

# A Novel Dynamic Model and Simulation of Gas Sweetening in Tray Beds

Sara. Pourkarimi, Ahmad. Hallajisani, Nasrollah. Majidian, and Sahar. Pourkarimi

**Abstract**—Contrary to the distillation towers, much research has not been fulfilled on dynamic treatment of absorption towers. Studying on dynamic treatment of absorption towers goes back to half a century ago. In order to fulfill such a thing, we have studied dynamic and static modeling of sweetening sour gas in a tray tower by using computational software (MATLAB). In the present study, we have written a model for static condition. we have obtained the amount of CO<sub>2</sub> mole fraction changes on each tray and pressure changes across the tower. we have determined temperature changes across the tower by writing energy balance on each tray. The result is conformed to industrial results and the used solvent is 45% MDEA. Although, in comparison with filled towers, modeling of tray towers has been less considered because of hydraulic problems and diversity in types of trays. Their modeling is so important, because of their widespread usage in industrial conditions. In order to create a dynamic simulation, we have suddenly changed the volumetric flow rate of inflow liquid solvent and the way of mole fraction changes on each tray. we have defined the exact time of getting a stable mode by fixing the number of trays.

**Index Terms**—Dynamic Model, modeling, sweetening, tray towers.

## I. INTRODUCTION

Gases which are produced by petroleum resources, gas and petrochemical industries, include different amounts of acid compositions such as hydrogen sulphide. That's why they are called sour gas idiomatically. The presence of small amounts of CO<sub>2</sub> and H<sub>2</sub>S in gas causes a lot of difficulties.

Acidic gases are very poisonous compositions and cause severe harm to the equipment and biological environment.

The interest in CO<sub>2</sub> retrieval has been increased in recent years for two major reasons: first, the possibility of using this gas as a product in different industries, in particular, for petroleum resources, second, needing to reduce greenhouse gases in the atmosphere because of climate changes and earth-heating. Generally, in order to separate CO<sub>2</sub> and H<sub>2</sub>S from natural gas, tray towers and solutions such as amines are used in gas industries and powerhouses. So, CO<sub>2</sub> and H<sub>2</sub>S should be omitted from gas flow. Different methods are used for separation of CO<sub>2</sub>. One of the most important of these methods is chemical absorption. The most common solvents which are used in this method are called Alkanolamines.

In general, there are two ways for absorption towers modeling and reclamation towers simulation.

- Equilibrium way.
- Non- equilibrium way (The way based on mass transfer).

In the equilibrium way, mass and energy balance equations are written for one stage entirely (each tray is considered as an equilibrium stage, that its outflows are together in equilibrium).

In 2007, Van loo and his colleagues used a non-equilibrium way for modeling CO<sub>2</sub> absorption, by using MDEA solvent. They modeled chemical absorption process in a tray tower [1]. In 1989 Potter and his colleagues studied dynamic treatment of packed absorbers and tray towers. In this model, absorption absorption is merely physical and the process is assumed to be Adiabatic and Isothermal [2].

## II. MODEL DEFINITION

In this model, mass transfer equations are obtained on the basis of film theory. In this theory it is assumed that resistance against mass transfer is just in two phases and there is no resistance in phase interface. Here we describe the two stable and unstable sections.

In a stable mode, no changes happen to gas and liquid conditions, and the model computes the number of trays and the quality of changes in transferable mole fraction, pressure changes and temperature changes across the tower.

In an unstable mode, mole fraction changes on each tray are studied by inflow liquid changes.

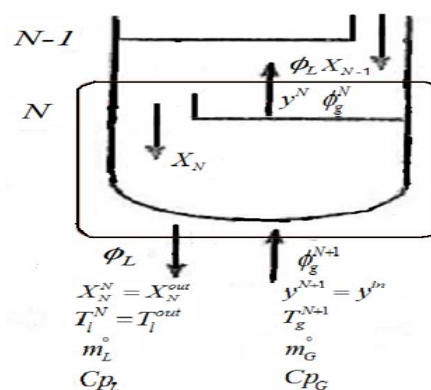


Fig. 1. Bottom of the tower scheme

### A. Stable mode studies

- Total mass balance equation:

Considered assumptions include:

- Mass transfer is assumed to be steady-state.
- Mass transfer should be done from gas phase to liquid

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Phase.

