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Towards practical optimal control of batch reactors

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Abstract

Instead of finding only the optimal temperature profile, the optimal flow rates of heating and cooling fluids are determined, so that the yield of a desired product in a batch reactor is maximized. The two additional differential equations that are introduced to handle the heat balances make the optimization more difficult, especially when constraints are placed on the reactor temperature. However, by using iterative dynamic programming (IDP) in multi-pass fashion, the optimal policy can be readily obtained. Optimization as carried out on two typical batch reactor problems shows that if the heat transfer coefficient is reasonably chosen, then the optimal yield can be significantly larger than what can be expected from the best isothermal operation. To prevent simultaneous flows of heating and cooling streams, we used for optimization a single heat flow term as a control variable. When positive, this heat flow term is equal to the heating stream flow rate; when negative, the magnitude of the heat flow term is equal to the coolant flow rate. An augmented performance index was used to handle state constraints resulting from the bounds on the reactor temperature in the second example. In both the examples, it was clear that significantly better yields than those possible from the best isothermal temperature profile can be obtained, even if the heat transfer coefficient is not known accurately at the start of the batch time. © 1999 Elsevier Science S.A. All rights reserved.

Keywords: Batch reactor control; Optimal control; Iterative dynamic programming

1. Introduction

There has been a growing interest in recent years in the use of optimization in the control of batch reactors. A large part of the recent developments in the optimal control of batch reactors has been aimed towards obtaining the theoretical optimal temperature profile [1–3]. An optimal temperature profile provides useful design information, by providing the upper limit for the expected yield of the reactor and showing how the temperature should change during the course of the reaction to achieve the maximum yield. For typical batch reactors, however, the best temperature profile is generally very difficult to obtain when Pontryagin's maximum principle is used [4,5]. Part of the difficulty is due to the existence of singular arcs and the low sensitivity of the control policy on the yield of the reactor [6]. However, iterative dynamic programming (IDP), as developed by Luus [7,8], offers a good alternative for obtaining the global optimum. IDP has the advantage of not requiring additional variables to be introduced, and therefore the method does not encounter such problems as singular control [9].

The optimal temperature profile, however, cannot be applied directly to the actual control of a reactor. This is quite obvious when the optimal control policy consists of very rapid changes in the temperature. Marroquin and Luyben [10] found that for typical situations, there is only a small difference between the yields obtained from the optimal temperature profile and the use of the best isothermal policy, and they recommended using the best constant temperature as the set point for practical control of a batch reactor. However, it is not possible to start the reactor at the desired temperature, and due to the heat effects during the chemical reaction, such control strategy is not always simple to implement. A better approach is to solve the original optimal control problem, using the flow rates of the heating and the cooling fluids as the control variables, but still keeping the objective of maximizing the yield or some other performance index. The purpose of this paper is to investigate such an approach in the control of typical chemical reactors by considering two examples.

As a starting point, we use the approach of obtaining the theoretical optimal temperature profile, which gives us the theoretical maximum yield that can be expected. This places the upper limit on the yield, and serves as a useful benchmark. The next step is to formulate the optimal control problem in terms of the control variables consisting of the physical elements that can be readily manipulated, such as the flow rates of some heating fluid and of coolant. Since at present the available digital computers are very fast, such an

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approach, although yielding an open-loop control policy, can be used on-line in feedback manner, where the problem is solved repeatedly with different initial conditions during the course of reaction. Appropriate changes can then be made in the control policy to reflect any inaccuracies in modelling of the system. This is illustrated by both of the examples.

2. Optimal control problems

2.1. Example 1

Let us first consider the consecutive chemical reaction A → B → C in a batch reactor, as was considered by Bilous and Amundson [11], used for optimal control studies by Jaspan and Coull [12] and Luus [13], and was used as an example for practical control by Marroquin and Luyben [10]. In the consecutive reaction scheme it is required to maximize the production of the desired component B. The reaction in each step is assumed to be first order, so that the system is described by the two differential equations

$$\frac{dx_1}{dt} = -k_1 x_1 \tag{1}$$

$$\frac{dx_2}{dt} = k_1 x_1 - k_2 x_2 \tag{2}$$

where x_1 is the concentration (mol/l) of the reactant A and x_2 is the concentration of the desired product B. The rate constants are given by

$$k_1 = 5.35 \times 10^{10} \exp\left(\frac{-9000}{T}\right) \text{ per min} \tag{3}$$

and

$$k_2 = 4.61 \times 10^{17} \exp\left(\frac{-15\,000}{T}\right) \text{ per min} \tag{4}$$

The initial state is specified as

$$\boldsymbol{x}(0)^{\mathrm{T}} = [0.95 \quad 0.05] \tag{5}$$

and the batch time is specified as $t_f = 30$ min. The performance index to be maximized is the concentration of component B at the specified final time, i.e.,

$$I = x_2(t_f) \tag{6}$$

The standard optimal control problem is then to find the temperature profile, such that the performance index in Eq. (6) is maximized.

Here we initially consider this formulation of the optimal control problem and then make the problem more realistic by adding two differential equations to this model to take into account how such a temperature profile can be approached in practice.

