When the acid gases are diffused into the liquid, they react with solvent and leads to unstable products after which the solvent is recovered [5]. In

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order to determine the capacity and rate of absorption, modeling of amine absorption process is carried out by using some known parameters such as; the percent of acid gases in feed, the amount of circulating solvent, operating temperature and pressure, amine concentration and amine loading [6].

Equilibrium method

In this method, vapor and liquid are entered a column, pass over the tray or flow through packed bed, exchange the materials and energy and then left in equilibrium [5].At this stage, the concentration of inlet gas and output liquidis calculated, using experimental data (as equilibrium curves) or using thermodynamic relation (such as equation of state).

Followings are equilibrium equations for H_2S and CO_2absorption in amine solvent that were presented by Dankwerts and Mc Neil for the first time [4]. Other researchers accounted for the constants of equilibrium equations, using empirical studies [7].

Generally for $H_2S/CO_2/amine/H_2O$ system, with two known parameters (α_{H2S}, α_{CO2}), the 13 following unknowns parameters could be calculatedby equation 10 to 20 [8].

The equations 17 to 20 are determined from mass and electric charge balance. K_1 to $K_7$are temperature dependent variables and can be calculated using empirical data. Considering equations 10 to 20, the following 3 equations can be written for calculating pressure of H_2S and CO_2 and also concentration of $[H^+]$.

$$RR'NH_2^+ \xleftrightarrow{K_1} H^+ + RR'NH \quad (1)$$

$$R'RNCOO \xleftrightarrow{K_2} R'RNH + HCO_3 \quad (2)$$

$$H_2O + CO_2 \xleftrightarrow{K_3} H^+ + HCO_3 \quad (3)$$

$$H_2O \xleftrightarrow{K_4} H^+ + OH^- \quad (4)$$

$$HCO_3^- \xleftrightarrow{K_5} H^+ + CO_3^{2-} \quad (5)$$

$$H_2S \xleftrightarrow{K_6} H^+ + HS^- \quad (6)$$

$$HS^- \xleftrightarrow{K_7} H^+ + S^{2-} \quad (7)$$

$$P_{CO_2} = H_{CO_2} * [CO_2] \quad (8)$$

$$P_{H_2S} = H_{H_2S} * [H_2S] \quad (9)$$

$[H_2S]$, $[S^{2-}]$, P_{CO_2}, P_{H_2S}, $[RR'NH_2^+]$, $[H^+]$, $[RR'NH]$, $[RR'NCOO^-]$, $[HCO_3^-]$, $[CO_2]$, $[OH^-]$,$[CO_3^{2-}]$, $[HS^-]$

$$K_1 = \frac{[H^+][RR'NH]}{[RR'NH_2^+]} \quad (10)$$

$$K_2 = \frac{[RR'NH][HCO_3^-]}{[RR'NCOO^-]} \quad (11)$$

$$K_3 = \frac{[H^+][HCO_3^-]}{[CO_2]} \quad (12)$$

$$K_4 = [H^+][OH^-] \quad (13)$$

$$K_5 = \frac{[H^+][CO_3^{2-}]}{[HCO_3^-]} \quad (14)$$

$$K_6 = \frac{\left[H^+\right]\left[HS^-\right]}{\left[H_2S\right]} \quad (15)$$

$$K_7 = \frac{\left[H^+\right]\left[S^{2-}\right]}{\left[HS^-\right]} \quad (16)$$

$$m = \left[RR'NH\right] + \left[RR'NH_2^+\right] + \left[R'RNCOO^-\right] \quad (17)$$

$$m\alpha_{H_2S} = \left[HS^-\right] + \left[H_2S\right] + \left[S^{2-}\right] \quad (18)$$

$$m_{CO_2} = \left[R'RNCOO^-\right] + \left[HCO_3^-\right] + \left[CO_2\right] + \left[CO_3^{2-}\right] \quad (19)$$

$$\left[RR'NH_2^+\right] + \left[H^+\right] = \left[RR'NCOO^-\right] + \left[HCO_3^-\right] + \left[OH^-\right] + 2\left[CO_3^{2-}\right] + \left[HS^-\right] + 2\left[S^{2-}\right] \quad (20)$$

$$P_{H_2S} = \frac{\left[\frac{H_{H_2S}}{K_6K_7}\right]\left[m\alpha_{H_2S} - \frac{P_{H_2S}}{H_{H_2S}}\right]\left[H^+\right]^2}{\left[1 + \frac{\left[H^+\right]}{K_7}\right]} \quad (21)$$

$$P_{CO_2} = \frac{\left[\frac{H_{CO_2}}{K_3K_5}\right]\left[m\alpha_{CO_2} - \frac{P_{CO_2}}{H_{CO_2}}\right]\left[H^+\right]^2}{\left[1 + \frac{\left[H^+\right]}{KS} + \frac{m\left[H^+\right]}{K_2K_5K''}\right]} \quad (22)$$

$$\left[H^+\right] = \frac{K_1K''}{m + K_1K''}\left[\left[m_{CO_2}\frac{P_{CO_2}}{H_{CO_2}}\right]\left[1 + \frac{K_2K_5}{K_2K_5 + K_2\left[H^+\right] + \frac{m\left[H^+\right]}{K''}}\right] + \frac{K_4}{\left[H^+\right]}\left[m\alpha_{H_2S}\frac{P_{H_2S}}{H_{H_2S}}\right]\left[1 + \frac{K_1}{K_1 + \left[H^+\right]}\right]\right] \quad (23)$$

