Two-Step Procedure for Data-Based Modeling for Inferential Control Applications

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A two-step procedure for building an inferential control model, which uses both historical operation data and plant test data, is proposed. Motivation for using the two types of data is given, and a systematic way to combine them in the model-identification step is proposed. Some potential problems associated with the procedure in practice and their solutions are discussed. The efficacy of the procedure is demonstrated in a case study involving a multicomponent distillation column simulated in HYSYS.

Introduction

For many chemical processes, control is greatly limited by process delays and measurement difficulties. For example, measurement of a stream composition often requires an on-line gas chromatograph, which introduces a large delay to the system and suffers from a high failure ratio. Most product property variables are similar in that they can only be analyzed in laboratories, requiring substantial processing time and limiting the frequency of analysis. Moreover, there are cases wherein key variables are measured in the downstream but can be affected only in the upstream. Some control of the variables of these types can be achieved by keeping the measurable process conditions (such as temperatures, pressures, flow rates) stable and implementing feedforward controllers, but the variability can still be quite substantial given the often-significant feed variations and other unmeasured disturbances. For these cases, *inferential control*, a control strategy based on the inferring of the composition or property variable(s) (referred to as the ‘‘primary variable(s)’’) based on the measurement of other variables (called ‘‘secondary variables’’), can be an attractive, viable alternative. A pictorial representation of the candidate process for inferential control is given in Figure 1.

The idea of inferential control has existed for a long time, but its industrial application is still at a nascent stage. Broadly speaking, there are two approaches to inferential control; the direct approach in which one builds a converter between the secondary measurements and the primary variables (usually through data regression of sorts) and couples it with a conventional feedback controller, and the indirect (or model-based) approach in which one builds a stochastic system model for the overall process and disturbances and designs a state estimator and a state-feedback controller based on it. These two approaches are depicted in Figure 2. Thus far, the direct approach has seen some application in the industry, but the indirect approach has received little attention from the practitioners. This can be attributed to the fact that building a model for the inferential controller design requires substantially more information and effort than that for the conventional control. Most importantly, such a model must quantify how the measured outputs are related to the unmeasured outputs. In the context of fundamental modeling, this means that the source(s) of disturbance must be identified and their temporal behavior characterized as a stochastic process. In the empirical modeling's context, this requirement calls for a *multiple-input, multiple-output (MIMO) stochastic system identification*, something that is inherently difficult and requires a high-level of expertise.

Despite the practical barriers, there is a significant incentive to further develop and tailor the indirect approach so that it can be practiced. The recent acceptance by the industry of model-predictive control (MPC) as the standard advanced control method is one reason. The indirect approach fits naturally into the scheme of MPC, as a multistep predictor of the primary variable that uses all the available measurements in an optimal manner can be easily developed given a stochastic system model. At a more general level, it provides a framework to predict and control the system behavior optimally, without the need to categorize the variables explicitly into the categories of primary and secondary variables. Multirate measurements and variable time delays that are common in practice can be handled straightforwardly and rigorously within this setting.

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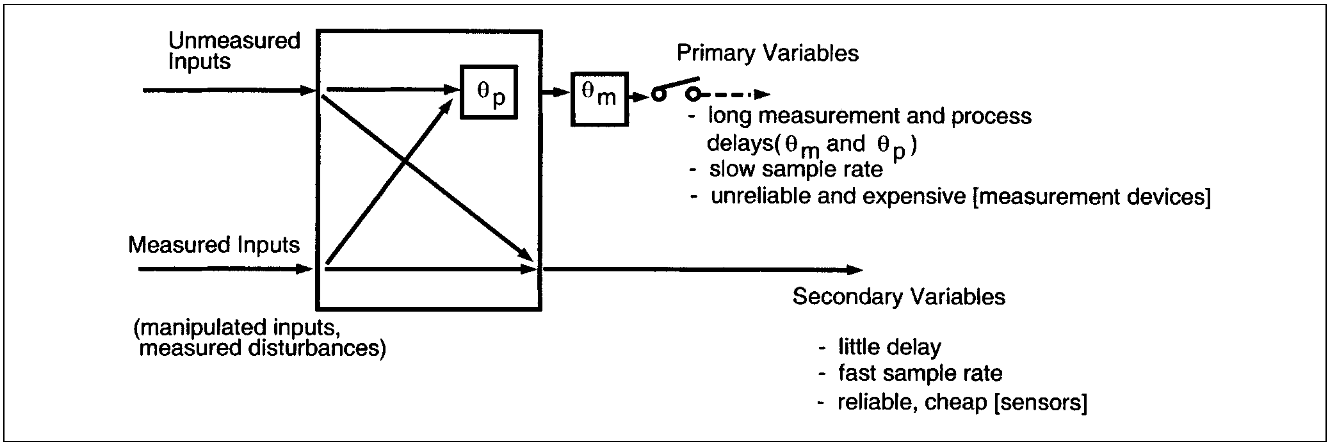

Figure 1. Candidate process for inferential control.

Since we pointed to the modeling difficulty as the main bottleneck in taking the indirect approach, it is natural to seek a systematic framework for a building a requisite model using plant data alone. The importance of such a framework in order for a widespread use of the approach is supported by the fact that almost all model-predictive controllers implemented today are designed based on data from plant tests. However, both data-collection and system identification methodologies for building an inferential control model need to be substantially different from those currently used. Since the effect of *unmeasured* disturbances and system noises on the future behavior of primary variables must be predicted from secondary measurements, we need to capture accurately into the model the *autocorrelation* and *cross-correlation* information. This is unlike in the conventional feedback-control case, where the quick and frequent feedback of errors for all output channels lessens the demand on the accuracy of model prediction.

Development of a data-based modeling framework for inferential control is the main topic of this article. The ensuing

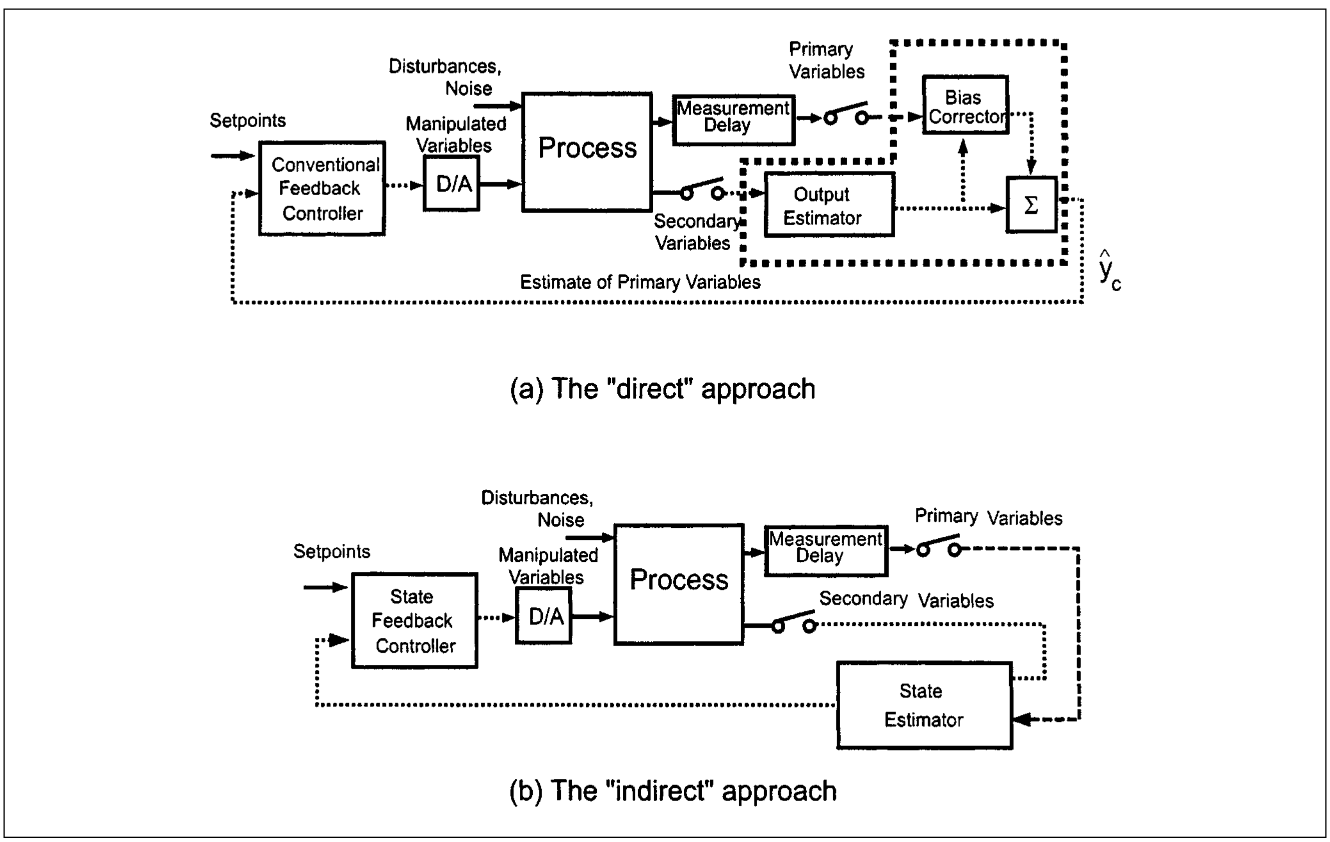

Figure 2. Two approaches to inferential control system design.

development stems from the issue of data requirement for system identification. In order to capture the requisite correlation information in the model, we need a large data set that is rich in effects of *unmeasured* disturbances and noises. Data from plant tests, the basis for model-building in current MPC applications, do not meet this criterion, as data records from plant tests are usually quite short and external conditions (such as disturbance variables) are made artificially ''quiet'' during the test period in an effort to ensure good signal-to-noise ratio. Hence, they seldom contain a sufficient amount of disturbance effects needed to build a good correlation model. For this, historical operation data are better suited, as they come in a more abundant quantity and usually contain disturbance effects that are more representative of real operation. On the other hand, one cannot build the entire control model with historical operation data alone. Since the manipulated inputs are likely to show very different correlation behavior once the inferential control loop is closed, we need a good *causal* model between the manipulated inputs and the outputs. Historical operation data rarely contain a sufficient amount of uncorrelated input changes necessary to build a good causal model. This information must be generated through a plant test.

