

Time (Energy) Requirements in Closed Batch Distillation Arrangements

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Abstract

Batch time (energy) requirements comparisons are provided for the separation of a ternary zeotropic mixture in three closed batch column configurations. Two multivessel column arrangements, with and without vapor bypass, and a regular batch column (rectifier) operated under the cyclic policy, were studied. First, the improvement achieved in the middle vessel dynamics by elimination of the vapor bypass is exhibited, through a base case study. The proposed modified multivessel column requires 30% less time than the conventional one, mostly studied in the literature. Next, the effect of the feed composition and product specification on the time requirements is discussed. The multivessel arrangements perform always better than the cyclic column, which requires from 35% - 100% more time to perform a given separation. All results are based on dynamic simulations of the processes.

1. Introduction

Batch distillation is known to be less energy efficient than its continuous counterpart. However, it has received renewed interests last years due to the flexibility it offers. In a batch column, multicomponent mixtures can be separated in one single column and variations in the feed, the separation difficulty and the product specifications can be handled efficiently. This makes batch distillation especially suitable for pharmaceutical, fine and specialty chemicals industry where the product demand and lifetime is both time varying and uncertain.

Following these trends, new batch column configurations, like the multivessel column, and non-conventional operation modes, like closed operations, has received lately strong attention both in the industry and the academia. In this work, two different multivessel column configurations are compared to a regular batch column (rectifier) in terms of batch time (energy) requirements. The results are based on dynamic simulations on the separation of a zeotropic system. To the best of our knowledge, this is the first study where the dynamics in the middle vessel of a multivessel configuration are discussed in detail, and two different multivessel configurations are compared to each other and to a conventional batch rectifier.

The multivessel batch column can be viewed as a generalization of a batch rectifier and a batch stripper. The column has both a rectifying and a stripping section and therefore it is possible to obtain a light and a heavy fraction simultaneously from the top and the bottom of the column, while an intermediate fraction is also recovered in the middle vessel. Two modifications of the multivessel are studied here. The first one is the vapor bypass modification in which the vapor from the stripping section bypasses the middle vessel and enters the rectifying section, as shown in Figure 1a. We refer to this configuration as conventional multivessel, since it is the one mostly studied in the

literature. The second multivessel configuration is the one where both the liquid and the vapor streams enter the middle vessel. This configuration is illustrated in Figure 1b and we refer to this one as modified multivessel. The third column, is a regular batch column (rectifier) operated with the cyclic policy. This column is called cyclic column and is shown in Figure 1c.

All columns are operated as closed systems, which simply means that there are no distillate or bottom streams out from the columns. The final products are accumulated in the vessel and discharged when the specifications are satisfied. In the multivessel column a ternary mixture can be separated simultaneously in one such close operation. No product change-overs are required and all products are accumulated in the three vessels at the end of the process. In the closed cyclic column the separation is sequential. The products are separated one at each time and for a ternary mixture a sequence of two such closed operations is needed. The sequence chosen here resembles to the direct split in continuous columns.

From the practical point of view, closed operation modes are preferable over traditional open operation modes, like constant reflux or constant distillate or optimal reflux ratio policies. The closed operation mode requires minimum operator intervention and monitoring. There is also a definite distinction between the product change-overs and it is easier to assure the product qualities. Surprisingly, closed operation modes can also exhibit advantages in terms of separation time or energy requirements. Sorensen and Skogestad (1994) studied the performance of the cyclic column compared to conventional open operation strategies and they found that the cyclic column requires significantly less batch time for difficult separations where a small amount of light product is to be recovered. In some cases the reduction in the operating time was more than 30%, which simply indicates the potential energy savings by changing the

operating policy. Sorensen and Prenzler (1997) applied the cyclic policy in an experimental batch column and they highlighted its much simpler operation and control. Noda et al. (1999) and Hasebe et al. (1999) provided comparisons between the cyclic column (referred as total reflux column in their work) and a rectifier or a stripper for a constant relative volatility system. They showed that the cyclic column performs equal or better than the other two columns when the operation in all columns is optimized.

Comparisons between the multivessel column and the regular (rectifier) batch column has also been provided in the literature. In a series of papers, Hasebe et al (1995, 1997 and 1999) investigated optimal operating modes for the multivessel column and compared the novel column with both batch rectifiers and continuous columns. The energy consumption of the multivessel was almost half of that of a rectifier. Wittgens and Skogestad (1998) also reached the same conclusion “a reduction of energy consumption of approximately 50% was found when using a multivessel column instead of a conventional batch distillation column”. The superiority of the multivessel column over the batch rectifier was further justified by the work of Furlonge et al. (1999). The regular column required twice as much mean rate energy consumption as those of the multivessel for the separation for an equimolar quaternary ideal mixture.