- 3) Each tray property is assumed to be equal with outflow conditions from each tray. It means it is assumed that gas or liquid gets to outflow conditions, as soon as their entrance. This is similar to ideal mixture storages.

$$y_n = y_{n+1} - \frac{\phi_L}{\phi_g} (x_n - x_{n-1}) \quad (1)$$

In above equation,  $Y, X, \phi_L, \phi_g$  are mole fraction of  $CO_2$  in bulk of gas and liquid phase, molar flow rates of liquid and gas in terms of ( $kgmol/hr$ ).

- *mass balance in the gas phase:*

In order to compute mole fraction in gas phase, consider the following assumptions:

- 1) Gas formation in the liquid on each tray is assumed global and separates from the other bubbles, so that each bubble movement doesn't have any effects on the shape of other bubbles and mass transfer in it.
- 2) The speed of gas movement into the liquid is stable.

Equation (2) is used to compute the molar flux, in which  $K_C$  is obtained from the mass transfer relationship, and total concentration  $C$  is obtained from the following equation.

$$N_A = K_C C (y_{n+1} - K x_{n-1}) \quad (2)$$

$$C = C_1 \frac{T_1}{T_2} \quad (3)$$

For computing the amount of  $K$  (slope of equilibrium curve), we used the method which is presented by Fischer in 2003 [3]. We also used the equation which is presented by Sharman and Donckwerts in 1970 for computing the Shroud number [4].

All physical properties are calculated in film condition, and these relationships are obtained after  $N_A$  is placed.

$$y_n = y_{n+1} - \frac{K_C C M A''}{m_G^\circ} (y_{n+1} - K x_{n-1}) \quad (4)$$

In the above equation,  $y_{n+1}, x_{n-1}, K_C, C, m_G^\circ, M, A$  are mole fractions of gas and liquid, mass transfer coefficient ( $Kmol/m^2.s (Kmol/m^3)$ ), total concentration ( $Kmol/m^2.s$ ), total molar flow rate of gas ( $kg/s$ ), gas molecular weight and mass transfer surface ( $m^2$ ), respectively.

Two of the equations (1&4), which have terms of two equations in two unknowns, the two unknown quantities  $y_n$  and  $x_{n-1}$  are computed and the number of trays turns out to be.

- *Equilibrium of the total tower energy and computation of  $T_l^N$  and  $T_g^N$ :*

The temperature across the tower is changed because of heat interchange between the two phases and also existence of heat effects caused by absorption and reaction in liquid phase. So, in order to obtain the quality of temperature changes, we can get the equation (5) by writing equilibrium of energy on a tray like shown in fig (2).

Considered assumptions include:

- 1) The tower is adiabatic and heat transfer is just done

between gas and liquid phases.

- 2) Liquid mass flow changes insignificant.
- 3) There is thermal equilibrium between outflow phases of trays, in other words, it is assumed that outflow gas and liquid phases on each tray have reached thermal equilibrium, and the temperature in outflow gas phase on each tray is equal to that of the outflow liquid phase on the same tray [1].

$$T_g^{(j+1)} = T_l^{(j+1)} \quad (j = 1 \text{ to } N) \quad (5)$$

$$T_l^{out} = T_l^{in} + \frac{(T_g^{in} \phi_g^{in} - T_g^{out} \phi_g^{out}) \rho_l c_{p_g}}{\phi_l \rho_l c_{p_l}} + \frac{\Delta H_{CO_2} \left( N_{total}^{(N)} \cdot \left( \frac{A}{L} \times 1000 \right) \right)}{\rho_l c_{p_l}} \quad (6)$$

$$\text{If } J = N \rightarrow T_l^{(N)} = T_l^{out}, \text{ So } T_g^N = T_l^N.$$

In order to calculate enthalpy in MDEA solution, the following equation presented by Kohl in 1997 was used [5].

