The Use of Secondary Measurements to Improve Control

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Many industrial processes are difficult to control because product quality cannot be measured economically on line. One solution to this problem is to use secondary measurements in conjunction with a mathematical model of the process to estimate product quality. This paper presents a method for designing a *static estimator which predicts product quality* from a linear combination of process input and output measurements. The design method includes procedures for selecting a subset of the available output measurements so as to obtain an estimator which is relatively insensitive to modeling errors and *measurement noise. Application* of the estimator to a simulated multicomponent distillation column shows that the composition control achieved with an estimator based on temperature, reflux, and steam flow measurements is comparable to that achieved with instantaneous composition measurements. The composition control using the estimator is far superior to the composition control achieved by attempting to maintain a constant temperature on any single stage of the column.

The control of many industrial processes is complicated by problems associated with the on-line measurement of the product quality. Occasionally, the required measurement technology simply does not exist. More frequently, the needed instrumentation is either prohibitively expensive and/or the measurement lags and sampling delays associated with the measurement are so large as to make it impossible to design an effective feedback control system. In such cases secondary measurements can be used to infer the effect of process disturbances on the product quality. This is relatively easily done when there is a thermodynamic or physical relationship between the available measurements and the unmeasurable product quality. For example, in binary distillation one can use either the temperature and pressure of a stage, or the output of a vapor pressure bulb inserted into the liquid on the stage, to estimate the composition of the liquid on the stage. When there is no direct physical relationship between the available measurements and the product quality, then the estimation of product quality from secondary measurements requires some knowledge of how the process operates. Feed-forward control systems use process input-output relationships and measurements of major process disturbances to estimate the effect of the measured disturbance on the product quality. The controller then adjusts the control effort so as to maintain the estimated product quality at the desired level. Usually, the estimation and control steps are combined and are not separately distinguishable.

The control strategy proposed in this paper is to use selected measurements of both process inputs and outputs to estimate the effect of measured and unmeasured disturbances on the product quality and to then use a standard control system to adjust the control effort so as to maintain the product quality at the desired level. This strategy reduces approximately to that of a feed-forward control system when there are no measurements of process outputs. The design of the estimator can be reduced to three steps: 1. the selection of the appropriate measurements from those available, 2. the inversion of the process model so as to obtain an estimate of the unmeasured process disturbances from the measurements, and 3. application of the process model to map the estimated and measured process inputs into the estimate of the product quality. Conceptually, steps 2 and 3 can be carried out even with very complex dynamic models. However, the calculations are correspondingly complex and the resulting estimator will generally be too expensive to implement.* Therefore, the approach adopted in this work is to reduce the process model to as simple a form as possible subject to the constraint that the combined estimator and controller system must yield satisfactory process regulation. The simplest conceivable process model is a set of linear, static input-output relationships. Somewhat surprisingly, it turns out that this simple model yields a static estimator, so called because it has no dynamic elements, which performs quite satisfactorily for a special but interesting class of processes. The next two sections develop methods for the design of the static estimator. The third section shows that the static estimator will yield good dynamic estimates for the class of processes which, when viewed by observing only their outputs, appear to move from one steady state to another through a sequence of steady states. Finally, the last section presents the results of applying the static estimator in combination with a standard P-I control system to the control of a simulated multicomponent distillation column. Future work will concentrate on extending the design methods presented below to include processes to which the static estimator cannot be successfully applied.