These considerations motivated us to consider a two-step approach, in which a stochastic system model is built first using historical operation data, after which the model is used as a prefilter in deterministic model identification conducted with plant test data. We point out a number of issues that arise within the two-step approach and propose some practical solutions. Finally, we apply the two-step approach to a multicomponent distillation column in order to demonstrate the feasibility of the approach and to bring to the surface some additional issues that are specific to this type of process.

The rest of the article is organized as follows. In the following section, two different inferential control approaches are introduced, with a higher emphasis given to the model-based approach. We also highlight some relevant developments in system identification and model-predictive control. In the third section, we present the two-step identification procedure. We first discuss a method for identifying a stochastic system model using historical operation data and the issues therein; we then present a method to obtain the overall system model for the inferential controller design, utilizing the developed stochastic system model and the data from the plant test. Again, some potential issues are identified and addressed. We briefly discuss how the identified model can be transformed into a prediction model that can utilize measurements of variable delays and multiple or nonuniform sampling rates. We also show how the state-space model can be implemented as a predictor in the conventional step-response-model-based MPC framework. In the fourth section, we present the result of the case study. We conclude the article in the fifth section with some final comments and suggestions.

Preliminaries

Inferential control

Inferential control techniques can be broadly classified into direct and indirect approaches. In the following we present the main ideas and compare the two. For a more detailed discussion and references, see Amirthalingam and Lee (1997, 1999).

Direct Approach. In the direct approach, an estimator for the primary variable is constructed and coupled with a regular feedback controller, as shown in Figure 2a. Typically, a static linear estimator is employed, which is either designed using the revelant steady-state gain matrices or identified directly through data regression. Least-squares (LS) or partial least-squares (PLS) regression techniques have been most commonly used for this purpose. Recently, the use of artificial neural networks (ANNs) for the estimator development has become popular in industrial applications in which the nonlinearity is a major issue. To account for the dynamics, time-series-based regression has also been suggested.

The main attraction for the direct approach is the conceptual simplicity. On the other hand, this approach does not render itself naturally to the implementation of advanced control methods like MPC. To implement a predictive controller using the direct approach, one has to build a separate prediction model that uses the output of the estimator as the main feedback variable. A potential problem with this is that, when the loop is closed and the inputs are manipulated, the estimator (designed in prior to the loop closure) may no longer provide good estimates. This is because the closing of the loop can significantly change the correlation behavior of the input and output signals (such as their power spectra).

Indirect (Model-Based) Approach. The root of this approach can be traced all the way to the general problem of designing an output feedback controller for a stochastic system. Theories for optimal prediction and control of linear stochastic systems are well established, mostly through the pioneering work of Kalman (Kalman, 1960; Kalman and Bucy, 1961). For articles that specifically address the topic of model-based inferential-control-system design, see the recent review by Doyle (1998). In the context of model-predictive control, several researchers (Lee and Morari, 1992; Lee et al., 1992; Ricker, 1991; Muske and Rawlings, 1993) suggested combining the Kalman filter with MPC formulated in state space. Similar approaches have been reported in various applications' context (Banerjee et al., 1997; Cambell and Rawlings, 1998; Yu et al., 1994). There also have been numerous articles reporting the success of the model-based approach in batch processes (Quintero-Marmol and Luyben, 1992; Lee and Datta, 1994; Russell et al., 1998; Tatiraju and Souroush, 1997; Tatiraju et al., 1999). These works employed the extended Kalman filters and other nonlinear observers to cope with the strong nonlinear behavior of most batch processes.

Despite the academicians' enthusiasm, the indirect approach has so far received little attention from the practitioners. The reason for this is that few articles shed light on the requisite traits of the model for inferential control and even fewer hint at any realistic way to obtain such a model when the necessary fundamental knowledge is lacking. An exception is the recent work by Amirthalingam and Lee (Amirthalingam and Lee, 1997, 1999), who discuss the data-based construction of an inferential model for a pulp digester.

Model-predictive control for inferential control problems

A convenient system representation for inferential controller design within the MPC framework is given by

$$x(k+1) = Ax(k) + Bu(k) + w(k)$$
$$\underbrace{\begin{bmatrix} y_c(k) \\ y_s(k) \end{bmatrix}}_{y(k)} = \underbrace{\begin{bmatrix} C_c \\ C_s \end{bmatrix}}_{C} x(k) + \underbrace{\begin{bmatrix} \upsilon_c(k) \\ \upsilon_s(k) \end{bmatrix}}_{\nu(k)}, \tag{1}$$

where u represents the manipulated input vector; y_c and y_s the primary and secondary output vectors, and $w(k)$, $\upsilon_c(k)$, and $\upsilon_s(k)$ are white noise sequences. Measured disturbances can be included in y_s without loss of generality.The preceding model can be thought of as a superposition of two models, the deterministic model

$$x^d(k+1) = Ax^d(k) + Bu(k)$$
$$y^d(k) = Cx^d(k), \tag{2}$$

expressing how the manipulated inputs affect the outputs, and the stochastic model

$$x^s(k+1) = Ax^s(k) + w(k)$$
$$y^s(k) = Cx^s(k) + \upsilon(k), \tag{3}$$

which summarizes the statistics of the residual (that is, the total effect of all the unknown inputs and model error). Here w and υ do not correspond to any physical input; rather, they are just mathematical instruments used to express the autocorrelation and cross-correlation of the residual. The superscripts d and s stand for ''deterministic'' and ''stochastic'' portions of the variables.

With such a model, an optimal state estimator (the Kalman filter) and the optimal prediction equation for y can be easily developed. Treatment of multiple sample rates, measurements delays, etc., is straightforward within the Kalman filtering. The future control input trajectory can be optimized at each sample time based on the prediction equation, which is easily derived from the Kalman filter equation, and the typical quadratic criterion used in MPC. Of course, any relevant constraints on the inputs and outputs can be entered into the optimization. The details of the approach can be found in several articles (Lee et al., 1992; Muske and Rawlings, 1993).

The point we stress here is that the state-space model of Eq. 1 represents a general and convenient vehicle for implementing an inferential control strategy within the already proven framework of model-predictive control. The main challenge in practice then lies in obtaining a model of such form, especially when the requisite knowledge for building a fundamental process model is lacking.

Relevant identification methods

There are several ways to obtain a model of the form in Eq. 1 using input/output data, but two methods are most relevant in the present context. The first is the prediction error method, where the model is first put in a predictor form and parameters are estimated by minimizing the prediction error for the available data (Ljung, 1987). This method requires some canonical parameterization of state-space matrices, which require significant prior knowledge, especially in the multiple output case. It also results in a nonconvex optimization. An alternative is the method of subspace identification, which consists of (1) the construction of data for two consecutive Kalman state vectors through an oblique projection involving appropriate input/output matrices, and (2) the fitting of model matrices through linear least squares (Larimore, 1990; Van Overschee and De Moor, 1994; Verhaegen, 1991; Ljung and McKelvey, 1996). This method only involves noniterative linear algebra operations and does not require any prior knowledge. The subspace identification is a major development in that it enables an easy, automatic construction of a multivariable stochastic system model needed for the inferential control system design. The prediction error method and the subspace identification method can be used in a complementary sense, for example, by using the result of subspace identification to obtain an appropriate parameterization and starting values for the prediction error minimization, which further improves the model fit.

Two-Step Identification Procedure

Why the two-step procedure?

Though the basic identification methods are already in place, practicing them to obtain an inferential control model is still not very straightforward. Most importantly, the issue of data requirement deserves our attention. Traditionally, data used for system identification are collected through a plant test, designed to generate information about all the relevant parts of system dynamics with an adequate signal-to-noise ratio. This practice is justifiable when the sole aim of the identification is to obtain a good causal model between the manipulated inputs and the measured outputs. However, modeling for inferential control has another dimension in that we must also capture the correlations of the residuals (due to unmeasured disturbances, system noise, etc.). For this, plant test data are seldom adequate, as they are typically short in length and rarely contain sufficient disturbance information, which is necessary to extract the correlation information that is representative of normal operation.

In many cases, such information is better drawn from historical operation data, which are available in more abundant quantity and contain bountiful disturbance effects. The premise here is that useful correlation information for predicting the behavior of future operations are contained in the data collected from previous operations. This is reasonable in view of the fact that autocorrelations and cross-correlations seen in the outputs are mostly due to the process dynamics and interactions. Barring any significant change in the process dynamics (due to large changes in the operating condition, etc.), a correlation model obtained through statistical averaging of previous operation data should be relevant for future operations.

