

SRC-TR-87-68

**CHEMICAL PROCESS SYSTEMS
LABORATORY**

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Moderate and High Purity Distillation
Towers

by

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CHEMICAL PROCESS SYSTEMS ENGINEERING LABORATORY

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APPLICATION OF DYNAMIC MATRIX CONTROL
TO MODERATE AND HIGH PURITY
DISTILLATION TOWERS

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Dynamic Matrix Control, a predictive computer control algorithm developed at Shell Oil Co. (Cutler, 1983) is applied to dual composition control of moderate and high purity, binary distillation towers. The composition control loops in these towers are highly interacting and, in addition, very nonlinear. The difficulty in obtaining a representative process model for nonlinear systems is demonstrated and methods to overcome this problem are suggested. Multivariable gain and time constant scheduling is evaluated using simple analytical models to update key process model parameters (process gains and time constants) on-line. This approach results in a significant improvement in regulatory control performance over the standard application of DMC.

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I. Introduction

In this study, predictive control techniques are applied to dual composition control (control of both top and bottom product compositions) of moderate and high purity, binary distillation towers. Composition control of distillation processes is a particularly challenging problem due to the extensive interaction between process variables. Because of the multivariable nature of the problem, dual composition control appears to be a prime candidate for predictive, multivariable control techniques. To date, there have been very few studies involving predictive control of a distillation process (Marchetti, 1982). One of the potential problems with the application of predictive control techniques is that they assume the processes are linear so that effects of process nonlinearity on predictive control performance must be considered. The objectives of this study are to quantitatively characterize the nonlinear nature of distillation systems and to develop and evaluate methods of compensating for the nonlinear behavior to improve regulatory control system performance.

Nonlinear steady state and dynamic behavior in distillation processes has been reported by several investigators. Tsogas and McAvoy (1982) have divided nonlinearity in distillation processes into three broad categories based on product purity specifications. Low purity towers often exhibit linear composition dynamics but as product purity is increased the composition gains may become more nonlinear even though time constants and dead times remain fairly constant. For high purity towers, nonlinear gains, time constants and dead times have been reported (Mizuno et al., 1972; Fuentes and Luyben, 1983; Tyreus and Luyben, 1976). A recent investigation of composition loop time constants for feed com-

position disturbances (Kapoor et al., 1986a) indicates that tower time constants change drastically when the tower is perturbed from the steady state design conditions. There are very few control system design techniques which attempt to account for nonlinear behavior typical of high purity distillation columns. In practice, control system design is based on a local linearization about an operating point. One approach which has been used to achieve consistent control system performance over a range of operating conditions is known as gain scheduling, gain compensation or variable controller gain tuning. This method has been applied by several investigators (Chiang and Durbin, 1980, 1983; Shinskey, 1977; Tsogas and McAvoy, 1985) to nonlinear processes in the chemical industry. In this approach, auxiliary measurements that reflect the changes in process dynamics are used to update the controller parameters on-line. The objective in this type of approach is to adjust the Gain scheduling differs from adaptive control in the gain adjustment algorithm is essentially open loop; there is no mechanism to compensate for incorrect scheduling. One difficulty with this method is in the determination of a scheduling algorithm to obtain good agreement over the entire set of operating points. An important advantage is that controller parameters can be changed rapidly in response to process changes, limited only by the response time of the auxiliary measurements. Tsogas and McAvoy (1982) evaluated a gain scheduling approach suggested by Shinskey (1977) for single-ended material balance control of moderate and high purity distillation towers. They used a simple scheduling approach in which they assumed that the process gain dropped off linearly with increasing product purity. The controller gain was then increased to compensate for this decrease in the process gain. This one-sided gain scheduling strategy resulted in a significant improvement in closed loop control performance for feed composition

disturbances for both of the towers. A multivariable (3×3) gain scheduled controller was developed by Kapasouris et al., (1985) for control of a highly nonlinear turbofan jet engine. In their approach, they approximated the nonlinear engine with a series of linear models throughout the operating region of the engine. A single output variable was used to adapt the controller gains and the process model to provide a nonlinear feedback control system over the entire operational envelope of the engine.

II. Case Study Towers

Two binary distillation towers, referred to as Towers B and D, were chosen as representative moderate and high purity towers exhibiting control problems due to interaction and nonlinearity. Tower B is a moderate purity ($x_D = 0.98$, $x_B = 0.02$) benzene/toluene tower with 18 stages. Tower D is a high purity ($x_D = 0.994$, $x_B = 0.0062$) isobutane/n-butane tower with 41 stages. Table 1 lists steady state design specifications for both of the towers. Tower B has been considered in a number of previous control studies (Weischedel, 1980; Weischedel and McAvoy, 1980; Tsogas and McAvoy, 1982; Marchetti, 1982; Stanley, 1985). Dual composition control of Tower D has been studied by Stanley (1986).

III. Interaction in Multiloop SISO Control Configurations

An analysis of the steady state relative gains (RGA) for the case study towers indicates the severity of the interaction when dual composition control is attempted using the traditional multiloop SISO control configuration. The relative gain gives a quantitative indication of how the closed loop behavior of a loop changes when the other loops in a multiloop system are activated (McAvoy, 1983). Table 2 shows the steady state values of the RGA for Towers B and D for several choices of manipulated variables. The steady state

process gains which were used to calculate the RGA values were accurately determined by averaging gains due to small (1×10^{-6} * steady state value) positive and negative perturbations in the manipulated variables using a steady state design package with a very tight convergence criteria (1×10^{-13}). From Table 2 it is evident that, for the multiloop control strategies considered, interaction problems will be severe. This is especially true for Tower D, since the RGA values are about 0.5 (maximally interacting for a 2×2 system) for two of the schemes and 141 (very sluggish) for the energy balance scheme. A multivariable controller, such as Dynamic Matrix Control, which bases control action on both output variable measurements and incorporates a process model which includes the interaction effects would be more appropriate for these towers. Unfortunately, these towers are also very nonlinear and the effects of process nonlinearity on the design and implementation of the DMC algorithm must be considered.

IV. Nonlinear Nature of Case Study Towers

For nonlinear processes, the scaled open loop step responses used to represent the process dynamics in the DMC algorithm will depend on the size and direction of the input step. If the open loop response can be approximated by simple first order dynamics, this nonlinearity is indicated by differences in the process gains, time constants and dead times. The asymmetry which results from the process nonlinearity presents a dilemma in the choice of the most appropriate step response to describe the process in the DMC algorithm.

Open loop step responses for Towers B and D were generated using a nonlinear dynamic simulation package. Details of the simulation package are given by McDonald (1985). The nonlinearity of the towers, particularly Tower D, was evident from the open loop step tests and made it very difficult to determine

representative open loop responses which could be used to construct a nominal process model. For Tower D, order of magnitude changes in the effective process time constant were observed as well as order of magnitude changes in the effective process gains. Although small perturbations in the input variables gave more accurate estimates of the process gains at the design point, the time constants obtained with the small input changes were extremely long. Figure 1 shows the bottoms composition response to 0.1, 0.5 and 2.0 percent changes in the reflux flow with constant vapor boilup. Depending on the size and direction of the input step, time constant estimates from the open loop step responses range from 50 min. to greater than 500 min. These large differences in time constants, as well as the corresponding differences in the process gains, illustrate the difficulty in experimentally determining open loop responses for high purity towers.

Tables 3-4 summarize the results of the open loop responses to step changes in energy balance input variables (L , V) for Towers B and D. The step responses were modeled by first order with deadtime dynamics and values of the effective process gains, time constants and deadtimes were estimated for each of the responses. The final product compositions are also given in the tables to indicate how far the tower has been perturbed from the initial design state. Typically, in the application of DMC to nonlinear systems, the open loop step responses are averaged to obtain a representative process model. Values of the dynamic parameters were therefore calculated from the averaged step responses and are given in the tables. The tables also show the steady state process gains which were accurately determined at the design state using the steady state design package. In addition, estimates of the time constants at the design point are given. These time constants were determined by linearizing a

simplified dynamic model and calculating the frequency response of the linear model using a stepping technique (Luyben, 1973).

The results in Tables 3-4 indicate a significant degree of nonlinearity particularly with respect to the process gains. In all cases, when the mole fraction of the impurity in one of the product streams approaches zero and the impurity in the other product stream increases (as is often the case for most disturbances), the gain corresponding to the pure stream decreases while the gain for the more impure stream increases. These process gain variations arise because input changes which increase distillate product purity, for example, cause the composition profile to move up the tower, towards the pinch zone whereas input changes which reduce distillate purity cause the profile to move away from the pinch zone. It is also apparent from these tables that differences between the gains for positive and negative input perturbations (as well as deviations from the "design" process gain) increase as the product compositions are perturbed farther away from their initial design values.

Nonlinearity is also evident from a comparison of closed loop responses to positive (increasing product purity) and negative (decreasing product purity) setpoint changes. A controller which is designed based on a process model at one operating point will exhibit sluggish or oscillatory performance when a setpoint change occurs. This is due to the fact that, as shown by the open loop responses, the process gains strongly depend on the product compositions. With fixed controller settings, an increase in the product composition setpoint (decrease in the process gain) will result in a sluggish response. Similarly, for a decrease in the setpoint, the increase in the process gains will produce an oscillatory response. Consider, for example, Tower B with distillate flowrate and vapor boilup chosen as manipulated variables. A DMC controller was designed based on the averaged open loop step responses. Figure 2 shows the

closed loop control performance for positive (x_D : 0.98 \rightarrow 0.99) and negative (x_D : 0.98 \rightarrow 0.97) setpoint changes in the distillate product purity with the DMC parameters given. For a positive setpoint change the distillate composition response appears to be a bit sluggish while for a negative setpoint change, the response is extremely oscillatory.

In general, the open loop step responses can be modeled as first order systems. Thus, the nonlinear behavior of the towers can be quantitatively analyzed by evaluating process gains and time constants as a function of operating point. There are two situations where this knowledge is useful. First, for setpoint changes, this information can be used to modify the process model to reduce plant-model mismatch when the desired operating point is changed. Secondly, the distillate and bottoms composition measurements reflect the important changes in the process dynamics (ie. changes in the process gains and time constants). If the relationship between product composition and effective process gain and time constants can be modeled, the product composition measurements can be used to update the process model on-line to improve control performance during a load upset.

Steady state gains were evaluated for Towers B and D at perturbed steady state operating points around the design point. These new operating points were systematically determined by making changes in one of the manipulative variables while keeping the second variable constant. These perturbations produce variations in product compositions which might be encountered during a closed loop transient response. "Local" process gains were then accurately determined at the perturbed operating points using the steady state design package. The ratios of the process gains at the perturbed point to the process gains at the

design point were then plotted as a function of product composition. Figures 3-6 show the gain characteristic curves for Tower B and Tower D under material (D,V) and energy balance (L,V) control schemes. In each figure, ratios of the process gains at perturbed steady state operating points to the process gains at the design point are plotted (shown by the symbols) as a function of distillate composition. Even though the results are presented as a function of distillate composition it is important to recognize that there is a specific bottoms composition which corresponds to each value of the distillate composition at the perturbed operating point.

Figures 3-6 provide a quantitative comparison of the degree of nonlinearity of the towers. In general, as the distillate product purity increases (and bottoms purity decreases) gains associated with the distillate composition decrease by approximately 50% for Tower B and 95% for Tower D over the composition ranges considered. It is also interesting to note that, for the energy balance control schemes, the x_D -L and x_D -V gain ratios are very close as are the x_B -L and x_B -V gains. This behavior greatly simplifies the additional computational burden introduced by updating the process model gains online in the DMC algorithm. In general, if each of the process gains is changing independently, updating the process model on-line will require on-line inversion of the Dynamic Matrix. For the energy balance control scheme, the gain scale ratios can be factored from the nominal Dynamic Matrix.

