

Optimizing Control of a Batch Reaction Process

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The batch chemical reaction is chosen as the process model to be optimized and the rate constants are functions of pressure only, as the reactions are assumed to occur isothermally. The time optimal control problem considered here means to determine the minimum time path from the given initial compositions to desired final compositions by manipulating the process pressure. A gradient method or a steepest-ascent method is applied to determine the control variable program by using the high speed digital computer. Numerical solutions are presented for the following three cases: (1) no constraint on the operating pressure open and matched terminal constraint. (2) constraint on the operating pressure open terminal constraint. (3) constant operating pressure open terminal constraint.

§ 1. Introduction

During the past decade, there has a remarkable development in optimization techniques which can be applied to the problem of optimal design and control. The most useful techniques are dynamic programming, quasilinearization method, Pontryagin's maximum principle and gradient methods.

The chemical process is one of the most complicated and multivariable system and has essentially nonlinear characteristic. The classical method of the calculus of variations can not solve such complex optimization problems even by using a digital computer, because it results in a two-point boundary value problem for a set of nonlinear ordinary differential equations. The maximum principle also can not avoid this computational difficulties. Dynamic programming has the disadvantage of the "curse of dimensionality" and can be applied to the system of only three state variables. The gradient method is a systematic and rapid computation technique to obtain numerical solutions of complex optimization problems^{1,2)}. This method is applied to solve the optimal control problem of the batch reaction process. This problem has been solved by the calculus of variations³⁾ and dynamic programming⁴⁾ but the gradient method has advantage in numerical computation over other methods.

§ 2. Gradient Method

Recently, Kelley⁵⁾ and Bryson⁶⁾ have deve-

loped the gradient method or the steepest-ascent method to solve the two-point boundary-value problems in the calculus of variations. The details of the gradient method are available in the literature in Refs 2 and 3 and the results of Bryson are outlined here. We desire to determine the control variable program $\alpha(t)$ in the interval $t_0 \leq t \leq t_f$ so as to maximize

$$\phi = \phi[x(t_f), t_f], \quad (1)$$

subject to the constraints

$$\frac{dx}{dt} = f[x(t), \alpha(t), t], \quad (2)$$

$$\psi = \psi[x(t_f), t_f] = 0, \quad (3)$$

$$t_0 \text{ and } x(t_0) \text{ given,} \quad (4)$$

$$t_f \text{ determined by } \Omega = \Omega[x(t_f), t_f] = 0 \quad (5)$$

where ϕ is the performance index and is a known function of $x(t_f)$ and t_f , $x(t)$ is an n-vector of state variables, f is an n-vector of known functions of $x(t)$, $\alpha(t)$ and t , $\alpha(t)$ is an m-vector of control variables, ψ is a p-vector of terminal constraint functions and $\Omega=0$ is the stopping condition.

This is the problem of Mayer in the calculus of variations. The gradient method procedure starts with a nominal control variable program $\alpha(t)$ and determines the change in the control variable program $\delta\alpha(t)$ that gives maximum increase in the performance index function for a given value of the integral

$$(dS)^2 = \int_{t_0}^{t_f} \delta\alpha^T(t) W^{-1}(t) \delta\alpha(t) dt, \quad (6)$$

while simultaneously changing the terminal quantities by desired amounts. A new control variable program is obtained as

$$\alpha_{NEW}(t) = \alpha_{OLD}(t) + \delta\alpha(t) \quad (7)$$

The process is continued until no further useful improvement can be made. The small perturbations can be expressed as follows:

$$\begin{aligned} \delta\alpha(t) = & \pm \mathbf{W}^{-1} \mathbf{G}^T (\lambda_{\varphi\Omega} - \lambda_{\psi\Omega} \mathbf{I}_{\psi\psi}^{-1} \mathbf{I}_{\psi\varphi}) \\ & \times \left[\frac{(dS)^2 - d\psi^T \mathbf{I}_{\psi\psi}^{-1} d\psi}{\mathbf{I}_{\varphi\varphi} - \mathbf{I}_{\varphi\psi}^T \mathbf{I}_{\psi\psi}^{-1} \mathbf{I}_{\psi\varphi}} \right]^{1/2} \\ & + \mathbf{W}^{-1} \mathbf{G}^T \lambda_{\psi\Omega} \mathbf{I}_{\psi\psi}^{-1} d\psi, \end{aligned} \quad (8)$$

