On-line Optimization of Batch Processes in the Presence of Measurable Disturbances

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Feedforward/state feedback laws are developed for on-line optimization of batch reactors in the presence of measurable disturbances. The degrees of singularity with respect to manipulated input and disturbance input are used to characterize the nature of the feedforward/state feedback laws. Explicit synthesis formulas are derived that relate the optimal manipulated input to the system states and the measurable disturbance. It is shown that when the degree of singularity with respect to the manipulated input is infinite, the end-point optimization problem reduces to a regulation problem in the presence of disturbances. For finite degrees of singularity, the optimal feedforward/state feedback law is, in general, dynamic. The proposed methodology is illustrated through several end-point optimization problems in batch reactors.

Introduction

During the past decade there has been an increasing use of *model-based* nonlinear control strategies. In the formulation of the control problem of *continuous* processes, the desired output is a *steady state* and known *a priori*. However, in the case of *batch* processes, there is no process steady state and the objective is to *optimize* a cost function (such as yield) at the *end* of the batch time. Such problems are called *end-point optimization problems*.

The classic approach to solving end-point optimization problems in batch reactors has been to convert the optimal control problem into a nonlinear optimization problem and solve this problem by standard nonlinear optimization numerical methods. These numerical techniques provide the *open-loop* time profile of the manipulated input. However, due to batch-to-batch variations in the system parameters and initial conditions (which is a typical characteristic of most commercial batch processes), the implementation of this open-loop profile can lead to suboptimal performance. For this reason, it is necessary to develop *closed-loop* optimization schemes for end-point optimization of batch processes. One approach used by several researchers in the literature is to *repeatedly* use an open-loop algorithm at each time step. This *numerical* procedure calculates the open-loop optimal input profile at each time step based on current values of the system states. For instance, Luus (1974) calculated the optimal control vector by employing a direct-search procedure on the feedback gain matrix. Cuthrell and Biegler (1989) used a sequential quadratic programming approach to solve the optimal control problem. Eaton and Rawlings (1990) used a combination of orthogonal collocation and successive quadratic programming for end-point optimization. In all these numerical techniques, it is necessary to integrate the state equations a large number of times at each iteration. Furthermore, these techniques cannot easily incorporate information on *measurable disturbances*. This is because the optimal solution requires the integration of the process model up to the final time at each step. For this integration, it is necessary to know how the disturbance would behave in *future time*. This information on future values of the disturbance would obviously not be available during actual on-line implementation.

The use of measurements of the disturbances has been recognized as an important problem in nonlinear process control. Hirshorn (1981) and Isidori et al. (1981) solved the disturbance decoupling problem for the class of nonlinear systems where the relative order of the disturbance with respect to the output is greater than the relative order of the input with respect to the output. In the context of the Su-Hunt-Myer method, Calvet and Arkun (1988) developed a methodology for eliminating the effect of measurable disturbances by adding feedforward action for the case where the disturbances and manipulated input enter the state-space model through the same scalar function. Daoutidis and Kravaris (1989) developed a methodology in the input-output lin-

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earization framework for synthesizing feedforward/state-feedback controllers that made the closed-loop system independent of the measurable disturbances. Thus, a survey of the literature shows that the effect of measurable disturbances on nonlinear systems has been studied extensively for the *regulation* problem. However, no results are available that explicitly account for the effect of disturbances that provide *end-point optimization* in batch processes.

The purpose of this article is to develop optimal feedforward/state-feedback laws for the end-point optimization of batch processes. Using tools from differential geometry, Palanki et al. (1993) developed optimal state feedback laws for end-point optimization of batch processes. This method will be extended to incorporate the effect of measurable disturbances. First, a brief overview of the problem is presented in the context of the classic Pontryagin's principle. It is shown that the first-order necessary conditions for optimality are linear functions of the adjoint states. The degrees of singularity with respect to the manipulated input as well as the disturbance input are defined in terms of the system Lie Brackets. Feedforward/state-feedback laws are derived by elimination of the adjoint states. It is shown that the optimal feedforward/state-feedback law is static or dynamic depending on the degrees of singularity with respect to manipulated input and the measurable disturbance. In the special case of infinite degree of singularity with respect to the manipulated input and the disturbance input, the end-point optimization problem reduces to the regulator problem that was considered in the literature by Calvet and Arkun (1988) and Daoutidis and Kravaris (1989). Finally, the application of the developed methodology is illustrated via three simulation examples.

Formulation of End-Point Optimization Problem: The Classic Optimal Control Perspective

The end-point optimization problem is formulated as follows:

Minimize the performance index

$$J = \phi[x(t_f)] \tag{1}$$

subject to the dynamics

$$\begin{aligned} \dot{x} &= f(x) + g(x)u + w(x)d \qquad 0 \le t \le t_f \\ x(0) &= x_0, \end{aligned} \tag{2}$$

where u is the (scalar) manipulated input; x is the n-vector of state; t_f is the final time; $f(x)$, $g(x)$ and $w(x)$ are smooth vector functions; $\phi(x)$ is a smooth scalar function; and d is the measured disturbance input. In this formulation, we consider a scalar disturbance input. Results for a vector of disturbances is a very straightforward extension.

By Pontryagin's principle, the preceding minimization problem is equivalent to minimizing the Hamiltonian:

$$H(x,\lambda,u,d) = \lambda^T(f(x) + g(x)u + w(x)d), \tag{3}$$

where λ is an n-vector of adjoint states and is the solution of

$$\begin{aligned} \dot{\lambda}^T &= -\lambda^T\left(\frac{\partial f}{\partial x} + \frac{\partial g}{\partial x}u + \frac{\partial w}{\partial x}d\right) \\ \lambda(t_f) &= \frac{\partial \phi}{\partial x(t_f)}. \end{aligned} \tag{4}$$

A necessary condition for minimizing the Hamiltonian is given by (Bryson and Ho, 1975):

$$\frac{\partial H}{\partial u} = 0 \qquad \forall t \in [0,t_f]. \tag{5}$$

This gives an infinite hierarchy of necessary conditions (Bourdache-Siguerdidjane and Fliess, 1985):

$$\frac{d^k}{dt^k}\left(\frac{\partial H}{\partial u}\right) = 0 \qquad \forall t \in [0,t_f], \qquad k \ge 0 \tag{6}$$

Because the Hamiltonian is affine in the control, u, the optimal control problem is *singular*. The optimal trajectory $u(t)$ will correspond to either hitting an input constraint or to a singular extremal. To solve for the optimal input $u(t)$ in the singular region, one has to solve both the state equations (Eq. 2) as well as the adjoint equations (Eq. 4). Since the boundary conditions of these two sets of differential equations are split, this results in a two-point boundary-value problem. The numerical solution of this problem has to be implemented in an *open-loop* fashion and so uncertainties in the process are not attenuated. Furthermore, since the optimal solution depends on the disturbance input, d, one has to know *a priori* how the disturbance will behave in the time interval $[0, t_f]$ which is an unrealistic assumption. These problems can be alleviated if the optimal solution is derived as a function of the system states and the disturbance input.

Development of Optimal Feedforward/ State-Feedback Laws in the Singular Region

In the previous section it was shown that the classic approach to end-point optimization leads to a two-point boundary-value problem. In this section, it is shown that the necessary conditions of optimality (Eq. 6) are linear functions of the adjoint states, λ. Feedforward/state-feedback laws will be developed by eliminating the n adjoint states from n necessary conditions.

The definition of Lie Brackets of a nonlinear system is reviewed as follows: Given $p(x)$, $q(x)$ C^∞ time-invariant vector fields on R^n, the Lie Bracket $[p, q](x)$ is a vector field defined by

$$[p,q](x) = \frac{\partial q}{\partial x}p(x) - \frac{\partial p}{\partial x}q(x),$$

where $\partial p/\partial x$ and $\partial q/\partial x$ are the Jacobians. The Lie Bracket $[p, q]$ is also a C^∞ vector field on R^n. One can define iterated Lie Brackets $[p, [p, q]]$, $[p, [p, [p, q]]]$, etc. The following notation is standard:

$$ad_p^0 q(x) = q(x)$$
$$ad_p^1 q(x) = [p,q](x)$$
$$ad_p^2 q(x) = [p,[p,q]](x)$$
$$\vdots$$
$$ad_p^k q(x) = \left[p,\, ad_p^{k-1} q\right](x). \quad (7)$$

If the vector fields p and q are time varying, it is necessary to modify the definition of Lie Brackets to take into account, the time-varying component of the functions: Given $p(x, t)$ and $q(x, t)$ C^∞ time-varying vector fields on R^n, modified Lie Brackets are defined as follows (Palanki et al., 1993):

$$\overline{ad}_p^0 q(x,t) = q(x,t)$$
$$\overline{ad}_p^1 q(x,t) = [p,q](x,t) + \frac{\partial q}{\partial t}$$
$$\overline{ad}_p^2 q(x,t) = \left[p,\overline{ad}_p^1 q\right](x,t) + \frac{\partial \overline{ad}_p^1 q}{\partial t}$$
$$\vdots$$
$$\overline{ad}_p^k q(x,t) = \left[p,\overline{ad}_p^{k-1} q\right](x,t) + \frac{\partial \overline{ad}_p^{k-1} q}{\partial t}. \quad (8)$$

In the definitions below, we propose an extension to the concept of *degrees of singularity* (Palanki et al., 1993) of the system with respect to the manipulated input, to include disturbance as well. This extension allows for a characterization of the dynamic interaction between the manipulated and disturbance inputs. Furthermore, this definition provides a key conceptual tool for developing optimal feedforward/state-feedback laws.