THE STATIC ESTIMATOR

The static estimator relates perturbations in measured quantities to perturbations in product quality. It is derived from a linear model of the process which is valid

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* The same is true of Kalman Filters (3) which will usually require too much computation to be economically feasable for most chemical plants.

in some region about a steady state operating point. This model is written as

$$x = Fv = Mm + Ju; \quad \dim(v) = \dim(u) + \dim(m) \tag{2.1}$$

$$y = Hx = Qm + Ru; \quad \dim(y) \geq \dim(u) \tag{2.2}$$

$$w = Gx = Pm + Ku \tag{2.3}$$

where v = process input perturbations
dim $(\cdot)$ = the dimension of the vector inside the brackets
u = unmeasured components of v
w = process product quality perturbations (assumed to be unmeasurable for purpose of control)
x = process state perturbations
y = measurable process output perturbations

Lower case letters in (2.1), (2.2) and (2.3) are vectors, capital letters in (2.1), (2.2) and (2.3) are matrices and

$$(M \vdots J) \equiv F; \quad Q = HM; \quad R = HJ; \quad P = GM; \quad K = GJ$$

Relations (2.1), (2.2), and (2.3) can be obtained either directly from perturbation tests on the process or by manipulation of the static relationships given in the process model.

The main restriction which we place on the static model given by (2.1) to (2.3) is that there be at least as many measurable outputs y as there are unmeasured inputs u [that is, dim $(y) \geq$ dim (u)]. If this restriction is not met by the process under consideration, then the process model should be re-examined to see if it can be recast with fewer unknown inputs. To illustrate how this might be done, consider a 20 component distillation. If one looks at this process as if the composition of each component in the feed is an unknown (the feed composition is not measured) then one must have a minimum of 19 secondary measurements to be able to estimate the composition of each component of feed and thus be in a position to estimate the product compositions. If, however, one views the feed as a distribution of components and the parameters describing the distribution are the unknowns, then there may be far fewer than 19 unknowns. (A good distribution to consider might be the cumulative mole fraction versus the component number, where the components are ordered by their relative volatilities.) It is highly unlikely that a feed distribution which arises from some natural or man made process will change so radically to have 20 degrees of freedom. It is more likely that all possible distributions will be describable by a distribution function having on the order of 5 free parameters. In this case the minimum number of secondary measurements is now 5 rather than 19.

Another restriction which we place on the model given by (2.1) to (2.3) is that the rank of the matrix R in (2.2) be equal to the number of unmeasured inputs [that is, Rank R = dim (u)]. If the rank of R is less than the dimension of u [it can never exceed dim (u)] then there exists a number of linear relationships between the unmeasured inputs equal in number to the difference between the dimension of u and the rank of R. In Appendix I* we show how to use these relationships to reduce the number of unmeasured inputs and the size of the matrix R so that the rank of R is equal to the dimension of u. Since the matrix R plays such a central role in the development of the static estimator which follows, we shall give it a special name.

$$R \equiv \text{the model matrix}$$

The main problem in designing the static estimator is to select that subset of measurable outputs y which will yield an effective, yet inexpensive, estimator. If there were no noise in the measurements, no modeling errors, and no limits on computational accuracy, then the design of the estimator would proceed as follows. First, select as many of the least expensive measurements as there are unmeasured inputs. Then solve for the unmeasured process inputs u in terms of the measurements, as in (2.2). Substituting this relationship into Equation (2.3) yields the following relationship between the product quality and the measurements.

$$w = Pm + K\hat{R}^{-1}[\hat{y} - \hat{Q}m] \tag{2.4}$$

where $\hat{y}$ = the vector of measurements selected for use in the estimator (the components of $\hat{y}$ are a subset of the components of y)
$\hat{R}$ = the reduced model matrix (that is, the square submatrix of R formed by selecting the rows of R corresponding to the measurements of $\hat{y}$)
$\hat{Q}$ = the submatrix of Q associated with the measurements $\hat{y}$.

