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Selection of Parameters for Updating in On-line Models

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Predictions from dynamic mechanistic models used for process monitoring and control often exhibit sustained offset from process measurements. This offset is caused by imperfect measurements and by model deficiencies that result from simplifying assumptions, unmodeled disturbances, and uncertain parameter estimates. Extended Kalman filter (EKF) state estimation can eliminate offset by on-line updating of a subset of the model parameters. Offset elimination is accomplished by incorporating nonstationary stochastic states in the model equations. A difficult problem faced by practitioners when implementing state estimators is deciding which model parameters to update using on-line measurements. In this article, simple screening tools are developed to aid in updateable parameter selection. These tools are extensions of the relative gain array (RGA), the relative disturbance gain (RDG), and the disturbance condition number (DCN), which have been used in multivariable control applications to determine appropriate manipulated variable/control variable pairings and to examine disturbance effects. The application of these techniques for updateable parameter selection is demonstrated using simulations of a gas-phase polyethylene reactor system. A benefit of these screening tools over past trial-and-error parameter screening practices is that neither tuning of the state estimator nor running of simulations is required. We show that the RGA is an effective tool for determining when problems will arise due to correlated effects of different parameters on model outputs. The RDG is shown to be an effective tool for reducing the number of adjustable parameters when only particular types of disturbances are anticipated. We demonstrate that the DCN can be used to screen out parameter sets that will lead to excessive and physically unrealistic adjustment of model parameters.

Difficulties arise when implementing model-based process monitoring and control schemes due to discrepancies between model predictions and measured process conditions. These discrepancies result from drifting measurements and from model deficiencies, which are often due to simplifying assumptions, unmodeled process changes and inaccurate parameter estimates. Parameter estimates can be inaccurate for a number of different reasons. If the model is a simplified representation of the true process or if the underlying nature of the process changes with time, then the optimal values of some parameters will vary with time and location in the operating space. In such situations, the model must be updated in some fashion to prevent sustained offset between model predictions and plant data. Even if the model structure is perfect and the parameters have fixed true values, experimentally determined estimates of the parameters will deviate from true values, leading to inaccuracy in the model predictions. State estimation techniques can be formulated to account for uncertainty in fixed model parameters and to adjust selected model parameters on-line to ensure that the model outputs track the process measurements without bias. Examples of these approaches include the extended Kalman filter[1] (EKF), in which parameters and states are estimated jointly, and decoupled observer/estimators,[2] in which parameters are updated distinctly from the states, and parameter estimates are then provided to the state estimator. Regardless of the approach used, a critical step in implementing such schemes is the choice of parameters that are to be updated from a larger set of possible candidates. This step is the focus of the current article, namely, the selection of appropriate parameters for on-line updating to eliminate plant/model mismatch. Although EKF state estimation is considered in this article, the updateable parameter-selection techniques developed here will also apply when other types of observer and parameter estimation schemes are used.

Combined state and parameter estimation has found numerous applications in chemical process engineering,[3−6] particularly in biochemical systems[7−9] and in polymerization reactors.[10−25] Models used for state estimation in polymerization processes are usually nonlinear, and some model parameters are expected to fluctuate over time[21,26] due to, for example, reactive impurities and catalyst variability. Many simulation studies using state estimation for polymerization reactors have been reported.[12−14,16,17,20,22−25] However, few actual industrial implementations[19] are described in the literature because effective application in a real process environment can be difficult and time-consuming. Kozub and MacGregor[16] note that one of the most common errors in implementing a state estimation procedure is neglecting to incorporate adequate nonstationary stochastic states or updateable parameters. If one fails to adequately incorporate such variables, the result is a proportional state estimator that has none of the integral action necessary to eliminate bias between the measured plant outputs and the model predictions. An EKF implementation on a batch methyl methacrylate polymerization by Ellis et al.[11,18] illustrates this problem. No nonstationary parameter states were included

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in their EKF formulation, and bias between measurements and on-line estimates is apparent in their results.

Examples of EKF state estimation using updateable parameters or nonstationary stochastic states have been presented by a number of authors.[10,13,16,17,22,27] Stengel[1] and Soroush[6] refer to EKF implementation with updateable parameters as parameter-adaptive filtering and adaptive EKF, respectively. Jo and Bankoff[10] reported one of the earliest applications of an EKF to a polymerization reactor. They considered updating two parameters, together and separately, to investigate the effects on the quality of predictions from their kinetic model for free-radical polymerization. Jo and Bankoff showed that there was little additional benefit when both parameters were updated. Parameter updating markedly increased the computational load of the filter, and they concluded that it was best to update only the most uncertain parameter. Jo and Bankoff did not have a specific strategy for selecting updateable parameters. They stated that the choice of parameters to be estimated in a given problem has to be made by experimentation under actual conditions. This approach was sufficient for the simple model they considered. For more complex models, however, arbitrarily choosing subsets of parameters and testing them experimentally can be a difficult and time-consuming process and may not be practical for plant environments.

The problem of the appropriate choice of updateable parameters raised by Jo and Bankoff has continued to receive attention. The most pervasive approach is to rely on trial-and-error simulations combined with qualitative process knowledge for selecting and testing parameter sets for on-line updating. Examples of this approach include Gagnon and MacGregor,[13] McAuley and MacGregor,[15,17] Kozub and MacGregor,[16] Semino et al.[21] and Clarke-Pringle and MacGregor.[22]

Recently, Scali et al.[24] proposed an alternative approach, which they used to analyze the performance of different Kalman filters for closed-loop control of a continuous solution polymerization reactor. They screened potential sets of updateable parameters by constructing observability matrixes, which were used to determine if the chosen parameters could be updated with the available measurements. The advantage of this approach is that it is a preliminary analysis, which can be performed prior to implementation of the state estimator, and can be used for complex models with many parameters. Limitations of this approach are that no information is provided about the anticipated uncertainty of the state estimates and no information is provided about the anticipated size of the parameter adjustments that will be required to eliminate offset. Patton[28] addressed the former problem using covariance matrixes computed off-line using prior noise covariance information to determine the effects of added stochastic states on the precision of model predictions. He showed that as the number of nonstationary parameter states is increased to eliminate bias, the precision of state estimates becomes worse. Patton also developed a structural test to determine whether a specified set of stochastic parameter states will be able to eliminate bias.

Patton's work focused on selection and updating of arbitrary nonstationary stochastic disturbance states that are added to the linearized model equations. However, process engineers often prefer to update meaningful parameters within their models that correspond to changes in actual physical characteristics (e.g., unmeasured impurity concentrations and heat transfer coefficients) because changes in these parameters can be monitored to provide useful information to detect and ultimately eliminate potential sources of process disturbances.[17] Process engineers usually have some information about the types and sources of disturbances to be expected, and they would benefit from a screening tool that can determine a priori whether particular types of disturbances can be handled effectively by a parameter-updating scheme, without excessive changes in updateable model parameters beyond their physically meaningful ranges.

Summarizing, updateable parameters are typically selected using a combination of trial-and-error simulations and physical insight, combined with structural tests to ensure that the parameters introduced into a state and parameter estimation scheme are in fact observable. The use of sensitivity information quantifying how output predictions are influenced by parameter perturbations has received relatively little attention. Sensitivity information is used indirectly in the covariance assessment of Patton[28] since the state covariance matrixes depend on the covariances of the parameter estimates via the sensitivities of the states to the parameters. Similarly, the decoupled state and parameter estimation approach proposed by Agarwal and Bonvin[2] relies on parametric sensitivities of the states to provide covariance information for the separately estimated parameters to the state estimator. The techniques proposed in the present paper use parametric sensitivities of the outputs to identify appropriate updateable parameters. Since sensitivity analysis is regularly used in regression analysis to guide the selection of parameters and since combined on-line state-and-parameter estimation can be considered as a recursive on-line regression, it is useful to consider the available sensitivity analysis techniques for regression analysis.

In regression analysis, parameter selection (or parametrization) for steady-state or dynamic models is accomplished by examining sensitivity information that describes the effects of parametric perturbations on the predicted responses. Conventional approaches examine first-order derivative information, either directly, in terms of the first-order sensitivity matrix, or indirectly, in terms of the Fisher Information Matrix (see, for example, Seber and Wild[29]). The elements of the first-order sensitivity matrix provide marginal sensitivity information, describing how predicted responses vary when individual parameters are perturbed. Unfortunately, the marginal sensitivities do not provide information about joint parameter effects. Information about joint effects can be obtained indirectly from the Fisher Information Matrix (FIM) since the approximate variance−covariance matrix of the parameter estimates is equal to the inverse of the FIM when the noise is normally distributed.[29] Parameter estimates having large variances signify parameters having a small influence on predicted responses. Large-magnitude covariances of parameter estimates indicate highly correlated effects of the particular parameters on model ouputs.

A related concept is parameter identifiability, which refers to the ability to uniquely resolve values for parameters in a model.[30] Poor conditioning of the FIM, indicated by its condition number, implies a potential

lack of identifiability. This lack of identifiability can result from individual parameters having negligible influence on model outputs or to highly correlated effects of some parameters. Under these conditions, only a subset of the model parameters can be estimated uniquely. Vajda et al.[30] used singular value decomposition of the FIM to identify subsets of parameters that can be jointly estimated with reasonable precision. In their analysis, some parameters may be dropped from estimation if they fail to contribute to the singular vectors associated with the dominant singular values.

First-order parametric sensitivities, which are evaluated at a particular operating point, depend on the model structure and the values of the independent variables at that operating point. On the other hand, the first-order sensitivity matrix, and hence the FIM, depend on the independent variable settings for the entire set of experimental runs to be used in parameter estimation. Thus, it is important to recognize that sensitivity-based parameter selection in regression analysis, using these techniques, is performed in the context of an experimental design, which consists of a prespecified set of experimental conditions under which data will be collected.[29]

Weijers and Vanrolleghem[31] have proposed a procedure for selecting identifiable parameters when calibrating dynamic models against plant data. Their procedure is off-line and combines sensitivity analysis and an examination of the Fisher Information Matrix to identify a set of parameters for estimation. The first step in their approach is to specify the model, the initial conditions, the outputs being measured, the candidate parameters, the manipulated variable input sequences, and the resulting experimental data. An initial prescreening, based on scaled marginal sensitivity coefficients, is then used to reduce the number of candidate parameters. Subsequently, two measures of the FIM are computed for all possible subsets of the candidate parameters, beginning with sets of two and ending with the entire set of candidate parameters identified from the sensitivity prescreening. Because calculations are performed for all the possible combinatorial subsets of parameters, this approach can be very time-consuming. When there are many candidate parameters, the initial prescreening step to remove noninfluential parameters is important for reducing computational effort.