Where in equation 22 and 23, K" is equal to:

$$K'' = 1 + \frac{\left[H^+\right]}{K_1}\frac{P_{CO_2}K_3}{K_2H_{CO_2}\left[H^+\right]}$$

It is important to note that with these equations, one can calculate the theoretical numbers of required trays, which can then be multiplied by tray efficiency to obtain the real numbers. The reported amount of efficiencies in such systems is 0.1 to 0.4 [3].Maddox et al worked on some gas purification units, using this method. Their results are shown in table 1[9-10].

It is obvious that the theoretical number of trays that were calculated with this method is quite different than those of real. This large discrepancy is due to the fact that the hydraulic parameters of absorption tower are not accounted for.

Table 1: Results of Maddox et al

Unit number	1	2	3	4
Real number of trays	25	20	15	30
Theoretical number of trays	2	4	2	2

Mass transfer method

In this method each tray is considered as a mass transfer stage between liquid and gas. The output stream conditions are calculated, using tray mass balance, while assuming the plug flow for gas phase and complete mixing of liquid on each tray. Variation of acid gas mole fraction in gas phase on tray K, are calculated by the following equations [10]:

$$\left.\begin{aligned} \frac{F}{1-y_j\sum_{i=1}^{n_A}\frac{N_i|_{y=0}}{N_j|_{y=0}}}\frac{dy_j}{dz} &= -N_j|_{y=0}\,A_v'\Omega_A \\ \frac{dF}{dZ} &= -\sum_{i=1}^{n_A}N_i|_{y=0}\,A_v'\Omega_A \end{aligned}\right\} For\ j=1,...,n_A \tag{24}$$

While for the components that is not absorbed; F_{yi}=Constant for $j=n_A+1,\ldots,n_G$

The boundary conditions are as follows:

$$\left.\begin{aligned} &For\ Z=0, y_i=y_{i,k}^{in} \\ &\qquad F=F_K^{in} \\ &and \\ &For\ Z=h_f, y_j=y_{j,k} \\ &\qquad F=F_K \end{aligned}\right\} For\ \ j=1,...,n_G \tag{25}$$

F_k^{in} *and* $y_{j,k}^{in}$ are the flow rate and the mole fraction of gas stream input to the tray respectively. They are obtained from output stream data of the next tray K+1.To calculate flow rate and composition of the liquid phase, the kinetics of reaction of acid gas-amine should be known. Generally this reaction could be as:

$$\alpha_{A_{1,1}}A_1^G+\sum_{j=1}^{n_R}\alpha_{R_{j,1}}R_j^L \Leftrightarrow \sum_{j=1}^{n_p}\alpha_{P_{j,1}}P_j^L \tag{26}$$

$$\alpha_{A_{2,2}}A_2^G+\sum_{j=1}^{n_R}\alpha_{R_{j,2}}R_j^L \Leftrightarrow \sum_{j=1}^{n_p}\alpha_{P_{j,2}}P_j^L \tag{27}$$

Liquid flow rate and the corresponding component concentrations are calculated according to reaction rate of acid gas and amine. Since acid gas reaction with different amines has different reaction rate, determination of $x_{j,K}$ is depended on Hatta number (Ha) which is defined as:

$$Ha=\frac{1}{K_{L.A}}\sqrt{\frac{2}{m_A+1}a_A K_1 C_A^{m_A-1}\left[\prod_{j=1}^{n_R}\left(CR_j\right)_b^{m_{Rj}}\right]D_A}$$

For 3<Ha; $x_{j,K}$=0 for $j=1,\ldots\ldots\ldots,n_v$

For 0.3<Ha <3

(28)

$$x_{j,k}\left(L_k'+w_{wk}\right)=x_{j,k-1}L_{k-1}'+x_{w_{j,k}}w_{vk}+N_j|_{y=y_L}A_v'\Omega h_F-a_{j,j}r_j\left(1-A_v y_L\right)\Omega h_F\varepsilon_L$$
$$For\ \ j=n_v+1,...,n_v+n_m \tag{29}$$

$$x_{j,k}\left(L_k'+w_{wk}\right)=x_{j,k-1}L_{k-1}'+x_{w_{j,k}}w_{vk}+y_{j,k}^{in}F_K^{in}-y_{j,k}F_k-a_{j,j}r_j\left(1-A_v y_L\right)\Omega h_F\varepsilon_L$$
$$For\ \ j=n_v+n_m+1,...,n_v+n_m+n_s \tag{30}$$

There are similar relations for other components which are not absorbed. Absorption flux of different species is also obtained from the equation 31:

$$N_j|_{y=0}=K_{G,j}\left(P_t\right)_k\left[y_i-H_j'\left(x_{j,k}\right)_i\right] \qquad For \quad j=1,...,n_A \tag{31}$$