To find the optimal temperature profile, we first divide the given time interval into P subintervals of equal length $(0, t_1)$, (t_1, t_2),…, (t_{P-1}, t_P), where $t_P = t_f$, so that the length of each subinterval is

$$L = \frac{t_f}{P} \tag{7}$$

We seek a piecewise linear continuous control policy for the temperature profile, so that in the time interval (t_k, t_{k+1}) the temperature is given by

$$T(t) = T(k) + \left(\frac{T(k+1) - T(k)}{L}\right)(t - t_k) \tag{8}$$

where $T(k)$ is the temperature at time t_k and $T(k+1)$ is the temperature at time t_{k+1}. The optimal control problem is to find the $P + 1$ values of $T(k)$, $k = 0, 1, 2,\ldots, P$, such that the performance index given in Eq. (6) is maximized.

This problem is readily solved by using IDP with a single grid point for the state at each time stage [14,15], by using the algorithm given in Appendix B. We chose $P = 50$ time stages, and an initial control policy of 335 K, with the initial region size $r^{(0)} = 50$ and region contraction factor $\gamma = 0.85$. Two passes were used, each consisting of 30 iterations, with a region restoration factor $\eta = 0.70$. Double precision was used throughout. It was found that even with three allowable values of control ($R = 3$), rapid convergence to $x_2(t_f) = 0.768367$ was obtained, as is shown in Fig. 1 for the first 15 iterations. The computation time on a Pentium/120 personal computer for $R = 5$ allowable values for control for the two passes was only 14.8 s. The resulting optimal temperature profile is shown in Fig. 2, and the concentration profiles for components A and B are given in Fig. 3.

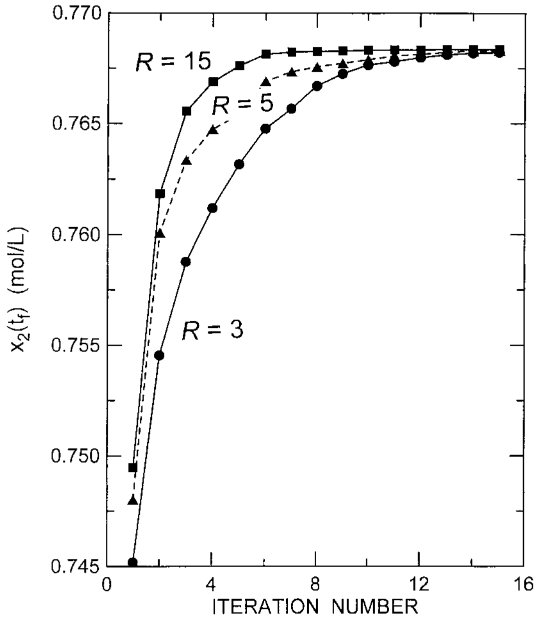

Fig. 1. Effect of the number of allowable values for control on the convergence rate of IDP for Example 1.

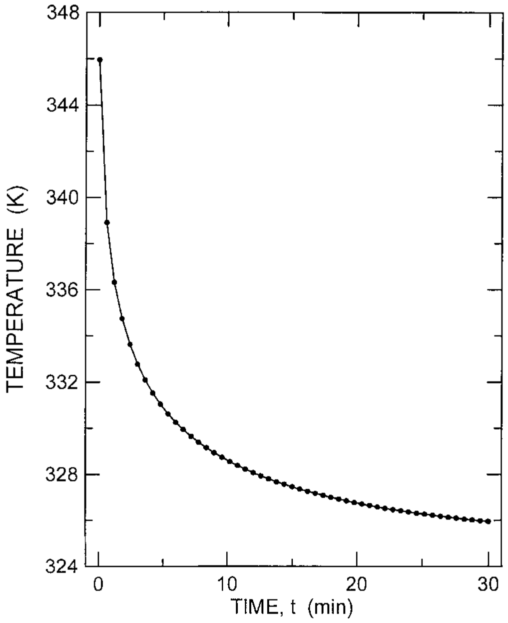

Fig. 2. Optimal temperature profile, giving $x_2(t_f) = 0.76837$ mol/l.

To obtain the best isothermal control policy, we simply consider a single stage and piecewise constant control policy. In a straightforward manner by using IDP with the single time stage, we obtained $x_2(t_f) = 0.763606$ at a constant temperature of 329.02 K. Therefore, the use of the optimal control policy rather than the best isothermal policy gives an increase of 0.6% in the yield of the desired product. These two values for the yield provide a benchmark when considering the practical attainment of the maximum yield.

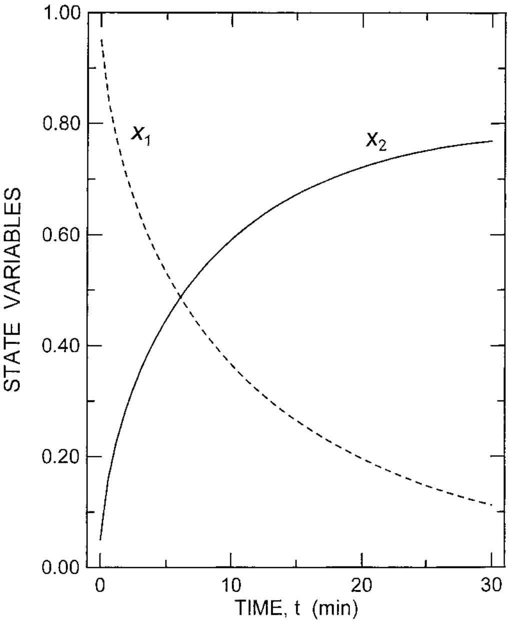

Fig. 3. Concentration profiles with the use of optimal temperature profile.