This reasoning serves as the motivation for the two-step approach, wherein we identify the stochastic part of the system model (given by Eq. 3) using historical data and the deterministic part (given by Eq. 2) using plant test data. It still remains to decide the best way to combine the two types of identification. One can envision two different paths with respect to this. In the first path, one identifies the deterministic part of the model first using the plant test data. Then, using the model, one subtracts the effect of the deterministic inputs from the historical operation data and fits a stochastic model to the residual. In the second path, one would first identify the stochastic part of the model using the normal operation data and then follow this by identification of the deterministic part using the test data. In this article, we pursue the second path.

Identification of stochastic system model using historical operation data

As previously mentioned, the first of the two-step procedure is to capture the autocorrelation and cross-correlation information contained in the historical operation data into a stochastic system model of Eq. 3. The method of subspace identification is convenient for this, as it enables us to capture this information without a difficult numerical optimization. It is also user-friendly in that it requires little input from the user. For example, the N4SID method, one of the most popular subspace identification algorithms (Van Overschee and De Moor, 1994), requires the user to give only an upper bound of the system order and it automatically yields the system model of the form

$$\begin{aligned} x(k+1) &= Ax(k) + Bu(k) + K\epsilon(k) \\ y(k) &= Cx(k) + \epsilon(k). \end{aligned} \tag{4}$$

From the preceding, we retain only

$$\begin{aligned} x^s(k+1) &= Ax^s(k) + K\epsilon(k) \\ y^s(k) &= Cx^s(k) + \epsilon(k), \end{aligned} \tag{5}$$

since the deterministic part of the model is hardly adequate given the usual lack of systematic input excitation in historical operation data. The subspace identification method requires a relatively large amount of data, a major drawback for regular system identification, but not so for our purpose, since historical operation data are usually available in bountiful quantity and at no cost.

Even though the methodology is well established in the literature, we found that applying it to chemical processes gives rise to some additional issues not covered in the literature, and thus requires some tailoring and care. These issues include:

- The N4SID method requires that the stochastic part of the system be stationary. On the other hand, most chemical processes show nonstationary characteristics, most notably the process variables drifting or experiencing jumps.
- Most inferential control problems involve multirate measurements, with the primary variables sampled at a substantially slower rate than the secondary variables. Measurements can also be made with substantial delays, which may vary with time.
- Most historical data contain input adjustments, made by operators or existing supervisory loops in response to some upsets or major disturbances. This means input data would be correlated with the residuals. The standard N4SID method gives a biased result in such a case.

In addition to these, there is the issue of data selection; not all historical data are appropriate for the stated purpose. Then, how do we select appropriate data from a huge database? We discuss these issues next.

Choosing Slices of Data from Historical Data Base. In general, historical data refer to huge piles of data stored in the computer for days, months, and years. Most importantly, slices of data corresponding to periods of *normal* operation should be selected. Recall that we are trying to draw from these data a correlation structure that can be used to predict the behavior of future operations. Any abnormal situations that are either one-time events or rare events should not be reflected in the statistical model. In addition, periods corresponding to unusually large upsets should be avoided, since they tend to make correlations nonlinear. These large or abnormal upsets may also be beyond the realm of automatic control, as they often require special actions by the operator. The following list can be used as a guideline in choosing the historical data.

- Select a period in which the system's production rate did not deviate significantly from the nominal value.
- Select a period in which the reliability of the critical measurements were high (such as after a shutdown maintenance).
- Select a period that includes no serious plant upset.
- Select a period where the disturbances were likely to be representative of most other times.
- Select a period where input manipulations were not unusually high.

Nonstationary Disturbances. Chemical processes commonly experience disturbances that make the process variables drift (or jump). This violates the basic requirement of the N4SID method that the stochastic part of the system be stationary (Van Overschee and De Moor, 1994). When the data used do not meet this requirement, these algorithms can behave badly, even creating artificial, unstable modes.

Assuming that the changes are not large, this nonstationary behavior is well approximated by including integrator(s) to the usual time-invariant stochastic system model (Morari and Stephanopoulos, 1980). Within this context, the presence of integrators is what makes the system nonstationary. A simple way to resolve this conflict is to ‘‘difference’’ the input/output data (to express the data in terms of their incremental change from the previous samples) which effectively removes the integrator from the system. In other words, differencing of the data before applying the subspace identification algorithm makes the assumption of stationarity more realistic and hence makes the algorithm better behaved. In fact, this feature of data-differencing can be found in the impulse-response identification modules of some commercial MPC packages (Cutler and Yocum, 1991) and is referred to as ‘‘detrending.’’ Along with the differencing, some low-pass filtering may be necessary, as the differencing tends to overaccentuate the portions of the data pertaining to the system's high-frequency dynamics.

The obtained model will be in the form of

$$\begin{aligned} x(k+1) &= Ax(k) + B\Delta u(k) + K\epsilon(k) \\ \Delta y(k) &= Cx(k) + \epsilon(k). \end{aligned} \tag{6}$$

Note that the inputs and outputs of the system model are incremental changes in the process inputs and outputs at each sample time instead of the usual deviation values. We will discuss later how we can use this model to form a predictor for MPC.

Let us support the preceding assertion by presenting a simple example. An output data set consisting of 1000 samples was generated from the following stochastic state-space system:

$$x(k+1) = 0.8\,x(k) + 0.4\eta(k)$$
$$y(k) = 0.2\,x(k) + \eta(k), \tag{7}$$

where $\eta(k)$ was obtained by integrating a white-noise sequence of variance 0.01. The application of the N4SID algorithm with y data resulted in the following stochastic system model:

$$x(k+1) = \begin{bmatrix} 1.0000 & -0.0136 \\ 0.0070 & 1.1836 \end{bmatrix} x(k) + \begin{bmatrix} 0.3918 \\ -7.0867 \end{bmatrix} \epsilon(k)$$
$$y(k) = [1.5144 \;\; -0.0037]\, x(k) + \epsilon(k). \tag{8}$$

Note the presence of unstable poles (1.005 and 1.1836), which resulted from the integrating nature of the external input η. We also applied the algorithm with Δy data, that is, after differencing the data. The resulting model was

$$x(k+1) = 0.7720\,x(k) + 0.4640\epsilon(k)$$
$$\Delta y(k) = 0.2\,x(k) + \epsilon(k), \tag{9}$$

where $\epsilon(k)$ is a white-noise sequence. We can see the clear improvement in the model fit.

Measurement Delays and Multiple Sample Rates. It is best that *known* delays be taken out before the identification algorithm is applied. Delays increase the system order, which makes system identification more difficult. This is especially true if the length of the delay is significant in relation to the sample time. The delay taken out can always be added back after the model is identified.

To eliminate delays due to the sampling and analysis, data can be marked with the time of sampling (rather than the time when the analysis is completed). This eliminates measurement delays from the data regardless of whether the delays are constant or time-varying. Any known process delay can also be taken out by shifting the output (input) data by that amount. If the length of the delay is not exactly known or time-varying, the data can still be shifted by a lower bound.

In addition, data for the primary variables can be available at much slower rates than those for the secondary variables. The model, on the other hand, should be developed at the faster of the two, in order to realize the benefits of the secondary measurements. One may be able to increase the sampling rate just for the purpose of system identification in some cases, but this may not always be possible. If the sampling rate for the primary variable cannot be increased, interpolation can be used to fill in the missing points. From our experience, simple linear interpolation works adequately given that the measurements are not very noisy. An alternative is to use ''lifting'' which is a technique to transform a multirate sampled-data system into a single-rate system (Friedland, 1960; Kranc, 1957; Lie et al., 1999).

Handling Closed-Loop Historical Data. Historical data often include changes in the manipulated inputs that are made by the operator in response to some observed output behavior. If such manipulations are recorded and the records are available in the historical data, it should be possible to remove their effect from the data. Because these moves are based on output behavior, however, they are correlated with the output data. With such correlated data, the conventional subspace identification method gives a biased result.

If input adjustments are minor and infrequent, they can be ignored without any substantial problem. If input adjustments are significant, there are extensions of the subspace identification method that can handle closed-loop data. For example, Ljung and McKelvey (1996) propose a method that uses multistep predictions of the output (based on a high-order ARX model) instead of actual output data in defining the state.

In order to further demonstrate this point, let us consider the simple system

$$x(k+1) = 0.8\,x(k) + 0.7u(k) + 0.4\epsilon(k)$$
$$y(k) = 0.2\,x(k) + \epsilon(k), \tag{10}$$

where $\epsilon(k)$ is a white-noise sequence of variance 0.01. We assumed that normal operation data (consisting of 1000 samples) are collected under the following intermittent closed-loop control strategy:

$$u(k) = -0.5 \times y(k) \quad \text{for} \quad k = 10, 20, 30, \text{etc.}$$
$$u(k) = u(k-1) \quad \text{otherwise.} \tag{11}$$

Application of the regular N4SID algorithm yielded the following stochastic system model:

$$x(k+1) = 0.7751\,x(k) - 1.2033u(k) - 0.925\epsilon(k)$$
$$y(k) = 0.2\,x(k) + \epsilon(k). \tag{12}$$

Clearly the identified model is extremely biased, having a gain of wrong sign. With the algorithm modified to handle closed-loop data, we obtained

$$x(k+1) = 0.6635\,x(k) + 0.7198u(k) + 0.3333\epsilon(k)$$
$$y(k) = 0.2\,x(k) + \epsilon(k), \tag{13}$$

which is a clear improvement.