Definition 1. The system governed by Eq. 2 has a finite degree of singularity, s_u, with respect to the manipulated input u, if

$$\left[g,\overline{ad}_{f+wdg}^{\nu}\right] \in \text{span}\left\{g,\overline{ad}_{f+wdg}^{1}, \ldots, \overline{ad}_{f+wdg}^{\nu}\right\} \quad \forall \nu \le s_u - 1$$
$$\left[g,\overline{ad}_{f+wdg}^{s_u}\right] \notin \text{span}\left\{g,\overline{ad}_{f+wdg}^{1}, \ldots, \overline{ad}_{f+wdg}^{s_u}\right\}. \quad (9)$$

The system 2 has an infinite degree of singularity with respect to manipulated input u ($s_u = \infty$) if

$$\left[g,\overline{ad}_{f+wdg}^{\nu}\right] \in \text{span}\left\{g,\overline{ad}_{f+wdg}^{1}, \ldots, \overline{ad}_{f+wdg}^{\nu}\right\} \quad \forall \nu \ge 0. \quad (10)$$

Definition 2. The system governed by Eq. 2 has a finite degree of singularity, s_d, with respect to the disturbance input d, if

$$\left[w,\overline{ad}_{f+wdg}^{\nu}\right] \in \text{span}\left\{g,\overline{ad}_{f+wdg}^{1}, \ldots, \overline{ad}_{f+wdg}^{\nu}\right\} \quad \forall \nu \le s_d - 1$$
$$\left[w,\overline{ad}_{f+wdg}^{s_d}\right] \notin \text{span}\left\{g,\overline{ad}_{f+wdg}^{1}, \ldots, \overline{ad}_{f+wdg}^{s_d}\right\}. \quad (11)$$

The degree of singularity of system 2 is infinite with respect to disturbance input d ($s_d = \infty$) if

$$\left[w,\overline{ad}_{f+wdg}^{\nu}\right] \in \text{span}\left\{g,\overline{ad}_{f+wdg}^{1}, \ldots, \overline{ad}_{f+wdg}^{\nu}\right\} \quad \forall \nu \ge 0. \quad (12)$$

These definitions of degrees of singularity can be used to develop the feedforward/state-feedback laws for various situations depending on the values of s_u and s_d.

Theorem 1. Consider a system of the form of Eq. 2 and a performance index of the form of Eq. 1. When the degree of singularity with respect to the manipulated input, s_u, is infinite (while the degree of singularity with respect to the disturbance input, s_d, may or may not be finite), the end-point optimization problem reduces to the following regulation problem in the singular region:

$$\dot{x} = f(x) + g(x)u + w(x)d$$
$$y = C(x,d), \quad (13)$$

where C is an algebraic function independent of the manipulated input and is given by

$$C(x,d) = \det\left[g \,\vdots\, \overline{ad}_{f+wdg}^{1} \,\vdots\, \cdots \,\vdots\, \overline{ad}_{f+wdg}^{n-1}\right] = 0. \quad (14)$$

Proof. When $s_u = \infty$, the first-order necessary conditions on the singular region (Eq. 6) can be written as

$$\lambda^T g = 0$$
$$\lambda^T \overline{ad}_{f+wdg}^{1} = 0$$
$$\lambda^T \overline{ad}_{f+wdg}^{2} = 0$$
$$\vdots$$
$$\lambda^T \overline{ad}_{f+wdg}^{n-1} = 0$$
$$\vdots \quad (15)$$

The first n equation can be written in compact form as

$$\lambda^T\left[g \,\vdots\, \overline{ad}_{f+wdg}^{1} \,\vdots\, \cdots \,\vdots\, \overline{ad}_{f+wdg}^{n-1}\right] = 0. \quad (16)$$

Since λ^T is a nonzero vector, it follows that

$$\det\left[g \,\vdots\, \overline{ad}_{f+wdg}^{1} \,\vdots\, \cdots \,\vdots\, \overline{ad}_{f+wdg}^{n-1}\right] = 0, \quad (17)$$

which is Eq. 14.

Corollary 1. When the degrees of singularity with respect to the *manipulated input* and the *disturbance input* is infinite ($s_u = s_d = \infty$), the algebraic function C in Eq. 13 is a function of x (and not d) only and is given by

$$C(x) = \det\left[g \,\vdots\, ad_f^1 g \,\vdots\, \cdots \,\vdots\, ad_f^{n-1} g\right] = 0. \tag{18}$$

For a proof of this corollary, see Appendix A1.1.

Note that for this special case, the end-point optimization problem is reduced to controlling the nonlinear system 2 to a function of the system states described by Eq. 18. When the disturbance free part of the model described by Eq. 2 is involutive and the disturbance and the manipulated input enter the state-space model through the same scalar functions, the preceding regulation problem can be solved by the methods described in Calvet and Arkun (1988). When this system has finite relative order, the regulation problem can be solved by the methods described in Daoutidis and Kravaris (1989).

Theorem 2. Consider a system of the form of Eq. 2 and a performance index of the form of Eq. 1. When the degree of singularity with respect to the manipulated input, s_u, is equal to $n-2$ (while the degree of singularity with respect to the disturbance input, s_d, may take any value), then the optimal feedforward/state feedback law in the singular region is given by

$$u = -\frac{\det\left[g \,\vdots\, \overline{ad}_{f+wd}^{1} g \,\vdots\, \cdots \,\vdots\, \overline{ad}_{f+wd}^{n-1} g\right]}{\det\left[g \,\vdots\, \overline{ad}_{f+wd}^{1} g \,\vdots\, \cdots \,\vdots\, \left[g, \overline{ad}_{f+wd}^{n-2} g\right]\right]}. \tag{19}$$

Proof. When $s_u = (n-2)$, the first-order necessary conditions in the singular region can be written as

$$\lambda^T g = 0$$

$$\lambda^T \overline{ad}_{f+wd}^{1} g = 0$$

$$\lambda^T \overline{ad}_{f+wd}^{2} g = 0$$

$$\vdots$$

$$\lambda^T \overline{ad}_{f+wd}^{n-1} g + \lambda^T\left[g, \overline{ad}_{f+wd}^{n-2} g\right] u = 0 \tag{20}$$

n adjoint states can be eliminated from Eq. 20 to obtain Eq. 19. Note that this feedforward/state-feedback law is *static* with respect to u but *dynamic*, in general, with respect to d.

Corollary 2. When $s_d = s_u = n-2$, the optimal feedforward/state-feedback law reduces to the following static law with respect to u and d:

$$u = -\frac{\det\left[g \,\vdots\, ad_f^1 g \,\vdots\, \cdots \,\vdots\, ad_f^{n-1} g\right]}{\det\left[g \,\vdots\, ad_f^1 g \,\vdots\, \cdots \,\vdots\, ad_f^{n-2} g \,\vdots\, \left[g, ad_f^{n-2} g\right]\right]} - \frac{\det\left[g \,\vdots\, ad_f^1 g \,\vdots\, \cdots \,\vdots\, ad_f^{n-2} g \,\vdots\, \left[w, ad_f^{n-2} g\right]\right] d}{\det\left[g \,\vdots\, ad_f^1 g \,\vdots\, \cdots \,\vdots\, ad_f^{n-2} g \,\vdots\, \left[g, ad_f^{n-2} g\right]\right]}. \tag{21}$$

For a proof of this corollary, see Appendix A2.1.

Corollary 3. When $s_d > s_u$ and $s_u = n-2$, the optimal feedforward/feedback law reduces to the following expression:

$$u = -\frac{\det\left[g \,\vdots\, ad_f^1 g \,\vdots\, \cdots \,\vdots\, ad_f^{n-1} g\right]}{\det\left[g \,\vdots\, ad_f^1 g \,\vdots\, \cdots \,\vdots\, ad_f^{n-2} g \,\vdots\, \left[g, ad_f^{n-2} g\right]\right]}. \tag{22}$$

For a proof, see Appendix A2.2.

Note that Eq. 22 is not a function of the measurable disturbance and the optimal operating policy is a state feedback with no feedforward action.

Theorem 3. Consider a system of the form of Eq. 2 and a performance index of the form of Eq. 1. When the degree of singularity with respect to the manipulated input, s_u, is finite and $s_u \le n-3$ (while the degree of singularity with respect to the disturbance input, s_d, may take any value), the feedforward/state-feedback law in the singular region is given by

$$\det\left[\left(I\frac{d}{dt} - \frac{\partial f}{\partial x} - \frac{\partial g}{\partial x}u - \frac{\partial w}{\partial x}d\right)^0 g \,\vdots\, \left(I\frac{d}{dt} - \frac{\partial f}{\partial x} - \frac{\partial g}{\partial x}u - \frac{\partial w}{\partial x}d\right)^1 g \,\vdots\, \cdots \,\vdots\, \left(I\frac{d}{dt} - \frac{\partial f}{\partial x} - \frac{\partial g}{\partial x}u - \frac{\partial w}{\partial x}d\right)^{n-1} g\right] = 0. \tag{23}$$

Proof. The first-order necessary conditions (Eq. 6) can be written as

$$\lambda^T\left(I\frac{d}{dt} - \frac{\partial f}{\partial x} - \frac{\partial g}{\partial x}u - \frac{\partial w}{\partial x}d\right)^0 g = 0$$

$$\lambda^T\left(I\frac{d}{dt} - \frac{\partial f}{\partial x} - \frac{\partial g}{\partial x}u - \frac{\partial w}{\partial x}d\right) g = 0$$

$$\vdots$$

$$\lambda^T\left(I\frac{d}{dt} - \frac{\partial f}{\partial x} - \frac{\partial g}{\partial x}u - \frac{\partial w}{\partial x}d\right)^{n-1} g = 0. \tag{24}$$

In the preceding equations, I is the identity matrix and $d(\cdot)/dt$ is the total time-derivative operator. Equation 23 can be obtained from Eq. 24 by eliminating the n adjoint states. Note that feedforward/state-feedback law given by expression 23 is *dynamic* with respect to the system states and the measurable disturbance.