Finally, Hilmen (2000) provided a detailed comparison between the multivessel and the cyclic column (referred as cyclic 2-vessel column) when both columns are operated as closed systems. The indirect split case was studied. The multivessel column required less operating time than the conventional batch column operated in two closed cycles. The time savings by using the multivessel were largest for difficult separations, reaching a total of 50%.

This paper is structured as follows. First, the model used in our simulation will be briefly presented along with the necessary information about the simulation procedure.

After this, the paper is divided in two parts. In the first part, the results for the base case of equimolar feed are presented. The way the mixture is separated in the different column configurations is explained. Then, the batch time comparisons are given. Emphasis is given to the elimination of the vapor bypass in the conventional multivessel. The great effect of this design modification in the dynamics of the middle vessel, and consequently the time requirements is discussed. In the second part of the paper, the effect of feed composition and product specification is investigated. Feeds rich in light, intermediate and heavy component are studied and the subsequent changes in the time requirements are presented. The paper ends with some concluding remarks.

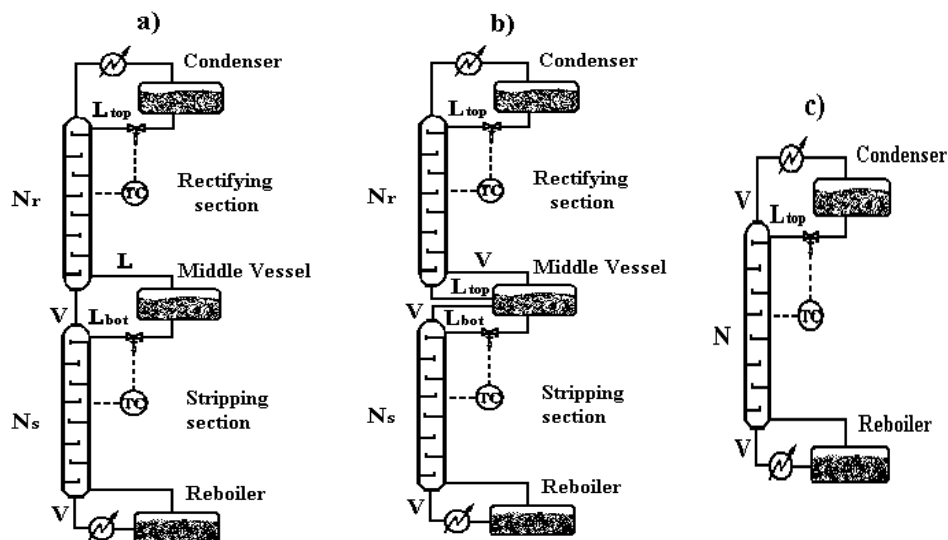


Figure 1. a) Conventional multivessel column with vapor bypass
b) Modified multivessel column without vapor bypass
c) Cyclic (2-vessel) column

2. Simulations

2.1 The model

The model used in our simulations consists of: overall and component material balances, vapor-liquid equilibrium modeled by NRTL activity coefficient model with binary parameters taken from the DECHEMA series, temperature estimations in each stage by a bubble point calculation under constant atmospheric pressure. The following assumptions have been made: staged column sections, constant vapor flows, constant liquid holdup on all stages, negligible vapor holdup, perfect mixing and equilibrium in all stages and ideal vapor phase.

The resulting mathematical model takes the form of a set of differential and algebraic equations (DAE system) with a total of $(N_c+1)*(N_T+3)$ state variables, where N_c is the number of components and N_T is the total number of stages in the column sections plus the vessels. The resulting DAE system is solved in Matlab with the DAE solver ODE15s.

2.2 Simulation aspects

Batch time (energy) comparisons are provided for the separation of a zeotropic system. The system under consideration is a ternary mixture of methanol/ethanol/1-propanol. A quick rough estimation of the relative volatilities of the system (4.4,2.3,1) indicates a medium difficulty separation. However, the assumption of constant relative volatilities is not used in our model and this is the reason we avoid the term 'ideal' mixture and we prefer the term 'zeotropic' which is used instead throughout the paper.

We consider batch time, as a direct indication of energy consumption since the heat input (boilup) in the reboiler is constant. In order to minimize batch time, all columns are operated at maximum boilup (reboiler capacity). Thus, in this work the vapor flow is

constant and equal in all three columns. The ratio of the vapor flow relative to the initial feed (V/F) is a measure of how many times the feed is boiled every hour. This is chosen to be close to unity (once per hour) and is the same for both the multivessel and the cyclic column.