We computed heat capacity and density of liquid phase for the solution "MDEA" by using relationships presented by Cheng and Meissen in 1996 [6].

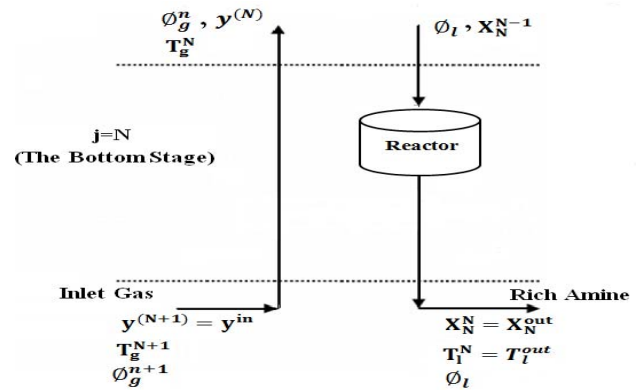


Fig. 2.  $N^{th}$  Tray (bottom of tower)

In the following equation,  $N_{tray}^{(N)}, \phi_g^{out}, G_{inert}$  and  $y_{in}$  are the total amount of absorbed  $CO_2$  from the first tray to the  $N^{th}$  tray ( $grmol/cm^2.s$ ), outflow gas from the tower, molar flux of inert gas entering into the tower and mole fraction of  $CO_2$  in input of the tower, respectively.

$$N_{tray}^{(N)} = G_{inert} \left( \frac{y^{in}}{1 - y^{in}} - \frac{y^{out}}{1 - y^{out}} \right) \quad (7)$$

$$\phi_g^{out} = \frac{\phi_g^{in} (1 - y^{in})}{1 - y_{CO_2}^{out}} \quad (8)$$

### B. Survey of Unstable Mode (Dynamic Model)

In this section, by fixing the number of trays, mole fraction changes on each tray, until they get new stable mode

conditions pursuant to sudden Changes in the volume flow rate of liquid and gas should be in a way that no critical mode of flooding and entrainment is established in tray column, so by using the chart presented by Smith and Delnick in 1975, changes of volume flow rate of liquid and gas Was obtained in a proper confines [7]. The amount of inflow liquid changes from  $L_0$  to  $L'_0$  abruptly but  $y_{N,\infty}$  (final mole fraction) is assumed stable in outflow gas. So, by using overall mass equilibrium, outflow mole fraction, which comes along the liquid, will be obtained.

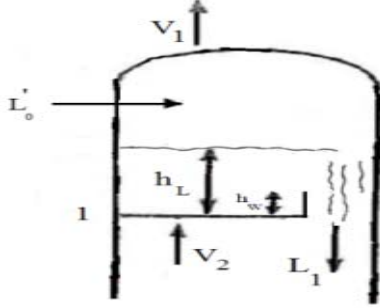


Fig. 3. volume flow rate changes on tray number one.

When the dike height ( $h_w$ ) is stable, the volume of liquid on each tray changes, and it equilibrates after some determined time. Its amount is determinable based on Manning equation [8].

It is assumed that in this model liquid volume changes on the tray is like exponential. ( $\tau$ ) is the response time which the following relationship is proposed for:

$$\tau = \frac{V_{1(\infty)} - V_{1(0)}}{L'_{(0)}} \quad (9)$$

Input of volume flow rate starts to change by phase changing volume starts to change by phase changing ( $\tau$ ) and contrary to the first tray, its changes are not in step form and are the function of time.