The two FIM measures used by Weijers and Vanrolleghem are the determinant and condition number of the FIM. The volume of the parameter joint-confidence ellipsoid is inversely proportional to the determinant of the FIM; thus, large values of the determinant are indicative of more precise estimation of the parameters. The condition number, as noted above, can indicate a potential lack of identifiability. The final selection of a parameter set is based on joint consideration of the determinant, which is desired to be large, and the condition number, which is desired to be small. Weijers and Vanrolleghem demonstrated the application of their procedure using a wastewater treatment plant model and industrial data.

The approach of Weijers and Vanrolleghem, which is applicable to parameter selection for dynamic models, could be applied in an off-line manner prior to implementation of a state estimator. To apply their approach (or indeed, to apply any approach utilizing the regression sensitivity matrix and FIM), it would be necessary to specify an operating profile consisting of input moves and to have a data set. If prior knowledge of the noise covariance matrix were available, together with initial conditions, Weijers and Vanrolleghem's procedure could be modified to eliminate the need for output data. However, detailed knowledge of the input moves and the sampling times would still be required. Finally, it is important to note that their approach does not address bias in the model predictions.

The tools for parameter-update selection proposed in this article are simple to use because they require steady-state parametric sensitivity information only at a nominal operating point rather than sensitivity information at a set of predefined experimental run conditions. They are aimed at selecting subsets of parameters for updating to eliminate bias between model predictions and on-line measurements. The proposed screening tools are extensions of the relative gain array (RGA),[32] the relative disturbance gain (RDG),[33] and the disturbance condition number (DCN).[34] These tools have been used in multiloop control systems to screen for interaction among the relationships between manipulated variables and controlled variables and to assess the effects of these interactions on rejection of particular disturbances.

The proposed diagnostic tools are particularly informative for choosing appropriate subset of parameters to update on-line because these tools account for and assess the joint effects of parameters on the outputs. For example, each element of the parameter-selection RGA is the ratio of the sensitivity of a predicted output to a particular parameter (conditional on adjusting the remaining parameters to obtain correct predictions of the remaining outputs) to the marginal sensitivity of the predicted output to the particular parameter. Under joint estimation, this measure provides a more informed assessment of the impact of parameters on predicted responses than marginal-sensitivity approaches provide. The need to properly account for joint effects when assessing parametric sensitivities was recently recognized by Sulieman et al.,[35] who developed a profile-based sensitivity coefficient for regression analysis that accounts for correlation among parameter estimates. Since their technique is defined in the context of an experimental design, it cannot be readily applied to the selection of updateable parameters for on-line dynamic models.

Since the proposed screening tools are based on steady-state parametric sensitivity information, there is an implicit assumption that the state estimator will be able to converge to steady-state state and parameter estimates. As a number of researchers have noted, divergence difficulties can be encountered when joint state and parameter estimation techniques such as the extended Kalman filter are used.[2] In such instances, the use of decoupled state and parameter estimation approaches should be considered.

The proposed screening tools and their application to parameter updating are illustrated using a gas-phase polyethylene reactor model. This model was chosen to illustrate the screening techniques because it is a simple dynamic mechanistic model with a number of physically meaningful parameters that can be adjusted on-line. The primary objective is not to gain insight into this particular system. Rather, our goal is to provide insight into the methods themselves so that they can be applied to larger systems and systems that are not well understood.

Gas-Phase Polyethylene Reactor Model

In commercial gas-phase polyethylene reactors, ethylene and α-olefins are copolymerized in fluidized-bed reactors using heterogeneous Ziegler−Natta, metallocene, or supported metal-oxide catalysts.[36] The model equations below are simplified dynamic material balances on hydrogen, butene comonomer, and catalyst sites, respectively:[17]

$$\frac{d[H_2]}{dt} = \frac{1}{V_g}\left\{F_{H2} - k_H Y[H_2] - \frac{[H_2](b + b_m)}{[C_T]} - g_l[H_2]\right\} \quad (1)$$

$$\frac{d[M_2]}{dt} = \frac{1}{V_g + V_s}\left\{F_{M2} - k_{p2} Y[M_2] - \frac{[M_2](b + b_m)}{[C_T]} - S[M_2]O_p\right\} \quad (2)$$

$$\frac{dY}{dt} = F_{cat}a_{cat} - \frac{YO_p}{B_w} - k_d Y \quad (3)$$

where $[H_2]$ and $[M_2]$ are the gas-phase concentrations of hydrogen and butene and Y is the number of moles of active catalyst sites in the reactor. Material balances for ethylene and polymer are not included in the model because it is assumed that accurate and fast measurements for ethylene concentration, $[M_1]$, and the weight of polymer in the bed, B_w, are available on-line and that these quantities are regulated by adjusting the ethylene feed rate to the reactor and the polymer outflow rate, respectively. Assuming that the mass of polymer in the fluidized bed is regulated at a particular set point, the polymer outflow rate,O_p, is equal to the polymer production rate, P_R:

$$O_p = P_R = Y(k_{p1}[M_1]m_{w1} + k_{p2}[M_2]m_{w2}) \quad (4)$$

Measured inputs, which can be adjusted by an operator or on-line control scheme, include the hydrogen feed rate, F_{H2}, the butene feed rate, F_{M2}, the catalyst feed rate, F_{cat}, and the outflow rate of gas, b, from the reactor system (in a bleed stream and interstitially with the polymer product). Measured process outputs are the hydrogen concentration, the production rate, and the comonomer concentration:

$$\mathbf{y} = \begin{bmatrix}[H_2] \\ P_R \\ [M_2]\end{bmatrix} \quad (5)$$

The gas concentrations are measured using an on-line gas chromatograph and P_R is determined from an on-line energy balance on the reactor.

The model contains a number of parameters.[17] V_g is the volume of the gas phase and S is a solubility parameter that accounts for unreacted butene dissolved in the polymer. S can be calculated using Henry's law, as can V_s, the equivalent volume of gas phase that would contain the quantity of butene dissolved in the polymer. $[C_T]$ is the total molar concentration of all species in the gas phase. The remaining parameters, which are known with less accuracy and are candidates for on-line updating using the EKF, are described in Table 1.

Table 1. Potential Parameters for On-line Updating

updateable parameter	description
a_{cat}	active site concentration in the catalyst feed
k_H	kinetic rate constant for consumption of hydrogen
k_{p2}	kinetic rate constant for consumption of comonomer
k_d	catalyst site deactivation rate constant
b_m	bleed stream flow rate uncertainty
g_l	mismatch factor accounting for uncertainty in the hydrogen mass balance

State and Parameter Estimation Using an Extended Kalman Filter

When an EKF is implemented with updateable parameters, the vector of modeled states is augmented by the set of parameters to be updated. For example, if we implement an EKF using the gas-phase polyethylene reactor model, and we decide to update parameters g_l, k_d, and k_{p2} on-line, the augmented state vector becomes

$$\mathbf{x_{aug}} = \begin{bmatrix}[H_2] \\ [M_2] \\ Y \\ g_l \\ k_d \\ k_{p2}\end{bmatrix} \quad (6)$$

The EKF updates the elements of this augmented state vector recursively,

$$\hat{\mathbf{x}}_{\mathbf{aug}}(t_{k+1}|t_{k+1}) = \hat{\mathbf{x}}_{\mathbf{aug}}(t_{k+1}|t_k) + \mathbf{K}(t_k)\{\mathbf{y}(t_{k+1}) - \hat{\mathbf{y}}(t_{k+1}|t_k)\} \quad (7)$$

where $\hat{\mathbf{x}}_{\mathbf{aug}}(t_{k+1}|t_{k+1})$ contains estimates of the model states and updateable parameters that have been updated using the measurements $\mathbf{y}(t_{k+1})$ available at time t_{k+1}. $\hat{\mathbf{x}}_{\mathbf{aug}}(t_{k+1}|t_k)$ is a vector of predicted states, which can be obtained by integrating the dynamic model from time t_k to t_{k+1}, starting at $\hat{\mathbf{x}}_{\mathbf{aug}}(t_k|t_k)$ and assuming that the values of the model parameters remain constant over this time interval. The vector of measurement predictions, $\hat{\mathbf{y}}(t_{k+1|k})$, is calculated from the predicted states. Gagnon and MacGregor[13] give detailed information about how to calculate the Kalman gain, $\mathbf{K}(t_k)$ and implement an EKF with updateable parameters.

As a motivating example of the application and utility of an EKF, a simulation is shown in Figure 1 wherein g_l, k_d, and k_{p2} in eqs 1−6 are updated on-line. McAuley and MacGregor[17] chose these parameters for updating because they each influence at least one of the outputs concerned, and they are expected to change values with changing process conditions. As shown in Figure 1a, an unmeasured (and hence unmodeled) step change in comonomer feed rate occurs at 4 h. The EKF adjusts the model by altering the updateable parameters to track this unmodeled disturbance. Solid lines indicate simulated plant data, and symbols (diamonds) show the response of the updated model at each time step. As shown in Figures 1b−d, the measured outputs are tracked without bias. Figures 1e−g show the adjustment of the parameters required to track the unmodeled disturbance in the butene feed rate. Sandink[37] provides details about how the EKF was implemented and tuned.

