On-Line Optimizing Control of a Packed-Bed Immobilized-Cell Reactor

On-line optimizing control has been used to find and track the economically optimal operating conditions of a packed-bed reactor. The continuous reactor under study converts the ammonium salt of fumaric acid to aspartic acid using whole cells immobilizing in K-carrageenan beads. The on-line optimizing control was performed using a least-squares recursive estimation algorithm with a variable forgetting factor to estimate the parameters in a linear discrete-time model. A Newton optimization procedure used these parameters to calculate the direction and distance to the optimal conditions. Features found to enhance the speed and stability of the algorithm included the use of a variable forgetting factor algorithm, both low- and high-pass filtering of the data, outlier rejection, and linearizing input-outupt transformations.

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Introduction

Optimizing control deals with the problem of changing the operating conditions of a continuous process to bring it to its economic optimum. The direct search methods are the simplest, and these can be implemented using either gradient- or pattern-type search methods; Edler et al. (1970) provide a review. These are steady state procedures requiring that the process be settled before observations can be made. For processes with long transients or disturbances resulting in drifts (such as catalyst deactivation), these methods work poorly.

In 1978, Bamberger and Isermann suggested recursively identifying a dynamic model of the system, thus characterizing the plant based on transient data and eliminating the need to wait for steady states. The dynamic model is then simplified to a steady state model and this is used to deduce the direction to the optimum.

Garcia and Morari (1981) showed in simulations that the advantages of high convergence speed and noise tolerance were retained in the multivariable extension of the algorithm.

Rolf and Lim (1984, 1985) applied this method to optimizing the volumetric productivity of a baker's yeast fermentation in a chemostat through the selection of the optimal dilution flow rate. At a residence time of about 4 h, a sampling interval of 8 min resulted in the maximum parameter convergence rate. The optimal flow rate was recalculated every 2 h. No excitation beyond changes in the optimum flow was used except for an initial 30 h period where an M (pseudorandom) sequence was used to excite the chemostat to get good initial parameter estimates. In their study, a recursive least-squares algorithm with a fixed forgetting factor was used for parameter estimation and the simple steepest descent algorithm performed the optimization. The ability of this algorithm to track changes in the optimum conditions was tested by changing the feed concentration. When the optimum moved to lower dilution rates (4.5 h residence time) convergence was slow (50 to 90 h) and considerable undershoot in dilution rate was experienced. When the optimum moved to higher residence times and smaller step sizes were used, convergence was faster (20 h) and much smoother.

The application of on-line optimizing control to a nonlinear distributed-parameter system was performed recently by Lee and Lee (1985). A pilot scale packed-bed reactor for the conversion of *n*-butane to maleic anhydride was optimized. Residence time and bed temperature were manipulated to maximize a simple profit function. The reactor had a residence time of 1 to 4 s; however, its thermal time constant may have been several minutes. The system was sampled once a minute with optimizations performed once every 100 min. Excitation in the form of a pseudorandom binary sequence was superimposed upon the levels selected by the optimizer throughout the experiments. The system was moved to the optimum conditions in a reasonable number of optimization steps (less than 10); but because 100 samples were required before each step, the overall rate of convergence was quite slow. Efforts to reduce the number of samples resulted in unacceptably large overshoots, perhaps because of the inability of the second-order Hammerstein model to represent the dynamics of the process.

These two papers indicate that on-line optimizing control using recursively estimated dynamic models does work, but convergence rates in practice often fall below those predicted by simulation. In our work, several improvements to these ideas were used to speed convergence, reject noise, and tolerate highly nonlinear processes.

Experimental Method

In this study the process to be optimized is the commercially important conversion of ammonium fumarate to 1-aspartic acid. This process uses the cells of whole *E. coli* immobilized in beads of K-carrageenan packed in a 1 × 12 in. (25 × 305 mm) glass column. The immobilization procedure is described by Nishida et al. (1979). Reactors of this type have a finite life owing to slow deactivation of the aspartase enzyme and mechanical degradation of the beads most probably due to a loss of crosslinking bonds. During the lifetime of a column, the optimal operating conditions drift; for example, the optimal flow rate moves from high flows at the start to low, marginally profitable flows at the end. In addition, disturbances in substrate composition, impurities, and column temperatures result in shifts in the optimum operating conditions.