We are now interested in considering the practical optimal control problem, where the batch is loaded initially at 310 K, and there is a heat exchanger jacket around the reactor. As a control, instead of the temperature profile, we use flow rates of hot water for heating and cold water for cooling the jacket surrounding the reactor. We assume that the water in the jacket is recirculated around the reactor sufficiently fast, so that the rate of inflow does not affect the heat transfer coefficient, which is taken to be constant. The water from the jacket is bled off at the same rate as the inflow.

If we denote the temperature inside the reactor by x_3 and the jacket temperature by x_4, we have two additional differential equations

$$\frac{dx_3}{dt} = \frac{(-\Delta H_1)k_1x_1}{\rho C_p} + \frac{(-\Delta H_2)k_2x_2}{\rho C_p} - \frac{UA(x_3 - x_4)}{V\rho C_p} \tag{9}$$

and

$$\frac{dx_4}{dt} = \frac{u_1(372 - x_4)}{V_j} + \frac{u_2(300 - x_4)}{V_j} + \frac{UA(x_3 - x_4)}{V_j\rho_j C_{pj}} \tag{10}$$

where u_1 and u_2 are the flow rates of hot and cold water, respectively. These flow rates are bounded by

$$0 \le u_j \le 2.85\ \mathrm{m^3/min}, \quad j = 1,\ 2. \tag{11}$$

The temperature of the hot water entering the jacket is arbitrarily set at 372 K and the cold water temperature is set at 300 K. The term ρC_p for the components inside the reactor and for the water in the jacket is taken to be 4.19×10^3 kJ/(m^3 K). Both of the reactions are exothermic with $(-\Delta H_1) = 79.2$ kJ/mol and $(-\Delta H_2) = 53.0$ kJ/mol. We also take the volume of the reactor to be $V = 1.2$ m^3 and of the jacket $V_j = 0.15$ m^3. With these parameters, Eqs. (9) and (10) become

$$\frac{dx_3}{dt} = 18.90k_1x_1 + 12.65k_2x_2 - 1.989 \times 10^{-4}UA(x_3 - x_4) \tag{12}$$

and

$$\frac{dx_4}{dt} = 6.67u_1(372 - x_4) + 6.67u_2(300 - x_4) + 1.591 \times 10^{-3}UA(x_3 - x_4) \tag{13}$$

The initial conditions for these variables are $x_3(0) = 310$ and $x_4(0) = 310$. The system now consists of Eqs. (1), (2), (12) and (13) with the initial state

$$\boldsymbol{x}(0)^T = [0.95 \quad 0.05 \quad 310 \quad 310] \tag{14}$$

It is noted that the reactor is started 19° below its best isothermal temperature, so part of the problem is to raise the temperature to some value which is not known ahead of time. Therefore, the optimal control problem we wish to consider is the determination of the controls u_1 and u_2 so that the performance index in Eq. (6) is maximized.

To avoid simultaneous heating and cooling, we introduce a heat flow term w with the bounds

$$-2.85 \leq w \leq 2.85 \tag{15}$$

such that

$$\begin{aligned} &u_1 = w, \ u_2 = 0 \quad \text{if } w \geq 0 \\ &u_2 = -w, \ u_1 = 0 \quad \text{if } w < 0 \end{aligned} \tag{16}$$

and carry out optimization on w. Thus for optimization there is really a single scalar variable to be determined. We are seeking a piecewise constant control over P time stages, and IDP is well suited for such optimization.

From the values of heat transfer coefficients reported by Geankoplis [16], a practical range for the heat transfer term UA appears to be between 400 and 4000 kJ/(min K). Runs were performed by increasing UA in multiples of 342 for different number of time stages P. As expected, the optimum yield increases as UA is increased, but the increase is determined very much by the number of time stages P when UA is large, as is shown in Fig. 4. When $P = 10$, the change in flow rates is done after every 3 min, whereas with $P = 30$, the flow rates are changed after each minute, allowing more accurate switching of the coolant flow rate, which is translated more directly into the change in the reactor temperature when UA is high. When $P = 10$, then no improvement in the yield is obtained if UA is increased beyond 1000, and when $P = 15$ no improvement is obtained if UA is increased beyond 1600. It is noted that when UA is greater than 1000 and P is greater than 10, then the yield obtained is greater than is possible by the best isothermal policy. With $UA = 2052$ kJ/(min K) the yield is approximately halfway between the yields obtained from the best isothermal temperature profile and the optimal temperature profile. The use of $P = 20$ rather than $P = 15$ gives only a slight improvement from $x_2(t_f) = 0.76560$ to $x_2(t_f) = 0.76605$, whereas the use of $P = 10$ gives a considerably lower value.