The simulation in Figure 1 employed one of many possible selections of the updateable parameters from Table 1. The maximum number of parameters that can be updated by the EKF is three, the number of mea-

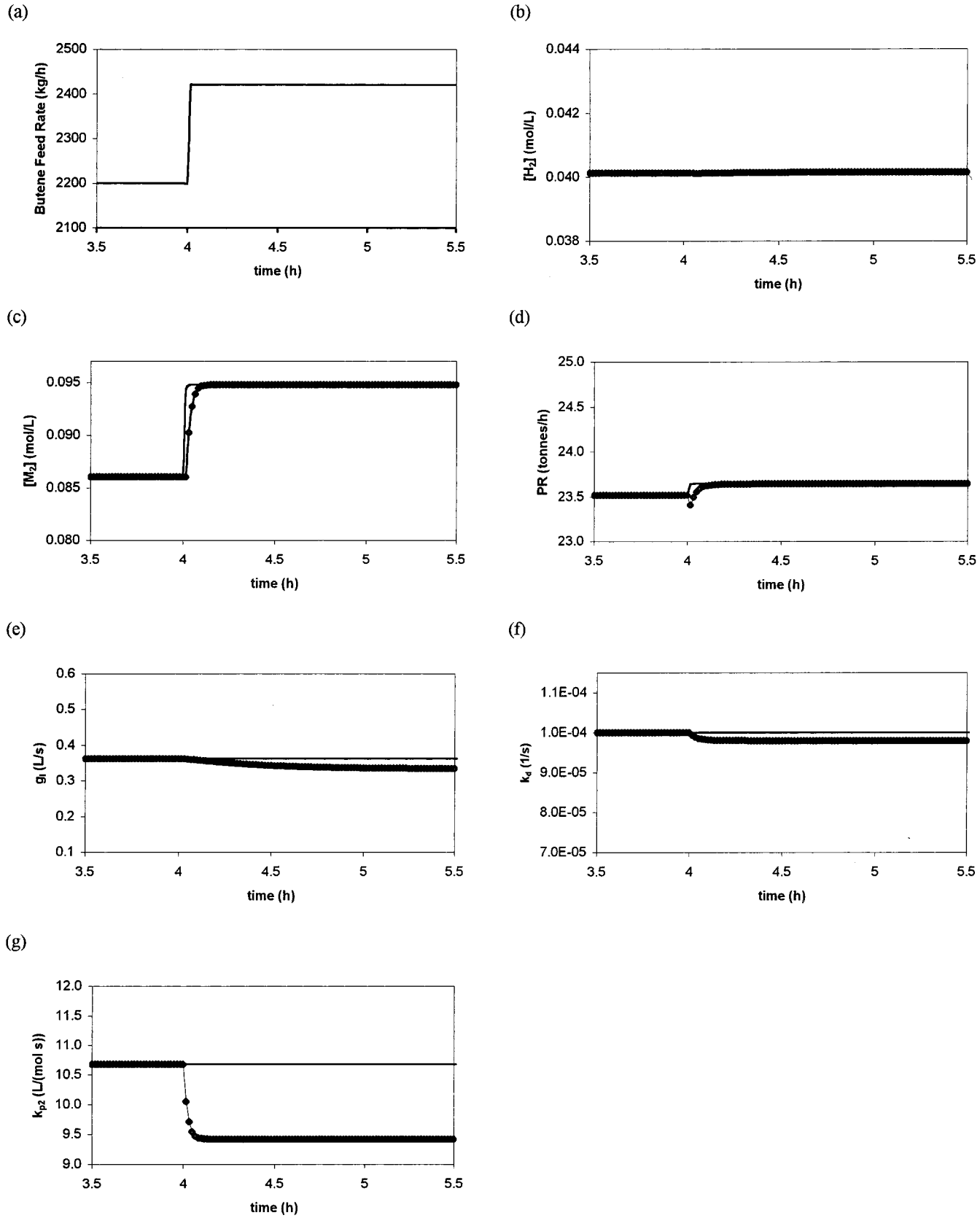

Figure 1. Updating of parameters g_l, k_d, and k_{p2} in response to an unmodeled step disturbance in comonomer feed rate at 4 h. —♦—, Updated values from EKF; —, simulated plant.

surements. Some groups of three parameters work well to eliminate bias, whereas others do not. Quick, reliable methods that can assist practitioners in selecting appropriate sets of parameters for updating are presented below.

Screening Diagnostics for Parameter Selection. An analogy can be drawn between an EKF state estimation problem and a multiloop/multivariable control problem. The EKF adjusts model parameters and states to ensure good dynamic model predictions and

to eliminate steady-state offset between model predictions and plant measurements. A multivariable control system adjusts manipulated variables to achieve good dynamic plant performance and to eliminate offset between plant measurements and desired set points. Diagnostics for determining interaction in multiloop and multivariable control situations include the relative gain array (RGA),[32] the relative disturbance gain (RDG),[33] and the disturbance condition number (DCN).[34] These diagnostics are useful for determining appropriate control loop pairings and for screening for interaction in the relationships between manipulated variables and controlled variables in multiloop control situations. The analogy between state estimation and multivariable control problems presents an opportunity to examine the suitability of these diagnostics for extension to EKF state and parameter estimation problems.

Relative Gain Array. In multiloop control problems, the RGA is used to screen for effects of transmission interaction in relationships between manipulated and controlled variables. λ_{ij}, the ijth element of the RGA, is the ratio of the open-loop gain between the ith output variable and the jth manipulated variable (with all other manipulated variables held constant) to the effective closed-loop gain (for the same pair of variables) with all other output variables fixed at nominal conditions by varying the remaining input variables:

$$\lambda_{ij} = \frac{\left.\frac{\partial y_i}{\partial u_j}\right|_{u_{k\neq j}}}{\left.\frac{\partial y_i}{\partial u_j}\right|_{y_{l\neq i}}} \tag{8}$$

When the RGA can be rearranged to give an identity matrix, the gain effect of all manipulated variables on the outputs is the same in both open- and closed-loop situations, and there is no steady-state transmission interaction. There may, however, be a one-way interaction between control loops. Elements that differ significantly from 1 indicate potential control difficulties using the specific pairing. Values that are less than 1 indicate gain amplification under closed-loop control, while values greater than 1 indicate gain attenuation. Negative values indicate gain reversal, which can be especially problematic.

In an analogous fashion, we can define an RGA for EKF parameter updating, which has elements $\lambda_{\theta ij}$:

$$\lambda_{\theta ij} = \frac{\left.\frac{\partial y_i}{\partial \theta_j}\right|_{\theta_{k\neq j}}}{\left.\frac{\partial y_i}{\partial \theta_j}\right|_{y_{l\neq i}}} \tag{9}$$

From a statistical point of view, the denominator in eq 9 is the conditional sensitivity when other parameters are adjusted to alleviate bias in other responses, similar in spirit to profiling in nonlinear regression, in which one parameter is varied while others are fixed at conditional least-squares estimates.[38]

RGA elements equal to 1 indicate that the effect of the parameter on its corresponding model output does not depend on whether the parameter is being estimated individually or jointly with the other parameters. RGA elements that are zero indicate that the parameter has no influence on the particular output. As such, RGAs that can be arranged to give identity matrixes suggest that on-line parameter estimation should be straightforward. RGA elements with magnitudes significantly different from 1 indicate that the effect of a particular parameter on the model response depends on whether the other parameters are also being updated and that bias in the particular model output can be addressed by adjusting more than one parameter. In this case, joint estimation of the particular set of parameters may be difficult because of correlated effects of the parameters on the model outputs. Although gain reversal associated with negative RGA elements is important for multiloop control systems where individual controllers can be taken off-line, the sign of RGA elements is less important in multivariable parameter updating problems. If RGA elements indicate that there is an extreme transmission interaction in the parameter-updating problem, the parametric gain matrix may be nearly singular and large updateable parameter adjustments may be required to track a process change.

The steady-state RGA can be determined readily from a linear steady-state gain matrix using the Hadamard product,[39]

$$\mathbf{\Lambda} = \mathbf{K} \circ \mathbf{K}^{-\mathrm{T}} \tag{10}$$

where the operator " o " indicates element-wise multiplication. For parameter updating, $\mathbf{K}$ is a matrix of steady-state gains between parameters and outputs, with individual elements corresponding to the numerator in eq 9. From a statistical perspective, $\mathbf{K}$ contains first-order sensitivity coefficients for steady-state predictions. Since the model outputs are, in general, functions of both states and parameters,

$$\mathbf{K} = \frac{\partial \mathbf{y}}{\partial \boldsymbol{\theta}} = \left.\frac{\partial \mathbf{y}}{\partial \mathbf{x}}\right|_{\boldsymbol{\theta}} \frac{\partial \mathbf{x}}{\partial \boldsymbol{\theta}} + \left.\frac{\partial \mathbf{y}}{\partial \boldsymbol{\theta}}\right|_{\mathbf{x}} \tag{11}$$

Matrixes $(\partial \mathbf{y}/\partial \mathbf{x})|_{\boldsymbol{\theta}}$ and $(\partial \mathbf{y}/\partial \boldsymbol{\theta})|_{\mathbf{x}}$ can be obtained by differentiating the output equations (eqs 4 and 5 in the gas-phase polyethylene reactor example). All partial derivatives on the right-hand side of eq 9 must be evaluated at a nominal operating point. The state-sensitivity matrix, $\partial \mathbf{x}/\partial \boldsymbol{\theta}$, can be obtained by differentiating the steady-state process model, $\mathbf{g}(\mathbf{x},\boldsymbol{\theta}) = \mathbf{0}$ (eqs 1−3 for the polyethylene reactor example, with derivatives set to zero),

$$\left.\frac{\partial \mathbf{g}}{\partial \mathbf{x}}\right|_{\boldsymbol{\theta}} \frac{\partial \mathbf{x}}{\partial \boldsymbol{\theta}} + \left.\frac{\partial \mathbf{g}}{\partial \boldsymbol{\theta}}\right|_{\mathbf{x}} = \mathbf{0} \tag{12}$$

and solving for $\partial \mathbf{x}/\partial \boldsymbol{\theta}$, which can be substituted into eq 11 to obtain the gain matrix $\mathbf{K}$. If the steady-state model is nonlinear, the elements of $\mathbf{K}$ may change with operating point.