To compensate for gain variations resulting from process nonlinearity, a simple method of updating process model gains on-line is required. One approach would be to fit the results for each of the process gains to a surface above the product composition (x_D , x_B) plane. The resulting empirical expressions could then be used to estimate the gain ratio (relative to the nominal or design point)

at any value of product composition. Another approach, taken in this study, is to use a simplified steady state model to estimate the process gains as a function of product composition. The approximate steady state distillation model which was chosen has been used by McAvoy (1983) to determine process gains for dual composition control of binary towers for a variety of control schemes. It uses Eduljee's (1975) empirical approximation to Gilliland's (1940) graphical correlation to relate product specification variables to tower design and operating variables. Analytical expressions for process gains relating product compositions to manipulated variables for material and energy balance control schemes are summarized in Table 5.

The solid and dashed curves in Figures 3-6 show the gain ratios calculated using the approximate analytical equations. The simple analytical model provides a good estimate of the gain ratios calculated from the rigorous steady state package. In most cases, the approximate gain expressions provide a conservative estimate of the magnitude of the process gain variations.

Process time constants and dead times were also evaluated at perturbed states to analyze the changes in the dynamic parameters with operating point. A frequency response "stepping" technique (Rippin and Lamb, 1960), based on a simplified binary distillation tower model presented by Luyben (1973), was used to estimate the dynamic parameters. At each steady state operating point, values of the time constants and dead times were estimated from the frequency response assuming the process transfer functions were first order with dead time.

Figures 7-8 show the energy balance time constants and dead times for Towers B and D at perturbed operating points as a function of the mole fraction of impurity in the product stream which has become more impure at the perturbed

steady state. To the right of the dashed line, for example, the dynamic parameters correspond to perturbed steady states such that the distillate product is becoming more pure and the bottoms product is becoming more impure.

From Figures 7-8 it is apparent that the dynamics of moderate and high purity distillation systems change drastically when the operating point is perturbed into a region where one of the product streams is becoming relatively impure. This behavior agrees with the results of Kapoor et al. (1985) which predict large time constants for moderate and high purity distillation towers at the design point. Their work has shown that distillation towers contain positive feedback recycle structures. Large time constants arise naturally because the gain of the positive recycle loop approaches unity at the high purity design state. Their analysis shows, however, that as the tower is perturbed away from the high purity design state (i.e. as one of the product streams becomes more impure) the gain of the positive feedback loop drops and tower time constants are greatly reduced. For Tower B, time constants decrease by about a factor of two, whereas for Tower D, they show almost an order of magnitude decrease over the composition range considered. In general, dead times associated with changes in the manipulative variables were small compared with the time constants and did not change very significantly.

As with process gain variations, the time constant variations could be empirically fit to a representative surface above the product composition plane. Another possibility is to use the stepping technique in conjunction with a simplified steady state model to evaluate the process time constants and dead times on-line. Work is currently underway (Kapoor, 1985) to develop analytical expressions for time constants and dead times at perturbed steady states.

In this study, as a first approach in modeling time constant variations, a simple analytical method was used. An analysis of the time constant results

from the numerical stepping technique indicate that, as process gains decrease (i.e. for increasing product purity), the time constants decrease at approximately the same rate. Therefore, knowledge of the time constant at the design point and an estimate of the process gain ratio at the perturbed state according to

$$(\tau_{ij})_P = \frac{(K_{ij})_P}{(K_{ij})_D} (\tau_{ij})_D \quad \begin{array}{l} P = \text{Perturbed state} \\ D = \text{Design state} \end{array} \quad (1)$$

The numerically evaluated time constants for the case study towers also predict that the time constants for distillate composition are approximately equal to the time constants for the bottoms composition (corresponding to the same input variable). Therefore, in our time constant scheduling approach, the time constant for the loop with an increased process gain (decreased purity) was set equal to the time constant for the other loop. For example, if the perturbed state was such that the distillate purity has increased (i.e. decreased process gain) then eqn. (1) would be used to estimate the time constants relating x_D to L and V. The time constants for the bottoms composition. Estimates of the process time constants for Towers B and D using this method are shown by the solid and dashed lines in Figures 7-8. For Tower B, the approximate time constants are fairly good estimates of the process time constants obtained by the stepping technique while for Tower D, the time constant estimates are off by as much as 50 min. For Tower D, it is probably on a process model with the large time constants (>150 min.) obtained at the design point and then adapt the model time constant using Eqn. (1). It is more reasonable perhaps to assume that larger

input steps (or input steps at a perturbed, low purity operating point) would be used to obtain a faster open loop response which would be more indicative of the speed of the system during a transient.

V. Gain and Time Constant Scheduled Dynamic Matrix Control

Since process gain and time constant changes can be modeled using measurements of the process outputs (the distillate and bottoms composition), a multi-variable gain and/or time constant scheduling technique can be used to compensate for these process changes during transients. The advantage of using a scheduling rather than an adaptive approach to compensate for process nonlinearity, is that the scheduling approach allows the controller parameters to change very quickly in response to changes in the product compositions during a disturbance upset. Adaptive techniques are better suited to compensate for slow variations in the process parameters and transitions to new operating points.

The DMC algorithm¹ calculates, based on a nominal process model \underline{A}_0 , sequences of input moves which minimize the squared deviation between the predicted trajectory and the setpoint by solving the least squares problem

$$\underline{\hat{A}} \underline{\Delta I} = \underline{E} \quad (2)$$

In addition, the process model is used to update the output projection vector. During a transient (or at a different operating point), the model will not be very accurate, however, due to the system nonlinearity. Using the approximate

1. For a detailed description of the DMC algorithm see Cutler (1983)

analytical expressions for the process gains and time constants, a better estimate of the process dynamics can be provided. The nominal open loop responses can be scaled to adjust for changes in the process gains, and the nominal responses can be contracted to adjust for the reductions in the time constants at perturbed operating points. Scheduling in this way (i.e. based on a nominal process model) allows for a smooth transition in the process model parameters as the product compositions move away from steady state and insures that the process model parameters return to their original values as the control system brings the process back to steady state. For the 2 x 2 dual composition control problem, only eight parameters (the gains and time constants for each of the responses) need to be estimated at each time step. Several different approaches to on-line gain and time constant scheduling were considered. The modified DMC algorithms included:

1) Gain scheduling only in one direction (no change in the process model time constants). Based on the product composition measurements from the analyzer, the analytical gain expressions are used to determine the gain scale factors (ratio of the gain at the current perturbed operating point to the design point) for each of the responses i.e.

$$(K_{ij})_{SF} = \frac{(K_{ij})_P}{(K_{ij})_D} \quad \begin{array}{l} P = \text{Perturbed state} \\ D = \text{Design state} \end{array} \quad (3)$$

If the gain at the current state has decreased (i.e. $K_{ijSF} < 1.0$) then the process model response is scaled to reflect this change. If the gain at the current state has increased, the nominal process model is used. This "one way" scheduling approach was first proposed by Tsogas and McAvoy (1985) to compensate

for the decrease in the process gain, but take advantage of increases in process gain to return the system to steady state more quickly.

2) "Two way" gain scheduling. With this modification, the algorithm compensates for both increases and decreases in the process gains. The nominal model coefficients are multiplied by the gain scale factors even when the gain scale factors are greater than 1.0.

3) One way gain and time constant scheduling. This method is similar to 1) except that, in addition to scaling the nominal step response coefficients, the responses are contracted in time as well. Thus, if a reduction in gain is calculated from the analytical equations at the perturbed state, the corresponding time constant is reduced according to Eqn. (1).

4) Two way gain and time constant scheduling. With this approach, the model gains and time constants are scheduled at every sampling time. For increasing product purity (i.e. decreasing gain), the time constants are evaluated using Eqn. (1). If the perturbed process gain is greater than the design point gain (i.e. gain scale factor > 1.0), then the corresponding time constant is set equal to the time constant for the opposite composition loop.

In general, updating the process model on-line will require on-line matrix inversion. Gain scheduling can be accomplished without on-line matrix inversion if the nominal process model can be factored from the updated process model i.e.

$$\underline{A}_p = \underline{D}_1 \underline{A}_0 \underline{D}_2 \quad (4)$$

where \underline{D}_1 and \underline{D}_2 are diagonal matrices. Solving the least squares problem at the perturbed state is therefore equivalent to solving the problem with the nominal model using "perturbed" error and input vectors

$$\underline{A}_{\approx 0} \underline{\Delta I}_p = \underline{E}_p \quad (5)$$

where

$$\underline{E}_p = \underline{D}_1^{-1} \underline{E}$$

$$\underline{\Delta I}_p = \underline{D}_2 \underline{\Delta I}$$

For energy balance control, the a_{11} and a_{12} gains change simultaneously, as do the a_{21} and a_{22} gains, so that gain scheduling can be easily accomplished by using a modified error vector in the standard DMC algorithm and updating the projection vector using the scheduled or perturbed process model.

VI. Nonlinear Simulation Results

Nominal process models for the towers were obtained by averaging the open loop step responses generated by the nonlinear dynamic simulation. These responses were then scaled so that the gains matched those calculated from the steady state package at the design point. A sampling time of 2.0 min. was chosen for Tower B and 4.0 min. for Tower D. Using the nominal process model, tuning parameters were selected according to the guidelines proposed by Cutler (1983). The same tuning parameters were used in both the modified and standard DMC algorithms for a particular tower and choice of manipulated variables. It should be stressed that the feedforward capability of the DMC algorithm was not used; the feed disturbances were assumed to be unmeasurable.

Figures 9-10 compare the different approaches to gain/time constant scheduling for Tower B using L and V as manipulated variables for a +20% step in feed composition. Figure 9 compares the gain scheduling approaches (methods 1

and 2) with the standard DMC application. As expected, the standard DMC approach produces a very sluggish distillate composition response. The one way and two way gain scheduling approaches are very similar and both result in an improvement in the distillate response without much effect of the bottoms composition response. Since the area under the distillate curve represents product give-away (i.e. producing a higher grade material) this improvement is significant. The peak in the bottoms composition response is also important since it determines how far the operating setpoint has to be moved to insure product specifications are satisfied during a "worst case" transient. In most of the simulations for Tower B, the peaks in the composition depended primarily on the analyzer deadtime, and were not affected very much by the scheduling approach. Figure 12 presents results comparing gain and time constant scheduling (methods 3 and 4) with standard DMC. Again, the scheduling approaches return the distillate composition to the setpoint much more quickly than with the standard DMC algorithm. Similar improvements in the bottoms composition loop are obtained for a negative 20% step in feed composition. Although all of the scheduling approaches improved control performance, particularly with respect to the distillate composition response, the one way gain scheduling and the one way gain and time constant scheduling appeared to be the most promising. Another important consideration is that the improvements in control performance did not require a drastic increase in control action. It should also be stressed that, in the case of gain scheduling only (methods 1 and 2), on-line matrix inversion is not required so that the additional computational burden is minimal.

Results for a -20% step in feed flowrate are shown in Figure 11. With standard DMC, the nonlinearity of the tower is very apparent. In this case the

distillate response is oscillatory while the bottoms response is very sluggish. Both of the one way scheduling approaches improve the bottoms composition response; the gain scheduling approach slightly reduces the peak in the distillate composition as well.

Similar improvements in performance were observed for +20% changes in feed flow, and -20% step changes in the feed composition. The gain/time constant scheduling DMC algorithms using D and V as manipulated variables also compared favorably to the standard method (McDonald, 1985). As would be expected, the largest differences between the scheduling approaches and the standard DMC were observed for cases in which product compositions deviated the farthest from the design point (i.e. larger step disturbances, tunings with larger move suppression factors, and larger analyzer deadtimes).