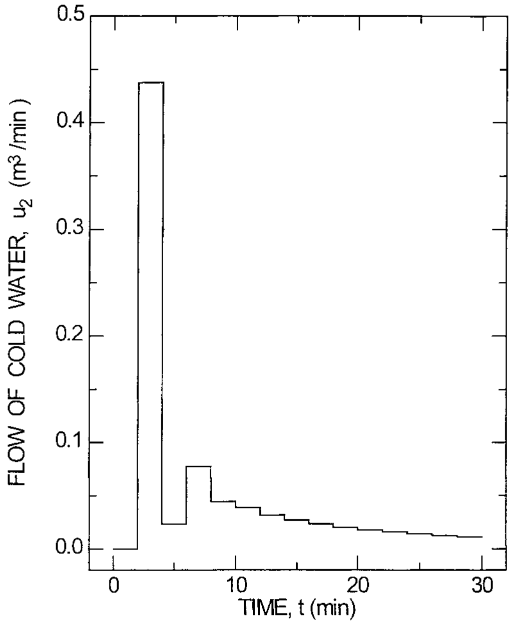

Fig. 5. Optimal flow rate of coolant as function of time for $UA = 2052$ kJ/min K with $P = 15$.

The optimal control policies for the coolant flow rate for $P = 15$ and $P = 20$ are given in Figs. 5 and 6. In each case, for the first stage, only heating was used and for the rest of the stages only coolant was used. With $P = 15$, for

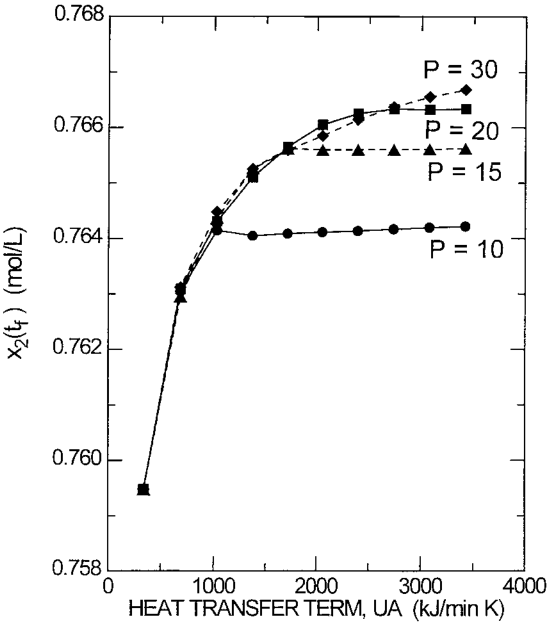

Fig. 4. Effect of the heat transfer term UA on $x_2(t_f)$ as a function of the number of stages P.

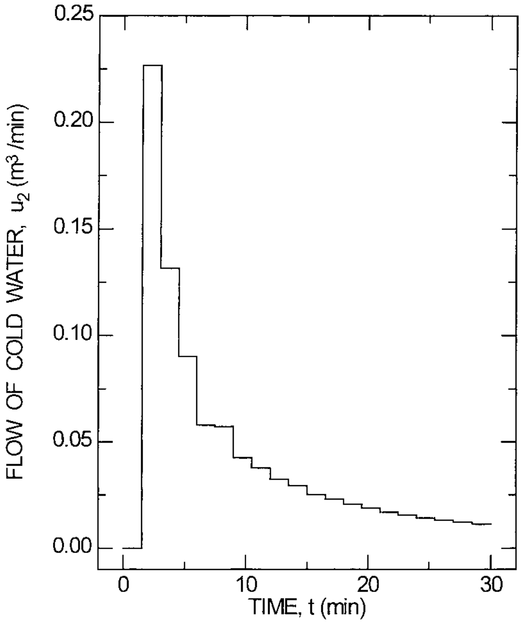

Fig. 6. Optimal flow rate of coolant as a function of time for $UA = 2052$ kJ/min K with $P = 20$.

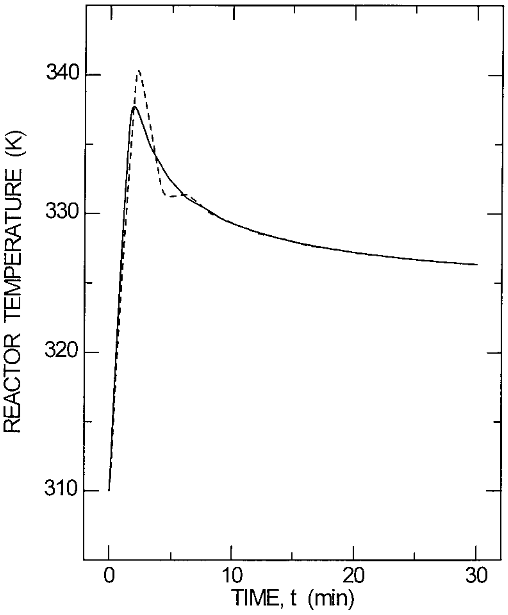

Fig. 7. Optimal temperature profile for the reactor with $UA = 2052$ kJ/min K with different number of stages: (- - -) $P = 15$, (———) $P = 20$.

