Effect of Feedback Controllers in State Estimation Schemes

Guillermo E. Eliçabe*

Departamento de Ingeniería Química, Facultad de Ingeniería, Universidad Nacional de Mar del Plata and INTEMA (CONICET, Universidad Nacional de Mar del Plata), J.B. Justo 4302, 7600 Mar del Plata, Argentina

Christos Georgakis

Chemical Process Modeling and Control Research Center and Department of Chemical Engineering, Lehigh University, Iacocca Hall #111, Bethlehem, Pennsylvania 18015

It is common practice in state estimation of chemical systems to include augmented states modeled as random-constant or random-walk processes. When process controllers with integral terms are present, undesirable interaction effects may occur between the augmented states and the controllers. If no attention is paid to this interaction, the resulting estimator may diverge. In this work the interaction between controller and augmented states is analyzed. Using the linear systems theory, it is shown that the unwanted interaction and final divergence are caused by lack of detectability of the augmented system. A specific test, based on the Popov−Belevitch−Hautus rank test, to check the detectability in the system under study is derived. In many cases the test can be performed by simple inspection. A series of examples are given where the concept of detectability is applied to help in discovering and preventing the negative interaction between controllers and augmented states. Finally, a discussion is presented comparing the results of the standard observability test, applied to a real problem, with those obtained with the test derived here and with the behavior of a real estimator for the same problem. It is concluded that the standard observability test is not able to discriminate between different estimator designs and consequently to produce practical results as those obtained with the alternative test, i.e., the disclosure of unfeasible estimator designs.

1. Introduction

State estimators are used to provide on-line predictions of those variables that describe the system dynamic behavior but cannot be directly measured. If a reasonably accurate model of the process is available, then it may be possible to estimate those states which are not measured, based on the values of those states, or a combination of them, which are.

One of the most popular state estimators is the Kalman filter.[1,2] In its basic form this type of estimator is based on the assumption that the unknown driving forces of the process are white noises. However, more often than not, the driving functions in the original problem are not white noises. Some of them are deterministic measurable inputs which can be incorporated directly into the estimator equations. Others must be modeled with differential equations relating these driving functions to fictitious white noise processes.[3] These differential equations add new states to the original state vector. These extra states are called augmented states and are appended to the original ones. The form that the appended differential equations take depends on the driving functions they model. In chemical process applications, the random-constant and random-walk models are commonly used.[4−6] Markov processes may also be a choice if slow changes are expected in the new states.[5] The random walk has the advantage that it may follow sudden changes and therefore is probably the most common choice of all.

* Corresponding author: Phone: 54 223 4816600. Fax: 54 223 4810046. E-mail: elicabe@fi.mdp.edu.ar.

In chemical processes it is normal to find automatic controllers. When an estimator is designed, those controllers must be formally treated as part of the process and the equations that represent their behavior included in the design.

In this paper the interaction between controller and augmented states will be analyzed. The case in which the controller contains integral terms and the augmented states are modeled as random-constant or random-walk processes will be considered. If no attention is paid to this interaction, the resulting estimator may diverge. This motivates questions like the following:

(1) What measurements can or cannot be used to drive the estimator?

(2) Can these measurements be the same as the controlled outputs?

(3) Is there a systematic approach to select the measurements to avoid undesirable behavior?

In what follows it will be shown that the unwanted interaction and final divergence are due to observability problems. First it will be shown that the estimator divergence is a consequence of the lack of detectability of the augmented system, and consequently a specific test to check the detectability will be developed based on the Popov−Belevitch−Hautus rank test.[7] Then a series of examples will be given where the concept of detectability is applied to help prevent the negative interaction between controllers and augmented states. Finally, a discussion will be presented comparing the results of the standard observability test, applied to a

10.1021/ie990361r CCC: $19.00
Published on Web 12/21/1999

real problem, with those obtained with the test derived here and with the behavior of an estimator for the same problem.

2. Problem Motivation: Jacketed CSTR

A simplified version of the problem that actually motivated this investigation will be analyzed in this section. This example, however, retains the main features of the actual problem, that will be analyzed later in another section.

Assume that a reaction A → products is carried out in a jacketed CSTR in which the reactor temperature is controlled by manipulating the inlet cooling flow through a PI controller. This process can be modeled after some common assumptions in the usual form

$$\frac{dC_A}{dt} = \frac{F_o}{V}(C_{A_o} - C_A) + kC_A \quad (1a)$$

$$\frac{dT}{dt} = \frac{F_o}{V}(T_o - T) + \frac{\lambda}{\rho C_p V}kC_A - \frac{UA_H}{\rho C_p V}(T - T_j) \quad (1b)$$

$$\frac{dT_j}{dt} = \frac{F_j}{V_j}(T_{j_o} - T_j) + \frac{UA_H}{\rho_j C_j V_j}(T - T_j) \quad (1c)$$

$$F_j = F_{j_o} + K(T^{set} - T) + \frac{1}{\tau_I}e_I \quad (1d)$$

$$\frac{de_I}{dt} = (T - T^{set}) \quad (1e)$$

$$\frac{dT_{j_o}}{dt} = 0 \quad (1f)$$

where C_A is the reactor concentration, C_{Ao} is the inlet concentration, F_o is the inlet flow, T_o is the inlet reactor temperature, T is the reactor temperature, T_j is the jacket temperature, F_j is the inlet jacket flow, F_{jo} is a base value for the inlet jacket flow, T_{jo} is the inlet jacket temperature, T^{set} is the reactor temperature set point, V and V_j are the reactor and jacket volumes, C_p and C_j are the reactor and jacket heat capacities, U is the heat-transfer coefficient, A_H is the heat-transfer area, e_I is the integrated error, τ_I is the integral time, K is the proportional gain, ρ and ρ_j are the reactor and jacket densities, k is the reaction rate constant, and λ is the heat of reaction. Equation 1f is included to model T_{jo} as an augmented state. This equation plays an important role when the model is used to design the state estimator.