By writing volume equilibrium on each tray ( $j$ ), liquid volume changes on each tray and volume flow rate of outflow liquid on each tray is computed using the following relationships:

$$V_{N,L(t)} = V_{0,N} + (V_{0,\infty} - V_{0,N}) \left[ 1 - \exp\left(\frac{-(t - (N-1)\tau)}{\tau}\right) \right] \quad (10)$$

$$L'_{N,t} = L'_{N-1,t} - \frac{dV_N}{dt} \quad (11)$$

$$\text{If } t > (N-1)\tau \rightarrow L_0 = L'_{N,t}$$

In order to compute mole fractions on each tray, two relationships (12&13) are used.

$$\begin{aligned} \frac{\rho_L}{M_L} \cdot V_{N(t)} \cdot \left( \frac{X_{N(t)}^{p+1} - X_{N(t)}^p}{\Delta t} \right) + X_{N(t)}^p \left[ \left( \frac{\rho_L}{M_L} \cdot \frac{dV_{N(t)}}{dt} \right) + \frac{L'_{N(t)}}{M_L} \right] &= \left( \frac{L'_{N-1}}{M_L} \times X_{N(t)}^p \right) + (N_{A_N} \cdot A) \end{aligned} \quad (12)$$

$$\begin{aligned} \frac{\varepsilon \times \rho_G}{M_G} \cdot V_{N(t)} \cdot \left( \frac{Y_{N(t)}^{p+1} - Y_{N(t)}^p}{\Delta t} \right) + Y_{N(t)}^p \left[ \left( \frac{\varepsilon \times \rho_G}{M_G} \cdot \frac{dV_{N(t)}}{dt} \right) + \frac{\phi_g}{M_G} \right] &= \left( \frac{\phi_g}{M_G} \times Y_{N(t)}^p \right) - (N_{A_N} \cdot A) \end{aligned} \quad (13)$$

In above equation,  $A$ ,  $C_p$ ,  $L$ ,  $M$ ,  $V$ ,  $\rho$  and  $\Delta H$ , are Cross sectional area of column ( $\text{cm}^2$ ), Volume flow rate of liquid phase ( $\text{m}^3/\text{s}$ ), molecular weight ( $\text{kg}/\text{kgmol}$ ), Volume of Liquid equilibrium ( $\text{cm}^3$ ), Density ( $\text{kg}/\text{m}^3$ ) and Heat absorption ( $\text{J}/\text{mol}$ ), respectively.

After simplifying,  $Y_N^{p+1}$  and  $X_N^{p+1}$  can be computed.  $\Delta t$  quantity is twice as much as ( $\tau$ ). Mole fraction on the tray  $N$  is compared with  $Y_{N,\infty}$ . If  $|y_N - y_{N,\infty}| < \varepsilon$ , (whenever the changes increase or decrease to the rate of  $0/01$ ), computations are finished.

### III. SIMULATION RESULT

In absorption tower, inflow sour gas comes into contact with Methyl diethanolamine solvent. The amount of inflow sour gas is 25988 ( $\text{Kgmol/hr}$ ) with the temperature  $25^\circ\text{C}$  and the pressure 6641 (kpa) and the amount of inflow amino equals 5311 ( $\text{Kgmol/hr}$ ) that enters into the tower with the temperature of  $41^\circ\text{C}$ . The input gas includes 0.36 percent moles of  $\text{H}_2\text{S}$  and 2.3 percent moles of  $\text{CO}_2$ .

Modeling of sour gas sweetening process is done in static and dynamic parts by using computational software [MATLAB] [9].

Fig. 4. Shows the concentration change curve of  $\text{CO}_2$  in gas phase and indicates that the maximum absorption by amino occurs in some trays below; this action is fulfilled from bottom to top the tower. So, in order to make sweet gas achieve the purity level (less than one percent moles of  $\text{CO}_2$ ), 28 trays should be used. It is done for this reason that the acid gas concentration in the outflow sweet gas from the tower, be in standard quantity.

