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by

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RESEARCH REPORT

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AN ANALYTICAL APPROACH TO APPROXIMATE DYNAMIC MODELING OF DISTILLATION TOWERS

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Abstract. This paper presents analytical expressions for predicting distillate and bottoms composition transient responses due to changes in manipulative and disturbance variables of a tower. The authors in an earlier paper showed that towers are inherently recyle structures and linearization techniques should be applied at perturbed conditions of tower models to evaluate realistic tower time constants. In this earlier paper, a numerical approach to estimating time constants was presented. The numerical approach is extended in this paper to an analytical approach that requires only steady state and design information of a tower. The analytical approach is relatively simple to use and much less time consuming compared to dynamic simulation. Further, the analytical technique gives insight into why towers respond nonlinearly.

Keywords. Distillation; dynamic modeling; modelling; approximate models; transfer functions.

INTRODUCTION

This paper presents analytical expressions for predicting distillate and bottoms composition transient responses due to changes in tower manipulative and disturbance variables. To date, published work on analytical techniques relates to predicting transient behavior of product compositions of an absorber section only (Lapidus and Amundson(1950), Amundson(1966) and Kim and Friedly(1974)). This paper deals with a complete distillation tower and presents simple analytical methods that may be used for short-cut dynamic modeling of high purity towers. The analytical expressions given in this paper require only steady state information to evaluate time constants and dead times of product composition responses for forcing in manipulative and disturbance variables. Further, they provide information necessary for identifying the key sections of a tower which are the major contributors to their dynamic behavior.

For predicting the transient responses of the product compositions Wahl and Harriott(1970) presented a numerical technique that utilizes the design conditions of a tower. Their predictions of time constants of product responses are unrealistically large for high purity towers. An earlier paper by Kapoor and McAvoy(1986) discusses the cause of such unrealistically large time constants. In this earlier paper a numerical approach to estimating time constants is presented. In the present paper an analytical approach is taken. To put the analytical approach into perspective the earlier numerical work is briefly reviewed here.

REVIEW OF PAST WORK

Kapoor et al.(1986) carried out a detailed study of six towers, discussed by Fuentes and Luyben (1983). The essential features of these towers are shown in Table 1. The time constants shown in the last column of Table 1, were obtained from numerically calculated frequency responses using a stepping technique, developed by Luyben(1973). The numerically evaluated time constants, relate response times of changes in distillate composition x_D to changes in feed composition x_F at design conditions. From the actual responses obtained from the non-linear simulation of tower models, the gain, time constant and dead time were estimated and are listed in Table 2. The time at which the

Table 1: Essential Features of Luyben's Towers

Case#	Feed $Kg\frac{moles}{min}$	α	$x_B = (1-x_D)$	N_T	N_S	$\frac{L}{D}$	$\Theta(min)$
1	65.8	4	.05	13	7	.53	10
2	61.7	4	.001	26	13	.73	450
3	61.7	4	.00001	40	20	.78	45400
4	36.3	2	.05	18	9	2.1	30
5	31.8	2	.001	40	20	2.4	1630
6	31.8	2	.00001	60	30	2.6	170000

Θ = Time constant

Table 2: Results from Open Loop Responses

Case#	Forcing: x_F =.6 Gain	Θ	τ	Forcing: x_F =.4 Gain	Θ	τ
1	.281	10.0	8.0	1.51	8.0	8.0
2	.007	23.0	15.0	1.99	13.0	26.0
3	.00006	25.0	22.0	2.0	10.0	36.0
4	.359	27.0	12.0	1.54	22.0	10.0
5	.007	25.0	22.0	1.99	23.0	50.0
6	.00006	28.0	28.0	2.0	30.0	85.0

Θ = Time constant τ = Dead time

response shows a noticeable change from the initial steady state conditions is used as an approximation to the dead time. The time required to reach 63% of the final conditions is approximated as the time constant. The gain is given by the change in x_D divided by the change in x_F . The highest purity towers respond much faster than the time constants, shown in Table 1, indicate. Observe also in Table 2 the asymmetric behavior of high purity towers 3, 5, and 6. The gains and time constants that approximate the x_D responses for increases in x_F are significantly different from the gains and time constants that approximate the x_D responses for decreases in x_F. To explain the asymmetric behavior of high purity towers and also to explain the discrepancy between the time constant estimates listed in Table 1 and time constants that approximate the non-linear responses(Table 2), a simplified dynamic model of a tower is analysed. Figure 1 shows the block diagram of a distillation column consisting of four sections of a tower namely, condenser, enriching section, stripping section and reboiler. The various transfer functions that can be defined for feed composition changes are shown in Fig. 1. The transfer functions relating $D\overline{x_D}$ and $B\overline{x_B}$ to $F\overline{x_F}$ can be derived from Fig. 1 and are given as eqns. 1 and 2.

