



## OPTIMAL CONTROL AND ON-LINE OPERATION OF REACTIVE BATCH DISTILLATION

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(Received 25 April 1995)

**Abstract**—While both the dynamic modelling, and to a lesser extent, the optimisation of reactive batch distillation have been studied in the past, issues related to control and on-line operation of such a process have not been properly addressed. In this study, *a priori* optimal profiles of the operating variables are established for an industrial reactive distillation process. The optimal profiles are found either by maximising the profitability or by minimising the operating time subject to constraints on the reactor temperature and the loss of volatile reactant in the distillate. The control properties at optimal and non-optimal conditions are assessed. A one-point column control scheme with a PI-controller is designed to implement the optimal profiles. The controller performance is tested using a simulation model including disturbances in the reaction model and in the reboiler heat duty. The fully automatic operation of the process according to the optimal policies is demonstrated in conjunction with both a continuous controller and a real time control system. Good performance is achieved in both cases.

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### 1. INTRODUCTION

Batch distillation is used in the chemical industry for the production of small amounts of products with high added value and for processes where flexibility is needed. A batch reactor can be combined with a distillation column as shown in Fig. 1. This combined unit operation, called *reactive batch distillation*, especially suits those chemical reactions where reaction equilibrium limits the conversion in a normal reactor to a low-to-moderate level. By continuously separating low-boiling products from the

reactants and other products while the reaction is in progress, the reaction can proceed to a much higher level of conversion. Also, removal of a light product results in a decrease in its concentration in the liquid phase which will increase the temperature and thereby the reaction rate.

While both the dynamic modelling of reactive batch distillation, and to a lesser extent, its optimisation has been studied in the past (e.g. Egly *et al.*, 1979; Cuille and Reklaitis, 1986; Albet *et al.*, 1991; Mujtaba and Macchietto, 1992), issues related to controllability and control of such a process have not been properly addressed. Some attention to the implementation of optimal control profiles for batch distillation has been given by Quintero-Marmol and Luyben (1992), and Bosley and Edgar (1992). So far, only Sørensen and Skogestad (1992, 1994) have considered controllability of reactive batch distillation.

This study addresses several aspects of optimal control of a reactive batch distillation process with reference to a specific industrial application. The control objective is either to maximise profitability or to minimise operating time. There are constraints on the maximum allowable reboiler temperature to avoid thermal decomposition of the product and on the maximum loss of volatile reactant in the distillate. Manipulated variables for control are the heat input to the reactor and the internal reflux ratio,  $Q_R$  and  $R$ , respectively. It is assumed that the condenser duty,  $Q_C$ , is used for pressure control and the

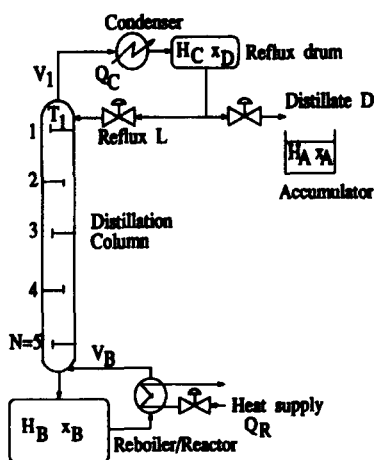


Fig. 1. Batch distillation column/reactor.

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Table 1. Process data for the industrial case study.