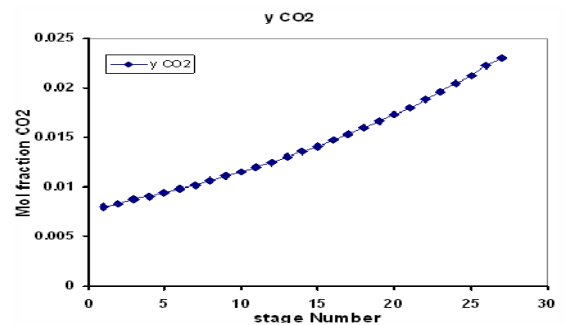


Fig. 4. mole fraction of  $\text{CO}_2$  in vapor phase across the tower.

Fig. 5. Shows the  $\text{CO}_2$  mole fraction in liquid phase. It represents that  $\text{CO}_2$  physical (molecular) dissolution occurs in the solvents. Driving Force of mass transfer is a lot because of high  $\text{CO}_2$  concentration in gas phase in bottom trays, so more  $\text{CO}_2$  is dissolved in liquid phase.

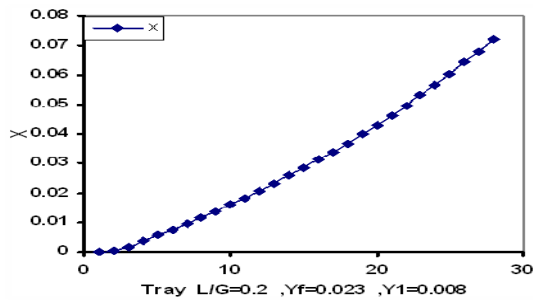


Fig. 5. mole fraction of  $\text{CO}_2$  in liquid phase across the tower

The simulated result is compared with the industrial data of Masjed Soleiman Gas Refinery and the results are shown in Fig 6 - 7. The results show that the changes are the same.

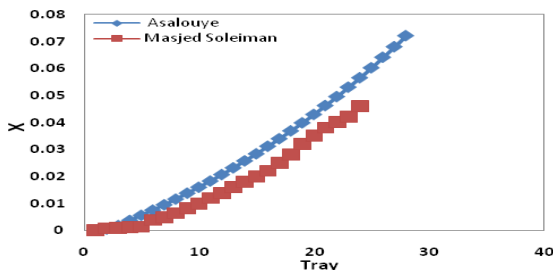


Fig. 6. Compare Mole fraction changes during  $\text{CO}_2$  absorption tower in liquid phase Between Assaluyeh refinery & refinery gas Masjed Soleiman.

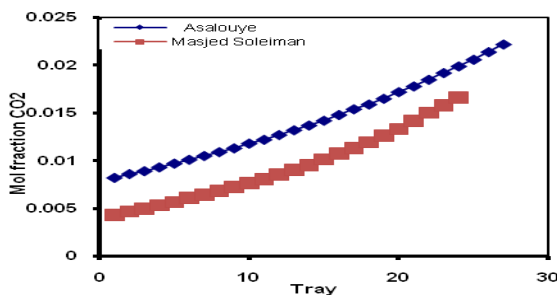


Fig. 7. Compare Mole fraction changes during  $\text{CO}_2$  absorption tower in vapor phase Between Assaluyeh refinery & refinery gas Masjed Soleiman

Considering gas inflow pressure 6641 kpa, as you see in Fig .8. the pressure is changed linearly across the tower. The amount of pressure loss is equal to all the trays and so the linear pressure loss occurs across the tower.