Corollary 4. When $s_d = s_u$ and $s_u \le n-3$, the preceding feedforward/state-feedback law reduces to

$$\det\left[g \,\vdots\, ad_f^1 g \,\vdots\, ad_f^2 g \,\vdots\, \cdots \,\vdots\, ad_f^{s_u} g \,\vdots\, ad_f^{s_u+1} g + [g, ad_f^{s_u} g]u + [w, ad_f^{s_u} g]d \,\vdots\, \left(I\frac{d}{dt} - \frac{\partial f}{\partial x} - \frac{\partial w}{\partial x}d - \frac{\partial g}{\partial x}u\right)^{s_u+2} g \,\vdots\, \cdots \,\vdots\, \left(I\frac{d}{dt} - \frac{\partial f}{\partial x} - \frac{\partial w}{\partial x}d - \frac{\partial g}{\partial x}u\right)^{n-1} g\right] = 0, \tag{25}$$

which is *dynamic* in nature.

For a proof of this corollary, see Appendix A3.1.

Corollary 5. When $s_d < s_u$ and $s_u \leq n-3$, Eq. 23 simplifies to

$$\det\Bigg[g \,\vdots\, ad_f^1 g \,\vdots\, \cdots \,\vdots\, ad_f^{s_d} g \,\vdots\, \overline{ad}_{f+wd}^{s_d+1} g \,\vdots\, \cdots \,\vdots\, \overline{ad}_{f+wd}^{s_u+1} g + \left[g, \overline{ad}_{f+wd}^{s_u} g \right] u \,\vdots\, \left(I\frac{d}{dt} - \frac{\partial f}{\partial x} - \frac{\partial w}{\partial x} d - \frac{\partial g}{\partial x} u \right)^{s_u+1} g \,\vdots\, \cdots \,\vdots\, \left(I\frac{d}{dt} - \frac{\partial f}{\partial x} - \frac{\partial w}{\partial x} d - \frac{\partial g}{\partial x} u \right)^{n-1} g \Bigg] = 0. \quad (26)$$

For a proof, see Appendix A3.2. A similar expression can be derived from Eq. 23 for the case where $s_d > s_u$.

Development of feedforward/feedback laws for a *vector* of measurable disturbances is a very straightforward extension. The main focus of this article is to show explicitly the effect of measured disturbance on the optimal solution and so we consider only the scalar disturbance case. In the case of a vector disturbance inputs, one would have to define a degree of singularity with respect to each disturbance input. The effect of each disturbance input on the optimal solution can be analyzed along the lines of Theorems 1, 2 and 3.

Implementation Issues

The results obtained in the previous sections provide optimal feedforward/state-feedback laws in the singular region for end-point optimization of batch reactors subject to a measurable disturbance. The feedforward/state-feedback laws require the calculation of Lie Brackets. This can involve the calculation of several derivatives, especially when the dimension of the problem is large. The use of symbolic manipulation software such as MAPLE or MATHEMATICA is highly recommended for the calculation of the feedforward/state-feedback laws.

For implementing the feedforward/feedback laws, one requires the switching times between the nonsingular and singular regions as discussed in Palanki et al. (1995) as well as estimates of the system states. In addition, since the feedforward/feedback laws are explicit functions of the measurable disturbance, it is necessary to have measurements or estimates of the measurable disturbance. The degree of singularity with respect to the manipulated input depends on the disturbance value. Thus, it is possible the structure of the feedforward/feedback law could change (e.g., from static to dynamic) due to changes in the disturbance value. For this reason it is necessary to monitor the degree of singularity on-line and use the appropriate feedforward/feedback law depending on the value of the degree of singularity. If the system is subjected to a state-inequality constraint, it is necessary to know the switching time to switch to the constraint as shown in Palanki et al. (1994).

The optimal feedforward/feedback laws developed in the previous section are based on a mathematical model of the batch process. However, there could be a mismatch between the parameters of the model and the actual process. Furthermore, the actual process could be subjected to unmeasured disturbances. Robustness to these errors in the parameters as well as to unmeasured disturbances has to be checked by simulation before implementation, as shown in Example 2 in the next section. A theoretical analysis of robustness of feedforward/feedback laws for nonlinear systems is an open research problem and is not considered in this article.

Illustrative Examples

The following simulation examples are studied to illustrate the application and to test the efficacy of the theory developed in the previous sections.

Example 1: Regulator problem

The following reaction is occurring in a semibatch reactor:

$$A \rightarrow B.$$

The reaction follows the Langmuir–Hishelwood type of kinetics. Component A is being fed to the reactor at a feed rate of u. To keep the viscosity from becoming too high, water is added at a feed rate of d. This situation is quite common in industrial fermentors where the viscosity of the fermentation broth becomes very high due to rapid growth of cell mass in complex media. Addition of water reduces the viscosity and aids in mixing as well as oxygen transfer, which is essential for growth and product formation.

The objective is to maximize the concentration of component B at the end of a batch cycle of 5 h. The manipulated input is u, the flow rate of species A. The flow rate of water, d, is subject to disturbances.

The end-point optimization problem can be stated as:

$$\text{Minimize } J = -C_{B0}\frac{V_0}{V} + C_A - C_{A0}\frac{V_0}{V} - S_A + S_A\frac{V_0}{V} \quad (27)$$

subject to

$$\frac{d}{dt}\begin{bmatrix} C_A V \\ V \end{bmatrix} = \begin{bmatrix} \dfrac{-k_1 C_A V}{k_2 + C_A^2} \\ 0 \end{bmatrix} + \begin{bmatrix} S_A \\ 1 \end{bmatrix} u + \begin{bmatrix} 0 \\ 1 \end{bmatrix} d. \quad (28)$$

Here, C_A and C_B are the concentration of component A and B, respectively; u and d are the flow rates of component A and water, respectively; V is the reactor volume; and the subscript 0 refers to initial conditions.

Defining

$$x_1 = C_A V$$
$$x_2 = V \quad (29)$$

the Eqs. 27 and 28 can be put in the form

$$\text{Minimize } J = -\frac{(C_{B0}V_0 + X_{10} + S_A X_2)}{X_2} + \frac{(X_1 + S_A X_{20})}{X_2} \quad (30)$$

subject to

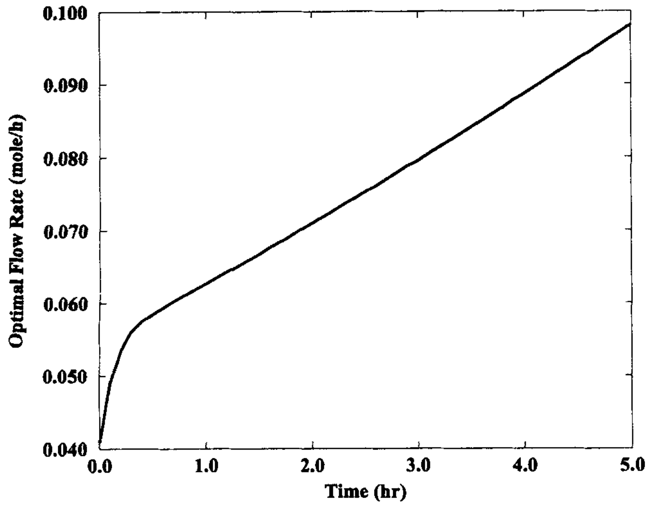

Figure 1. Optimal-input profile—constant d (Example 1).

$$\frac{d}{dt}\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} -k_1x_1x_2^2 \\ \overline{k_2x_2^2 + x_1^2} \\ 0 \end{bmatrix} + \begin{bmatrix} S_A \\ 1 \end{bmatrix}u + \begin{bmatrix} 0 \\ 1 \end{bmatrix}d. \quad (31)$$

For this system

$$x = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}, \quad f(x) = \begin{bmatrix} -k_1x_1x_2^2 \\ \overline{k_2x_2^2 + x_1^2} \\ 0 \end{bmatrix},$$

$$g(x) = \begin{bmatrix} S_A \\ 1 \end{bmatrix}, \quad w(x) = \begin{bmatrix} 0 \\ 1 \end{bmatrix}. \quad (32)$$

It can be shown that the degrees of singularity with respect to the manipulated input and the disturbance are equal to ∞; therefore, Eq. 18 leads to

Table 1a. Initial Conditions (Example 1)