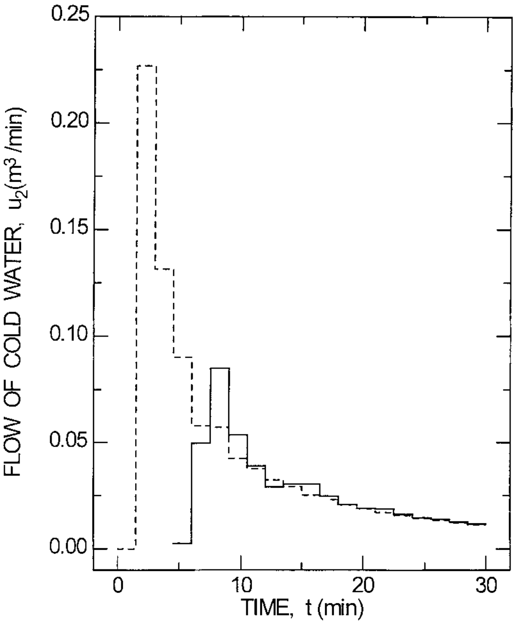

Fig. 8. Coolant flow rate policy after the first two stages: (- - -) original policy based on $UA = 2052$ kJ/min K, (———) recalculated control policy based on $UA = 1800$ kJ/min K.

the first stage $u_1 = 1.4858$, whereas with $P = 20$, for the first stage $u_1 = 2.8500$. It is noted that with $P = 20$, the coolant flow rate policy is smoother than with $P = 15$. The resulting temperature profiles are shown in Fig. 7. It is observed that a higher reactor temperature results with $P = 15$, but the value of the performance index is slightly lower than with $P = 20$.

To obtain these results, an initial value for w of 1.0 was used, with an initial region size of 2.85. Three grid points were used ($N = 3$) and 21 allowable values for control ($R = 21$) were used at each iteration. The region reduction factor $\gamma = 0.90$ was used in every iteration. Region restoration factor $\eta = 0.75$ was used for each pass. Each run consisted of 40 passes, each consisting of 30 iterations. For integration, the subroutine DVERK [17] was used with local error tolerance of 10^{-6}. On PentiumII/300 each run took approximately 25 min with $P = 15$ and 40 min with $P = 20$.

Now let us consider the application to a realistic situation. Suppose that the optimal control policy as determined for $UA = 2052$ is applied with $P = 20$, but in reality $UA = 1800$. Then with this control policy we should get $x_2(t_f) = 0.7611$. Suppose that such an error in the heat transfer term is detected after the second time stage when $\boldsymbol{x} = [0.74846 \quad 0.24664 \quad 333.42 \quad 322.29]^T$. We can use this as the initial condition and, while the reactor is operating at the previously determined control policy, we carry out optimization over the remaining 18 stages, each of length 1.5 min. We specify the control for the first stage to be $w = -0.1314$, i.e., $u_1 = 0$ and $u_2 = 0.1314$, because this is used while carrying out the optimization calculations. Since for this optimization problem we have already a good initial control policy available, we used $N = 1$ and $R = 11$ and carried out 9 passes of 30 iterations each, using as the initial region size 0.285 on PentiumII/300 to yield $x_2(t_f) = 0.76548$. The computation time of 86 s is within the length of the sampling time of 90 s, so the newly recalculated control policy as given in Fig. 8 can be implemented at the beginning of the fourth stage to give the higher yield. Thus optimal control as calculated here can be used to give in essence a feedback control policy where inaccuracies of the model can be taken into account, since the optimization can be carried out within a single sampling period. As the reaction proceeds, further updates can be carried out. Each successive update requires less computational effort since the number of stages becomes smaller as the reaction proceeds. Although it could be argued that here the improvement in the concentration of the desired product is quite small, in the next example we shall see that significant improvement in the yield can be realized by using optimal control, rather than trying to run the reactor at some best isothermal condition.

2.2. *Example 2*

We next consider the bitumen pyrolysis problem first considered for optimal control studies by Wen and Yen [4], and the problem has been used for optimal control studies by Luus [5], Rosen and Luus [18,19], and Bojkov and Luus [3]. There are five chemical reactions taking place among four chemical species, giving the system of equations

$$\frac{dx_1}{dt} = -k_1x_1 - (k_3 + k_4 + k_5)x_1x_2 \qquad (17)$$

$$\frac{dx_2}{dt} = k_1x_1 - k_2x_2 + k_3x_1x_2 \tag{18}$$

$$\frac{dx_3}{dt} = k_2x_2 + k_4x_1x_2 \tag{19}$$

$$\frac{dx_4}{dt} = k_5x_1x_2 \tag{20}$$

with the initial state $\boldsymbol{x}(0) = [1 \quad 0 \quad 0 \quad 0]^T$. The standard optimal control problem studied by many researchers has been to determine the temperature profile that will maximize the yield of the desired bitumen concentration; i.e., to maximize

$$I = x_2(t_f) \tag{21}$$

subject to the temperature constraints

$$698.15 \le T \le 748.15 \tag{22}$$

The temperature enters the equations implicitly through the reaction rate constants

$$k_i = k_{i0}\exp\left(\frac{-E_i}{RT}\right), \quad i = 1, 2\ldots, 5 \tag{23}$$

where the activation energy E_i and k_{i0} are given in the literature [2,4]. The residence time or batch time t_f is specified as 9.3 min. This optimal control problem to establish the optimal temperature profile is readily solved with IDP [3]. The solution consists of keeping the temperature at the lower boundary until about $t = 3.59$ min and then switching to the upper boundary and keeping it there for about 1.29 min and then bringing the temperature rapidly but not abruptly to the lower boundary and keeping it there for about 4.04 min [3].This optimal control policy gives $x_2(t_f) = 0.35382$ mol/l which is 1.8% better than the yield $x_2(t_f) = 0.34763$ mol/l obtained by the best isothermal policy of $T = 712.5$.