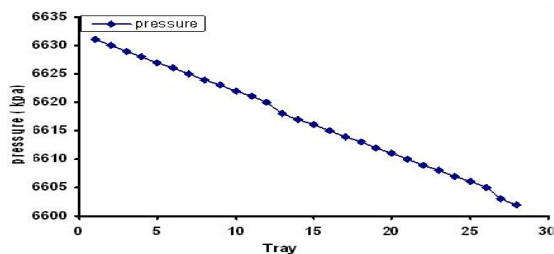


Fig. 8. Pressure changes across the tower

Temperature changes across the tower are surveyed in static condition. And also the results taken from simulation are represented in fig .9. temperature chart. To get these results, HYSYS and ASPEN [10], [11] soft ware's that respectively used Kent – Eisenberg and Electrolyte – NRTL models are used to compute equilibrium. So increasing heat is reasonable across the tower, and the result taken from this model, besides conformity with the other simulated models in

fig. 9, shows the same prediction.

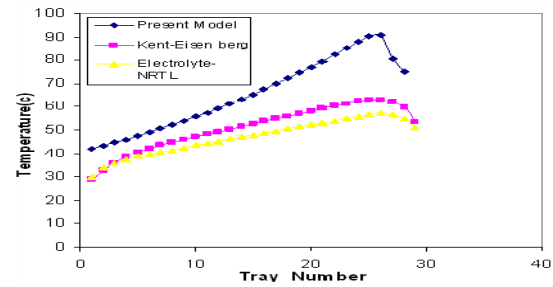


Fig. 9. temperature changes during the tower and Comparison with model results Kent-Eisen berg and Electrolyte-NRTL

The simulated result is compared with the industrial data of Masjed Soleiman Gas Refinery and the result is shown in Fig. 10.

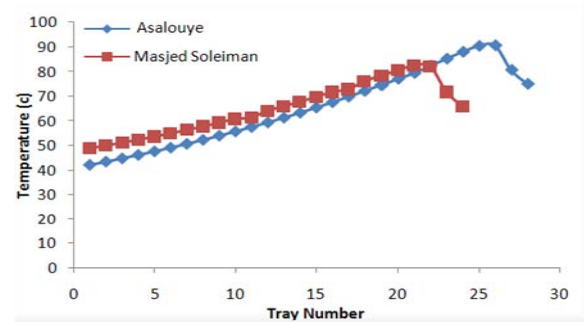


Fig. 10. Compare the temperature profile during the absorption tower Between Assaluyeh refinery & refinery gas Masjed Soleiman.

The number of tray changes in terms of the two phases volume ratio is depicted in fig .11. The amount of changes in the two phases volume ratio is chosen in the way that no disturbance phenomenon such as Flooding and Entrainment is presented. So, by using Smith and Delnick chart presented in 1975, volume ratio changes of liquid and gas flow in a proper confines is obtained [7].

By increasing in the volume ratio between the two phases, the number of necessary trays is increasing in the end to get one determined mole fraction. The reason is that, by increasing volume flow rate of liquid phase, the tower diameter stays stable, so linear speed of liquid movement increases, and as a result the time of contact between the two phases decreases.

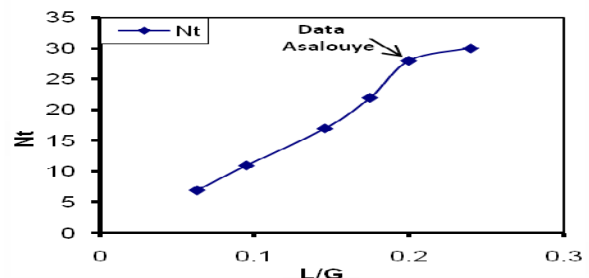


Fig. 11. The number of trays changes in terms of volume ratio of the two phases gas and liquid

In dynamic section, we can survey the quality of mole fraction changes on each tray and the time to achieve a stable mode by sudden change in the volume of inflow liquid solvent and fixing the number of trays.



Sudden change in the amount of inflow liquid volume to the tower causes that the inflow liquid volume of each tray is formed as a time function, so transfer coefficient changes by time changing. Change in liquid volume from its internal site starts suddenly and is seen across the tower gradually.

The mole fraction changes of CO<sub>2</sub>, on various trays in gas phase according to the two quantum are depicted in fig 12 - 13.