For Tower D, the nominal model time constants were more representative of the perturbed operating point than the design point since they were obtained from relatively large step input changes. For this reason, time constant scheduling was not attempted for Tower D; the one way and two way gain scheduling approaches were used and resulted in a very significant improvement in control performance. Figure 12 compares the standard DMC approach with the gain scheduling algorithms for a +10% step in feed composition. With the standard DMC algorithm, it takes about 400 min. to approach steady state. When smaller move suppression factors were used the results were more oscillatory. For this tower, the scheduling approach reduces the peak in the bottoms composition as well as returning the distillate composition to steady state more quickly.

For larger disturbances, increasing analyzer deadtime and increasing move suppression factors, the improvement obtained with the scheduling approach was more drastic. Figure 13 compares one way gain scheduling with standard DMC for

a +20% change in feed composition. The peak in the bottoms composition is reduced by about 25% with the gain scheduled DMC algorithm.

VII. Conclusions and Recommendations

One of the primary considerations in the application of DMC to nonlinear processes such as moderate and high purity distillation towers is the selection of an appropriate process model. For these systems, a nominal process model obtained from open loop step testing of the process will depend heavily on the size and direction of the step input which is used. In general, the open loop step responses for the case study towers could be approximated by first order systems. However, the effective process gains and time constants changed significantly over the operating regions of the towers. A quantitative analysis of process gain and time constant variations at perturbed operating points is presented and simple analytical expressions to predict these variations are also given. These analytical expressions are used for on-line gain and time constant scheduled DMC. An essential feature of this approach is to estimate these parameters relative to the process parameters at the design point. The advantages of using this type of an approach as compared with an adaptive DMC method (Freedman et al. 1985; Asbjornsen, 1984) is that the controller parameters can be changed much more quickly to improve performance during a transient. In addition, by assuming a first order dynamic response, the number of parameters which need to be estimated at each time step are greatly reduced.

The nonlinear simulation results presented for the case study towers indicate the potential for using multivariable scheduling techniques to compensate for process nonlinearities during a transient response to unmeasurable disturbances. In comparison with the standard DMC approach based on the same nominal

process model, the scheduling approaches reduce product give-away by returning the product stream which increases in purity to steady state more quickly and may also lower the peak in product impurity (enabling operation closer to product specifications). This improvement is obtained, however, at the additional computational expense of the on-line evaluation of the process model parameters, and in most cases, on-line matrix inversion.

Simulation results were presented for dual composition control of simple, symmetric, binary distillation towers equipped with composition analyzers. More work is required to evaluate the gain/time constant scheduling approach on more complicated distillation towers. In addition, better approximations are needed for the dynamic parameters (i.e. time constants) of high purity towers at perturbed operating points.

Acknowledgment

Financial support from the National Science Foundation under Grant CPE-8025301 is gratefully acknowledged. K. McDonald is also grateful to the Graduate School at the University of Maryland for a research fellowship and the Computer Science Center for generously supplying the computer time required for the dynamic simulations.

Nomenclature

A = Dynamic Matrix

B = molar flowrate of bottoms product (lbmol/min)

D = molar flowrate of distillate product (lbmol/min)

E = vector of future errors

I = vector of future input moves

K_{ij} = process gain relating ith output to jth input

L = molar flowrate of reflux (lbmol/min)

V = molar flowrate of vapor boilup (lbmol/min)

x_B = mole fraction of volatile component in bottoms product

x_D = mole fraction of volatile component in distillate product

x_F = mole fraction of volatile component in feed

Greek Symbols

τ_{ij} = process time constant relating ith output to jth input

Subscripts

o = nominal or design state

P = perturbed state

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TABLE CAPTIONS

Table 1:	Steady State Design Conditions for Towers B and D
Table 2:	Steady State RGA Values For Towers B and D
Table 3:	Tower B - Energy Balance Control
Table 4:	Tower D - Energy Balance Control
Table 5:	Approximate Analytical Expressions for Process Gains in Material and Energy Balance Control Schemes

TABLE 1
Steady State Design Conditions for Towers B and D

	Tower B	Tower D
Components	Benzene/Toluene	Isobutane/n-Butane
Number of Stages	18	41
Product Specifications x_D, x_B	0.98, 0.02	0.994, 0.0062 ¹
Feed Stage ² , n_F	9	21
Feed Flowrate, F (lb-mol/min)	1.5	1.0
Feed Composition, x_F	0.5	0.5
Feed Temperature, °R	662.5	573.8
Product Flowrates (lb-mol/min)		
Distillate, D	0.750	0.50
Bottoms, B	0.750	0.50
Reflux Ratio	1.697	12.78
Vapor Boilup (lb-mol/min)	1.965	6.415
Reboiler Heat Duty (Btu/min)	2.75×10^4	5.52×10^4
Reboiler Holdup (moles)	3.1	2.8
Condenser Holdup (moles)	3.1	2.8
Tray Holdup (moles)	0.31	0.28

¹ These product specifications are slightly higher than those reported by Stanley (1985).

² Counting from the bottom of the tower upward, including the reboiler

TABLE 2

Steady State RGA Values For Towers B and D

Control Scheme	Tower B	Tower D
$x_D - D, x_B - V$	0.652	0.543
$x_D - L, x_B - V$	4.719	141
$x_D - L, x_B - B$	0.403	0.459

TABLE 3

Tower B - Energy Balance Control

Process Gains, Time Constants and Dead Times from Open Loop Step Responses

Initial Steady State: $x_D = 0.98$, $x_B = 0.02$

Perturbation in Input (%SS)	Final Product Compositions		x_D Response		
			Gain ¹ (lb-mole/min) ⁻¹	Time Constant (min)	Dead Time (min)
+1% ΔL	0.9872	0.02612	0.564	16.8	< 1
-1% ΔL	0.9706	0.01656	0.772	19.1	< 1
Averaged	0.9789	0.02134	0.668	17.9	< 1
Design point	0.9800	0.02000	0.620	23.3	2.7
+1.13% ΔV	0.9652	0.01426	-0.668	18.0	< 1
-1.24% ΔV	0.9893	0.03270	-0.330	16.2	< 1
Averaged	0.9773	0.02348	-0.524	17.1	< 1
Design point	0.9800	0.02000	-0.586	23.6	3.9

Perturbation in Input (%SS)	Final Product Compositions		x_B Response		
			Gain (lb-mole/min) ⁻¹	Time Constant (min)	Dead Time (min)
+1% ΔL	0.9872	0.02612	0.479	21.5	< 1
-1% ΔL	0.9706	0.01656	0.273	12.5	< 1
Averaged	0.9789	0.02134	0.376	17.0	< 1
Design point	0.9800	0.02000	0.330	22.2	0.1
+1.13% ΔV	0.9652	0.01426	-0.260	9.0	< 1
-1.24% ΔV	0.9893	0.03270	-0.521	20.7	< 1
Averaged	0.9773	0.02348	-0.390	14.8	< 1
Design point	0.9800	0.02000	-0.395	21.5	0

TABLE 4

Tower D - Energy Balance Control

Process Gains, Time Constants and Dead Times from Open Loop Step Responses

Initial Steady State: $x_D = 0.99400$, $x_B = 0.006200$

Perturbation in Input (%SS)	Final Product Compositions		x_D Response		
			Gain (lb-mole/min) ⁻¹	Time Constant (min)	Dead Time (min)
+2% ΔL	0.99965	0.395865	0.044	11.8	0.0
-2% ΔL	0.88922	0.001653	0.820	17.8	17.9
Averaged	0.94443	0.198754	0.435	17.8	17.9
Design point	0.99400	0.006200	0.465	184.0	1.2
+2% ΔV	0.88279	0.001546	-0.867	16.4	17.7
-2% ΔV	0.99965	0.402036	-0.044	11.0	0.0
Averaged	0.94122	0.201791	-0.456	16.4	17.7
Design point	0.99400	0.006200	-0.494	184.0	1.1

Perturbation in Input (%SS)	Final Product Compositions		x_B Response		
			Gain (lb-mole/min) ⁻¹	Time Constant (min)	Dead Time (min)
+2% ΔL	0.99965	0.395865	3.050	27.9	33.7
-2% ΔL	0.88922	0.001653	0.036	10.0	30.0
Averaged	0.94443	0.198754	1.565	27.9	33.75
Design point	0.99400	0.006200	0.392	184.0	0.0
+2% ΔV	0.88279	0.001546	-0.036	8.73	0.0
-2% ΔV	0.99965	0.402036	-3.090	26.7	30.3
Averaged	0.94122	0.201791	-1.584	26.7	30.3
Design point	0.99400	0.006200	-0.419	184.0	0.0

TABLE 5
Approximate Analytical Expressions for Process Gains
in Material and Energy Balance Control Schemes

(McAvoy, 1983)

Material Balance Control

$$\begin{aligned}\left. \frac{\partial x_D}{\partial D} \right|_V &= \frac{1}{F} \left[-\frac{C_{11}V}{D^2} + C_{12} \right] & \left. \frac{\partial x_D}{\partial V} \right|_D &= \frac{C_{11}}{FD} \\ \left. \frac{\partial x_B}{\partial D} \right|_V &= \frac{1}{F} \left[-\frac{C_{21}V}{D^2} + C_{22} \right] & \left. \frac{\partial x_B}{\partial V} \right|_D &= \frac{C_{21}}{FD}\end{aligned}$$

Energy Balance Control

$$\begin{aligned}\left. \frac{\partial x_D}{\partial L} \right|_V &= \frac{1}{F} \left[\frac{C_{11}V}{D^2} - C_{12} \right] & \left. \frac{\partial x_D}{\partial V} \right|_L &= \frac{1}{F} \left[-\frac{C_{11}L}{D^2} + C_{12} \right] \\ \left. \frac{\partial x_B}{\partial L} \right|_V &= \frac{1}{F} \left[\frac{C_{21}V}{D^2} - C_{22} \right] & \left. \frac{\partial x_B}{\partial V} \right|_L &= \frac{1}{F} \left[-\frac{C_{21}L}{D^2} + C_{22} \right]\end{aligned}$$

Where

$$C_{11} = \frac{BK_3}{B(K_1 - K_4) - DK_2}$$

$$C_{21} = \frac{-DK_3}{B(K_1 - K_4) - DK_2}$$

$$C_{12} = -\frac{K_2(x_B - x_D)}{B(K_1 - K_4) - DK_2}$$

$$C_{22} = \frac{(K_1 - K_4)(x_B - x_D)}{B(K_1 - K_4) - DK_2}$$

$$K_1 = \frac{-1}{(N+1) \ln \alpha x_D (1-x_D)}$$

$$K_2 = \frac{1}{(N+1) \ln \alpha x_B (1-x_B)}$$

$$K_3 = \frac{0.5668(R_m + 1)}{(R+1)(R-R_m)} \left[\frac{N-N_m}{N+1} - 0.75 \right]$$

$$K_4 = -K_3 \frac{R+1}{R_m+1} \frac{1+x_F(\alpha-1)}{x_F(\alpha-1)(1-x_F)}$$

$$N_m = \frac{\ln \left(\frac{x_D}{1-x_D} \frac{1-x_B}{x_B} \right)}{\ln \alpha}$$

$$R_m = \frac{1}{(\alpha-1)} \left(\frac{x_D}{x_F} - \frac{\alpha(1-x_D)}{1-x_F} \right)$$

FIGURE CAPTIONS

- Figure 1: Open Loop Step Responses for Tower D: Effect of Input Variable Step Size
- Figure 2: Asymmetric Setpoint Responses for Tower B with Standard DMC Control
- Figure 3: Gain Characteristics for Tower B, Material Balance: Perturbations in D
- Figure 4: Gain Characteristics for Tower B, Energy Balance: Perturbations in L
- Figure 5: Gain Characteristics for Tower D, Material Balance: Perturbations in D
- Figure 6: Gain Characteristics for Tower D, Energy Balance: Perturbations in L
- Figure 7: Time Constant and Dead Time Characteristics for Tower B, Energy Balance: Perturbation in L
- Figure 8: Time Constant and Dead Time Characteristics for Tower D, Energy Balance: Perturbations in L
- Figure 9: Tower B, Energy Balance Control: Comparison of One-Way and Two-Way Gain Scheduled DMC for a +20% Step in x_F .
- Figure 10: Tower B, Energy Balance Control: Comparison of One-Way and Two-Way Gain and Time Constant Scheduled DMC for a +20% Step in x_F .
- Figure 11: Tower B, Energy Balance Control: Comparison of One-Way and Two-Way Gain Scheduled for a -20% Step in F.
- Figure 12: Tower D, Energy Balance Control: Comparison of One-Way Gain Scheduled DMC for a +10% Step in x_F .
- Figure 13: Tower D, Energy Balance Control: Comparison of One-Way Gain Scheduled DMC for a +10% Step in x_F .