Closed-loop identification is still at an evolving stage and many issues have not been resolved to a satisfactory level at this point. Several recent articles (Ljung and Forssell, 1999; Forssell and Ljung, 1999) address the issue of closed identification and its importance. Undoubtedly, better closed-loop identification algorithms for stochastic systems will come along in the future, and these algorithms can be readily used in the overall model-building strategy.

Identification of the deterministic part using plant test data

The next step after identifying the correlation structure is to generate a data set that is rich in input excitation by conducting a plant test. The usual rules for plant testing apply here as well. However, there is an issue that arises because we difference our data before model fitting. We will also discuss what role, if any, the stochastic part of the system model (which is already fixed) should play in obtaining the deterministic part.

Test Signal Design. Since we have obtained the stochastic model in terms of the differenced variable (Δy), it is convenient also to identify the deterministic model in terms of the differenced variables (Δy and Δu). This should also be done in view of the fact that process means do drift even during a plant test, which often lasts for several days. While the use of random (white-noise) signals or pseudorandom binary-sequence (PRBS) signals is recommended in the literature, these signals, once differenced, contain zero power at the zero frequency. The implication is poor accuracy for the low-frequency part of the model.

To combat this problem, we can generate $\Delta u(k)$ as a PRBS sequence. Integrating the sequence then gives the desired result. The generated sequence must be scaled to fit within the allowed magnitude bounds for the test signal. Different realizations of PRBSs give different maximum deviations from the mean, once integrated. Here, one should choose the realization that yields the lowest maximum deviation in order to maximize the power of Δu.

Another common problem encountered in identifying strongly interactive systems such as a high-purity distillation column is the problem of ill-conditioning. Directional input design, which requires information on the directionality of the system, has been suggested as a remedy (Andersen et al., 1989; Jacobsen and Skogestad, 1994; Li and Lee, 1995; Cooley and Lee, 2000).

Identification of the Deterministic Part Using Output Error Identification. After applying the N4SID method to historical operation data, we are left with the stochastic system model in the form of

$$x^s(k+1) = Ax^s(k) + K\epsilon(k)$$
$$\Delta y^s(k) = Cx^s(k) + \epsilon(k). \tag{14}$$

The overall system model we are seeking can be reexpressed in an input/output operator form as

$$\Delta y(k) = G(q)\Delta u(k) + H(q)\epsilon(k), \tag{15}$$

where $G(q)$ is the transfer matrix between $u(k)$ and $y(k)$. The noise model $H(q)$ is already set by the stochastic system model of Eq. 14 according to

$$H(q) = C(qI - A)^{-1}K + I. \tag{16}$$

Premultiplying the Eq. 15 with $H^{-1}(q)$ gives

$$\underbrace{H^{-1}(q)\Delta y(k)}_{\Delta y_f(k)} = \underbrace{H^{-1}(q)G(q)}_{G_f(q)}\Delta u(k) + \epsilon(k). \tag{17}$$

This is an output error (OE) structure. In prediction error minimization, $G_f(q)$ can be estimated by minimizing the output error $\Delta y_f(k) - G_f(q)\Delta u(k)$. The data from a plant test are to be used for this purpose.

The preceding requires the inverse of $H(q)$ to be stable. Recall that the stochastic system model is obtained through the N4SID method, which in effect identifies the model in the form of a Kalman filter (the innovation form). It can be shown that $H(q)$ generated from a Kalman filter (or any stable observer) of a stochastic system according to Eq. 16 is always stably invertible. If $H(q)$ happens to contain unstable zeros due to some identification error, one can always design the Kalman filter based on the model to readjust $H(q)$, which gives the desired result.

The OE identification can be conducted with the regular polynomial transfer function structure or the finite impulse response (FIR) structure. The use of a MIMO structure is not required since correlation information necessary for the inferential control design has already been captured. Once $G_f(q)$ is identified, $G(q)$ can be extracted out, using the relationship

$$G(q) = H(q)G_f(q). \tag{18}$$

We can then perform a minimal realization on the overall model of Eq. 15 to obtain a state-space model of the form

$$x(k+1) = Ax(k) + B\Delta u(k) + K\epsilon(k)$$
$$\Delta y(k) = Cx(k) + \epsilon(k). \tag{19}$$

Why Output Error Identification? One might ask why we advocate OE identification here. After all, it seems more convenient to apply the subspace identification just one more time. One could also consider fitting an ARMAX structure afterward to further improve the result. A key dilemma here is what to do with the stochastic part of the system model. It is tempting to simply "throw away" the stochastic part and retain only the deterministic part. However, there are some potential risks associated with this. To demonstrate the risk, we have applied N4SID, ARMAX, and OE identification methods to the following system:

$$y(k) = \frac{0.5q^{-1}}{(1-0.98q^{-1})^2}u(k) + \frac{1-0.4q^{-1}+0.04q^{-2}}{(1-0.98q^{-1})^2}\epsilon(k), \tag{20}$$

where $\epsilon(k)$ is a white-noise sequence of variance 0.1 and the test signal is a uniformly distributed random signal between ± 0.5. The results we obtained with a data set consisting of 500 samples were as follows:

ARMAX

$$y(k) = \frac{0.3535}{1-1.0024q^{-1}}u(k) + \frac{1+0.8104q^{-1}+0.59q^{-2}}{1-1.0024q^{-1}}\epsilon(k). \tag{21}$$

N4SID

$$y(k)=\frac{0.7071}{1-1.0033q^{-1}}u(k)+\frac{1-1.2294q^{-1}}{1-1.0033q^{-1}}\epsilon(k). \quad (22)$$

OE

$$y(k)=\frac{3.877}{1-0.9842q^{-1}}u(k)+\epsilon(k). \quad (23)$$

Notice that both the ARMAX identification and the N4SID method created an unstable pole in the deterministic model. This is not a problem of any practical relevance if the stochastic system model is used together with the deterministic model in the predictive controller design. In that case, the unstable pole gets stabilized by the same pole in the noise model in forming the optimal predictor. However, if the stochastic part of the system model is abandoned and replaced with something else (such as the one obtained in the previous step), the optimal predictive controller becomes internally unstable. The same problem cannot occur in the OE identification. Although this is a simplistic example designed for the sole purpose of demonstrating the point, we experienced similar problems in identifying higher-order systems, including the one we discuss later in the case study.

In summary, fixing the noise model ahead of identification means that we are *a priori* fixing the observer (or the state estimator) that will be used in the real application. It is then sensible to minimize the prediction error under that very observer. And this objective leads to OE identification.

Turning the model into a multistep predictor for MPC

Implementation in State Space. The two-step approach yields a combined model of the form given in Eq. 19. Since our goal is to predict the behavior of y (rather than Δy), it is convenient to use the following augmented form of Eq. 19:

$$\begin{bmatrix} x(k+1) \\ y(k+1) \end{bmatrix}=\begin{bmatrix} A & 0 \\ CA & I \end{bmatrix}\begin{bmatrix} x(k) \\ y(k) \end{bmatrix}+\begin{bmatrix} B \\ CB \end{bmatrix}\Delta u(k)+\begin{bmatrix} 0 \\ I \end{bmatrix}\epsilon(k+1)+\begin{bmatrix} k \\ Ck \end{bmatrix}\epsilon(k)$$

$$y_m(k)=[0 \;\; H(k)]\begin{bmatrix} x(k) \\ y(k) \end{bmatrix}, \quad (24)$$

where $y_m(k)$ represents the subset of y measured at the k_{th} sample time and $H(k)$ is the matrix that extracts $y_m(k)$ from $y(k)$. For convenience, let us denote the preceding as

$$z(k+1)=\Phi z(k)+\Gamma\Delta u(k)+w(k)$$
$$y_m(k)=\Xi(k)z(k). \quad (25)$$

Measurement delays not included in Eq. 19 can be incorporated into the preceding model using the standard procedure, that is, by augmenting the state with delayed outputs (see Åström and Wittenmark, 1997, pp. 38–41). In some cases, analysis delay can vary from one sample to the next. In this case, the number of delayed outputs augmented should correspond to the maximum delay. This way, one always has the delayed measurement appearing as a part of the state. One simply has to choose $\Xi(k)$ at each time to pick out the appropriate output. Even with the augmentation, the form of the equation will still remain the same as Eq. 25.

The preceding is in the standard state-space form and is ready for the design of the Kalman filter. Also, one can develop a multistep prediction equation for $y(k)$ based on the Kalman filter equation that serves as the basis for MPC calculation. For details, the readers are referred to Lee et al. (1992), Amirthalingam and Lee (1997, 1999).

Implementation as a Step-Response-Based Predictor. Most commercial MPC packages are based on the step-response representation of system dynamics. Hence, it is of interest to find a simple way to implement the model that results after the identification into these packages. For this, we show that Eq. 19 can be converted directly into a step-response predictor in the form of

$$Y(k+1)=MY(k)+S^u\Delta u(k)+\mathcal{K}\epsilon(k) \quad (26)$$

$$y(k)=NY(k)+\epsilon(k), \quad (27)$$

where $Y(k)$ is the state vector of the step-response model with the meaning of

$$Y(k)\triangleq\left[y^T(k),\ldots,\ldots,y^T(k+n-1)\right]^T \text{ for } \Delta u(k+i)=0 \text{ and } \epsilon(k+i)=0, \quad i\geq 0, \quad (28)$$

M represents the usual shift operator for the step-response model (Lee et al., 1994), N is the matrix extracting $y(k)$ from $Y(k)$, and

$$S^u=\begin{bmatrix} CB^u \\ \Sigma_{i=0}^{1}CA^iB^u \\ \vdots \\ \vdots \\ \Sigma_{i=0}^{n-1}CA^iB^u \end{bmatrix}, \quad \mathcal{K}=\begin{bmatrix} CK+I \\ \left(\Sigma_{i=0}^{1}CA^iK\right)+I \\ \vdots \\ \vdots \\ \left(\Sigma_{i=0}^{n-1}CA^iK\right)+I \end{bmatrix}, \quad (29)$$

where n should be chosen large enough so that $CA^nB^u\approx 0$ and $CA^nK\approx 0$. Note that this model can be implemented directly as a state estimator, since $\epsilon(k)=y(k)-NY(k)$.