Column	reboiler + 5 trays + total condenser + accumulator
Reaction	$1.0 R_1 + 0.7 R_2 + 0.3 R_3 \leftrightarrow P(s) + 2.0 W$
Reaction rate	$r_N = r_{R_1} = k_1 c_{R_1} (c_{R_2} + c_{R_3}) - k_2 c_W$
Rate constants	$k_r = k_{r,0} \exp\left(-\frac{E_r}{E_g} * \left(\frac{1}{T_B} - \frac{1}{T_0}\right)\right)$
Activation energies	$E_1 = E_2 = 18 \text{ kcal/mol} = 7.5 \times 10^4 \text{ kJ/kmol}$
Frequency factors	$k_{0,1} = 0.03$ and $k_{0,2} = 0.25 \cdot k_{0,1} = 0.0075$
Reference temperature	$T_0 = 500.0 \text{ K}$
Pressure in column and reactor	$P = 1 \text{ atm}$
Hydraulic time constant	$\tau = 0.0018 \text{ h} = 6.5 \text{ s}$
Initial holdups (reboiler, each tray, and condenser)	20.6, 0.1 and 1.7 kmol
Initial reboiler composition	$x^0(W, R_2, R_3, R_1) = [0.0097, 0.3544, 0.1505, 0.4854]$
Initial tray compositions, $j = 1, N$	$x^0(W, R_2, R_3, R_1) = [0.999999, 0.000001, 0.0, 0.0]$
Value of product $P$	$C_{\text{prod}} = 50 \text{ \$/kmol}$
Cost of steam	$C_{\text{heat}} = 3 \text{ \$/}10^6 \text{ BTU} = 2.844 \times 10^{-6} \text{ \$/kJ}$
Total cost of raw material	$C_{\text{raw}} = 200 \text{ \$}$
Charging and cleaning time	$t_c = 0.5 \text{ h}$
Total reaction time	specified or optimised, $t_r$ hr
Reboiler heat duty	specified or optimised, $Q_R \in [0, 0.9] \times 10^6 \text{ kJ/h}$
Reflux ratio	specified or optimised, $R \in [0, 1.0]$

distillate flow,  $D$ , for condenser level control. Of particular interest are:

1. Establishing *a priori* optimal profiles of the operating variables.
2. Assessing the controllability properties at the optimal conditions.
3. Designing controllers to implement the optimal profiles.
4. Verifying stability and control performance of the controller.

## 2. REACTIVE BATCH DISTILLATION MODEL

The procedure used in this study to solve the optimisation problem involves repeated solutions of the dynamic model of the system. The procedure is computationally expensive and the dynamic model is therefore rather simplified. The model is valid under the following assumptions:

1. Staged batch distillation column with trays numbered from the top and down (accumulator =  $A$ , condenser =  $C$ , reboiler =  $B$ ).
2. Perfect mixing and equilibrium on all trays.
3. Constant stage pressures and tray efficiencies.
4. Negligible vapour holdup.
5. Negligible changes in liquid enthalpies ( $dh^L/dt \approx 0$ ) (algebraic energy balance).
6. Total condensation with no subcooling in the condenser.
7. Chemical reaction limited to the reboiler.
8. Raoult's law for the vapour-liquid equilibrium.
9. Immediate heat input.
10. Constant molar holdup in the condenser (perfectly controlled).
11. Constant molar holdup on the trays (during optimisation).

## 12. Linear tray hydraulics (during simulation).

The molar holdup on the trays was assumed constant for the open-loop optimisation while a more complex model including linear tray hydraulics was used for simulations and control studies. The linear hydraulics model has the form  $L_j = L_j^0 + (H_j - H_j^0)/\tau$ , where  $L_j^0$  and  $L_j$  are the initial and current liquid flows and  $H_j^0$  and  $H_j$  the initial and current molar tray holdup, respectively. The parameter  $\tau$  is the hydraulic time constant.

The reaction considered is a condensation polymerisation reaction between a dibasic aromatic acid ( $R_1$ : terephthalic acid) and two glycols ( $R_2$ : 1,2-propanediol and  $R_3$ : 1,6-hexanediol) which form a polymer [ $P$ : poly(propylene/hexylene)-terephthalate] and water ( $W$ ). The polymer forms a separate, solid phase and is, therefore, not included in the distillation model. High conversion is achieved by distilling off the water. The physical properties data for the liquid components were taken from Coulson *et al.* (1983) for water and 1,2-propanediol and from Daubert and Danner (1985) for 1,6-hexanediol and terephthalic acid. A summary of the process data is given in Table 1.

The thermodynamic model used is a rather simple representation of the actual thermo behaviour. In particular, it is possible that strong non idealities may be present. For the purpose of the present paper (to demonstrate a method) the actual components are irrelevant and could be taken simply as representative of a generic mixture  $A$ ,  $B$ ,  $C$ , etc. However, reaction data are specific to the components indicated.

