Design of Reactive Distillations for Acetic Acid Esterification with Different Alcohols

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Abstract-

*In this work, the esterifications of acetic acid with five different alcohols, ranging from C_1 to C_5 are studied. First, qualitative relationships between macroscopic process flowsheet and microscopic phase equilibria are established and the process flowsheets are classified into type I, II, and III for these five systems. Next, a systematic design procedure is devised to optimize the design based on the total annual cost (TAC) and dominant design variables are identified for different flowsheets. The results clearly indicate that it is possible to systemize the design of reactive distillation by qualitatively generating flowsheet from phase equilibria and by quantitativ*ely completing the process flow diagram from a sequential design procedure.

Keywords: esterification, acetate, reactive distillation, process design

1. Introduction

Reactive distillation provides an attractive alternative for process intensification, especially for reaction/separation systems with reversible reactions. The literature in reactive distillation has grown rapidly in recent years and the books by Doherty and Malone (2001) and Sundmacker and Kienle (2003) give updated summaries in the field. As pointed out by Doherty and Buzad (1992) the concept of combining reaction and separation has long been recognized but rarely put into commercial practice, not until the successful application for the production methyl acetate (Agreda et al., 1990). Despite clear advantages of simultaneous reaction/separation (Kaymak and Luyben, 2004), commercializing of reactive distillation processes is still quite limited for several reasons. After the management and technical levels were convinced by the clear edge of reactive distillation, is that the process flowsheets seem to change from case to case.

The esterification reactions are studied in this work. Esters are of great importance to chemical process industries and esters are typically produced from the reactions of acid and alcohols under acidic condition. In order to provide possible generalization to the design procedure, in this work, we explore the esterifications of acetic acid with different alcohols ranging from C_1 to C_5. The objective of this work is intended to provide possible generalization for the design of reactive distillation for esterification reactions with acetic acid. The design procedures are proposed for different process configuration to determine, quantitatively, the tray numbers in each section of reactive distillation systems and design is optimized based on the total annual cost (TAC). Finally, process characteristics of these 5 optimally designed reactive distillations are studied followed by the conclusion.

2. Reaction Kinetics

The easterification of the acetic acid with different alcohols can be expressed in the following general form:

$$acid + alcohol \underset{k_{-1}}{\overset{k_1}{\Leftrightarrow}} acetate + water \qquad (1)$$

The alcohols studied in this work include methanol (MeOH), ethanol (EtOH), iso-propanol (IPOH), n-butanol (BuOH), and n-pentanol (amyl alcohol, AmOH) and corresponding products are methyl acetate (MeAc), ethyl acetate (EtAc), isopropyl acetate (IPAc), n-butyl acetate (BuAc), and amyl acetate (AmAc), respectively. In this work, we are interested on the solid-catalyzed reaction kinetics for an obvious reason that one can place the reactive zone in different sections of the reactive distillation columns. It is clear that this provides flexibility in process design as opposed to using homogeneous catalysis (e.g., sulfuric acid).

We have not seen too many kinetics data on solid-catalyzed easterfication reactions until recently. Literature surveys indicate that most of these data have become available in last 5 years (Pöpken et al., 2003; Hangx et al. 2001; Gadewar et al. 2002; Gangadwala et al.; 2003, Lee et al., 1999) and Table 1 lists the reaction kinetics used in this study. The reaction rates are expresses in the pseudo-homogeneous model or Langmuir-Hinshelwood and, generally, with the component represented in terms of activity. Moreover, they are all catalyst-weight (m_{cat}) based kinetics. Despite the fact that the kinetic experiment were performed by different groups with somewhat different type of catalysis, we observe certain degree of consistency in the kinetic data (Table 1), The equilibrium constant (K_{eq}, at 363 K) ranges from 1.6 to 16.8, the forward rate constant (k_1, at 363 K) changes from 1.73×10^{-4} to 2.5×10^{-3}, and activation energy of the forward reaction varies from 44000 kJ/kmol to 70000 kJ/kmol, and the heat of reactions are almost negligible except for the methyl acetate and ethyl acetate systems. Note that for the isopropyl acetate, the $[H^+]$ concentration of 4.6×10^{-3} (mol H^+/kg_{cat}) is assumed to convert the catalyst weight-based expression. Table 1 also shows that the methyl acetate system has the most favorable reaction kinetics catalyst an order of magnitude larger than the rest of the systems.

In applying the reaction kinetics to a reactive distillation, it is assumed that the solid catalyst occupies 50% of the tray holdup volume and a catalyst density of 770 kg/m^3 is used to convert the volume into catalyst-weight (m_{cat}).