After linearizing eqs 1a−1f and defining deviation variables, denoted with an overbar, the system can be rewritten as

$$\begin{Bmatrix} \dot{\bar{C}}_A \\ \dot{\bar{T}} \\ \dot{\bar{T}}_j \\ \dot{\bar{e}}_I \\ \dot{\bar{T}}_{j_o} \end{Bmatrix} = \underbrace{\begin{Bmatrix} a_{11} & 0 & 0 & 0 & 0 \\ a_{21} & a_{22} & a_{23} & 0 & 0 \\ 0 & a_{32} & a_{33} & a_{34} & a_{35} \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{Bmatrix}}_{\mathbf{A}} \begin{Bmatrix} \bar{C}_A \\ \bar{T} \\ \bar{T}_j \\ \bar{e}_I \\ \bar{T}_{j_o} \end{Bmatrix} = \begin{Bmatrix} a_{11} & \mathbf{0}^T \\ \mathbf{a} & \mathbf{A}' \end{Bmatrix} \mathbf{x} \quad (2)$$

If the available measurement T is used to drive the estimator, the measurement equation will be

$$y \equiv \bar{T} = \underbrace{(0 \,|\, 1\ 0\ 0\ 0)}_{\mathbf{c}^T} \begin{Bmatrix} \bar{C}_A \\ \bar{T} \\ \bar{T}_j \\ \bar{e}_I \\ \bar{T}_{j_o} \end{Bmatrix} = \{0 \,|\, \mathbf{c}'^T\} \mathbf{x} \quad (3)$$

Let us consider the following state estimator applied to the process described above:

$$\dot{\hat{\mathbf{x}}} = \mathbf{A}\hat{\mathbf{x}} + \mathbf{m}(y - \mathbf{c}^T\hat{\mathbf{x}}) \quad (4)$$

where $\hat{\mathbf{x}} = [\hat{C}_A\ \hat{T}\ \hat{T}_j\ \hat{e}_I\ \hat{T}_{jo}]^T$ is a vector of estimates of $\bar{\mathbf{x}} = [\bar{C}_A\ \bar{T}\ \bar{T}_j\ \bar{e}_I\ \bar{T}_{jo}]^T$, and $\mathbf{m}$ is a vector of estimator gains. When the estimator is a Kalman filter, this vector of gains will be determined by the Riccati equation and will be, in general, time varying.[1] Other designs set the entries of $\mathbf{m}$ at fixed values. The following analysis will be based on the assumption that $\mathbf{m}$ is fixed. Only the zero-pole structure of the estimator transfer matrix will be considered. This transfer matrix can be calculated for this example after a few manipulations with the following result:

$$\hat{\mathbf{x}}'(s) = \begin{pmatrix} \hat{C}'_A(s) \\ \hat{T}'(s) \\ \hat{T}_j'(s) \\ \hat{e}_I'(s) \\ \hat{T}_{j_o}'(s) \end{pmatrix} = \begin{pmatrix} \dfrac{b_{11}s^3 + b_{12}s^2 + b_{13}s + b_{14}}{s^4 + d_1s^3 + d_2s^2 + d_3s + d_4} \\ \dfrac{b_{21}s^3 + b_{22}s^2 + b_{23}s + b_{24}}{s^4 + d_1s^3 + d_2s^2 + d_3s + d_4} \\ \dfrac{b_{31}s^3 + b_{32}s^2 + b_{33}s + b_{34}}{s^4 + d_1s^3 + d_2s^2 + d_3s + d_4} \\ \dfrac{b_{41}s^4 + b_{42}s^3 + b_{43}s^2 + b_{44}s + b_{45}}{s(s^4 + d_1s^3 + d_2s^2 + d_3s + d_4)} \\ \dfrac{b_{51}s^4 + b_{52}s^3 + b_{53}s^2 + b_{54}s + b_{55}}{s(s^4 + d_1s^3 + d_2s^2 + d_3s + d_4)} \end{pmatrix} \bar{T}'(s) \quad (5)$$

where the primes indicate Laplace transforms of the respective variables. The d_i's and b_{ij}'s are related to the

a_{ij}'s of matrix **A** and to the elements of the gain vector **m**. Equation 5 shows clearly that some of the transfer functions of the estimator have a pole at zero. As a result of this, the noise always present in the measurement $\bar{T}$, which drives the estimator, will make the variances of the states whose transfer functions have a pole at zero grow without bounds,[3] and the estimator will diverge.

To show the connection between stability and observability in this case, the standard observability test can be applied to this example. Recall that the system will be observable if and only if the observability matrix has complete rank.[2] It can be easily shown that if the following matrix does not have complete rank

$$\begin{pmatrix} \mathbf{c}'^{T} \\ \mathbf{c}'^{T}\mathbf{A}' \\ \mathbf{c}'^{T}\mathbf{A}'^{2} \\ \mathbf{c}'^{T}\mathbf{A}'^{3} \end{pmatrix} = \begin{pmatrix} 1 & a_{11} & a_{11}^2 + a_{12}a_{21} & a_{11}(a_{11}^2 + a_{12}a_{21}) + a_{12}[a_{21}(a_{11} + a_{22}) + a_{23}] \\ 0 & a_{12} & a_{12}(a_{11} + a_{22}) & a_{12}(a_{11}^2 + a_{12}a_{21}) + a_{22}(a_{11}a_{12} + a_{12}a_{22}) \\ 0 & 0 & a_{23}a_{12} & a_{23}(a_{11}a_{12} + a_{12}a_{22}) \\ 0 & 0 & a_{24}a_{12} & a_{24}(a_{11}a_{12} + a_{12}a_{22}) \end{pmatrix}^{T} \tag{6}$$

then the observability matrix **O** of the complete system (eqs 2 and 3) does not have it either. Because the third and fourth rows of the matrix in eq 6 are collinear, then the rank of this matrix is not complete and the system is unobservable. Here a connection between stability and observability can be anticipated. In this example the design is unfeasible (unstable) and the system unobservable. However, the observability test is too exigent and is not able to discern between an unfeasible (unstable) design, like that of the example presented here, and cases in which the estimator can be acceptably implemented (stable design) even when the system is not observable.

In the next section, detectability, a relaxed type of observability, will be used to study the interaction between augmented states and process controllers in systems with the same characteristics as the one presented in this section.

3. Observability and Detectability of Closed-Loop Systems

Consider a dynamic system (**A**, **C**) described by the following state space equations:

$$\frac{d\mathbf{x}}{dt} = \mathbf{A}\mathbf{x} + \mathbf{B}\mathbf{u} + \mathbf{D}\mathbf{d} \qquad \text{with } \mathbf{y} = \mathbf{C}\mathbf{x} \tag{7}$$

where $\mathbf{x} \in \mathbf{R}^n$, $\mathbf{u} \in \mathbf{R}^m$, $\mathbf{d} \in \mathbf{R}^p$, and $\mathbf{y} \in \mathbf{R}^q$ are the state, control, disturbance, and output vectors. Matrices **A**, **B**, **C**, and **D** are of appropriate dimensions. For the moment neglect the presence of the **u** and **d** inputs and consider the following state estimator:

$$\frac{d\hat{\mathbf{x}}}{dt} = \mathbf{A}\hat{\mathbf{x}} + \mathbf{M}(\mathbf{y} - \mathbf{C}\hat{\mathbf{x}}) \tag{8}$$

where $\hat{\mathbf{x}}$ is the state estimate of **x** and **M** is the estimator's gain matrix. Depending on the method by which the gain matrix is calculated, it could be a fixed matrix (as in state observers) or it could be a varying one (as in Kalman filters). In any case, the condition for the estimator to be stable is that the pair of matrices (**A**, **C**) is detectable. This is a weaker condition than the better known one of observability. By use of the Popov–Belevitch–Hautus rank test,[7] the observability condition is equivalent to

$$\text{rank}\begin{pmatrix} \mathbf{A} - \lambda\mathbf{I} \\ \mathbf{C} \end{pmatrix} = n \tag{9}$$

for all of the eigenvalues λ of matrix **A**. Then the detectability condition can be expressed in a manner similar to that above for all of the eigenvalues of **A** that do not have a negative real part. If the only eigenvalues with a nonnegative real part are the zero eigenvalues of matrix **A**, then the detectability condition above translates to the following condition:

$$\text{rank}\begin{pmatrix} \mathbf{A} \\ \mathbf{C} \end{pmatrix} = n \tag{10}$$