By using a reactor of volume 1.2 m^3 and realistic parameters, the heat balance on the reactor gives us the differential equation for the reactor temperature

$$\frac{dx_5}{dt} = \frac{[602.4k_1x_1 - 0.833(UA/\rho)(x_5 - x_6)]}{C_p} \tag{24}$$

where the slurry density is given by

$$\rho = 2139x_1 + 760x_2 + 560x_3 + 1800x_4 \tag{25}$$

and the heat capacity is given by

$$C_p = 1.16x_1 + 0.827(1 - x_1) + [3.4x_1 + 0.92(1 - x_1)] \times (x_5 - 298) \times 10^{-3} \tag{26}$$

The differential equation describing the temperature of the jacket surrounding the reactor is

$$\frac{dx_6}{dt} = u_1(873 - x_6) + u_2(373 - x_6) + 0.01357UA(x_5 - x_6) \tag{27}$$

where u_1 is the hot steam flow rate and u_2 is the 'cold' steam flow rate (m^3/min), bounded by

$$0 \le u_j(t) \le 5.0, \quad j = 1, 2. \tag{28}$$

As in the first example, to avoid simultaneous flows of heating steam and coolant, we introduce again the heat flow term w with bounds from -5 to 5, and carry out optimization using w as the control variable. Then the result is translated to the values of u_1 and u_2 as before.

To handle the upper and lower constraints on the reactor temperature, we use the penalty function method as used for state constraints by Luus [20] and by Mekarapiruk and Luus [21], where we introduce two additional differential equations

$$\frac{dx_7}{dt} = \begin{cases} 698.15 - x_5 & \text{if } x_5 < 698.15 \\ 0 & \text{if } x_5 \ge 698.15 \end{cases} \tag{29}$$

$$\frac{dx_8}{dt} = \begin{cases} x_5 - 748.15 & \text{if } x_5 > 748.15 \\ 0 & \text{if } x_5 \le 748.15 \end{cases} \tag{30}$$

with zero initial condition. Whenever the constraints are violated, these auxiliary variables become positive. To prevent constraint violation, therefore, we construct the augmented performance index

$$J = x_2(t_f) - \theta[x_7(t_f) + x_8(t_f)] \tag{31}$$

where θ is a penalty function factor. The problem is now to choose w to maximize J. The initial condition for the state vector is

$$\boldsymbol{x}(0) = [1 \quad 0 \quad 0 \quad 0 \quad 698.15 \quad 698.15 \quad 0 \quad 0]^T \tag{32}$$

As in the first example, we used DVERK with local error tolerance of 10^{-6} to integrate the differential equations. For this example we used $P = 20$ time stages, each of length 0.465 min and piecewise constant control. Here we found that in order to get convergence from an initial choice of $w = 1.0$, we had to use a relatively large number of grid points. By taking $\theta = 0.01$, $N = 21$, $R = 15$, $\gamma = 0.90$, $\eta = 0.85$, $UA = 1000$, $w^{(0)} = 1.0$, $r^{(0)} = 5.0$, in 10 passes of 20 iterations each, the resulting value of the performance index was $J = I = 0.35193$. By using the resulting control policy as the initial starting point and initial region size of 0.1, another run was performed to yield a refined value of $I = 0.35211$. The computation time for the initial run was approximately 4 h on Pentium/120. The large computation time is mostly due to the need for a large number of grid points to obtain convergence from a poor initial starting point. Once a good starting policy is obtained, there is no longer the need for such a large number of grid points. This is illustrated later, where we show that a single grid point can be used to enable optimization to be carried out 'on-line'.

The resulting control policy as given in Fig. 9, shows that initially there is an attempt to bring the reactor temperature up to a high value, but full heating is not applied immediately. Then, halfway through the reaction, cooling is applied to reduce the temperature to the lower bound and to keep the reactor temperature then at the lower bound until the final

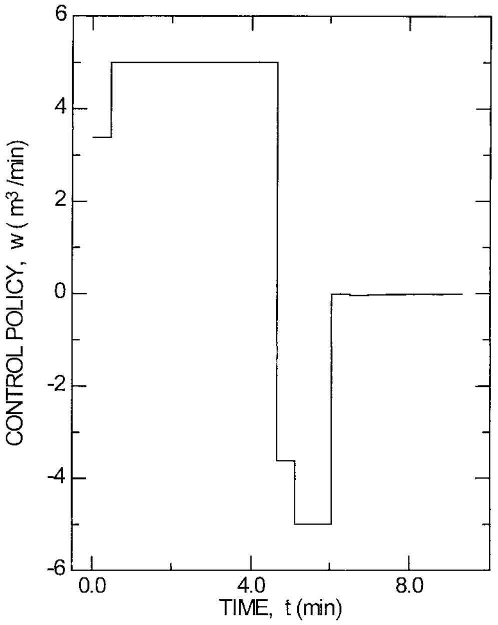

Fig. 9. Optimal control policy for $UA = 1000$ for Example 2, giving $x_2(t_f) = 0.35211$ mol/l.

time is reached. The temperature profile is given in Fig. 10. Although the ideal temperature profile cannot be achieved, the yield of 0.35211 is within 0.5% of the theoretical optimum of 0.35382 and is 1.3% above the best isothermal yield of 0.34763 mol/l.