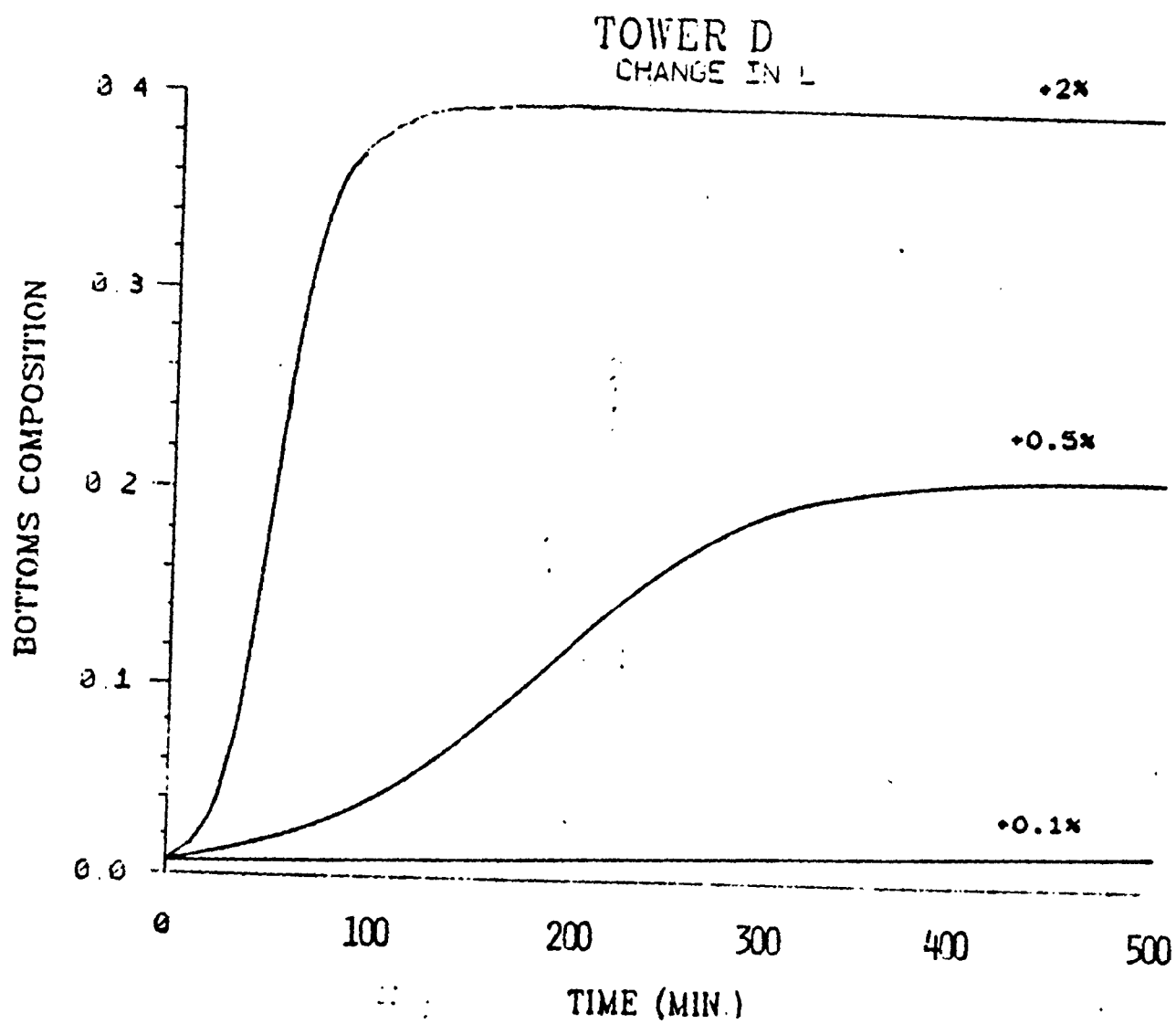
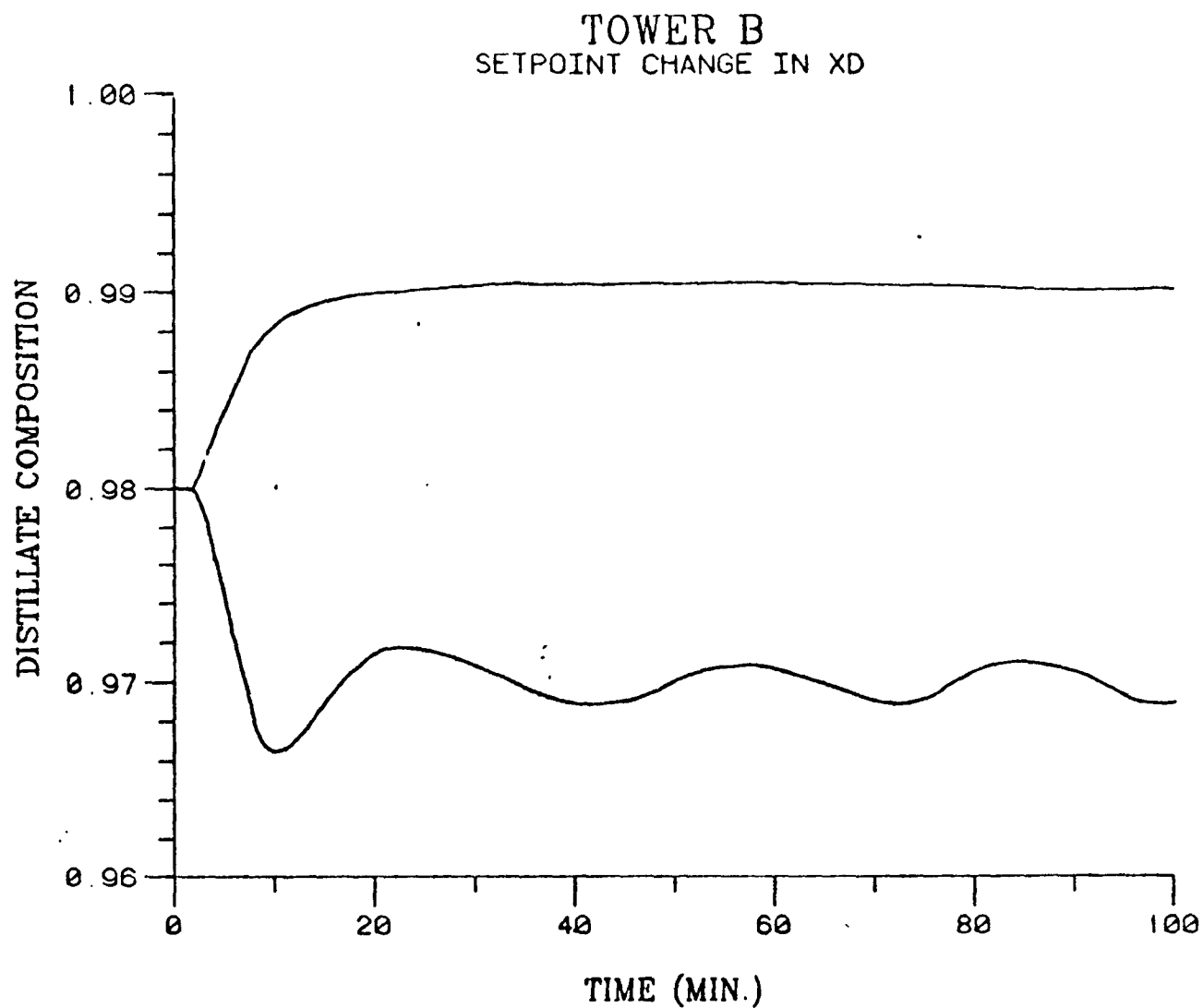


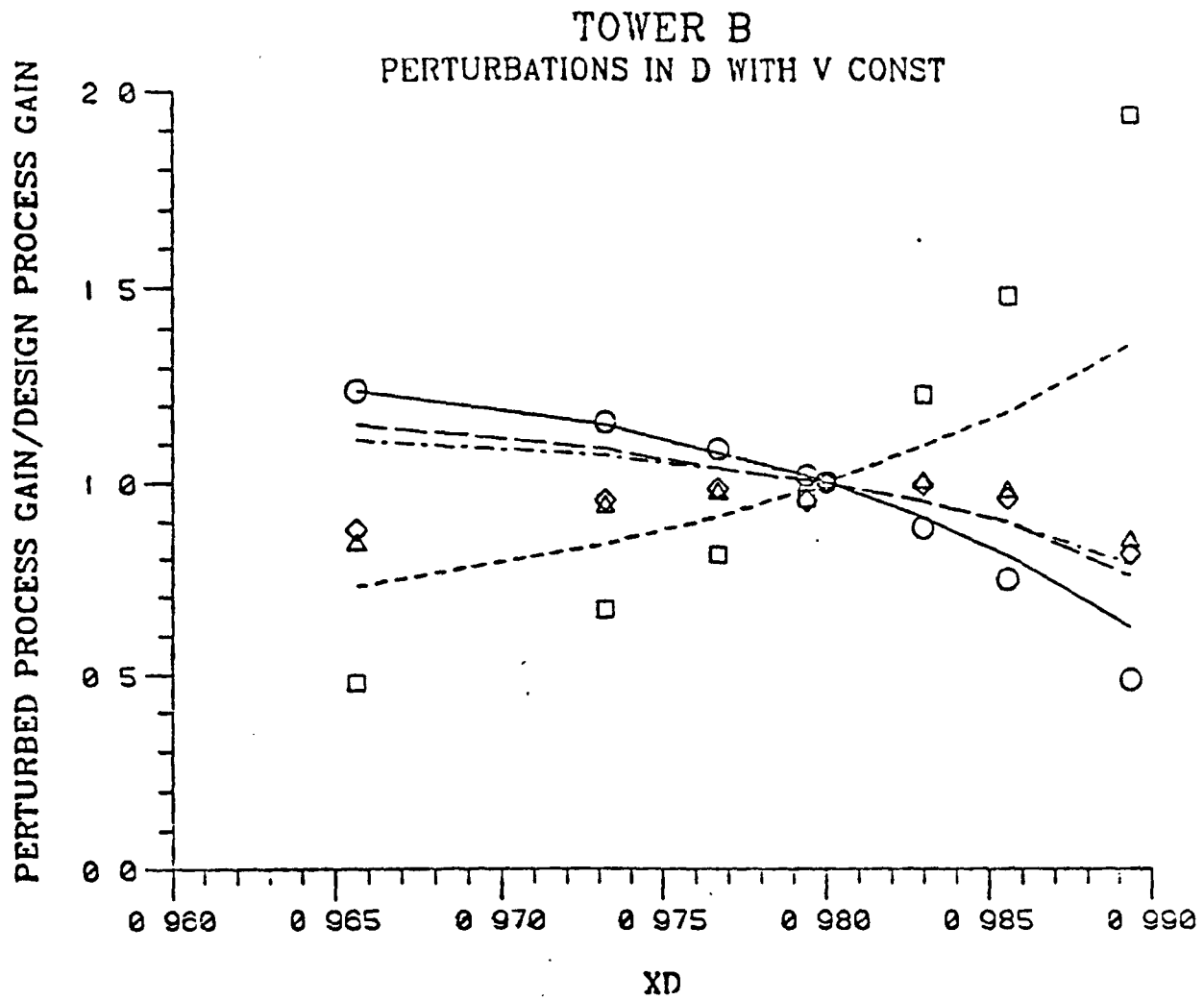
Figure 1 Open Loop Step Responses for Tower D; Effect of Input Variable Step Size