Theoretically, the minimum batch time is achieved for infinite number of stages. In practice, in our simulations, each column section has sufficient number of trays for the given separation and therefore the time calculations are not depended on the number of stages. Same number of stages was used in both the conventional multivessel and the cyclic column. Thus, the number of stages in the cyclic column is the sum of the stages in the two sections of the multivessel. The modified multivessel has one stage less than the conventional since the middle vessel is actually an additional equilibrium stage in this case. Simulation data for all three columns are given in the Appendix.

The effect of the column liquid holdup is not included in this study. All columns have constant very small liquid holdup negligible compared to the initial feed (total 2% of the charge). In practice, this means that almost all the initial charge is recovered in the vessels at the end of the process. It also means that the dynamics inside the column sections are neglected and a change in the holdup in one of the vessel is almost instantaneously anticipated by a change in the holdup of another vessel.

The initial distribution of the feed in the vessels affects the separation time and no try has been done in this work to optimize the initial feed distribution in the vessels. However, our simulation experience indicates that it either optimal or close to optimal, in terms of minimum batch time, to charge most of the feed in the reboiler. In the multivessel column, 94% of the total charge is fed in the reboiler, 5% in the middle vessel and only 1% in the top vessel. In the cyclic column, 99% if the charge is fed in the reboiler and 1% in the top vessel. Hasebe et al. (1995 and 1999) and Furlonge et al.

(1999) provide optimization studies on this issue. In many cases the simple 'feed in the reboiler' policy proved to be either optimal or close to optimal for the closed multivessel. In his experimental work in the multivessel column Wittgens (1999) found that it is easier to establish a good initial composition profile in the column by charging the feed in the reboiler. Finally, this feed policy resembles to the one used in the batch rectifier or the cyclic column with the feed charged in the reboiler. Based again on our simulation experience, the worst is to charge the feed in the middle vessel, while an equal distribution of the feed in the vessels is close to the 'feed in the reboiler' policy. The results from Hilmen (2000) also support this simple feed policy. In case of thermal decomposition or thermal sensitivity of the products it is wise to avoid the 'feed in the reboiler' policy and implement other feed policies.

Four different feed compositions are considered. The base case presented first is for an equimolar feed. After the base case, feeds rich in light, intermediate and heavy component will be subsequently discussed. In the simulations initial compositions in all stages are equal to that of the feed mixture $x_{i,n}=z_F$ and initial temperature estimations are that of the feed in boiling conditions. The solver ODE15s in Matlab was proved to be very robust in initializing the simulations in all cases and no problems were experienced, on this issue.

A simple indirect level control in the vessels based on temperature feedback control loops is implemented in all columns, as proposed by Skogestad et al. (1997). The feasibility of this control strategy was verified for ideal mixtures both by simulations and experiments in the multivessel column by Wittgens et al. (1996). The same simple control approach can be implemented for the cyclic column, as shown in Figure 1c, and it is surprising that only Hilmen (2000) has implemented this control scheme in a regular column. The main advantage of this feedback control strategy is the robustness

in facing uncertainties in the feed composition. Furlonge et al. (1999) agreed on this issue but mentioned that this method is not always the best in terms of batch time (energy) consumption. The temperature measurements for the T-controllers are situated in the center of the column section for both the multivessel and the cyclic column, as shown in Figure 1. Temperature setpoints are set to the average of the boiling point of the two components separated in this column section.

The criterion for terminating the simulations was the fulfillment of the product specifications in the vessels. However, the product recoveries are also an important factor. In order to obtain comparable results, we tried to take care of the recoveries in the vessels but this was not always possible because of the different way the separation is performed in the columns. The separation is simultaneous in the multivessel and sequential in the cyclic column, which implies that it is much easier to handle the recoveries of the products, independently, in the cyclic column

The batch time calculations do not include charging of the columns, preheating, product discharging and shutdown. These are considered to be the same for both the multivessel and the cyclic column. The only exception is the product discharging period, which is higher for the cyclic column because of the time required to discharge the top vessel holdup between the two cycles. This is an additional advantage for the multivessel column.

3. Results

A) Base case - Equimolar feed

The system methanol/ethanol/1-propanol is studied. An equimolar feed $z_F=[1/3,1/3,1/3]$, which is mainly placed in the reboiler, is considered and will be used as a base case in our work. Since this system exhibits no azeotropic behavior, the separation is proceeding according to the boiling temperatures of the components.

In the conventional multivessel column (Fig. 1a) the mixture is separated simultaneously in one closed operation. The three components are accumulated in the vessels at the end of the process. Methanol is the light component and is recovered in the top vessel, while ethanol and 1-propanol are the intermediate and heavy components recovered in the middle and bottom vessel, respectively. Figure 2 shows how the separation is evolving with time. The top vessel is steadily enriched in methanol, the middle vessel in ethanol and the propanol is staying in the bottom vessel. The column liquid profile, at the end of the process, is also shown with open circles. The rectifying (top) section of the column is performing the binary separation between methanol and ethanol. The top section liquid profile is therefore in the binary edge between methanol and ethanol. The stripping (bottom) section of the column is performing the binary separation between ethanol and 1-propanol and the bottom liquid profile is mainly in the binary edge between these two components.