Case A	
$C_A(0)$	0.15 mol·L^{-1}
$C_B(0)$	0.075 mol·L^{-1}
$V(0)$	1.0 L
d	0.1 L h^{-1}
Case B	
$C_A(0)$	0.15 mol·L^{-1}
$C_B(0)$	0.075 mol·L^{-1}
$V(0)$	1.0 L
d	$\begin{cases} 0.1\ \text{Lh}^{-1} & t \le 2\ \text{h} \\ 0.2\ \text{Lh}^{-1} & t > 2\ \text{h} \end{cases}$

Table 1b. Model Parameters (Example 1)

k_1	0.5 mol^2·L^{-2}·h^{-1}
k_2	0.1 mol^2·L^{-2}
t_f	5 h
S_A	10 mol·L^{-1}
V_{max}	5 L

$$C(x_1,x_2) = S_Ax_2(k_2x_2^2 - x_1^2) + 2x_1^3 = 0. \quad (33)$$

Thus, the optimization problem reduces to regulating the function $C(x_1, x_2)$ to zero where the system states x_1 and x_2 are described by Eq. 28. We use the following nonlinear feedforward/feedback law (see Daoutidis and Kravaris, 1989) for this regulator problem.

$$u = -\frac{S_A(k_2x_2^3 - x_2x_1^2) + 2x_1^3}{S_A(5x_1^2 - 2x_1x_2S_A + 3k_2x_2^2)} - \frac{S_A[(3k_2x_2^2 - x_1^2)]}{S_A(5x_1^2 - 2x_1x_2S_A + 3k_2x_2^2)}d \quad (34)$$

Figures 1 and 2 show the optimal feeding profile and corresponding product concentration profile for the system parameters in Table 1a and initial conditions in Table 1b for

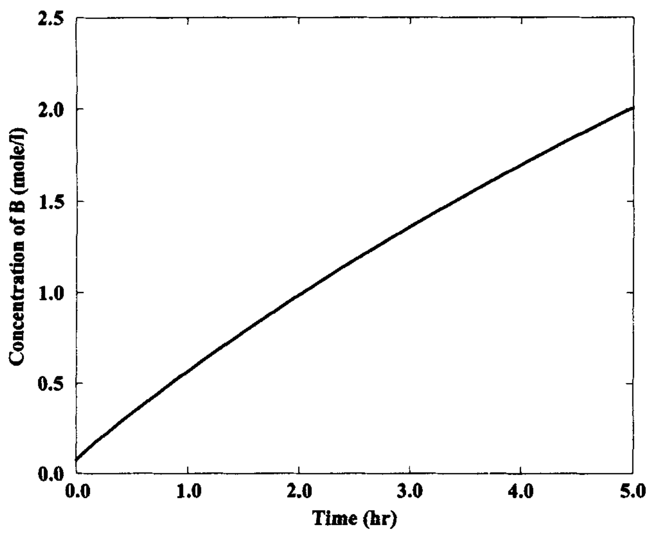

Figure 2. Product-concentration profile—constant d (Example 1).

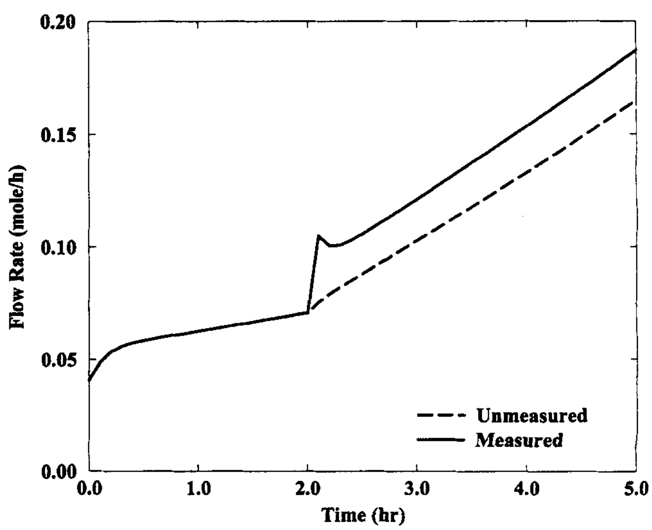

Figure 3. Optimal-input profiles—step disturbance (Example 1).

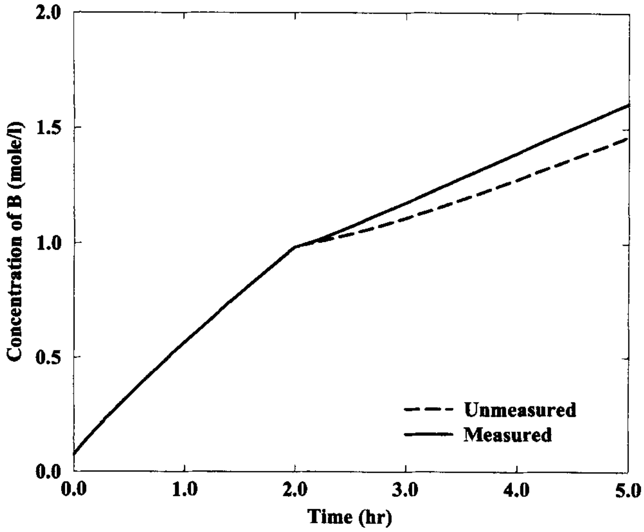

Figure 4. Product-concentration profiles—step disturbance (Example 1).

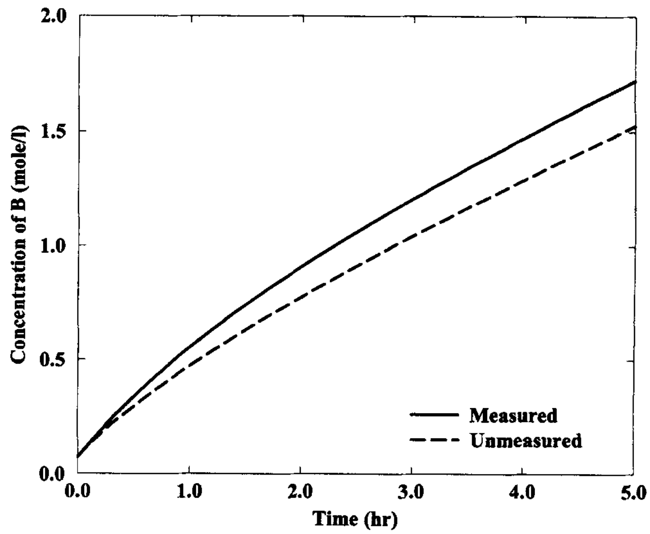

Figure 6. Product-concentration profiles—random disturbance (Example 1).

Table 1c. Effect of Measurement of Disturbance on Performance Index (Example 1)

Step disturbance	
Type	Performance index
Measured	− 1.65 mol/L
Unmeasured	− 1.45 mol/L
Random disturbance	
Type	Performance index
Measured	− 1.75 mol/L
Unmeasured	− 1.55 mol/L

the case where d is constant. The case where the system is subject to a *step disturbance* of magnitude 0.1 L/h after two hours of operation is studied. Two different cases are analyzed; the first is the case where the disturbance is *not* measured and the second is the case where the disturbance is measured. The optimal manipulated input profiles are shown in Figure 3, and the corresponding product concentration profiles are shown in Figure 4. It is evident from Figure 4 and Table 1c that the product concentration is 11.5% more in case where the disturbance is measured. The case where the disturbance input is subject to random fluctuations as shown in Figure 5 is studied. Once again, the case where the disturbance is not measured is compared with the case where the disturbance is measured. The optimal manipulated input profiles are shown in Figure 5 and the corresponding product concentration profiles are shown in Figure 6, respectively. It is observed from Figure 6 and Table 1c that the product concentration is 15% more in the case where the disturbance input is measured.

The effect of open-loop implementation of optimal profile on the performance index is studied. The optimal input profile of the system without disturbance (Case A in Table 1a) is implemented in open-loop fashion to the system with a step change in disturbance input (Case B in Table 1a). This open-loop policy is compared with the closed-loop case where the states as well as the disturbance inputs are measured and

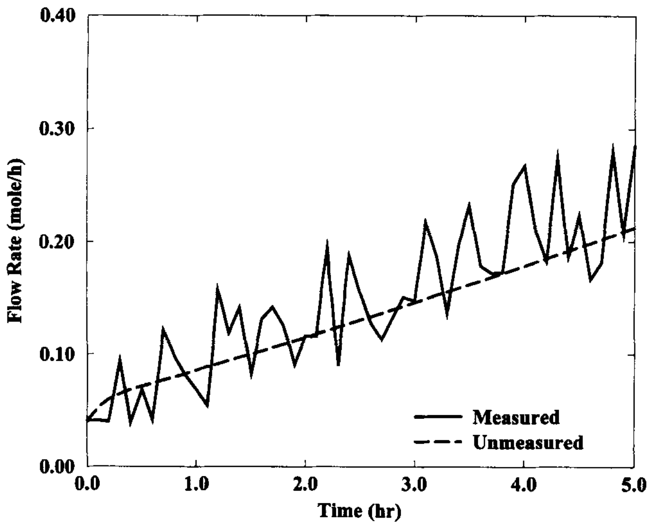

Figure 5. Optimal-input profiles—random disturbance (Example 1).

