Steady-State and Dynamic Simulations of Gas Absorption Column Using MATLAB and SIMULINK

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Abstract. Separation is one of the most important process in all the chemical industries and the gas absorption is the simplest example of separation process which is generally used for the absorption of dilute components from a gaseous mixture. In the present work, a dynamic system of mathematical equation (algebraic and differential) is modeled to predict the behavior of the absorption column using matrix algebra. The dynamic model was programmed using MATLAB/SIMULINK and S function was used for building user define blocks to find out the liquid and the gas composition using the standard MATLAB ode45 solver. As a case study, fermentation process is taken as an example to separate CO_2 from a mixture of alcohol and CO_2 in a tray gas absorber using water as absorbent. The steady state solution was first solved to give the initial condition for the dynamic analysis. Dynamic outcomes for stage compositions was figure out for step changes in the vapor and liquid feed compositions. The model results show good agreement with the practical situation and also compared favorably with results obtained by Bequette. With this work, we are able to provide a readily available simulation that can be used as a test bed for advanced process monitoring.

1. Introduction

Separation Process is a vital part of any process industries while absorption is the most mature technology available for chemical and allied industries [5, 6, 9, 14, 17, 18 and 20]. Although theoretical understanding of absorption has reached up-to nearly saturation level but the comprehension of dynamic part is still lacking,

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which contribute much to the economy of the process [4]. Absorption being versatile operation amongst the various processes of chemical engineering disciplines interest in the field grows rapidly. A wide range of the gases being absorbed in different alternative solvents opening the scope for substitution to the fossil fuels, like bioethanol as a substitute of petroleum in some countries [7].

Steady state conception of chemical equipment is confronted by dynamic issues [4]. Thus, design of chemical processes under steady state conditions is generally unrealistic. For the acceptance of a plant design and process synthesis, and to ensure safety and stability of plant operations (start up and shutdown), it is imperative to know the dynamic behavior of the relevant unit of plant. Dynamic simulation is considered a slow process. However, it provides new approaches in terms of memory and computational speed.

Kvamsdal et al. (2009) [10] built up a dynamic rate-based model of an absorber column for CO_2 seizure utilizing gPROMS. The mass and heat transfer were depicted by the two-film theory. Constant values of heat of absorption and heat of vaporization were assumed in that review. The model was validated at steady state utilizing information acquired from a pilot plant (Dugas, 2006). Both inlet gas flow rate and column height were adjusted to match the percentage of CO_2 removal and liquid temperature profile with the corresponding pilot plant data. The dynamic simulation results were presented for partial load reduction (reduced the base load from 100% to 50%) and start up. It was found that L/G ratio significantly affects the performance of the absorption process during partial load reduction.

Liu et al. [12] built up a model for absorption and desorption by employing Aspen HYSYS. The controllability issues of absorption model implemented in MATLAB were discussed by Bedelbayev [15], while Greer [16] used MATLAB to develop a full scale model of column.

Robinson and Luyben (2011) used ASPEN simulator for dynamic simulation of H2S and CO2 absorption/stripping process and watergas shift reactors for plantwide control structure design and dynamic simulation in hybrid/chemical plant, which are vital for the advancement of stable and vigorous plantwide control structures of their hybrid plant [13].

From the above perspective, it is important to integrate the dynamic simulation of a gas absorption process to steady state. Dynamic simulation of gas absorption process has captivated many researchers. Like in other classical unit operations, absorption is technically, theoretically and economically well developed. [19] But because of the older technology, out dated apparatus and limited parameters, the attractiveness of absorption in young researchers is decreasing, that raised the need of dynamic simulation. This process is typically brought out through tray columns that contain numerous quantity of trays, which bring gas and liquid into insinuate contact. The hypothetical stage is given, if the gas leaving the tray is in thermodynamic equilibrium with the liquid leaving the tray. The hypothetical stages are determined trialed by real stages by using tray efficiency [1]. The gas absorption process is demonstrated through an arrangement of mathematical equations to forecast the process behavior [11]. These equations do not have a general analytical solution and a few estimations and numerical strategies can be utilized for solving them [4]. The purpose of any dynamic system is to know the process response with respect to time so that the effect of external disturbances is suppressed, the stability of the process is ensured and to optimize process performance.

In the packed tower, because of the poor distribution of liquid there always some uncertainty remains, because of which it is hard to determine the efficiency of packed tower. In this study a plate tower was used in which the liquid and gas were contacted in stage-wise manner on the trays; whereas in packed column there

is a continuous contact between gas and liquid. The primary aim of this work is the use of MATLAB and SIMULINK programing to the absorption columns of bioethanol production process by sugar cane fermentation. The purpose is to keep the alcohol concentration low in the outflowing gas from the top of absorption column.

This work has been categorized into two parts namely steady state and dynamic solution. The steady state solution has been achieved using MATLAB to calculate the composition of outlet gas and liquid stream. The steady state results provides the initial conditions to the dynamic analysis. A complete dynamic model comprising a system of linear differential and mathematical equations was solved and coordinated with standard MATLAB ode45 solver.

The objective of this study is to formulate a steady state and dynamic model of a gas absorption column to lower the concentration of alcohol in the exit vapor stream to a level of minimum and to analyze the dynamic response of the absorber.