3. Process Flowsheets

In this section, attempts are made to generate flowsheet for high purity acetates using the combination of stripper, rectifier, reactive section, and possibly a decanter. That is to device hybrid reactive distillation systems to produce commercial grade acetates.

3.1 Type I Flowsheet - MeAc

In reactive distillation, typically, the *heavy* reactant is fed from the *top* of the reactive section and the *light* reactant goes into the *bottom* part of the reactive zone. For methyl acetate system, the heavy reactant is the acid (HAc) and the light reactant is the alcohol (MeOH). If the reactive zone consumes all the acid, we are dealing with the separation of the H_2O/MeOH/MeAc, an almost ternary system, in the stripping section. This process flowsheet can be understood from the boiling point (including azeotropes) temperatures ranking (Table 2). The heavy product of the reaction, H_2O, is with

drawn from the bottoms and the light product, MeAc, is taken out from the top. The azeotropes play little role in the separation sections except that the top product is a saddle (ultimately the RCM will end at the MeAc/H_2O azeotrope, 56.43°C). This will cause some problem in control and operation. Nevertheless, at design stage, it is possible to achieve high purity products at both ends with the type I flowsheet (Figure 1A).

3.2 Type II Flowsheet – EtAc & IPAc

The boiling point temperature ranking may suggest that we can use the type I flowsheet for the EtAc production with the EtAc and H_2O withdrawn the top and the bottom of the column. Indeed, it was simulated by several researchers (Komatsu and Holland, 1977; Vora and Daoutidis, 2001), but the purity level (~80%) is far from the product specification and further purification is needed. In analogy to the MeAc system, we are looking at the H_2O/EtOH/EtAc ternary system for the stripping section. It becomes obvious that, the EtAc system has a much complicated phase behavior with 3 distillation boundaries. Moreover, we also have EtOH/H_2O (78.18°C) azeotrope that may prevent obtaining high purity H_2O if one is performing the separation along the EtOH-H_2O edge. However, we also observe the ternary azeotrope, EtOH/EtAc/H_2O, has the lowest temperature (70.09°C) (Table 2). Furthermore, the azeotrope lies on the edge of the LL envelope with the tie lines slop towards relatively high purity H_2O. A decanter is placed to remove the heavy product H_2O from the aqueous with the organic phase further processed to obtain high purity EtAc in a stripper, with the top recycled back to the decanter. This is the flowsheet presented by Burkett and Rossiter (2000) and Tang et al. (2003) which is denoted as type II process hereafter (Figure 1). Note that the products of both the first column (reactive zone + rectifier) and the second column (stripper) are all nodes (stable or unstable) and they possess much better operability as compared to the MeAc system.

In contrast to MeAc and EtAc synthesis, the information about isopropyl acetate synthesis with acetic acid in a reactive distillation process can hardly be found in the literature except for the VLE and kinetics data (Lee and Kuo, 1996; Doherty and Malone, 2001). IPAc system is even more favorable with the type II flowsheet than the EtAc system for the reasons that it has a larger LL envelope with a minimum boiling ternary azeotrope (74.22°C) located further inside the LL zone with tie lines mostly point to the high-purity H_2O corner. Once the H_2O is removed from the aqueous phase of the decanter, part of the organic distillate is fed to a stripper by removing high purity IPAc from the bottoms and the top product of the stripper is recycled back to the decanter (Figure 1).

3.3 Type III Flowsheet – BuAc & AmAc

The boiling point temperature rankings in Table 2 reveal that butyl acetate differs from the IPAc in that the acetate is the highest boiling component. That implies that we can remove the acetate from the column base, even from a hybrid reactive distillation. Moreover, the minimum boiling azeotrope between BuOH and H_2O is a heterogeneous one and this leads to a type II LL envelope in the However, the BuAc and IPAc systems also share a common characteristic: a minimum boiling ternary azeotrope exists in the acetate/alcohol/water ternary system and it locates inside the LL envelope. This immediately suggests a decanter

should be placed in the column top by removing almost pure water from the aqueous phase. Unlike type II flowsheet, the heavy boiling acetate implies that we can totally recycle the organic phase back to the column and withdraw the acetate from the bottoms. The scenario suggests the type III flowsheet for the BuAc as shown in Figure 1. That is quite similar to a typical column with the reactive zone locates in the middle with a decanter to perform LL separation.

The amyl acetate system also shows a similar VLLE characteristic with an even larger LL envelope for the acetate/alcohol/water system. The larger LL zone suggests that the LL separation could be even easier for the AmAc system (as compared to the BuAc system). This naturally leads to the type III flowsheet by removing rather pure water from the top and heavy acetate from the bottoms. It is also observed that amyl alcohol is the second highest boiling pure component, which is different from the BuAc system where the acid is the one.