And with application of Fick's law it could be written as:

$$N_j|_{y=0}=-D_j C_K\left.\frac{dx_j}{dy}\right|_{y=0} \qquad For \quad j=1,...,n_A \tag{32}$$

$$N_j|_{y=y_L}=-D_j C_K\left.\frac{dx_j}{dy}\right|_{y=y_L} \qquad For \quad j=n_i+1,...,n_A \tag{33}$$

To determine the amount of flux, the concentration profile of absorption species is obtained from the following second order differential equation:

$$D_j\frac{d^2x_j}{d_y^2}=\frac{a_{j,j}}{c_k}r_j \qquad For\ \ j=1,...,n_v+n_M \tag{34}$$

For solving equation 34, boundary conditions should be determined.
Tray temperature is calculated by enthalpy balance around each tray as equations 35 to 38:

$$T_{K-1}L'_{K-1}\sum_{j=1}^{n_L}x_{j,K-1}Cp_{L,j}-T_K\left[F_K\sum_{j=1}^{n_G}y_{j,k}Cp_{G,j}+\left(w_{wk}+L'_K\right)\sum_{j=1}^{n_L}x_{j,k}Cp_{L,j}\right]+T_{K+1}\left[\left(F_{K+1}-V_{wk+1}\right)\sum_{j=1}^{n_G}y_{j,K+1}Cp_{G,j}\right]+$$

$$T_{vK+1}V_{VK+1}\sum_{j=1}^{n_G}y_{Vj,K+1}Cp_{G,j}+T_{wk}w_{VK}\times\sum_{j=1}^{n_L}x_{w_{j,K}}Cp_{L,j}=Q_K^C-\sum_{j=1}^{n_A}Q_{j,K}^{abs}-\sum_{j=1}^{n_G}Q_{j,K}^R \quad (35)$$

(36)

$$Q_{j,K}^{abs}=\left(-\Delta H_j^{abs}\right)\left(F_K^{in}y_{j,k}^{in}-F_K y_{j,k}\right) \quad For \quad j=1,\ldots,n_A \quad (37)$$

$$Q_{j,K}^R=\left(-\Delta H_j^R\right)\frac{1}{a_{j,j}}\left\{\left(F_K^{in}y_{j,k}^{in}-F_K y_{j,k}\right)-\left[x_{j,k}\left(L'_k+w_{wk}\right)-\left(L'_{K-1}x_{j,K-1}+w_{vk}x_{w_{j,k}}\right)\right]\right\} \quad For \quad j=1,...,n_E \quad (38)$$

The above equations planned for all trays in the tower and are solved simultaneously. A computer program is written to solve such equations [11-18].

Artificial neural network

An artificial neural network (ANN) is a mathematical model that is inspired by the biological neural networks and it is mostly an adaptive network whose structure can be modified basing on the information that flows through the network during the learning period [19]. In the learning process, neural networks are subjected to a set of training data together with corresponding outputs. After a sufficient number of training, the neural network learns the patterns of input data and creates an internal model which is then used to make predictions for new inputs. The foundation of ANN is the neuron or processing element (PE) (Fig .1).

Each processing element, receives an input vector I, (I_{i1}, I_{i2}, I_{i3}…I_{in}].The processing element calculates an output O_i, by using a sigmoid function.

$$O_i=f\left(I_i\right)=\frac{1}{1+\exp(-I_i)}$$

The PEs are arranged in a special topology or architecture. Several possible architectures have been used, however the most common one is the multi – layer back – propagation architecture.

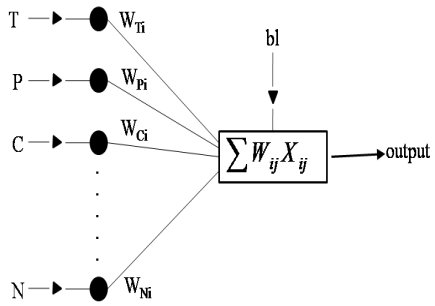

Figure 1: A typical neuron in the hidden layer

The back propagation algorithm is used in layered feed-forward ANN. This algorithm is applicable to a wide range of problems and is the predominant supervised training algorithm. The term back propagation indicates the method by which the network is trained, and the term supervised learning, implies that the network is trained through a set of available input – output patterns. In this algorithm the neurons are organized in some layers, and send their signals forward, and then the errors are propagated backwards.

Initially, all the weights are set randomly and input data are multiplied by weights and entered to the input layer of network, and the output of the network is given by a function which determines the activation of the neuron. Supervised learning is used in the back propagation algorithm to provide the algorithm with examples of the desired inputs and outputs, and then the error is calculated. The network is repeatedly exposed to these input – output relationships and the weights among the neurons are continuously adjusted until the network learns the correct input – output behavior.

The back propagation algorithm is desired to reduce the error that is propagated back through the network and is used to update the weights among neurons iteratively. This update process is repeated for all patterns many times until the network becomes capable of reproducing the input – output relationships to within an acceptable small tolerance. There may be some intermediate hidden layers (Fig 2) [16-19].