Using RGA for Screening of Updateable Parameter Sets. In Figure 1, the parameter set (g_l, k_d, k_{p2}) was shown to be effective for eliminating offset due to a butene feed rate disturbance. Using this particular parameter set, we find that the RGA for parameter updating is

$$\mathbf{\Lambda}_{\boldsymbol{\theta}} = \begin{array}{c} \begin{matrix} g_l & k_d & k_{p2} \end{matrix} \\ \begin{bmatrix} 1.00 & 0 & 0 \\ 0 & 1.01 & -0.01 \\ 0 & -0.01 & 1.01 \end{bmatrix} \end{array} \begin{matrix} [H_2] \\ P_R \\ [M_2] \end{matrix} \tag{13}$$

This RGA is essentially an identity matrix, indicating

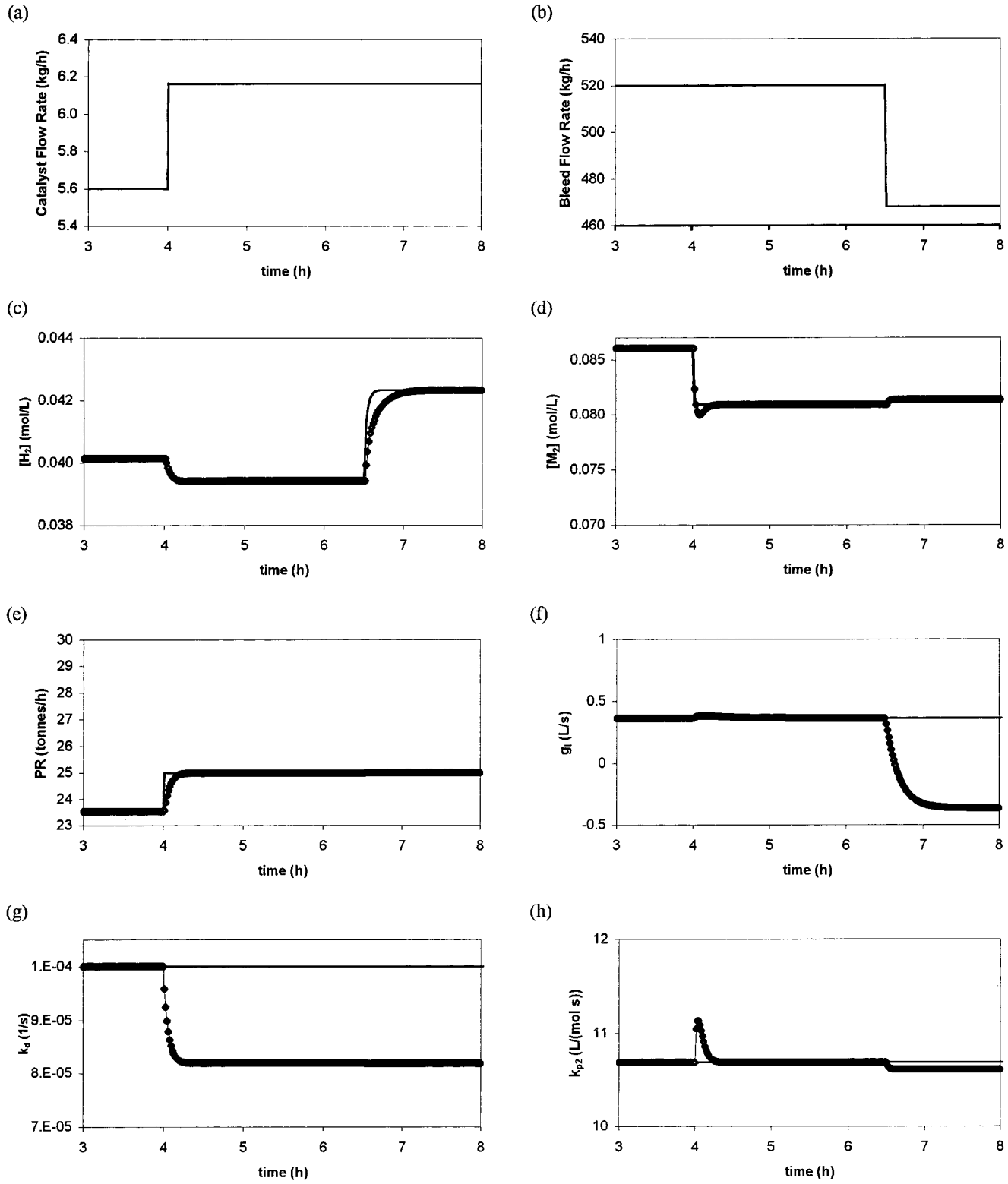

Figure 2. Updating of parameters g_l, k_d, and k_{p2} in response to unmodeled step disturbances in catalyst feed rate and bleed flow rate at 4 and 6.5 h, respectively. —♦—, Updated values from EKF; —, simulated plant.

that there will be very little transmission interaction between parameter and output pairings and that there will be little correlation among the effects of the parameters on the outputs at steady state. As such, it is not surprising that this parameter set was effective for tracking the butene feed rate disturbance. As shown in Figure 2, this parameter set is also effective for tracking unmodeled disturbances in catalyst feed rate and bleed-stream flow rate. The EKF is able to adjust g_l, k_d, and k_{p2} so that there is no steady-state offset between the simulated plant outputs and the model predictions. It is apparent from Figures 2f−h that k_d is the only parameter required to eliminate steady-state offset due to the catalyst feed disturbance. Parameters g_l and k_{p2} deviate slightly from their original steady-state values and then regain them. Because the RGA analysis uses only a steady-state model, we were unable to anticipate the small dynamic changes in g_l and k_{p2}

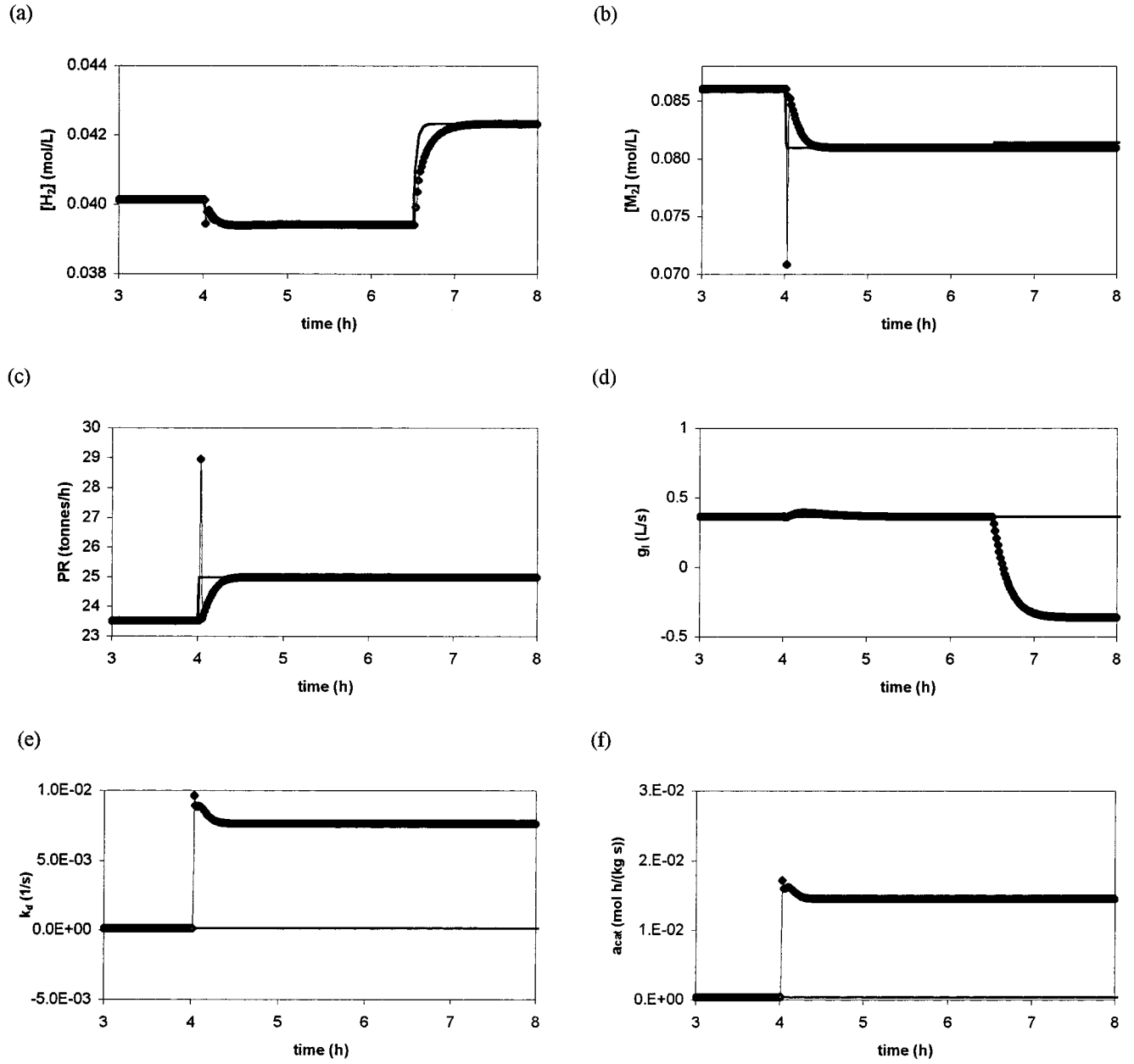

Figure 3. Updating of parameters g_l, k_d, and a_{cat} in response to unmodeled step disturbances in catalyst feed rate and bleed flow rate at 4 and 6.5 h, respectively. —♦—, Updated values from EKF, —, simulated plant.

immediately following the catalyst feed rate disturbance. The unmodeled bleed flow disturbance required both g_l and k_{p2} to achieve new steady-state values, while k_d did not change at all. The RGA predicted very little transmission interaction, and it is evident that the EKF tracked the unmodeled process changes well. An unbiased steady state was achieved with reasonable parameter adjustments and very little interaction between the three parameters, which is consistent with the RGA results.

If an alternative set of three updateable parameters (g_l, k_d, a_{cat}) is chosen from Table 1, the RGA that results is

$$\Lambda_\theta = \begin{array}{c} \begin{matrix} g_1 & k_d & a_{cat} \end{matrix} \\ \begin{bmatrix} 1.0 & 0 & 0 \\ 0 & 0.33(10^{10}) & -0.33(10^{10}) \\ 0 & -0.33(10^{10}) & 0.33(10^{10}) \end{bmatrix} \end{array} \begin{matrix} [H_2] \\ P_R \\ [M_2] \end{matrix} \quad (14)$$

This RGA predicts an extreme level of transmission interaction, indicating that the parameter-updating problem is ill-conditioned. The RGA elements indicate that g_l has an independent effect on the predicted hydrogen concentration, but that k_d and a_{cat} have highly correlated effects on P_R and $[M_2]$ and can be expected to interact severely when tracking disturbances. Since the relative gains are significantly greater than 1, there is severe attenuation of the parametric sensitivities under joint estimation. The sensitivity vectors for k_d and a_{cat} are nearly collinear and point in opposite directions.