The separation is performed exactly in the same way in the modified multivessel column (Fig. 1b). One closed operation is needed and the final products are simultaneously accumulated in the vessels. The reason for investigating this new multivessel configuration will become evident later after the analysis of the dynamics in the vessels.

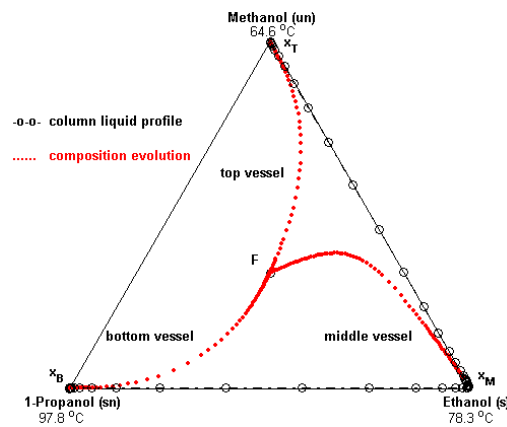


Figure 2. Simultaneous separation of a zeotropic mixture in the multivessel column

In the cyclic column (Fig 1c) the separation is proceeding differently. The column has two vessels, which means that it is not possible to separate all three components simultaneously, as in the multivessel. Two closed operations, which will be called cycles hereafter, are needed and the separation resembles to the direct split in continuous columns. During Cycle 1 the light component (methanol) is accumulated in the top vessel, as shown in figure 3a. The still (bottom vessel) is following a linear path away from the component (methanol) accumulated in the top vessel. Cycle 1 is terminated when the specification for methanol is fulfilled. Then the vessel is emptied and the accumulated methanol is discharged in the product tank, instantaneously. A small amount of methanol still remains in the column and can contaminate the future products. Thus, a small off-cut fraction has to be removed. The off-cut fraction is a closed operation operated for very short time with the same indirect level control and control parameters same as for the second cycle. The off-cut fraction removed from the top vessel is equal to the total column's holdup (0.1 kmol). Cycle 2 is, then, an almost binary separation of the two components (ethanol and 1-propanol) left in the still (x_{F1} in

fig. 3a). The intermediate component (ethanol) is accumulated in the top vessel, while the heaviest one (1-propanol) remains in the still, as shown in figure 3b.

The simulations were terminated when the composition specifications for all the products in the vessels were fulfilled. Results are provided for three specification sets. $x_{\text{spec}}^1 = [0.99, 0.97, 0.99]$, $x_{\text{spec}}^2 = [0.99, 0.99, 0.99]$ and $x_{\text{spec}}^3 = [0.995, 0.995, 0.995]$. In the second set, the specification in the middle vessel is becoming stricter (0.97 to 0.99). In the third set the specifications are tighter in all vessels (0.99 to 0.995). The results are presented in the following Table 1.

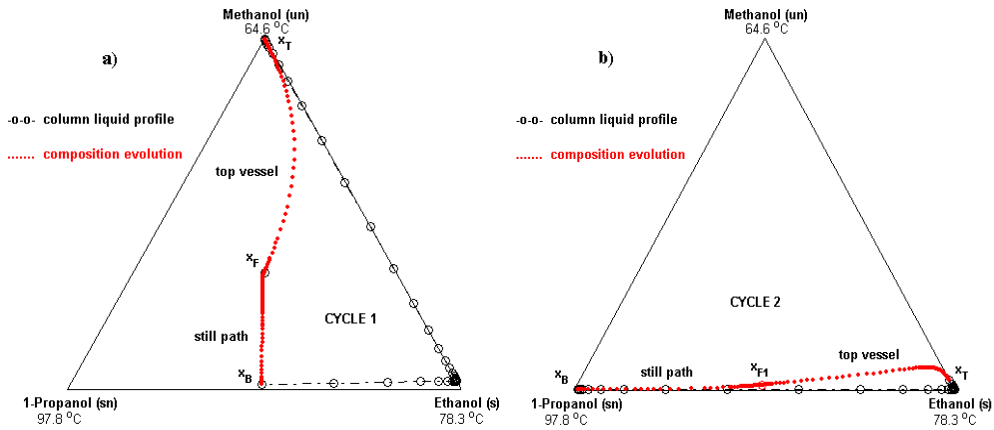


Figure 3. a) Separation of a zeotropic mixture in the cyclic column (Cycle 1)
b) Separation of a zeotropic mixture in the cyclic column (Cycle 2)