2. Process description

A fermentation process is taken as a contextual analysis [7] to apply the developed steady state and dynamic model. Some alcohol formed during sugar cane fermentation is lost by vaporization. In the recuperation process, this vapor containing the most part alcohol and carbon dioxide is gathered at the highest point of fermentation tanks and delivered to absorption column [3]. Referring to Fig. 1, the blend of CO_2 and alcohol gathered from the sugarcane fermentation tanks is fed at the base and the absorbent liquid (water) at the top of the alcohol recuperation column, where the two phases counter each other.
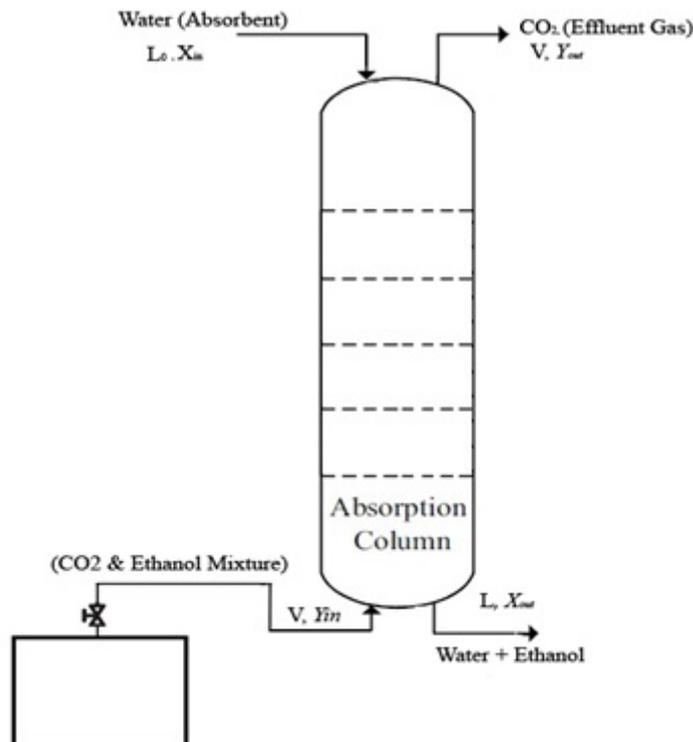
Figure 1. Bioethanol process flow diagram.

A distillation column supplies the retentive liquid, comprising of water containing no or few alcohol. This absorption column is made out of ten stages and operates at 40 °C and 1 atm. The column must process 1.2 mol/s of gas blend in order to decrease the alcohol concentration.

The inlet concentration depends on the conditions of fermentation broth and furthermore on particular features of the fermentation tanks. Subsequently, this is considered as an unsettling influence to absorption process and for a high alcohol recuperation the absorbent flow rate must be manipulated. The outflowing gas from the top of the column, mostly made out of carbon dioxide and a little measure of alcohol [7]. The disturbances (y_{in}, x_{in}) and manipulated variable (L_0) are the inputs while, output variable (y_{out}) and uncontrolled variables (L and x_{out}) are outputs.

3.   Absorption tower model development

Nowadays, dynamic simulation has become essential tool in the process industries for a number of reasons: operability studies, risk assessment and safety analysis, depth thinking of start-up and shut-down procedures and methodical optimization of process using optimal control techniques. Hence, it is the foundation for preliminary application of process control system and for the design of standard [8].

3.1   *Dynamic Modeling of Absorption Column*

A global mass balance is applied at each stage for the computational simulation of the alcohol recuperation retention column to obtain a mathematical model, equilibrium equation, and Francis equation for hydrodynamic computing. Consider the gas absorption column shown in figure 2. The liquid gas mixture in the vapor feed stream are captivated by the water entering from top of the column, so that the vapor product coming out from the top of the column are more pure. The trays are often modeled as equilibrium stages. At the operating conditions, the dissolution of alcohol in water is estimated by the equation,

$$y_i = kx_i \tag{1}$$

in light of Van Laar equation for vapor pressure information of isothermal framework [3]. Where x is the liquid phase molar fraction of alcohol and y is the gas phase molar fraction of alcohol.

The following are the assumptions taken into account for mathematical models:

(1) Liquid is incompressible and perfectly mixed on each tray.
(2) Gas holdup is negligible.
(3) Each stage of the process is in thermodynamic equilibrium however not in phase equilibrium. A Murphree tray efficiency is used to depict the departure from equilibrium.
(4) Overall flow rate of gas (G) is constant.
(5) Equilibrium relationship is linear.

We assume that most of the component of gas and liquid stream are inert and does not assimilate into each other. By applying the above assumptions, a mathematical model under unsteady state dynamic condition is inferred for the tray type absorption column using material balances on the ith tray as given in Fig. 2. The water flow from every tray is predicted using Francis equation [16].
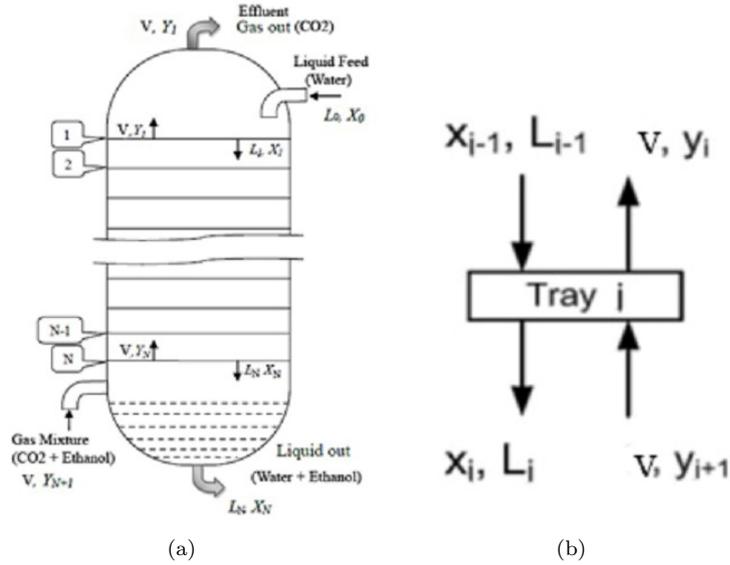
Figure 2. Tray Absorption Column focusing on a single tray.

$$M_i = A_p \rho_L \left[h_w + c \left(\frac{L_i}{L L_w} \right)^{2/3} \right] \tag{2}$$

For deviation from ideal demeanor, Murphree tray efficiency is employed:

$$\eta = \frac{y_i - y_{i+1}}{y_i^* - y_{i+1}} \tag{3}$$

Where y_i^* is the gas phase solute concentration in equilibrium leaving stage i while y_i is the actual gas phase (non-equilibrium) solute concentration leaving stage i.