Figure 3 shows how the EKF responds to the catalyst feed and bleed flow disturbances in parts a and b of Figure 2, using this alternative set of updateable parameters. We see that the EKF has particular difficulty in updating the parameters and the states. There is an initial large downward spike in the state estimate for $[M_2]$ and an upward spike in the estimate of P_R

(shown in parts b and c of Figure 3, respectively) after the catalyst disturbance is introduced. Examining parts e and f of Figures 3, we see that the EKF made very large steady-state upward adjustments to both a_{cat} and k_d to track the catalyst disturbance. These adjustments are consistent with collinear and opposite sensitivity vectors that were noted above. In this simulation, large simultaneous increases in both parameters have very little net effect on the model predictions. The steady-state change in k_d was ≈400 times the corresponding change shown in Figure 2g. Figure 3b shows that there is a small bias in the estimated steady-state butene concentration after the bleed stream flow rate disturbance because parameters k_d and a_{cat} cannot eliminate bias in both P_R and $[M_2]$ simultaneously. As was predicted by the RGA analysis, this would be a poor set of parameters to choose for updating due to excessive interaction between parameters k_d and a_{cat}. Such interaction could have been anticipated by examining the structure of eq 3. However, for more complex models, predicting interactions among parameters by inspection can be difficult, and RGA analysis would be particularly helpful in such situations.

One shortcoming of the RGA analysis is that it did not provide any information about which types of disturbances could be easily tracked by a particular set of parameters and which disturbances might lead to large or unrealistic changes in updateable parameters. The utility of the relative disturbance gain (RDG) and disturbance condition number (DCN) for addressing these issues will be demonstrated for screening sets of updateable parameters when specific types of disturbances are anticipated by the practitioner.

Relative Disturbance Gain. The RDG [33,40] provides a steady-state measure of the ease with which a particular disturbance can be rejected by a multiloop control scheme. The RDG element for the output/input pair *ij* is defined as the ratio of the effort required for manipulated variable *j* to reject the effect of a disturbance on output *i* with all control loops closed, divided by the analogous effort with only the *ij* control loop closed:

$$\beta_{ij} = \frac{\left.\frac{\partial u_j}{\partial d}\right|_{\mathbf{y}}}{\left.\frac{\partial u_j}{\partial d}\right|_{y_i, u_{k,k\neq j}}} \tag{15}$$

Like the elements of the RGA, RDG elements are dimensionless and are therefore scale-independent. An RDG element with magnitude greater than unity indicates that interaction among the control loops hinders rejection of the particular disturbance, whereas an RDG with magnitude smaller than unity indicates that interaction among the control loops helps disturbance rejection so that smaller manipulated variable moves will be required to reject the disturbance than if the other control loops were not operating. An RDG element of zero indicates that the other control loops are able tocompletely reject the disturbance and that no manipulated variable move will be required for the specific input/output pair. Marino-Galarraga et al.[40] suggest as a rule of thumb for good multiloop controller design that the sum of the absolute values of the RDGs for a specific configuration be less than *n*, where *n* is the number of control loops. When combined with the RGA, the RDG provides a valuable screening tool that allows control practitioners to screen out undesirable manipulated variable/controlled variable pairings prior to dynamic evaluation of candidate control schemes. The particular value of the RDG lies in assessing the impact of disturbance directions relative to the gain structure of the process, which is not addressed by the RGA.

We have defined a new RDG for analysis of state and parameter estimation as follows:

$$\beta_{\theta ij} = \frac{\left.\frac{\partial \theta_j}{\partial d}\right|_{\mathbf{y}=\mathbf{y_D}}}{\left.\frac{\partial \theta_j}{\partial d}\right|_{\theta_{k,k\neq j}; y_i = y_{Di}}} \tag{16}$$

The *ij*th element of this RDG is the gain between disturbance-variable *d* and parameter θ_j when all the updateable parameters are being adjusted to force the model to track the disturbed outputs, $\mathbf{y_D}$, divided by the analogous gain that results when only the *i*th disturbed output is tracked and all other parameters are held constant. The extended RDG is the ratio of the perturbation in parameter θ_j that is obtained when all parameters are updated jointly, to the perturbation in θ_j when the parameter is estimated singly using only the *i*th output. If the magnitude of a particular RDG element is greater than 1, then interaction among the effects of parameters hinders disturbance tracking when the parameters are estimated jointly, and larger adjustments to the particular parameter are required than if it were adjusted singly to eliminate bias in the output of interest.

It is preferable to look for candidate sets of updateable parameters that give small RDG values for key disturbances. Smaller RDG values, and hence small adjustments in parameters, are preferable because large parameter changes can lead to physically unrealistic parameter values (e.g., negative values for kinetic rate constants or excessively large heat-transfer coefficients), which will cause unreliable model predictions. The RDG defined in eq 16 is particularly useful for determining when a specific parameter in a candidate set has no influence for steady-state tracking of key disturbances. It is highly desirable for practitioners to remove unnecessary updateable parameters from the state-estimation procedure. The fewer updateable parameters required in an EKF application, the easier the design and implementation of the EKF and the smaller the uncertainty in the resulting state estimates.[28]

The RDG is computed using a model that describes the way the disturbance variable, *d*, affects the behavior of the process states and outputs at steady state. This model is usually in implicit form:

$$\mathbf{g_D}(\mathbf{x_D}, d) = \mathbf{0}$$
$$\mathbf{y_D} = \mathbf{h_D}(\mathbf{x_D}, d) \tag{17}$$

The states, outputs, and functions in eq 17 have been written with the subscript "D" to indicate that eq 17 can be different from the model used to implement the EKF because the EKF model might not contain specific information on the effects of the particular disturbance of interest. Note that the states contained in $\mathbf{x_D}$ may differ from those in $\mathbf{x}$. However, the elements of $\mathbf{y_D}$ must be the same as the elements of $\mathbf{y}$.

After a change in *d*, the values of some states and outputs will change. The steady-state gains between *d*

and the states can be determined by differentiating the steady-state model (17) and then solving eq 18 for $\partial \mathbf{x_D}/\partial d$:

$$\frac{\partial \mathbf{g_D}}{\partial d} = \mathbf{0} = \frac{\partial \mathbf{g_D}}{\partial \mathbf{x_D}}\Big|_d \frac{\partial \mathbf{x_D}}{\partial d} + \frac{\partial \mathbf{g_D}}{\partial d} \tag{18}$$

The steady-state gains between the disturbance and the outputs are given by

$$\frac{\partial \mathbf{y_D}}{\partial d} = \frac{\partial \mathbf{h_D}}{\partial \mathbf{x_D}}\Big|_d \frac{\partial \mathbf{x_D}}{\partial d} + \frac{\partial \mathbf{h_D}}{\partial d}\Big|_{\mathbf{x_D}} \tag{19}$$

To determine the effect that the disturbance will have on the jointly updated model parameters, consider the steady-state model that is used by the EKF:

$$\mathbf{g}(\mathbf{x},\theta) = \mathbf{0}$$
$$\mathbf{y} = \mathbf{h}(\mathbf{x},\theta) = \mathbf{0} \tag{20}$$

When all the parameters are estimated, the effects of output changes on the values of the updateable parameters are given by the elements of

$$\frac{\partial \boldsymbol{\theta}}{\partial \mathbf{y}} = \left(\frac{\partial \mathbf{y}}{\partial \boldsymbol{\theta}}\right)^{-1} = \mathbf{K}^{-1} \tag{21}$$

where **K** is the same gain matrix that was used to compute the elements of the RGA. The numerator of each RDG element is the corresponding element of the vector:

$$\frac{\partial \boldsymbol{\theta}}{\partial d}\Big|_{\mathbf{y}=\mathbf{y_D}} = \frac{\partial \boldsymbol{\theta}}{\partial \mathbf{y}} \frac{\partial \mathbf{y_D}}{\partial d} \tag{22}$$

$\partial \mathbf{y_D}/\partial d$ is used in place of $\partial \mathbf{y}/\partial d$ in eq 22 because the parameters are adjusted to force the outputs from the EKF model in eq 20 to match the disturbed outputs from eq 17. The denominator for the ijth element of the RDG can be obtained from

$$\frac{\partial \theta_j}{\partial d}\Big|_{y_i=y_{\mathrm{D}i},\theta_{k,k\neq j}} = \frac{\partial \theta_j}{\partial y_i}\Big|_{\theta_{k,k\neq j}} \frac{\partial y_{\mathrm{D}i}}{\partial d} \tag{23}$$

where $\partial\theta_j/\partial y_i|_{\theta_{k,k\neq j}}$ is the reciprocal of $\partial y_i/\partial \theta_j|\theta_{k,k\neq j}$, which is an element of the gain matrix, **K**, in eq 11. Therefore, the elements of the RDG for parameter updating can be readily obtained using eqs 17−23.