For the purpose of this study, the manipulated variable was the flow rate through the reactor since it had the largest effect on operating profit. The overall profit function included the feed costs, reactor costs, and drying costs. The feed costs are proportional to throughput, whereas for crystallization and drying operations, second-order response surfaces were used to relate product purity and yield to the outlet composition and column throughput. When these costs are combined the following profit function results:

$$p = a_1 + a_2 f + a_3 fc + a_4 fc^2 + a_5 fc^3 \tag{1}$$

where p is the profit, f is the flow rate, and c is the conversion of fumaric acid. The values of the coefficients given in the Notation section have been scaled to represent the economics of a larger column.

The concentration of residual fumaric acid was measured online using a UV detector at 280 nm. The feed was nominally a 1 molar ammonium fumarate solution at pH 8.5, and containing 200 mg/L of MgCl as an enzyme cofactor.

The real-time data acquisition was performed by a Hewlett-Packard A600 minicomupter. The software was written inhouse and simultaneously controls much of our pilot-scale and laboratory-scale equipment.

Column performance

There are a number of features of this column that make it challenging for on-line optimizing control. First, the operating range is wide; the optimal feed flow varies from less than 1 to more than 5 mL/min. The conversion, even at steady state, is not a linear function of flow over this range. Several simple input-output linearizing transformations were tried and the one that best linearized the steady state operating curves was the logarithm of the residual fumaric acid concentration vs. the logarithm of the residence time. This is shown in Figure 1. The reason for transforming the input and output variables such that the steady state operating curve becomes a straight line is to make the steady state gain independent of operating point (i.e., residence time) and more indicative of the overall column performance. This results in steadier parameter estimates, which reduces the time for parameter convergence, which in turn contributes to faster convergence to the optimum.

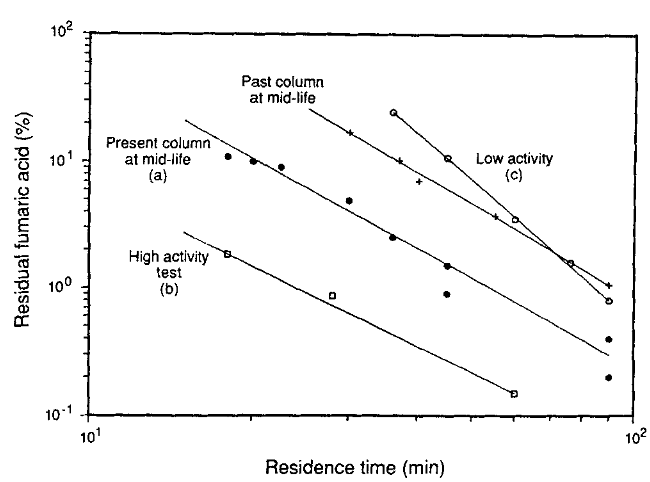

Figure 1. Steady state operating curves.

The residence times were based on a nominal void volume of 90 mL. The actual liquid void volume varied widely, mainly owing to trapped gas bubbles, which displaced the liquid. Periodic removal of these bubbles was necessary and was accomplished by rapidly depressurizing the column.

The results of step tests are shown in Figure 2, and a number of features deserve mention. First is the pure delay, which is due to the volume of the exit line between the top of the column and the detector (approx. 15 mL). The actual delay depends on the flow rate (3 to 15 min, assuming plug flow). The second feature is the approximate first-order response following the delay, and finally the long transients and noise, which delay the settling to steady state for a considerable time. It is these transients, along with the drifting nature of the column, which make optimization techniques based on steady states unattractive.

In order to model the dynamic response using a linear model, the model output y was based on the log of the residual fumaric acid concentration, and the input u was based on the log of the time duration that the detector sample had spent in the packed-bed portion of the column. This time duration was calculated simply from a stack of the flow rates that had been used and an assumption of plug flow through the nominal volumes in both the bed and the exit line. Thus the variable dead time is explicitly accounted for as a pure transport delay. Identification experiments were performed using pseudorandom binary sequence inputs. An off-line time series analysis of these data using the transformed inputs and outputs showed that a first-order linear discrete-time model could adequately describe the data.

$$y(k+1) = \theta_1 y(k) + \theta_2 u(k) + \theta_3 \tag{2}$$

A sample interval of 5 min placed the pole in the range of 0.3 to 0.8, depending mostly on the age of the column.