## 3. OPTIMAL A PRIORI OPERATION

The optimal operating values for reflux ratio and reboiler heat duty can be found based on some

optimisation criterion. In this study the optimisation problem has been solved according to a maximum profit or a minimum time control objective. In general, an optimal control problem can be stated as (Vassiliadis, 1993):

$$\min_{\dot{x}(\cdot), x(\cdot), y(\cdot), u(\cdot), v, x(t_0), t_f} \Phi(\dot{x}(t_f), x(t_f), y(t_f), u(t_f), v, t_f) \quad (1)$$

subject to

$$g(\dot{x}(t), x(t), y(t), u(t), v, t_f, t) = 0 \quad (2)$$

$$h_1(\dot{x}(t_f), x(t_f), y(t_f), u(t_f), v, t_f) = 0 \quad (3)$$

$$h_2(\dot{x}(t_f), x(t_f), y(t_f), u(t_f), v, t_f) \geq 0 \quad (4)$$

where  $g$  are the dynamic model equations, and  $h_1$  and  $h_2$  are the equality and inequality constraints, respectively. In addition there are upper and lower bounds on the state ( $x, y$ ), design ( $v$ ) and control ( $u$ ) variables and also on the final time ( $t_f$ ).

The optimal control problem is often referred to as an infinite dimensional problem because the control variable  $u$  is a function of time rather than a specific value at the optimum. This type of problem can be solved using Pontryagin's maximum principle. However, this solution method is usually time consuming. Therefore, it is more efficient to employ nonlinear programming rather than the maximum principle to compute the optimal control. The optimisation problem can then be solved by numerical techniques that convert the problem into a nonlinear programming problem (NLP). Two general approaches have appeared in the chemical engineering literature in recent years. These are either based on

1. Control vector parameterisation (e.g. Vassiliadis, 1993).
2. Full parameterisation of both control and states variables; often referred to as the collocation method (e.g. Logsdon and Biegler, 1989).

Comprehensive comparisons between control vector parameterisation and the collocation method have not been published. It is therefore difficult to make definite statements about their relative merits (Macchietto and Mujtaba, 1992).

The solution of the optimal control problem is in this paper based on control vector parameterisation and is solved using the optimisation program DAEOPT (Vassiliadis, 1993). The control vector  $u$  is parameterised into a finite number of variables which are optimised using a standard nonlinear optimisation technique (SQP). The solution method includes two levels. The first level performs an integration of the differential and algebraic equations for fixed values of the decision variables. The second level optimises these decision variables and

satisfies end point constraints. A complete solution of the dynamic model for each trial value of the decision variables is required. Note that the term *optimal control* does not involve control in the sense in which we discuss control later in this paper. The solution to the optimal control problem is a set of *optimal operating parameters* (here reflux ratio and reboiler heat duty) which may subsequently be used as set points for the actual controllers in on-line operation.

At the time when this work was performed, the optimisation software DAEOPT (Vassiliadis, 1993) was still in its initial phases of development. Optimal solutions with more than one discretisation interval for the control variables were difficult to obtain for this problem due to computational problems. The results shown here are therefore based on a single discretisation interval with either constant or linear control variables. Optimal solutions with up to four intervals using constant or linear control variables have been obtained later but are not presented in this paper. However, the optimal solutions using multiple intervals show only slightly higher optimal profitability than those for only one discretisation interval.

In the following we will consider two formulations of the maximum profit problem where zero cost of raw material is assumed in the first but not in the latter. Also, a minimum time control objective is considered.

#### *Maximum profit problem I—zero cost of raw material*

The optimal operating policy in terms of maximum profit can be determined by optimising the overall hourly profit [\$/h]:

$$\max_{R, Q_R, t_f} P^s = \frac{C_{\text{prod}} A_{\text{prod}} - C_{\text{heat}} \int_0^{t_f} Q_R(t) dt}{t_f} - C_{\text{fixed}}, \quad (5)$$

where  $C_{\text{prod}}$  is the value of product  $P$  (\$/kmol monomer block),  $A_{\text{prod}}$  is the amount of product  $P$  at  $t_f$  (kmol),  $C_{\text{heat}}$  is the cost of steam to the reboiler (\$/kJ),  $Q_R$  is the reboiler heat duty (kJ/h),  $t_f$  is the final time (h),  $C_{\text{fixed}}$  are the fixed costs (\$/h) and  $P^s$  is the profitability (\$/h). Zero cost of raw material is assumed (this cost is included in the next example). Note that since the initial charge is fixed, and we assume all unreacted feed is recycled to the next batch at no cost, this will not affect the location of the optimum. We use  $C_{\text{fixed}} = 0$  since the optimum will also be independent of the fixed costs. A single discretisation interval is used with constant control variables resulting in three operating parameters ( $R, Q_R$  and  $t_f$ ) for the optimisation. The constraints are:

1. Negligible loss of reactant  $R_2$  in the accumulated distillate

$$x_{A,w}(t_f) \geq 0.999. \quad (6)$$

2. Reboiler temperature below  $240^\circ\text{C} = 513.15\text{ K}$  to avoid thermal decomposition of the end-product

$$T_B(t_f) \leq 513.15\text{ K}. \quad (7)$$

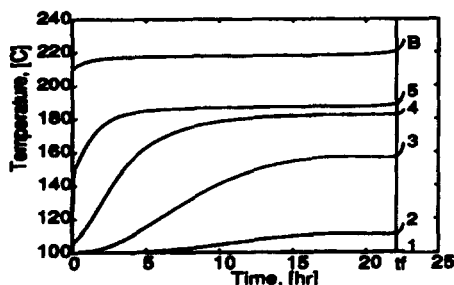
Experiments and simulations have shown that the reboiler temperature is highest at the end of the reaction, so keeping the endpoint temperature constraint is sufficient. If this was not the case, the constraint on the reboiler temperature could be added as a path constraint instead of as an end-point constraint.

With the process data given in Table 1 the optimal values are:

Optimal parameters			Optimal results			
$R$	$Q_R$ (kJ/h)	$t_f$ (h)	$P(t_f)$ (\$/h)	$x_{A,w}(t_f)$	$T_B(t_f)$ (K)	$\chi_{R_1}(t_f)$
0.950	$0.747 \cdot 10^6$	22.1	19.9	0.9997	494.4	0.97

The parameter  $\chi_{R_1}$  is the conversion of reactant  $R_1$ . Solutions with different values of the monomer product, e.g.  $C_{\text{prod}} = 100$  \$/kmol or  $C_{\text{prod}} = 25$  \$/kmol, give almost the same optimal results.

The temperature profiles for the process, given the optimal operating parameters, are presented to the left in Fig. 2. The reboiler temperature is more or less constant during the whole batch but the temperature in the top section of the column increases slowly. There is a sudden increase in temperature on all trays immediately after the optimal final time. The end of the reaction in the real plant can therefore be easily detected using temperature measurements on any one of the trays or in the reboiler.



When using sub-optimal values for  $R$  and  $Q_R$  (e.g.  $R = 0.954$  and  $Q_R = 0.691 \times 10^6$  kJ/h), a different response is obtained (right in Fig. 2). The constraints are still satisfied but the previous optimal conversion is only reached at  $t = 25.8$  h. The profitability is 15% lower, at 16.9 \$/h. The temperatures for this sub-optimal operation are lower than under optimal conditions showing that we are over-refluxing the column. Also, detection of the termination conditions based on temperature alone is much more difficult.

Note that the optimum with respect to time is very flat. Indeed, ending the batch after 16 h (25% time saving) still yields 99% of the optimal profitability with a conversion of  $R_1$  of  $\chi_{R_1}(t_f) = 0.71$ . The reason for this insensitivity to the value of  $t_f$ , is that we have assumed that there is no cost involved in recycling the unreacted feed since the cost of raw material is neglected.

#### Maximum profit problem II—fixed cost of raw material

Next consider a slightly different objective function where the cost of raw material is taken into consideration. Also a charging and cleaning time of  $t_s = 0.5$  h is included:

$$\max_{R, Q_R} P^s = \frac{-C_{\text{raw}} + C_{\text{prod}} A_{\text{prod}} - C_{\text{heat}} \int_0^{t_f} Q_R(t) dt}{t_f + t_s} - C_{\text{fixed}}, \quad (8)$$

where  $C_{\text{raw}}$  is the total cost of raw material (\$) and  $t_s$  is the charging and cleaning time (h). With this objective function, the constraints in equations (6)–(7) and the process data given in Table 1 the optimal values are given below for the case with one discretisation interval and constant or linear operating parameters where  $t_0 = 0$  is the start of the batch and  $t_f$  the final time:

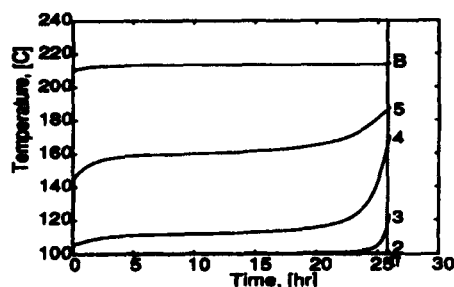


Fig. 2. Temperature profiles for (left) optimal and (right) sub-optimal conditions. The trays are numbered from the top and down and B is the reboiler/reactor (Maximum profit problem I—zero cost of raw material).

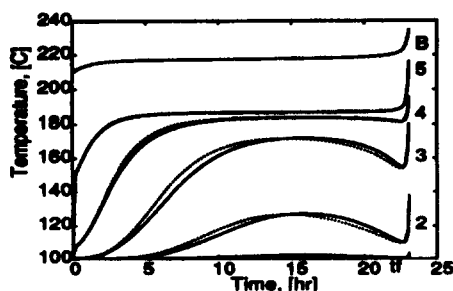


Fig. 3. Temperature profiles for optimal conditions with constant (dotted lines) and linear control parameters (solid lines). The trays are numbered from the top and down and B is the reboiler/reactor (Maximum profit problem II—fixed cost of raw material).

Optimal parameters				
	R	$Q_R$ (kJ/h)	$t_f$ (h)	
Constant	0.933	$0.545 \times 10^6$	23.0	
Linear	$0.9317(t_0) \rightarrow$ $0.9325(t_f)$	$0.533(t_0) \rightarrow$ $0.548(t_f) \times 10^6$	23.0	
Optimal results				
	$P(t_f)$ (\$/h)	$x_{A,w}(t_f)$	$T_B(t_f)$ (K)	$\chi_{R_1}(t_f)$
Constant	10.990	0.9990	508.5	1.00
Linear	10.993	0.9990	508.0	0.998

The temperature profiles for both cases are given in Fig. 3. With the cost of raw material included in the objective function, the optimum is no longer flat. When compared to the optimal results from the previous problem (equation 5), it can be seen that both the reflux ratio and the reboiler heat duty are reduced. However, the total operating time is increased from 22.1 h to 23.0 h. The reboiler heat duty is reduced by more than 25%. This is because the relative influence of the energy consumption is larger when the cost of raw material is included with the same costs as in the previous problem. Note that the reaction is now run almost to complete conversion. As a result, the final reactor temperature has increased.

The optimal solutions for constant or linear operating parameters are very similar. However, the energy consumption is slightly reduced for linear parameters. Optimal solutions with up to four intervals have also been found with optimal profitabilities slightly higher than those presented here (not shown).

#### Minimum time problem

Above, the optimal performance of the process was defined in terms of maximum profit. Alternatively, a minimum operating time can be used as optimisation criterion:

$$\min_{R, Q_R} t_f, \quad (9)$$

where  $t_f$  is the minimum operating time, subject to the same constraints on the maximum loss of reactant  $R_2$  and maximum reactor temperature (equations 6 and 7). In addition there is a constraint on the minimum conversion

$$\chi_{R_1}(t_f) \geq 0.99 \quad (10)$$

With the process data given in Table 1, the optimal solution to the minimum time problem is given below for the case with one discretisation interval and constant operating parameters:

Optimal parameters			Optimal results			
R	$Q_R$ (kJ/h)	$t_f$ (h)	$P(t_f)$ (\$/h)	$x_{A,w}(t_f)$	$T_B(t_f)$ (K)	$\chi_{R_1}(t_f)$
0.957	$0.9 \times 10^6$	22.1	10.576	0.9990	508.5	0.99

In Fig. 4, the temperature profile for the minimum time solution is compared to the optimal profile from the maximum profit problem with fixed cost of raw material (equation 8). The reboiler heat duty is now at its maximum value which is as expected since the objective is to run the batch in minimum time regardless of costs. As a result, the reflux ratio is also increased to maintain the specified product purity. However, the profitability is slightly decreased which is mainly due to the higher energy consumption but also to the lower conversion [ $\chi_{R_1}(t_f) = 0.99$  versus  $\chi_{R_1}(t_f) = 1.00$  for the maximum profit problem]. The temperature profiles in the column are slightly increased compared to the maximum profit solution.