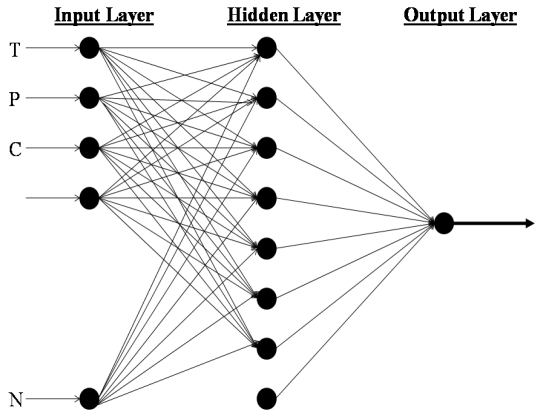

Figure 2: A one hidden layer feed and neural network

The output neuron from the hidden layers and the output layers are also given by the following equation. In this case the input I_i to a neuron in these layers is calculated by:

$$I_i = \left(\sum_j W_{ij} O_j \right) + W_{iB} O_B$$

Where the sum over j represents all neurons in the previous layer and O_B is an invariant output from the bias neuron. The weight W_{ij} represents the connection weight between neurons I and j and the weight W_{iB} is the connection weight between neuron i and the bias neuron.

Data Analysis

Effective parameters for the design of amine absorption tower are classified into several categories. The first ones are the parameters related to the absorbent solvent such as; the type, concentration, allowable loading amount and the solvent smell. The second category consists of parameters related to input sour gas such as; flow rate, temperature, pressure and the third category is about parameters related to how to use sweet gas which is, the percentage of allowable concentration of acid gas in output sweet gas and so on. In designing an amine absorption tower, with application of amines mixture, the optimized percent of amine mixture in water is also a significant parameter.

In this study all the above parameters for amine mixture absorption tower were extracted fromvarious gas refineries all over the world, which covers nearly 1200 data. These data contain designing conditions, operating conditions and test runs of sweetening units[20-22]. In network training, back propagation was used and the applied network was a 2-4-6-4 with figure 3in which sigmoid function has been chosen as neuron logistic function.

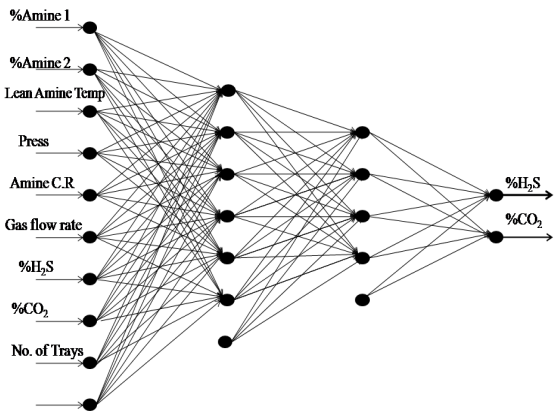

Figure 3: Structure of applied artificial neural network in this study

Network parameters such as number of layers, number of neurons in each layer, learning rate, error factor and etc, are utilized in various conditions and are simulated to reach the maximum rate of convergence and accuracy of calculation.

Result and discussion

Fajr jam refinery was chosen as a case study and three methods (equilibrium, mass transfer and artificial neural network) were used for simulation of absorption tower. Table 2presents the characteristics parameters together with operating conditions of amine absorption tower in the Fajr Jam refinery.

The test run data of Fajr Jam refinery (1999) for amine mixture in absorption tower are shown in table 3. These were used as reference data in current simulation [20].

Table 2: Characteristics parameters and operating conditions of amine absorption tower in the Fajr Jam refinery

Parameter	Value
Diameter (m)	3.7
Number of Trays	32
Tray	Valve
Tray Spacing (m)	0.61
Passes	1,2
Diameter of Valve (m)	0.048
Weir Height (m)	0.076
Down Comer Clearance (m)	0.038
Down Comer Width (m)	0.297
Feed Tray	1, 32

Table 3: Data of Fajr Jam refinery for amine mixture absorption

Sour gas flow rate (MMSCMD)	Amine C. R. (Cu m/hr)	Reboiler Steam (ton/hr)	MDEA (%wt)	DEA (%wt)	H_2S (mg/scm)	CO_2 (ppm)
5	252	25	22.42	11.6	1.84	-
10	252	25	22.42	11.6	1.8	354
14	252	25	24.8	12.3	1.8	1300
14	252	32	23.4	11.8	1.8	1450
14	270	32	26.62	12.18	1.6	763
14	300	34.5	26.61	13.4	1.84	426
14	300	38.4	25.7	14.3	1.6	403
14	300	38.4	25.1	17	0.92	136
14	300	38.4	26	18.24	1.8	25.5
14	300	38.4	26.2	18	0.87	47.4
14	300	38.4	26.3	18.2	0.9	40
14	300	38.4	24.82	17.65	1.5	49
14	300	38.4	25.99	17.75	1.8	14.5
14	300	38.4	26.52	18.27	1.57	-
14	300	38.4	24.77	17.77	0.9	24.6
14	300	38.4	24.41	20.1	1.2	22.58
14	300	38.4	25.2	20.32	1.1	26
14	300	38.4	23.32	19.51	1	15.32
14	280	35.32	25.37	19.84	1	14.7
14	252	34	22.47	19.41	1	23.1

Modeling and simulation results

Equilibrium method:

Simulation and modeling result of Fajr jam refinery and five other gas sweetening refineries (case 1 to 6) which was done by equilibrium method, are shown in table 4. The calculation basis of amine circulation rate in each case was concentration of CO_2 and H_2S in output stream.