Recursive Estimation Algorithm

A recursive least-squares algorithm was used to estimate the parameters in the discrete-time dynamic model. Recent papers describing on-line optimizing control have both used least-squares and instrumental-variables methods, the latter giving less biased estimates. Simulations by Garcia and Morari (1981) and Rolf and Lim (1984) showed little difference between these

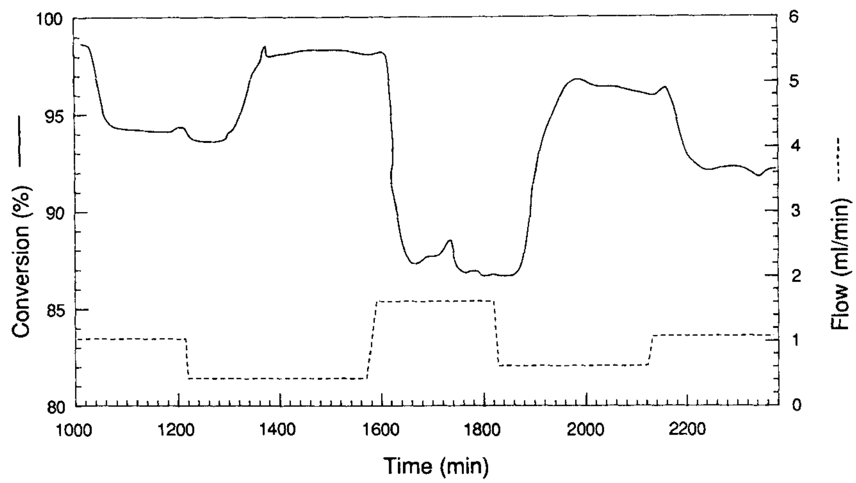

Figure 2. Step-test data.

methods when used in on-line optimizing control, so the simpler least-squares algorithm was used. Potter's square-root algorithm (Ljung and Soderstrom, 1983) was required to maintain a positive definite covariance matrix while using single precision calculations. The recursive estimation was examined with both fixed and variable forgetting factors, and the algorithm with the variable forgetting factor (Fortescue et al., 1981) was selected because it converged to steady parameter estimates faster. This agrees with the simulations done by Harmon et al. (1985).

To reduce the level of high-frequency noise present in the output, 36 samples were taken 1 s apart and their average was used every 5 min in the estimation. The variable forgetting-factor algorithm remained vulnerable to the apparently high information content of large disturbances passing through the detector. To solve this problem, a maximum error bound (0.15) was placed on the prediction error, and when the error exceeded this bound the prediction was used in place of the observation (Ljung and Soderstrom, 1983).

In on-line optimizing control, the model is used primarily as a means to obtain the steady state process gain. This depends on all parameters in the model except one, the bias or offset parameter. Unfortunately, changes in true system gain can be partly explained by changing the model bias, and vice versa. Faster convergence to the correct steady state gain was found if both the input and output sequences were passed through a high-pass digital filter to remove the steady component. No first- or second-order filter was found to work better than simple differencing. In this form, the value of the steady state gain was found robust to variations in the assumed orders of the numerator and denominator of the model. It was also reasonably insensitive to small (i.e., $\pm 20\%$) variations in the assumed column volume and the assumed exit-line volume.