It is interesting to see the gradual transition in the VLLE system (e.g., Figures 1 and 3) as the carbon number in the alcohols increases, despite via discrete change between chemical species. It is even more interesting to find out the jumps between process flowsheets (Figure 1) as the VLLE characteristics (e.g., ranking of boiling points in Table 2) pass through some critical points. Qualitatively, it seems that we can determine the type of flowsheet by simply examining the VLLE behavior. These observations will be examined carefully in the next section.

Finally, it is also observed that, despite of seemingly different process configurations, these three flowsheets (Figure 1) share a common characteristic. That is they all consist of three major elements: a reactive section, a rectifier, and a stripper with somewhat different arrangement.

4. Steady State Design

The total annual cost (TAC) of Douglas (1988; Chiang et al., 2002; Huang and Yu, 2003) is used to evaluate different designs. The TAC is defined as:

$$\text{TAC} = \text{operating cost} + \frac{\text{capital cost}}{\text{payback year}} \quad (2)$$

where the operating cost includes the costs of steam, cooling water, and catalyst, and the capital cost covers the cost of the column, trays, heat exchangers.

4.1 Design Procedure

As pointed out earlier, despite having different process configurations, these flowsheets all consist of a rectifier, a stripper, and a reactive section. Obvious design parameters are the number of rectifying tray (N_R), the number of stripping trays (N_S), and the number of reactive trays (N_{rxn}). In addition to the tray numbers, another set of important design parameters are the feed tray locations (NF_{Acid} & $NF_{Alcohol}$; Huang and Yu, 2003; Huang et al., 2004). In theory the equalmolar feed flow rates ($F_{Acid} = F_{Alcohol}$) should be economically optimal, but for the type II flowsheet, the feed ratio ($FR = F_{Acid} / F_{Alcohol}$) is also an important design variable.

For a system with a given production rate with product specifications, the design steps are:

(1) Set the reactants feed ratio to 1 initially (i.e., $FR = F_{Acid} / F_{Alcohol} = 1$).
(2) Fix a number of reactive trays (N_{rxn}).
(3) Place the heavy reactant feed (NF_{heavey}) on the top of the reactive zone and introduce the light reactant feed (NF_{light}) on the lowest tray of the reactive zone.

(4) Guess the tray numbers in the rectifying section (N_R) and the stripping section (N_S).
(5) Change the reflux flow (R) and heat input (Q_R) (type I flowsheet) or organic reflux flow (R) and stripper heat input ($Q_{R,S}$) (type II flowsheet) or heat input (Q_R) (type III flowsheet) until the product specification is met.
(6) Go back to (4) and change N_R and N_S until the TAC is minimized.
(7) Go back to (3) and vary N_{rxn} until the TAC is minimized.
(8) Go back to (2) and find the feed locations ((NF_{heavey} & NF_{light}) until the TAC is minimized.
(9) Go back to (1) and change the feed ratio (FR) until the TAC is minimized (for type II flowsheet only).

It seems strange to devise a sequential design procedure when it may be done simultaneously. Extensive experience on reactive distillation simulation indicates that the algorithm for the reactive distillation is much less robust as compared to typical distillation. It is more practical to carry out the simulation sequentially. Because in the work we assume the catalyst occupies 50% of the holdup volume in a reactive tray, the column diameter is sized using the short-cut method of Douglas (1988) and a weir height of 10.16 cm (Type I & II) or 5.08 cm (Type III) is assumed for the reactive tray. That is the catalyst weight is fixed once the column diameter is determined.

4.2 Optimal Design

4.2.1 Type I - MeAc

For the MeAc system, we assume an equalmolar feed rates (FR = 1), thus the dominant variables for optimization become: N_R & N_S, N_{rxn}, and NF_{Heavy} & NF_{light}. Figure 2 shows that N_R & N_S have little impact on the TAC, despite showing a minimum as N_S varies. Flat profiles are also observed as we change the number of reactive trays. The most dominant optimization variables are the *feed tray locations* as shown in Figure 2. The results indicate that the light reactant (MeOH) should be fed to tray 13 (counting the tray number from bottoms up) and the heavy reactant (HAc) should be introduced to tray 36. Note that these two trays lie inside the reactive zone (but not on the top & bottom).