Table 1. Batch time calculations and time savings (*basis: conventional multivessel*)

		Conventional multivessel	Modified multivessel	Cyclic column
		(vapor bypass)	(no vapor bypass)	
Base case-Equimolar	Specification			
	$Z_F=[1/3,1/3,1/3]$			
	[0.99,0.97,0.99]	3.8 hr	-26%	+32%
	[0.99,0.99,0.99]	4.9 hr	-31%	+16%
Rich in light	$Z_F=[0.7,0.15,0.15]$			
	[0.99,0.97,0.99]	3.6 hr	-19%	+8%
	[0.99,0.99,0.99]	4.1 hr	-22%	+2%
	[0.995,0.995,0.995]	4.5 hr	-22%	+2%
Rich in intermediate	$Z_F=[0.15,0.7,0.15]$			
	0.99,0.97,0.99]	4.0 hr	-33%	+28%
	[0.99,0.99,0.99]	6.6 hr	-36%	-2%
	[0.995,0.995,0.995]	7.9 hr	-34%	-8%
Rich in heavy	$Z_F=[0.15,0.15,0.7]$			
	[0.99,0.97,0.99]	2.4 hr	0%	+71%
	[0.99,0.99,0.99]	2.4 hr	0%	+104%
	[0.995,0.995,0.995]	2.8 hr	0%	+104%

Conventional multivessel vs cyclic column

The batch time comparisons in Table 1 show that the conventional multivessel performs always better than the cyclic column for equimolar feeds. The cyclic column requires from 16% to 32% more time than the multivessel in order to perform the same separation. The most important difference here is that the separation is performed simultaneously in the multivessel, in contrast to the cyclic column, where two closed operations are required.

The time advantages of the multivessel are becoming smaller, as the specification in the middle vessel becomes stricter. For example, when the specification in the middle vessel increases from 0.97 to 0.99, the time advantages of the multivessel decrease from 32% to 16%. However, when the specification becomes strict in all vessels (third specification set) no more time gains can be expected for the cyclic column. This happens because the increase in the separation time for the multivessel column, from 4.9h to 5.8h, is outweighed by a proportionally equal increase mainly in Cycle 1 of the cyclic column. Cycle 1 has to be run for longer time in order to achieve the strict specification of 0.995 for the methanol in the top vessel.

Conventional multivessel vs modified multivessel

Table 1 shows clearly that the elimination of the vapor bypass in the multivessel column has a great effect in the batch time (energy) requirements. The modified multivessel is always faster than the conventional multivessel for equimolar feeds. The time savings vary from 26% to 33% depending on the specification, which indicate a weak dependence on the specifications. In average, the modified multivessel exhibits time advantages of around 30% over the conventional multivessel.

This is a rather surprising result since, someone would expect minor differences, mainly attributed to the one additional equilibrium stage of the modified multivessel compared

to the conventional. However, the situation is a bit more complicated. The middle vessel should not be considered simply as an additional equilibrium stage. It has a significant holdup compared to the stages inside the column and the dynamics in the vessels are playing a decisive role in the separation time requirements.

Dynamics in the vessels

Figure 4 illustrates what is happening in the vessels of the multivessel during the process. Figure 4a shows the composition dynamics of the main component in each vessel for the conventional multivessel. The case of the first specification test [0.99,0.97,0.99] is considered. The methanol in the top vessel reaches the specification very fast, after 0.5h, mainly because of the very small amount of initial holdup in the vessel. The bottom vessel is responding slowly the first 1 hour. This is because it carries 94% of the total feed. However, the evolution is almost exponential after the first hour and finally, the propanol reaches its specification after 2.5hr. The middle vessel, which has the lowest specification, exhibits the slowest dynamics. It takes actually 3.8hr for ethanol to reach its low specification (0.97). At this time, all specifications are met and the separation task is ended. It is clear that the dynamics of the middle vessel are decisive for the whole process, since the middle vessel is the last one to reach the specification.

Figure 4b provides even more insight into the process. The composition dynamics of the light component (methanol) in all vessels are shown. We see that the light methanol starts accumulating very fast in the top vessel and it is depleted rather fast (practically after 1.5h) from the bottom vessel. However, the methanol insists on appearing in the middle vessel, which indicates an inherent inability, of the middle vessel, to 'boil-off' the light component. The light component is in a sense trapped in the middle vessel and the process is significantly delayed. Why this is happening is becoming clear by looking

in the design characteristics of the conventional multivessel in Figure 1a. The vapor bypass from the stripping section to the rectifying section of the column is responsible for this. The light component in the middle vessel is depleted in a slow rate because there is no vapor phase coming in contact with the liquid holdup in it. This disadvantage of the conventional multivessel is removed in the so-called modified multivessel, where the vapor stream from the stripping section is entering the middle vessel.