In practice, none of the foregoing assumptions are true; therefore, an estimator designed as described above will more often than not give very poor estimates. This is due to the fact that estimation errors caused by errors in modeling, measurement, and numerical roundoff can be greatly amplified by a poor choice of measurements. To show how this comes about, we first rewrite (2.2) explicitly incorporating modeling errors and measurement noise as follows:

$$(\hat{\mathcal{R}} + \hat{E})u = \hat{\mathbf{b}} + \hat{\epsilon} \tag{2.5}$$

where $\hat{\mathcal{R}} \equiv$ the error free reduced model matrix
$\hat{E} \equiv$ error matrix associated with $\hat{R}$
$\hat{\mathbf{b}} \equiv \hat{y} - \hat{Q}m =$ the noise free measurement vector
$\hat{\epsilon} \equiv$ vector sum of the measurement noise in $\hat{y}$ and $\hat{Q}m$
u = noisy estimate of the true process inputs

The error matrix $\hat{E}$ arises both from uncertainties in our knowledge of the elements of $\hat{R}$ and from changes in the steady state operating point of the process (that is, changes in u and m).

In general, there will be more measurements $\hat{b}$ than unmeasured inputs u and (2.5) will not have a solution for u which satisfies the equality. One can, however, obtain a generalized solution of the form

$$u = \hat{R}^{+}\hat{b} \tag{2.6}$$

$$\hat{R}^{+} \equiv (P\hat{R})^{-1}P \tag{2.6a}$$

* Appendices I and II have been deposited as Document No. 01763 with the National Auxiliary Publications Service (NAPS), c/o CCM Information Corp., 866 Third Ave., New York 10022 and may be obtained for $2.00 for microfiche or $5.00 for photocopies.

where $\hat{R} \equiv \hat{\mathcal{R}} - \hat{E}$

$\hat{R}^+$ = a generalized inverse of $\hat{R}$

P = any matrix such that $P\hat{R}$ is nonsingular

$\hat{b} = \hat{\mathbf{b}} + \hat{\epsilon}$

If P in Equation (2.6a) is taken as the transpose of $\hat{R}$ then the generalized solution of (2.5) given by (2.6) is the classical "least squares" solution.

The error in the process inputs estimated from (2.6) which is caused by the errors in modeling and measurement, is shown in Appendix II to be bounded as follows:

$$||u - \mathbf{u}|| \leq ||\hat{R}^+||\ ||\hat{E}\mathbf{u} + \hat{\epsilon}|| \tag{2.7}$$

and

$$\frac{||u - \mathbf{u}||}{||u||} \leq \{||\hat{R}^+||\ ||\hat{R}||\} \frac{||\hat{E}\mathbf{u} + \hat{\epsilon}||}{||\hat{b}^*||} \tag{2.8}$$

where

$$||R|| \equiv \sup_x \left\{ \frac{||Rx||}{||x||} \right\}$$

$\mathbf{u}$ = true process inputs = error free, unique, solution of $\mathcal{R}\mathbf{u} = \mathbf{b}$

$\hat{b}^*$ = projection of $\hat{b}$ on the space spanned by the columns of $\hat{R}$

$||\hat{R}^+||\ ||\hat{R}|| \equiv$ condition number of $\hat{R}$

The error bounds given in (2.7) and (2.8) are the best possible in the sense that the equality will be attained for some values of the vectors $\hat{E}\mathbf{u} + \hat{\epsilon}$ and $\hat{b}^*$ ($||\hat{b}^*|| \neq 0$).

We will henceforth take the vector norms in (2.7) and (2.8) to be the Euclidian norm. In this case the term $||\hat{R}^+||\ ||\hat{R}||$ in (2.8) is called the spectral condition number of $\hat{R}$. The spectral condition number (which we will often refer to simply as the condition number) is equal to the square root of the ratio of the maximum eigenvalue to the minimum eigenvalue of the symmetric matrix $(\hat{R})^T(\hat{R})$ as shown in Appendix II.* The term $||\hat{R}^+||$ in (2.7) is equal to the square root of the reciprocal of the minimum eigenvalue of $(\hat{R})^T(\hat{R})$.

The error bounds given by (2.7) and (2.8) can be used to aid in the selection of a good set of measurements for the static estimator. Whether the absolute error given by (2.7) or the fractional error given by (2.8) should be used as the criterion for selection will depend upon the particular problem. In the following discussion we will use the fractional error, but the same considerations apply to the absolute error. From (2.8) it is quite clear that the condition number of the reduced model matrix should be kept as small as practicable to avoid the possibility of error amplification. Indeed, if the condition number of the reduced model matrix were much above 100 then one would expect that the inevitable modeling errors would be amplified into unacceptably large errors in the estimate of $\mathbf{u}$.