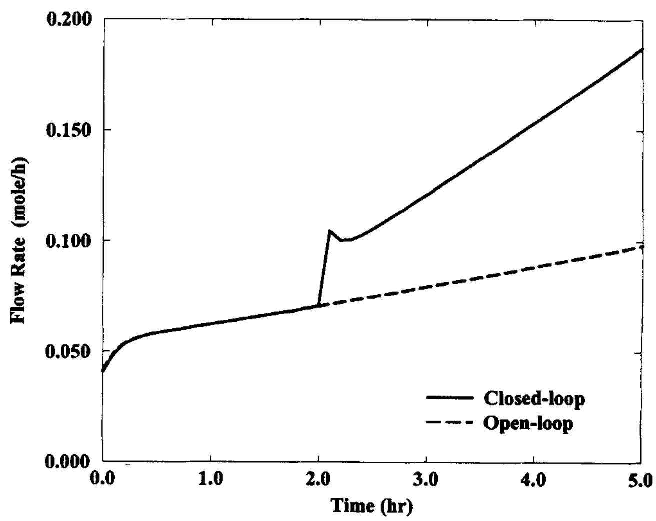

Figure 7. Closed- and open-loop input profiles—step disturbance (Example 1).

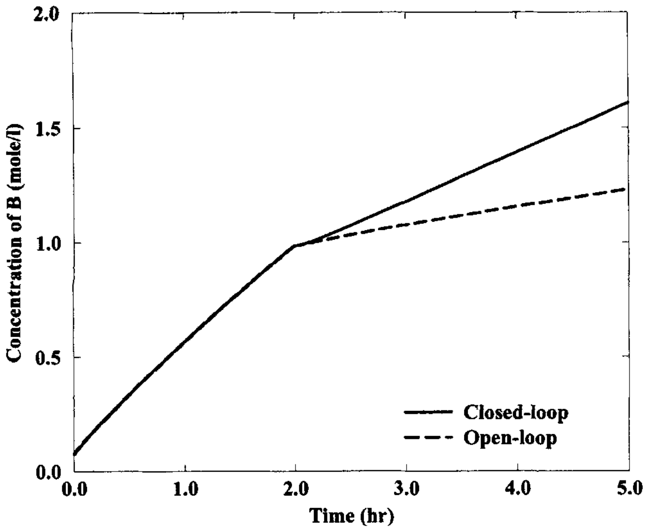

Figure 8. Closed- and open-loop product profiles—step disturbance (Example 1).

accounted in Eq. 34. The open-loop and closed-loop manipulated input profiles are shown in Figure 7, and the corresponding product profiles are shown in Figure 8. It is observed from Figure 8 and Table 1d that implementing the state-feedback profile in a closed-loop fashion leads to 37.5% more product concentration than the open-loop case.

Example 2: Static state feedback

The following irreversible reaction is occurring in a semibatch reactor:

$$A \rightarrow B.$$

The reaction follows the Langmuir–Hinshelwood type of kinetics. Component A is being fed to the reactor at a feed rate of d that is subject to disturbance. The objective is to find the optimal temperature profile to maximize the concentration of product B at the end of a batch cycle of one hour.

The end-point optimization problem can be stated as:

$$\text{Minimize } J = -C_B(t_f) \tag{35}$$

subject to

$$\frac{d}{dt}\begin{bmatrix} C_A \\ V \\ T \end{bmatrix} = \begin{bmatrix} \dfrac{-k_1 C_A}{k_2 + C_A^2} \\ 0 \\ 0 \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} u + \begin{bmatrix} \dfrac{(S_A - C_A)}{V} \\ 1 \\ 0 \end{bmatrix} d, \tag{36}$$

Table 1d. Open-loop vs. Closed-loop Implementation (Example 1)

Open-loop implementation	
Initial conditions	Case B in Table 1a
Input profile	Optimal solution for case A
Performance index at t_f	-1.25 mol·L^{-1}
Closed-loop implementation	
Initial conditions	Case B in Table 1a
Input profile	State-feedback law
Performance index at t_f	-1.65 mol·L^{-1}

where

$$k_1 = k_{10} e^{-\frac{E_1}{RT}}$$

$$k_2 = k_{20} e^{-\frac{E_2}{RT}}.$$

Here, C_A and C_B represent the concentrations of components A and B, respectively; k_1 and k_2 are reaction-rate constants; T is the temperature; V is the volume of the reactor; u is the manipulated input and d is the feed rate of component A (disturbance input). The system model is of the form

$$\dot{x} = f(x) + g(x)u + w(x)d, \tag{37}$$

where

$$x = \begin{bmatrix} C_A \\ V \\ T \end{bmatrix}; \quad f(x) = \begin{bmatrix} \dfrac{-k_1 C_A}{k_2 + C_A^2} \\ 0 \\ 0 \end{bmatrix}; \quad g(x) = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix};$$

$$w(x) = \begin{bmatrix} \dfrac{(S_A - C_A)}{V} \\ 1 \\ 0 \end{bmatrix}.$$

It can be shown that the degrees of singularity with respect to u and d are equal to $n-2$. Using Eq. 21, the optimal feedforward feedback law is given by

$$u = \frac{2 C_A E_1 R T^2}{(E_1 - E_2) E_2 k_2}\left[\frac{k_1 C_A}{k_2 + C_A^2} - \frac{(S_A - C_A) d}{V}\right]. \tag{38}$$

Table 2a. Initial Conditions (Example 2)

Case A	
$C_A(0)$	1.0 mol·L^{-1}
$C_B(0)$	0.01 mol·L^{-1}
$T(0)$	349.2 K
$V(0)$	1.0 L
d	1 L h^{-1}
Case B	
$C_A(0)$	1.0 mol·L^{-1}
$C_B(0)$	0.01 mol·L^{-1}
$T(0)$	349.2 K
$V(0)$	1.0 L
d	$\begin{cases} 1\ \text{Lh}^{-1} & t \le 0.2\ \text{h} \\ 2\ \text{Lh}^{-1} & t > 0.2\ \text{h} \end{cases}$

Table 2b. Model Parameters (Example 2)

k_{10}	12,500.0 mol^2·L^{-2}·h^{-1}
k_{20}	1,000.0 mol^2·L^{-2}
E_1	5,000.0 cal·mol^{-1}
E_2	9,500.0 cal·mol^{-1}
t_f	1 h
S_A	10.0 mol·L^{-1}
V_{max}	5.0 L

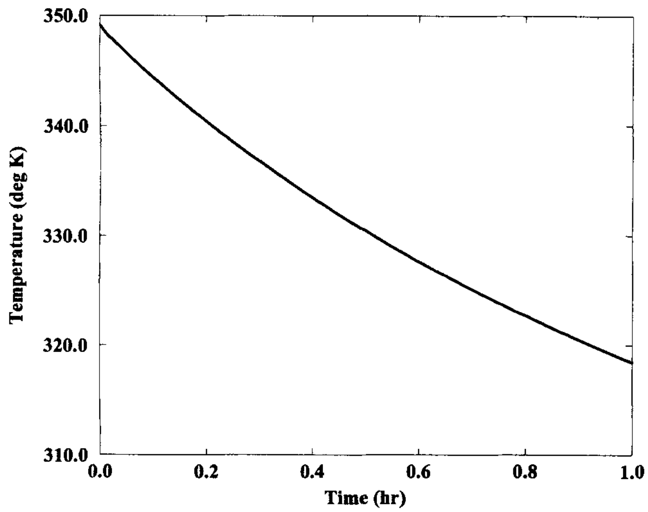

Figure 9. Optimal-input profile—constant *d* (Example 2).

Note that the preceding state feedback is an explicit function of the system states as well as the disturbance *d*. Simulation studies were conducted using the initial conditions given in Table 2a and the model parameters given in Table 2b. Figures 9 and 10 show the optimal temperature profile and corresponding product-concentration profile, respectively, for the case where *d* is constant. The effect of measuring the disturbance input *d*, is studied. A step disturbance of magnitude 1 L/h is introduced in the input flow stream of component *A* after 12 minutes of operation. Figure 11 shows the manipulated input profiles for two situations: one where the disturbance input is measured and corrected for in Eq. 38 and the other where the disturbance input is not measured and left unchanged in Eq. 38. The corresponding product concentration profiles are shown in Figure 12. It is observed from Figure 12 and Table 2c that the product concentration of component *B* is 115% higher in the case where the disturbance input is measured and accounted for in the optimal feedback law. A similar study is done for the case where there are random fluctuations in the disturbance input as shown in Figures 13 and 14. The results are tabulated in Table 2c. As in the case with the step disturbance, it is observed that when the disturbance input is measured and accounted for in the optimal state-feedback law, this leads to a much higher concentration of the product.

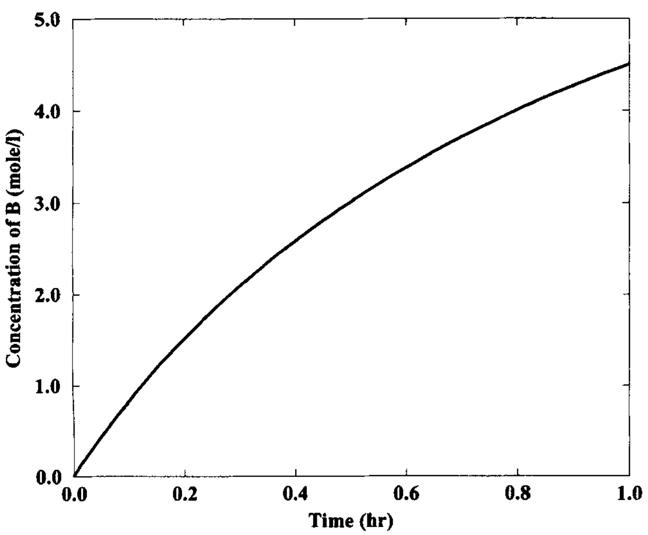

Figure 10. Product-concentration profile—constant *d* (Example 2).