4.2.2 Type II – EtAc & IPAc

The type II flowsheet differs from the type I in that the reactive zone extends to the column base of the first column (called RD column) and, therefore, a much larger holdup is expected in the bottom of the RD column (Figure 1). In this work, the column base holdup is taken to be 10 times of the tray holdup. We also assume the feed ratio of the reactant can be changed and this lead to the following optimization variables: N_R & N_S, N_{rxn}, NF_{Heavy} & NF_{light}, and FR. For EtAc, the results (Figure 3) indicate that the *number of trays in the rectifying section* in the RD column (N_R) is one of the dominant optimization variables while the N_S shows little impact on the TAC once N_R is fixed. As for the feed tray locations, the optimal feed tray for the heavy reactant (HAc) is the column base, despite with small difference in the TAC's. This is understandable because we have the largest catalyst holdup in the reboiler and this leads the same feed location for both reactants. Surprisingly, another dominant variable for optimization is the *feed ratio* (FR) and result shows that a little alcohol excess is preferred because this facilitates the top of the RD column falls inside the LL envelope leaving trace amount of acid. The reboiler duty in the RD

column reveals this fact as shown in Figure 3.

For the IPAc system, we have the same optimization variables for the type II flowsheet. Again, the results (Figure 4) reveal that N_S has little impact on the TAC and, as expected, both reactant feeds should be introduces to the reboiler. Again, the *number of trays in the rectifying section* (N_R) is one dominant variable for optimization and the other is the *feed ratio* (*FR*) as shown in Figure 4. The results also indicate a little alcohol excess is favorable to obtain as easier LL separation.

4.2.3 Type III – BuAc & AmAc

The type III flowsheet has been studied by several researchers (Chiang et al., 2002; Huang and Yu, 2003). In theory, we have the following optimization variables: N_R & N_S, N_{rxn}, and NF_{Heavy} & NF_{light}. For the BuAc system, the results clearly show that the *feed locations* are the most important optimization variables as shown in Figure 5 where significant TAC is saved by simply varying the feed locations. This can be understood because we need to arrange the feeds such that optimal reactant and temperature profiles can be achieved in the reactive section.

Similarly, for the AmAc system, Figure 6 clearly indicates that, again, the feed locations are the dominant optimization variables as compared to other variables such as N_R & N_S and N_{rxn}.

The optimization results show an interesting fact that different flowsheets give rise to different dominant optimization variables. They are: (1) NF_{Heavy} & NF_{light} for the type I flowsheet, (2) N_R and *FR* for the type II flowsheet, and (3) NF_{Heavy} & NF_{light} for the type III flowsheet. Table 3 summarizes the optimal designs for these five systems

4.3 Results and Discussion

The analyses of the esterfication of the acetic acid with five alcohols ranging from MeOH to AmOH (C_1~C_5) are intended to gain insight for the design of reactive distillation by varying the chemical species discretely. As the carbon number in the alcohol increases, the flowsheet changes from type I, to type II, and then to type III (Figure 1). The determinant factors in the flowsheet selection are the ranking of the pure component/azeotrope temperatures (Table 2) and the size of the LL envelope (Figure 1). That implies the structure of the flowsheet can be determined once the VLLE data become available. The flowsheets may look different in the arrangement; they all include the following units: a stripping section, a reactive zone, and a rectifying section. Once the flowsheet structure is determined, the design can be carried out in a sequential manner by minimizing the TAC. It is interesting to note that most of the dominant design variables are mostly associated with the feed: the feed tray locations (for type I & III) and the feed ratio (for type II). This can be understood because the reactants composition distribution is important for the kinetically controlled reactive distillation. It is also observed that the function of the reactive zone goes beyond providing necessary conversion. The reactive section also facilitates the separation by reacting away the heavy reactant toward the lower part of the reactive zone and by consuming most of the light reactant toward the upper part.

Finally, the MeAc system (type I) only boils up components necessary to achieve desired product purity and, therefore, much smaller energy consumption is expected. Another reason for the MeAc to have the lowest TAC is that the purity level of the acetate is 0.98 (mole fraction) which is typically seen in the

literature as compared to 0.99 the other four cases. However, the purity level difference will not lead to such significant reduction in the TAC.

5. Conclusion

In this work, the acetic acid esterifications with five different alcohols, ranking from methanol to amyl alcohol (C_1 to C_5), using the reactive distillation are explored. Two important factors in the flowsheet determination are: (1) the ranking of the pure component/azeotope boiling point temperature, and (2) the size and the location of the liquid-liquid phase zone. Next, a systematic design procedure is devised to optimize the *quantitative* design based on the total annual cost (TAC). This sequential design procedure overcomes the fragility of the simulation algorithm even with the state-of-the-art process simulator for the reactive distillation. The dominant design variables are also identified and they are: feed locations for the type I flowsheet, feed ratio and the number of trays in the rectifying section for the type II flowsheet, and feed locations for the type III flowsheet. Then, the characteristics of the optionally designed reactive distillation for these three types of flowsheets are investigated explanations are given. Finally, the TAC's of different flowsheets are compared, the economic potential is ranked, and the explanation is given. The results presented in this provide insight for the conceptual design of reactive distillation systems

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Table 1 Kinetic equations for five esterification systems.

