Profitability Analysis for Batch Reactive Distillation Process Based on Fixed Product Demand

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Profit maximisation for batch reactive distillation process involving ethanol esterification reaction was conducted in this work using optimisation technique. The optimisation parameters considered are: vapour load (V) reflux ratio (R) and batch time (t_b). Here, two cases were considered. In Case 1 the feed is composed of only the reactants (pure feed) and in Case 2 the feed is composed of reactants as well as a small fraction of one of the reaction products (diluted feed). The profit is maximised with fixed product demand ranging from 800 to 1200 kmol/year. For Case 1, the sensitivity of raw materials and or product prices is also investigated.

For a given product demand, the optimization results show that, operating with Case 2 is always more profitable compared to the Case 1. This is due to low cost diluted feed and significant change in design and operation for Case 2 compared to Case 1. Also, changes in feed/product prices lead to different design and operation as well as production target.

1. Introduction

The combination of batch reactor with a batch distillation column is called batch reactive distillation. It is an interesting alternative process to increase the conversion of equilibrium limited reactions such as etherification and esterification reactions. An extensive literature survey shows that optimal design and operation based on fixed market demand received very limited attention in the past. Diwekar *et al.* (1989) maximised annual profit for single and multi fraction batch distillation columns, operating under constant and variable reflux conditions. They applied an extended shortcut method for the solution of simple model equations and maximum principle to solve the optimization problem. Mujtaba and Macchietto (1997) presented computationally efficient framework for dynamic optimization of batch reactive distillation for ethanol esterification process. The polynomial curve fitting techniques were proposed and applied to the results of the dynamic optimization problem. These polynomials were used to formulate a maximum profit problem. Hanke and Li (2000) applied a variant Simulated Annealing method to the optimization of batch distillation processes. For a given purity with different prices of the product, the optimization problem was formulated with profit as an objective function.

Miladi and Mujtaba (2004) discussed the optimal design and operation policies of binary batch distillation under fixed product demand scenario. They showed that for fixed market demand, the maximum profit could be achieved with optimum vapour load and number of stages. Also they concluded that the maximum profit does not make sense without the consideration of product demand in the optimisation problem formulation, as it can lead to over or under production of the desired products. Most recently, Mahmud *et al.* (2008) considered optimal design and operation of multivessel batch distillation column (*Multi*VBD) under fixed product demand and strict product specification.

In this work, profitability analysis for batch reactive distillation process (synthesis of ethyl acetate) based on fixed product demand is investigated. The optimisation problem with maximum profit as the objective function, incorporating a detailed dynamic model, is formulated and solved using Control Vector Parameterization (CVP) and Successive Quadratic Programming (SQP) technique in gPROMS modelling software (2004).

2. Process Model

Figure 1 shows a detailed dynamic model (Edreder *et al.*, 2008) including mass and energy balance equations, column holdup, rigorous phase equilibria, and chemical reaction taking on the plates, in the reboiler and in the condenser.

3. Optimization Problem Formulation

The optimization problem can be stated as follows:
Given: the column configuration (N number of stages), the feed mixture, and a separation task (i.e. achieve the product with purity specification); production horizon (H, h/yr); product demand
Determine: the optimum design (vapour load, V) and operating decisions (reflux ratio, R and batch time, t_b)
So as to maximize: the objective function P
Subject to: equality and inequality constraints.

Mathematically the optimisation problem (OP) can be stated as shown in Figure 2. A profit function, P ($/year) for ethanol esterification problem can be defined (Miladi and Mujtaba, 2004) as follows:

$$P \ (\$/yr) = (C_1 D_1 - C_2 B_0 - OC) \times N_B - ACC \tag{1}$$

$$OC = (\frac{K_3 V}{A}) \times (t_b + t_s) \tag{2}$$

$$ACC = K_1 (V)^{0.5} (N)^{0.8} + K_2 (V)^{0.65} \tag{3}$$

$$N_B = \frac{(H / year)}{(t_b + t_s)} \tag{4}$$

Where, OC is operating cost ($/batch), ACC is Annualised capital cost ($/year), $K_1 = 1500$; $K_2 = 9500$; $K_3 = 180$; $A = 8000$; Set-up time (t_s) = 0.5 hr; H = 8000 hr/yr. The cost

parameters for ethanol esterification reaction are shown in Table 1, the feed prices have been assumed and the price of the product was taken from Greaves *et.al* (2003).