The prediction equation can also be developed easily based on the preceding model and takes the form of

$$\mathcal{Y}(k+1\,|\,k)=M_pY(k)+\mathcal{S}^{\epsilon}[y(k)-NY(k)]+\mathcal{S}^{\mathcal{U}}\Delta\mathcal{U}(k). \quad (30)$$

Basically, this equation adds to $Y(k+1)$ the effect of future input moves [$\Delta u(k+1)$, $\Delta u(k+2)$, etc.]. The future values of ϵ are assumed to be zero since it is a zero-mean variable. The symbol M_p is used instead of M for the shift operator, since the prediction horizon p may be different from n.

Table 1. The Nominal Operating Condition of the Depropanizer

Feed Compositions		Distillate Compositions	
Ethane	0.0300	Ethane	0.0517
Propene	0.4000	Propene	0.6863
Propane	0.1500	Propane	0.2562
i-Butane	0.1500	*i*-Butane	0.0050
*cis*2-Butene	0.2700	*cis*2-Butene	0.0007
Bottoms Compositions		**Flow Rates**	
Ethane	0.0000	Feed	3,000 kmol/h
Propene	0.0048	Distillate	1,740 kmol/h
Propane	0.0033	Bottoms	1,260 kmol/h
i-Butane	0.3501	Reflux	6,105 kmol/h
*cis*2-Butene	0.6417	Boilup	7,622 kmol/h
		(Reboiler duty—8.516×10^7 kJ/h)	
Temperatures		**Others**	
Feed	90°C	Column pressure	2,600 kPa
Distillate	59.27°C	Feed enthalpy	-1.259×10^8 kJ/h
Bottoms	125.1°C		

Case Study

Description of the case study

In this section, we present the result of applying the two-step approach to a multicomponent distillation column, a depropanizer, studied by Yiu et al. (1990). The column has 29 trays and is designed to fractionate a feed stream consisting of 3% ethane, 40% propene, 15% propane, 15% *i*-butane, and 27% *cis*-2-butene (on molar basis) into a distillate stream containing the lighter components, ethane, propene, and propane, and a bottom stream containing the heavier components, *i*-butane and *cis*-2-butene. We simulated this column using HYSYS, a dynamic simulation software. The input and output stream compositions and column conditions are summarized in Table 1.

Given the goal of reducing the heavier components in the distillate stream and lighter components in the bottom stream, we defined our controlled variables to be the concentration of the light-key component (propane) in the bottom and the concentration of the heavy-key component (*i*-butane) in the distillate. We assumed that three types of unmeasured disturbances can occur at the feed, namely, feed-composition variations, feed-enthalpy variations, and feed flow-rate variations. The inferential control was aimed at reducing the variability in the controlled variables in the presence of these disturbances. The manipulated variables were the reflux flow rate and the reboiler duty. The secondary measurements for inferential control were the temperature measurements at the first, fifth, tenth, fifteenth, twentieth, twenty-fifth, and twenty-ninth trays.

HYSYS and MATLAB were interfaced using the digital data exchange (DDE) capability of the two software programs. Hence, all the mathematical calculations except for the simulation of the column were carried out in MATLAB. At every sample time, the values of the output variables of the depropanizer column were transferred to MATLAB from HYSYS and the calculated input moves and the stored disturbance sequences were transferred back to HYSYS. The basic sample interval was chosen as 3 min. This means all the temperature measurements were read in and new control moves were implemented every 3 min. The end composition measurements were assumed to be available every 30 min, with a 30-min delay.

There are several reasons why the multicomponent distillation column makes for a good case study. First, unlike binary columns, a direct one-to-one relationship between tray temperatures and tray compositions is missing. In the presence of feed disturbances, the well-known industrial practice of regulating selected tray temperatures, no matter how well placed the thermocouples are, may not deliver a satisfactory result. This point is illustrated in Figure 3, which shows the time profiles of the endpoint compositions of the lean key components when the seventh and twenty-fourth trays are controlled. When a step disturbance occurs in the feed composition, despite the fact that the temperatures are successfully returned to their respective setpoints, the endpoint compositions show significant offsets. There are some case-specific solutions in the literature, such as those involving differentials and double differentials of certain tray temperatures (Yu and Luyben, 1984), but these are merely point solutions that do not generalize.

Data generation

Historical Operation Data. In generating the historical operation data, we assumed the maximum feed flow-rate disturbance to be ±150 kmol/h. To simulate the feed-composition variations, we added an external stream of propylene with a maximum flow rate of 10 kmol/h to the feed stream. This external stream was added to the feed stream before the feed flow-rate control valve. Feed-enthalpy variations introduced were $\pm1\times10^5$ kJ/h, which changed the vapor fractions of the feed stream from 0 to 0.0046 (the nominal value of 0.0016). These values for the disturbances were chosen after studying the effect of the individual disturbances on the controlled variables. The bounds were chosen such that all disturbances contribute about the same to the output variations. All three disturbances were simulated as integrated white-noise sequences.

In order to simulate the operation more realistically, a proportional controller $[u(k)=-60{,}000\,y(k)]$ was assumed to have been in place (prior to the inferential controller implementation), which controls the composition of *i*-butane in the distillate by manipulating the reflux flow rate every 30 min. Input/output data were collected for a duration of 3,000 min, with a sample time of 3 min. The data matrix used in the closed-loop subspace identification algorithm was a 1000×11 matrix containing 7 temperature measurements, 2 composition measurements, and 2 inputs (the reflux flow rate and the reboiler duty).

Plant Test Data Generation. In generating the plant test data, we faced an issue that is specific to ill-conditioned systems like the high-purity distillation column. The process gain for such a system depends strongly on the input direction. In the distillation column, the direction of $[1\ -1]$ (that is, increasing one of the manipulated variables and decreasing the other) induces a large response in the compositions, while the direction of $[1\ 1]$ (that is, a simultaneous increase or decrease of both manipulated variables) induces a much smaller response. If both inputs are perturbed independently with an equal amount of energy, the output response will be predom-

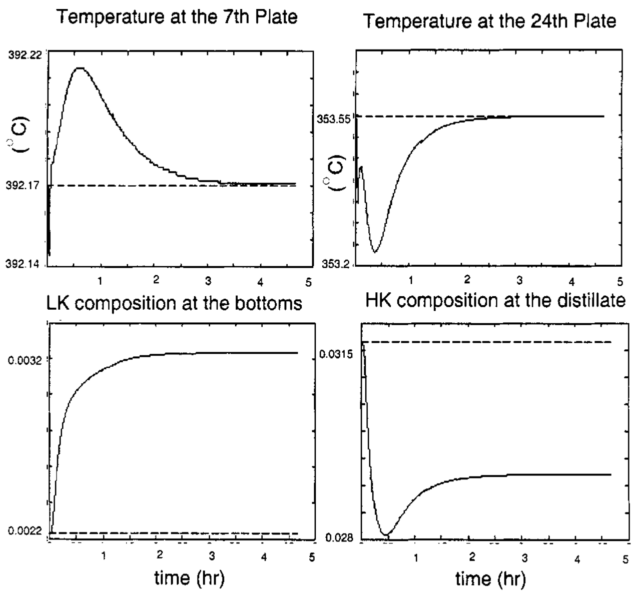

Figure 3. Behavior of compositions under the control of tray temperatures for a step change in feed composition of −0.05 in propylene and +0.05 in cisobutene.

Steady-state feed composition: ethane (0.03), propylene (0.40), propane (0.15), isobutane (0.15), cisobutene (0.27).

inantly along the high gain direction, causing a poor fit of the dynamics along the low gain direction.

For the depropanizer column, the condition number was about 25. Although this is not a severely ill-conditioned system, by experience, we realized that the process's gain directionality must be taken into account in the test signal design in order to identify a good causal model needed for two-point composition control. Since we knew that the large gain direction is [1 −1] and the small gain direction [1 1], we first generated an integrated white-noise sequence in the [1 −1] direction, with the constraints on the reflux rate and the reboiler duty set as ± 45 kmol/h and $\pm 1\times 10^5$ kJ/h. After generating another integrated white-noise input sequence in the [1 1] direction, with the constraints relaxed to ± 225 kmol/h and $\pm 2.5\times 10^6$ kJ/h, we superimposed the two and used that as the test input. The disturbances introduced during the plant test were similar to those introduced during the historical data generation. The plant test was conducted for 600 min, and a data set consisting of 200 data points was obtained.