DMC PARAMETERS

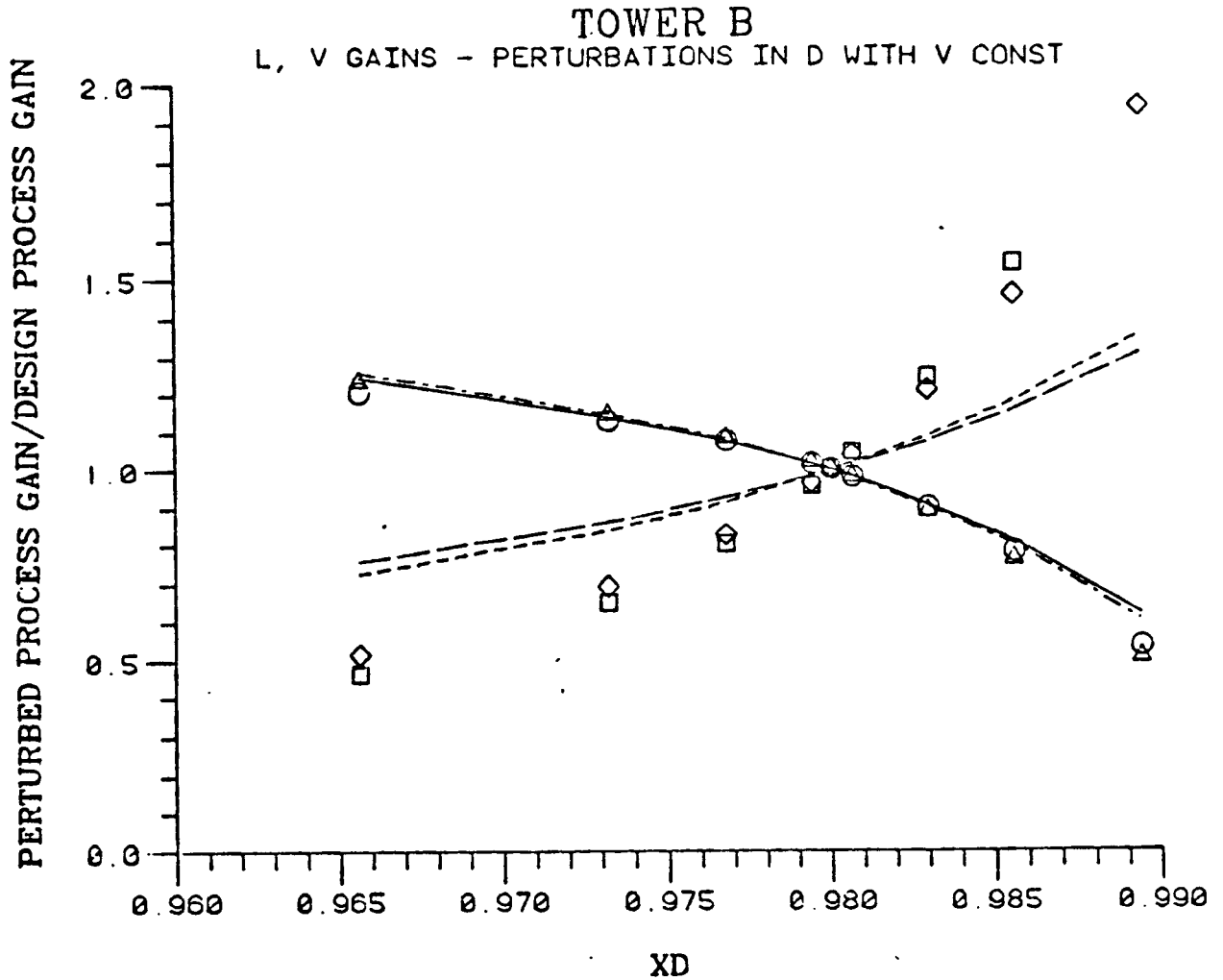
Sampling Time = 2.0 min.
Analyzer Dead Time = 2.0
Output Prediction Horizon = 51
Input Move Horizon = 13
Move Suppression Factors = 0.05

Figure 2 Asymmetric Setpoint Responses for Tower B with Standard DMC Control



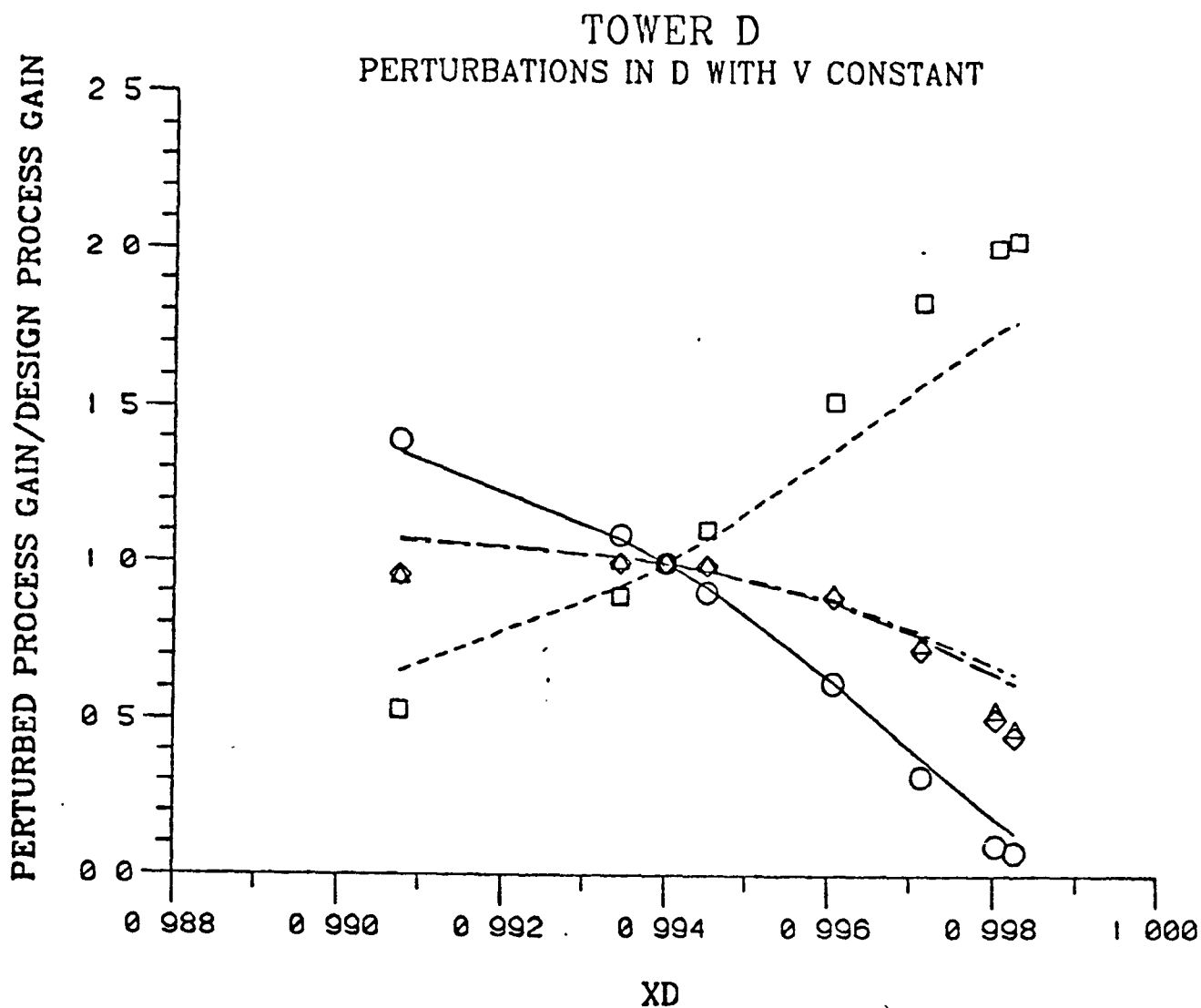
Gain Ratio For	Steady State Program	Approximation Using Analytical Model
$\frac{\partial x_D}{\partial D} \Big _V$	O	————
$\frac{\partial x_D}{\partial V} \Big _D$	Δ	- · - · -
$\frac{\partial x_B}{\partial D} \Big _V$	□	-----
$\frac{\partial x_B}{\partial V} \Big _D$	◇	-----

Figure 3 Gain Characteristics for Tower B, Material Balance: Perturbations in D



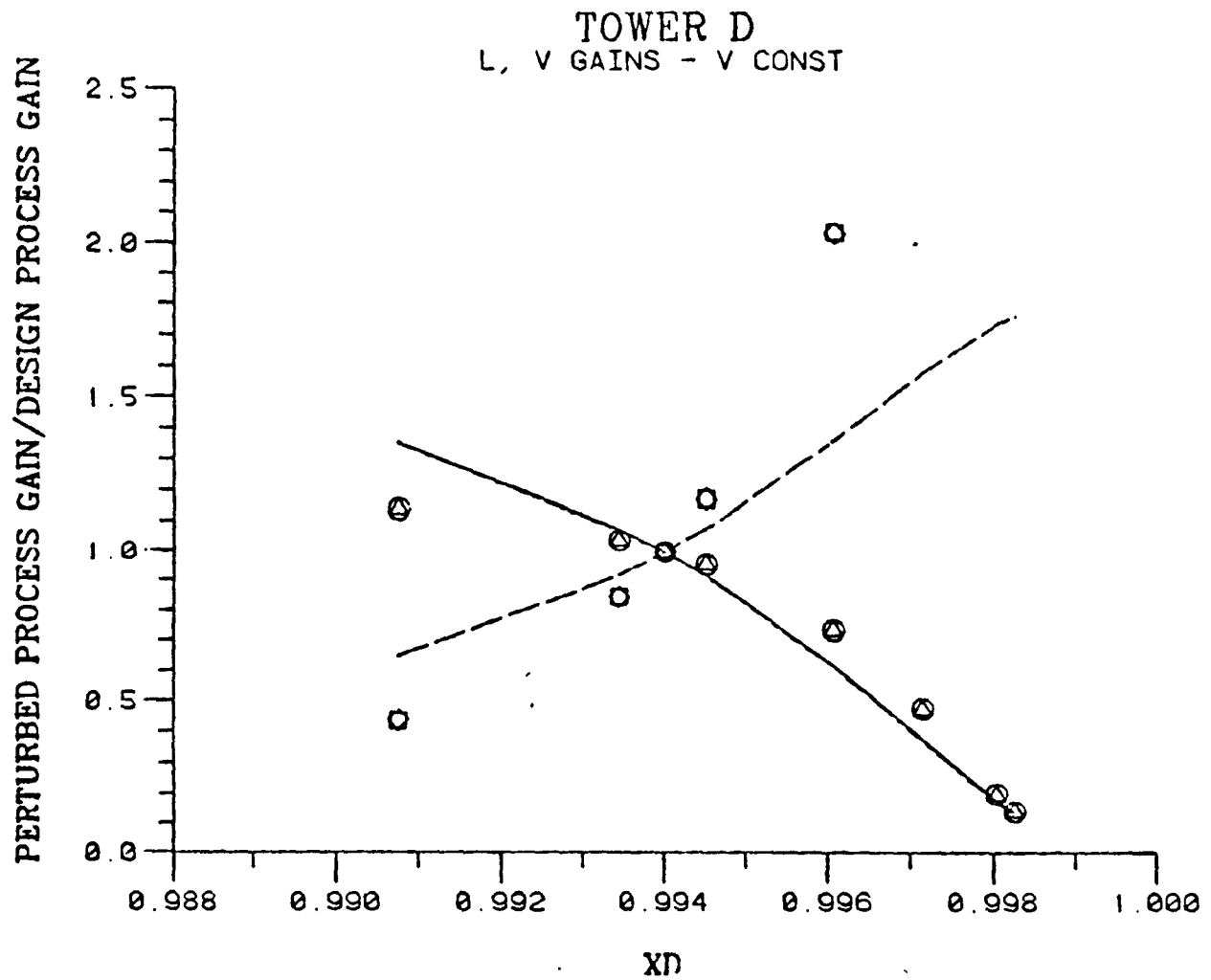
Gain Ratio For	Steady State Program	Approximation Using Analytical Model
$\frac{\partial x_D}{\partial L} \Big _V$	O	————
$\frac{\partial x_D}{\partial V} \Big _L$	Δ	- - - -
$\frac{\partial x_B}{\partial L} \Big _V$	□	- · - ·
$\frac{\partial x_B}{\partial V} \Big _L$	◇	- - - -