This condition will be used extensively in the following analysis. It is well-known that if the system (**A**, **C**) is observable, the poles of the estimator can be placed where desired by proper selection of the gain matrix **M**. If the system is not observable but is detectable, then the gain matrix **M** can relocate at least the unstable or marginally stable (i.e., with zero real part) eigenvalues of the matrix **A** and the estimator will be stable.

To facilitate the analysis that will follow, let us assume that the number of control variables is smaller than the number of measured variables, $m < q$. Furthermore, the state vector **x** can always be appropriately transformed so that it consists of two components $\mathbf{x}_1$ and $\mathbf{x}_2$ with the following properties. The first n_1 $(=m)$ states, $\mathbf{x}_1$, are the controlled ones and are directly measured. The other component, $\mathbf{x}_2$, is of dimension n_2 $(=n - m)$. Thus, the system equations are given by

$$\frac{d}{dt}\begin{pmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \end{pmatrix} = \begin{pmatrix} \mathbf{A}_{11} & \mathbf{A}_{12} \\ \mathbf{A}_{21} & \mathbf{A}_{22} \end{pmatrix}\begin{pmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \end{pmatrix} + \begin{pmatrix} \mathbf{B}_1 \\ \mathbf{B}_2 \end{pmatrix}\mathbf{u} + \begin{pmatrix} \mathbf{D}_1 \\ \mathbf{D}_2 \end{pmatrix}\mathbf{d} \tag{11}$$

and

$$\mathbf{y} = \mathbf{C}\mathbf{x} \qquad \text{with } \mathbf{C} = \begin{pmatrix} \mathbf{I}_{n_1} & \mathbf{0} \\ \mathbf{C}_1 & \mathbf{C}_2 \end{pmatrix} \tag{12}$$

here $\mathbf{I}_k$ represents the k-dimensional identity matrix.

3.1. Open-Loop Estimates of Nonstationary Disturbances. Here we briefly examine a well-known base case, in which we do not have any controllers active ($\mathbf{u} = \mathbf{0}$), but we wish to estimate the value of the nonstationary disturbances **d**. This is achieved by appending the state vector with a component $\mathbf{x}_3$ that represents these disturbances, $\mathbf{x}_3 = \mathbf{d}$. The dynamical system becomes

$$\frac{d}{dt}\begin{pmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \\ \mathbf{x}_3 \end{pmatrix} = \begin{pmatrix} \mathbf{A}_{11} & \mathbf{A}_{12} & \mathbf{D}_1 \\ \mathbf{A}_{21} & \mathbf{A}_{22} & \mathbf{D}_2 \\ \mathbf{0} & \mathbf{0} & \mathbf{0} \end{pmatrix}\begin{pmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \\ \mathbf{x}_3 \end{pmatrix} \tag{13}$$

with

$$\mathbf{y} = \begin{pmatrix} \mathbf{I}_{n1} & \mathbf{0} & \mathbf{0} \\ \mathbf{C}_1 & \mathbf{C}_2 & \mathbf{C}_3 \end{pmatrix} \begin{pmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \\ \mathbf{x}_3 \end{pmatrix} \tag{14}$$

In this case the detectability condition (10) requires that the following rank condition on a $(n_2 + q) \times (n_2 + p)$ matrix be satisfied:

$$\operatorname{rank} \begin{pmatrix} \mathbf{A}_{12} & \mathbf{D}_1 \\ \mathbf{A}_{22} & \mathbf{D}_2 \\ \mathbf{C}_2 & \mathbf{C}_3 \end{pmatrix} = n_2 + p \tag{15}$$

A necessary condition for the above to be true is the well-known condition that we should have at least as many measurements as the number of disturbances that we wish to estimate; i.e., $p \leq q$.

3.2. Closed-Loop Estimates of Nonstationary Disturbances. We will assume that a multivariable PI controller has been designed between the measured outputs $\mathbf{x}_1$ and the controlled variables, $\mathbf{u}$, in the following form

$$\mathbf{u}(t) = -\mathbf{K}_C \mathbf{x}_1(t) - \mathbf{K}_I \int_0^t \mathbf{x}_1(\tau)\, d\tau \tag{16}$$

We assume that the proportional and integral gain matrices, $\mathbf{K}_C$ and $\mathbf{K}_I$, respectively, can be and are appropriately selected so that the closed-loop system has the desired stable dynamics. Because of its integral action, this controller introduces n_1 new states that will be denoted here by $\mathbf{x}_3$ and will be equal to $\int \mathbf{x}_1(\tau)d\tau$. Then the closed-loop dynamics of the system are characterized by the following matrix:

$$\begin{pmatrix} \mathbf{A}_{11} & -\mathbf{B}_1\mathbf{K}_C & \mathbf{A}_{12} & -\mathbf{B}_1\mathbf{K}_I \\ \mathbf{A}_{21} & -\mathbf{B}_2\mathbf{K}_C & \mathbf{A}_{22} & -\mathbf{B}_2\mathbf{K}_I \\ & \mathbf{I}_{n_1} & \mathbf{0} & \mathbf{0} \end{pmatrix} \tag{17}$$

If we append the nonstationary disturbances $\mathbf{d}$ to the above states, denoted here by $\mathbf{x}_4 = \mathbf{d}$, then the overall dynamic system will be described by the following equations:

$$\frac{d}{dt}\begin{pmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \\ \mathbf{x}_3 \\ \mathbf{x}_4 \end{pmatrix} = \begin{pmatrix} \mathbf{A}_{11} & -\mathbf{B}_1\mathbf{K}_C & \mathbf{A}_{12} & -\mathbf{B}_1\mathbf{K}_I & \mathbf{D}_1 \\ \mathbf{A}_{21} & -\mathbf{B}_2\mathbf{K}_C & \mathbf{A}_{22} & -\mathbf{B}_2\mathbf{K}_I & \mathbf{D}_2 \\ & \mathbf{I}_{n_1} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \end{pmatrix} \begin{pmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \\ \mathbf{x}_3 \\ \mathbf{x}_4 \end{pmatrix} \tag{18}$$