As shown in the table, the simulation results have an average accuracy. However the main problem the method is its inability of computing temperature, pressure and concentration profile of the components along the tower [7]. In fact, this method can just calculate the acid gas percentage in output sweet gas using of known input data. Because of trial and error procedure used in this method, the calculation speed was low.

Mass transfer method:

By applying film theory and mass transfer method procedure, absorption tower of Fajr jam refinery and five other gas sweetening refineries (case 1 to 6) has been simulated. Results are shown in table 5. As shown in the table, the results have very good accuracy that is due to the fact that in the simulation, the hydraulic condition of the absorption tower is also taken into account. The speed of this method is lower than equilibrium method, because of complicated equations. The determining basic parameter of amine circulation rate in each case was the concentration of CO_2 and H_2S in output stream.

Table 4: Simulation results for various refineries by equilibrium method

Case	%H_2S	%CO_2	%MDEA	%DEA	%MEA	Amine C. R	
						Actual	Sim
1	2.5	1.2	35	15	-	290	278
1	2.1	1.1	35	15	-	240	230
1	2.6	1.6	34	16	-	310	301
2	0.8	4.1	24.4	17.65	-	65	83
3	16.1	1	32	18	-	43	51
4	4.5	2.3	45	5	-	155	140
5	0.81	3.1	40	10	-	120	115
5	0.77	2.5	38	12	-	143	150
6	3.2	1.8	35	-	15	21	30

Table 5: Simulation results for various refineries by mass transfer method

Case	%H_2S	%CO_2	%MDEA	%DEA	%MEA	Amine C. R	
						Actual	Sim
1	2.5	1.2	35	15	-	290	292
1	2.1	1.1	35	15	-	240	235
1	2.6	1.6	34	16	-	310	318
2	0.8	4.1	24.4	17.65	-	65	66
3	16.1	1	32	18	-	43	40
4	4.5	2.3	45	5	-	155	149
5	0.81	3.1	40	10	-	120	118
5	0.77	2.5	38	12	-	143	150
6	3.2	1.8	35	-	15	21	25

Temperature, pressure and H_2S concentration profiles along the absorption tower are shown in figures 4 - 6. As shown in fig 4, the tower temperature rises sharply and then decrease gradually till reach to a stable condition at the top of the tower. This is due to a large absorption heat of reaction that is released in lower trays and its gradual decrease long the tower.

Artificial neural network method:

By building a 2-4-6-9 network, followed by its training using more than 700 input data, the weights between neurons are clarified. This network has been surveyed by all existing parameters such as the number of neurons in each layer, the amount of hidden layers and the error factor in the network. Then it is optimized to the minimum error.
This network has also been used for simulation of absorption tower of Fajr jam refinery and five other refineries (case 1 to 6) and the obtained result have been demonstrated in table 6.

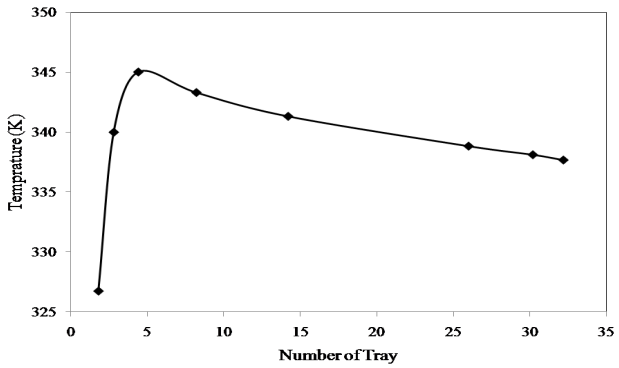

Figure 4:Temperature profile along the absorption tower

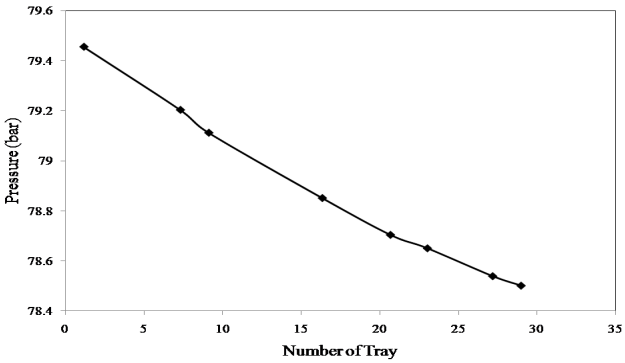

Figure 5:Pressure profile along the absorption tower

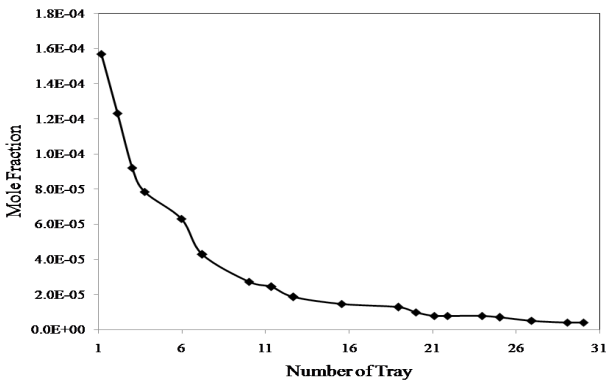

Figure 6: H2S Concentration profile along the absorption tower

As shown in table 6, data conformity with the actual data is much better than those in the equilibrium method and has as good accuracy as in mass transfer method. Also ANN can present all profiles of temperature, pressure and H_2S concentrations (figures 7, 8, 9).

