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## PROCESS DESIGN AND CONTROL

### Dual Composition Control in a Novel Batch Distillation Column

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The newly emerging batch column called the middle vessel column presents the problem of dual composition control similar to the continuous distillation column. The degree of interaction between the two composition control loops can be assessed using the relative gain array technique. This paper presents the RGA analysis for the middle vessel column dual composition control problem. The analysis shows that the interaction between the two loops for this new column is mostly negligible due to the large time constant of the middle vessel. Furthermore, with the middle vessel column, there is a greater likelihood of reducing the interaction between control loops by varying the parameter  $q'$  (the ratio of the vapor rate in the rectification section of the column to the vapor rate in the stripping section of the column).

#### 1. Introduction

Batch processing technologies, specifically batch distillation, have seen a renewed interest in the past few years. This is due in part to the production of low-volume specialty products such as pharmaceuticals as well as the desire for industry to maintain lower raw material inventories. Batch distillation offers increased flexibility over continuous distillation and a variety of operating modes. The two well-known operating modes of a conventional batch distillation column (a rectifier) include (1) constant reflux and variable product composition and (2) variable reflux and constant product composition of a key component. The variable reflux mode is the only candidate for closed-loop composition control. Optimal reflux policy represents the third mode of operation which is neither constant reflux nor constant product composition and usually involves an open-loop control problem. With the advent of new column designs, the number of possible operating modes has increased dramatically. Some of the new column configurations include a batch stripper, a middle vessel column, and a multivessel column. The stripper, similar to the rectifier, can be operated in the constant, variable, or optimal reboil policy modes. The middle vessel column proposed by Bortolini and Guarise<sup>2</sup> is composed of rectifying and stripping sections with a large middle vessel between the two sections. This column was first suggested in the English literature by Devidyan et al.<sup>4</sup> The middle vessel can be operated with even greater flexibility and includes the constant reflux/constant reboil, constant reflux/variable reboil, constant reflux/optimal reboil, variable reflux/constant reboil, variable reflux/variable reboil, variable reflux/optimal reboil, optimal reflux/constant reboil, optimal reflux/variable reboil, and optimal reflux/optimal reboil operating modes. The variable reflux/variable reboil mode of the

middle vessel is similar to a continuous column and, hence, is posed with the challenge of dual composition control.

Meski and Morari<sup>8</sup> compared the performance of the middle vessel column with the conventional batch columns and concluded that the middle vessel was always better in terms of producing a constant product composition with respect to time. These authors also showed that the solution to the maximum product problem for the middle vessel column was one in which the column was operated at steady state, with the composition in the middle vessel equal to the composition of the initial feed charge to the vessel.

Hasebe et al.<sup>7</sup> determined when a middle vessel column will perform better than a conventional batch column. They concluded that the middle vessel column will outperform a conventional column when the heavy impurity is easy to remove as compared to a light impurity. In this case, the column is operated in such a way that the light impurity is taken off the top and the heavy impurity is taken off the bottom. This operation is sustained until the desired product is reached in the middle vessel.

Skogestad et al.<sup>9</sup> analyzed the performance of a multivessel batch distillation column under temperature control. The multivessel column is different from the middle vessel in that the multivessel column will have more than one intermediate holding vessel. The results for this column showed that the steady-state compositions in the intermediate holding vessels could be maintained regardless of the initial feed composition by controlling the liquid rate from the holding vessel so that the temperature of the tray just below the holding vessel remained constant. The control structure was such that proportional controllers could be used and no offset occurred. Thus, as many compositions could be controlled as there are intermediate vessels.

Barolo et al.<sup>1</sup> verify some computation results shown in the literature with an experimental middle vessel column. They show that two of the column levels must be controlled when a middle vessel is used and there is

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no impurity to be removed. In this case, the authors suggest running the column at total reflux and total reboil. The specified products are recovered once steady-state operation has been established. In this case, the control structure is such that the condenser level is maintained with the reflux flow rate and the reboiler level is maintained with the liquid feed rate from the middle vessel. If an impurity is present, the authors suggest two possible control strategies. The first structure is the same as the total reflux case with an additional valve in the bottoms line that controls the bottoms flow rate. The other configuration controls the level in the reboiler with the bottoms flow rate and the ratio of the withdrawal rate from the column to the feed rate to the column is decreased stepwise. The authors show experimental results of the proposed control structures for both dual composition control with an impurity and dual composition control with no impurity.