Stochastic model identification

The historical operation data matrix included 1000 samples of the 7 temperatures, the 2 compositions, the reflux flow rate, and the reboiler duty. After differencing the data to create a data matrix containing $\Delta y(k)$ and $\Delta u(k)$, we scaled the data by dividing the elements of each differenced input and output vector by its standard deviation. The scaling is critical since the choice of state space and model fitting in the N4SID algorithm is based on the total prediction error for the given data. Because these data had been generated in the presence of the proportional control loop, we programmed the modified N4SID algorithm suggested by Ljung and McKelvey (1996) in MATLAB and used it to obtain a stochastic system model. In the identification, the maximum order we gave was 20, and the model order of 10 was chosen after the singular values of the predicted output block-Hankel matrix were inspected (Van Overschee and De Moor, 1994). A model in the form of Eq. 6 was then obtained, and the B matrix was discarded, since the level of input excitation in these data was judged too low. The model was then scaled back to the original units using the input/output scaling factors.

Determinstic model identification

In the deterministic model identification, our strategy involved filtering the differenced output data with the stochastic model, followed by an OE identification for each output. In the present case study, we needed to identify nine MISO models using the plant test data. First, the input and output data were differenced. Then, the inverse of the noise model was computed and the differenced output data were filtered by it. The filtered output vectors and input vectors were scaled similarly as before. We then identified $G_f(q)$ using the scaled data for $\Delta u(k)$ and $\Delta y_f(k)$. For this, we used the following MISO OE structure for each output:

$$
\begin{aligned}
[\Delta y_f]_i(k) &= \frac{b_{1_{i,1}}q^{-1} + b_{2_{i,1}}q^{-2} + b_{3_{i,1}}q^{-3} + b_{4_{i,1}}q^{-4}}{1 + a_{1_i}q^{-1} + a_{2_i}q^{-2}}\Delta u_1(k) \\
&+ \frac{b_{1_{i,2}}q^{-1} + b_{2_{i,2}}q^{-2} + b_{3_{i,2}}q^{-3} + b_{4_{i,2}}q^{-4}}{1 + a_{1_i}q^{-1} + a_{2_i}q^{-2}}\Delta u_2(k) \\
&+ e_i(k), \quad i = 1,\dots,9. \qquad (31)
\end{aligned}
$$

This structure was chosen by comparing the mean square of the output error for several different structures. After scaling back $G_f(q)$ to correspond to the original variables, we determined the deterministic transfer matrix $G(q)$ by premultiplying $G_f(q)$ with $H(q)$ (as in Eq. 15). The transfer matrix $G(q)$ was then realized as a state-space system and put together with the stochastic system to form the overall system model.

Estimation results

Using the identified model for the development of a multirate Kalman filter was already discussed in the third section. After augmenting the state with the outputs and 10 additional delayed outputs (to account for the 30-min delays in the primary measurements), we designed a multirate Kalman filter and tested its estimation performance through simulation. Since the primary measurements were assumed to be available every 30 min and the temperature measurements every 3 min, a periodic Kalman filter with the period of 10 sample steps was used. We compared the estimation performance of the multirate Kalman filter against that of the single-rate Kalman filter which was only the temperature measurements and that which uses only the delayed composition measurements. For the latter, we identified a separate state-space model (of sample time of 30 min), which had the composition variables as the only outputs. The estimation was performed only once every 30 min in this case.

First, the performances of the three estimators were simulated when deterministic step disturbances occurred in the feed enthalpy, feed composition, and feed flow rates. Estimation results were also generated by varying all the three disturbances in a stochastic fashion (that is, as independent integrated white-noise sequences). The results are shown in Figures 4–7 and Tables 2–5.

The simulation results show that reasonable predictions of the composition variables can be made using the temperature measurements alone, but the predictions can be improved further by using the delayed infrequent composition measurements in addition to the temperature measurements. Using the delayed composition measurements alone, on the other hand, gives a poor estimation performance.

Closed-loop control results

The next step was to design a model-predictive controller and simulate its closed-loop performance. At each sample time, the controller used the result from the Kalman filter to build a prediction of future outputs and calculated a sequence of optimal input moves based on the quadratic criterion (Lee et al., 1992; Lee et al., 1994; Muske and Rawlings, 1993) of

$$\min_{\Delta u(k),\ldots,\Delta u(k+m-1)} \sum_{i=1}^{p} y^T(k+i\mid k)\Lambda_y y(k+i\mid k) + \sum_{j=0}^{m-1} \Delta u^T(k+j)\Lambda_u \Delta u(k+j), \quad (32)$$

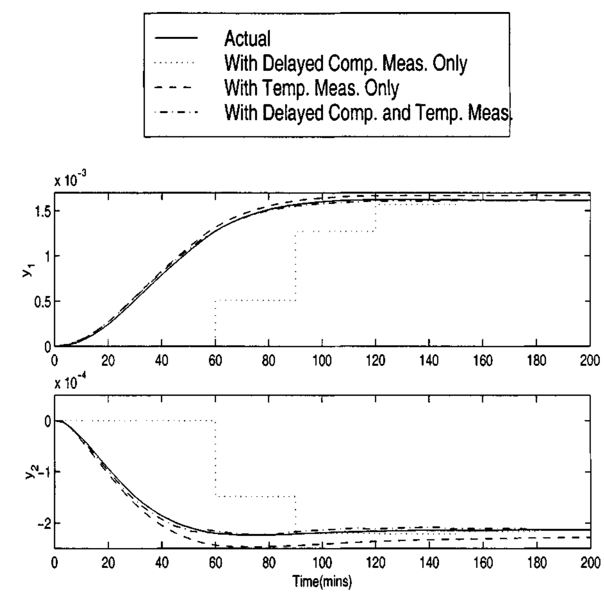

Figure 4. Evaluation of the estimators' performances for a step change (1×10^5kJ/h) in the feed enthalpy with a change in vapor fraction from 0.016 to 0.019.

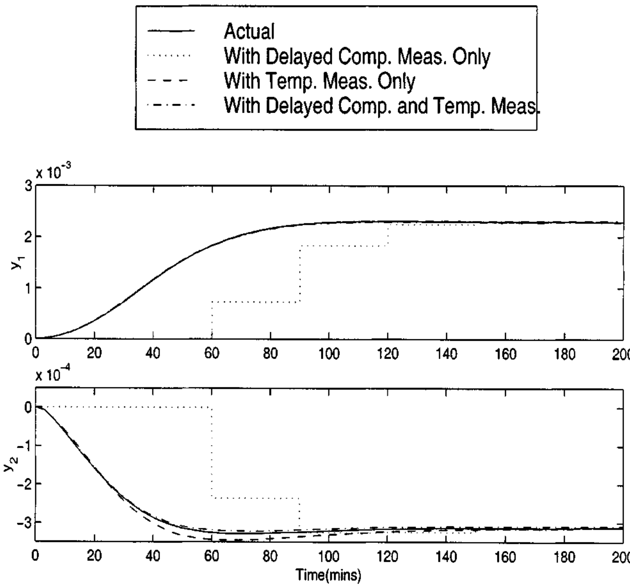

Figure 5. Evaluation of the estimators' performance for a step change in the composition (external propylene stream flow rate + 10 kmol/h).

where Λ_y was chosen as diag(1, 1, 0, 0, 0, 0, 0, 0, 0), given the equal importance of the compositions and the absence of control requirements for the temperatures. Since the system's gain exhibited a strong dependence on the input direction, we tuned the input weighting matrix with the structure

$$\Lambda_u = \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} \lambda_{u_1} & 0 \\ 0 & \lambda_{u_2} \end{bmatrix} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}. \quad (33)$$

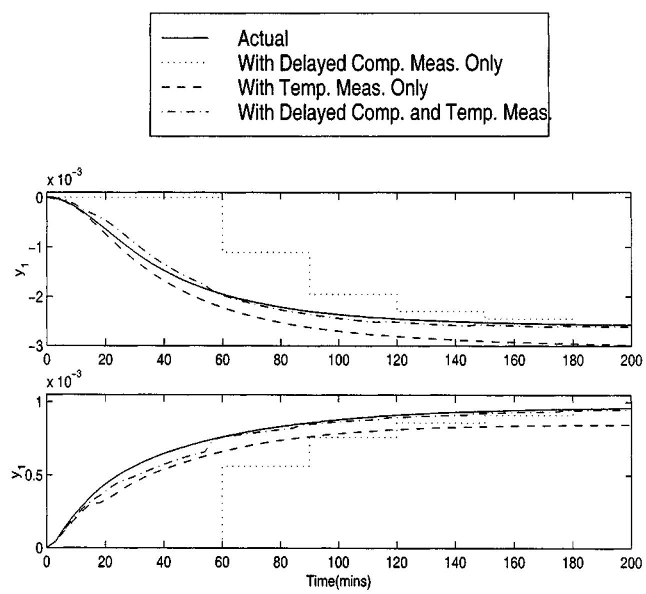

Figure 6. Evaluation of the estimators' performances for a step change in the feed flow rate (+150 kmol/h).