Figure 4 Gain Characteristics for Tower B, Energy Balance: Perturbations in L



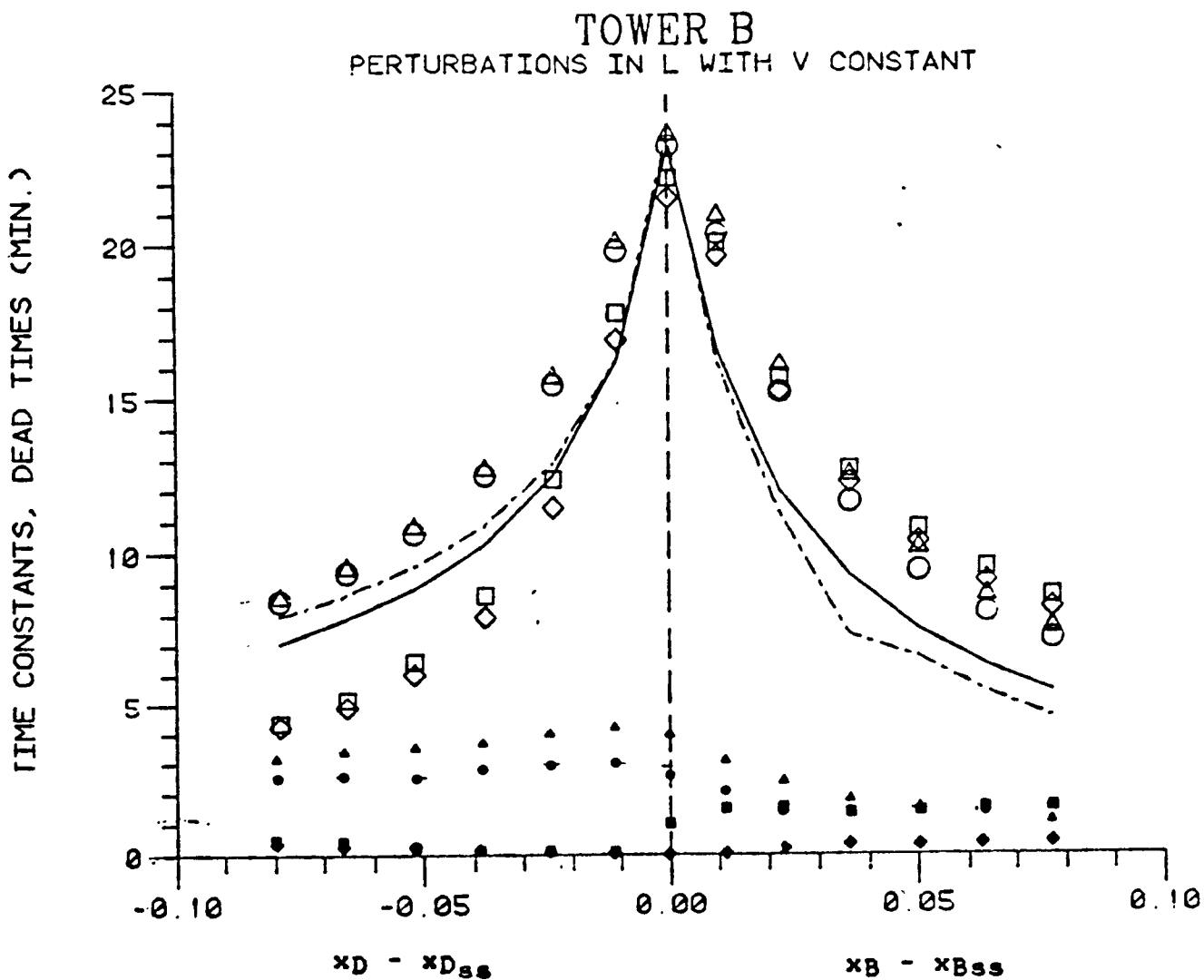
Gain Ratio For	Steady State Program	Approximation Using Analytical Model
$\left. \frac{\partial x_D}{\partial D} \right _V$	○	_____
$\left. \frac{\partial x_D}{\partial V} \right _D$	Δ	- - - - -
$\left. \frac{\partial x_B}{\partial D} \right _V$	□	- - - - -
$\left. \frac{\partial x_B}{\partial V} \right _D$	◇	- - - - -

Figure 5 Gain Characteristics for Tower D, Material Balance: Perturbations in D



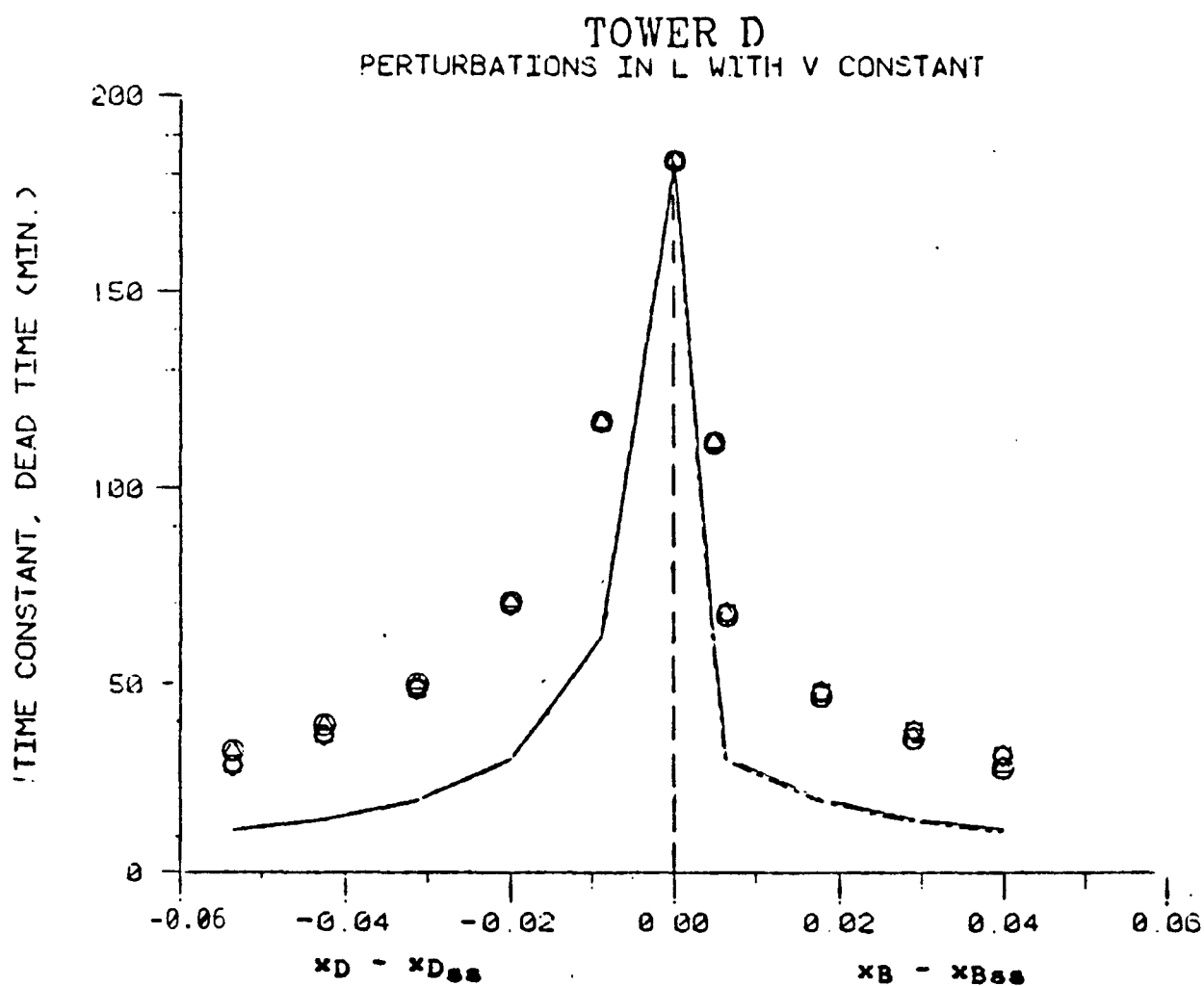
Gain Ratio For	Steady State Program	Approximation Using Analytical Model
$\frac{\partial x_D}{\partial L} _V$	O	_____
$\frac{\partial x_D}{\partial V} _L$	Δ	- - - - -
$\frac{\partial x_B}{\partial L} _V$	\square	- - - - -
$\frac{\partial x_B}{\partial V} _L$	\diamond	- - - - -

Figure 6 Gain Characteristics for Tower D, Energy Balance: Perturbations in L



Transfer Function Relation	Time Constant (min)	Dead Time (min)	Approximation Using Equation 7.1
$x_D - L$	○	•	_____
$x_D - V$	△	▲	- - - - -
$x_D - L$	□	■	_____
$x_B - V$	◇	◆	- - - - -

Figure 7 Time Constant and Dead Time Characteristics for Tower B, Energy Balance: Perturbation in L



Transfer Function Relation	Time Constant (min)	Dead Time (min)	Approximation Using Equation 7.1
$x_D - L$	○	•	_____
$x_D - V$	△	▲	- - - - -
$x_B - L$	□	■	_____
$x_B - V$	◇	◆	- - - - -

Figure 8 Time Constant and Dead Time Characteristics for Tower D, Energy Balance: Perturbations in L