#### 4. IMPLEMENTATION OF OPTIMAL POLICIES

Since the formation of product resembles a continuous feed to the reboiler (Sørensen and

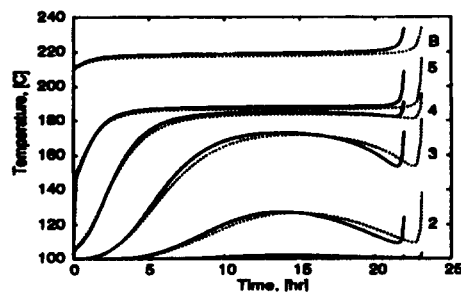


Fig. 4. Temperature profiles for optimal conditions with constant operating parameters. The trays are numbered from the top and down and B is the reboiler/reactor (solid lines: Minimum time problem, dotted lines: Maximum profit problem II—fixed cost of raw material).

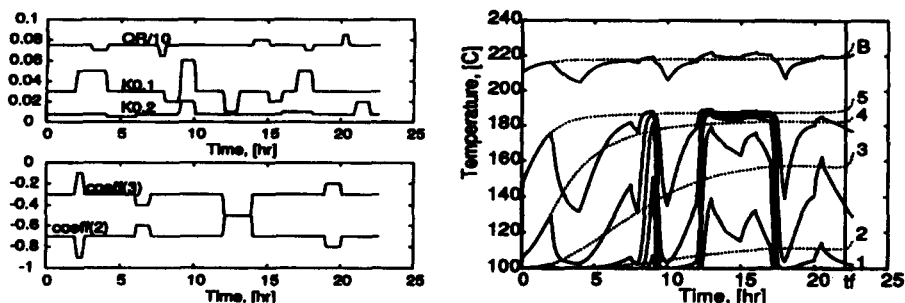


Fig. 5. (a) Disturbances in the process and (b) temperature profiles for the uncontrolled process. The trays are numbered from the top and down and  $B$  is the reboiler/reactor (dotted lines: undisturbed optimal profiles).

Skogestad, 1992, 1994), the issues involved in control of a reactive batch column are more similar to conventional continuous distillation control than to batch distillation control. In a conventional batch column one may usually implement the optimal values of  $R$  and  $Q_R$  in an “uncontrolled” open-loop fashion. However, for reactive distillation the operation is usually much more sensitive to the exact value of the reflux ratio  $R$ . A slightly too low  $R$  may result in a distillate flow which is larger than the amount of light component ( $W$ ) formed in the reaction and the difference must be provided by loss of the intermediate boiling reactant ( $R_2$ ). Therefore, there is a need to implement the optimal policy in some feedback fashion which maintains control of the distillate composition.

In order to implement the optimal policy, we propose to keep  $Q_R$  constant at its optimal value and adjust  $R$  to control the temperature on some tray inside the column. The temperature measurement should be placed on a tray with a large response to changes in the controller input. By controlling the temperature on one of the trays one will also to some extent indirectly control the reactor temperature since there is a strong coupling between the compositions in the column (Sørensen and Skogestad, 1992, 1994).

##### 5. ONE-POINT COLUMN CONTROL

We now consider implementing the optimal solution to the maximum profit problem I (where cost of raw material was neglected). Various disturbances are introduced in the simulation model to test the sensitivity to process changes (left in Fig. 5). The disturbances are assumed to be in:

1. Reboiler heat duty,  $Q_R$ .
2. Frequency factors for the forward and reverse reaction,  $k_{0,1}$  and  $k_{0,2}$ .
3. Stoichiometric coefficients of the alcohols (reactant 2 and 3) in the rate equation.

Disturbances 2 and 3 are used to represent some uncertainty in the reaction mechanism.