Although the papers by Skogestad et al.,<sup>9</sup> Hasebe et al.,<sup>7</sup> and Barolo et al.<sup>1</sup> all dealt with various control issues, none of these papers analyzed the specific control interactions between the control loops. The purpose of this paper is to analyze the interactions between the control loops.

Some of the difficulties surrounding dual composition control pertain to the interaction between competing control loops. The degree of interaction can be assessed with the relative gain array technique.<sup>3</sup> This paper presents the RGA analysis of this new column operating in the variable reflux/variable reboil mode. The study is restricted to ideal binary systems so as to separate the complexity associated with the nonideal thermodynamics and the complexity associated with the transient behavior of the new batch distillation column.

The paper is organized as follows: Section 2 briefly describes the dynamic model with the PI controllers for the two composition loops followed by the RGA analysis for the middle vessel column in section 3. Section 4 provides the simulation results validating the theory presented in section 3, and section 5 presents the conclusions.

## 2. Middle Vessel Column Dynamics

The rigorous model for the middle vessel column is presented below. The model is based on the assumptions of negligible vapor holdup, theoretical trays, and adiabatic operation. A schematic for the middle vessel column is shown in Figure 1.

The systems studied assumed ideal binaries, where the separation is based on constant relative volatilities. Thus, an energy balance for the column was not performed, and the constant molar overflow assumption is used.

For the plates, the component balances are written as

$$\frac{dx_j}{dt} = \frac{1}{H_j} [V(y_{j+1} - y_j) + L(x_{j-1} - x_j)] \quad (1)$$

where  $H_j$  is the total molar holdup of tray  $j$ ,  $V$  is the vapor flow rate,  $L$  is the liquid flow rate, and  $y_j$  and  $x_j$  are the mole fractions in the vapor and liquid leaving tray  $j$ , respectively. The plate balances are valid for each plate in the top and bottom sections of the column (numbered from the top). The vapor rate  $V$  is equal to

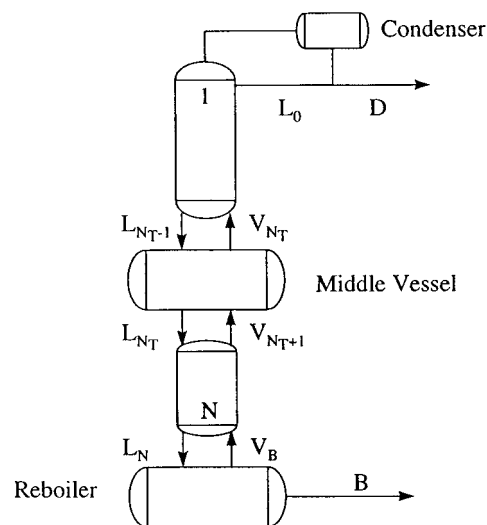


Figure 1. Schematic of middle vessel column.

$V_T$  for the top section of the column and is equal to  $V_B$  for the bottom section of the column. Similarly the liquid flow rate  $L$  at the top is equal to  $L_T$  and the bottom liquid flow rate is  $L_B$ . The overall material balance equation for the plate is eliminated as the constant molar holdup assumption is used.

The material balance around the condenser is described by

$$L_T = RD \quad (2)$$

$$V_T = D(R + 1) \quad (3)$$

and the composition balances are

$$\frac{dx_D}{dt} = \frac{V_T}{H_D} (y_1 - x_D) \quad (4)$$

where  $R$  is the reflux ratio,  $H_D$  is the condenser holdup, and  $x_D$  is the distillate composition.

The material balance for the reboiler is described by

$$V_B = R_B B \quad (5)$$

and the composition balances are

$$L_B = V_B \left( \frac{R_B + 1}{R_B} \right) \quad (6)$$

$$\frac{dx_{BOT}}{dt} = \frac{1}{H_B} [L_B(x_N - x_{BOT}) - V_B(y_{BOT} - x_{BOT})] \quad (7)$$

where  $R_B$  is the reboil ratio. There is one differential equation for each component in the system.