Optimization Algorithm

The optimization algorithm takes the estimated steady state gain, the conversion, and the nominal residence time associated with each sample and predicts the flow rate that would optimize Eq. 1. Use is made of the nonlinearities captured in the input-

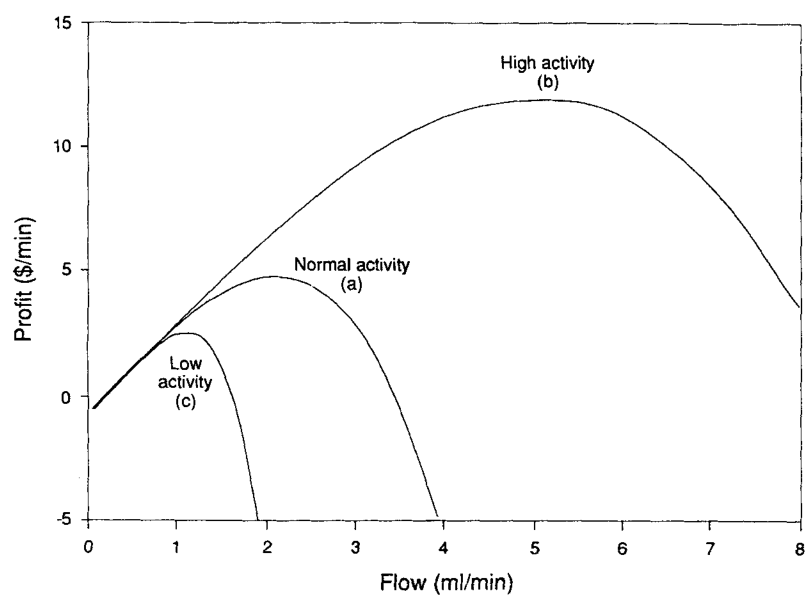

Figure 3. Steady state profit curves.

output transformations. The first and second derivatives of conversion with respect to flow are

$$\frac{dc}{df} = \frac{e^u e^y}{V_\epsilon}\frac{dy}{du} \tag{3}$$

$$\frac{d^2c}{df^2} = -\frac{e^{2u}e^y}{(V_\epsilon)^2}\frac{dy}{du}\left(1 + \frac{dy}{du}\right) \tag{4}$$

where V_ϵ is the nominal reactor void volume occupied by fluid, u is the logarithm of the residence time, and y is the logarithm of the residual fumaric acid. Quantity dy/du is the steady state gain in transformed variables as shown by the slope of the operating curve in Figure 1. These equations are then used in calculating the first and second derivatives of the profit with respect to flow

$$\frac{dp}{df} = a_2 + a_3c + a_3f\frac{dc}{df} + a_4c^2 + 2a_4fc\frac{dc}{df} + a_5c^3 + 3a_5fc^2\frac{dc}{df} \tag{5}$$

$$\frac{d^2p}{df^2} = 2a_3\frac{dc}{df} + a_3f\frac{d^2c}{df^2} + 4a_4c\frac{dc}{df} + 2a_4f\left(\frac{dc}{df}\right)^2 + 2a_4fc\frac{d^2c}{df^2} + 6a_5c^2\frac{dc}{df} + 6a_5fc\left(\frac{dc}{df}\right)^2 + 3a_5fc^2\frac{d^2c}{df^2} \tag{6}$$

Since first- and second-order information is available, a full Newton optimization method is employed to determine the optimum flow rate.

$$f_{opt} = f_{sample} - \alpha\frac{\dfrac{dp}{df}}{\dfrac{d^2p}{df^2}} \tag{7}$$

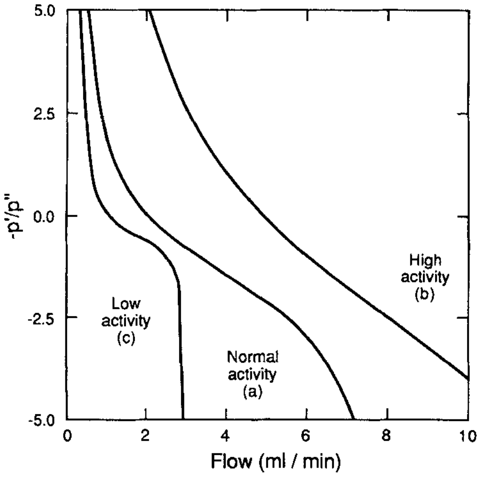

Figure 4. Predicted distance from optimal flow as a function of operating condition.