As is shown in Fig. 11, the effect of UA is noticeable but not overwhelming. Even with $UA = 400$, we get substantially better yield than can be expected from best isothermal operation.

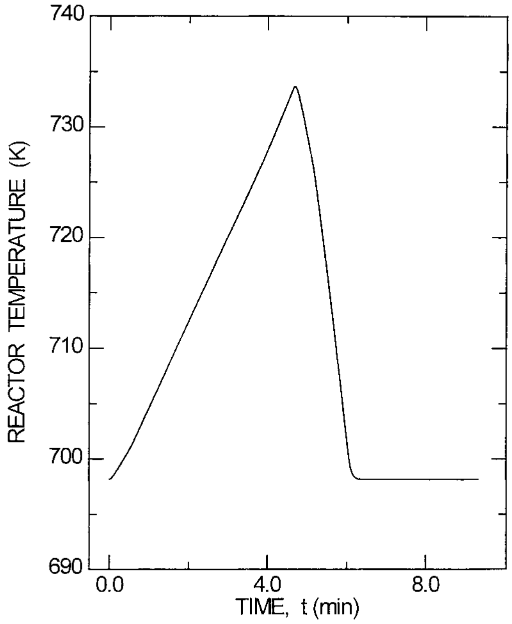

Fig. 10. Temperature profile resulting from the optimal control policy for $UA = 1000$ kJ/min K.

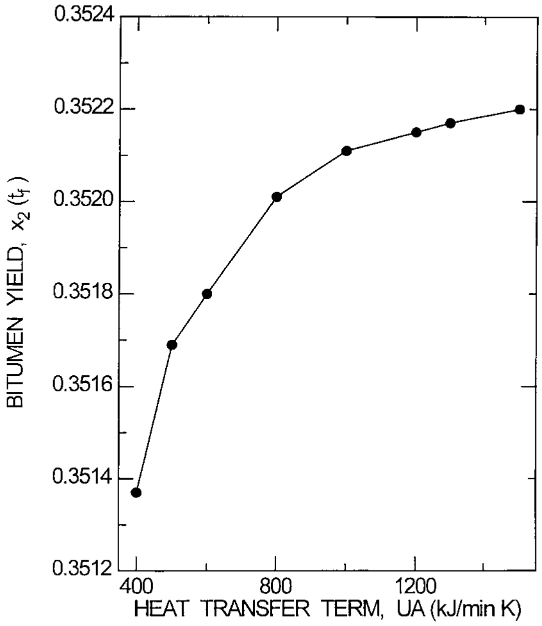

Fig. 11. Effect of the heat transfer term UA on the yield $x_2(t_f)$ using $P = 20$.

Now consider the situation where the optimal control policy for $UA = 1200$ is used, when after two sampling periods it is found that in reality $UA = 800$. If no correction is made, then the final yield will be 0.35127. If the control policy is switched over to the one obtained for $UA = 800$ then a final yield of 0.35133 is obtained. Although these yields may be considered acceptable, we can improve the result by recalculating the control policy. The cooling phase starts at around $t = 4.65$ min, so the computations will have to be done in less than 3.7 min, since the first two sampling times have used up 0.93 min of the batch time. The optimal control policy that has been established for $UA = 1200$ as applied to $UA = 800$ will give in time 4.65 the following state

$$x(4.65) = [0.71504 \;\; 0.14675 \;\; 0.08248 \;\; 0.05573 \;\; 730.72 \;\; 775.22 \;\; 0 \;\; 0]^{\mathrm{T}} \tag{33}$$

Now we can perform the optimization over the remaining 10 stages, by using Eq. (33) as the initial condition with initial time of 4.65 min. We can use the previously calculated optimal control policy as the initial control policy. Therefore, a single grid point and a small number of passes could be used for the optimization to save computation time. The computation time for one such run consisting of two passes, each consisting of 20 iterations, was 14.3 s on PentiumII/300 computer. After six runs, taking 1.5 min of computation time in total, a reoptimized control policy was calculated for $UA = 800$ with a resultant yield of 0.35192 mol/l. This is quite close to 0.35201 if the optimal control policy for $UA = 800$ would have been used for the entire time interval. The differences in the control policies for the latter half of the batch time are apparent in Fig. 12. As the computers become faster, optimization by IDP will be possible 'on-line' for even more complex problems.

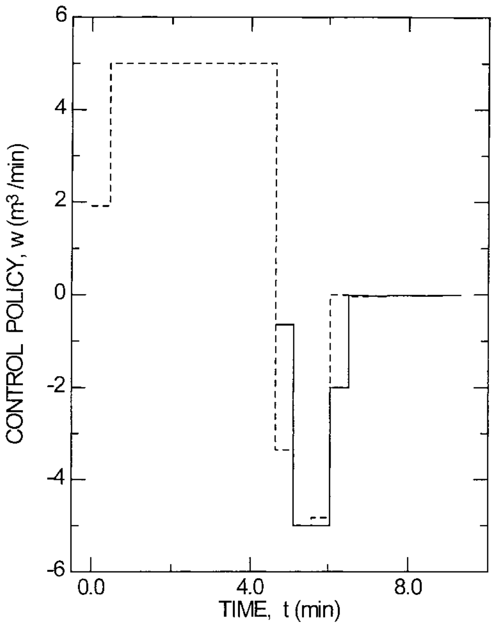

Fig. 12. Control policies for $UA = 800$ kJ/min K: (- - -) optimal policy for $UA = 1200$, giving $x_2(t_f) = 0.35127$ mol/l, (———) control policy as recalculated from the state at $t = 4.65$ min, giving $x_2(t_f) = 0.35192$ mol/l.