Using RDG for Screening of Updateable Parameter Sets. Consider a disturbance in the comonomer consumption rate experienced by the plant. The comonomer consumption rate may vary as a result of a change in reactor operating temperature or a change in the properties of the catalyst. k_{p2} in eq 2 is a pseudo rate constant for butene consumption, which would be expected to change as the relative number of each type of active site on the catalyst changes.[41] The RDG values corresponding to an unmodeled disturbance, $d = k_{p2}$, are given by the elements of $\mathbf{B}_{\boldsymbol{\theta}}$:

$$\mathbf{B}_{\theta} = \begin{matrix} g_1 & k_d & k_{p2} \\ \end{matrix} \begin{bmatrix} 0.3(10^{-9}) & 0.8(10^{-9}) & 1.0 \\ 0 & -0.4(10^{-9}) & 1.0 \\ 0 & -0.4(10^{-11}) & 1.0 \end{bmatrix} \begin{matrix} [H_2] \\ P_R \\ [M_2] \end{matrix} \tag{24}$$

Since the columns of $\mathbf{B}_{\boldsymbol{\theta}}$ associated with parameters g_l and k_d are essentially 0, the RDG analysis indicates that adjustment of parameter k_{p2} can compensate for the effect of the disturbance on all three outputs. As a general rule, tracking of a disturbance that corresponds directly to one of the updateable parameters in the EKF model will require only that parameter be updated. There are also cases when only a single parameter is required to compensate for a disturbance that is not directly associated with an updateable parameter. For example, if a disturbance occurs in the concentration of active sites on the catalyst being fed to the reactor, the RDG elements for the updateable parameter set (g_l, k_d, k_{p2}) are

$$\mathbf{B}_{\boldsymbol{\theta}} = \begin{matrix} g_1 & k_d & k_{p2} \\ \end{matrix} \begin{bmatrix} -0.1(10^{-8}) & 1.0 & 0 \\ 0 & 1.0 & 0 \\ 0 & 1.0 & 0 \end{bmatrix} \begin{matrix} [H_2] \\ P_R \\ [M_2] \end{matrix} \tag{25}$$

indicating that disturbances in a_{cat} can be addressed by updating only k_d. These results were confirmed by simulation.[37]

If an unmeasured disturbance in the flow rate of comonomer occurs, using updateable parameters g_l, k_d, and k_{p2}, the RDG values are

$$\mathbf{B}_{\boldsymbol{\theta}} = \begin{matrix} g_1 & k_d & k_{p2} \\ \end{matrix} \begin{bmatrix} 3.9 & -2.7 & -0.2 \\ 0 & 1.2 & -0.2 \\ 0 & -0.1 & 1.1 \end{bmatrix} \begin{matrix} [H_2] \\ P_R \\ [M_2] \end{matrix} \tag{26}$$

indicating that there is interaction among the parameters when they are estimated jointly to track the comonomer feed rate disturbance. This interaction causes some of the parameters to require more adjustment during joint estimation than would have been required for single estimation. For example, to track $[H_2]$ and the other outputs, g_l must be changed by an amount that is 3.9 times greater than if only $[H_2]$ were being tracked by updating g_l alone. None of the elements in the RDG matrix in eq 26 are particularly large, so excessively large changes in parameters are not anticipated using the particular set of parameters to track the disturbance. The plots in Figure 1 show that, as anticipated by the RDG analysis, adjustments in all of the parameters were required at steady state to track this disturbance. RDG analysis is useful for determining whether there will be significant interaction among the parameters and which parameters will require adjustment to track the particular disturbance. RDG analysis does not provide much information on the absolute size of the parameter adjustments that will be required since it is a ratio of adjustments under different circumstances. For example, we were not able to predict from the RDG analysis that a fairly large change in k_{p2} would be required (compared to the size of the range or realistic values for k_{p2}), and only minor adjustments would be required for parameters g_l and k_d. Disturbance condition number (DCN) analysis, presented below, can give information on the extent of parameter adjustments and can thus be used to complement the RDG analysis when screening candidate sets of parameters for on-line updating.

Disturbance Condition Number. In its conventional form, the DCN[34] provides information about the effects of output disturbances on multivariable con-

Table 2. Disturbance Condition Numbers for Three Candidate Parameter Sets

parameter set	$\gamma_{\theta d}$ catalyst feed rate ($d = F_{cat}$)	$\gamma_{\theta d}$ catalyst sites ($d = a_{cat}$)	$\gamma_{\theta d}$ butene feed rate ($d = F_{M2}$)	$\gamma_{\theta d}$ butene consumption ($d = k_{p2}$)	$\gamma_{\theta d}$ hydrogen flow rate ($d = F_{H2}$)	$\gamma_{\theta d}$ bleed flow rate ($d = b$)	γ_θ worst case
1: (g_l, k_d, k_{p2})	1.001	1.001	65.06	75.32	178.4	178.7	181.9
2: (k_H, k_d, k_{p2})	1.001	1.001	65.06	75.32	234.9	235.3	239.4
3: (g_l, k_d, b_m)	1.001	1.001	1739	2018	178.4	89.17	2303

trolled processes, indicating the degree of difficulty for steady-state rejection of a particular disturbance relative to other types of disturbances. Conceptually, the DCN is the ratio of the effort required to reject a particular disturbance relative to the effort required to reject a disturbance in the best-case direction in which the least amount of adjustment is required. The control efforts computed for the ratio are each first normalized by the magnitudes of the respective output disturbances to remove effects of disturbance size.

The expression for the DCN can be determined by considering a small change in a disturbance variable, d, which would cause a steady-state change, $\boldsymbol{\delta}$, in the process outputs if no control action were taken. To eliminate the effects of this disturbance, the control system must adjust the manipulated variables by d$\mathbf{u}$,

$$\mathrm{d}\mathbf{u} = -\left(\frac{\partial \mathbf{y}}{\partial \mathbf{u}}\right)^{-1}\boldsymbol{\delta} \tag{27}$$

where $\partial\mathbf{y}/\partial\mathbf{u}$ evaluated at the nominal conditions represents the matrix of steady-state gains relating changes in manipulated variables to output changes (this is the same gain matrix used to compute the RGA). The DCN for this disturbance is defined as

$$\gamma_d = \frac{||\mathrm{d}\mathbf{u}||_2}{||\boldsymbol{\delta}||_2}\sigma_{max} \tag{28}$$

where the numerator and denominator in eq 28 are defined using Euclidean norms of the manipulated variable adjustments and the output changes, respectively, and σ_{max} is the largest singular value of the gain matrix $\partial\mathbf{y}/\partial\mathbf{u}$. The best-case disturbance direction corresponds to the direction in which the process gain is largest, i.e., the direction associated with the maximum singular value. As a result, the normalized best-case output change required is $1/\sigma_{max}$ which, when introduced into the denominator of the ratio of control efforts, leads to eq 28.

The DCN is valuable to control practitioners because it can identify types of disturbances that are difficult to reject because they require large steady-state adjustments in manipulated variables. Comparing the control adjustments for the specific disturbance against the best-case effort provides a useful benchmark that accounts for inherent process structure.

The DCN is bounded between unity (when the disturbance is in the best-case direction) and the plant condition number, $\gamma = \sigma_{max}/\sigma_{min}$ (when the disturbance is in the worst-case direction). Unlike the RGA and the RDG, the DCN is scale-dependent, so it is helpful to scale each manipulated variable and output variable by the size of its appropriate operating range before computing the Euclidean norms in eq 28. Matrix scaling can also be used to find the minimum condition number over all possible scalings;[34] however, the use of such techniques can result in the loss of physical insight.

The DCN supplements the plant condition number as a diagnostic for assessing the difficulty of controlling a process. While large plant condition numbers signify processes that are ill-conditioned and hence difficult to control in general, it is still possible that key disturbances could be readily rejected using modest control actions, even for an ill-conditioned plant. This possibility is reflected in the fact that the DCN is bounded between unity and the plant condition number. Thus, the DCN is an important tool beyond the plant condition number when considering disturbance rejection capabilities.

The DCN for Parameter Updating. The DCN can be extended and used as a screening tool for selecting sets of adjustable parameters in state-estimation problems. Consider a small change in disturbance variable, d, which would cause a steady-state bias, $\boldsymbol{\beta}$, between model predictions and plant outputs if model parameters were not updated. To eliminate this steady-state bias, the state estimator must adjust the vector of updateable parameters by d$\boldsymbol{\theta}$ where

$$\mathrm{d}\boldsymbol{\theta} = -\mathbf{K}^{-1}\boldsymbol{\beta} \tag{29}$$

The DCN for parameter updating can be calculated from

$$\gamma_{\theta d} = \frac{||\mathrm{d}\boldsymbol{\theta}||_2}{||\boldsymbol{\beta}||_2}\sigma_{\theta max} \tag{30}$$

where the numerator and denominator in eq 30 are Euclidean norms of the steady-state parameter adjustments and the output bias, respectively, and $\sigma_{\theta max}$ is the maximum singular value of the parametric gain matrix $\mathbf{K}$. $\gamma_{\theta d}$ is the ratio of the magnitude of steady-state parameter adjustments necessary to eliminate bias when a particular disturbance occurs to the magnitude of adjustments required for bias occurring in the best-case direction. The steady-state parameter adjustments used to determine this ratio are first normalized by the magnitudes of the respective bias vectors, which is analogous to the normalization used for conventional DCN calculations for control. Large values of $\gamma_{\theta d}$ indicate that substantial changes in updateable parameters will be required to track the disturbance, whereas small values indicate that only minor steady-state parameter adjustments will be required. The value of $\gamma_{\theta d}$ is bounded by unity (for the best-case bias direction) and by γ_θ, the condition number of $\mathbf{K}$ (for the worst-case bias direction).[37] Like the DCN for control, $\gamma_{\theta d}$ is scale-dependent, so each parameter and output-bias value should be scaled appropriately. Otherwise, choices of units for states, outputs, and parameters will influence the Euclidean norms, giving potentially misleading results.

Using Disturbance Condition Numbers for Screening of Updateable Parameter Sets. $\gamma_{\theta d}$ was computed for three candidate sets of updateable parameters and six different disturbances to illustrate the use of the DCN for parameter-set screening. The results are shown in Table 2. Before DCNs were calculated, pa-

Table 3. Scaling Factors Applied to Parameters and Outputs

variable	scaling factor	variable	scaling factor
b_m	52.0 kg h^{-1}	k_{p2}	1.068 L mol^{-1} h^{-1}
g_l	0.363 L s^{-1}	$[H_2]$	0.040 mol L^{-1}
k_d	0.0000 80 s^{-1}	P_R	23.5 T h^{-1}
k_H	0.028 L mol^{-1} s^{-1}	$[M_2]$	0.086 mol L^{-1}

rameters and outputs were first scaled by dividing by the corresponding factors in Table 3 to make each variable dimensionless. b_m was scaled by 10% of the nominal bleed stream flow rate used in the simulations in Figures 1−3 because the uncertainty in the bleed flow should rarely exceed 10%. Since the mismatch in the hydrogen mass balance can be considerable and even negative values of g_l are physically reasonable, g_l was scaled by its nominal value. k_d was scaled by 80% of its nominal value because, although it does not make physical sense for k_d to become negative, fluctuations in impurity levels within the reactor can have a large effect on catalyst-site deactivation rates. Kinetic parameters k_H and k_{p2} were each scaled by 10% of their nominal values because large changes in these kinetic parameters are not anticipated for the range of catalysts and operating conditions encountered in the reactor. The three output variables, $[H_2]$, P_R, and $[M_2]$, can change considerably during normal plant operation, especially during grade changeovers, so each output variable was scaled by its nominal value.