We will initially assume that the measured outputs remain the same as before, described by eq 14, but with the addition of a measurement matrix ($\mathbf{C}_{2'}$) that takes into account the contribution of the integrated error to the output vector. Then, assuming the controller ensures closed-loop asymptotic stability, the detectability condition should address only the zero eigenvalues introduced by the appended disturbances.

$$\operatorname{rank} \begin{pmatrix} \mathbf{A}_{11} & -\mathbf{B}_1\mathbf{K}_C & \mathbf{A}_{12} & -\mathbf{B}_1\mathbf{K}_I & \mathbf{D}_1 \\ \mathbf{A}_{21} & -\mathbf{B}_2\mathbf{K}_C & \mathbf{A}_{22} & -\mathbf{B}_2\mathbf{K}_I & \mathbf{D}_2 \\ & \mathbf{I}_{n_1} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ & \mathbf{I}_{n_1} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ & \mathbf{C}_1 & \mathbf{C}_2 & \mathbf{C}_{2'} & \mathbf{C}_3 \end{pmatrix} = n + n_1 + p \tag{19}$$

This condition easily translates to the following simpler one:

$$\operatorname{rank} \begin{pmatrix} \mathbf{A}_{12} & -\mathbf{B}_1\mathbf{K}_I & \mathbf{D}_1 \\ \mathbf{A}_{22} & -\mathbf{B}_2\mathbf{K}_I & \mathbf{D}_2 \\ \mathbf{C}_2 & \mathbf{C}_{2'} & \mathbf{C}_3 \end{pmatrix} = n_1 + n_2 + p \tag{20}$$

A necessary condition needed to fulfill eq 20 is that $p \leq q - n_1$. Thus, the maximum number of appended states cannot exceed the number of measured but not controlled outputs of the process; i.e., $q - n_1$. This is a much more restricted condition compared to the one of the open-loop case expressed in eq 15. If $q = n_1$, then no disturbances can be appended in the state vector and thus estimated. This result indicates that there is a potential pitfall that state estimation schemes can encounter in their application to closed-loop systems.

This is caused by the presence of the integral action of the controller, which indirectly estimates the magnitude of step disturbances so it is able to achieve zero steady-state offset in the controlled outputs $\mathbf{x}_1$. To verify this, one can calculate the detectability condition of a closed-loop system with only proportional action ($\mathbf{K}_I = \mathbf{0}$), which does not yield a zero offset in the controller outputs. In such a case, in which $\mathbf{C}_{2'} = \mathbf{0}$, the detectability condition of eq 20 becomes that of eq 15, implying again that $p \leq q$.

The limitation brought about by the integral action of the controller might be remedied by considering the control variable $\mathbf{u}$ as part of the system output. This vector, which is the output of the controller, has dimension n_1 and is easily measured if the controller is a digital one. In such a case the output matrix is

$$\mathbf{y} = \begin{pmatrix} \mathbf{I}_{n_1} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{C}_1 & \mathbf{C}_2 & \mathbf{C}_{2'} & \mathbf{C}_3 \\ -\mathbf{K}_C & \mathbf{0} & -\mathbf{K}_I & \mathbf{0} \end{pmatrix} \begin{pmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \\ \mathbf{x}_3 \\ \mathbf{x}_4 \end{pmatrix} \tag{21}$$

leading to the detectability condition of interest

$$\operatorname{rank} \begin{pmatrix} \mathbf{A}_{11} & -\mathbf{B}_1\mathbf{K}_C & \mathbf{A}_{12} & -\mathbf{B}_1\mathbf{K}_I & \mathbf{D}_1 \\ \mathbf{A}_{21} & -\mathbf{B}_2\mathbf{K}_C & \mathbf{A}_{22} & -\mathbf{B}_2\mathbf{K}_I & \mathbf{D}_2 \\ & \mathbf{I}_{n_1} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ & \mathbf{I}_{n_1} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ & \mathbf{C}_1 & \mathbf{C}_2 & \mathbf{C}_{2'} & \mathbf{C}_3 \\ & -\mathbf{K}_C & \mathbf{0} & -\mathbf{K}_I & \mathbf{0} \end{pmatrix} = n + n_1 + p \tag{22}$$

which reduces to

$$\operatorname{rank} \begin{pmatrix} \mathbf{A}_{12} & -\mathbf{B}_1\mathbf{K}_I & \mathbf{D}_1 \\ \mathbf{A}_{22} & -\mathbf{B}_2\mathbf{K}_I & \mathbf{D}_2 \\ \mathbf{C}_2 & \mathbf{C}_{2'} & \mathbf{C}_3 \\ \mathbf{0} & -\mathbf{K}_I & \mathbf{0} \end{pmatrix} = n_1 + n_2 + p \tag{23}$$

and requires that, once more, $p \leq q$.

Consequently, we can say that when a PI controller is present in the closed-loop system, the number of nonstationary disturbances that can potentially be estimated is larger (q instead of $q - n_1$) if the controller outputs are also measured. In other words, the inclusion of the control variable **u** in the measured outputs leads to the maximum number of disturbances that can be estimated. If this is not realized, as it might have been in many industrial applications, then the estimator will run the risk of being unstable. This type of failure to achieve the desired estimates might lead the practitioner to claim that state estimation is not appropriate for the chemical industry because of the prevalent use of integral control action. As the above analysis demonstrated, this can be easily remedied by including the control variable in the set of output measurements.

4. Examples

4.1. Jacketed CSTR. The example of section 2, in which $n_1 = 1$, $n_2 = 2$, $q = 1$, and $p = 1$, will now be analyzed using eq 20. To do so, the following matrix must be examined:

$$\begin{pmatrix} a_{12} & a_{13} & 0 & 0 \\ a_{22} & 0 & 0 & 0 \\ 0 & a_{33} & a_{34} & a_{35} \\ 0 & 0 & 0 & 0 \end{pmatrix} \qquad (24)$$

It can be readily verified that this matrix has rank three, and then the system is not detectable and consequently the estimator unstable. As in section 2, it can be concluded that the system is unobservable. With this test, however, this conclusion can be arrived at without performing any computation.

In this example the number of measurements ($q = 1$) is equal to the number of variables controlled with integral controllers ($n_1 = 1$), and then from section 3, the maximum number of states that can be appended to estimate disturbances is zero. If the states are appended, the estimator will be unstable, as concluded in the previous paragraph.