$$\frac{D\overline{x_D}}{F\overline{x_F}} = \left(\frac{H_S}{1-H_EH_S}\right)G_9\left(\frac{G_{12}}{1-G_{10}G_{11}}\right) \quad (1)$$

$$\frac{B\overline{x_B}}{F\overline{x_F}} = \left(\frac{1}{1-H_EH_S}\right)G_2\left(\frac{G_6}{1-G_4G_5}\right) \quad (2)$$

where

$$H_E = G_7 + \frac{G_8G_9G_{11}}{1-G_{10}G_{11}} \quad (3)$$

and

$$H_S = G_1 + \frac{G_2G_3G_5}{1-G_4G_5} \quad (4)$$

Since the gains of all G_i's are positive, Fig. 1 indicates that there are a number of positive feedback loops in a tower's dynamic structure. The $1 - H_EH_S$ term in eqn. 1, $1 - G_{10}G_{11}$ term in eqn. 2 and $1 - G_4G_5$ term in eqn. 3 indicate positive feedback loops resulting from the recycle structure of a distillation column. In fact, each tray involves a positive feedback loop. By lumping the enriching and stripping sections of a tower into H_E and H_S it is possible to elucidate the underlying reason for the large time constants which result from a linear analysis. The authors in another paper(Kapoor et al. (1986b)) showed that extremely large time constants will result if the gain of any of the positive feedback loops, i.e. H_EH_S, G_4G_5 or

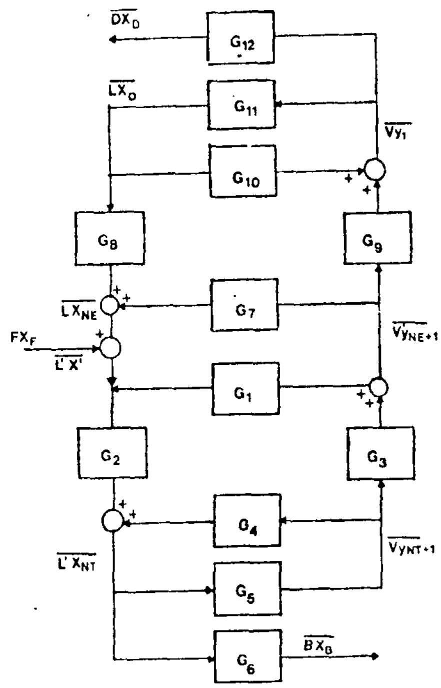

Fig. 1. Block transfer function

$G_{10}G_{11}$, approaches unity. They also showed that the gains of G_4G_5 and $G_{10}G_{11}$ rarely approach unity in most towers. However, the loop gain of the H_EH_S transfer function, K_EK_S, approaches unity in a very small region around the design conditions of high purity towers and indeed around any steady state where high purity is achieved at both ends of a tower. Figure 2a is a plot of K_EK_S versus x_F for the high purity tower 3. As can be seen from Fig. 2a near the design condition of x_F = .5 the K_EK_S loop gain approaches 1.0. It was shown in Kapoor et al.(1986b) that for K_EK_S approaching unity the dynamic response of a tower will be extremely sluggish. Figure 2a illustrates that K_EK_S is close to 1.0 in a very small region near x_F = .5. Therefore we expect the towers dominant time constants to be large only in this small region. However, outside this small region, i.e. at slightly perturbed conditions of the tower, the loop gain K_EK_S drops off drastically from 1.0 resulting in a much smaller and realistic time constant. This result suggests that one should use a perturbed value of x_F to estimate effective tower time constants from a linearized model. The authors accordingly used a perturbed steady state to estimate time constants using the same approach as Fuentes and Luyben(1983). These estimates are plotted in Fig. 2b for case 3 at various values of x_F . Figure 2b shows that the time constants are extremely large at design conditions of x_F =.5. However, outside a very small region the time constants are much smaller and reasonably constant for x_F > .5 and x_F < .5. For the transients shown in Fig. 1, large x_F changes were used to force the towers and the towers operated at x_F values substantially different from the design values. Since time constants change drastically with x_F , time constants must be evaluated at perturbed conditions of a tower. Fig. 2b shows that the time constants change in a fairly linear fashion with respect to x_F at perturbed conditions. If an average value of