System	Kinetic model (Catalyst)	k_1 (T=363K)	K_{eq} (T=363K)
(i) MeAc	Pseudo-homogeneous model (Amberlyst 15) $r = m_{cat}\left(k_1 a_{HAc} a_{MeOH} - k_{-1} a_{MeAc} a_{H_2O}\right)$ $k_1 = 2.961\times10^{4}\exp(\frac{-49190}{RT})$ $k_{-1} = 1.348\times10^{6}\exp(\frac{-69230}{RT})$	2.49×10^{-3} [kmol/(kg$_{cat}$*s)]	16.76
(ii) EtAc	Pseudo-homogeneous model (Purolite CT179) $r = m_{cat}\left(k_1 x_{HAc}^{1.5} x_{EtOH} - k_{-1} x_{EtAc} x_{H_2O}\right)$ $k_1 = 4.24\times10^{3}\exp(\frac{-48300}{RT})$ $k_{-1} = 4.55\times10^{5}\exp(\frac{-66200}{RT})$	4.78×10^{-4} [kmol/(kg$_{cat}$*s)]	3.50
(iii) IPAc	Langmuir-Hinshelwood / Hougen-Watson model (Amberlyst 15) $r = m_{cat}\frac{k_1\left(a_{HAc}a_{IPOH} - a_{IPAc}a_{H_2O}/K_{eq}\right)}{\left(1+K_{HAc}a_{HAc}+K_{IPOH}a_{IPOH}+K_{IPAc}a_{IPAc}+K_{H_2O}a_{H_2O}\right)^2}$ $k_1 = 7.667\times10^{-5}\exp(23.81-\frac{68620.43}{RT})$ $K_{eq}=8.7$, $K_{HAc}=0.1976$, $K_{IPOH}=0.2396$, $K_{IPAc}=0.147$, $K_{H_2O}=0.5079$ Assumption: mol H$^+$/kg$_{cat}$=4.6×10^{-3}	2.26×10^{-4} [kmol/(kg$_{cat}$*s)]	8.7
(iv) BuAc	Pseudo-homogeneous model (Amberlyst 15) $r = m_{cat}\left(k_1 a_{HAc} a_{BuOH} - k_{-1} a_{BuAc} a_{H_2O}\right)$ $k_1 = 3.3856\times10^{6}\exp(\frac{-70660}{RT})$ $k_{-1} = 1.0135\times10^{6}\exp(\frac{-742417}{RT})$	2.32×10^{-4} [kmol/(kg$_{cat}$*s)]	10.9
(v) AmAc	Quasi-homogeneous model (Amberlyst 15) $r = m_{cat}\left(k_1 C_{HAc} C_{AmOH} - k_{-1} C_{AmAc} C_{H_2O}\right)$ $k_1 = 31.1667\exp(\frac{-51740}{RT})$ $k_{-1} = 2.2533\exp(\frac{-45280}{RT})$	1.13×10^{-6} [m^6/(kmol*kg$_{cat}$*s)]	1.6

*R=8.314 [kJ/kmol/K], T[K], r[kmol/s], m_{cat}[kg$_{cat}$], C_i[kmol/m^3], x_i[mole fraction]