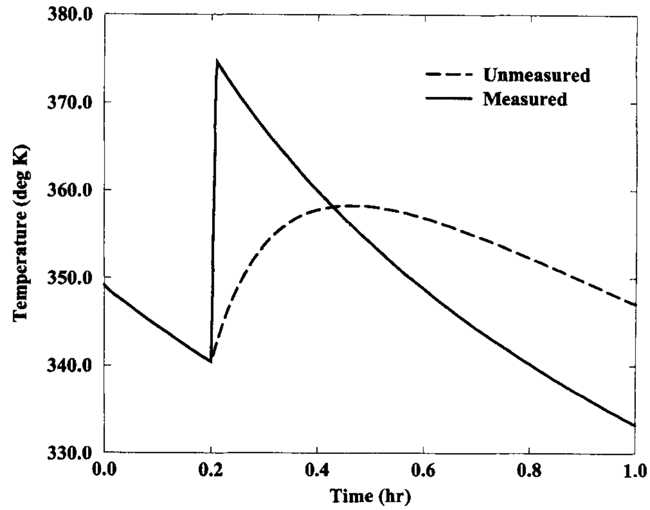

Figure 11. Optimal-input profiles—step disturbance (Example 2).

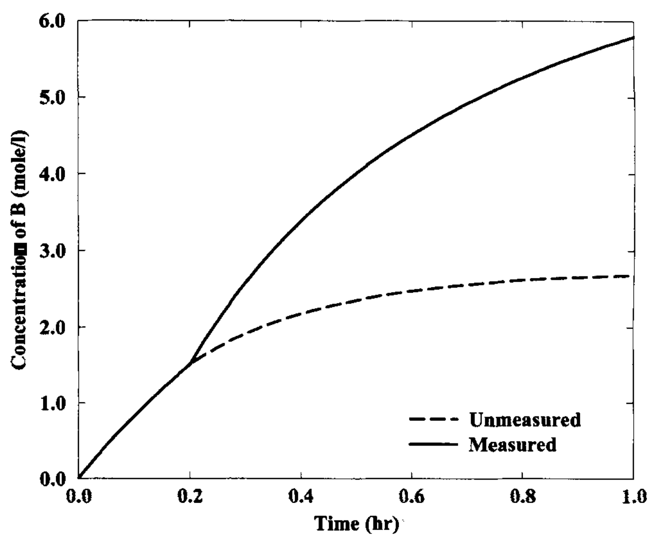

Figure 12. Product-concentration profiles—step disturbance (Example 2).

Table 2c. Effect of Measurement of Disturbance on Performance Index (Example 2)

Step disturbance	
Type	Performance index
Measured	−5.6 mol/L
Unmeasured	−2.6 mol/L
Random disturbance	
Type	Performance index
Measured	−4.8 mol/L
Unmeasured	−4.5 mol/L

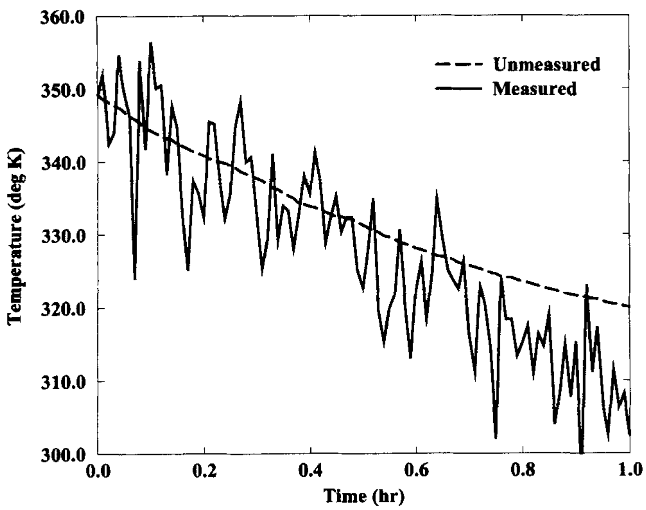

Figure 13. Optimal-input profiles—random disturbance (Example 2).

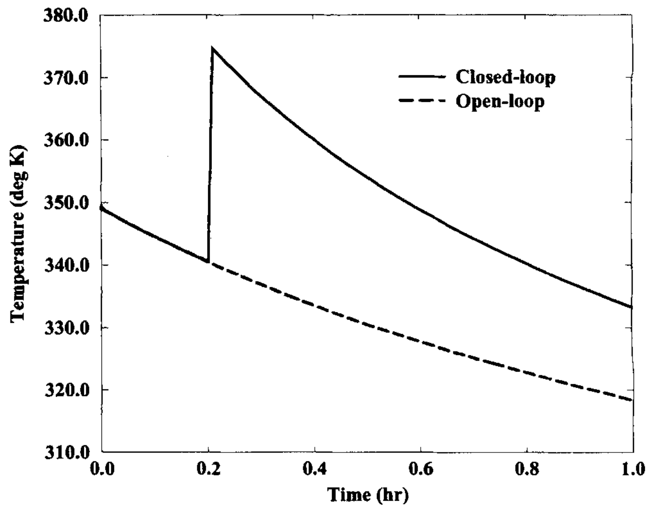

Figure 15. Closed- and open-loop optimal input profiles—step disturbance (Example 2).

The effect of open-loop implementation of optimal profiles on the performance index is studied. The optimal input profiles of the system without disturbance (Case A in Table 2a) is implemented in open-loop fashion to the system subject to a step change in disturbance input (Case B in Table 2a). This open-loop policy is compared with the closed-loop case where the states as well as disturbance input are measured and accounted for in Eq. 38. The open-loop and closed-loop manipulated input profiles are shown in Figure 15 and the corresponding product profiles are shown in Figure 16. The performance indices obtained in these two cases is compared in Table 2d. It is observed that the closed-loop implementation results in an increment of about about 117% in product formation as compared to the open-loop case. Robustness to plant/model mismatch in kinetic parameters was tested via simulations. The results are shown in Table 2e. It is observed that the performance index is robust to an error of $\pm 10\%$ in the parameter E_1. A similar analysis can be conducted for all the system parameters as well as unmeasured disturbances.

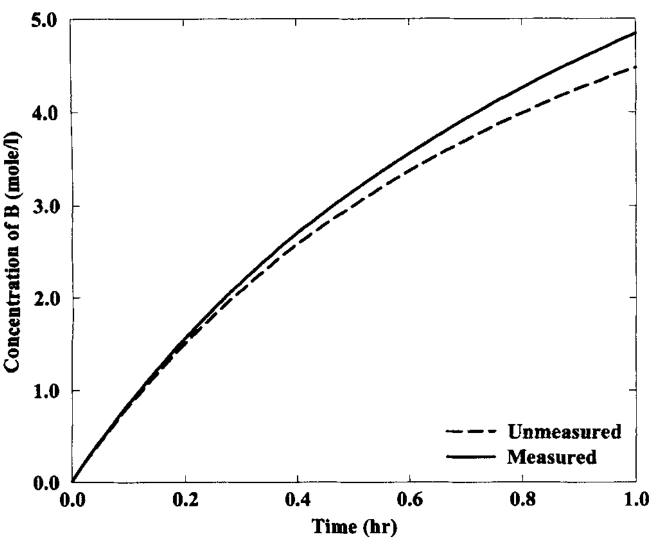

Figure 14. Product-concentration profiles—random disturbance (Example 2).

Example 3: Dynamic state feedback

The following series reaction is occurring in a semibatch reactor:

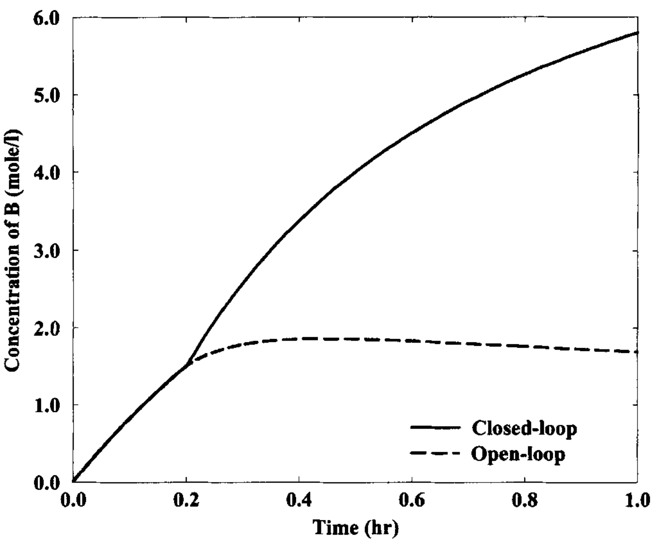

Figure 16. Closed- and open-loop product formation profiles—step disturbance (Example 2).