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Internal Plates, j = 2, N-1

Total Mass Balance:
$$0 = L_{j-1} + V_{j+1} - L_j - V_j + \Delta n_j H_j$$
Component Mass Balance:
$$H_j \frac{dx_{ji}}{dt} = L_{j-1} x_{j-1,i} + V_{j+1} y_{j+1,i} - L_j x_{ji} - V_j y_{ji} + r_{ji} H_j$$
Energy Balance:
$$0 = L_{j-1} h^L_{j-1} + V_{j+1} h^V_{j+1} - L_j h^L_j - V_j h^V_j$$
Equilibrium:
$$y_{ji} = K_{ji} x_{ji} \,,$$
Restrictions:
$$\sum y_{ji} = 1$$
Relations defining physical properties:
$$K_{ji} = K_{ji}(y_j, x_j, T_j, P)$$
$$h^L_j = h^L_j(x_j, T_j, P), \, h^V_j = h^V_j(y_j, T_j, P)$$
$$r_{ji} = r_{ji}(k_{ji}, x_{ji}), \, \Delta n_j = \sum r_{ji}$$

Reboiler: j = N

Total Mass Balance:
$$\frac{dH_N}{dt} = L_{N-1} - V_N + \Delta n_N H_N$$
Component Mass Balance:
$$H_N \frac{dx_{Ni}}{dt} = L_{N-1}(x_{N-1,i} - x_{Ni}) - V_N(y_{Ni} - x_{Ni})$$
$$+ r_{Ni} H_N - \Delta n_N H_N x_{Ni}$$
Energy Balance:
$$0 = L_{N-1}(h^L_{N-1} - h^L_N) - V_N(h^V_N - h^L_N) + Q_R$$

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Condenser and Distillate Accumulator: j=1
Accumulator Total Mass Balance:
$$\frac{dH_a}{dt} = L_D$$
Component Mass Balance:
a) Accumulator:
$$H_a \frac{dx_a}{dt} = L_D(x_{D,i} - x_{a,i})$$
b) Condenser Holdup Tank
$$H_c \frac{dx_{Di}}{dt} = V_2 y_{2,i} + r_{1,i} H_c - (V_2 + \Delta n_1 H_c) x_{Di}$$
Energy Balance:
$$0 = V_2 h^V_2 - (V_2 + \Delta n_1 H_c) h^L_1 - Q_c$$
Other Equation
$$L_1 = R(V_2 + \Delta n_1 H_c), \, L_D = (V_2 + \Delta n_1 H_c)(1 - R)$$
$$T_1 = T_1(x_{D,i}, P), \, h^L_1 = h^L_1(x_{D,i}, T_1, P)$$
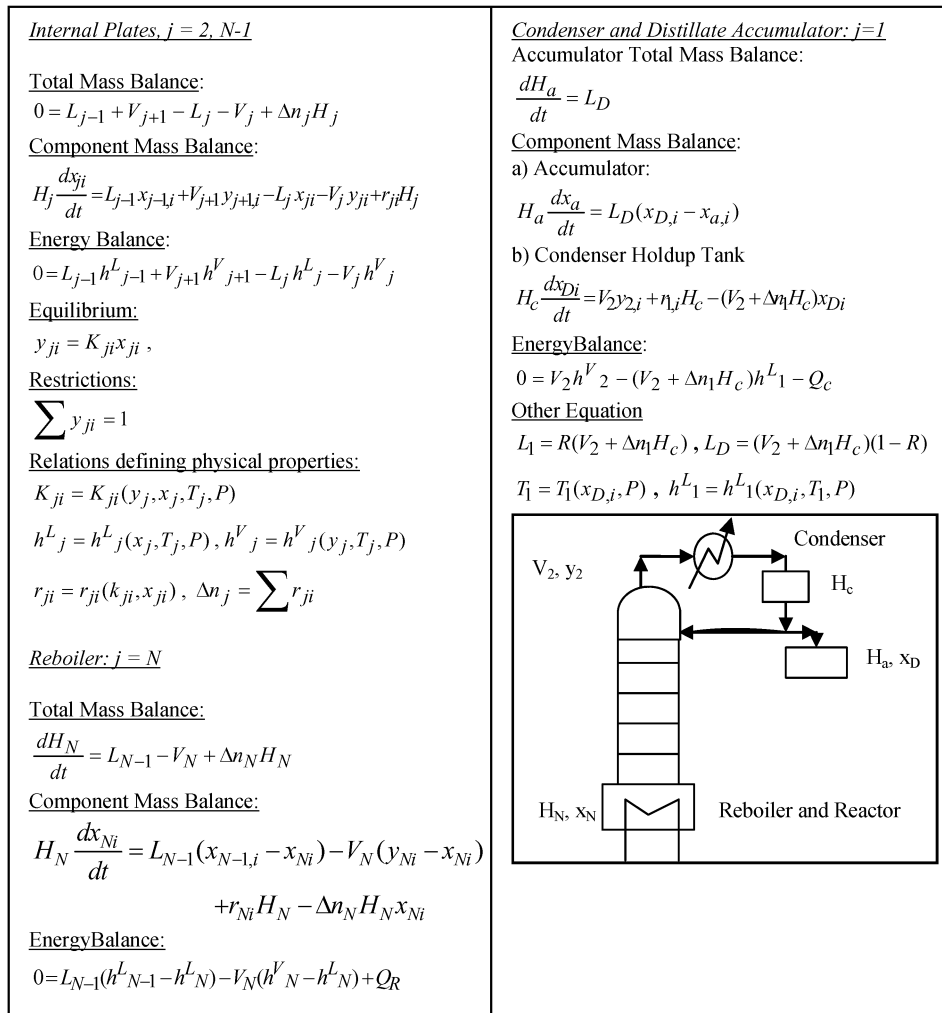