(i) Pöpken et al., 2003 (ii) Hangx et al. 2001 (iii) Gadewar et al. 2002

(iv) Gangadwala et al., 2003 (v) Lee et al., 1999

Table 2 Ranking of azeotropic temperatures and pure component NBP temperatures

(i)MeAc	(ii)EtAc	(iii)IPAc	(iv)BuAc	(v)AmAc
MeOH/MeAc 53.65 °C	EtOH/EtAc/H_2O 70.09 °C	**IPOH/IPAc/H_2O** **74.22** °C	**BuOH/BuAc/H_2O** **90.68** °C	**AmOH/AmAc/H_2O** **94.71** °C
MeAc/H_2O 56.43 °C	**EtAc/H_2O** **70.37** °C	**IPAc/H_2O** **76.57** °C	**BuAc/H_2O** **90.94** °C	**AmAc/H_2O** **94.90** °C
MeAc 57.05 °C	EtOH/EtAc 71.81 °C	IPOH/IPAc 78.54 °C	**BuOH/H_2O** **92.62** °C	**AmOH/H_2O** **95.80** °C
MeOH 64.53 °C	EtAc 77.20 °C	IPOH/H_2O 80.06 °C	H_2O 100.02 °C	H_2O 100.02 °C
H_2O 100.02 °C	EtOH/H_2O 78.18 °C	IPOH 82.35 °C	BuOH/BuAc 116.85 °C	HAc 118.01 °C
HAc 118.01 °C	EtOH 78.31 °C	IPAc 88.52 °C	BuOH 117.68 °C	AmOH 137.68 °C
	H_2O 100.02 °C	H_2O 100.02 °C	HAc 118.01 °C	HAc/AmOH/AmAc 139.89 °C
	HAc 118.01 °C	HAc 118.01 °C	HAc/BuOH/BuAc 121.58 °C	HAc/AmOH 140.07 °C
			HAc/BuOH 123.21 °C	AmAc 147.71 °C
			BuAc 126.01 °C	

* Heteroazeotropes in boldface.

Table 3 Steady-state operating condition and total annual cost (TAC) for reactive distillation designs of five esterification systems.

System	(i)MeAc	(ii)EtAc		(iii)IPAc		(iv)BuAc	(v)AmAc
Column configuration	RD	RD	Stripper	RD	Stripper	RD	RD
Total No. of trays including the reboiler	39	22	10	27	8	33	36
No. of trays in stripping section (N_S)	3		9		7	9	12
No. of trays in reactive section (N_{rxn})	34	11		13		20	22
No. of trays in rectifying Section (N_R)	1	9		13		4	2
Reactive tray	4~37	0~10		0~12		10~29	13~34
Acetic acid feed tray	36	0		0		25	30
Alcohol feed tray	13	0		0		29	34
Feed folw rate of acid (kgmol/hr)	50.00	48.40		48.20		50.00	50.00
Feed flow rate of alcohol(kgmol/hr)	50.00	50.00		50.00		50.00	50.00
Top product flow rate (kgmol/hr)	50.35	50.30		49.94		50.38	49.98
Bottom product flow rate(kgmol/hr)	49.65		48.10		48.26	49.62	50.02
X_D or $X_{D,aq}$							
m.f. acid	0.00087	0.00001		2.5E-6		0.01670	0.00221
m.f. alcohol	0.00556	0.02337		0.02665		0.00688	0.00643
m.f. acetate	0.98000	0.01533		0.00835		0.00076	0.00019
m.f. water	0.01357	0.96129		0.96500		0.97566	0.99117
X_B							

m.f. acid	0.01237		0.00010		0.00002	0.00004	0.00711
m.f. alcohol	0.00763		0.00912		0.00993	0.01006	0.00289
m.f. acetate	$<10^{-8}$		0.99000		0.99000	0.98990	0.99000
m.f. water	0.98000		0.00078		0.00005	$<10^{-8}$	$<10^{-8}$
Condenser duty (kW)	-1280.22	-4265.71	-1860.54	-3428.58	-1129.89	-2857.92	-1483.15
Subcooling duty (kW)		-833.82		-506.51		-461.35	-227.42
Reboiler duty (kW)	1035.71	4523.98	2195.68	3473.31	1370.90	3085.41	1532.48
Column diameter (m)	1.03	1.95	1.45	1.89	1.23	1.88	1.34
Weir height (m)	0.1016	0.1016	0.0508	0.1016	0.0508	0.0508	0.0508
Decanter temperature (°C)		40		50		50	50
Condenser heat transfer area (m^2)	80.03	157.62	68.99	107.37	36.78	57.06	27.63
Subcooling heat transfer area (m^2)		170.24		96.06		57.89	21.82
Reboiler heat transfer area (m^2)	38.63	168.72	92.80	129.53	57.94	115.07	57.15
Damköhler number (*Da*)	28.88	29.61		13.08		16.86	4.35
Total capital cost ($1000)	730.78	2051.44		1731.74		1277.26	854.62
Column	323.30	511.57		539.56		547.92	408.93
Column trays	50.60	88.10		97.02		111.55	71.85
Heat exchangers	356.888	1451.77		1095.16		617.79	373.84
Total operating cost ($1000/year)	122.49	613.08		466.35		319.06	190.10
Catalyst cost	30.94	64.97		67.06		29.80	16.61
Energy cost	91.55	548.11		399.29		289.26	173.49
TAC ($1000/year) (50 kmol/hr)	366.08	1296.89		1043.60		745.01	474.97
TAC ($1000/year) (52825 ton/year)	644.96	1993.64		1377.95		840.74	474.97