Where

$$\begin{aligned} \lambda_{\varphi\Omega} &= \lambda_{\varphi} - \frac{\dot{\phi}}{\dot{\Omega}} \lambda_{\Omega}, & \lambda_{\psi\Omega} &= \lambda_{\psi} - \lambda_{\Omega} \frac{\dot{\psi}}{\dot{\Omega}}, \\ \dot{\phi} &= \left(\frac{\partial \phi}{\partial t} - \frac{\partial \phi}{\partial \mathbf{x}} \mathbf{f} \right), & \dot{\Omega} &= \left(\frac{\partial \Omega}{\partial t} - \frac{\partial \Omega}{\partial \mathbf{x}} \mathbf{f} \right), \\ \dot{\psi} &= \left(\frac{\partial \psi}{\partial t} - \frac{\partial \psi}{\partial \mathbf{x}} \mathbf{f} \right), & & \\ \mathbf{F} &= \left(\frac{\partial \mathbf{f}}{\partial \mathbf{x}} \right), & \mathbf{G} &= \left(\frac{\partial \mathbf{f}}{\partial \alpha} \right), \end{aligned} \quad (9)$$

$$\mathbf{I}_{\varphi\varphi} = \int_{t_0}^{t_f} \lambda_{\varphi\Omega}^T \mathbf{G} \mathbf{W}^{-1} \mathbf{G}^T \lambda_{\varphi\Omega} dt,$$

$$\mathbf{I}_{\psi\psi} = \int_{t_0}^{t_f} \lambda_{\psi\Omega}^T \mathbf{G} \mathbf{W}^{-1} \mathbf{G}^T \lambda_{\psi\Omega} dt,$$

$$\mathbf{I}_{\psi\varphi} = \int_{t_0}^{t_f} \lambda_{\psi\Omega}^T \mathbf{G} \mathbf{W}^{-1} \mathbf{G}^T \lambda_{\varphi\Omega} dt,$$

λ is an n -vector of influence functions, the Lagrange-multiplier functions and the solution of the adjoint differential equations

$$\frac{d\lambda}{dt} = -\mathbf{F}(t)\lambda \quad (10)$$

with boundary conditions

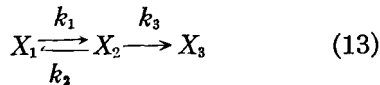
$$\begin{aligned} \lambda_{\varphi}^T(t_f) &= \left(\frac{\partial \phi}{\partial \mathbf{x}} \right)_{t_f}, & \lambda_{\psi}^T(t_f) &= \left(\frac{\partial \psi}{\partial \mathbf{x}} \right)_{t_f}, \\ \lambda_{\Omega}^T(t_f) &= \left(\frac{\partial \Omega}{\partial \mathbf{x}} \right)_{t_f} \end{aligned} \quad (11)$$

If there is no terminal constraint $\psi = 0$, Eq. (8) is reduced to the following simple form

$$\delta\alpha(t) = \pm \mathbf{W}^{-1} \mathbf{G}^T \frac{dS}{(I_{\varphi\varphi})^{1/2}} \quad (12)$$

§ 3. System Model and Statement of Problem

We choose the following batch reaction as the system model³⁾



where x_2 is the desired product. The equations of this process are given

$$\dot{x}_1 = -k_1 x_1 + k_2 x_2, \quad (14)$$

$$\dot{x}_2 = k_1 x_1 - (k_2 + k_3) x_2, \quad (15)$$

$$\dot{x}_3 = k_2 x_2, \quad (16)$$

where x_1 , x_2 and x_3 represent the concentration of X_1 , X_2 and X_3 respectively and k_1 , k_2 and k_3 are the rate constants of the reaction. The reactions are assumed to occur isothermally. Therefore, the rate constants are functions of pressure $p(t)$ only and given by

$$\begin{aligned} k_1 &= 1.000 \times p^{0.5}, \\ k_2 &= 5 \times 10^{-4} \times p^2, \\ k_3 &= 1.2594 \end{aligned} \quad (17)$$

We consider the time optimal control problem to determine the minimum time path from the given initial compositions of x_1^0 , x_2^0 , x_3^0 to the desired final compositions of x_1^f , x_2^f , x_3^f by manipulating the pressure. Numerical solutions were obtained for the following three cases,

1) no constraint on operating pressure x_2 only is fixed (open terminal constraint) and, x_1 , x_2 and x_3 are fixed respectively (matched terminal constraint).