If, on the other hand, the condition number of $\hat{R}$ were between 1 and 10, then it is unlikely that error amplification would be a significant problem. Thus, it is easy to select between measurement sets whose associated reduced model matrices have very widely differing condition numbers; one selects that set which is associated with the lower condition number. However, when selecting between measurement sets whose associated condition numbers vary between 20 and 100 or so, then it is necessary to consider the noise and error statistics of the measurements and model matrices as well as the condition number of the model matrix in order to obtain a precise ordering of the various measurement sets. Unfortunately, in many practical situations the required statistics will be unavailable. This is especially true of the modeling error statistics. In such cases condition number considerations can be used to get at least a qualitative ordering between various measurement sets. A complete discussion of the techniques to be used when the required statistics are available is beyond the scope of this paper. However, when the measurements are statistically independent and the measurement noise is Gaussian and much larger than the modeling noise, then it is a fairly simple matter to modify the measurement selection procedure to account for the different noise levels on the various measurements. One approach is to modify (2.2) by premultiplying each side by a diagonal matrix of reciprocal standard deviations. This gives

$$S\mathcal{R}u = S(\mathbf{b} + \epsilon) = S\mathbf{b} + \epsilon^* \tag{2.2a}$$

where ϵ^* = transformed noise vector, each component of which has a standard deviation of 1.

The measurement sets can now be compared by comparing the condition numbers of the submatrices of SR rather than of the original model matrix R.

Since there is a significant computational expense associated with the calculation of condition numbers, and since in most cases condition number considerations lead only to a qualitative ordering of measurement sets, it is desirable to have a simpler heuristic for selecting measurements. Economics dictate that any such heuristic start by comparing all combinations of measurements equal in number to the number of unmeasured inputs. In terms of the model matrix R this means that the initial search is over all square submatrices of R of order equal to the dimension of the unknown inputs u. Clearly, one will not choose a submatrix in which two of the row vectors are parallel since such a submatrix would be singular, and the noise and error amplification is infinite. Carrying this idea one step further, one would not choose a submatrix in which two vectors were almost parallel since such a matrix would be almost singular, and the error and noise amplification would be almost infinite. These considerations lead one to a heuristic, called the minimax row dot product heuristic, which selects that set of measurement vectors which have the largest angles between each other. The cosine of the angle between two vectors is given by their normalized dot product which is defined by (2.9) below.

$$DP(i,j) \equiv \frac{\langle r_i, r_j \rangle}{\langle r_i, r_i \rangle^{1/2} \langle r_j, r_j \rangle^{1/2}}, \quad i,j = 1 \ldots n \tag{2.9}$$

where $\langle r_i, r_j \rangle$ = inner product of r_i with r_j

r_j = jth row of R

n = the number of feasible measurements

If $DP(i,j) = 1$ the vectors i and j are parallel and if $DP(i,j) = 0$ the vectors are orthogonal. In order to compare various sets of measurements, we define

$$MDP_k \equiv \max_{i,j \epsilon S_k} DP(i,j) \tag{2.10}$$

$\equiv$ maximum row dot product for the kth set of measurements, S_k

The sets of measurements with the smallest maximum row

* See footnote on page 615.

dot product are candidates for use in the estimator. If one or more of these sets has a reduced model matrix with a relatively low condition number then the set with the lowest noise level is chosen as the measurement set and the search is over. If the condition numbers are all very high then the number of measurements in the sets S_k is increased by one and (2.10) is recomputed. Again, the sets of measurements with the smallest maximum row dot product are candidates for use in the estimator. This procedure is continued until a set of measurements with an acceptable condition number is found. It is not difficult to construct examples where the above algorithm fails to yield a good set of measurements even though such a set does indeed exist. This occurs when the Euclidian length of the row vectors of the model matrix R vary substantially. Such variations are likely to occur when one is selecting between different types of measurements, as for example between flow and temperature measurements. For this reason we recommend using the minimax row dot product heuristic only when selecting between large numbers of like measurements as is the case in the selection of temperature measurements in the distillation column example of the last section.