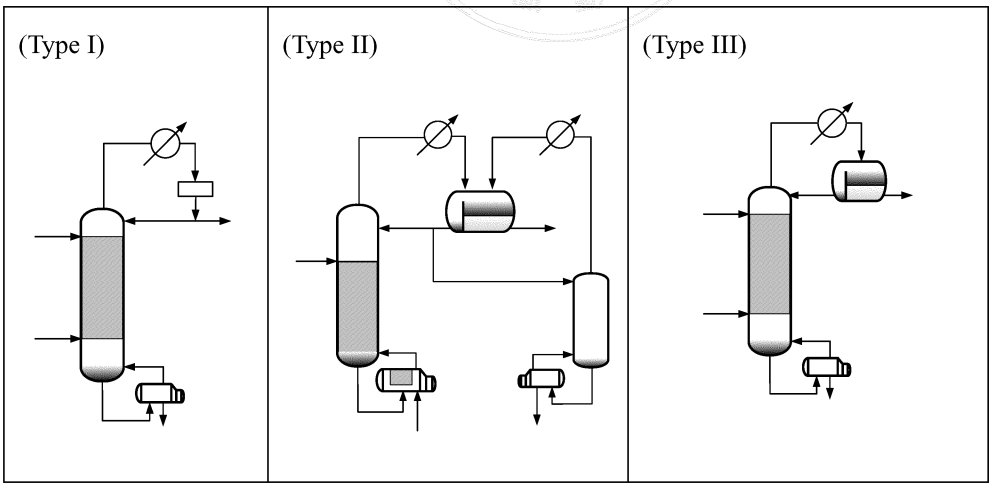

Figure 1. Three possible flowsheets for these five esterification system

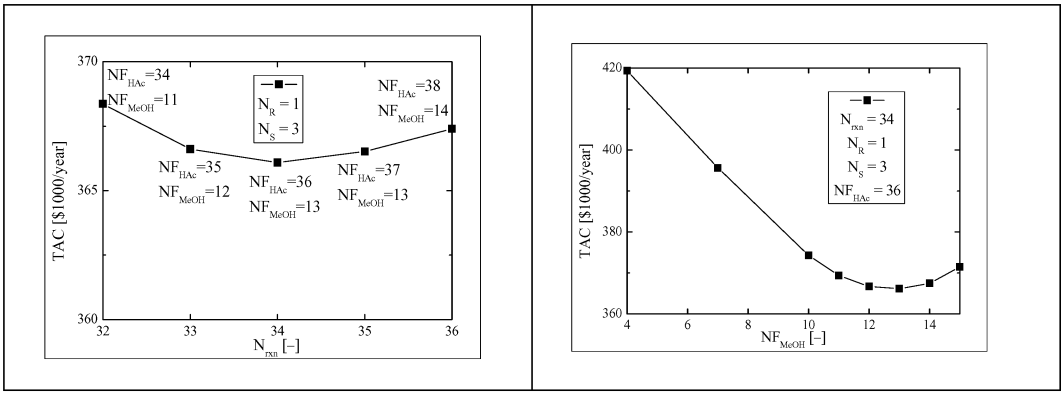

Figure 2. Effects of design variables on TAC for the MeAc system.

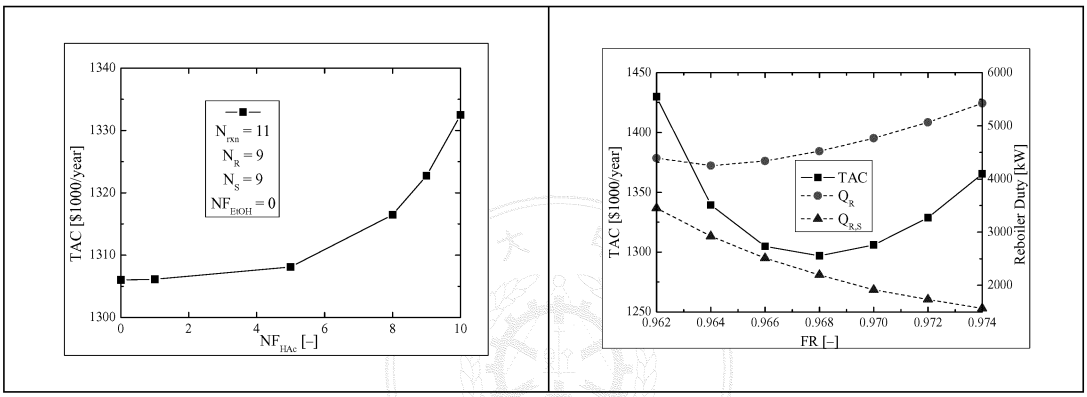

Figure 3. Effects of design variables on TAC for the EtAc system.