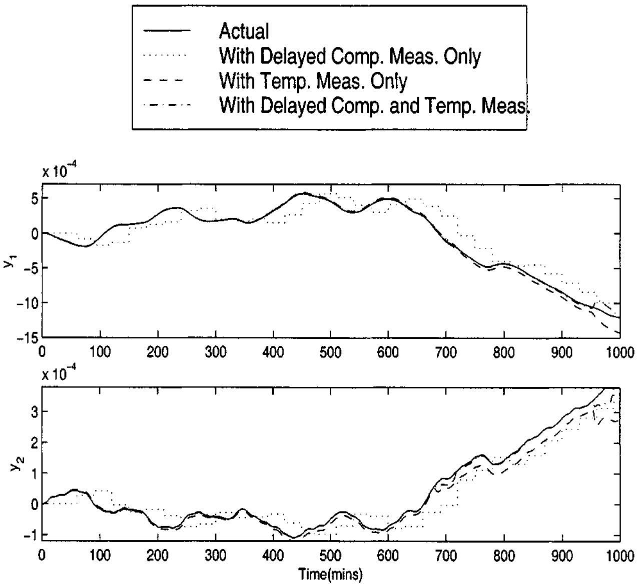

Figure 7. Evaluation of the estimators' performance for stochastic changes in the feed composition, feed temperature, and feed flow rate.

Table 2. Evaluation of the Estimators' Performance for a Step Change (1×10^5kJ/h) in the Feed Enthalpy with a Change in Vapor Fraction from 0.016 to 0.019

Mean Square Error in Estimation	y_1	y_2
With delayed comp. meas.	$7.7741e-008$	$1.3020e-006$
With temp. meas. only	$1.8137e-009$	$3.4625e-010$
With delayed comp. meas. and temp. meas.	$2.6687e-010$	$2.0517e-011$

Table 3. Evaluation of the Estimators' Performance for a Step Change in the Composition

Mean Square Error in Estimation	y_1	y_2
With delayed comp. meas.	$1.6038e-007$	$2.6637e-006$
With temp. meas. only	$9.5158e-011$	$1.0132e$-010
With delayed comp. meas. and temp. meas.	$9.9340e-011$	$2.0562e-011$

Note: External propylene stream flow rate +10 kmol/h.

Table 4. Evaluation of the Estimators' Performance for a Step Change in the Feed Flow Rate

Mean Square Error in Estimation	y_1	y_2
With delayed comp. meas.	$1.7402e-007$	$4.3230e-006$
With temp. meas. only	$9.8302e-008$	$9.6829e-009$
With delayed comp. meas. and temp. meas.	$6.9290e-009$	$1.0766e-009$

Note: +150 kmol/h.

This way, we could penalize input movements along the low-gain direction less than those along the high-gain direction (see Table 6). This is logical, as the choice of input weight needed to achieve a certain speed of response directly depends on the size of the gain. The values we used for the tuning parameters are summarized in Table 6.

Table 5. Evaluation of the Estimators' Performance for Stochastic Changes in the Feed Composition, Feed Temperature, and Feed Flow Rate

Mean Square Error in Estimation	y_1	y_2
With delayed comp. meas.	$1.4606e-008$	$3.6739e-007$
With temp. meas. only	$2.4351e-009$	$7.5129e-010$
With delayed comp. meas. and temp. meas.	$4.8160e-010$	$7.2304e-011$

We simulated the same three scenarios (that is, with the three different measurement combinations) as before. In the cases where the temperature measurements were used either by themselves or together with the delayed composition measurements, the input calculations were performed and the optimal input moves were implemented every 3 min. When only the composition measurements were used, this was done once every 30 min. As before, we first simulated the closed-loop responses for various deterministic changes in the feed and then introduced stochastic disturbances. The simulation results for a step change in the feed temperature, feed composition, and feed flow rate, and for stochastic changes in all three disturbances, are shown in Figures 8–11 and Tables 7–10 .

Although not shown here, we made several painstaking attempts to build an inferential control model using the plant test data alone. In general, the combined deterministic/stochastic model, which we obtained from applying the subspace identification method to the plant test data, showed poor estimation *and* control performance. Even when we gave a very high signal-to-noise ratio by eliminating most of the disturbances during the plant test, the results did not improve. In this case, even though the deterministic part of the obtained model was fairly accurate, the captured correlation between the temperatures and the compositions, critical for inferential control, was poor since such data contained little disturbance information. On the other hand, when we increased the level of disturbances during the plant test, identification of the deterministic model became a problem. The estimation performance improved, but the control performance became extremely poor, often showing instability. Only by combining the historical operation data and the plant test data in the proposed manner could we derive an inferential control model that delivered satisfactory estimation and control results.

Conclusion

In this article, we examined the feasibility of using plant data to build a stochastic system model that can be used to

Table 6. MPC Tuning Parameters

Control horizon: $m=3$
Prediction horizon: $p=10$
Input weight: $(\lambda_{u_1}, \lambda_{u_2})=(0.02, 0.1)$

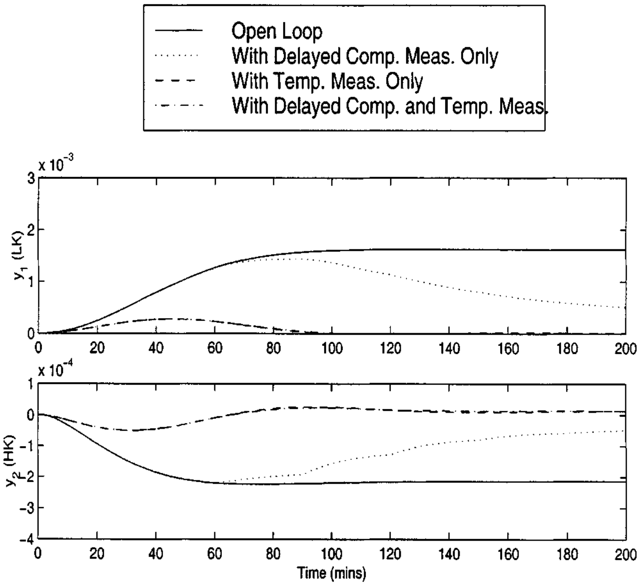

Figure 8. Evaluation of the controller performance for a step change (1×10^5kJ/h) in the feed enthalpy.

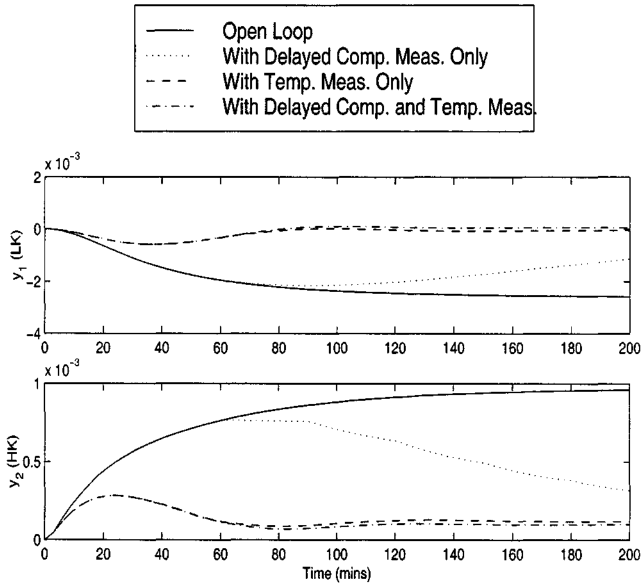

Figure 10. Evaluation of the controller performance for a step change in the feed flow rate (+150 kmol/h).

design an inferential controller. The focus was given to the requirements for the data, specifically what information the data are required to possess and which data types are the most appropriate. Our conclusion is that, for many systems, both historical operation data and plant test data are needed to build an adequate model for inferential control. This is in contrast to the conventional feedback controller design for which plant test data alone are usually adequate. We proposed a two-step procedure for building a model using both

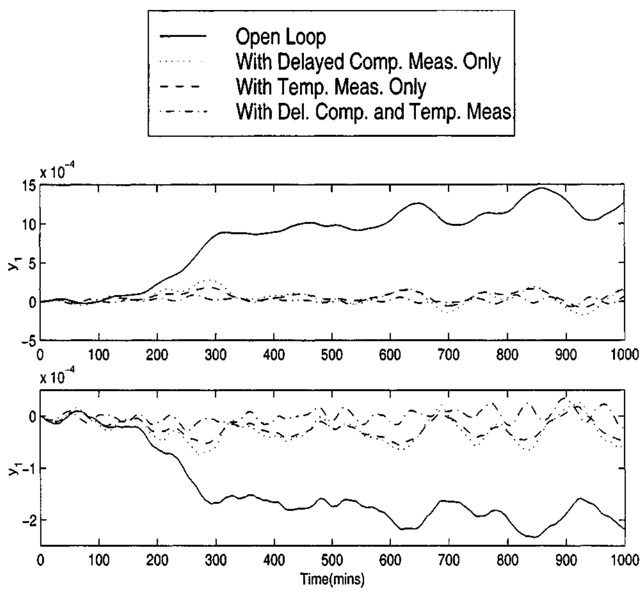

Figure 11. Evaluation of the controller performance for stochastic changes in the feed composition, feed temperature, and feed flow rate.

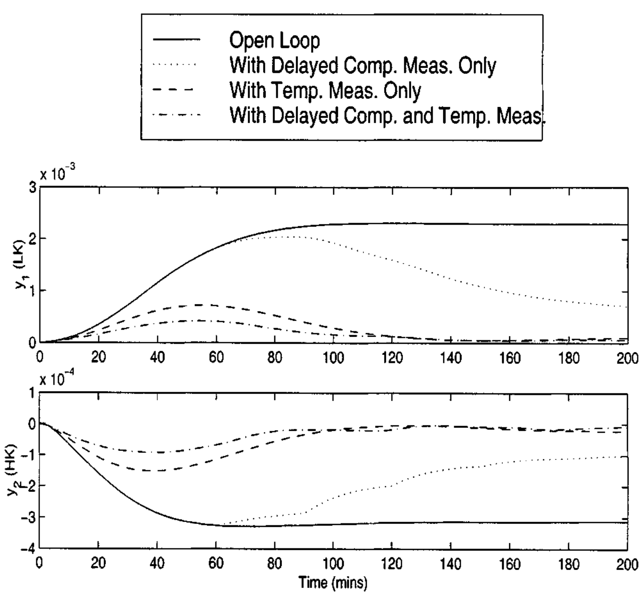

Figure 9. Evaluation of the controller performance for a step change in the composition (external propylene stream flow rate + 10 kmol/h).