Table 6: Simulation results for various refineries by artificial neural network method

Case	%H_2S	%CO_2	%MDEA	%DEA	%MEA	Amine C. R	
						Actual	Sim
1	2.5	1.2	35	15	-	290	288
1	2.1	1.1	35	15	-	240	242
1	2.6	1.6	34	16	-	310	315
2	0.8	4.1	24.4	17.65	-	65	75
3	16.1	1	32	18	-	43	45
4	4.5	2.3	45	5	-	155	152
5	0.81	3.1	40	10	-	120	123
5	0.77	2.5	38	12	-	143	150
6	3.2	1.8	35	-	15	21	19

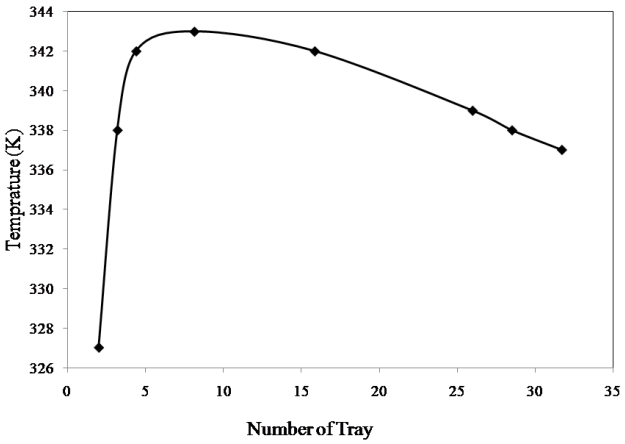

Figure 7: Temperature profile along the absorption tower

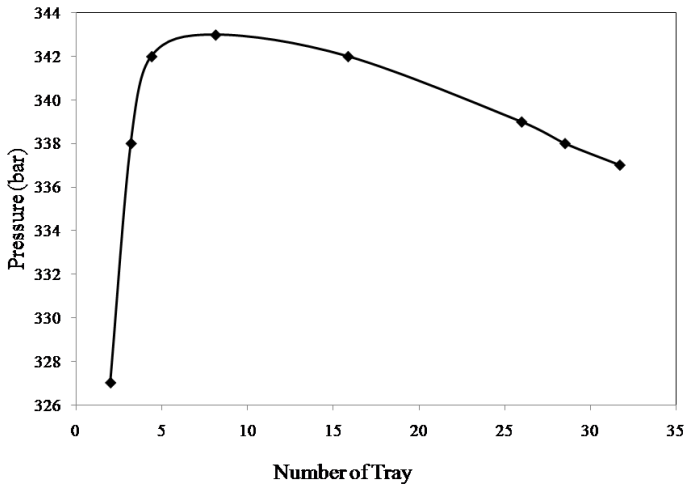

Figure 8: Pressure profile along the absorption tower

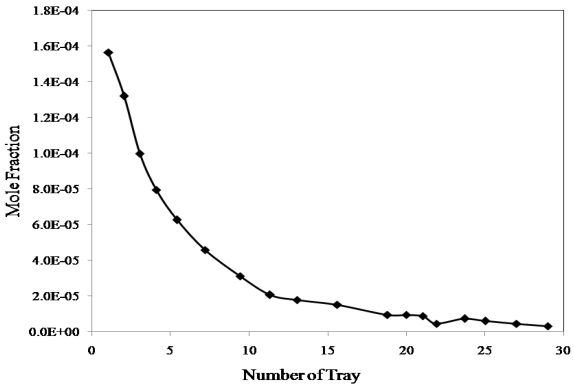

Figure 9: H_2S Concentration profile along the absorption tower

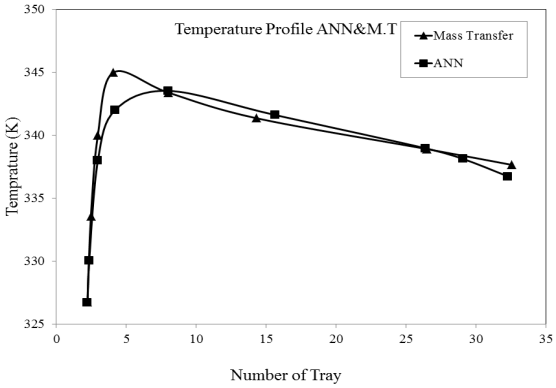

Figure 10a: Temperature profile along the absorption tower

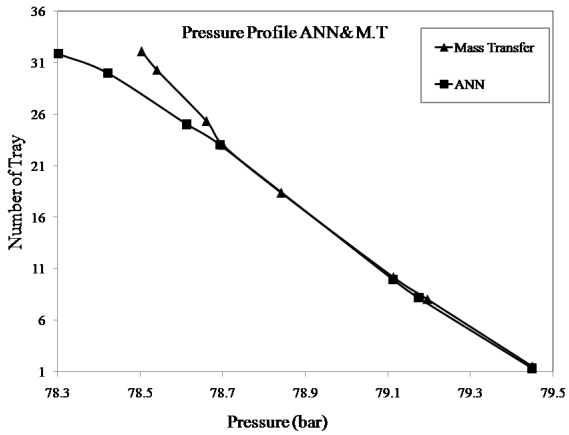

Figure 11: Pressure profile along the absorption tower

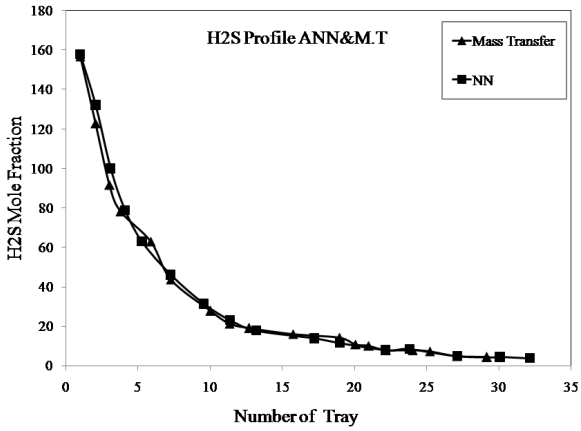

Figure 12: H2S Concentration profile along the absorption tower

Convergence rate of calculation in this method is approximately in the order of millisecond and by doing some simple modification, simulation results are obtainable for other absorption tower.

Figures10a-calso; show the comparison of mass transfer method with neural network methods for calculating absorption tower profiles. As shown in these figures, the results obtained by artificial neural network are as good as mass transfer method.

Conclusion

Considering this comparative survey, it has been clarified that neural network method is a good new method in simulating absorption towers of amine units. Its accuracy is better than that in equilibrium method while it is comparable to mass transfer method.

Neural network method is also able to compute temperature, pressure and concentration profiles of components. This specification is in contrast to the equilibrium method. On the other hand, the simplicity of calculation and convergence rate of neural networks method is much better when compared with those in equilibrium and mass transfer methods. Finally, sigmoid logistic function is capable for information processing of absorption tower.