If T_j would be added to the measured outputs, $q - n_1 = 1$, and then it might be possible to estimate one disturbance. However, it can be easily verified that in this case the system would still not be detectable. Instead, as demonstrated in section 3, the inclusion of the controller output in the output measurements leads, according to eq 24, to the following matrix to be analyzed:

$$\begin{pmatrix} a_{12} & a_{13} & 0 & 0 \\ a_{22} & 0 & 0 & 0 \\ 0 & a_{33} & a_{34} & a_{35} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & -k_I & 0 \end{pmatrix} \qquad (25)$$

This matrix has rank four, and then the system is detectable and consequently the estimator design feasible.

From this example it can be concluded that even if the system can be checked using the standard observability test, the conclusions of this test may not be as useful as those obtained with the detectability test. In fact, if the system is unobservable the estimator could still be implemented as far as the system is detectable, which guarantees a stable estimator. Considering that the observability test is often difficult to conduct in practice and that does not allow one to predict instability, it becomes clear that for practical purposes the detectability test, a test that is easier to conduct, gives more information about the behavior of the estimator, at least in the context analyzed here.

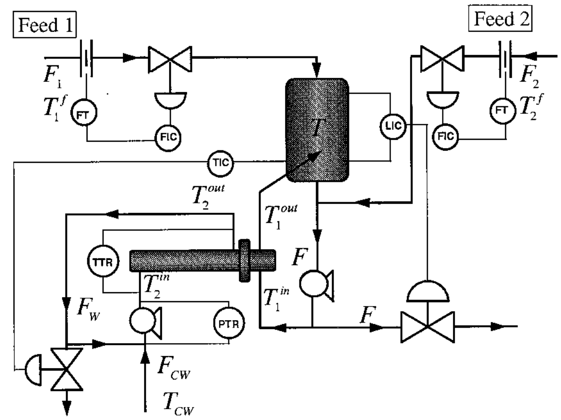

Figure 1. Schematic diagram of the reactor with instrumentation.

In what follows the detectability of two other systems, in which augmented states and process controllers interact as described by eq 18, will be studied. The results developed in the previous sections will be used to predict the estimator behavior and eventually correct unfeasible estimator designs.

4.2. Externally Refrigerated CSTR. A Simplified Model. A more complex example is the process sketched in Figure 1. It consists basically of two units. The main unit is a continuous chemical reactor fed by two currents automatically controlled. The second unit is an external concentric tube heat exchanger used to remove the heat of reaction from the reactor. This is accomplished by circulating the reaction mixture through the heat exchanger at a very high flow rate using a rotary pump and then returning the cooled mixture to the reactor. Although no agitator is used in this reactor, the high flow rate at which the reacting mixture is recirculated keeps it well mixed inside the reactor. This type of operation allows one to consider the reactor as homogeneous. (This process is a generalized version of a process operated by Union Carbide which was the focus of detailed study at the Chemical Process Modeling and Control Research Center at Lehigh University where (G.E.E.) spent a 2-year stay.)

The temperature inside the reactor is controlled through a PI controller by manipulating the flow rate of cold water entering a closed loop of circulating water driven by a second rotary pump (see Figure 1). A second controller is used to regulate the level in the reactor by manipulating the opening of a downstream valve.

With the focus on the detectability problem and if rate constants are assumed to be independent of temperature, the heat removal section of the reactor can be considered independently of the mass balance, and then the system is analyzed through the equations corresponding to the energy balances. To obtain a simple model for demonstration purposes, the temperature inside each part of the heat exchanger is considered to be homogeneous. In addition, the three flow controllers that determine the reactor holdup are considered to be fast enough such that the assumption of a constant reactor level is valid. A model contemplating these simplifications could be written as follows:

$$\rho_M C_{p_M} V \frac{dT}{dt} = \rho_1 C_{p_1} F_1 T_1^{\ f} + \rho_2 C_{p_2} F_2 T_2^{\ f} + \rho' C'_p (F' - F''') T_1^{out} - F''' T_1^{in} \rho' C'_p - r\Delta H V \quad (26a)$$

$$\frac{dT_1^{out}}{dt} = \frac{F' - F'''}{V_1}(T_1^{in} - T_1^{out}) - \frac{UA_H}{\rho' C'_p V_1}(T_1^{out} - T_2^{out}) \quad (26b)$$

$$\frac{dT_2^{out}}{dt} = \frac{F_{CW}}{V_2}(T_{CW} - T_2^{out}) + \frac{UA_H}{\rho_w C_{p_W} V_2}(T_1^{out} - T_2^{out}) \quad (26c)$$

$$\frac{de_I}{dt} = T - T^{set} \quad (26d)$$

$$T_1^{in} = \frac{F_2 \rho_2 C_{p_2} T_2^f + (F' - F_2)\rho_M C_{p_M} T}{F' \rho' C'_p} \quad (26e)$$

$$F_{CW} = F_{CW_o} + K(T^{set} - T) + \frac{1}{\tau_I} e_I \quad (26f)$$

$$F''' = \frac{F_1 \rho_1 C_{p_1}}{\rho' C'_p} + \frac{F_2 \rho_2 C_{p_2}}{\rho' C'_p} \quad (26g)$$

Three candidates for augmented states are considered, T_{CW}, F_W, and U. The corresponding equations are

$$\frac{dT_{CW}}{dt} = 0 \quad (27a)$$

$$\frac{dF_W}{dt} = 0 \quad (27b)$$

$$\frac{dU}{dt} = 0 \quad (27c)$$

Besides the controlled variable, T, another measurement, $\Delta T = T_2^{out} - T_2^{in}$, is considered. This measurement is related to the states through the following equation:

$$\Delta T = \frac{F_{CW}}{F_W}(T_2^{out} - T_{CW}) \quad (28)$$

Equation 26 involve a fairly large number of variables and parameters. The meaning of most of them is obvious from the diagram of the process. Others were defined in the previous example in more or less the same form. Finally r and ΔH are the reaction rate and heat of reaction, respectively.