##### Uncontrolled case

First consider the uncontrolled case where  $R$  is kept constant. The temperature profiles (right in Fig. 5, solid lines) deviates significantly from the optimal profiles (right in Fig. 5, dotted lines). The disturbances yield breakthrough of the intermediate component  $R_2$  resulting in some loss of this reactant [ $x_{A,W}(t_f) = 0.989$  for the accumulated distillate] and the batch, therefore, does not satisfy the specifications. More severely, the reboiler temperature deviates up to  $12^\circ\text{C}$  from the optimal one which may result in a varying quality of the product  $P$  between batches.

##### Implementing the optimal policy

Next consider implementing the optimal policy in a feedback fashion by varying the reflux ratio  $R$  to keep a selected tray temperature constant. The reflux ratio  $R$  is the manipulated variable and  $Q_R$  is kept at its optimal value. The temperature measurement is placed on tray 3. The selection of measurement point is based on a comparison of the responses in tray temperatures to changes in the controller input  $R$ . Figure 6 illustrates typical responses at a given operating point. A further discussion of the selection of measurement points for

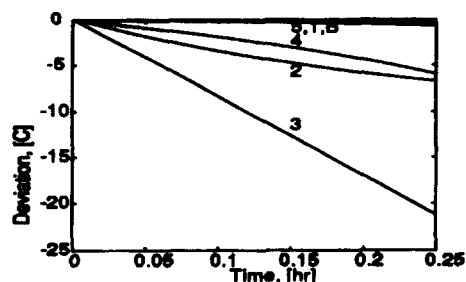


Fig. 6. Linear temperature responses for a 1% step in reflux ratio  $R$  (dynamic model linearised at  $t = 15$  h with the optimal temperature profile in Fig. 2, left). The trays are numbered from the top and down and  $B$  is the reboiler/reactor.

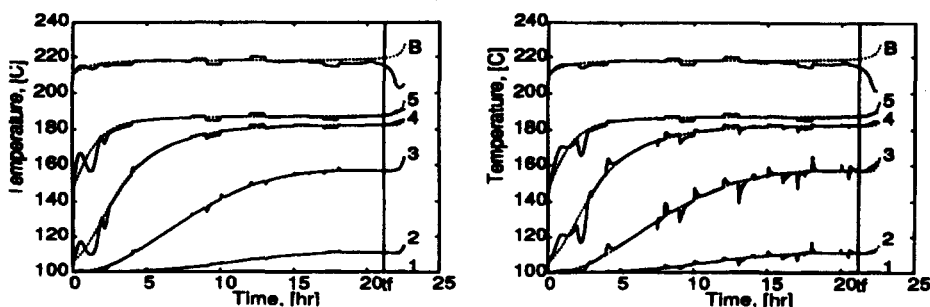


Fig. 7. Temperature profiles using (left) continuous controller and (right) real time control system. The trays are numbered from the top and down and *B* is the reboiler/reactor (solid lines: controlled profile, dotted lines: optimal profile).

control of this reactive batch distillation column is given by Sørensen and Skogestad (1994).

The set point for the PI-controller is the optimal temperature profile for tray 3 as a function of time (in the simulations fitted to a polynomial). A time delay of 15 s was added to the temperature measurement and the controller settings used are  $K_p = -0.01$  and  $\tau_i = 0.1$ . The controller is tuned using a linearised model at given operating points.

As can be seen from the results in Fig. 7 (left, solid lines), good control is achieved. The deviation in the reboiler temperature from the optimal profile (dotted lines) is small during most of the batch, but increases up to 20 °C towards the end. The optimal conversion ( $\chi_{R1} = 0.97$ ) is reached at  $t = 21.2$  h. After this time the reboiler temperature starts drifting away from the optimal value. For the controlled process (solid lines), the reboiler temperature is decreasing instead of increasing as for the optimal process (dotted lines). This is because the controller maintains the temperature on tray 3 at its set point as given by the optimal profile. However, due to the disturbances, the reaction rate is quicker than under optimal conditions. Keeping the temperature at the optimal set point will therefore hold light component back in the lower part of the column causing the reboiler temperature to decrease.

Detecting the end of the reaction based on the criteria from the optimal temperature profile, that the reaction is ended when the temperatures start rising rapidly, cannot be applied in this case. However, the fact that the reboiler temperature is drifting away from the optimal in either direction is an indication that the reaction is ended. The end point can therefore be estimated to when the reboiler temperature deviates from the optimal value on either side by an amount greater than, for example 5 °C.