Table 2d. Open-Loop vs. Closed-loop Implementation (Example 2)

Open-loop implementation	
Initial conditions	Case B in Table 2a
Input profile	Optimal solution for case A
Performance index at t_f	-1.75 mol·L^{-1}
Closed-loop implementation	
Initial conditions	Case B in Table 2a
Input profile	State-feedback law
Performance index at t_f	-5.75 mol·L^{-1}

Table 2e. Robustness Analysis (Example 2)

Parameter in Control Law	Parameter in Process	Performance Index
No Disturbance		
$E_1 = 5{,}000.000$ All other parameter values from Table 2b	$E_1 = 5{,}000.00$ All other parameter values from Table 2b	$-4.505\ \text{mol}\cdot\text{L}^{-1}$
$E_1 = 5{,}000.00$ All other parameter values from Table 2b	$E_1 = 4{,}500.00$ All other parameter values from Table 2b	$-4.505\ \text{mol}\cdot\text{L}^{-1}$
$E_1 = 5{,}000.00$ All other parameter values from Table 2b	$E_1 = 5{,}500.00$ All other parameter values from Table 2b	$-4.505\ \text{mol}\cdot\text{L}^{-1}$
Step Disturbance		
$E_1 = 5{,}000.00$ All other parameter values from Table 2b	$E_1 = 5{,}000.00$ All other parameter values from Table 2b	$-5.59\ \text{mol}\cdot\text{L}^{-1}$
$E_1 = 5{,}000.00$ All other parameter values from Table 2b	$E_1 = 4{,}500.00$ All other parameter values from Table 2b	$-5.59\ \text{mol}\cdot\text{L}^{-1}$
$E_1 = 5{,}000.00$ All other parameter values from Table 2b	$E_1 = 5{,}500.00$ All other parameter values from Table 2b	$-5.59\ \text{mol}\cdot\text{L}^{-1}$

$$A \rightarrow B \rightarrow C. \tag{39}$$

The first reaction is second order with respect to A and the second reaction is first order with respect to B. The reaction-rate constants follow the Arrhenius rate expression. Component A is being fed to the reactor at a feed rate of d that is subject to disturbances. The objective is to find the optimal temperature profile to maximize the product B at the end of one hour.

The end-point optimization problem can be stated as:

$$\text{Minimize } J = -C_B(t_f) \tag{40}$$

subject to

$$\frac{d}{dt}\begin{bmatrix} C_A \\ C_B \\ V \\ T \end{bmatrix} = \begin{bmatrix} -k_1C_A^2 \\ k_1C_A^2 - k_2C_B \\ 0 \\ 0 \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix} u + \begin{bmatrix} \frac{(S_A - C_A)}{V} \\ -\frac{C_B}{V} \\ 1 \\ 0 \end{bmatrix} d, \tag{41}$$

where

$$k_1 = k_{1_0} \exp\left(\frac{-E_1}{RT}\right)$$

$$k_2 = k_{2_0} \exp\left(\frac{-E_2}{RT}\right). \tag{42}$$

Here, C_A and C_B represent the concentration of component A and B, respectively; k_1 and k_2 are reaction rate constants; T is the temperature; V is the volume of the reactor; u is the manipulated input; and d is the disturbance input.

The system model is of the form

$$\dot{x} = f(x) + g(x)u + w(x)d, \tag{43}$$

where

$$x = \begin{bmatrix} C_A \\ C_B \\ V \\ T \end{bmatrix}; \quad f(x) = \begin{bmatrix} -k_1C_A^2 \\ k_1C_A^2 - k_2C_B \\ 0 \\ 0 \end{bmatrix}; \quad g(x) = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix};$$

$$w(x) = \begin{bmatrix} \frac{(S_A - C_A)}{V} \\ \frac{-C_B}{V} \\ 1 \\ 0 \end{bmatrix},$$

For this system $n = 4$, and it can be easily verified that $s_u = s_d = 1$. Thus, the optimal state feedback in the singular region will be dynamic. Substituting $n = 4$ and $s = 1$ in Eq. 23 we get the following dynamic state feedback law:

Table 3a. Initial Conditions (Example 3)

Case A	
$C_A(0)$	$1.0\ \text{mol}\cdot\text{L}^{-1}$
$C_B(0)$	$0.01\ \text{mol}\cdot\text{L}^{-1}$
$T(0)$	300.0 K
$V(0)$	1.0 L
d	$1\ \text{L}\,\text{h}^{-1}$
Case B	
$C_A(0)$	$1.0\ \text{mol}\cdot\text{L}^{-1}$
$C_B(0)$	$0.01\ \text{mol}\cdot\text{L}^{-1}$
$T(0)$	300.0 K
$V(0)$	1.0 L
d	$\begin{cases} 1.0\ \text{Lh}^{-1} & t \le 0.2\ \text{h} \\ 0.5\ \text{Lh}^{-1} & t > 0.2\ \text{h} \end{cases}$

Table 3b. Model Parameters (Example 3)

k_{10}	$7{,}000.0\ \text{L mol}^{-1}\cdot\text{h}^{-1}$
k_{20}	$6.2\times10^5\ \text{h}^{-1}$
E_1	$5{,}000.0\ \text{cal}\cdot\text{L}^{-1}$
E_2	$10{,}000.0\ \text{cal}\cdot\text{L}^{-1}$
t_f	1 h
S_A	$10.0\ \text{mol}\cdot\text{L}^{-1}$
V_{max}	2.0 L

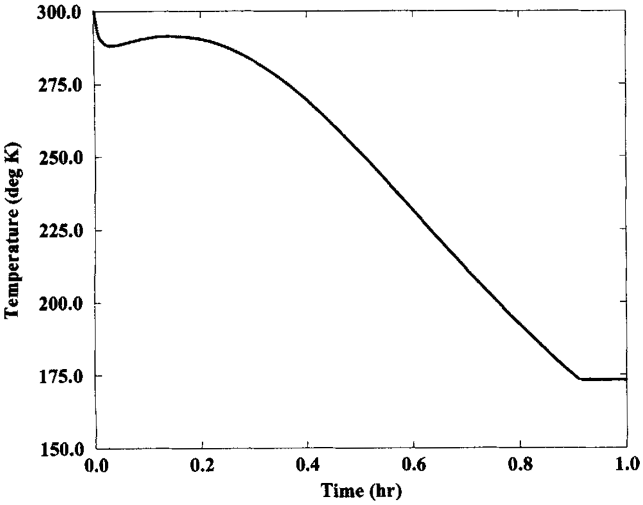

Figure 17. Optimal-input profile—constant *d* (Example 3).

$$\frac{du}{dt} - \frac{2}{T}u^2 + E_1 Z_1 u + RT^2 Z_1\left[k_2 - \frac{k_1 C_A}{C_B}(2C_B + C_A)\right]$$
$$+ Z_2[2Z_1 S_A(E_1 - E_2) - Z_1 C_A(E_1 - E_2) + 2k_1 S_A C_A$$
$$- \{2S_A(S_A - C_A + 1) - C_A\}d/V]\frac{d}{V} = 0, \quad (44)$$

where

$$Z_1 = \frac{k_1 C_A^2}{E_2 C_B}$$
$$Z_2 = \frac{RT^2}{C_A(E_1 - E_2)}. \quad (45)$$

Simulation studies were conducted using the initial conditions and process parameters given in Table 3a and 3b, respectively. Optimal input and corresponding optimal product concentration profiles for the case where d is constant are shown in Figures 17 and 18, respectively. The effect of measuring the disturbance input d, is studied. A step disturbance of magnitude 0.5 L/h is introduced in the input flow stream of component A after 12 minutes of operation. Figure 19 shows the manipulated input profiles for two situations: one where the disturbance input is measured and corrected for in Eq. 44, and the other where the disturbance input is not measured and left unchanged in Eq. 44. The corresponding

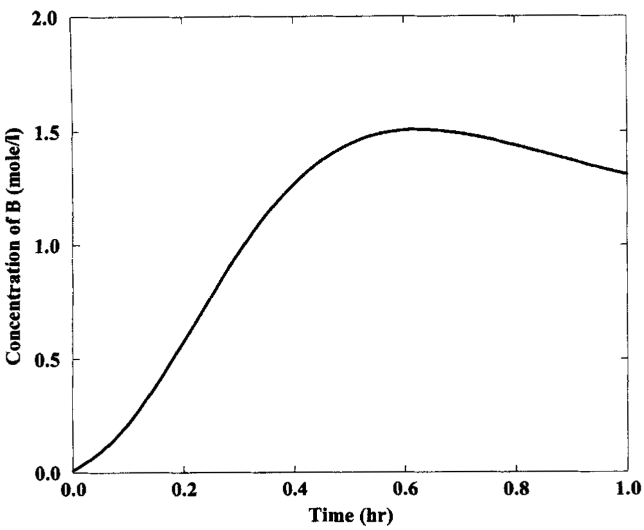

Figure 18. Product-formation profile—constant *d* (Example 3).

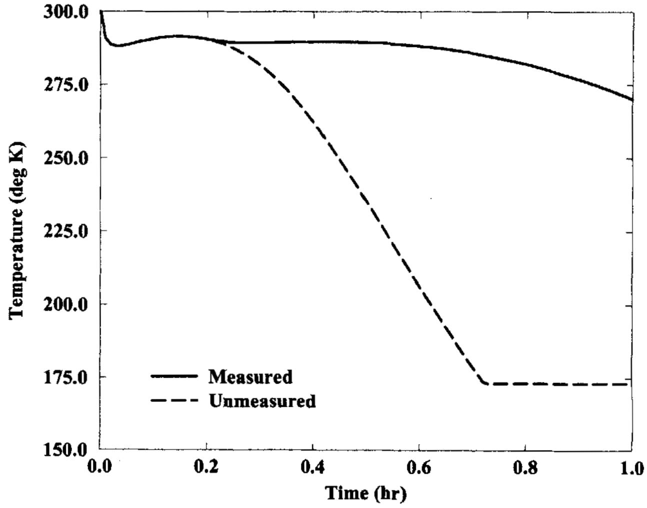

Figure 19. Optimal-input profiles—step disturbance (Example 3).