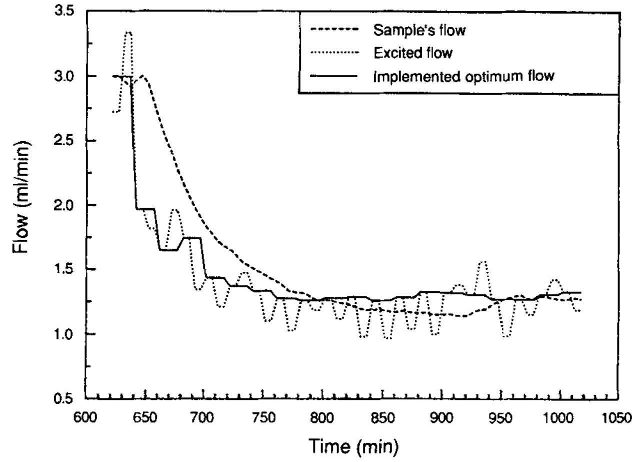

Figure 5. Flow rate at start-up of on-line optimization.

where f_{sample} is the steady flow rate that would produce the nominal residence time spent by the sample in the packed bed.

If the straight-line operating curves marked in Figure 1 are assumed, the profit functions shown in Figure 3 would exist and the correction to obtain the optimal flow rate given in Eq. 7 would be as shown in Figure 4. Figure 4 shows that the algorithm is expected to overshoot possibly when increasing the flow to achieve the optimum, but to have no problems when reducing the flow. For this reason α in Eq. 7 was chosen as 0.5, and the maximum step size in flow rate was limited to ± 1.0 mL/min.

Because of the nonlinear input-output transformations, Eqs. 3–6 depend on conversion and flow as well as steady state gain. The conversion referred to should actually be the conversion that would result at steady state at the residence time of the sample. Since the steady state offset parameter is not being estimated at the same time as the other parameters, estimating steady state conversion requires a second estimation step. This does not affect the convergence speed of the algorithm, but it does affect the steadiness of the predicted optimum. Tests performed with and without the correction to the steady state conversion showed little difference, since the bounce in the predicted optimum flow due to the dynamics of the output was less than the excitation added to the optimum to make the system observable in the presence of noise.

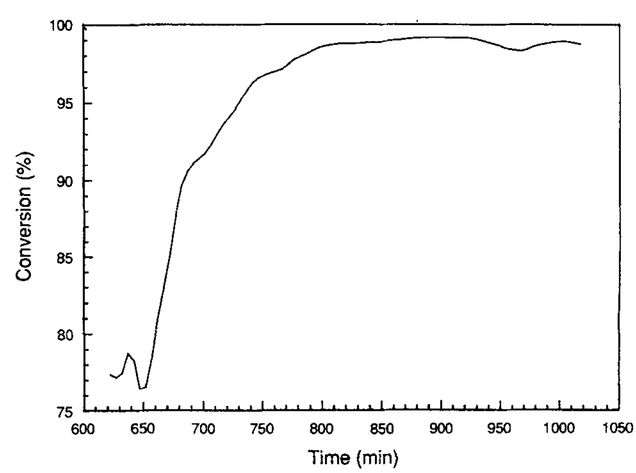

Figure 6. Conversion at start-up of on-line optimization.

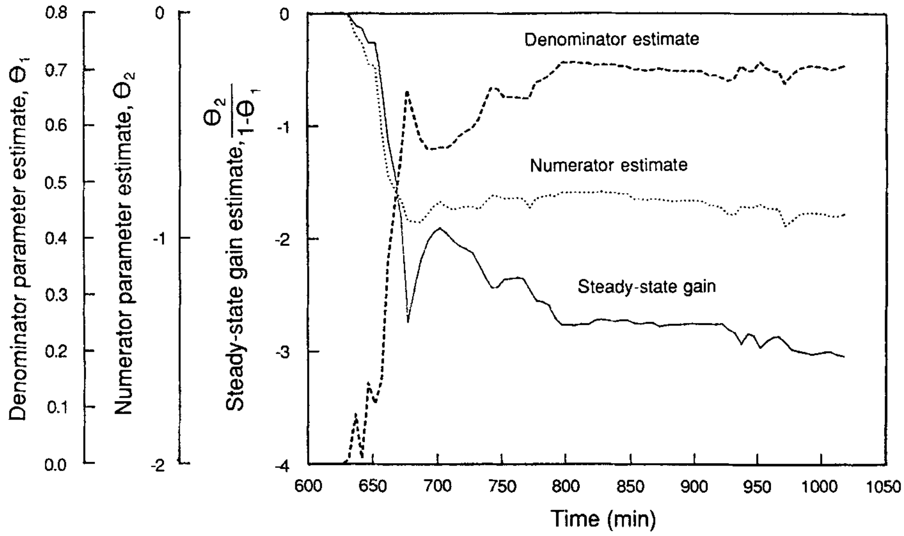

Figure 7. Parameter estimates at start-up of on-line optimization.