2) constraint on operating pressure open terminal constraint.

3) constant operating pressure open terminal constraint.

The initial and final conditions of state variables are

Initial conditions	Final conditions	
	(open terminal constraint)	(matched terminal constraint)
$x_1^0 = 0.88000$	$x_1^f = \text{open}$	$x_1^f = 0.60000$
$x_2^0 = 0.11365$	$x_2^f = 0.29765$	$x_2^f = 0.29765$
$x_3^0 = 0.00635$	$x_3^f = \text{open}$	$x_3^f = 0.10235$

(18)

§ 3. Approach to the Problem Solution

The performance index for the time optimal control problem is

$$\phi = - \int_{t_0}^{t_f} dt = -(t_f - t_0) \quad (19)$$

The stopping condition is

$$\Omega = x_2 - x_2^f = x_2 - 0.29765 = 0 \quad (20)$$

The terminal constraint is

$$\psi = x_1 - x_1^f = x_1 - 0.60000 = 0 \quad (21)$$

The adjoint differential equations are

$$\frac{d\lambda_1}{dt} = k_1(\lambda_1 - \lambda_2) \tag{22}$$

$$\frac{d\lambda_2}{dt} = k_3(\lambda_2 - \lambda_1) + k_2(\lambda_2 - \lambda_3), \tag{23}$$

$$\frac{d\lambda_3}{dt} = 0 \tag{24}$$

The boundary conditions on the adjoint variables are

$$\begin{aligned} \lambda_\phi(t_f) &= \left[\frac{\partial \phi}{\partial x} \right]_{t_f} = [0, 0, 0] \\ \lambda_\psi(t_f) &= \left[\frac{\partial \psi}{\partial x} \right]_{t_f} = [1, 0, 0], \\ \lambda_\Omega(t_f) &= \left[\frac{\partial \Omega}{\partial x} \right]_{t_f} = [0, 1, 0] \end{aligned} \tag{25}$$

To begin with successive improvement process, a nominal control variable program $p(t)$ is chosen and the terminal time t_f is determined by Eq. (20) using the initial conditions. The adjoint equations are integrated backward with the boundary conditions Eq. (25) and $I_{\phi\phi}$, $I_{\psi\psi}$ and $I_{\psi\phi}$ are computed along the nominal trajectory. Using the given value of dS and the desired terminal condition changes $d\psi$, $\delta p(t)$ can be calculated from Eq. (8) and the new control variable program $p_{NEW}(t)$ is obtained by Eq. (7).

If $(dS)^2 - d\psi^T I^{-1}_{\psi\psi} d\psi$ is negative, $d\psi$ are automatically scaled down to make this quantity vanish. The process is repeated until the terminal constraint $\psi=0$ is satisfied and the square of the gradient $(I_{\phi\phi} - I_{\phi\psi}^T I_{\psi\psi}^{-1} I_{\psi\phi})$ tends to zero.

§ 4. Results and Discussion

4-1 No constraint on operating pressure

When there are no terminal constraints $\psi=0$, the optimal control variable program can be obtained by using Eq. (12). We take the substantially different operating pressure $p=100$ and 200 as the nominal path. Figs. 1 and 2 show the approach of the control variable from the nominal path to the minimum time solution. From these Figures, it is clear that the same operating

pressure is obtained after 8 and 11 iterations respectively. The results of computations are $t_f=2.7481 \times 10^{-2}$ and $x^*_1=0.64258$ in Fig. 1. $t_f=2.7481 \times 10^{-2}$ and $x^*_1=0.64252$ in Fig. 2.