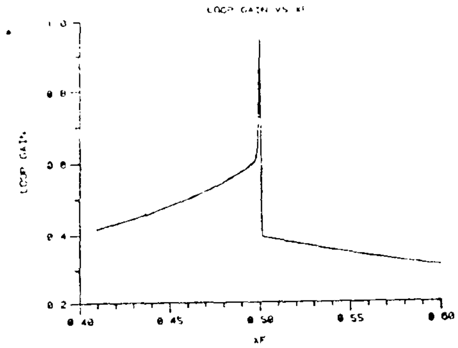

Fig. 2a. $K_E K_S$ vs x_F

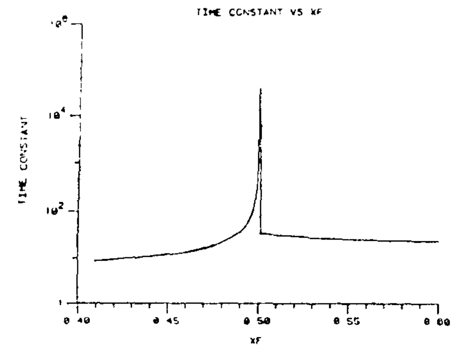

Fig. 2b. Θ vs x_F

the time constants is estimated over the linear zone then a better approximation to the simulation results can be expected. Such an average value of the time constants can be obtained approximately half way between the design and perturbed conditions. For example, if the tower models are forced from x_F =.4 to .5 then the time constants should be estimated at x_F =.45. The results presented in this paper are obtained by linearizing tower models at conditions half way between the initial and final steady state values.

To this point this paper has presented a review of the numerical technique of Kapoor et al.(1986). Our objective is to develop analytical expressions for all the composition tranfer functions of a tower for all forcing variables. Further we want to reduce the final complicated transfer functions (for example eqns. 1 and 2 for x_F changes) to a first order with dead time model by the method of moments(Gibilaro and Lees(1969)). A reduction in order of final transfer functions will provide simple analytical relationships between a tower's dynamic model and its physical variables. The next section presents analytical expressions for x_D respones for forcing in x_F . Additional analytical transfer function expressions for other forcing variables are given in Kapoor and McAvoy(1986).

REDUCING THE FINAL TRANSFER FUNCTION

To obtain a simple dynamic model for the x_D response due to x_F changes we will make the following assumption. first order model with dead time approximates the pro composition responses for x_F changes. Equation 1 is transfer function of the x_D response due to x_F change it can be divided, into 3 terms. The first term of eqn $H_S/(1-H_EH_S)$ and it gives the change in the compos of the vapor entering the enriching section due to a ch in x_F. The second term in eqn. 1 is G_9. Referri Fig. 1, G_9 gives the change in the composition of the entering the condenser to a change in the compositi the vapor entering the enriching section. The third te eqn. 1 is $G_{12}/(1-G_{10}G_{11})$ and it gives the change i x_D response due to a change in the composition of the entering the condenser. The effective time constant x_D response for x_F changes will therefore be a com effect of all three terms. To develop low order tr functions the first step is to reduce the order of G_i's and H_S in eqn. 1. After substituting the reduced of G_i's, H_E and H_S in eqn. 1 the moments of eqn. 1 are equated to the moments of a first order transfer function with dead time, the form of which is given as:

$$\frac{D\overline{x_D}}{F\overline{x_F}} = \frac{Ke^{-\tau_D(x_F)s}}{\Theta(x_F)s+1} \qquad (5)$$

To reduce eqn. 1 to eqn. 5, the gain K, the dead time $\tau_D(x_F)$ and the time constant $\Theta(x_F)$ are related to the parameters in eqn. 1 by the method of moments. A detailed derivation for $K, \Theta(x_F)$ and $\tau_D(x_F)$ is given in Kapoor(1986). The final expressions are:

$$K = \left(\frac{K_7}{1-K_EK_S}\right) K_9 \left(\frac{\frac{1}{RR+1}}{1-K_{10}K_{11}}\right) \qquad (6)$$

$$\Theta(x_F) = \overbrace{\frac{T_1+l_1T_7}{1-l_1}}^{\text{Loop 1(Enr. Sect.)}} + T_9 + \overbrace{\frac{T_C+l_2T_7}{1-K_{10}K_{11}}}^{\text{Loop 2}} \qquad (7)$$