Quantum is the ratio of liquid height on each tray in the stable state, before and after the sudden change in its volume. Primary trays achieve the stable state early, whereas, final trays in which volume changes happen, achieve the stable state later by. Primary trays achieve the stable state early, whereas, final trays in which volume changes happen, achieve the stable state later by and Potter's studies confirm that [2].

In Potter's researches, dynamic condition of trays towers was studied

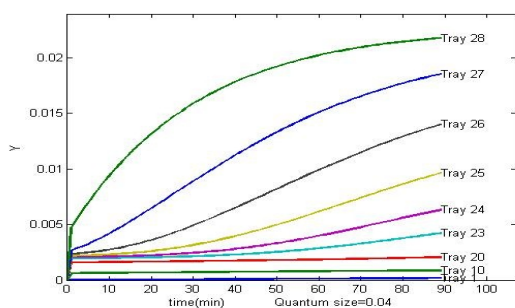


Fig. 12. Dynamic response of a tray absorber (Gas phase) for a quantum size of 0.04. The tray numbers are shown.

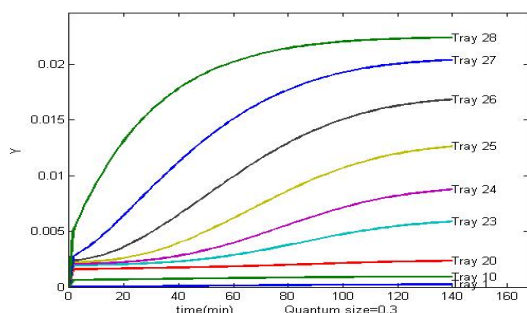


Fig. 13. Dynamic response of a tray absorber (Gas phase) for a quantum size of 0.3. The tray numbers are shown.

#### IV. CONCLUSION

From the simulations the following are concluded:

1. The absorption process is heat-producing. So increasing heat is reasonable across the tower, and the result taken from this model, conformity with the other simulated models shows the same prediction.
2. By increasing in the volume ratio between the two phases, the number of necessary trays is increasing in the end to get one determined mole fraction. The reason is that, by increasing volume flow rate of liquid phase, the tower diameter stays stable, so linear speed of liquid movement increases, and as a result the time of contact between the two phases decreases
3. Driving Force of mass transfer is a lot because of high CO<sub>2</sub> concentration in gas phase in bottom trays, so more

CO<sub>2</sub> is dissolved in liquid phase.

4. By increasing volume and the amount of quantum, the time to achieve the stable state increases too.

#### REFERENCES

- [1] S. Van Loo, E.P. Van Elk, G.F. Versteeg, "The Removal of Solutions of methyl -diethanol-amine," *Journal of petroleum science and Engineering*, 55 (2007) 135-145.
- [2] C.C. Lakshmanan and O.E. Potter, "Dynamic Simulation of packed and Tray- Type Absorbers," *Ind. Eng. Chem. Res.*, 28, 1397-1405, 1989.
- [3] K. Fischer, R. Sidi-Boumedine, S. Horstmann, "Experimental determination of carbon dioxide solubility data in aqueous alkanolamine solutions," *Fluid Phase Equilibria*, 218 (2004) 85-94.
- [4] P.V. Danckwerts, F.R.s., *Gas -Li quid Reaction*, McGraw-Hill, 1970.
- [5] A. Kohl, R.B. Nielson, *Gas publisher* 5<sup>th</sup> Ed., 1997.
- [6] S. Cheng, A. Meisen, *predictAmine Solution properties Accurately. Hydrocarbon processing*, 81-83, 1996.
- [7] V.C. Smith, and W.V. Delnicki: *Chem. Eng. Prog.*, 71, 1975.
- [8] F.M. Handerson, "Open Channel Flow" *Mecmillan, New York*, 1966.
- [9] MATLAB Software version, R2009a.
- [10] HYSYS Software version, 7.1. 2007.
- [11] ASPEN Software version, 7.1. 2007.



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