The total unsteady state mass balance at the ith stage:

$$\frac{dM_i}{dt} = L_{i-1} + G - L_i - G \tag{4}$$

Similarly, the absorbed component mass balance at i^th stage is given by

$$\frac{d(M_i * x_i)}{dt} = x_{i-1} L_{i-1} - x_i L_i + G(y_{i+1} - y_i) \tag{5}$$

Where Mi = total liquid holdup at i^{th} tray kmol, L_{i-1}, L_i are the absorbent flow rates re in mol/s, G = overall constant gas flow rate in mol/s.

The associated working parameters used for calculation are taken from [4].

In order to ease the initialization process of dynamic simulations, the steady-state model was used to provide initial values for process variables for the system of Eqs. (4) and (5).which is stated as:

At $t = 0$;

$$Mi = M_{0,i} \qquad L_i = L_{0,i} \qquad x_i = x_{0,i} \qquad y_i = y_{0,i} \tag{6}$$

$\forall$ 1,2,...,N.

Since the control process was not incorporated in this model but rather from control designing perspective, only two factors that can be controlled here: The inlet liquid flow rate and its composition. The inlet liquid composition (x_{in}) is assigned from the upstream unit, therefore it is considered as a disturbance. Consequently, the only manipulated variable left is liquid flow rate (L_0).

3.2 *Steady State Model Development*

Steady-state simulation is important for the design or process synthesis because most processes operate around a nominal (steady-state) condition.

Combining equations (4) and (5) with the algebraic system given in equation (3) to acquire a tray type absorption column model in steady state form ($L_{i-1} = L_i = L$). For simplification, the above model is compacted to a matrix form as given below:

$$A_x x = Bu - \triangle y \tag{7}$$

Equation (7) is acquired by merging Eqs. (4) and (5),

Also the equation (3) for murphy tray efficiency is compacted in matrix form as

$$A_y y = -\eta \kappa x \left(1 - \eta\right) y_{in} v \tag{8}$$

In the above equations, the elements of Ax and Ay are given by:

$$(a_x)_{i,j} = \begin{bmatrix} -\frac{L_0}{G} & if & i = j \\ \frac{L_0}{G} & if & j = i+1 \end{bmatrix}$$

$$(a_x)_{i,j} = \begin{bmatrix} -1 & if & i = j \\ 1 - \eta & if & j = i+1 \end{bmatrix}$$

$$\forall_{i,j} \ 1,2,3,4...,N.$$

Where the element of B, U, y, x, v and y are as follows:

$$B = \begin{bmatrix} -1 & 0 \\ 0 & 0 \\ ... & ... \\ ... & ... \\ 0 & 1 \end{bmatrix} \qquad U = \begin{bmatrix} \frac{L_0 * x_{in}}{G} \\ y_{in} \end{bmatrix}$$

$$\triangle y = \begin{bmatrix} \triangle y_1 \\ \triangle y_2 \\ ... \\ ... \\ \triangle y_{n-1} \\ -y_n \end{bmatrix} \qquad \triangle y_j = (y_{i+1} - y_i), \quad i = 1, 2, ...N$$

$$v = \begin{bmatrix} 0 \\ 0 \\ 0 \\ \ldots \\ \ldots \\ 1 \end{bmatrix} \qquad x = \begin{bmatrix} x_1 \\ x_2 \\ \ldots \\ \ldots \\ x_{n-1} \\ x_n \end{bmatrix} \qquad y = \begin{bmatrix} y_1 \\ y_2 \\ \ldots \\ \ldots \\ y_{n-1} \\ y_n \end{bmatrix}$$

It ought to be noticed that the entire input variable (manipulated, L_0 and disturbances, G, $x_i n$, and $y_i n$) are accommodated in a vector U, whereas the composition of gas and the liquid phase of ethanol are put in vector x and y respectively. At steady state,

$$Ax_0 = BU \qquad (9)$$

The elements of the matrix A are as follows:

$$(a)_{i,j} = \begin{bmatrix} -(\eta \mathrm{K} + \frac{L_0}{G}) & if\ i = j \\ \frac{L_0}{G} & if\ i = j + 1 \end{bmatrix}$$

And the elements of B and U are the same as those given in Eq. (9)

3.3 *Dynamic Model Derivation and Solution Algorithm*

The left hand side derivative vector of Eq. (5) is expanded and the dynamic model given by Eqs. (2) - (5) is thrown into the accompanying state-space frame, which is appropriate for MATLAB/SIMULINK execution:

$$\frac{dx}{dt} = A_x' x + Bu \qquad (10)$$

Where the elements of A_x' and B' are

$$\left(a_x'\right) = \begin{bmatrix} \frac{-(L+GK)}{M} & i = j \\ \frac{L}{M} & i = j + 1 \\ \frac{GK}{M} & j = i + 1 \end{bmatrix} \ ;\ B' = \begin{bmatrix} \frac{L}{M} & 0 \\ 0 & 0 \\ \ldots & \ldots \\ \ldots & \ldots \\ 0 & \frac{G}{M} \end{bmatrix}$$

The dynamic methodology begins by considering the L_i (mol/s) of the absorbent flow rate entering from the highest point of the column with $\eta = 1$, trialed by solving the steady state system given by Eqs. (7) and (8) applying the calculation offered above to give the initial condition to the dynamic model. Then, the system of ODEs given by Eq. (10) is incorporated using the standard MATLAB ordinary differential Equation solver ode45.