$$K_EK_S = K_1K_7 = l_1 \qquad (8)$$

$$\tau_D(x_F) = (\tau_D)_9 \qquad (9)$$

The expressions for the gains K_i's, T_i's and τ_{D9} are given in Table 3. Equation 7 shows that the time constant of the x_D response due to x_F changes is comprised of three parts. The first term, labeled Loop 1, is due to the recycle structure formed by integration of the enriching and the stripping sections. The Loop 1 time constant refers to the response time of the composition of the vapor entering the enriching section due to a change in x_F. The Loop 1 time constant can be extremely large if the variable l_1 which is the product of the enriching and stripping section gains, K_EK_S, is very close to 1.0. In Fig. 2a it is shown that at design conditions of high purity towers $l_1 \longrightarrow 1.0$ and therefore the Loop 1 time constant in eqn. 7 is extremely large. The Loop 1 time constant is the major contributor to the time constant of x_D in the small neighborhood near steady state. As can be seen from Fig. 2a, the loop gain l_1 drops off drastically from 1. at perturbed conditions, implying that the Loop 1 time constant is not necessarily the major contributor to the time constant of the x_D response at perturbed conditions of a tower. This behavior agrees with our numerical results.

The time constant T_9 refers to the response time of y_1 due to a change in y_{N+1} (See Fig. 1). The time constant T_9 is usually much larger than the Loop 1 time constant at perturbed conditions of a tower. The third term in eqn. 7, labeled Loop 2, is a result of the feedback loop formed by integration of the condenser with the enriching section. As shown in Kapoor et al. (1986) the loop gain l_2 rarely approaches unity. Therefore, the contribution by the Loop 2 time constant to the effective time constant of the x_D response will be approximately of the order of the sum of the condenser time constant, T_C, and T_7.

Equation 9 is the expression for the dead time of the x_D response for x_F changes. The dead time is a sum of all but the largest lag of the enriching section. All the lags of an enriching section can be evaluated using analytical expressions developed by Kim and Friedly(1974) and are presented in Table 3. Equations 7 and 9 were used for the evaluation of time constants and dead times of the x_D responses for x_F changes. Results obtained from eqns. 7 and 9 for tower 3 are compared with the the non-linear simulation results in Fig. 3. The tower model starts at a perturbed initial steady state corresponding to $x_F = .4$ and the response to the design condition corresponding to $x_F = .5$ is shown. As can be seen from Fig. 3 the agreement between the analytical responses and non-linear simulation results is very good. We studied all the six towers illustrated in Table 1 in detail(Kapoor (1986)) and compared the analytical expression results with the non-linear simulation results for forcing in x_F from design to perturbed conditions and back. Both positive and negative perturbations in x_F were considered. The analytical expressions compared very well with the non-linear simulation results for all the cases except for forcing in x_F from design to a decreased value. A significant error in the dead time was obtained for this case. This error may not be a serious problem since one is normally interested in determining response times of towers responding from upset conditions back to their design specifications.

Equations 6-9 are analytical expressions that relate the gains, time constants and dead-times of the enriching and stripping sections to x_D response times for forcing in x_F. Table 3 shows that the gains, time constants and dead-times of the enriching and stripping sections can be related to the physical variables of a tower. Further, the relationships presented in Table 3 provide a method for relating the product composition response time to the physical variables such as holdup on a tray, in the condenser and reboiler, flow variables, relative volatility, etc.. The expressions for x_B responses to changes in x_F can be derived in the same manner as for the x_D case and are presented in the following section.

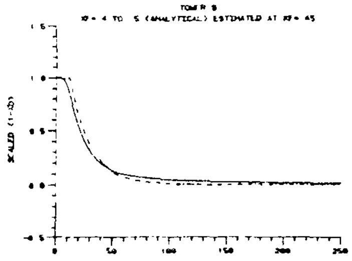

Fig. 3. x_D response for x_F changes

Table 3: Gains, Leads and Lags

$$A_S = \frac{(1+(\alpha-1)x_F)^2}{\alpha}\frac{RR+\frac{F}{D}}{RR+1} \qquad A_E = \frac{\alpha x_F RR}{1+x_F RR}$$

$$D_S = A_S^{N_S+1} - 1 \qquad D_E = A_E^{N_E+1} - 1$$

$$K_1 = \frac{A_S^{N_S} - 1}{D_S} \qquad K_7 = \frac{A_E^{N_E+1} - A_E}{D_E}$$

$$K_2 = \frac{A_S^{N_S+1} - A_S^{N_S}}{D_S} \qquad K_9 = \frac{(A_E - 1)}{D_E}$$

$$K_4 = \frac{A_S^{N_S+1} - A_S}{D_S} \qquad K_{10} = \frac{A_E^{N_E} - 1}{D_E}$$