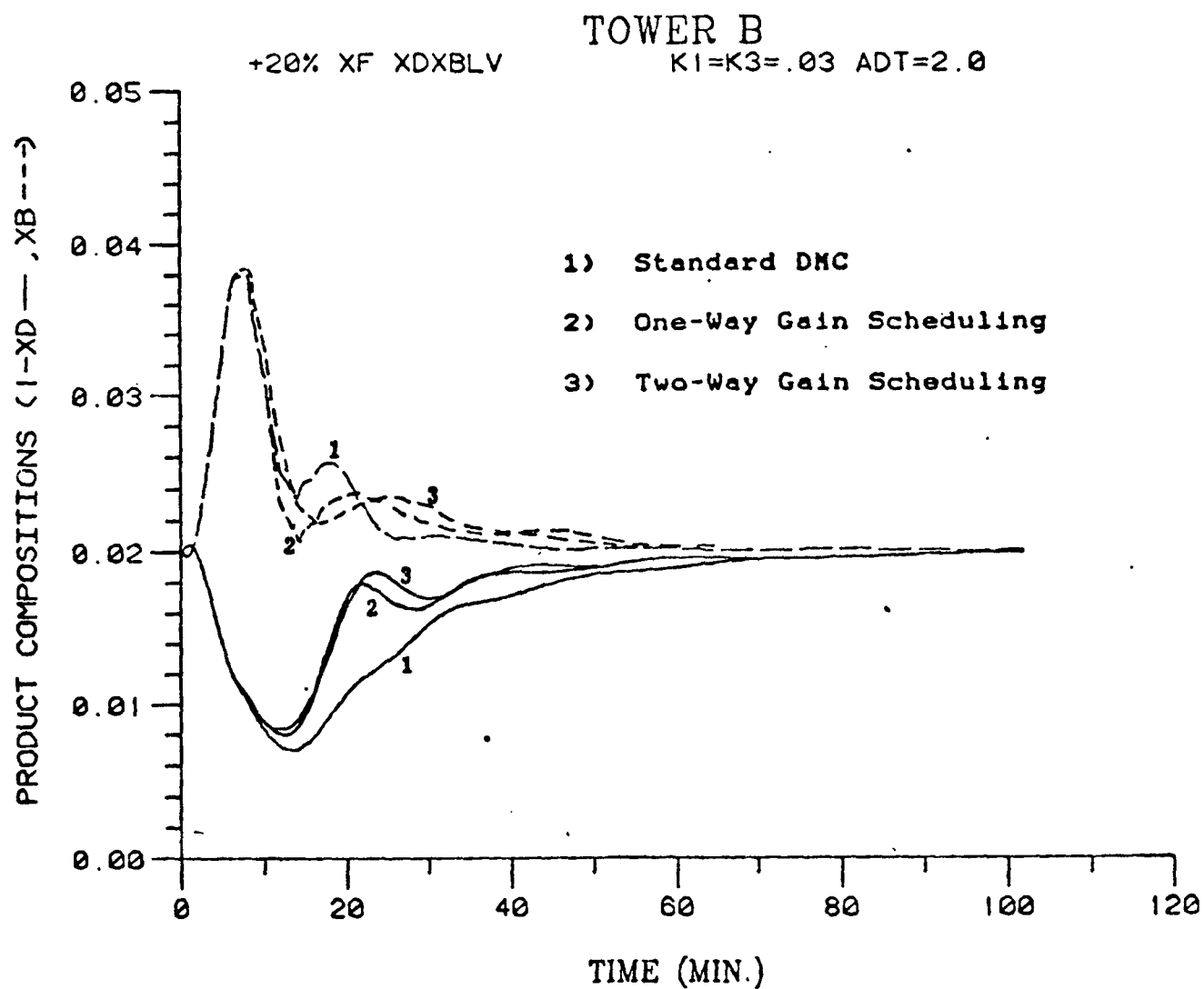


Figure 9 Tower B, Energy Balance Control: Comparison of One-Way and Two-Way Gain Scheduled DMC for a +20% Step in x_F .

DMC PARAMETERS

$$T_s = 2.0 \text{ min.}$$

$$N = 13 \quad k_1 = k_2 = 0.03$$

$$M = 38 \quad W = I$$

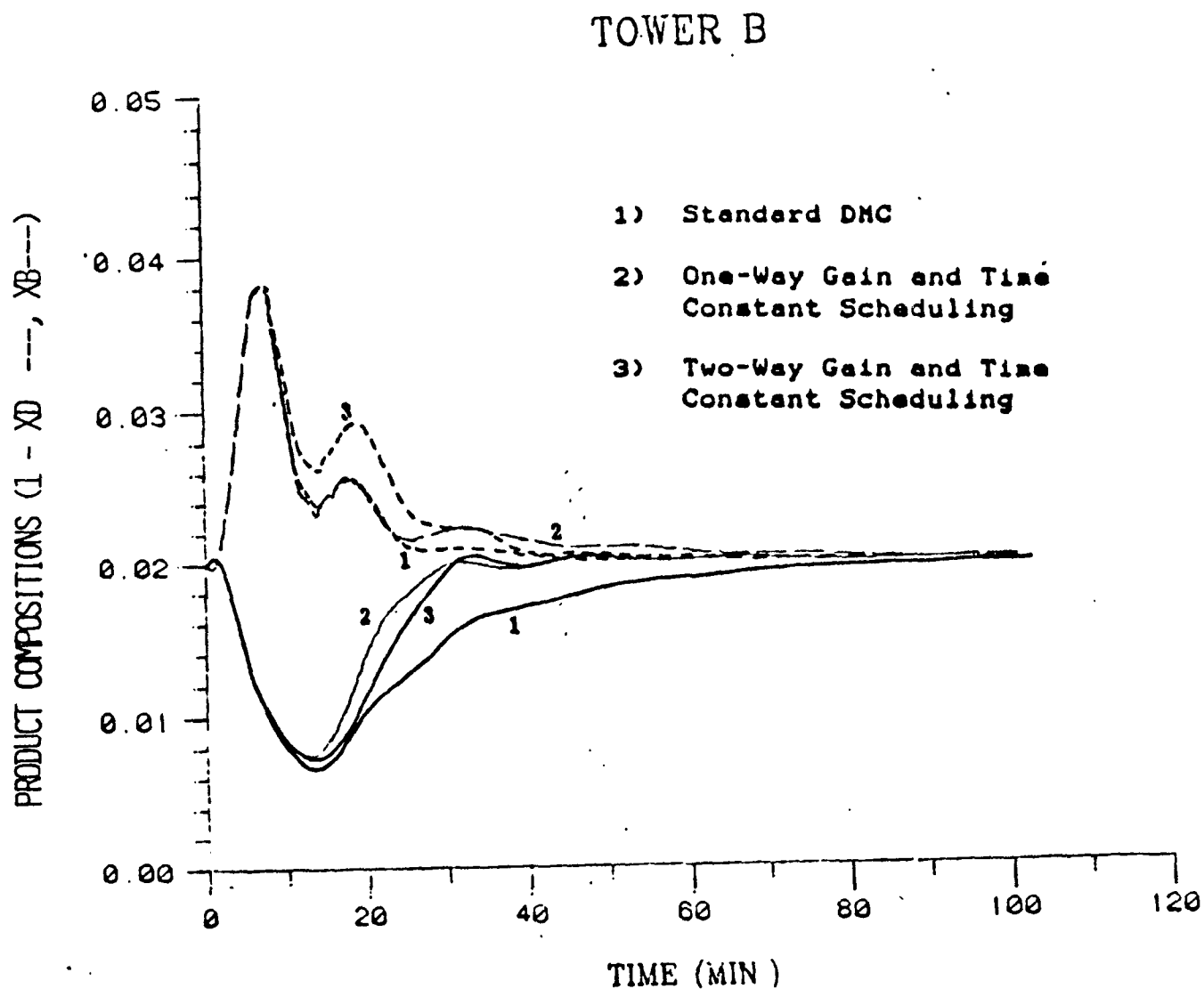


Figure 10 Tower B, Energy Balance Control: Comparison of One-Way and Two-Way Gain and Time Constant Scheduled DMC for a +20% Step in x_F .

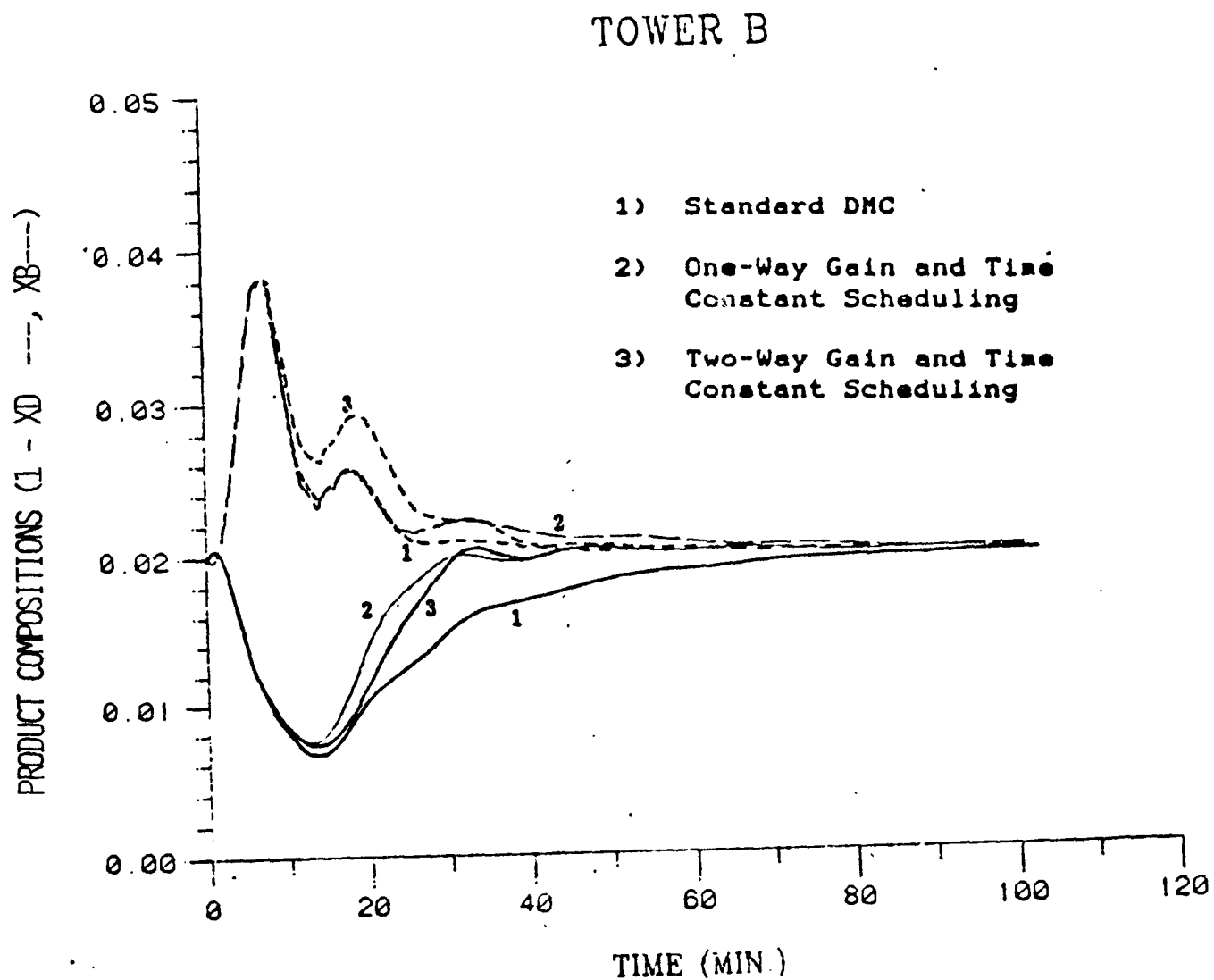


Figure 10 Tower B, Energy Balance Control: Comparison of One-Way and Two-Way Gain and Time Constant Scheduled DMC for a +20% Step in x_F .