#### Implementation using a real time control system

The simulated process including disturbances was also interfaced to an industrial real-time control

system Paragon (1991). All controllers were implemented using Paragon's own facilities. Instead of using a polynomial to describe the simulation temperature set point profile, only 16 set points were used. The sampling time was 1 min. As shown to the right in Fig. 7, good control is achieved and the responses are very similar to those obtained with the simulated continuous controller.

## 6. CONCLUSIONS

Optimal operating values for reflux ratio and reboiler heat duty have been determined according to a maximum profit and a minimum time control objective for a batch distillation column with reaction in the reboiler. The optimal policy must be implemented using feedback control to avoid loss of reactant ("break-through") in the distillate waste product. We select to control an intermediate column temperature, the location of which is selected based on a sensitivity analysis of the optimal temperature profiles. The column has been controlled using both a simple continuous PI-controller and a real time control system, with disturbances in the reaction parameters and in the reboiler heat duty. Good performance has been achieved in both cases. For this industrial application it has been found that the end of the reaction can be detected based on temperature measurements in the reboiler.

## NOMENCLATURE

- $A_{\text{prod}}$  = Amount of product *P* (kmol)
- $c_i$  = Concentration of component *i* in the reactor (kmol/m<sup>3</sup>)
- $C_{\text{fixed}}$  = Fixed costs (\$/h)
- $C_{\text{heat}}$  = Cost of steam (\$/kJ)
- $C_{\text{prod}}$  = Value of product *P* (\$/kmol)
- $C_{\text{raw}}$  = Total cost of raw material (\$)
- $D$  = Distillate flow (kmol/h)
- $E_r$  = Activity coefficient for reaction *r* (kJ/kmol)
- $g$  = Dynamic model equations in the general optimisation problem
- $h_1$  = Equality constraints in the general optimisation problem

$h_2$  = Inequality constraints in the general optimisation problem  
 $H_j$  = Liquid holdup on tray  $j$  (kmol)  
 $H_j^0$  = Initial liquid holdup on the trays (= 0.1 kmol)  
 $k_r$  = Rate constant for reaction ( $r$ )  
 $k_{or}$  = Frequency factor for reaction  $r$   
 $K_p$  = PI-controller gain  
 $L$  = Reflux flow (kmol/h)  
 $L_j$  = Internal liquid flow (kmol/h)  
 $L_j^0$  = Initial liquid flow (= 15 kmol/h)  
 $L_D$  = Distillate flow (kmol/h)  
 $N$  = Number of theoretical stages  
 $n_c$  = Number of components  
 $P$  = Pressure (atm)  
 $P^S$  = Profitability (\$/h)  
 $Q_C$  = Condenser duty (kJ/h)  
 $Q_R$  = Reboiler heat duty (kJ/h)  
 $r_N$  = Reaction rate (kmol/h)  
 $R_g$  = Ideal gas constant (= 8.314 kJ/kmol K)  
 $\bar{R}$  = Internal reflux ratio (=  $L/V$ )  
 $t$  = Time (h)  
 $t_0$  = Start time (h)  
 $t_f$  = Final operating time (h)  
 $t_s$  = Charging and cleaning time (h)  
 $T_B$  = Temperature in reactor (K)  
 $T_j$  = Temperature on tray  $j$  (K)  
 $T_0$  = Reference temperature (K)  
 $u$  = Control variables in the general optimisation problem  
 $v$  = Design variables in the general optimisation problem  
 $V_j$  = Vapour flow from tray  $j$  (kmol/h)  
 $x^0$  = Initial composition  
 $x_{A,w}$  = Mole fraction of component  $W$  in the accumulator  
 $x$  = State variables in the general optimisation problem  
 $y$  = Algebraic variables in the general optimisation problem

#### Greek letters

$\tau$  = Hydraulic time constant ( $h^{-1}$ )  
 $\tau_1$  = Integral time for PI-controller (h)  
 $\Phi$  = Objective function in the general optimisation problem  
 $\chi_{R_1}$  = Conversion of reactant  $R_1$

#### Scripts

$A$  = accumulator  
 $B$  = reactor/reboiler  
 $C$  = condenser  
 $i$  = component number

$j$  = tray number  
 $r$  = reaction number

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