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Fig. 1 Model Equations

4. Case Study

4.1 Specifications

Ethyl acetate is produced by the reversible reaction between the acetic acid and ethanol:
Acetic Acid + Ethanol ⇔ Ethyl Acetate + Water in a 10-stage batch distillation column. The total column holdup is 4 % of the initial feed (50 % is taken as the condenser hold up and the rest is equally divided in the plates) and the reboiler capacity is 5 kmol. The feeds (kmol) <Acetic Acid, Ethanol, Ethyl Acetate, Water> are: Case 1 - <2.5, 2.5, 0.0, 0.0> and Case 2 -<2.25, 2.25, 0.0, 0.5>. The kinetic and thermodynamic models are given in Edreder *et al.* (2008). For Case 1, the sensitivity of feed and or product prices

on the design, operation and profitability is carried out. In Scenario 1, the price of the feed is increased by 5% while the product price is kept constant; in Scenario 2, both feed and the product prices are increased by 5%.

OP	Max	P
	V, R, t_b	
	s.t. $x_c \geq x_c^*$	(inequality constraint)
	Product demand	fixed
	Process model equations	(equality constraint)
	Linear bounds on V, R	(inequality constraint)

Fig. 2 Optimization problem formulation

Table 1. Cost Parameters

	Case 1 (pure feed)	Case 2 (diluted feed)
Acetic acid, $/kmol	50	40
Ethanol, $/kmol	20	18
C_2 = raw material cost, $/kmol	35	26.1
Ethyl acetate at 70 % purity, $/kmol	96	96

4.2 Results and Discussions

Case 1: The results in terms of optimal design, operation, operating cost, annualised capital cost, amount of distillate and the maximum profit ($/yr) for each fixed product demand (ranging from 800 to 1200 kmol /yr) are summarized in Table 2. It is clear from the results that the optimal vapour load (V) and reflux ratio (R) are increased while the batch time (t_b) decreases with increasing product demand and consequently leads to increases the number of batches (N_B) according to Equation 4. The maximum profit ($/yr) has been achieved for product demand of 1100 kmol/yr with optimum (V=2.11 kmol/hr, R= 0.933, t_b = 18.8 hr and N_B= 414.5). The results are indicating that, operating cost and annual capital cost are directly proportional to increases in vapour load. For the given column configuration (i.e. N=10), it was not possible to further improve on profitability for other product demands.