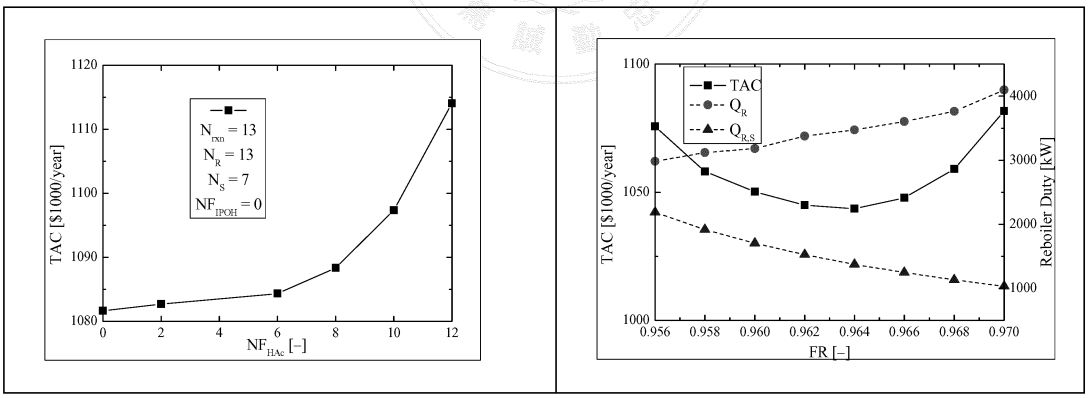

Figure 4. Effects of design variables on TAC for the IPAc system.

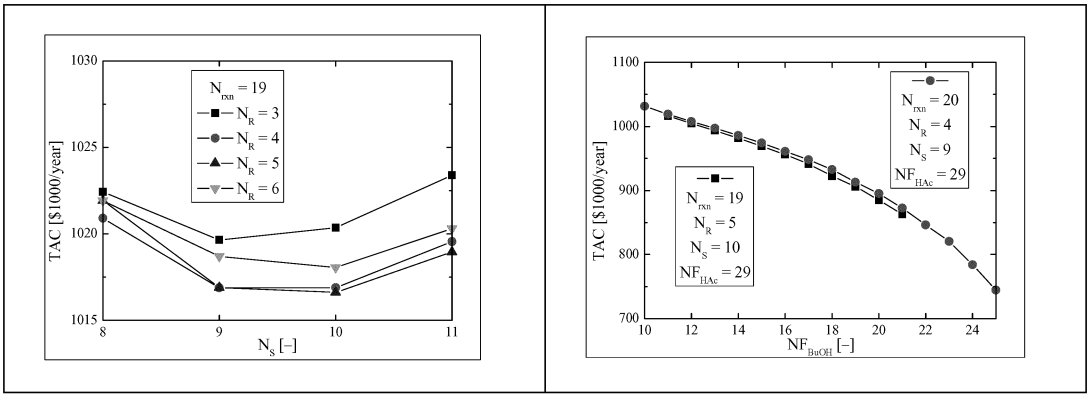

Figure 5. Effects of design variables on TAC for the BuAc system.

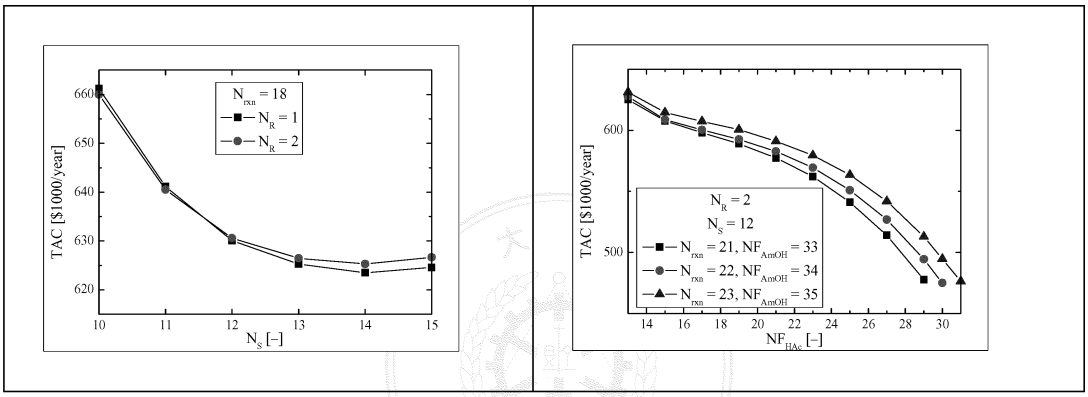

Figure 6. Effects of design variables on TAC for the AmAc system..