For the middle vessel, the holdup is a function of time; therefore, we have the following equations

$$q' = V_T/V_B \quad (8)$$

$$\frac{dH_m}{dt} = V_B + L_T - V_T - L_B \quad (9)$$

where  $H_m$  is the holdup of the middle vessel and for the components we have

$$\frac{dH_m x_m}{dt} = V_B V_{N_{T+1}} + L_T x_{N_{T-1}} - V_T V_{N_T} - L_B x_{N_T} \quad (10)$$

where  $N_T$  is the middle vessel tray number and  $x_m = x_{NT}$ .

The separation is described by the following vapor–liquid equilibria.

$$y_j = \frac{\alpha x_j}{(\alpha - 1)x_j + 1} \quad (11)$$

where  $\alpha$  is the relative volatility.

The column is operated initially at the total reflux and total reboil condition ( $L = V$  for both sections of the column). Before the startup operation, the feed is charged from the top so that initially the middle vessel composition as well as the composition on each plate is equal to the feed composition. Once the steady state is reached at the total reflux condition, the normal operation is started with the following controllers.

The controllers used in the simulation studies are simple proportional–integral controllers. These controllers are described by the following equations.

$$R = R^* + K_{cl} \left[ e_T + \frac{1}{\tau_{I1}} \int e_T dt \right] \quad (12)$$

$$R_B = R_B^* + K_{c2} \left[ e_B + \frac{1}{\tau_{I2}} \int e_B dt \right] \quad (13)$$

$$e_T = (x_D^* - x_D) \quad (14)$$

$$e_B = (x_{BOT}^* - x_{BOT}) \quad (15)$$

where  $K_c$  is the gain for the controller and  $\tau_I$  is the integral time constant for the controller. These parameters are determined off-line before the simulations are performed. In each case, the setpoint values for the reflux and reboil ratios are taken from the previous time step. The setpoints for the distillate and bottoms compositions are fixed for all time. For the cases where the controller predicted negative values for the reflux or the reboil ratio, the corresponding reflux/reboil ratio is replaced by a small fixed value. Since the levels in the condenser and reboiler are assumed to be constant, no controller equations are included for these variables.

### 3. Relative Gain Array Analysis

The interaction between the control loops can be determined by evaluating the relative gain array (RGA). If the liquid holdup on each plate is negligible as compared to the holdup in the middle vessel, then the batch distillation column can be considered as a continuous distillation column with changing feed at each time step. This assumption leads to the semirigorous model (Diwekar<sup>5</sup>) for the batch distillation column. It is also assumed that the holdups of the condenser and reboiler are negligible compared to the holdup of the middle vessel. This assumption is followed by deriving the expression for the RGA at each time step. The detailed derivation for binary mixtures is presented below.

The minimum number of trays in the rectifying section of the middle vessel column can be described by

$$\frac{\ln \left[ \frac{x_D}{1 - x_D} \frac{1 - x_m}{x_m} \right]}{\ln \alpha} = N_{\min}^T \quad (16)$$

Rearranging this expression and solving for  $x_D$  yields

$$x_D = \alpha^{N_{\min}^T} \frac{x_m}{1 - x_m} (1 - x_D) \quad (17)$$

Defining the separation factor  $S_T$  for the top of the column as

$$S_T = \alpha^{N_{\min}^T} \quad (18)$$

and solving for  $x_m$  yields

$$x_m = \frac{x_D / S_T}{1 + \left( \frac{1}{S_T} - 1 \right) x_D} \quad (19)$$

By the same reasoning, a separation factor for the bottom of the column can be defined by

$$S_B = \alpha^{N_{\min}^B} \quad (20)$$

Solving for  $x_m$  yields

$$x_m = \frac{S_B x_{BOT}}{1 + x_{BOT} (S_B - 1)} \quad (21)$$

Using the separation factors for the top and the bottom of the middle vessel column, we can define a separation factor for the entire column. Thus, the overall separation factor  $S_{TOT}$  is

$$S_{TOT} = \alpha^{N_{\min}^B + N_{\min}^T} \quad (22)$$

or

$$S_{TOT} = \frac{x_D}{1 - x_D} \frac{1 - x_{BOT}}{x_{BOT}} \quad (23)$$

The degree of interaction between the distillate and bottoms control loops will be determined by the use of the relative gain array (RGA) technique. The RGA is defined by Bristol<sup>3</sup> as the ratio of the open-loop gain to the closed-loop gain and is designated as  $\Lambda$ . This can be written for the middle vessel batch distillation column.

$$\Lambda|_t = \frac{\left. \frac{dR}{dx_D} \right|_{x_{BOT}}}{\left. \frac{dR}{dx_D} \right|_{R_B}} \quad (24)$$