Case 2: The results are summarised in Table 3. For each product demand comparison of the results with those in Table 2 clearly shows the effect of feed dilution on the design, operation and profitability. Although the maximum profit is achieved for the product demand of 1100 kmol/yr (same as Case 1), feed dilution not only reduces the raw material costs but results in much higher profit for each product demand. For example, for product demand 800 kmol/yr, the profitability has improved by almost 70%. Note for Case 2, the column needs to operate at higher reflux ratio but with higher V and thus decreasing the batch time compared to those in Case 1. This results in producing

less amount of distillate (on specification) per batch and more number of batches in the production campaign.

Price Sensitivity: The optimisation results of Scenario 1 are presented in Table 4. The optimal design and operation are found to be very close to that of Case 1. Since feed prices are increased, it directly reduces the maximum profit for each case (almost by 60% compared to Case 1). From the manufacturer point view, the production target should be reduced to 1000 kmol/yr to make most money.

The optimisation results of Scenario 2 are presented in Table 5. It is observed that the profit has been improved by 28 % compared to Case 1 due to increase in product price and raw material prices. Also it reveals that the production target should remain the same as in Case 1 (1100 kmol/year). Also similar observations are made in terms of the other optimisation parameters such as (V, R, t_b).

Table 2. Summary of the results – Case 1

Demand	t_b (hr)	V	R	OC($/year)	ACC($/year)	N_B	D	P($/year)
800	26.49	1.29	0.921	231.3	20154.0	296.5	2.70	4556.8
900	23.36	1.52	0.924	275.0	22236.9	335.4	2.68	5203.1
1000	20.79	1.77	0.928	319.3	24312.6	375.7	2.66	5621.6
1100	18.80	2.11	0.933	381.3	26926.3	414.5	2.65	5757.9
1200	16.77	2.28	0.934	407.7	28167.4	463.3	2.59	5542.3

Table 3. Summary of the results – Case 2

Demand	t_b(hr)	V	R	OC($/year)	ACC($/year)	N_B	D	P($/year
800	22.36	1.63	0.937	294.0	23135.5	350.0	2.29	7702.6
900	19.66	1.95	0.941	353.2	25743.9	396.8	2.27	8527.2
1000	17.48	2.32	0.945	418.3	28507.3	445.0	2.25	9002.3
1100	15.66	2.75	0.948	494.9	31468.0	494.9	2.22	9051.2
1200	14.13	3.24	0.952	585.0	34676.5	546.7	2.19	8595.4

Table 4. Summary of the results – Scenario 1 (5% increase of feed price)

Demand	t_b (hr)	V	R	OC($/year)	ACC($/year)	N_B	D	P($/year)
800	26.55	1.30	0.921	233.7	20256.1	295.8	2.70	1965.7
900	23.41	1.54	0.925	277.7	22364.9	334.6	2.69	2270.7
1000	20.87	1.80	0.929	32.5.7	24544.4	374.4	2.67	2341.6
1100	18.77	2.09	0.933	377.7	26812.8	415.1	2.63	2133.9
1200	16.95	2.39	0.935	430.9	28942.9	458.4	2.62	1591.6

Table 5. Summary of the results - Scenario 2 (5% increase in feed and product price)

Demand	t_b (hr)	V	R	OC($/year)	ACC($/year)	N_B	D	P($/year)
800	26.55	1.30	0.921	233.6	20266.3	295.7	2.71	5804.1
900	23.41	1.54	0.925	277.7	22365.1	334.6	2.69	6589.7
1000	20.87	1.80	0.929	325.7	24544.3	374.4	2.67	7140.2
1100	18.60	2.01	0.931	372.6	26210.7	418.7	2.63	7370.8
1200	16.98	2.40	0.936	430.2	29068.6	457.7	2.62	7354.4

Note: D is the amount of distillate product per batch, kmol/batch

5. Conclusion

In this work, profitability analysis has been conducted for esterification reaction of ethanol to produce ethyl acetate based on fixed product demand in batch reactive distillation process. An optimisation problem is formulated with profit as an objective function to maximize and a number of design and operation parameters to optimize subject to product demand and strict product specification. The results indicate that the operation with diluted feed is more profitable compared to the case with undiluted feed. Also price increase in feed, although does not affect the design and operation significantly, it can lead to reduced production target to make a profitable operation. On the other hand prices increase in feed and product (by equal percentage amount) will not lead to reduced production target but can enhance profitability significantly.

6. References

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