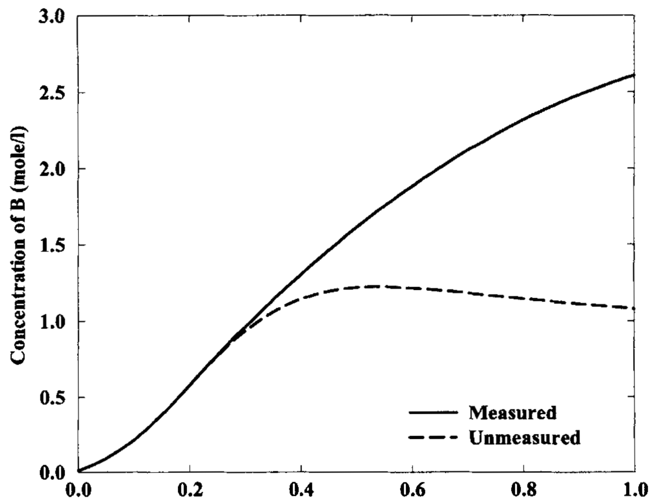

Figure 20. Product-concentration profiles—step disturbance (Example 3).

Table 3c. Effect of Measurement of Disturbance on Performance Index (Example 3)

Step disturbance Type	Performance index
Measured	−2.6 mol/L
Unmeasured	−1.1 mol/L

product concentration profiles are shown in Figure 20. It is observed from Figure 20 and Table 3c that the product concentration of component B is 150% higher in the case where the disturbance input is measured and accounted for in the optimal feedback law.

Acknowledgment

Financial support from the Florida State University as well as NSF Research Grant CTS 9409577 is gratefully acknowledged.

Notation

det = determinant
F = flow rate of reactant A, L/h
S_A = concentration of feed, mol/L

Literature Cited

Bourdache-Siguerdidjane, H., and M. Fliess, "On-line Computation of Optimal Nonlinear Feedback Controls," *IFAC Workshop on Control Application of Nonlinear Programming and Optimization*, Capri, Italy (1985).
Bryson, A. E., and Y. C. Ho, *Applied Optimal Control*, Wiley, New York (1975).
Calvet, J. P., and Y. Arkun, "Feedforward and Feedback Linearization of Nonlinear Systems and Its Implementation Using Internal Model Control (IMC)," *Ind. Eng. Chem. Res.*, **27**, 1822 (1988).
Cuthrell, J. E., and L. T. Biegler, "Simultaneous Optimization Methods for Batch Reactor Control Profiles," *Comp. Chem. Eng.*, **13**, 49 (1989).
Daoutidis, P., and C. Kravaris, "Synthesis of Feedforward/State Feedback Controllers for Nonlinear Processes," *AIChE J.*, **35**, 1602 (1989).
Eaton, J. W., and J. B. Rawlings, "Feedback Control of Nonlinear Processes Using On-Line Optimization Techniques," *Comp. Chem. Eng.*, **14**, 469 (1990).
Hirschorn, R. M., "(A-B) Invariant Distributions and Disturbance Decoupling of Nonlinear Systems," *SIAM J. Contr. Opt.*, **19**, 1 (1981).
Isidori, A., A. J. Krener, C. Gori-Giorgi, and S. Monaco, "Nonlinear Decoupling via Feedback: A Differential Geometric Approach," *IEEE Trans. Automat. Contr.*, **AC-26**, 331 (1981).
Luus, R., "Optimal Control by Direct Search on Feedback Gain Matrix," *Chem. Eng. Sci.*, **29**, 1013 (1974).
Palanki, S., C. Kravaris, and H. Y. Wang, "Optimal of State Feedback Control of Batch Reactors with a State Inequality Constraint and Free Final Time," *Chem. Eng. Sci.*, **49**(1), 85 (1994).
Palanki, S., C. Kravaris, and H. Y. Wang, "Synthesis of State Feedback Laws for End-Point Optimization in Batch Processes," *Chem. Eng. Sci.*, **48**(1), 135 (1993).
Palanki, S., S. Feteih, and D. Sadhukhan, "On-line Optimization of Batch Processes Using Neural Networks Coupled with Optimal State Feedback," *Proc. Amer. Control Conf.*, Seattle, WA, p. 1772 (1995).

Appendix: Proofs of Corollaries

Proofs of corollaries of Theorem 1

Proof of Corollary 1. When $s_u = \infty$, the first-order necessary conditions on the singular region (Eq. 6) can be written as

$$\begin{aligned} \lambda^T g &= 0 \\ \lambda^T ad_f^1 g &= 0 \\ \lambda^T ad_f^2 g &= 0 \\ &\vdots \\ \lambda^T ad_f^{n-1} g &= 0 \\ &\vdots \end{aligned} \tag{A1}$$

The first n equation can be written in compact form as

$$\lambda^T \left[g \,\vdots\, ad_f^1 g \,\vdots\, \cdots \,\vdots\, ad_f^{n-1} g \right] = 0. \tag{A2}$$

Since λ^T is a nonzero vector, it follows that

$$\det \left[g \,\vdots\, ad_f^1 g \,\vdots\, \cdots \,\vdots\, ad_f^{n-1} g \right] = 0, \tag{A3}$$

which is Eq. 18.

Proofs of corollaries of Theorem 2

Proof of Corollary 2. When $s_u = s_d = (n-2)$, the first-order necessary conditions are as follows:

$$\begin{aligned} \lambda^T g &= 0 \\ \lambda^T ad_f^1 g &= 0 \\ \lambda^T ad_f^2 g &= 0 \\ &\vdots \\ \lambda^T ad_f^{n-2} g &= 0 \\ \lambda^T ad_f^{n-1} g + \lambda^T \left[g, ad_f^{n-2} g \right] u + \lambda^T \left[w, ad_f^{n-2} g \right] d &= 0. \end{aligned} \tag{A4}$$

Eliminating n adjoint states from Eq. A4 leads to Eq. 21.

Proof of Corollary 3. When $s_d > s_u$ and $s_u = (n-2)$, the first-order necessary conditions in the singular region can be written as

$$\begin{aligned} \lambda^T g &= 0 \\ \lambda^T ad_f^1 g &= 0 \\ \lambda^T ad_f^2 g &= 0 \\ &\vdots \\ \lambda^T ad_f^{n-2} g &= 0 \\ \lambda^T ad_f^{n-1} g + \lambda^T \left[g, ad_f^{n-2} g \right] u &= 0. \end{aligned} \tag{A5}$$

Eliminate n adjoint states from Eq. A5 to obtain Eq. 22.

Proofs of corollaries of Theorem 3

Proof of Corollary 4. When $s_u = s_d$ and $s_u \le (n-3)$, the first-order necessary conditions can be given as

$$\begin{aligned} \lambda^T g &= 0 \\ \lambda^T ad_f^1 g &= 0 \\ \lambda^T ad_f^2 g &= 0 \\ &\vdots \end{aligned}$$

$$\lambda^T ad_f^{s_u} g = 0$$

$$\lambda^T ad_f^{s_u+1} g + \lambda^T [g, ad_f^{s_u} g] u + \lambda^T [w, ad_f^{s_u} g] d = 0$$

$$\lambda^T \left(I\frac{d}{dt} - \frac{\partial f}{\partial x} - \frac{\partial w}{\partial x} d - \frac{\partial g}{\partial x} u \right)^{s_u+2} g = 0$$

$$\vdots$$

$$\lambda^T \left(I\frac{d}{dt} - \frac{\partial f}{\partial x} - \frac{\partial w}{\partial x} d - \frac{\partial g}{\partial x} u \right)^{n-1} g = 0. \qquad \text{(A6)}$$

Equation 25 can be obtained from Eq. A6 by eliminating n adjoint states.

Proof of Corollary 5. When $s_d < s_u$ and $s_u \leq (n-3)$, the first-order necessary conditions are as follows:

$$\lambda^T g = 0$$

$$\lambda^T ad_f^1 g = 0$$

$$\lambda^T ad_f^2 g = 0$$

$$\vdots$$

$$\lambda^T ad_f^{s_d} g = 0$$

$$\lambda^T \overline{ad}_{f+wd}^{s_d+1} g = 0$$

$$\vdots$$

$$\lambda^T \overline{ad}_{f+wd}^{s_u+1} g + \lambda^T \left[g, \overline{ad}_{f=wd}^{s_u} g \right] u = 0$$

$$\lambda^T \left(I\frac{d}{dt} - \frac{\partial f}{\partial x} - \frac{\partial w}{\partial x} d - \frac{\partial g}{\partial x} u \right)^{s_u+1} g = 0$$

$$\vdots$$

$$\lambda^T \left(I\frac{d}{dt} - \frac{\partial f}{\partial x} - \frac{\partial w}{\partial x} d - \frac{\partial g}{\partial x} u \right)^{n-1} g = 0. \qquad \text{(A7)}$$

Equation 26 can be obtained by eliminating n adjoint states from Eq. A7.

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