3.4 *Step Responses*

Further, the MATLAB function step is used to determine the responses to a step change in inlet composition. The step function needs a linear state space model in

deviation variable form.

$$\Delta \dot{x} = A\Delta x + B\Delta u$$

4.   Results and discussion

4.1   *Steady State Results:*

Figure 3 shows the variation of the output variable (y_{out}) as a function of changes in inlet liquid flow rate (L_0). The graph shows that the outlet of gas phase composition is less sensitive when the change in the liquid flow rate (L_0) is high. It shows that the above process is linear only up to the absorbent flow rate of about 1.5 mol/s.
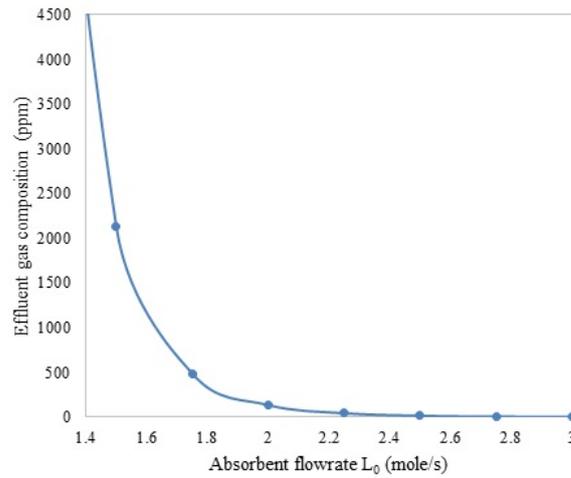
Figure 3. Variation of the exit gas phase composition to a step change in liquid flow rate.
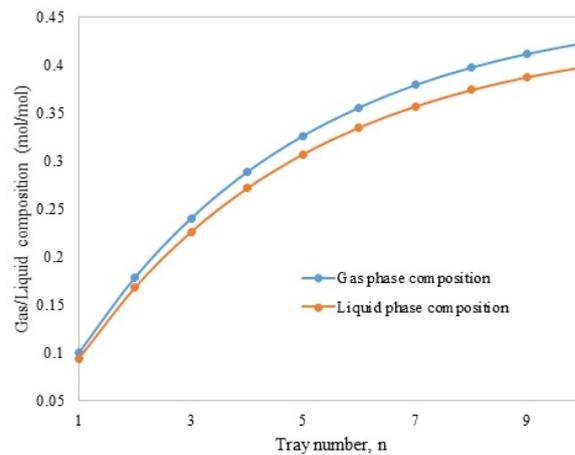
Figure 4.   Gas and Liquid phase concentration profile as a function of tray number for Liquid flow rate 1.0 (mol/s)

Graphical displays of the steady state results for the absorber simulation are shown in figures 4 - 12. All the steady state simulation results of the tray gas absorber shows that the gas phase composition profile is a function tray number when the liquid flow rate varies from 1.0 to 3.0 mol/s.

Fig. 4 only shows a convex plot that means at very low liquid flow rate (i.e. L=1.0mol/s) vapors get enough time to reach upto the top plate and the rate of absorption is more only in the upper portion of the column. The relationship is almost linear for Liquid flow rate of 1.25 mol/s as shown in fig. 5.

Further increase in the liquid flow rate absorbs more alcohol from the gas phase at a faster rate as the liquid reaches to the bottom more rapidly and the graphs become more deepens as we move on up to L = 3 (mol/s).
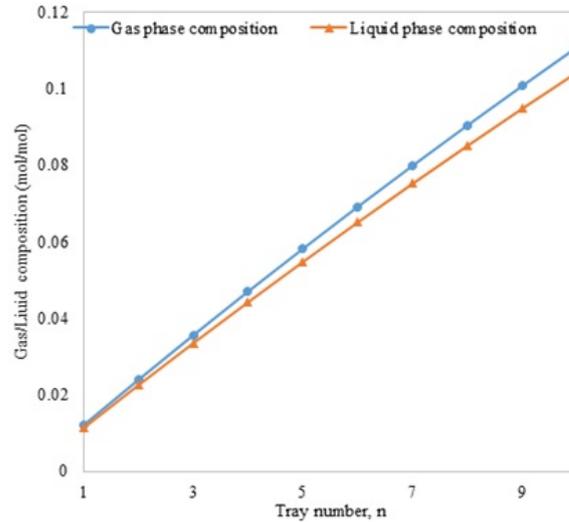
Figure 5. Gas and Liquid phase concentration profile as a function of tray number for Liquid flow rate 1.25 (mol/s).
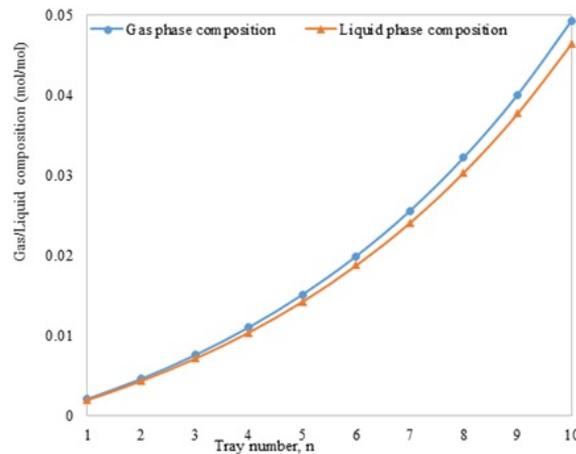
Figure 6. Gas and Liquid phase concentration profile as a function of tray number for Liquid flow rate 1.5 (mol/s).