Since this is a two by two system, it is only necessary to evaluate one of the interaction parameters  $\Lambda$  and all the others can be determined from that. The zero holdup model for the middle vessel involves differential mass balance equations for the middle vessel and a quasi-steady-state assumption for the rest of the col-

umn. Therefore, the dynamics of the middle vessel are described by

$$-\frac{dH_m}{dt} = \frac{V_T}{R+1} + \frac{V_B}{R_B} \quad (25)$$

$$-\frac{H_m}{\Delta t}(x_m - x_{m,old}) = \frac{V_T}{R+1}(x_D - x_m) + \frac{V_B}{R_B}(x_{BOT} - x_m) \quad (26)$$

Rewriting (25) in discrete form and substituting into (26) yields

$$-\frac{H_m - H_{m,old}}{\Delta t}x_m - \frac{H_m}{\Delta t}(x_m - x_{m,old}) = \frac{V_T}{R+1}x_D - \left[ \frac{H_m - H_{m,old}}{\Delta t} + \frac{V_T}{R+1} \right]x_{BOT} \quad (27)$$

Rearranging (27) for  $R$  and differentiating with respect to  $x_D$  at constant  $x_{BOT}$  yields

$$\left. \frac{dR}{dx_D} \right|_{x_{BOT}} = \frac{\left[ \frac{H_m}{\Delta t} + \frac{H_m - H_{m,old}}{\Delta t} \right] \frac{dx_m}{dx_D} + \frac{V_T}{R+1}}{\frac{V_T}{(R+1)^2}(x_D - x_{BOT})} \quad (28)$$

It is assumed in the derivation above that the change in the distillate composition with respect to the mass holdup in the middle vessel is negligible. This is the numerator for the relative gain array. Rearranging (27) for  $R$  and differentiating with respect to  $x_D$  at constant  $R_B$  yields

$$\left. \frac{dR}{dx_D} \right|_{R_B} = \frac{\left[ \frac{H_m - H_{m,old}}{\Delta t} + \frac{H_m}{\Delta t} \right] \frac{dx_m}{dx_D} + \left[ \frac{V_B}{R_B} \right] \frac{dx_{BOT}}{dx_D}}{\frac{V_T}{(R+1)^2}(x_D - x_{BOT})} \quad (29)$$

This is the denominator for the relative gain array. In order to evaluate the RGA, we must determine the two remaining differential equations. Differentiating  $x_m$  with respect to  $x_D$  in (19) yields

$$\frac{dx_m}{dx_D} = S_T \left[ \frac{x_m}{x_D} \right]^2 \quad (30)$$

Differentiating  $x_{BOT}$  with respect to  $x_D$  in (26) yields

$$\frac{dx_{BOT}}{dx_D} = S_{TOT} \left[ \frac{x_{BOT}}{x_D} \right]^2 \quad (31)$$

Finally, substituting (30) into (28), (30) and (31) into (29), and (28) and (29) into the relative gain array expression, we get

$$\Lambda|_t = \frac{\left[ \frac{H_m}{\Delta t} + \frac{\Delta H_m}{\Delta t} \right] \frac{dx_m}{dx_D} + \frac{V_T}{R+1}}{\left[ \frac{H_m}{\Delta t} + \frac{\Delta H_m}{\Delta t} \right] \frac{dx_m}{dx_D} + \left[ \frac{V_B}{R_B} \right] \frac{dx_{BOT}}{dx_D}} \quad (32)$$

It can be seen that the middle vessel holdup  $H_m$  has to be significantly greater than  $|\Delta H_m|$  (except toward the end of simulation when the middle vessel starts drying)

**Table 1. Controller Parameters for Fixed Tuning**

$q'$	distillate		bottoms	
	$K_c$	$\tau_1$	$K_c$	$\tau_1$
0.1	2.5155	0.001	2.9124	1.8188
0.2	1.0277	1.0141	1.0126	1.0106
0.5	3.326	0.79268	0.64971	0.018124
1.0	1.0004	1.0001	1.0002	1.0001

resulting in the following equations.

$$\frac{H_m}{\Delta t} \gg \left| \frac{\Delta H_m}{\Delta t} \right| \quad (33)$$

$$\frac{H_m}{\Delta t} \gg \frac{V_T}{R+1} \quad (34)$$

$$\frac{H_m}{\Delta t} \gg \frac{V_B}{R_B} \quad (35)$$

From the above equations and the RGA expression (eq 32), it is obvious that the first square bracket term in the numerator and the denominator of the RGA expression dominates the expression. Therefore, the RGA is near unity, signifying negligible interactions between the two loops. Furthermore, it should be remembered that whenever  $V_T/(R+1)$  is greater than  $[V_B/R_B] dx_{BOT}/dx_D$ , the resulting RGA is above one suggesting a possibility of controller instability. However, this can be easily taken care of by manipulating the variable  $q'$ . The following section presents the numerical simulation results which support the above argument.