Therefore the value of the reaction time is proved to be minimum and this policy is optimal. The value of dS is determined by choosing $\delta p(t)$ in Eq. (6) as $p(t)/10$ and kept constant during the computations. If $\delta p(t)$ is too large to give the more unsuccessful results in some trial than the preceding one, the value of $\delta p(t)$ is automatically scaled down to $\delta p(t)/2$ in each trial and this procedure is repeated until the successful result is obtained. The computing time for the one iteration is about 40 sec. on KDC-1 (HITAC-102). The saving in the reaction time for the nominal path is $(t_0 - t_8)/t_0 = 5\%$ in Fig. 1 and $(t_0 - t_{11})/t_{11} = 28\%$ in Fig. 2.

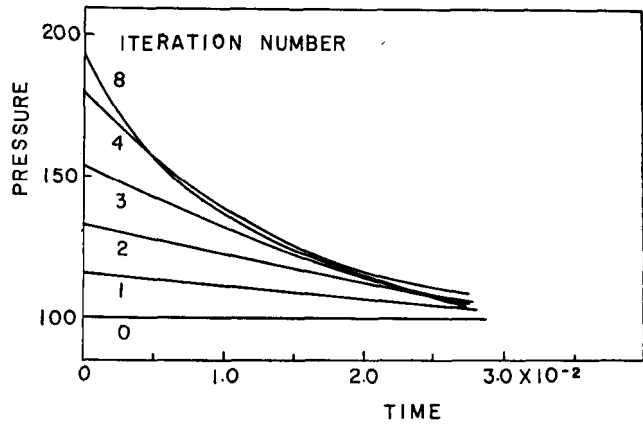


Figure 1. Successive approximations to optimal operating pressure, terminal constraints open.

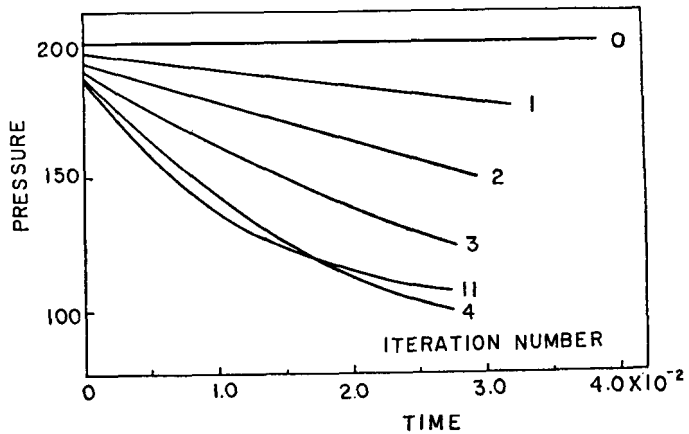


Figure 2. Successive approximations to optimal operating pressure, terminal constraints open.

Figs. 3 and 4 show the approach of control variable on successive iterations from the nominal path of $p=150$ and 200 to optimal one in the problem where there is a terminal constraint. The small perturbations $\delta p(t)$ is computed from Eq. (8) and it is necessary to scale down $\delta p(t)$ and dS simultaneously. In this example, $\delta p(t)$ is scaled down to $\delta p(t)/2$ for the one failure of some trial and dS is scaled down to $dS/2$ for the two consecutive failures of trials. When $[(dS)^2 - d\psi^T I^{-1} \psi d\psi]$ is negative and $d\psi$ is determined to make this quantity vanish, $\delta p(t)$ is never scaled down. This case is the iteration No. 1 in Fig. 3. As shown from Figs. 3 and 4, the good agreement is obtained on the final operating pressure starting from the different nominal path.

The results of computations are $t_f = 2.9029 \times 10^{-2}$ and $x_1^f = 0.59941$ after 14 iterations in Fig. 3.

$t_f = 2.9029 \times 10^{-2}$ and $x_1^f = 0.59955$ after 24 iterations in Fig. 4.

4-2 Constraint on operating pressure

Chemical process usually involve inequality constraints on control variables. Recently, Bryson presented the computation procedure by the gradient method to solve the optimization problem with inequality constraints on the function of the control and/or state variables⁷). The details of this method will not be shown here.

We consider the following inequality constraint on the operating pressure in the time optimal control problem

$$110 \leq p(t) \leq 160 \quad (26)$$

This inequality constraint has no term of the state variables and the adjoint differential equations is same as Eq. (10). Fig. 5 shows the approach of the control variable to the optimal one.