Initially at low liquid flow rate, the rate of absorption is very slow and the outlet gas composition is very high. The minimum outlet concentration is evident that as the liquid flow rate increases, the degree of absorption also increases stage by stage. As expected the solute removal is highest when the flow rate is 3.0mol/s. From the above graphs, it is clear that the shift in gas composition profile is almost nonlinear along the column.
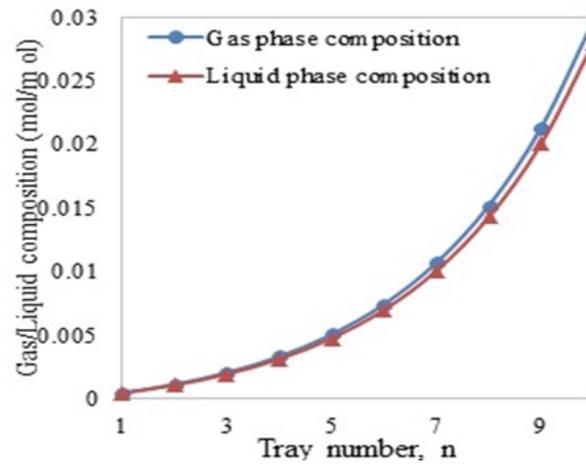
Figure 7. Gas and Liquid phase concentration profile as a function of tray number for Liquid flow rate 1.75 (mol/s).
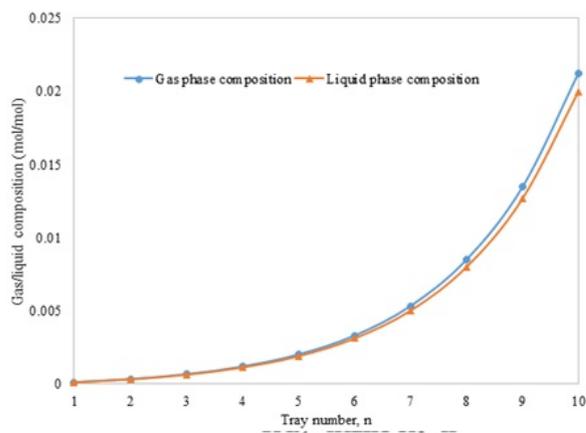
Figure 8. Gas and Liquid phase concentration profile as a function of tray number for Liquid flow rate 2.0 (mol/s).
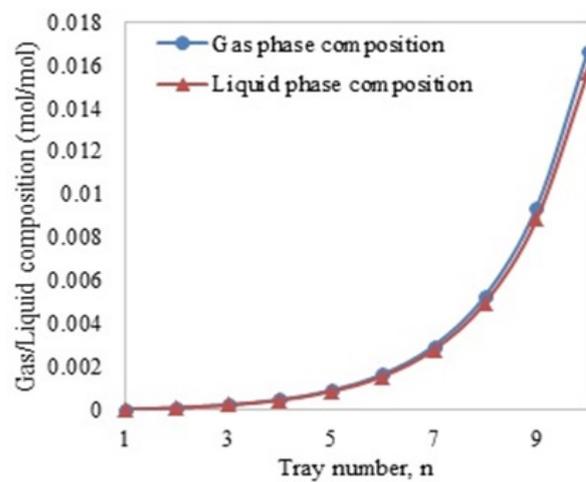
Figure 9. Gas and Liquid phase concentration profile as a function of tray number for Liquid flow rate 2.25 (mol/s).

4.2 Dynamic Simulation Results:

The simulation was run for 18000 seconds. Dynamic analysis of the gas absorption column was done to investigate the column response due to the step change in the
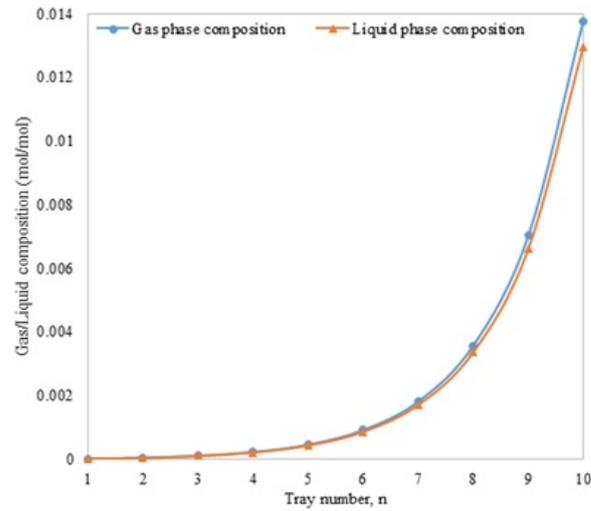
Figure 10. Gas and Liquid phase concentration profile as a function of tray number for Liquid flow rate 2.50 (mol/s).
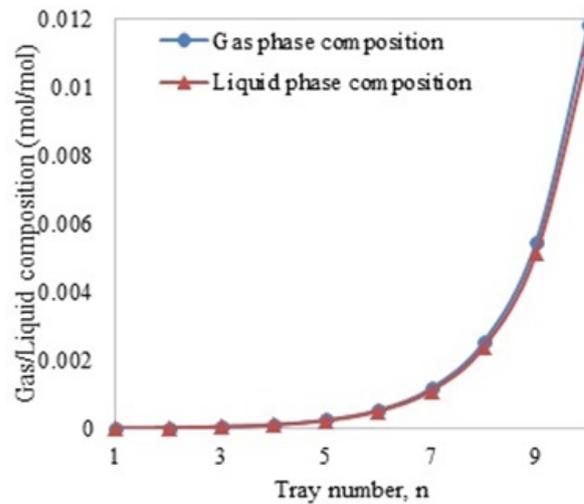
Figure 11. Gas and Liquid phase concentration profile as a function of tray number for Liquid flow rate 2.75 (mol/s).

inlet gas composition at a liquid flow rate of 2.25 mol/s. The graph shows (fig. 13) a stage wise response to a step change in the inlet gas composition. The magnitude of the change in stage composition is greatest on the bottom stage. The rate of absorption is faster to a stage at the bottom of the column. In other words we can say that the non-linearity increases from bottom to the top tray due to the non-symmetric profile.

A comparison of fig 14 and fig 15 shows that the bottom composition (y_{10}) responds more quickly to the vapor feed change than the top vapor composition (y_{exit}). This is obvious because the disturbance must propagate through ten stages (from the bottom to the top of the column) to affect the top composition. Fig 14 shows the more sluggish response to the step change.

The similar plots can be observed from the Simulink scope block as shown in fig. 16 – 18.