The effect of the elimination of the vapor bypass is obvious in figure 4c, where the evolution of the compositions in the middle vessel is shown for both the conventional and the modified multivessel. The methanol is boiled-off faster when there is no vapor bypass and the main component (ethanol for the middle vessel) is reaching its specification faster. Almost 30% less time is required for performing this separation in the modified multivessel compared to the conventional one.

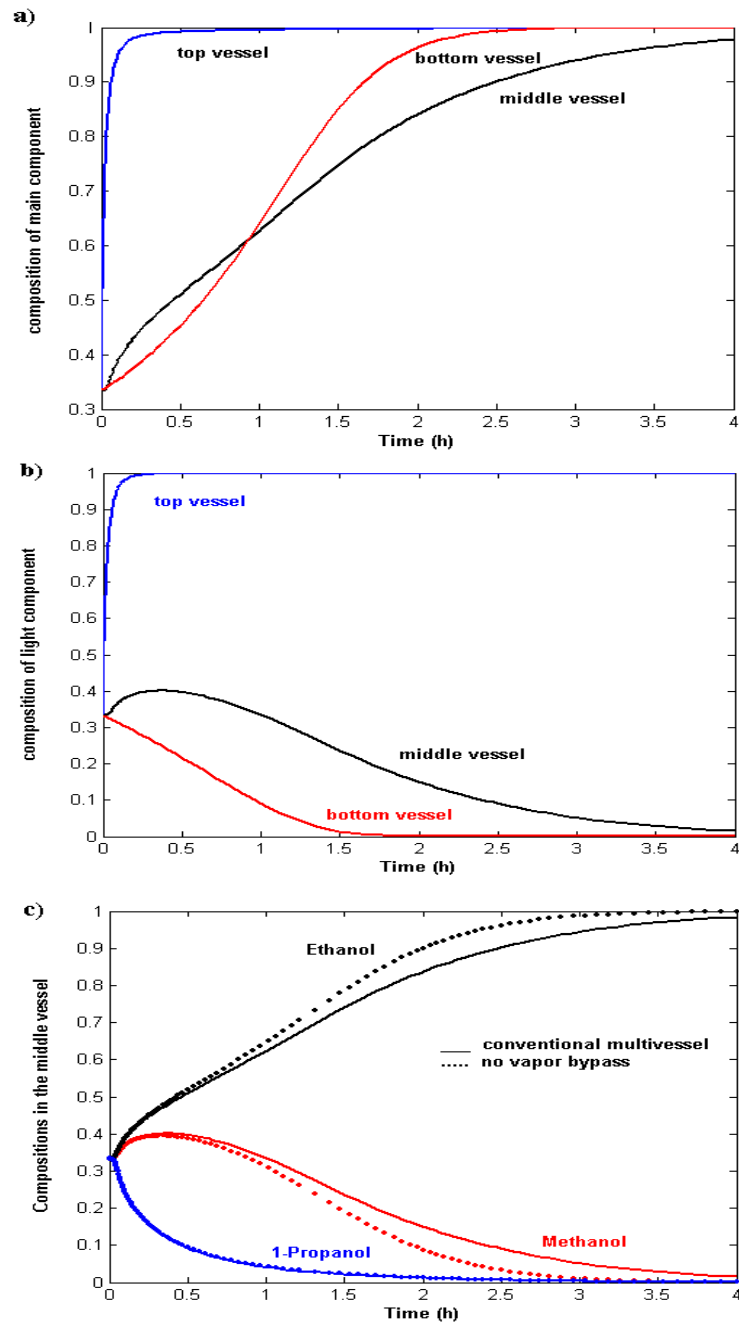


Figure 4. a) Composition dynamics of the main component in each vessel
 b) Composition dynamics of the light component in each vessel
 c) Composition dynamics in the middle vessel with and without vapor bypass

General comments

In Figure 4c it is obvious that the elimination of the vapor bypass has negligible effect in the composition dynamics of the heavy component (1-propanol). This is reasonable since the liquid flow out from the middle vessel remains almost unchanged in the two multivessel configurations. The problem however can be important in liquid bypass configurations. In this case, we would observe the reverse situation. The heavy component, entering the middle vessel, will be stripped away in a very slow rate.

The results presented in Hasebe et al. (1995) and Wittgens et al. (1997) are indicating the slow dynamics in the middle vessel are slow. In figure 7 of Hasebe et al. (1995) the middle vessel product satisfies its specification last. Wittgens et al. (1997) provided results for a quaternary mixture in a multivessel column with four vessels. In Figures 3 and 4 of this work the light impurities in the two middle vessels persist for long time, thus delaying the process. The elimination of the vapor bypass enhances the composition dynamics in the middle vessel, thus making the process faster. In the work of Hasebe, a set of existing batch rectifiers connected sequentially is proposed for a practical realization of the multivessel column. In this case it would be impractical to eliminate the vapor bypass since this will require significant changes in the existing rectifier columns. Nevertheless, in the case of a new multivessel column, built from scratch, the no vapor bypass configuration would be the best choice.