#### 4. Numerical Simulations

Simulation studies were performed to determine the flexibility of the middle vessel column for the purpose of dual composition control. Two separate cases were run: one where a single set of tuning parameters was used for the entire run and the other where two sets of tuning parameters are used. The aim of the two types of tuning was to show that the interactions are negligible in the two composition loops. The simulation results also present the effect of  $q'$  on the dual composition control.

As stated earlier, a middle vessel column is controlled with two proportional–integral (PI) controllers. Various other control structures were considered in ref 1. The tuning parameters for these controllers were determined a priori using a nonlinear programming optimizer based on sequential quadratic programming (SQP). The values of the controller gains and integral time constants for each of the simulations are shown in Tables 1 and 2 assuming that the composition is always known. In an actual column, the composition would either have to be analyzed directly or estimated from the temperature in the column. In either case, there would be deadtimes associated with the corresponding measurements and the model would have to be adjusted accordingly. Once the model is changed, the optimization routine will inevitably return with different controller tuning parameters from those shown below. Since we are more interested in analyzing the interactions in the control loops as opposed to estimating the actual compositions, the compositions were assumed to be known.

The objective of the optimization problem was to minimize the sum of the squares of the errors between the distillate composition and its setpoint and the

**Table 2. Controller Parameters for Scheduled Tuning**

$q'$	first half of batch				second half of batch			
	distillate		bottoms		distillate		bottoms	
	$K_c$	$\tau_I$	$K_c$	$\tau_I$	$K_c$	$\tau_I$	$K_c$	$\tau_I$
0.1	1.6307	0.58351	2.0766	1.2531	1.5649	0.16385	1.2047	0.78651
0.2	1.0215	1.0101	1.0119	1.0116	1.0137	0.99899	0.99691	1.0041
0.5	3.1686	0.049264	0.5716	0.14761	3.2959	2.0658	0.82403	0.60124
1.0	2.8412	0.063295	1.8666	0.67698	2.0386	0.001	0.92315	1.0732

**Table 3. Value of Objective Function: Sum of Squares of Errors**

$q'$	fixed tuning	scheduled tuning
0.1	0.009 773 1	0.017 380
0.2	0.029 365	0.029 567
0.5	0.027 997	0.029 504
1.0	0.374 86	0.329 72

bottoms composition and its setpoint. Bounds were placed on all of the tuning parameters so that an appreciable amount of product would be obtained at the end of the run. The values of the objective functions for the simulations are shown in Table 3.

We see that, in both cases, the objective function was best for the case where the value of  $q'$  is smallest and worst for the case where the value of  $q'$  is largest. The intermediate values of  $q'$  show similar trends.

The objective of the control scheme is to simultaneously control the distillate and bottoms compositions. Since this is a batch column, the changing composition in the middle vessel is treated as the disturbance to the system. The level control in the condenser and the reboiler is assumed to be perfect. The holdup on the trays was also assumed to be constant. The resulting system then corresponds to the semi-rigorous model as described in ref 5. A degrees of freedom analysis for the middle vessel column can also be found in ref 5. The resulting degrees of freedom analysis shows that there are six possible manipulated variables: the vapor flow rate in the rectification section ( $V_T$ ), the vapor flow rate in the stripping section ( $V_B$ ), the reflux ratio ( $R$ ), the reboil ratio ( $R_B$ ), the number of trays in the rectification section, and the number of trays in the stripping section. Since the vapor flow rates in the rectification and stripping sections are fixed and the number of trays are fixed, the only remaining manipulated variables are the reflux and reboil ratios.