The graph shows a sharp profile at high liquid flow rate with increase of absorption rate. Since at high liquid flow rate the liquid reaches to the bottom stage more rapidly and the absorption takes place from the bottom of the column. Whereas
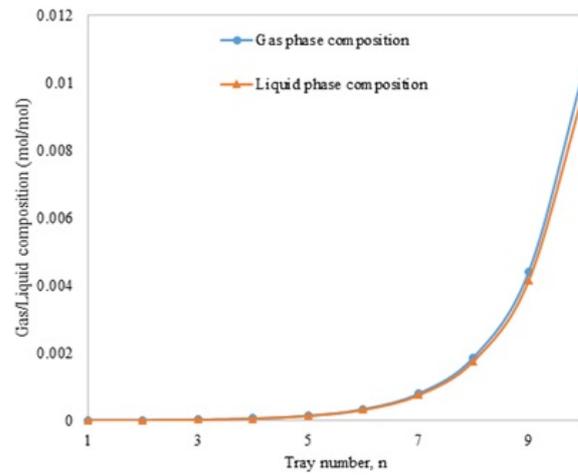
Figure 12. Gas and Liquid phase concentration profile as a function of tray number for Liquid flow rate 3.0 (mol/s).
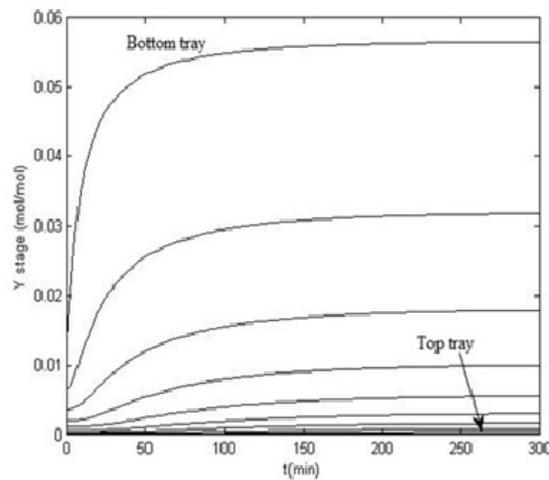
Figure 13. stage wise response of gas phase composition to a step increase in vapor feed composition of 0.1, at t=0.

at low liquid flow rate, the vapor phase has enough time to reach up to the top and the vapor-liquid contact should be less that decreases the rate of absorption. From the above result, it is clear that the exit vapor composition is more sensitive to the inlet liquid flow rate.

The model results show the good agreement with the practical situation and also compared favorably with standard results obtained by Bequette [2]. With this work we are able to provide a readily available simulation that can be used as a test bed for advanced process monitoring.