The knowledge of the slow dynamics in the middle vessel can serve as a very simple guideline for the initial feed distribution in the vessels. If the objective is to minimize batch time (energy demand) the advice we give is not to place the feed in the middle vessel. In the opposite case, e.g. placing the feed in the middle vessel, the dynamic response of the vessel is even slower, because of the large holdup to be accomplished and the large amount of light component that has to be boiled off in a slow rate. Hilmen

(2000) supports this simple intuitive guideline. “For medium difficulty separations...charging the feed to the intermediate vessel was worst in all cases of feed composition” and “...for easy separations we found large time savings for feeds charged to the reboiler instead of the middle vessel”. In contrast, for difficult separations the initial distribution of the feed is not very important anymore. This happens because the actual batch time is determined by the difficulty of the separation task itself and not by the dynamics of the vessels.

In conclusion, the results for the base case indicate that the modified multivessel is the best alternative. The modified column requires 30% less time than the conventional one. By comparing now the cyclic column with the modified multivessel, we see that the former requires around 70% more time than the latter for the same separation.

B) Effect of the feed composition

Feed rich in light component

For a feed rich in light component the results in Table 1 reveal that the elimination of the vapor bypass is advantageous also in this case. The modified multivessel requires around 20% less time than the conventional multivessel and the time savings are independent of the specification.

The striking result for such feeds is the minor advantages of the multivessel column compared to the cyclic column, which is marginally slower (8%-2%) than the multivessel. This result is in agreement with the results presented by Hilmen, (2000) that mentions “for medium difficult separations, the benefits of the multivessel column are low for feeds rich in light components and feed low in heavy component”. The comparison in Hilmen, (2000) refers to the indirect split in the cyclic column but our results show that it holds also for the direct split.

However, we see that there is a potential to save separation time (energy) by using multivessel configurations as long as the modified multivessel is employed, instead of the conventional one. Then, the potential savings in the modified multivessel compared to the cyclic are around 25%.

Feed rich in intermediate component

Intuitively, the results for this case should reflect the fact that the middle vessel has slow dynamics and delays the separation task in multivessel configurations. Indeed, the results in Table 1 prove this fact. The first thing to observe is the increase in the absolute separation time values for the conventional multivessel. Notice, for example, the time requirements for the second specification set. The actual separation times increase from 4.1h to 4.9h and finally to 6.6h, as the intermediate component increase in the feed. This happens because of the large amount of intermediate component

accumulated in the middle vessel during the process. The middle vessel has anyway very slow dynamics and the large holdup to be processed in the vessel is making the situation even worse.

As expected, the elimination of the vapor bypass is very effective in this case. The modified multivessel requires around 35% less time than the conventional one and this is the maximum time savings achieved with the modified configuration, in this study. Consequently, the modified multivessel is strongly recommended for such feeds.

The comparison between the conventional multivessel and the cyclic column is in favor of the former only for the first specification set. When the specifications become stricter in the middle vessel (from 0.97 to 0.99) or to all the vessels (from 0.99 to 0.995) then the cyclic column requires slightly less time than the conventional multivessel.

The same was mentioned by Meski et al. (1998), who compared the multivessel column with the direct and indirect split (or combinations) in regular batch columns. They found that regular columns (like the cyclic column) were best for feeds rich in the intermediate component. In contrast, Hasebe et al. (1992) claimed that the multivessel column is more effective in removing light and heavy impurities from a feed than ordinary distillation. Our results, certainly do not support such a statement, neither do the results from other sources like Meski et al. (1998) and Hilmen, (2000).

By comparing now the modified multivessel with the cyclic column we see that even in this case, which is the ‘waterloo’ of the conventional multivessel, the modified multivessel is superior and requires around 35% less time than the cyclic column.

Feed rich in heavy component

The results for this last case studied here are very interesting. This case represents the ‘ultimate’ situation for multivessel configurations. The last rows in Table 1 show that

the separation task is accomplished very fast in the conventional multivessel. It takes only 2.4h (for the second specification set) for the separation to be finished, compared to 6.6h or 4.9hr or 4.1h in previous cases.

The secret behind these numbers is that the separation is governed by the dynamics of the bottom vessel. The middle vessel is not anymore the slowest vessel and therefore the inherent disadvantage of the middle vessel is vanishing. The fact that the middle vessel dynamics are playing no role in this case is illustrated clearly by the zero time savings of the modified multivessel. The elimination of the vapor bypass has no effect in the separation task, which is determined by the bottom vessel dynamics.