Results

Two features of the on-line optimizing algorithm that affected the convergence rate and performance were the excitation used to make the system observable and the frequency at which the optimization was performed. Both of these variables were investigated experimentally. The level of excitation was determined by a random number from a uniform distribution, which was scaled to be a fixed percentage of the optimum flow rate. When the excitation level was changed every 5 min, it was found that very little signal was reaching the detector. Rather than increasing the magnitude of the excitation, we extended its duration to 10 min, with the parameter estimation still being done every 5 min.

The frequency of the optimization can limit the rate at which the algorithm can track the optimum. Rolf and Lim (1985) found it necessary to wait for 15 estimations between optimizations, and Lee and Lee (1985) found that 100 were necessary. Various optimization intervals were tested, and good results were obtained by optimizing after every other excitation, or after every fourth estimation. In our algorithm, no excitation is added in the period immediately following the optimization; instead the suggested optimum flow rate itself is used.

It was found that it was possible to start both estimation and optimization algorithms together with no special warm-up period for the estimation routine. Rolf and Lim (1985) and Lee and Lee (1985) found 225 and 300 estimation steps necessary for start-ups in their respective algorithms.

An example of a start-up is shown in Figures 5–7. The column is initially steady at 3 mL/min. The excitation was limited at ±25% of the flow level. In this first-order model, both parameters are started at zero and the diagonal of the covariance matrix is set to 100. The flows are shown in Figure 5. The sample flow plotted is the steady state flow that would result in the same residence time as that of the fluid element just sampled. The excitation in flow begins at 612 min and it is not until 20 min later that any changes show up in the calculated residence time of the material leaving the column. The optimal flow rate is calculated as a change from the calculated residence time, Eq. 7, and hence the first two optimization steps at 632 and 652 min are constrained by the bound of 1 mL/min on the step size.

After 100 min, or five optimization steps, the optimization flow has settled at the correct value of 1.3 mL/min as deter-

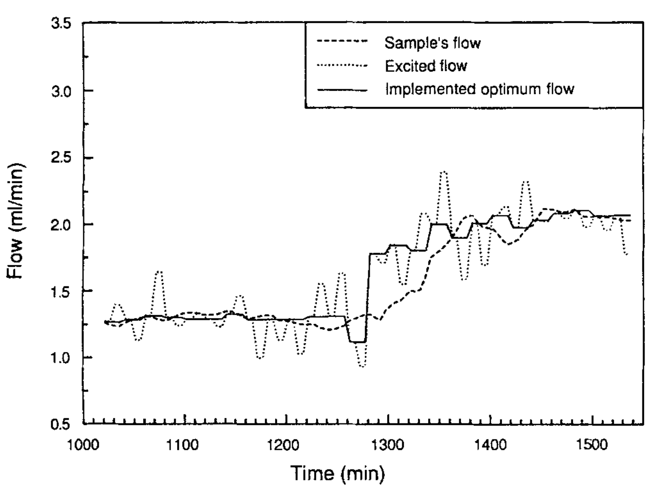

Figure 8. Response of on-line optimizing controller to changes in temperature.