5.   Conclusion and recommendation

The main contribution of this work was the application of MATLAB/SIMULINK software to the absorption column. In this work, a mathematical model was proposed to predict the steady state and dynamic behavior of a sieve tray gas absorption column by the powerful combination of MATLAB and SIMULINK software.
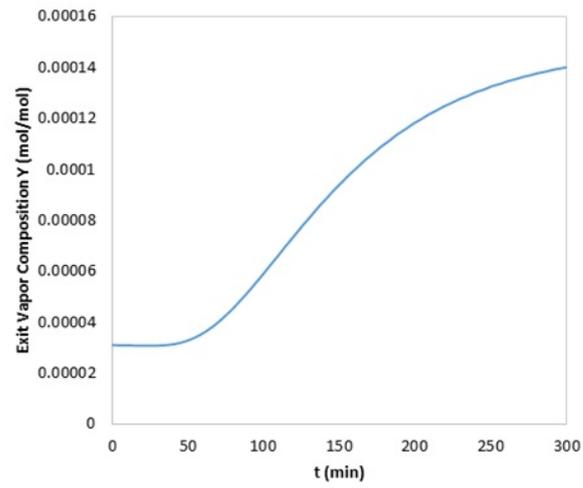
Figure 14. Response of exit vapor composition to a step increase in vapor feed composition of 0.1, at t=0.
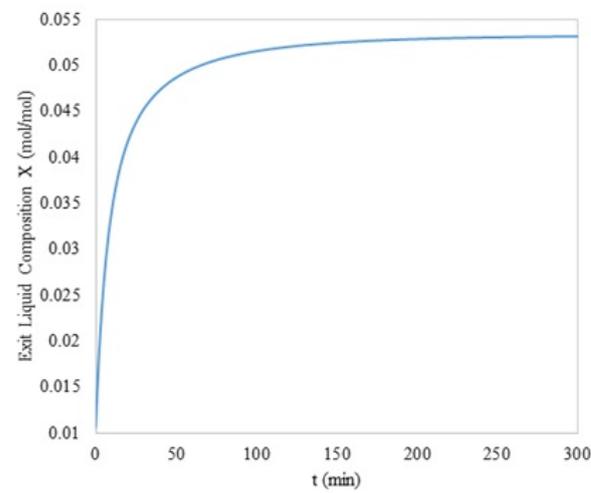
Figure 15. Response of bottom composition to a step increase in vapor feed composition of 0.1, at t=0.
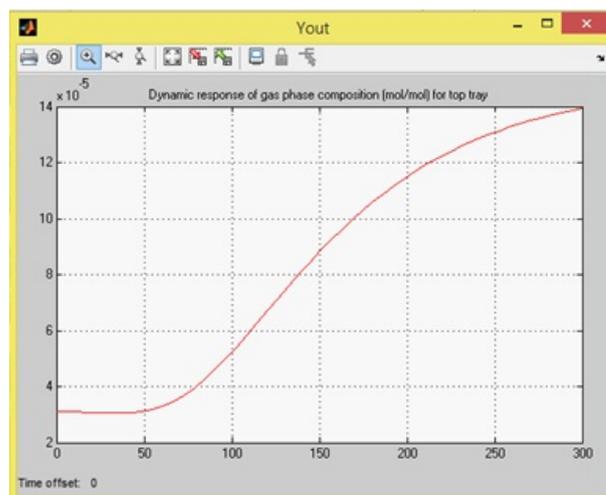
Figure 16. Stage wise response to a step increase in vapor feed of 0.1 SIMULINK plot.
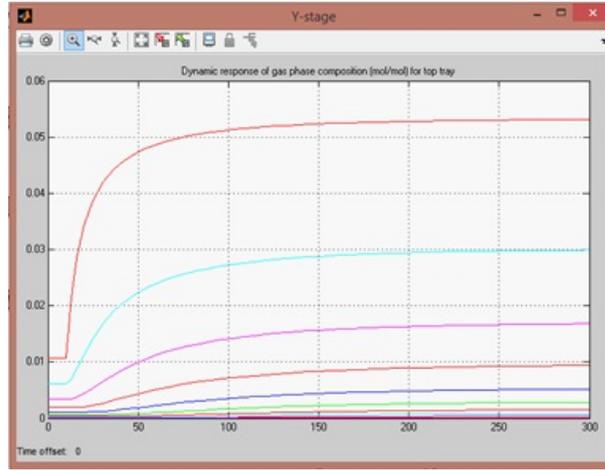
Figure 17. Response of exit vapor composition to a step increase in vapor feed of 0.1 SIMULINK plot.
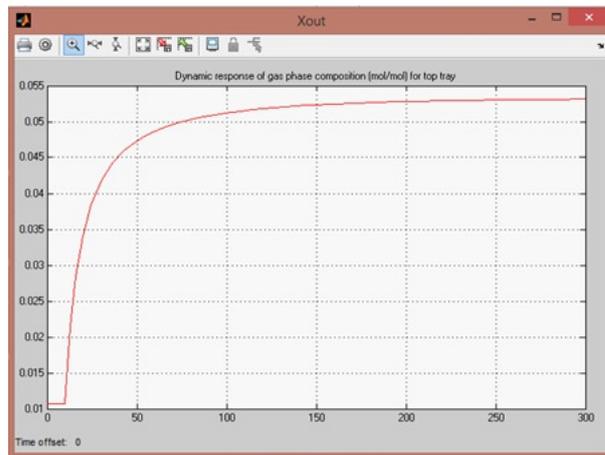
Figure 18. Response of bottom composition to a step increase in vapor feed of 0.1 SIMULINK plot.
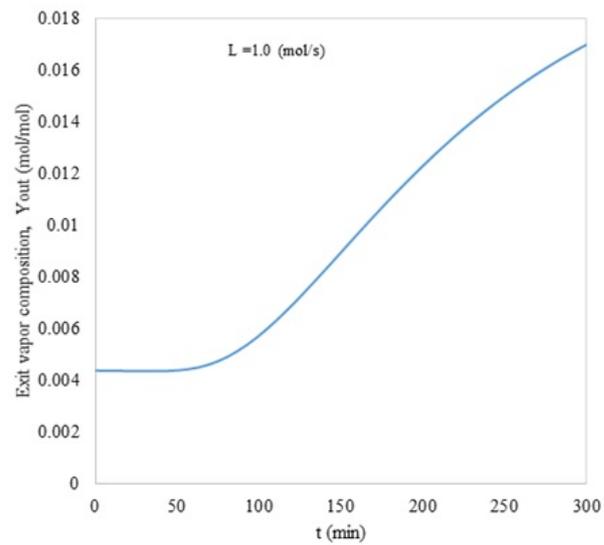
Figure 19. Dynamic response of exit vapor composition due to the step increase in the inlet vapor phase composition at L = 1.0 (mol/s).
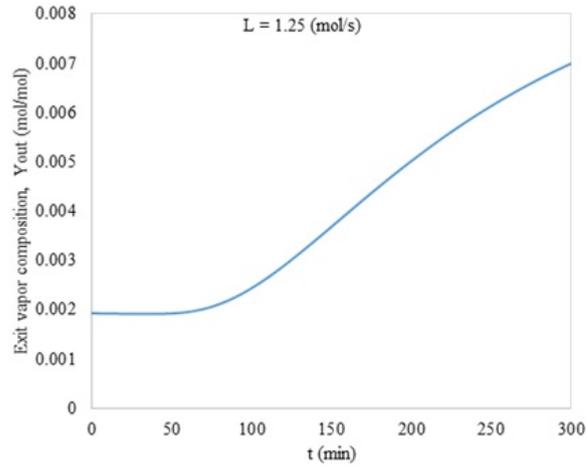
Figure 20. Dynamic response of exit vapor composition due to the step increase in the inlet vapor phase composition at L = 1.25 (mol/s).
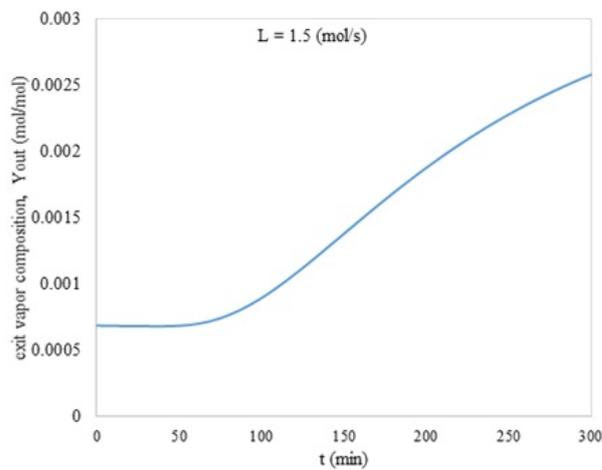
Figure 21. Dynamic response of exit vapor composition due to the step increase in the inlet vapor phase composition at L = 1.5 (mol/s).
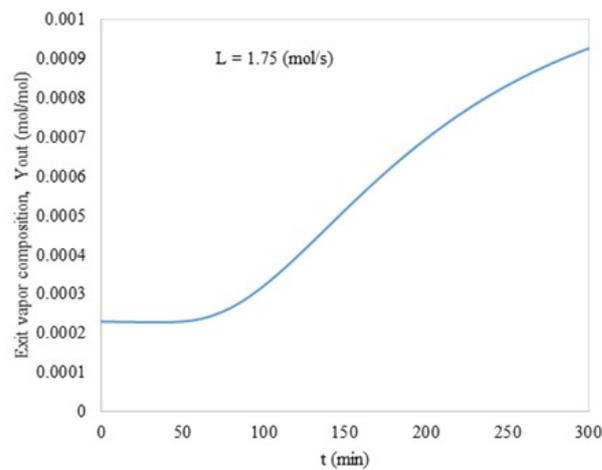
Figure 22. Dynamic response of exit vapor composition due to the step increase in the inlet vapor phase composition at L = 1.75 (mol/s).