In this case $n_1 = 1$, $n_2 = 2$, and $q = 2$. Because $p = q - n_1$, the maximum number of disturbances that could be estimated is one. Therefore, the possibility of estimating either T_{CW}, F_W, or U from these measurements cannot be ruled out. If T_{CW} is chosen as the augmented state, the equations can be arranged in linearized form using deviation variables following the steps given previously.

$$\begin{pmatrix} \dot{\bar{T}} \\ \dot{\bar{T}}_1^{out} \\ \dot{\bar{T}}_2^{out} \\ \dot{\bar{e}}_I \\ \dot{\bar{T}}_{CW} \end{pmatrix} = \begin{pmatrix} a_{11} & a_{12} & 0 & 0 & 0 \\ a_{21} & a_{22} & a_{23} & 0 & 0 \\ a_{31} & a_{32} & a_{33} & a_{34} & a_{35} \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \bar{T} \\ \bar{T}_1^{out} \\ \bar{T}_2^{out} \\ \bar{e}_I \\ \bar{T}_{CW} \end{pmatrix} \quad (29a)$$

$$\begin{pmatrix} \bar{T} \\ \Delta T \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ c_1 & 0 & c_3 & c_4 & c_5 \end{pmatrix} \begin{pmatrix} \bar{T} \\ \bar{T}_1^{out} \\ \bar{T}_2^{out} \\ \bar{e}_I \\ \bar{T}_{CW} \end{pmatrix} \quad (29b)$$

To test if indeed this estimator design is feasible, the rank of the following matrix is considered:

$$\begin{pmatrix} a_{12} & 0 & 0 & 0 \\ a_{22} & a_{23} & 0 & 0 \\ a_{32} & a_{33} & a_{34} & a_{35} \\ 0 & c_3 & c_4 & c_5 \end{pmatrix} \quad (30)$$

Here a_{34}, a_{35}, c_4, and c_5 are according to eqs 26–28

$$a_{34} = \left[\frac{\partial \dot{T}_2^{out}}{\partial e_I}\right]_{\mathbf{x}=\mathbf{x}_o} = \frac{T_{CW_o} - T_{2_o}^{out}}{V_2 \tau_I} \quad (31a)$$

$$a_{35} = \left[\frac{\partial \dot{T}_2^{out}}{\partial T_{CW}}\right]_{\mathbf{x}=\mathbf{x}_o} = \frac{F_{CW_o}}{V_2} \quad (31b)$$

$$c_4 = \left[\frac{\partial \Delta T}{\partial e_I}\right]_{\mathbf{x}=\mathbf{x}_o} = \frac{(T_{2_o}^{out} - T_{CW_o})}{F_W \tau_I} \quad (31c)$$

$$c_5 = \left[\frac{\partial \Delta T}{\partial T_{CW}}\right]_{\mathbf{x}=\mathbf{x}_o} = -\frac{F_{CW_o}}{F_W} \quad (31d)$$

It can be easily verified that $a_{34}c_5 = a_{35}c_4$. This implies that the matrix defined by eq 30 has rank equal to $3 < 4 = n_1 + n_2 + p$, and then the system is not detectable. Detectability could not be restored by using T_1^{out} or T_2^{out} in place of ΔT as it can be easily verified from eq 30. However, if the output from the controller, e_I, is used to drive the estimator, as suggested before, the rank of the matrix defined by eq 30 would be four and the system would be detectable.

If now the augmented state is F_W, the rank test will be performed with the following matrix:

$$\begin{pmatrix} a_{12} & 0 & 0 & 0 \\ a_{22} & a_{23} & 0 & 0 \\ a_{32} & a_{33} & a_{34} & 0 \\ 0 & c_3 & c_4 & c_5 \end{pmatrix} \quad (32)$$

It can be confirmed by simple inspection that this matrix has four linearly independent rows. Therefore, the system is detectable. If, instead of ΔT, either T_1^{out} or T_2^{out} or the output from the controller were used as the output measurement, the system would not be detectable.

Finally the augmented state U will be analyzed. The rank test must be performed in this case on the following matrix:

$$\begin{pmatrix} a_{12} & 0 & 0 & 0 \\ a_{22} & a_{23} & 0 & a_{25} \\ a_{32} & a_{33} & a_{34} & a_{35} \\ 0 & c_3 & c_4 & 0 \end{pmatrix} \quad (33)$$

After a few manipulations it can be shown that $a_{23}c_4a_{35} - a_{25}(a_{33}c_4 - a_{34}c_3) = 0$, and then the rank of the matrix is three and the system undetectable. If, instead of ΔT, T_2^{out} is used to drive the estimator, a simple inspection to the matrix of eq 33 reveals that the system is detectable. The same result is valid if the output from the controller is used in place of ΔT. This can be verified by checking that $a_{23}a_{35} - a_{33}a_{25} \neq 0$.

4.3. Externally Refrigerated CSTR. A More Realistic Model. The process presented in this example is the same as that in Figure 1. The design of an estimator for this reactor system (a section of a real plant) originally motivated this investigation.[8] The same model used in the real application will be analyzed next.

The more realistic model was obtained considering the mass balances coupled with the energy balances, on the one hand, and the existence of a temperature profile inside the tubes of the exchanger, on the other hand.

The set of main and side reactions described below is assumed to occur inside the reactor

$$\begin{gathered} \text{A} + \text{B} \rightarrow \text{C} + \text{E} \\ \text{B} + 3\text{A} \rightarrow 3\text{E} + \text{G} \\ \text{A} \rightarrow \frac{1}{2}\text{F} + \text{E} \end{gathered} \quad (34)$$

To describe the dynamics of the concentrations of components A and B (C_A and C_B) inside the reactor, the following equations are used:

$$\frac{dC_A}{dt} = \frac{F_1}{V}C_A^f - \frac{F' - F_2}{F'}\frac{F'''}{V}C_A - r_1 - 3r_2 - r_3 \quad (35a)$$

$$\frac{dC_B}{dt} = \frac{F_2}{V}C_B^f\frac{F' - F'''}{F'} - \frac{F' - F_2}{F'}\frac{F'''}{V}C_B - r_1 - r_2 \quad (35b)$$

The reaction rates of the main and side reactions depend on the concentrations of the components inside the reactor and on temperature in the following way:

$$r_1 = k_1 e^{-E_1/RT}C_AC_B \quad (36a)$$

$$r_2 = k_2 e^{-E_2/RT}C_AC_B \quad (36b)$$

$$r_3 = k_3 e^{-E_3/RT}C_A \quad (36c)$$

where k_1, k_2, k_3, E_1, E_2, and E_3 are kinetic parameters and R is the gas constant.

The energy balance for the heat exchanger is described by two equations with state variables T_1^* and T_2^*. These variables are the arithmetic averages of the inlet temperature and the outlet temperature on both sides of the heat exchanger. The heat transferred from the reacting mix in the tubes of the process side of the heat exchanger to the cold water in the tubes of the water side of the heat exchanger is represented using a rigorous expression that takes into account the temperature profile along the tubes of the exchanger. With these assumptions the equations for the average temperatures on both sides of the heat exchanger are as follows:

Process Side:

$$\frac{dT_1^*}{dt} = \frac{F' - F'''}{V_1}2(T_1^{\text{in}} - T_1^*) - \frac{UA_H}{\rho' C_p' V_1} \times 2\frac{T_1^* - T_1^{\text{in}} + T_2^* - T_2^{\text{in}}}{\ln \dfrac{2T_1^* - T_1^{\text{in}} - T_2^{\text{in}}}{-2T_2^* + T_1^{\text{in}} + T_2^{\text{in}}}} \quad (37)$$