The ratio of the vapor rates in the rectifying and stripping sections of the middle vessel column could be an additional control variable. Although we looked at various values of  $q'$ , we did not specifically use  $q'$  as another control variable. An additional product stream could be drawn from the middle vessel and the  $q'$  ratio could be used to control the composition in the vessel. Thus, the RGA matrix would have nine  $\Lambda$ 's as opposed to four for the dual composition case. The  $q'$  could also be used as a variable in the optimization routine, as will be seen in the results presented below.

In all the test cases, the column specifications and the feed composition specifications were the same. A ten-tray column with five trays in the rectification section and five trays in the stripping section was used. The initial feed charge to the middle vessel was 100 mol of a mixture containing 70% A and 30% B. The feed was distributed throughout the column in such a way that the plate holdup is 1 mol on each tray and the remaining charge was in the middle vessel. The vapor

**Table 4. Accumulated Products and Compositions for Fixed Tuning**

$q'$	distillate		bottoms	
	accumulated	avg. comp.	accumulated	avg. comp.
0.1	22.5879	0.9515	10.4655	0.946
0.2	20.2883	0.9511	9.1671	0.944
0.5	19.8328	0.9522	4.0106	0.9434
1.0	26.2942	0.9433	0.6454	0.9016

**Table 5. Accumulated Products and Compositions for Scheduled Tuning**

$q'$	distillate		bottoms	
	accumulated	avg. comp.	accumulated	avg. comp.
0.1	22.8940	0.951	12.7955	0.9424
0.2	20.4023	0.9505	9.0965	0.9445
0.5	20.1506	0.9521	3.8209	0.9439
1.0	19.5390	0.9507	0.4443	0.9023

rate in the rectification section of the column  $V_T$  was fixed at 10 mol/h, and the vapor rate in the stripping section of the column  $V_B$  was calculated from the  $q'$  equation. Various binary systems having volatilities ranging from 1.5 to 3.0 and setpoints varying from 0.95 to 0.98 were considered for the case studies. The following paragraphs describe the results for a case where the relative volatility is 2.0 and the setpoints for both of the compositions are 0.95.

The amounts of distillate and bottoms collected and the average compositions of these fractions are shown in Tables 4 and 5.

Figure 2 shows the distillate and bottoms composition profiles for the batch run where the tuning parameters were fixed for the duration of the run. It should be noted that the initial distillate composition for all of the runs is approximately constant whereas the bottoms composition varies. This is due to the fact that the vapor flow rate in the rectification section is the same in each case and the vapor flow rate in the stripping section is different. As can be seen in Table 4, both the controllers are very effective for  $q'$  values less than 1. Furthermore, it can be seen that changes in  $q'$  can change the control action significantly. For example, in Figure 2 the bottom composition profile for  $q' = 1$  takes longer to reach the setpoint as compared to other values of  $q'$ . A  $q'$  value greater than 1 means that the temperature of the middle vessel is greater than the bubble point temperature of the feed. Thus, more of the feed is vaporized. A  $q'$  less than 1 means that the temperature is lower than the dewpoint temperature of the vapor entering the middle vessel. Thus, some of the entering vapor is condensed. A  $q'$  equal to 1 means that the liquid in the middle vessel is at its bubble point.

Figure 3 shows the profiles for the reflux ratio and the reboil ratio necessary to obtain the composition profiles in Figure 2. The column was first run in the total reflux mode for 1 h before the normal operation began. Once the normal operation started, the reflux ratio was set to 2.2 and the reboil ratio was set to 20.

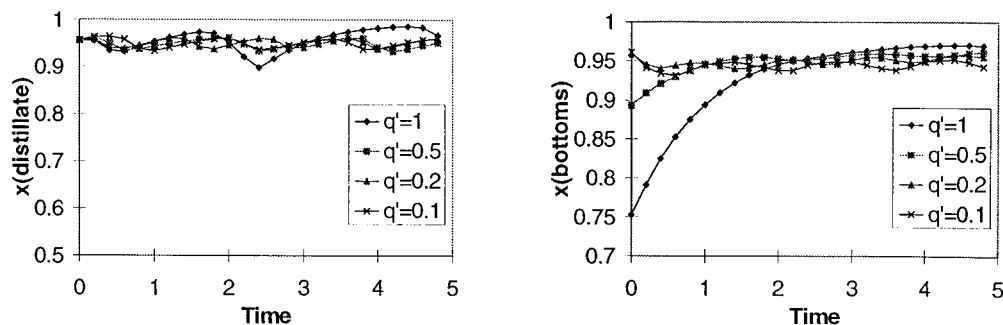


Figure 2. Distillate and bottoms compositions with fixed tuning.