The steady state and dynamic model was first solved in the MATLAB to predict the behavior of the column then implemented into SIMULINK by the use of
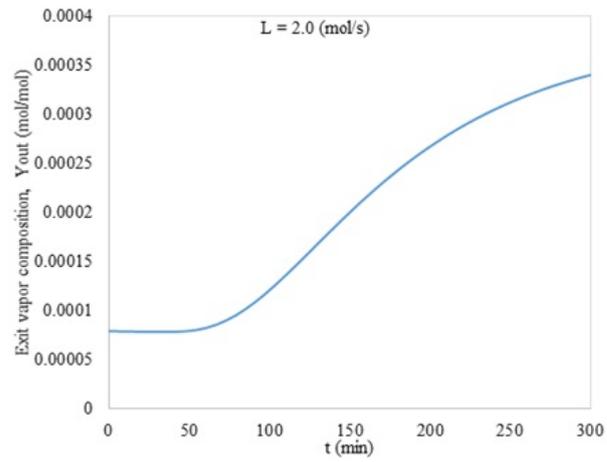
Figure 23. Dynamic response of exit vapor composition due to the step increase in the inlet vapor phase composition at L = 2.0 (mol/s).
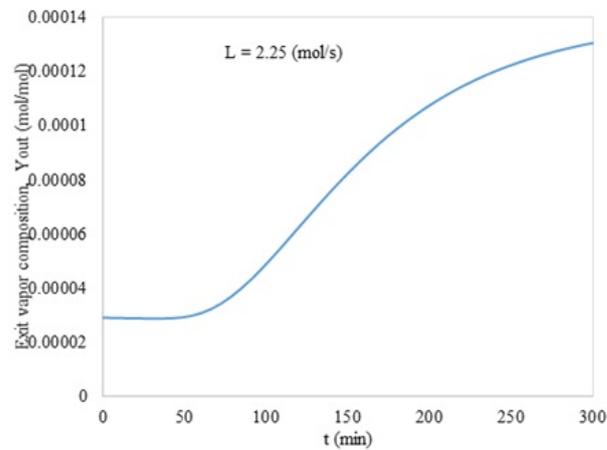
Figure 24. Dynamic response of exit vapor composition due to the step increase in the inlet vapor phase composition at L = 2.25 (mol/s).
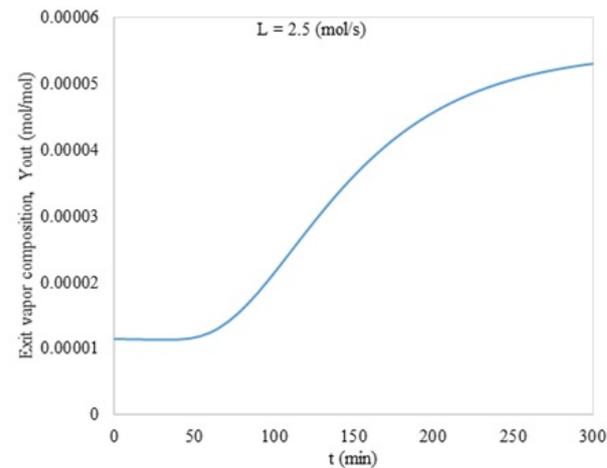
Figure 25. Dynamic response of exit vapor composition due to the step increase in the inlet vapor phase composition at L = 2.50 (mol/s).

inbuilt user defined block S-Function and compared with the result obtained by the MATLAB. The steady state mathematical model was solved to calculate the
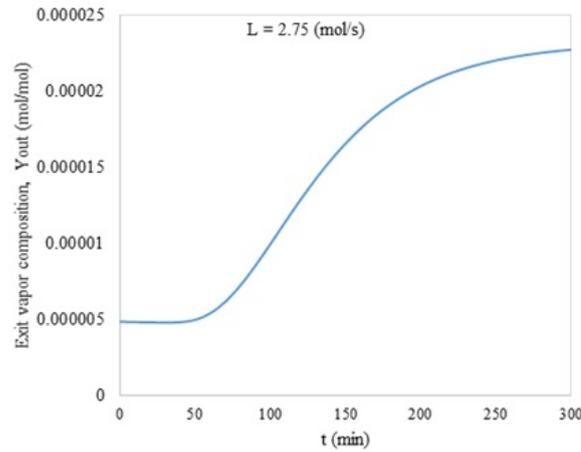
Figure 26. Dynamic response of exit vapor composition due to the step increase in the inlet vapor phase composition at L = 2.75 (mol/s).
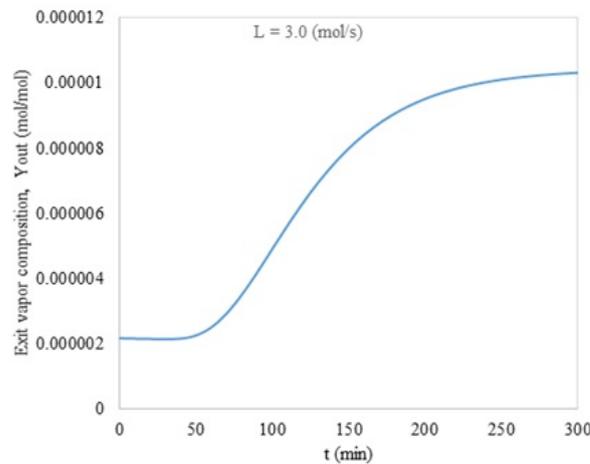
Figure 27. Dynamic response of exit vapor composition due to the step increase in the inlet vapor phase composition at L = 3.0 (mol/s).

composition of the outlet liquid and gas stream with the inlet liquid flow rate as a parameter. It was concluded that exit gas and liquid composition was non-linear with respect to the stage number. The exit vapor composition is less sensitive when the liquid flow rate is high. The main focus of this work was to minimize the concentration of alcohol in the exit vapor stream. A step change in the inlet gas phase composition was introduced to analyze the stage wise response of the gas absorption column at a liquid flow rate of 2.25 mol/s. The outlet gas phase composition is strongly influenced by the inlet liquid flow rate and change in the inlet gas phase composition. With the increase in liquid flow rate, the concentration of alcohol in the exit vapor stream reaches to minimum. The magnitude of composition change was greatest on the stages closest to the step input change. From the dynamic point of view the plot of exit vapor composition becomes sharper when the flow rate is high. In this work only liquid flow rate and gas phase composition were studied simultaneously. The model was proposed for the binary system only. A similar model can be formulated for a multicomponent system. Also modelling and simulation of the process with the incorporation control strategy has a scope for further work.

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