USING OCCASIONAL PRIMARY MEASUREMENTS TO UPDATE THE STATIC ESTIMATE

In many industrial systems where primary measurements are available, the designer may still wish to make use of secondary measurements for control purposes. This happens when the primary measurements are only infrequently available or when the time required to process the primary measurements is too large to allow them to be used in an efficient control scheme. In such cases, the primary measurements can be used to correct the estimated product quality for the steady state offset induced by modeling errors and measurement bias. One method for doing this is to add a correction term to the estimate which is the difference between the last primary measurement and the estimate corresponding to the time of the last primary measurement. That is, let

$$\delta(t_k) \equiv w_m(t_k) - w_e(t_k) \tag{3.1}$$

where

$w_e(t_k)$ = the estimate of w obtained from the static estimator at time t_k

$w_m(t_k)$ = the measurement of w at time t_k

From (2.6) and (2.3) $w_e(t_k)$ is given by

$$w_e(t_k) = Pm(t_k) + K\hat{R}^+ [\hat{y}(t_k) - \hat{Q}m(t_k)] \tag{3.2}$$

The corrected estimate $w_{ec}(t)$ is then given by

$$w_{ec}(t) = w_e(t) + \delta(t_k)\ ; \quad t_k \leq t \leq t_{k+1}\ . \tag{3.3}$$

ANALYSIS OF THE DYNAMIC PERFORMANCE OF THE STATIC ESTIMATOR

In this section we show that there exists a class of processes for which the static estimator of the last section will give a satisfactory estimate of the dynamic state of the process without the addition of any dynamic compensation. Unfortunately, the development will *not* permit determination of whether a particular process is in the above class without a prohibitive amount of computation. Thus, the results of this section are of interest mainly because they indicate that the results of the next section, where the static estimator is applied to a multicomponent distillation, are not restricted to the particular example process, which was chosen more or less at random from the literature, but rather extend to a large number of distillation processes and perhaps other processes as well. For the purposes of our analysis we take the process equations to be of the form

$$\dot{x}(t) = Ax(t) + Bu(t) \tag{4.1}$$

$$y(t) = Hx(t) \tag{4.2}$$

where $x(t)$ = process state vector

A, B, and H are constant matrices

In order to keep the notation simple, we assume that there are no measured inputs. In order to keep the analysis simple we assume that there are no model errors or measurement noise. Under these assumptions the static estimator for $x(t)$ is

$$x_e(t) = J\hat{R}^+ \hat{y}(t) = J\hat{R}^+ \hat{H}x(t) \tag{4.3}$$

$$J = A^{-1}B$$

$$\hat{R} = -\hat{H}A^{-1}B = \hat{H}J$$

The error involved in using the static estimator for dynamic estimation is then given by

$$x(t) - x_e(t) = (I - J\hat{R}^+H)x(t) \tag{4.4}$$

$$= \Gamma\, x(t)$$

where $\Gamma \equiv I - J\hat{R}^+ \hat{H}$

The matrix Γ in (4.4) will be called the distortion matrix. This matrix has the important property that it annihilates the matrix J as can be seen from the following

$$\begin{aligned}\Gamma J &= J - J\hat{R}^+HJ \\ &= J - J\hat{R}^+\hat{R} \quad \text{(by the definition of } \hat{R}) \\ &= J - J \qquad (\text{since } \hat{R}^+\hat{R} = I) \\ &= 0\end{aligned}$$

The above property of the distortion matrix allows us to rewrite (4.4) as

$$x(t) - x_e(t) = \Gamma(x(t) - Jd(t)) \tag{4.5}$$

where d = any vector in Euclidian m space E^m

m = dimension of the input vector $u(t)$

Since $d(t)$ can be any vector in E^m we will choose it so that the quantity $||x(t) - Jd||$ is a minimum.