Nomenclature

A_j Absorbed component j

A Stoichiometric coefficient

A_v Gas – liquid interfacial area per unit volume of liquid (m^2/m^3)

A_v' Gas – liquid interfacial area per m^3 froth on the plate (m^2/m^3)

a_v' Interfacial area per unit volume of packed column (m^2/m^3)

C_A Molar concentration of component A ($kmol/m^3$)

C_k Total molar concentration in the liquid on plate k ($kmol/m^3$)

c_p Specific heat (kJ/kmole K)

D Molecular diffusivity (m^2/h)

d_k Column diameter (m)

F Total molar gas flow (kmol/h)

F_A Enhancement factor

F_k Molar gas flow rate leaving plate k (kmol/h)

H_j Henry's coefficient for absorbed component j ($bm^3/kmol$)

Ha, Hatta Number

Ha" Modified Hatta number

$-\Delta H_j^{abs}$ Heat of absorption of component j (kJ/kmol)

$-\Delta H_j^{R}$ Heat of reaction of component j (kJ/kmol)

h_F Froth height on plate (m)

K_j Equilibrium constant of component j

k_j Reaction – rate coefficient of component j

k_G, A_j Gas – solid mass –transfer coefficient for absorbed component A_j (m/h)

L Volumetric liquid flow rate (m^3/h)

L' Molar liquid flow rate (kmol/h)

L_0' Molar flow rate of liquid feed to column (kmol/h)

L_k' Molar flow rate of liquid stream leaving plate k (kmol/h)

$m_{j,I}$ Reaction order with respect to component j in reaction i

M Molecular weight (kg/kmol)

m Reaction order

$N_j\big|_{y=0}$ Interfacial flux of component j per unit gas – liquid interfacial area ($kmol/m^2h$)

n_A Number of absorbing components

n_E Number of reactions in the liquid phase

n_G Total number of components in gas phase

n_L Total Number of components in liquid phase

n_M Number of gas – phase components involved in moderately fast reactions

n_P Number of reaction products in the liquid phase

n_R Number of reactants in liquid phase.

n_S Number of gas – phase components involved in very slow reactions

n_V Number of gas – phase components involved in very fast reactions

p Partial pressure (b)

p_t Total pressure (b)

P_j Product j

r Reaction rate ($kmol/m^3h$)

R_j Liquid – phase reactant j

$Q_{j,k}^{abs}$ Total heat of absorption of component j on plate k (kJ/h)