Table 7. Evaluation of the Controller Performance for a Step Change (1×10^5kJ/h) in the Feed Enthalpy

	Mean Square Error	
	y_1	y_2
Open loop	$1.8717e-006$	$3.9123e-008$
With delayed comp. meas.	$9.3407e-007$	$1.8915e-008$
With temp. meas. only	$1.5466e-008$	$5.5139e-010$
With del. comp. meas. and temp. meas.	$1.5481e-008$	$5.5108e-010$

Table 8. Evaluation of the Controller Performance for a Step Change in the Composition

	Mean Square Error	
	y_1	y_2
Open loop	3.7981e−006	8.5512e−008
with delayed comp. meas.	1.8714e−006	4.4615e−008
With temp. meas. only	1.3615e−007	5.1916e−009
With del. comp. meas. and temp. meas.	4.7393e−008	1.9616e−009

Note: External propylene stream flow rate +10 kmol/h.

Table 9. Evaluation of the Controller Performance for a Step Change in the Feed Flow Rate

	Mean Square Error	
	y_1	y_2
Open loop	4.4710e−006	6.5296e−007
With delayed comp. meas.	2.8145e−006	3.3486e−007
With temp. meas. only	6.1400e−008	2.3039e−008
With del. comp. meas. and temp. meas.	4.1067e−008	2.0032e−008

Note: +150 kmol/h.

Table 10. Evaluation of the Controller Performance for Stochastic Changes in the Feed Composition, Feed Temperature, and Feed Flow Rate

	Mean Square Error	
	y_1	y_2
Open loop	8.5288e−007	2.5188e−008
With delayed comp. meas.	1.1139e−008	1.2428e−009
With temp. meas. only	7.0732e−009	8.0135e−010
With del. comp. meas. and temp. meas.	9.4616e−010	1.3526e−010

types of data. We also brought out some practical issues that may arise during an application of the procedure and proposed solutions. Finally, we showed the efficacy of the method in a case study involving a mulitcomponent distillation column simulated in HYSYS.

As industries continue to invest heavily in new sensors and information-management systems, the volume of plant data being collected is rising rapidly. While data may come cheap, unlocking values hidden in them takes a great many resources. The proposed method can serve as a tool for extracting value from collecting data.

Acknowledgment

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Literature Cited

Amirthalingam, R., and J. H. Lee, "Subspace Identification Based Inferential Control of a Continuous Pulp Digester," *Comput. Chem. Eng.*, **21**, S1143 (1997).

Amirthalingam, R., and J. H. Lee, "Subspace Identification Based Inferential Control Applied to a Continuous Pulp Digester," *J. Process Control*, **9**, 397 (1999).

Andersen, H. W., M. Kummel, and S. B. Jorgensen, "Dynamics and Identification of a Binary Distillation Column," *Chem. Eng. Sci.*, **44**, 2571 (1989).

Åström, K. J., and B. Wittenmark, *Computer-Controlled Systems: Theory and Design*, Prentice Hall, Upper Saddle River, NJ (1997).

Banerjee, A., Y. Arkun, B. Ogunnaike, and R. Pearson, "Estimation of Nonlinear Systems Using Linear Multiple Models," *AIChE J.*, **43**, 1204 (1997).

Cambell, H. C., and J. B. Rawlings, "Predictive Control of Sheet and Film Forming Processes," *AIChE J.*, **44**, 1162 (1998).

Cooley, B., and J. H. Lee, "Control-Relevant Experiment Design," *AIChE J.* (2000).

Cutler, C. R., and F. H. Yocum, "Experience with the DMC Inverse for Identification," *CPC-IV, AIChE Symp. Ser.*, **P-67**, 297 (1991).

Doyle, F. J., III, "Nonlinear Inferential Control for Process Applications," *J. Process Control*, **8**, 339 (1998).

Forssell, U., and L. Ljung, "Closed-Loop Identification Revisited," *Automatica*, **35**, 1215 (1999).

Friedland, B., "Sampled-Data Control Systems Containing Periodically Varying Members," *Proc. IFAC Cong.*, (1960).

Jacobson, E. W., and S. Skogestad, "Inconsistencies in Dynamic Models for Ill-Conditioned Plants: Application to Low-Order Models of Distillation Columns," *Ind. Eng. Chem. Res.*, **33**, 631 (1994).

Kalman, R. E., "A New Approach to Linear Filtering and Prediction Problems," *Trans. ASME, Ser. D: J. Basic Eng.*, **82**, 35 (1960).

Kalman, R. E., and R. S. Bucy, "New Results in Linear Filtering and Prediction Theory," *Trans. ASME, Ser. D: J. Basic Eng.*, **83**, 95 (1961).

Kranc, G. M., "Input-Output Analysis of Multi-Rate Feedback Systems," *IRE Trans. Automat. Contr.*, **AC-3**, 21 (1957).

Larimore, W. E., "Canonical Variate Analysis in Identification, Filtering, and Adaptive Control," *Proc. IEEE Conf. on Decision and Control*, Hawaii, 596 (1990).

Lee, J. H., and A. K. Datta, "Nonlinear Inferential Control of Pulp Digester," *AIChE J.*, **40**, 50 (1994).

Lee, J. H., M. Morari, and C. E. García, "State Space Interpretation of Model Predictive Controll," *Automatica*, **30**, 707 (1994).

Lee, J. H., M. S. Gelormino, and M. Morari, "Model Predictive Control of Multi-Rate Sampled-Data Systems: A State-Space Approach," *Int. J. Control*, **55**, 153 (1992).

Lee, J. H., and M. Morari, "Robust Inferential Control of Multi-rate Sample-data Systems," *Chem. Eng. Sci.*, **47**, 865 (1992).

Li, D., S. L. Shah, T. Chen, and R. Patwardhan, "System Identification and Long-Range Predictive Control of Multi-Rate Systems," *Proc. Amer. Control Conf.*, San Diego, California, p. 336 (1999).

Li, W., and J. H. Lee, "Control Relevant Identification of Ill-Conditioned Systems: Estimation of Gain Directionality," *Comp. Chem. Eng.*, **20**(8), 1023 (1995).

Ljung, L., *System Identification: Theory for the User.*, Prentice Hall, Englewood Cliffs, NJ (1987).

Ljung, L., and T. McKelvey, "Subspace Identification from Closed Loop Data," *Signal Process.*, **52**, 209 (1996).

Ljung, L., and U. Forssell, "An Alternative Motivation for the Indirect Approach to Closed-Loop Identification," *IEEE Trans. Automat. Contr.*, **AC-44**, 2206 (1999).

Morari, M., and G. Stephanopoulos, "Minimizing Unobservability in Inferential Control Schemes," *Int. J. Control*, **31**, 367 (1980).

Muske, K. R., and J. B. Rawlings, "Model Predictive Control with Linear Models," *AIChE J.*, **39**, 262 (1993).

Quintero-Marmol, E., and W. L. Luyben, "Inferential Model-Based Control of Multicomponent Batch Distillation," *Chem. Eng. Sci.*, **47**, 887 (1992).

Ricker, N. L., "Model Predictive Control: State of the Art," *Proc. Int. Conf. on Chemical Process Control—CPC IV*, Y. Arkun and W. Ray, eds., South Padre Island, TX, p. 271 (1991).

Russell, S. A., D. G. Robertson, J. H. Lee, and B. A. Ogunnaike, "Quality Monitoring and Control of Nylon 6,6 Autoclave," *Chem. Eng. Sci.*, **53**, 3685 (1998).

Tatiraju, S., M. Souroush, and R. Mutharasan, "Multi-Rate Nonlinear State and Parameter Estimation in a Bioreactor," *Biotechnol. Bioeng.*, **63**(1), 22 (1999).

Tatiraju, S., and M. Souroush, "Nonlinear State Estimation in a

Polymerization Reactor,'' *Ind. Eng. Chem. Res.*, **36**, 2679 (1997).
Van Overschee, P., and B. De Moor, ''N4SID: Subspace Algorithms for the Identification of Combined Deterministic Stochastic Systems,'' *Automatica*, **30**, 75 (1994).
Verhaegen, M., ''A Novel Non-iterative MIMO State Space Identification Technique,'' *Preprints 9th IFAC/IFORS Symp. on Identification and System Parameter Estimation*, Budapest, Hungary (1991).
Yiu, Y., G. A. Carling, and R. K. Wood, ''Dynamic and Control Behaviour of Multicomponent Distillation Columns,'' *Simulation*, 201 (1990).
Yu, C. C., and W. L. Luyben, ''Use of Multiple Temperatures for the Control of Multicomponent Distillation Columns,'' *Ind. Eng. Chem. Process Des. Dev.*, **23**, 590 (1984).
Yu, Z., W. Li, J. H. Lee, and M. Morari, ''State Estimation Based Model Predictive Control Applied to Shell Control Process: A Case Study,'' *Chem. Eng. Sci.*, **18**, 15 (1994).

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