The comparison between the conventional multivessel and the cyclic column is, of course, strongly in favor of the former. The cyclic column requires from 70% to 104% more time depending on the specification. In addition, as the specification becomes stricter the comparison is even worse for the cyclic column, a trend that is opposite of what we have seen until now. This case verifies the 50% time savings by using the multivessel column in comparison to the cyclic column, reported before in the literature and mentioned in the introduction of the paper.

Hilmen, (2000) also mentioned that large time savings are expected for the multivessel column compared to the cyclic for medium difficult and feeds rich in heavy components. Sorensen and Prenzler (1997) mention that this is a common separation task in the pharmaceutical and fine chemical industries where light solvents must be recovered from waste water streams and the specifications are very tight (usually in the order of ppm for the solvent). The common practice is to perform these separations sequentially in conventional batch rectifiers. However, as the results indicate here, a multivessel configuration of serially connected existing rectifiers is actually a much

better alternative. The potential time (energy) savings of such a rearrangement of existing rectifiers in the plant are remarkable (around 50%) and indicate that valuable process time can be saved.

4. Conclusions

Batch time (energy) requirements, based on simulations, were provided for the separation of a zeotropic mixture in closed batch distillation arrangements. The batch arrangements studied were a conventional multivessel column with a vapor bypass, a modified multivessel without a vapor bypass and a cyclic column (rectifier). The task was to separate a mixture of methanol/ethanol/1-propanol. The effect of the feed composition and the product specifications were studied, based on simulations.

The base case of equimolar feed was used for illustrating an important disadvantage of conventional multivessel configurations namely, the slow dynamics in the middle vessel. Elimination of the vapor bypass in the middle was proposed in order to remedy this disadvantage. The results for the so-called modified multivessel support this intuitive design modification.

Multivessel configurations, either conventional or modified, perform always better than traditional configurations like the cyclic column, in terms of batch time (energy) consumption.

In the comparison between the modified multivessel (without vapor bypass) and the conventional multivessel (with vapor bypass), the former is superior to the latter, with the exception of feeds rich in heavy components when no differences, in the time requirements, are noticed.

The conventional multivessel performs worst for feeds rich in the intermediate component. This is the only case where the cyclic column is faster and reflects the slow

dynamic response of the middle vessel. However, even in this case, the modified multivessel is the best alternative.

Feeds rich in the heavy component are the ultimate case for multivessel configurations.

The potential time savings of processing such feeds in multivessel configurations instead of in regular batch columns are around 50%. This result should be of great practical importance in the pharmaceutical, fine and specialty chemicals industries.

5. Nomenclature

N	Number of stages
M	Liquid holdup (kmol)
x	compositions
K _c	Controller gains
T _{sp}	Temperature setpoints
1,2	Separation cycles

Subscripts

F	Feed
T	Top vessel
M	Middle vessel
B	Bottom vessel
R	Rectifying section
S	Stripping section
0	Initial values

6. References

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APPENDIX

Table 1: Column data

	Conventional multivessel	Modified multivessel	Cyclic column
Stages per section	$N_r = 25, N_s = 25$	$N_r = 25, N_s = 24$	$N_{\text{total}} = 50$
Initial feed	$M_F = 5.385 \text{ kmol}$	$M_F = 5.385 \text{ kmol}$	$M_F = 5.385 \text{ kmol}$
Initial condenser holdup	$M_{T0} = 0.035 \text{ kmol}$	$M_{T0} = 0.035 \text{ kmol}$	$M_{T0} = 0.035 \text{ kmol}$
Initial middle vessel holdup	$M_{F0} = 0.250 \text{ kmol}$	$M_{F0} = 0.250 \text{ kmol}$	No middle vessel
Initial reboiler holdup	$M_{B0} = 5.000 \text{ kmol}$	$M_{B0} = 5.000 \text{ kmol}$	$M_{B0} = 5.250 \text{ Kmol}$
Trays holdup	$M_i = 1/500 \text{ kmol}$	$M_i = 1/500 \text{ kmol}$	$M_i = 1/500 \text{ kmol}$
Vapor flow	$V = 5 \text{ kmol/h}$	$V = 5 \text{ kmol/h}$	$V = 5 \text{ kmol/h}$

Table 2: Proportional temperature controller data

$K_{c,r} = 0.365 \text{ kmol/h}^\circ\text{C}$ (Cycle 1)	$T_{\text{sp},r} = 71.45 \text{ }^\circ\text{C}$ (Cycle 1)
$K_{c,s} = 0.256 \text{ kmol/h}^\circ\text{C}$ (Cycle 2)	$T_{\text{sp},s} = 88.05 \text{ }^\circ\text{C}$ (Cycle 2)