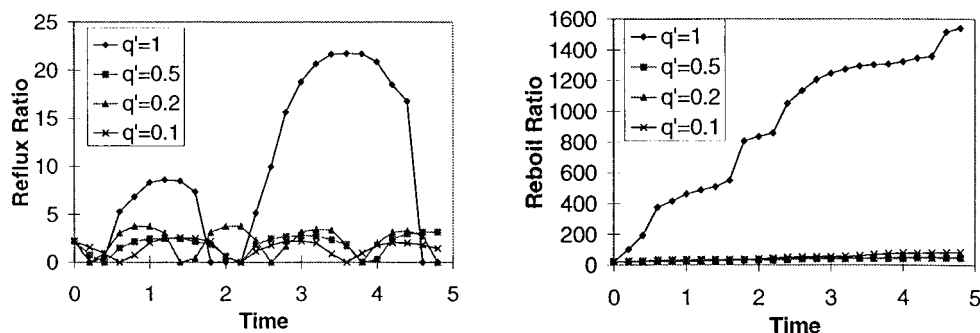


Figure 3. Reflux and reboil ratios with fixed tuning.

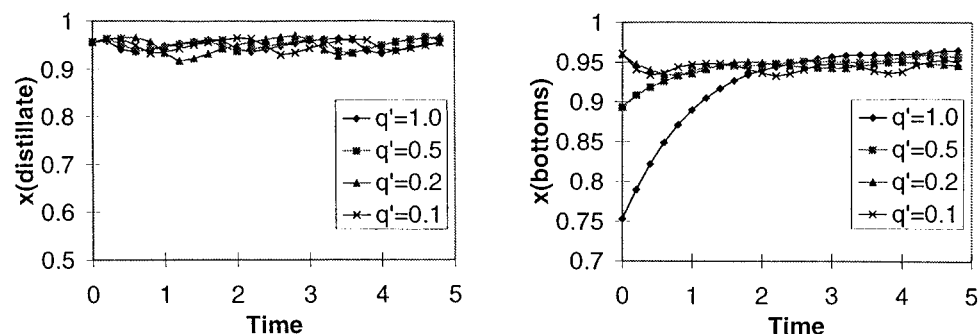


Figure 4. Distillate and bottoms compositions with scheduled tuning.

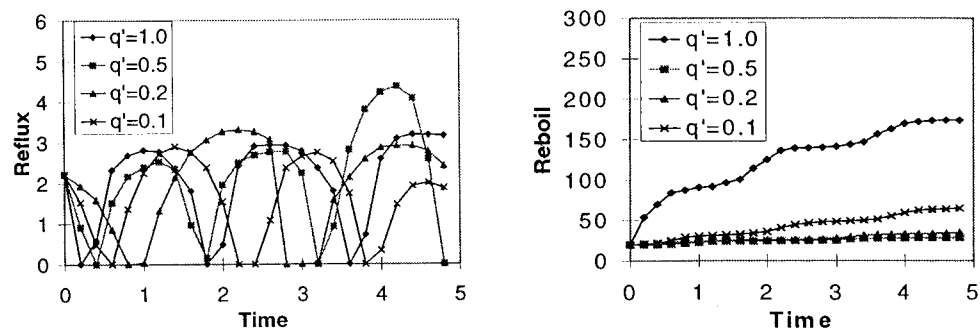


Figure 5. Reflux and reboil ratios with scheduled tuning.

It has been shown in the case of a batch rectifier that using one set of tuning parameters over the entire batch run may not be as effective as scheduling the tuning parameters (Finefrock et al.<sup>6</sup>). Simulation studies were performed to determine whether or not better composition control could be achieved by varying the tuning parameters at intermediate times during the batch run. The batch time was divided into two equal sections, and the optimal tuning parameters were determined for each section. Figure 4 shows the distillate and bottoms compositions for the scheduled tuning run. The parameters for the simulation are the same as those of the previous example. It is difficult to tell from this

example whether or not gain scheduling does in fact provide better control. However, by comparing the results in Tables 4 and 5, we see that the amounts of accumulated products and their corresponding compositions are similar in all cases except for  $q' = 1$ . For  $q' = 1$ , the scheduled tuning results show distillation compositions that are within specifications as opposed to the fixed tuning where the resulting product is below specification. Although, the amount of product is less in the scheduled case than in the fixed case. Also, the composition of the bottoms product is slightly greater in the scheduled case than in the fixed case, again with less accumulation. These results seem to suggest that

scheduled tuning may be advantageous for simulations involving larger values of  $q'$ . Simulation results from the case where the setpoints are 0.98 indicate that gain scheduling does in fact provide better control.