Water Side:

$$\frac{dT_2^*}{dt} = \frac{F_W}{V_2}2(T_2^{\text{in}} - T_2^*) + \frac{UA_H}{\rho_W C_{p_W} V_2} \times 2\frac{T_1^* - T_1^{\text{in}} + T_2^* - T_2^{\text{in}}}{\ln \dfrac{2T_1^* - T_1^{\text{in}} - T_2^{\text{in}}}{-2T_2^* + T_1^{\text{in}} + T_2^{\text{in}}}} \quad (38)$$

The inlet temperature on the process side of the heat exchanger (T_1^{in}) is given, as in the previous example, by eq 26e. The inlet temperature on the water side (T_2^{in}) is given by

$$T_2^{\text{in}} = \frac{F_{CW}(T_{CW} - 2T_2^*) + 2F_WT_2^*}{2F_W - F_{CW}} \quad (39)$$

The flow of cold water entering the heat removal system is determined by the PI controller used to control the temperature inside the reactor as in the previous example. The equations describing the dynamics of the controller are thus the same as before (eqs 26d,f). As before F''' is modeled by eq 26g. The heat balance inside the reactor is, in a manner similar to that of the previous example, given by

$$\rho_M C_{p_M} V\frac{dT}{dt} = \rho_1 C_{p_1} F_1 T_1^f + \rho_2 C_{p_2} F_2 T_2^f + \rho' C_p'(F' - F''')2(T_1^* - T_1^{\text{in}}) - F'T_1^{\text{in}}\rho' C_p' - r_1\Delta H_1 V - r_2\Delta H_2 V - r_3\Delta H_3 V \quad (40)$$

where T_1^f is the temperature of the feed stream no. 1 and ΔH_i ($i = 1-3$) are the heats of reaction of the main and side reactions. The remaining variables are according to the previous example and to Figure 1.

The available output measurements are T and $\Delta T = T_2^{\text{out}} - T_2^{\text{in}}$. The first measurement coincides directly with one of the states, namely, T, and ΔT is related to the states through the following equation:

$$\Delta T = \frac{2F_{CW}}{2F_W - F_{CW}}(T_2^* - T_{CW}) \quad (41)$$

Again T_{CW}, F_W, and U are chosen as potential augmented states. As in the example before no more than one of them can be potentially included in the estimator scheme with the measurements that are available ($p = q - n_1 = 1$). These augmented states will be analyzed one at a time to check the detectability as done before. The linearized model equations arranged in matrix form using deviation variables are

$$
\begin{pmatrix} \dot{\bar{T}} \\ \dot{\bar{C}}_{\mathrm{A}} \\ \dot{\bar{C}}_{\mathrm{B}} \\ \dot{\bar{T}}_1^* \\ \dot{\bar{T}}_2^* \\ \dot{\bar{e}}_{\mathrm{I}} \\ \dot{\bar{T}}_{\mathrm{CW}} \\ \dot{\bar{F}}_{\mathrm{W}} \\ \dot{\bar{U}} \end{pmatrix} = \begin{pmatrix} a_{11} & a_{12} & a_{13} & a_{14} & 0 & 0 & 0 & 0 & 0 \\ a_{21} & a_{22} & a_{23} & 0 & 0 & 0 & 0 & 0 & 0 \\ a_{31} & a_{32} & a_{33} & 0 & 0 & 0 & 0 & 0 & 0 \\ a_{41} & 0 & 0 & a_{44} & a_{45} & a_{46} & a_{47} & a_{48} & a_{49} \\ a_{51} & 0 & 0 & a_{54} & a_{55} & a_{56} & a_{57} & a_{58} & a_{59} \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \bar{T} \\ \bar{C}_{\mathrm{A}} \\ \bar{C}_{\mathrm{B}} \\ \bar{T}_1^* \\ \bar{T}_2^* \\ \bar{e}_{\mathrm{I}} \\ \bar{T}_{\mathrm{CW}} \\ \bar{F}_{\mathrm{W}} \\ \bar{U} \end{pmatrix} \tag{42}
$$

$$
\begin{pmatrix} \bar{T} \\ \Delta T \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ c_1 & 0 & 0 & 0 & c_5 & c_6 & c_7 & c_8 & 0 \end{pmatrix} \begin{pmatrix} \bar{T} \\ \bar{C}_{\mathrm{A}} \\ \bar{C}_{\mathrm{B}} \\ \bar{T}_1^* \\ \bar{T}_2^* \\ \bar{e}_{\mathrm{I}} \\ \bar{T}_{\mathrm{CW}} \\ \bar{F}_{\mathrm{W}} \\ \bar{U} \end{pmatrix} \tag{43}
$$

To perform the detectability test, the following matrix must be examined with either the sixth, seventh, or eighth column, with the sixth column to check the feasibility of estimating T_{CW}, with the seventh to check that of F_{W}, and with the eighth to check that of U.

$$
\begin{pmatrix} a_{12} & a_{13} & a_{14} & 0 & 0 & 0 & 0 & 0 \\ a_{22} & a_{23} & 0 & 0 & 0 & 0 & 0 & 0 \\ a_{32} & a_{33} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & a_{44} & a_{45} & a_{46} & a_{47} & a_{48} & a_{49} \\ 0 & 0 & a_{54} & a_{55} & a_{56} & a_{57} & a_{58} & a_{59} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & c_5 & c_6 & c_7 & c_8 & 0 \end{pmatrix} \tag{44}
$$

If T_{CW} is to be estimated, the system will not be detectable if the corresponding matrix (eq 45 without columns 7 and 8) has rank less than $n_1 + n_2 + p = 6$. After the row of zeroes is eliminated, the rank of the resulting 6×6 matrix has to be analyzed. After some manipulations, it can be verified that $c_5(a_{46}a_{57} - a_{56}a_{47}) - c_6(a_{45}a_{57} - a_{55}a_{47}) + c_7(a_{45}a_{56} - a_{55}a_{46}) = 0$. This condition makes the analyzed 6×6 matrix have rank ≤ 5, and the system is not detectable. It is clear from eq 44 that the detectability could not be achieved by using T_1^* or T_2^* as measured outputs. With T_2^* the reason is obvious, and with T_2^* the condition $a_{46}a_{57} - a_{56}a_{47} = 0$ prevents detectability. However, if the output from the controller was used to feed the estimator, the condition $a_{45}a_{57} \neq a_{55}a_{47}$ guarantees a detectable system.

The same analysis can be performed when F_{W} is the augmented state instead. The matrix to be analyzed is now that of eq 44 without columns 6 and 8. This matrix will have full rank if

$$
\begin{vmatrix} a_{45} & a_{46} & a_{48} \\ a_{55} & a_{56} & a_{58} \\ c_5 & c_6 & c_8 \end{vmatrix} \neq 0
$$

This can be verified analytically as well as numerically. In this case after a few calculations it can be shown that the determinant is different from zero and that the system is detectable. Detectability could also be obtained with T_2^* and/or the output from the controller as output measurements.