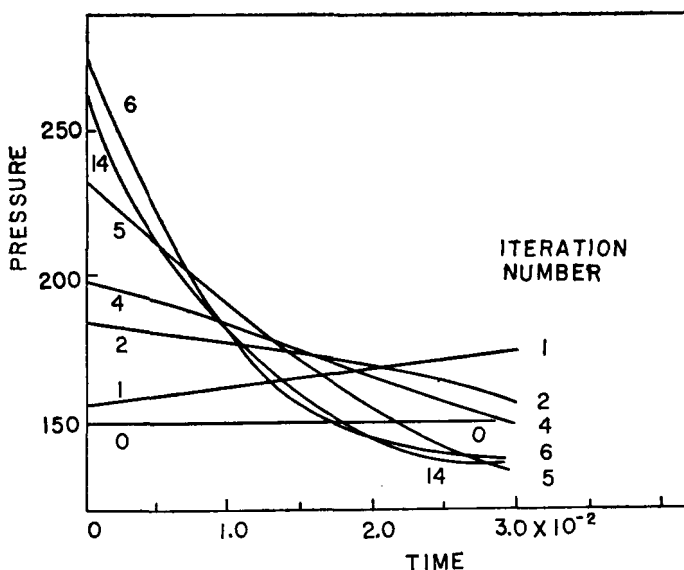


Figure 3. Successive approximations to optimal operating pressure, matched terminal constraints.

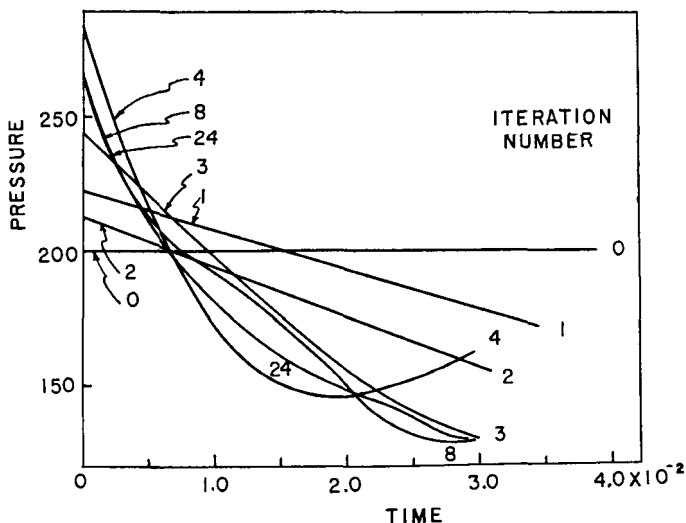


Figure 4. Successive approximations to optimal operating pressure, matched terminal constraints.

As compared with the result without inequality constraint on the operating pressure, the reaction time is somewhat long and the increase in the time is only $(2.7513 - 2.7487) / 2.7487 = 0.1\%$. It follows that inequality constraint on the operating pressure has quite small effect on the reaction time in this batch reaction process.

4-3 Constant operating pressure

The problem treated here is the time optimal control by constant operating pressure. The gradient method is modified to obtain the constant control variable in other paper⁸). However,

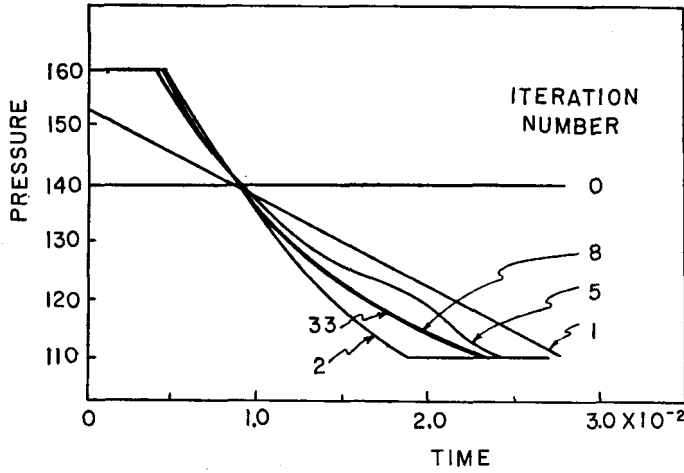


Figure 5. Successive approximations to optimal operating pressure with inequality constraint, terminal constraints open.