The DCN results in Table 2 are particularly helpful in deciding which set of parameters might be best for eliminating bias when key disturbances occur. The three parameter sets considered are (g_l, k_d, k_{p2}), (k_H, k_d, k_{p2}), and (g_l, k_d, b_m). Nearly diagonal RGA results were obtained for all three parameter sets,[37] indicating that they show promise for online updating because there is little two-way correlation among the effects of the parameters on the outputs.

As shown in Table 2, all three parameter sets require only small parameter changes to track disturbances in catalyst feed rate and active-site concentration. $\gamma_{\theta d}$ for these disturbances is close to unity, indicating that these disturbances result in bias in the best-case direction for parameter updating. It is not surprising that all three parameter sets give best-case DCN values for tracking these disturbances because RDG analysis indicates that k_d, which is included in all three parameter sets, is the only parameter that must be updated to account for disturbances in either F_{cat} or a_{cat}.[37] The scaling, prescribed in Table 3, reduces the effect of k_d on $||d\boldsymbol{\theta}||_2$ so that changes in k_d are penalized very little in DCN calculations. As a result of the prescribed scaling, and also the large sensitivity of outputs P_R and $[M_2]$ to changes in k_d, bias that can be addressed by updating k_d occurs in the best-case direction. An important feature of DCN analysis is that it allows the practitioner to appropriately scale changes in different model parameters to reflect whether it is physically realistic for large changes to occur in each parameter. Analogous information about appropriate sizes of parameter adjustments can be incorporated into the state-estimation scheme via elements of the model-uncertainty covariance matrix once a particular parameter set has been chosen for on-line updating and the state estimator has been implemented.

The DCNs for butene feed and consumption-rate disturbances in Table 2 indicate that parameter sets 1 and 2 require significantly less parameter-updating effort than parameter set 3 to track these disturbances, which affect $[M_2]$ and P_R. As such, either set 1 or set 2 would be preferable to set 3 for tracking the disturbances. The results for parameter sets 1 and 2 are identical because butene feed rate and consumption rate disturbances have very little effect on $[H_2]$ (see Figure 1), and $[H_2]$ is the only output that is influenced by parameters g_l and a_{cat}. The values of $\gamma_{\theta d}$ for parameter set 3 are very large, and similar to the worst-case DCN for this parameter, indicating that tracking of butene feed and consumption-rate disturbances using parameter set 3 would require large changes in the updateable parameters.

The DCNs in Table 2 indicate that unmeasured disturbances in the bleed flow rate and hydrogen feed rate lead to bias in what is essentially the worst-case direction for parameter sets 1 and 2 since the values of $\gamma_{\theta d}$ are similar to those of the plant condition numbers. The values of $\gamma_{\theta d}$ and γ_θ for parameter set 1 are smaller than those for set 2 because smaller adjustments to the scaled value of g_l, compared to corresponding changes to the scaled value of k_H, would be required to track the disturbances. The bleed flow and hydrogen feed disturbances occur in a more favorable direction for parameter set 3, leading to less parameter-updating effort than if set 1 were used. On the basis of the steady-state DCN results in Table 2, it appears that parameter set 1 shows the most promise for tracking these particular disturbances.

The DCN provides useful information, beyond that provided by the plant condition number, and should be considered during the selection of updateable parameters. Note that, for parameter set 1 in Table 2, assessing the ability to track a catalyst feed rate disturbance strictly on the basis of the plant condition number (specifically, the condition number of the parametric sensitivity matrix) would lead to the conclusion that the estimation problem is ill-conditioned since the condition number is 181.9. However, as noted in the preceding discussion, the catalyst feed rate disturbance enters in essentially the best-case direction and can thus be tracked readily, as is indicated by the DCN of 1.0 for this disturbance.

DCN analysis complements RGA and RDG analysis for screening candidate sets of parameters for on-line updating. It is a helpful tool for screening sets of parameters because it can flag parameter sets that will result in large parameter adjustments when specific types of disturbances are encountered.

Parameter Selection in Larger Scale and Highly Nonlinear Systems. For the polyethylene example in this paper, the goal was to select three parameters for updating from the six possible candidates in Table 1. As a result, there are

$$\binom{6}{3} = 20$$

possible combinations of parameters that could be selected and analyzed using RGA, DCN, and RDG. In larger scale systems, with more outputs and more candidate parameters to choose from, the number of combinations that the practitioner may choose to analyze can become very large. We recommend that the calculations be performed using a symbolic computation package such as Maple, which we have used to perform the RGA, RDG, and DCN computations in this article. We also recommend that RGA analyses be performed

first to screen out the majority of unacceptable parameters sets before considering responses to key disturbances using RDG and DCN analyses. In large-scale systems, it is more difficult for practitioners to gain intuitive knowledge about interactions among parameters and outputs in their models. It is also more difficult and time-consuming to screen candidate sets of parameters using EKF simulations. As a result, we anticipate that RGA, RDG, and DCN will be particularly useful for parameter selection in large-scale models, even though the proposed screening method can require analysis of a large number of candidate parameter sets.

A nominal steady-state operating point is required to compute the sensitivity matrix, **K** (eq 11) used to determine the RGA, RDG, and DCN. If the process model is highly nonlinear (so that elements of **K** change significantly over the intended range of operation), then analyses for the most promising candidate sets of parameters should be repeated at several steady-state points from different parts of the operating region to confirm that the most promising parameter sets will be effective. A more comprehensive view of local steady-state parameter updating behavior can be obtained by plotting a surface of RGA, RDG, or DCN numbers over the operating region, as suggested by Piette et al.[42] It may be possible to extend nonlinear interaction measures such as those proposed by Guay et al.[43] to the parameter updating case; however, the complexity of the computations and interpretation would be significantly increased.

Finally, since the RGA, RDG, and DCN are computed using steady-state information only, dynamic simulations should be performed before the EKF is implemented to ensure that the combined state-estimation and parameter-updating scheme is properly tuned and provides good dynamic performance. However, a benefit of using the diagnostics proposed in this article is that a smaller number of simulations should be required to test the parameter and state-estimation scheme compared to a traditional trial-and-error parameter-selection approach.

Conclusions

This article demonstrates the utility of extending diagnostic tools traditionally used for design of control schemes to the design of on-line state and parameter-estimation schemes. The RGA, RDG, and DCN were extended by drawing analogies between manipulated-variable/controlled-variable relationships in multivariable process control and updateable-parameter/output-variable relationships in on-line parameter estimation. A polyethylene reactor example was used to illustrate the application of the new tools for screening candidate sets of updateable parameters.

The steady-state RGA was extended from its standard use for assessing transmission interaction between controlled and manipulated variables to a new use for assessing transmission interaction between updateable parameters and model outputs. In this new setting, the RGA can be used to assess whether correlation among the effects of updateable parameters on the model outputs will lead to difficulties during joint parameter estimation. The polyethylene reactor example was used to show that parameter sets exhibiting minor transmission interaction could be updated successfully by an EKF and that parameter sets that exhibit large transmission interaction were unable to track process changes successfully.

The RDG was extended from a process-control setting to a new state-estimation setting where it can be used to examine the effects of interaction on the tracking of disturbances. RDG analysis was shown to be useful for determining whether adjustments in all of the updateable parameters are required to track particular disturbances. If the types of disturbances that will be encountered by a state estimator are known a priori, RDG analysis can be used to determine whether the number of parameters that are updated on-line can be reduced, leading to a simplified state estimator and improved precision of state and parameter estimates.

The steady-state DCN was successfully extended from its multivariable control setting where it is used to assess the ease of disturbance rejection to a state- and parameter-estimation setting where it is used to determine the extent of updateable parameter adjustments required to track disturbances. The DCN can be used to screen out parameter sets that will require excessive adjustment of parameters when important disturbances are encountered. Unlike the RGA and RDG, DCN results are scale-dependent. Appropriate scaling of parameters and output variables ensures that meaningful results are obtained.

The RGA, RDG, and DCN for parameter updating are easy to use, requiring computations involving gains from steady-state process models that can readily be computed using symbolic computation programs such as Maple. Together, the RGA, RDG, and DCN can be used to screen out undesirable sets of updateable parameters before the practitioner conducts simulations to test the dynamic performance of proposed state-estimation schemes. The parameter screening results obtained using a gas-phase polyethylene reactor model example agreed well with the results of dynamic simulations and our prior physical understanding of parameter effects in the model, confirming the predictions from the screening tools.

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Nomenclature

a_{cat} = concentration of sites on the fresh catalyst fed to the reactor
b = measured bleed stream flow rate
B_{ij} = RDG element for a specific input/output pair
b_m = bleed stream flow rate uncertainty
B_w = mass of polymer in the fluidized bed
$[C_T]$ = total concentration of all gas-phase components
d = disturbance variable
F_{cat} = fresh feed rate of catalyst
F_{H2} = fresh feed rate of hydrogen
F_{M2} = fresh feed rate of comonomer
$\mathbf{g}$ = vector of right-hand sides of dynamic model
$\mathbf{g_D}$ = vector of right-hand sides of dynamic model that describes the effect of the disturbance
g_l = mismatch factor accounting for uncertainty in the hydrogen mass balance
$\mathbf{h}$ = vector of output functions
$\mathbf{h_D}$ = vector of output functions that describe the effect of the disturbance
$[H_2]$ = concentration of hydrogen

$\mathbf{K}(t_k)$ = Kalman gain matrix computed using information available at time k
k_d = catalyst site deactivation rate constant
k_H = kinetic rate constant for the consumption of hydrogen
k_{p1} = kinetic rate constant for the consumption of ethylene
k_{p2} = kinetic rate constant for the consumption of comonomer
$[M_1]$ = concentration of ethylene
$[M_2]$ = concentration of comonomer
m_{w1} = molecular weight of ethylene
m_{w2} = molecular weight of comonomer
O_p = polymer outflow rate
P_R = production rate
S = solubility of butene in the polymer
t = time
t_k = time at which the kth set of process measurements is made
$\mathbf{u}$ = vector of manipulated variables
u_j = jth element of the vector of manipulated variables
V_g = volume of gas phase in the polyethylene reactor
V_s = equivalent volume of butene that is dissolved in polyethylene
$\mathbf{x}$ = vector of states
$\mathbf{x_{aug}}$ = state vector augmented by updateable parameters
$\mathbf{x_D}$ = state vector from the model that describes the effects of the disturbance
y_i = ith output variable
$\mathbf{y}$ = vector of outputs
$\mathbf{y_D}$ = vector of outputs from the model which describes the effects of the disturbance
Y = moles of active catalyst sites in the reactor