$$K_5 = \frac{1}{1+\frac{B(1+(\alpha-1)x_B)^2}{V\alpha}} \qquad K_{11} = \frac{RR}{RR+1}$$

$$K_6 = 1 - K_5 \qquad K_{12} = \frac{1}{RR+1}$$

From Kim and Friedly's analysis:

$$Lag_j = \frac{H}{L}\frac{1}{(1+\frac{1}{A_E}) - 2\sqrt{\frac{1}{A_E}}\cos(\frac{\pi j}{N+1})} \qquad j = 1,\ldots,N \quad (Enr.Sect.)$$

$$Lead_j = \frac{H}{L}\frac{1}{(1+\frac{1}{A_E}) - 2\sqrt{\frac{1}{A_E}}\cos(\frac{\pi j}{N})} \qquad j = 1,\ldots,N-1 \quad (Enr.Sect.)$$

$$Lag_i = \frac{H}{L'}\frac{1}{(1+\frac{1}{A_S}) - 2\sqrt{\frac{1}{A_S}}\cos(\frac{\pi i}{N+1})} \qquad i = 1,\ldots,N \quad (Str.Sect.)$$

$$Lead_i = \frac{H}{L'}\frac{1}{(1+\frac{1}{A_S}) - 2\sqrt{\frac{1}{A_S}}\cos(\frac{\pi i}{N})} \qquad i = 1,\ldots,N-1 \quad (Str.Sect.)$$

X_B RESPONSES FOR X_F CHANGES

The transfer function relating x_B responses due to changes in x_F is given as eqn. 2. Equation 2 can be reduced by the method of moments, to a simple first order transfer function with dead time following the same approach used for the x_D case. The final expressions for the dynamic parameters of x_B responses for forcing in x_F are given as:

$$\Theta_{x_B}(x_F) = \overbrace{\frac{l_1(T_1+T_7)}{1-l_1}}^{\text{Loop 1(Stripp.Sect.)}} + T_2 + \overbrace{\frac{T_R + l_3 T_1}{1-l_3}}^{\text{Loop 3}} \qquad (10)$$

$$l_3 = K_4 K_5 \qquad (11)$$

and

$$\tau_B(x_F) = (\tau_D)_2 \qquad (12)$$

The Loop 1(Stripp. Sect.) time constant in eqn. 10 gives the effect of the first term of eqn. 2. The Loop 3 time constant gives the effect of the loop formed by the reboiler and the stripping section on the x_B response time. The time constant T_2 gives the response time of x_{N_T} due to changes in x_N'. Equation 12 gives the dead time of the x_B responses due to changes in x_F . The analytical expressions are used to evaluate the time constants and dead times of the towers when forced from increased values of x_B to design values. Figure 4 gives the x_B response for case study tower 3. Analytical expression results for all the

Table 3 continued

$$T_1 = (\sum_{i=1}^{N_S} Lag_i - \sum_{i=1}^{N_S-1} Lead_i)$$

$$T_7 = (\sum_{j=1}^{N_E} Lag_j - \sum_{j=1}^{N_E-1} Lead_j)$$

$$T_2 = (Lag_1)$$

$$T_9 = (Lag_1)$$

$$(\tau_D)_2 = (\sum_{j=2}^{N_S} Lag_i)$$

$$(\tau_D)_9 = (\sum_{j=2}^{N_E} Lag_j)$$

$$T_5 = T_R = \frac{H_R}{V + B/\alpha}$$

$$T_C = \frac{H_C}{V}$$

$H_R = Reboiler\ Holdup$

$H_C = Condenser\ Holdup$

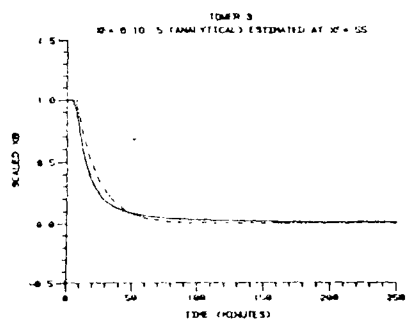

Fig. 4. x_B response for x_F changes

cases listed in Table 1 are compared with non-linear simulation results in Kapoor(1986). The agreement between the simulation and the analytical expressions is good for all the cases studied.