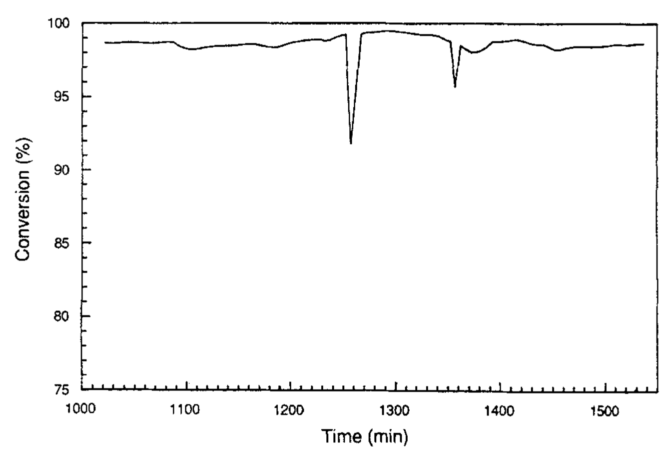

Figure 9. Conversion during transition in temperature.

mined by steady state analyses performed just prior to turning on the on-line optimizer; see curve c in Figures 1, 3, and 4. Note that the optimizer has settled even before the conversion in Figure 6 has reached its final level. The parameters and steady state gain from the linear dynamic model are shown in Figure 7. In this case the time required for the parameters to converge is at least that required for the optimum to settle. This indicates that for this system it is unnecessary to wait for parameter convergence before beginning optimization, either at start-up or while tracking shifts in the optimum. In other words, intermediate parameter estimates result in an improving series of predicted optimum operating points so that the parameter estimates and the optimization can converge simultaneously.

To demonstrate the ability of the algorithm to track a changing optimum, the set point on the temperature controller was increased by 10°C at 1,217 min. From steady state analyses done before and after the shift, this change was expected to move the optimum flow rate up to about 2.1 mL/min—see curve a in Figures 1, 3, and 4—and increase the steady state gain from -3.2 to approximately -2.7. The on-line optimizing control did well at recognizing the change in operating conditions and increased the flow to the new level over a period of 100 min, less than half the time required to establish one steady state operating point, Figure 8. The algorithm accomplished this in spite of the large disturbances that were seen at the detector at 1,250 and 1,350 min, Figure 9. These points were correctly identified as outliers and so disturbed the parameter estimates very little, Figure 10.

This test was repeated with no excitation signal added to the optimum flow rate. When the temperature was changed, the optimizer began moving the flow rate toward the new optimum; however, the time required for the change was double that required when using an excitation signal. In addition, the flow rate changes produced by the optimizer were insufficient signal for good tracking of the parameters, so that the parameter estimates were far less steady. When the flow rate had settled at the new values, the estimate of the pole had only moved half the anticipated amount, leaving the parameters with considerable bias. It was concluded that although the on-line optimizing control algorithm could work using only the signals provided by the optimizer for excitation, superior convergence rates for both the optimizer and the estimator were obtained when an *additional* excitation signal was provided.

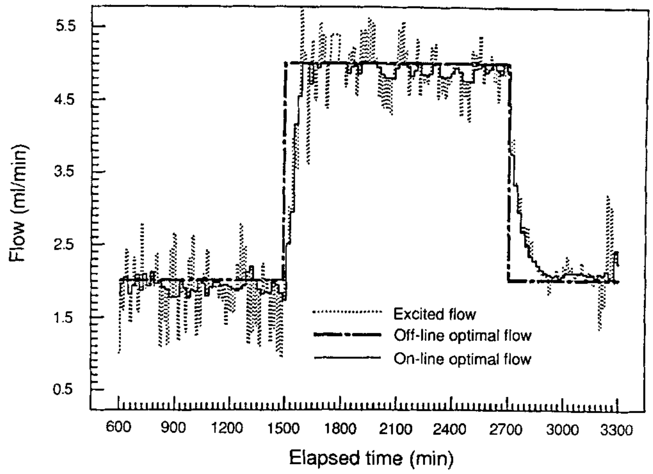

Figure 11. Response of on-line optimizing controller to changes in activity (simulated by changing detector calibration).

In a second test of the ability of the on-line optimizing algorithm to track a shifting optimum, a different type of disturbance was introduced. In this test, shown in Figure 11, the calibration of the detector was changed at time 1,496 and changed back at 2,702. This shifted the operating curve as shown in Figures 1, 3, and 4 from curve a to curve b with corresponding changes in the optimum flow rate from 2.1 to 5.0 mL/min. The test began with the excitation level bounded at ±50% of the flow level. The shift in the optimum was detected and tracked quite well, settling at the new conditions in less than 100 min, with the steps used in the first 60 min being the maximum allowable size.