Q_k^C Total heat of cooling taken away from plate k (kJ/h)
$Q_{j,k}^R$ Total heat of reaction of reaction j on plate k (kJ/h)
T_k Temperature of intermediate gas feed to plate k (K)
T_{vk} Temperature of intermediate gas feed to plate k (K)
T_{wk} Temperature of intermediate liquid feed to plate k (K)
V_{vk} Flow rate of intermediate gas feed to plate k (kmol/h)
V_{wk} Flow rate of intermediate gas withdrawal from plate k (kmol/h)
x_j Mole fraction of component j in the liquid bulk
$x_{j,k}$ Mole fraction of component j in the bulk of the liquid stream leaving plate k
$x_{w_{j,k}}$ Mole fraction of component j in the intermediate liquid feed to plate k
y Coordinate perpendicular to the gas – liquid interface (m)
y_{F_j} Location of reaction front of reaction j (m)
y_G Gas – film thickness (m)
y_j Mole fraction of component j in the bulk of the gas phase
$y_{j,k}$ Mole fraction of component j in the bulk of the gas stream leaving plate k
y_L Liquid – film thickness (m)
$y_{v_{j,k}}$ Molar fraction of component j in the intermediate gas feed to plate k
z Axial coordinate in the froth on the plate (m)

Greek symbols

ε_L Liquid hold – up of packing or fraction of liquid in the froth
ρ_L Liquid density (Kg/m^3)
Ω_A Active area of plate (m^2)
α Loading of acid gas

References:

1- Mandal, B. P. and Bandyopadhyay, S. S. (2005). “Simultaneous absorption of carbon dioxide and hydrogen sul?de into aqueous blends of 2-amino-2-methyl-1-propanol and diethanolamine.” *Chemical Engineering Science*., Vol. 60, No. 22, PP. 6438 – 6451.

2- Lu, J. G., Zheng, Y. F. and He, D. L. (2006). “Selective absorption of H2S from gas mixtures into aqueous solutions of blended amines of methyldiethanolamine and 2-tertiarybutylamino-2-ethoxyethanol in a packed column.” *Separation and Puri?cation Technology*., Vol. 52, No. 2, PP. 209–217.

3- Kohl. A. L. and Nielsen. R. B. (1997). Gas purification. 5th. Ed. Gulf publishing company , Houston , TX.

4- Danckwerts, P. V. (1995). “Gas absorption accompanied by chemical reaction.” *AIChE Journal*, Vol. 1, No. 4, PP. 456–463.

5- Vickery, D. J., Adams, J. T. and Wright, R. D. (1992). “Benefits from the rigorous mass transfer rate approach to modeling acid gas absorption using mixed amines.” *Conf. Distillation and Absorption '92*, Birmingham, England, PP. B241-B252.

6- Mohamadirad, R., Hamlehdar, O., Boor, H., Fattahi-Monavar, A. and Rostami, Sh. (2011). “Mixed amines application in gas sweetening plants.” *Chemical Engineering Transactions*, Vol. 24, PP. 265-270.

7- Kent, R. L. and Eisenberg, B. (1976)."Better data for amine treating." *Hydrocarbon Processing*. Vol. 55, No. 2, PP. 87-90.

8- Moshfeghian, M. and Maddox, R. N. (1991). "Optimization of chemical reaction parameter for sour gases and alkanol amine system." *AL. Azhar Engineering 2nd Int. Conf*. Egypt.

9- Maddox, R. N. (1982). Gas sweetening. 3rd. ED. McGraw Hill.

10- Leye, L. D and Froment, G. F. (1986). "Rigorous simulation and design of columns for gas absorption & chemical reaction 2." *Computer and Chemical Engineering*, Vol. 10, No. 5, PP. 505-515.

11- Baghli, N. A., Pruess, S. A., Yesavage, V. F. and Selim, M. S. (2000). "A rate based model for the design of gas absorbers for the removal of CO_2 and H_2S using aqueous solution of MEA & DEA."*14thsym of Thermophysical Properties*, USA.

12- Ouwerkerk, C. (1978). "Design for selective H_2S absorption." *Hydrocarbon Processing*, Vol. 57, No. 4, PP. 89-94.

13- Cornelissen, R. and Beenackers, A. C. (1986). "Numerical accompanied by complex reversible reactions." *Chemical Engineering Science*, Vol. 35, PP. 740-741.

14- Finlayson, B. A. (1981). Nonlinear analysis in chemical engineering. McGraw Hill.

15- Demidorich, B. P. and Maron, I. A. (1981). Computational mathematics. Mir publishers.

16- Picton, P. (2000). "Neural networks," 2th. ED. McGraw Hill.

17- Bulsari, A. B. (1995). "Neural networks for chemical engineering." Elsevier, Amsterdam.

18- Stein, R. (1993). "Pre-Processing data for neural networks." AI expert, 33 – 37.

19- Roman, M. B. and Ekaterina I. L. (2009). "Neural network approach to quantum-chemistry data: Accurate prediction of density functional theory energies." *J. Chem. Phys.* Vol. 131, No. 7, 074104.

20- Saremi, H. S. and Abdi, N. (2001). "Blending amines debottlenecks Iranian gas plant." *OGJ*, Vol. 98, No. 46, PP. 60-61.

21- Spears, M. L., Kathy, M. H., Jerry, A. B. and Carl, J. M. (1996). "Converting to DEA/MDEA mix UPS sweetening capacity." *OGJ*, Vol. 63, No. 2, PP. 63-67.

22- Mc. H.Y. (1994). "New MDEA design in gas plant improves sweetening reduces CO_2 ." *OGJ*, Vol. 83, No. 29, PP. 83-86.