The corresponding reflux and reboil ratio profiles are shown in Figure 5. In all the cases significant changes in the values of the reflux ratios are observed as compared to the reboil ratio profiles. For example, in the case of  $q'$  equal to 1.0, the reflux ratio profile and hence the distillate composition profile is changed considerably. However, the bottom composition profile is not affected by this change, supporting the earlier argument that in a middle vessel column the interaction between the control loops is mostly negligible. As expected, the RGAs for the two cases are found to be closer to unity. In all our studies, a similar behavior was observed. Very rarely the RGA at some time step for a specific  $q'$  was found to be higher than 1 (making the complimentary RGA negative). However, the control interactions remained unaffected as the negative RGA is found to be significantly small.

## 5. Conclusion

The batch distillation middle vessel column is similar to the continuous distillation column and faces the problem of dual composition control when operated in the variable reflux and variable reboil mode. There are cases when dual composition control will not work, and the analysis of the RGA is used to determine which combinations of controlled and manipulated variables are not realistic. As the holdup in the middle vessel becomes on the order of the holdup on the plates, the decoupling effect of the middle vessel will be lost. For tight composition objectives, this will probably not happen because the batch run will be much shorter than that for loose composition objectives. Thus, the amount of accumulated products will be smaller for tight objectives as opposed to loose objectives. This paper analyzed the interactions of the two composition control loops in this newly emerged batch distillation column. At first, the relative gain array expression for each time step is derived for this new column dual composition control. It was shown that the RGAs for this column are likely to be closer to 1 because of the large time constant of the middle vessel column. The simulation studies confirm the interactions between the two loops to be negligible and the RGAs to be closer to unity for all the time steps. It was observed that the variable  $q'$ , the ratio of vapor rate for the top section to the vapor rate for the bottom section of the column, plays an important role in control action. Further, the scheduled tuning appeared to perform better than fixed tuning.

The analysis of the interactions between the control loops will become more difficult as the assumption of perfect level control in the condenser and reboiler is dropped and the ratio of the vapor flow rate in the rectification section to the vapor flow rate in the stripping section is allowed to vary. This will provide a number of different possible control strategies that were not available previously. By dropping this assumption, we would be able to analyze the control structures suggested in ref 1. There would then be five possible control valves to control the two objectives as opposed to the two control valves to control the two objectives as seen in this paper.

A detailed analysis of all of the possible controller pairings would have to be investigated in order to determine which of the possible pairings is best for a given set of components and feed conditions.

## Nomenclature

- $B$ : bottoms flow rate (mol/h)
- $D$ : distillate flow rate (mol/h)
- $e_B$ : error used in the bottom composition controller equations
- $e_T$ : error used in the distillate composition controller equations
- $H_m$ : holdup in the middle vessel (mol)
- $K_C$ : proportional gain for the controller
- $L_B$ : liquid flow rate in the stripping section (mol/h)
- $L_T$ : liquid flow rate in the rectification section (mol/h)
- $N_B$ : number of trays in the stripping section
- $N_T$ : number of trays in the rectification section
- $N_{\min}^B$ : minimum number of trays in the stripping section
- $N_{\min}^T$ : minimum number of trays in the rectification section
- $q'$ : ratio of  $V$  and  $V_B$
- $R$ : reflux ratio
- $R_B$ : reboil ratio
- $S_B$ : separation factor for the bottom of the column
- $S_T$ : separation factor for the top of the column
- $S_{TOT}$ : separation factor for the entire column
- $\tau_I$ : integral time constant for the controller (h)
- $V_B$ : vapor flow rate in the bottom section of the column (mol/h)
- $V_T$ : vapor flow rate in the top section of the column (mol/h)
- $x_{BOT}$ : composition of the light key component in the bottoms
- $x_D$ : composition of the light key component in the distillate
- $x_m$ : composition of the light key component in the middle vessel
- $\alpha$ : ratio of the relative volatility of component B to component A
- $\Lambda$ : relative gain array parameter

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