At the high flow rate, the level of excitation appeared excessive and so the bound was reduced to ±12.5% of the flow. Even at this reduced level of excitation, the change in operating performance was detected immediately and the algorithm con-

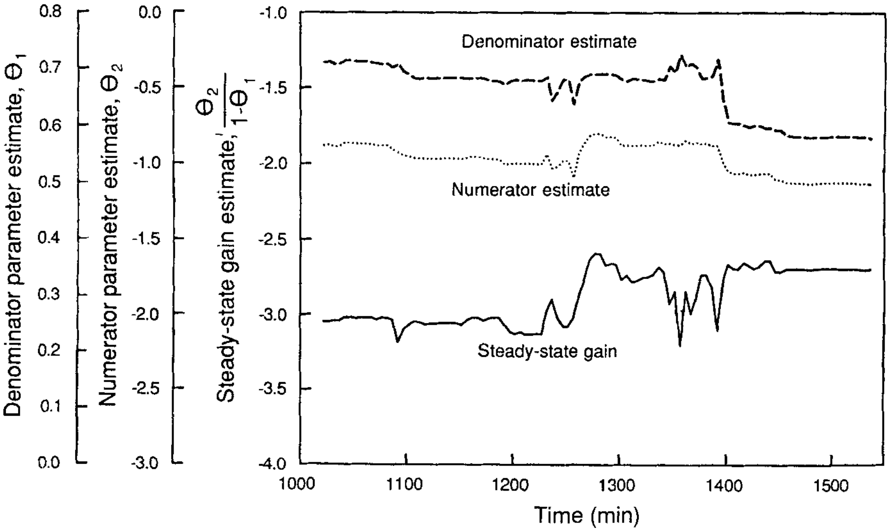

Figure 10. Parameter estimates during transition in temperature.

verged smoothly back to the original level. This transition took 180 min, the increase in transition time being due partly to the dramatic slowdown in the column dynamics as the flow rate decreases from 5 to 2 mL/min.

To put into perspective the time of 100–200 min for the on-line optimizing control to converge to the new steady operating point, note from Figure 2 that this is not much longer than the time it takes to establish a single steady state. Hence, compared with a conventional optimization method requiring several steady state points to converge to an optimum, the on-line optimization method converges to the optimum much faster.

Conclusions

On-line optimizing control has been shown to be a useful tool for finding and following optimal economic operating conditions for continuous processes. As a model system, the packed-bed immobilized-cell reactor used here was a nonlinear, noisy, distributed-parameter system. And yet, once certain enhancements were made to the basic algorithm, the on-line optimizing control handled this system with no difficulties, operating over a wide range of conditions, achieving convergence rates and tracking speeds greater than any found in previous experimental studies. One enhancement was the use of nonlinear input-output transformations, which linearized the steady state operating curves, making the parameters less sensitive to the operating point. Another enhancement was the use of a variable forgetting-factor algorithm to control forgetting during periods when very little new information was being received. Coupled with this was the use of outlier detection and error limiting. High-pass filtering of the data eliminated the need to estimate a bias parameter, allowing the recursive estimation algorithm to focus on those parameters affecting the gain. The optimization algorithm was enhanced by using the curvature information from the nonlinear input-output transformations to obtain second-order information so that a full Newton method could be used, increasing the accuracy of the predicted distance to the optimum.

We demonstrated that convergence of the parameter estimates could be done concurrently with optimization and hence long delays between optimization steps and an initial estimation warm-up period were not required. This leads to great improvements in performance, making on-line optimization using recursive estimation of a dynamic model clearly more efficient than on-line optimization based on steady state evaluations.

Notation

a_i = coefficients in profit equation
a_1 = -4.25
a_2 = -26.51
a_3 = -3.49×10^{-2}
a_4 = 2.949×10^{-3}
a_5 = 4.349×10^{-6}
c = conversion of fumaric acid, %
f = feed flow rate, mL/min
p = scaled profit rate, dollars/min
u = logarithm of nominal time sample spent in reactor
V_ϵ = volume of column occupied by moving fluid
y = logarithm of residual fumaric acid in sample
θ_i = parameters in linear dynamic model

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