Greek Symbols

$\boldsymbol{\beta}$ = bias vector
β_{ij} = ijth RDG element
$\beta_{\theta ij}$ = ijth RDG element for parameter updating
$\mathbf{B}_\theta$ = relative disturbance gain matrix
$\boldsymbol{\delta}$ = vector of changes in process outputs
λ_{ij} = ijth element of the relative gain array
$\lambda_{\theta ij}$ = ijth element of the relative gain array for parameter updating
$\boldsymbol{\Lambda}$ = relative gain array
$\boldsymbol{\Lambda_\theta}$ = relative gain array for parameter updating
$\mathbf{K}$ = gain matrix between parameters and outputs
$\boldsymbol{\theta}$ = updateable parameter vector
θ_j = jth updateable parameter
γ_d = disturbance condition number
$\gamma_{\theta d}$ = disturbance condition number for updateable parameter adjustments
σ_{min} = smallest singular value
σ_{max} = largest singular value
$\sigma_{\theta max}$ = largest singular value of parametric gain matrix $\mathbf{K}$

Acronyms

DCN = disturbance condition number
EKF = extended Kalman filter
RDG = relative disturbance gain
RGA = relative gain array

Literature Cited

(1) Stengel, R. F. *Optimal Control and Estimation;* Dover: New York, 1994.

(2) Agarwal, M.; Bonvin, D. Improved State Estimator in the Face of Unreliable Parameters. *J. Procress Control* **1991**, *1*, 251.

(3) Venkateswarlu, C.; Gangiah, K. Dynamic Modeling and Optimal State Estimation Using Extended Kalman Filter for a Kraft Pulping Digester. *Ind. Eng. Chem. Res.* **1992**, *31*, 848.

(4) Ricker, N. L.; Lee, J. H. Nonlinear Modeling and State Estimation for the Tennessee Eastman Challenge Process. *Comput. Chem. Eng.* **1995**, *19*, 983.

(5) Yang, D. R.; Lee, D. S. Monitoring of a Distillation Column Using Modified Extended Kalman Filter and a Reduced Order Model. *Comput. Chem. Eng.* **1997**, *21*, S565.

(6) Soroush, M. State and Parameter Estimations and their Applications in Process Control. *Comput. Chem. Eng.* **1998**, *23*, 229.

(7) Bastin, G.; Dochain, D. *On-Line Estimation and Adaptive Control of Bioreactors*; Elsevier: Amsterdam, 1990.

(8) Gudi, R. D.; Shah, S. L.; Gray, M. R. Adaptive Multirate State and Parameter Estimation Strategies with Application to a Bioreactor. *AIChE J.* **1995**, *41*, 2451.

(9) Myers, M. A.; Kang, S.; Luecke, R. H. State Estimation and Control for Systems with Delayed Off-Line Measurements. *Comput. Chem. Eng.* **1996**, *20*, 585.

(10) Jo, J. H.; Bankoff, S. G. Digital Monitoring and Estimation of Polymerization Reactors. *AIChE J.* **1976**, *11*, 361.

(11) Ellis, M. F.; Taylor, T. W.; Gonzalez, V.; Jensen, K. F. Estimation of the Molecular Weight Distribution in Batch Polymerization. *AIChE J.* **1988**, *34*, 1341.

(12) Adebekun, D. K.; Schork, F. J. Continuous Solution Polymerization Reactor Control. 2. Estimation and Nonlinear Reference Control during Methyl Methacrylate Polymerization. *Ind. Eng. Chem. Res.* **1989**, *28*, 1846.

(13) Gagnon, L.; MacGregor, J. F. State Estimation for Continuous Emulsion Polymerization. *Can. J. Chem. Eng.* **1991**, *69*, 648.

(14) Kim, J. K.; Choi, K. Y. On-line Estimation and Control of a Continuous Stirred Tank Polymerization Reactor. *J. Process Control* **1991,** *1*, 96.

(15) McAuley, K. B.; MacGregor, J. F. On-Line Inference of Polymer Properties in an Industrial Polyethylene Reactor. *AIChE J.* **1991**, *37*, 825.

(16) Kozub, D. J.; MacGregor, J. F. State Estimation for Semi-Batch Polymerization Reactors. *Chem. Eng. Sci.* **1992**, *47*, 1047.

(17) McAuley, K. B.; MacGregor, J. F. Nonlinear Product Property Control in Industrial Gas-Phase Polyethylene Reactors. *AIChE J.* **1993**, *39*, 855.

(18) Ellis, M. F.; Taylor, T. W.; Jensen, K. F. On-Line Molecular Weight Distribution Estimation and Control in Batch Polymerization. *AIChE J.* **1994**, *40*, 445.

(19) Ogunnaike, B. A. On-line Modeling and Predictive Control of and Industrial Terpolymerization Reactor. *Int. J. Control* **1994**, *50*, 711.

(20) Elicabe, G. E.; Ozdeger, E.; Georgakis, C.; Cordeiro, C. On-Line Estimation of Reaction Rates in Semicontinuous Reactors. *Ind. Eng. Chem. Res.* **1995**, *34*, 1219.

(21) Semino, D.; Morretta, M.; Scali, C. Parameter Estimation in Extended Kalman Filters for Quality Control in Polymerization Reactors. *Comput. Chem. Eng.* **1996**, *20*, S913.

(22) Clarke-Pringle, T.; MacGregor, J. F. Nonlinear Adaptive Temperature Control of Multi-Product Semi-Batch Polymerization Reactors. *Comput. Chem. Eng.* **1997**, *21*, 1395.

(23) Mutha, R. K.; Cluett, W. R.; Penlidis, A. A New Multirate-Measurement-Based Estimator: Emulsion Copolymerization Batch Reactor Case Study. *Ind. Eng. Chem. Res.* **1997**, *36*, 1036.

(24) Scali, C.; Morretta, M.; Semino, D. Control of the Quality of Polymer Products in Continuous Reactors: Comparison of Performance of State Estimators with and without Updating of Parameters. *J. Process Control* **1997**, *7*, 357.

(25) Tatiraju, S.; Soroush, M. Nonlinear State Estimation in a Polymer Reactor. *Ind. Eng. Chem. Res.* **1997**, *36*, 2679.

(26) MacGregor, J. F. Control of Polymerization Reactors. *Polym. Process Eng.* **1984**, *2*, 179.

(27) Keller, J. Y.; Darouach, M. Optimal Two-Stage Kalman Filter in the Presence of Random Bias. *Automatica* **1997**, *33*, 1745.

(28) Patton, M. S. Describing Uncertainty in State Estimates. M.Sc. (Eng.) Thesis, Queen's University, Kingston, Canada, 2000.

(29) Seber, G. A. F.; Wild, C. J. *Nonlinear Regression*; Wiley: New York, 1989.

(30) Vajda, S.; Rabitz, H.; Walter, E.; Lecourtier, Y. Qualitative and quantitative identifiability analysis of nonlinear chemical kinetic models. *Chem. Eng. Commun.* **1989**, *83*, 191.

(31) Weijers, S. R.; Vanrolleghem, P. A. A Procedure for Selecting Best Identifiable Parameters in Calibrating Activated Sludge Model No. 1 to Full-Scale Plant Data. *Water Sci. Technol.* **1997**, *5*, 69.

(32) Bristol, E. On a New Measure of Interaction for Multivariable Process Control. *IEEE Trans. Autom. Control* 1**966**, AC-11, 133.

(33) Stanley, G.; Marino-Galarraga, M.; McAvoy, T. J. Shortcut Operability Analysis. 1. The Relative Disturbance Gain. *Ind. Eng. Chem. Process Des. Dev.* **1985**, *24*, 1181.

(34) Skogestad, S.; Morari, M. Effect of Disturbance Directions on Closed-Loop Performance. *Ind. Eng. Chem. Res.* **1987**, *26*, 2029.

(35) Sulieman, H.; McLellan, P. J.; Bacon, D. W. A profile-based approach to parametric sensitivity analysis of nonlinear regression models. *Technometrics* **2001**, in press.

(36) Xie, T.; McAuley, K. B.; Hsu, J. C. C.; Bacon, D. W. Gas-Phase Ethylene Polymerization: Production Processes, Polymer Properties and Reactor Modeling. *Ind. Eng. Chem. Res.* **1994**, *33*, 449.

(37) Sandink, C. A. Screening Diagnostics for Parameter Selection in Extended Kalman Filter Implementations. M.Sc. (Eng.) Thesis, Queen's University, Kingston, Canada, 1999.

(38) Bates, D. M.; Watts, D. G. *Nonlinear Regression Analysis and Its Applications*; Wiley: New York, 1988.

(39) McAvoy, T. J. *Interaction Analysis: Principles and Applications*; Instrument Society of America: Research Triangle Park, NC, 1983.

(40) Marino-Galarraga, M.; McAvoy, T. J.; Marlin, T. E. Short-Cut Operability Analysis. 3. Short-Cut Methodology for the Assessment of Process Control Designs. *Ind. Eng. Chem. Res.* **1987**, *26*, 521.

(41) McAuley, K. B.; MacGregor, J. F.; Hamielec, A. E. A Kinetic Model for Industrial Gas-Phase Ethylene Copolymerization. *AIChE J.* **1990**, *36*, 837.

(42) Piette, R.; Harrist, T. J.; McLellan, P. J. Graphical interpretations of steady-state interaction measures. *Ind. Eng. Chem. Res.* **1995**, *34*, 4436.

(43) Guay, M.; McLellan, P. J.; Bacon, D. W. Measure of Closed-Loop Nonlinearity and Interaction for Nonlinear Chemical Processes. *AIChE J.* **1997**, *43*, 2261.

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