Finally the analysis is performed with U as the augmented state. Columns 6 and 7 are not considered now. The identity $c_5(a_{46}a_{59} - a_{56}a_{49}) - c_6(a_{45}a_{59} - a_{55}a_{49}) = 0$, which can be easily verified, makes the matrix given in eq 44 without columns 6 and 7 have rank ≤ 5. Again the system is in this case not detectable. If instead of ΔT, T_2^* and/or the output from the controller are used to feed the estimator, the fact that $a_{46}a_{59} - a_{56}a_{49} \neq 0$ and $a_{45}a_{59} - a_{55}a_{49} \neq 0$ makes in this case the system detectable.

In all cases the condition $a_{22}a_{33} \neq a_{32}a_{23}$ needed to have a detectable system is also verified.

Table 1. Singular Values (SV) and Rank of the Observability Matrix Corresponding to Two Different Choices of Augmented States in the Example: Externally Refrigerated CSTR. A More Realistic Model

SV	F_{W} and T_{CW}	T_{CW}	F_{W}
1	3.39×10^{19}	3.39×10^{19}	3.39×10^{19}
2	8.55×10^{12}	8.55×10^{12}	8.55×10^{12}
3	4.31×10^{7}	4.31×10^{7}	4.31×10^{7}
4	4.35×10^{5}	4.35×10^{5}	4.35×10^{5}
5	8.89×10^{2}	8.89×10^{2}	8.89×10^{2}
6	2.29×10^{1}	2.29×10^{1}	2.29×10^{1}
7	2.29×10^{1}	1.64×10^{-3}	7.29×10^{-6}
8	3.47×10^{-6}		
rank	4	4	4

5. Numerical Results

The results of the previous sections were numerically verified by implementing a state estimator in a system modeled as in the third example presented above. Although the actual estimator was a hybrid extended Kalman filter,[2] the results anticipated by the theoretical analysis performed with the assumptions of linearity and fixed gain were completely confirmed; i.e., (i) the estimator diverges when both F_{W} and T_{CW} are included as augmented states even if the output from the controller is also used to drive the estimator; (ii) the estimator diverges when T_{CW} is included as the augmented state alone, except when the output from the controller is used to drive the estimator; (iii) the estimator behaves well when F_{W} is the single augmented state, even if the output from the controller is not used; and (iv) the estimator behaves as in (ii) if U is the augmented state. In all cases the initially proposed output measurements T and ΔT are considered.

A second numerical verification was performed to confirm what it was claimed before with regard to how undependable the standard observability test can be. The test was performed on the same example as before for the cases in which F_{W} and T_{CW} are used as augmented states. The rank of the corresponding observability matrix (eq 6) was determined numerically using the MATLAB software. The results are listed in Table 1. In MATLAB the rank is calculated as the number of singular values (SV) ν_i ($i = 1, ..., n$) of $\mathbf{O}$ that are greater than $\{\mathrm{Max}(\nu_i)[\sum_{i=1}^{n}(\nu_i)^2]^{1/2}\mathrm{eps}\}$, with the machine-dependent parameter eps $= 2.2204 \times 10^{-16}$ in this case. According to this test (see Table 1), the system is unobservable without discrimination between the different choices of augmented states. In addition, it can be noticed that the ratio of the largest to the smallest singular values is higher with F_{W} as the augmented state than with T_{CW}. These numbers may suggest the following: *Although in all cases the system is unobserv-*

able, there could be more chances of having a "more" observable system when T_{CW} is the augmented state. This possible conclusion may lead to the presumption that T_{CW} is more appropriate as the augmented state than F_W. This completely contradicts the results found using the detectability test and the practical experience. It also shows how inaccurate the standard observability test may be when several variables of different magnitudes are involved and the test is performed numerically.

6. Conclusions

It is common practice in state estimation of chemical systems to include augmented states modeled as random-constant or random-walk processes. When in these systems process controllers with integral terms are present, undesirable interaction effects may occur between the augmented states and the process controllers. This undesirable interaction, when present, results in estimator divergence.

In this work it is shown that the undesirable behavior is caused by a lack of detectability caused by the implicit disturbance estimation role of the integral action. A specific detectability test is derived as a convenient tool of analysis for the type of system under study. To resolve this issue, it is suggested that the control variables $\mathbf{u}$ are considered as a system output and treated likewise in the closed-loop estimator. This is different from the way these variables are treated in open-loop systems, namely, as measured inputs.

To demonstrate how the concept of detectability is applied to help in discovering and preventing the negative interaction between controllers and augmented states, three examples are presented and analyzed. In all of them, different choices of augmented states and output measurements are discussed. In all cases the test clearly reveals if the choice of the augmented state and measurement is adequate or not. In case one choice is not satisfactory, different options can be easily examined.

The third example, the real application that motivated this investigation, was used to test numerically the predictions of the theoretical analysis. In all cases the performance of the estimator in practice corroborated the results anticipated by the detectability test. In this example the standard observability test was also performed, and its results were contrasted against those of the detectability test. The observability test was unable to distinguish the difference between the various estimator designs.

Literature Cited

(1) Maybeck, P. S. *Stochastic Models, Estimation and Control*; Academic Press: New York, 1982; Vol. 2.

(2) Stengel, R. F. *Stochastic Optimal Control. Theory and Application*; John Wiley & Sons: New York, 1986.

(3) Brown, R. *Introduction to Random Signal Analysis and Kalman Filtering*; John Wiley & Sons: New York, 1984,

(4) Dalle Molle, D. T.; Himmelblau, D. M. Fault Detection in a Single Stage Evaporator via Parameter Estimation Using the Kalman Filter. *Ind. Eng. Chem. Res.* **1987**, *26*, 2482.

(5) Schuler, H.; Schmidt, C. Calorimetric-State Estimation for Chemical Reactor Diagnosis and Control: Review of Methods and Applications. *Chem. Eng. Sci.* **1992**, *47*, 899.

(6) Agarwal, M.; Bonvin, D. Limitations of the Extended Kalman Filter for Batch Reactors. IFAC Symposium DYCORD, Maastricht, NL, 1989.

(7) Kailath, T. *Linear Systems*; Prentice Hall, Inc.: Englewood Cliffs, NJ, 1980.

(8) Eliçabe, G.; Georgakis, C. *State Estimation in a Continuous Reactor: The Union Carbide Problem*; Research Progress Report No. 16; Chemical Process Modeling and Control Research Center: Lehigh University, PA, 1993.

Received for review May 25, 1999
Revised manuscript received September 29, 1999
Accepted October 12, 1999

IE990361R