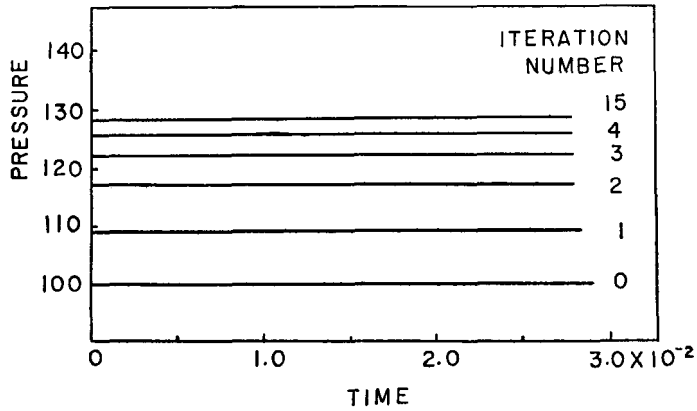


Figure 6. Successive approximations to optimal constant operating pressure, terminal constraints open.

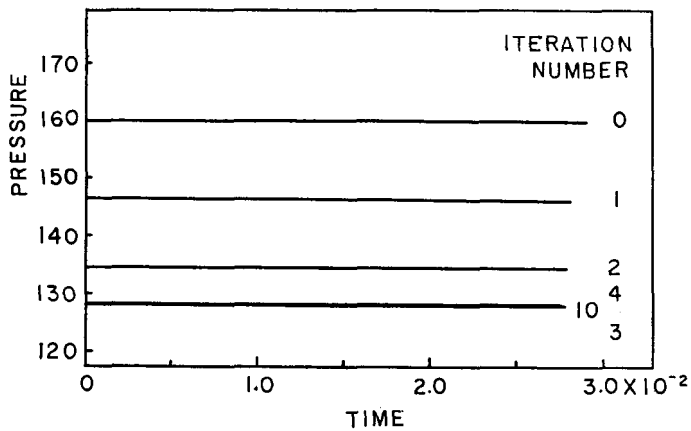


Figure 7. Successive approximations to optimal constant operating pressure, terminal constraints open.

the constant operating pressure can be determined by using the values of $\delta\alpha(t)$ in each iteration as follows ;

$$\delta\alpha_m = \int_{t_0}^{t_f} \delta\alpha(t) dt / \int_{t_0}^{t_f} dt = \left(\int_{t_0}^{t_f} \mathbf{W}^{-1} \mathbf{G}^T \lambda_{\varphi} \mathbf{Q} dt \right) \times [dS / (t_f - t_0) (I_{\varphi\varphi})^{1/2}] \quad (27)$$

Figs. 6 and 7 show the approach of the constant operating pressure to optimal one and the final results of computations are

$t_f = 2.786 \times 10^{-2}$, $p = 128.41$ and $x_1^f = 0.64621$ in each experiment.

As compared with the result of varying operating pressure, the increase in the reaction time is only 1.8% and the deviation of x_1^f results in 0.5%. It follows that control by the constant operating pressure is a good and simple method for the time optimal control of this batch reaction process with open terminal constraints.

References

- 1) E. S. Lee: I. E. C. Fundamentals **3**, (1964) 373.
- 2) M. M. Denn and R. Aris: I. E. C. Fundamentals **4**, (1965) 7, 213 and **4**, (1965) 248.
- 3) P. Eckman and I. Lefkowitz: Control Eng. **4**, (1957) No. 9, 197.
- 4) S. M. Robert and J. D. Mahoney: C. E. P. Symposium Series **58**, (1962) No. 37, 1.
- 5) H. J. Kelley: in "Optimization Techniques with Applications to Aero-space Systems", G. Leitman, ed., Academic Press, New York, (1962).
- 6) A. E. Bryson and W. F. Denham: J. Appl. Mech. **29**, (1962) 247.
- 7) A. E. Bryson et al.: A. I. A. A. Journal **1**, (1963) 2544 and **2**, (1964) 25.
- 8) Y. Sawaragi, T. Takamatsu, H. Fukawa and H. Sayama in PREPRINT of IFAC TOKYO SYMPOSIUM on SYSTEMS ENGINEERING FOR CONTROL DESIGN (1965).