3. Conclusions

Although the inclusion of additional differential equations to handle the flow rates as control increases the computational effort quite significantly, the computation time with IDP is not excessive. The effect of the heat transfer coefficient is quite important, and therefore, accurate modelling is required when implementation of optimal control is considered in practice. However, even with inaccurate modelling, the parameters can be updated while running the reactor. With the updated parameters reoptimization can be carried out over the rest of the batch time even with complex systems.

Since personal computers are now very fast and will be even faster in the future, the optimal control approach as outlined here appears to be quite practical. Although the resulting control policy is open loop in nature, during the course of reaction the parameters can be updated and the optimization problem can be solved repeatedly. This means that appropriate changes can be made during the operation of the reactor. In essence then the optimal control will be feedback in nature, where the control action is determined from the knowledge of the state of the system at any particular time.

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Appendix

Nomenclature

A	reactant
A	area (m^2)
B	desired product
C	waste product
C_p	heat capacity (kJ/(kg K))
E_i	activation energy of reaction i
ΔH	molar enthalpy change used in Eq. (9) (kJ/mol)
I	performance index to be maximized
J	augmented performance index
k_i	rate constant (per min)
L	length of time step (min)
N	number of grid points used in IDP
P	number of time stages
q	pass number
r	region size used for allowable control
R	number of allowable values for control used at each grid point, gas constant
t	time (min)
t_f	residence time or batch time (min)
T	temperature (K)
u_1	flow rate of heating fluid (m^3/min)
u_2	flow rate of coolant (m^3/min)
U	heat transfer coefficient (kJ/(m^2 min K))
V	volume of the reactor (m^3)
V_j	volume of the jacket (m^3)
w	heat flow term used for optimization to eliminate simultaneous cooling and heating (m^3/min)
x_i	state variable
$\mathbf{x}$	state vector

Greek letters

γ	region contraction factor used after every iteration
η	region restoration factor
θ	penalty function factor
ρ	density (kg/m^3)

Subscripts/superscripts

f	final
j	jacket
T	transpose
(0)	initial value

Appendix B

Iterative dynamic programming algorithm

1. Divide the given time interval into P time stages, each of equal length L.

2. Choose the number of test values for the temperature T (control) denoted by R, an initial control policy and the initial region size r_{in}; also choose the region contraction factor γ used after every iteration and the region restoration factor η used after every pass.
3. Choose the number of iterations to be used in every pass and the number of passes.
4. Set the pass number index $q = 1$, and the iteration number index $j = 1$.
5. Set $r^{(j)} = \eta^{q-1} r_{\text{in}}$.
6. With the best control policy (the initial control policy for the first iteration of the first pass), integrate Eqs. (1) and (2) to generate the **x**-trajectory and store the values of **x** at the beginning of each time stage, so that $\mathbf{x}(k\text{-}1)$ corresponds to the value of **x** at the beginning of stage k.
7. Starting at stage P, corresponding to time $t_f - L$, integrate Eqs. (1) and (2) from $t_f - L$ to t_f, using as the initial state the stored value $\mathbf{x}(P-1)$ from step 6, with each of the R allowable sets of control, by using the piecewise linear control in Eq. (8) where for the last stage

   $$T(P-1) = T(P-1)^{*(j)} + D_1 r^{(j)}$$

   and

   $$T(P) = T(P)^{*(j)} + D_2 r^{(j)}$$

   Here $T(P-1)^{*(j)}$ and $T(P)^{*(j)}$ are the best values obtained in the previous iteration and D_1 and D_2 are different random numbers between -1 and 1. Out of the R values of the performance index I as calculated from Eq. (6), choose the temperature values that give the maximum value, and store these as $T(P\text{-}1)$ and $T(P)$.
8. Step back to stage $P-1$, corresponding to time $t_f - 2L$. Choose R values for $T(P-2)$ as in step 7, and by taking as the initial state $x(P-2)$ integrate Eqs. (1) and (2) over one stage length by using Eq. (8) for the control. Continue integration over the last time stage by using Eq. (8) with the stored values of $T(P-1)$ and $T(P)$ from step 7. Compare the R values for the performance index I and store the $T(P-2)$ that gives the maximum value.
9. Continue the procedure until stage 1, corresponding to the initial time $t = 0$ and the given initial state, is reached. As before, integrate Eqs. (1) and (2) and compare the R values of I and store the value $T(0)$ corresponding to the maximum value of I.
10. Reduce the region for allowable control

    $$r^{(j+1)} = \gamma r^{(j)}$$

    where j is the iteration number index.
11. Increment the iteration index by 1, use the superscript* to denote the best control values from step 9, and go to step 6. Continue the procedure for the chosen number of iterations specified in step 3 to finish the pass.
12. Increment the pass number index q by 1 and go to step 5. Continue the procedure for the specified number of passes and interpret the results.

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