Since space does not permit the presentation of additional analytical expressions for the product composition responses for forcings in V and B and L and D, they are given in Kapoor and McAvoy (1986). However, results for tower 3 for forcing in V and L are given in Figs. 5 and 6. Figures 5 and 6 give a comparison of the approximate x_D and x_B responses determined from the analytical expressions and the non-linear responses. The agreement between the analytical expression results and the simulation results is excellent for the V case and very good for L case. In Kapoor(1986) analytical expression results for all the six towers and a number of towers with non-ideal and multicomponent features are compared with non-linear simulation results. A reasonably good comparison is obtained for most of the cases studied. As a result the analytical expressions derived in Kapoor(1986) present an approximate and short-cut approach to modeling towers in a timely manner. Additionally, the expressions provide insight for high purity towers where the existing linearization techniques fail.

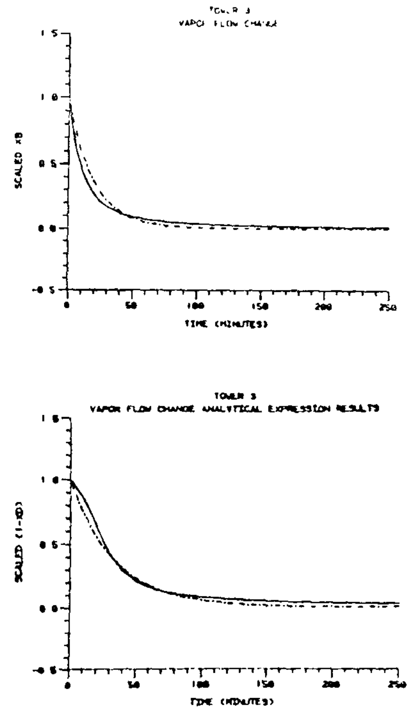

Fig. 5. x_D & x_B responses for V changes

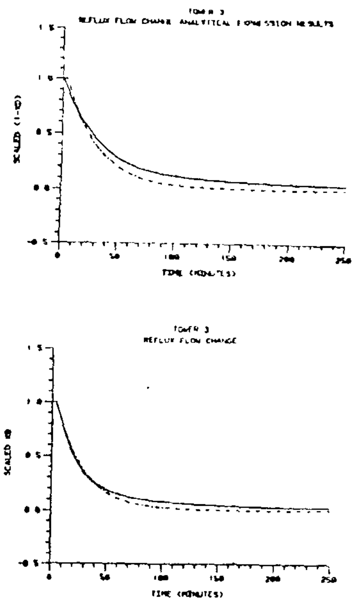

Fig. 6. x_D & x_B responses for L changes

Conclusion

The analytical expressions presented in this paper are an extension of the analysis technique employed in Kapoor and McAvoy(1986). In this earlier paper, it is shown that distillation tower models can be modeled by block transfer functions integrated to each other in a recycle processing configuration. In this paper analytical expressions for the various block transfer functions are developed and reduced to first order transfer functions with or without dead times by the method of moments. These reduced order transfer functions are used to predict response times of towers for forcing in manipulative and disturbance variables. The results obtained from the analytical expressions are compared with the non-linear simulation results. The agreement between the responses obtained from the analytical expressions and the non-linear responses is good for a number of cases studied in Kapoor(1986). In this paper, results for a high purity tower are presented. The high purity tower is forced from perturbed conditions back to its design specifications. The reason for studying this forcing is that for control and operability studies one is insterested in determining the response times of towers for forcing from upset conditions back to the normal operating setpoints.

The analytical expressions presented in this paper require only steady state and design information of the tower to evaluate tower time constants. Further, the analytical expressions help in determining which sections of a tower, namely, condenser, enriching and stripping sections and reboiler, are the major contributors to the response times. Finally, these expressions provide insight into the effect of a change in design on the response times of a tower.

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Nomenclature

A_E	Effective Absorption Factor
B	Bottoms Flow
D	Distillate Flow
F	Feed Flow
G_i	Transfer function
H_E	Transfer function for enriching section
H_S	Transfer function for stripping section
K_E	Gain for enriching section
K_S	Gain for stripping section
L	Reflux Flow in the Enriching Section
L'	Reflux Flow in the Stripping Section
N_E	Trays in the Enriching Section
N_S	Trays in the Stripping Section
RR	Reflux Ratio
S_S	Effective Stripping Factor
V	Vapor Flow
x_B	Bottoms mole Fraction
x_F	Feed mole Fraction
x_D	Distillate mole Fraction

Greek Letters

α	Relative volatility
Θ	Time Constant
τ	Dead Time