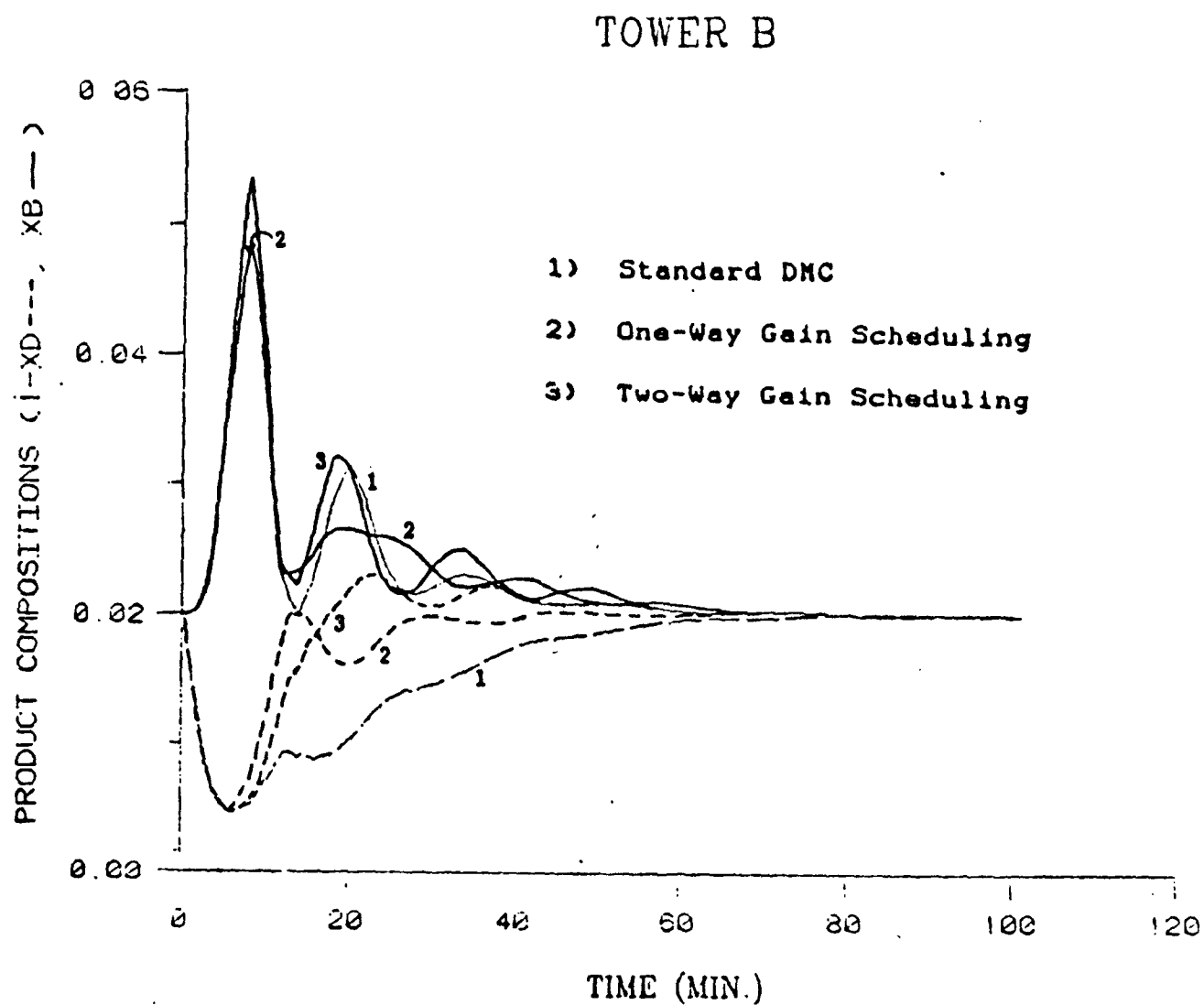


Figure 11 Tower B, Energy Balance Control: Comparison of One-Way and Two-Way Gain Scheduled for a -20% Step in F .

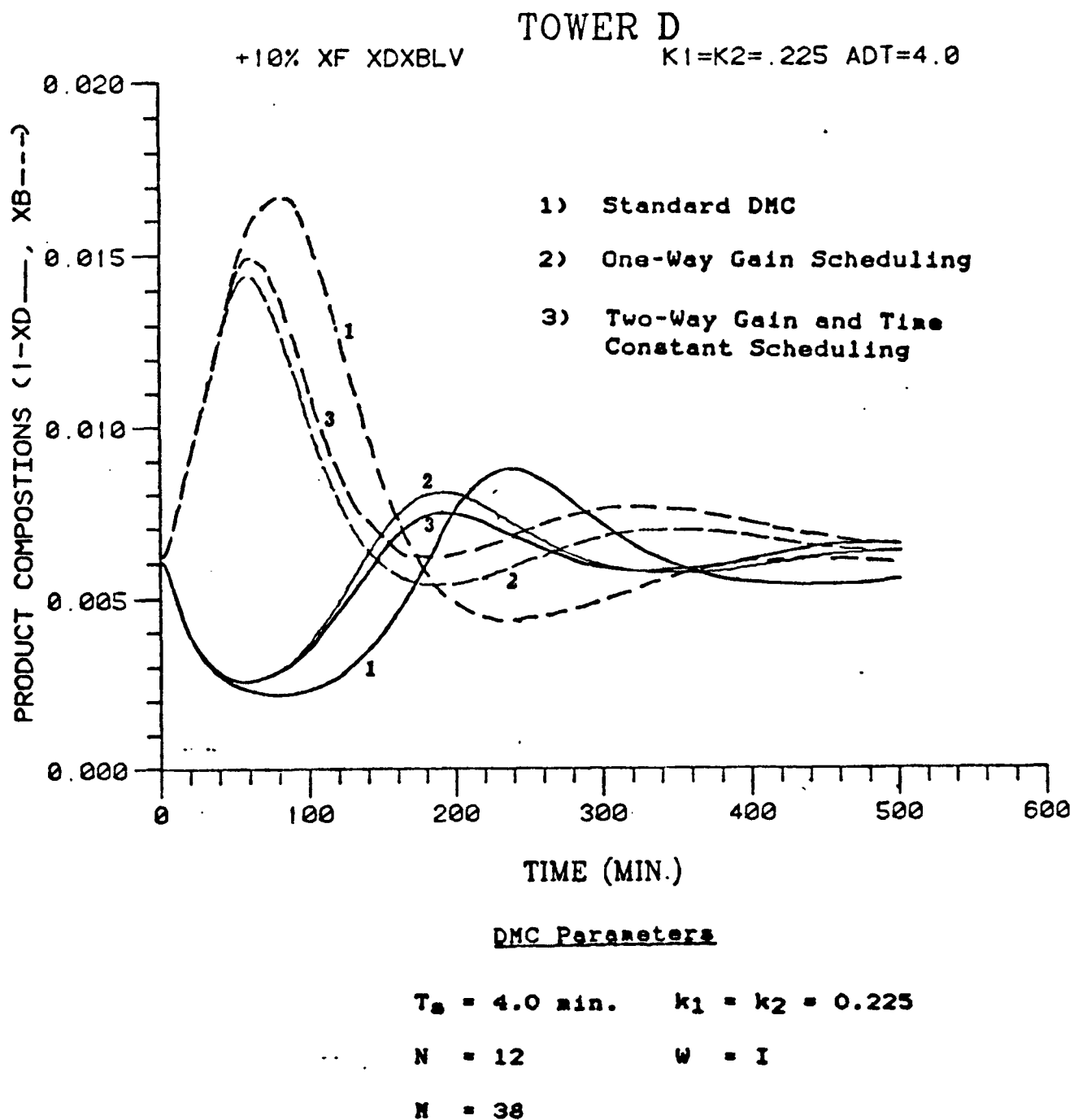


Figure 12 Tower D, Energy Balance Control: Comparison of One-Way Gain Scheduled DMC for a +10% Step in x_F .

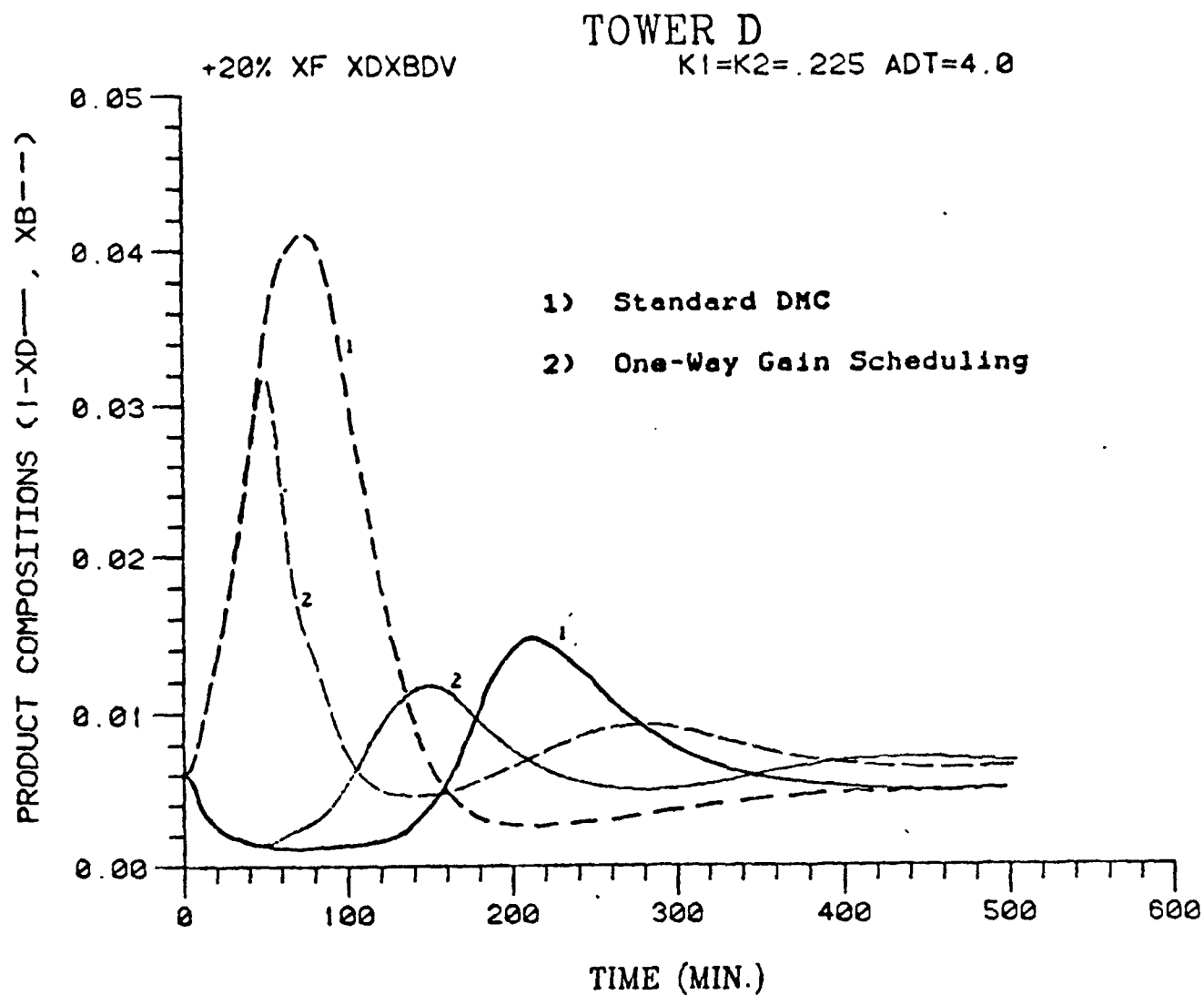


Figure 13 Tower D, Energy Balance Control: Comparison of One-Way Gain Scheduled DMC for a +20% Step in x_F .