Let d^* ≡ the vector which minimizes $||x(t) - Jd(t)||$ at time t

$$\mathcal{E}^*(t) \equiv x(t) - Jd^*(t)$$

We call the quantity $\mathcal{E}^*(t)$ the local transient error.

Now (4.5) can be rewritten as

$$x(t) - x_e(t) = \Gamma\mathcal{E}^*(t) \tag{4.7}$$

and from (4.7) it follows that

$$||x(t) - x_e(t)|| \leq ||\Gamma||\ ||\mathcal{E}^*(t)|| \tag{4.8}$$

To get an error bound which is independent of time and the particular inputs to the system we define a global transient error $\mathcal{E}(U)$ as

$$\mathcal{E}(U) \equiv \max_{\substack{0\leq t\leq T<\infty \\ u(0)\in U}} \{||\mathcal{E}^*(t)||\}$$

U ≡ the set of allowable $u(\cdot)$ in interval $0 \leq t \leq T$.

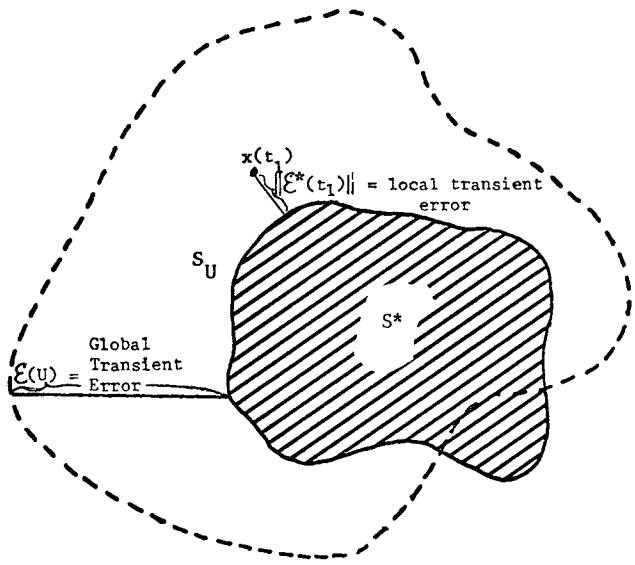


Fig. 1. Local and global transient errors.

It then follows immediately from (4.8) that

$$||x(t) - x_e(t)|| \leq ||\Gamma||\, \mathcal{E}(U) \qquad (4.9)$$

An interesting pictorial interpretation of the local and global transient errors is obtained if one defines the following sets.

Definition: The steady state vector space S° is

$$S^\circ \equiv \{x | x = Jd, \quad d \epsilon E^m\}$$

Definition: The space of all reachable system states from x_0 is

$$S_U \equiv \{x |\, \dot{x}(t) = Ax(t) + Bu(t),\ x(0) = x_0;\ u(\cdot) \epsilon U,\ t \geq 0\}$$

The sets S° and S_U are depicted in Figure 1. The local transient error at time t_1 is the minimum distance between the system state $x(t_1)$ and the boundary of the set S°. The global transient error is the maximum distance from the boundary of S_U to the closest point on the boundary of S°. Notice that S° need not be contained in S_U since some steady states may not be reachable from x_0 with the inputs $u(t)$ restricted to lie in the set U.

A bound on the error in the estimate of the product quality similar to that of (4.9) is obtained directly from (4.7) and the relationship between the product quality and the state of the system. From (2.2) and (2.3)

$$w(t) = G\, x(t)$$

$$w_e(t) = G\, x_e(t)$$

where $w_e(t) =$ the estimate of the product quality
Therefore

$$||w(t) - w_e(t)|| \leq ||\Gamma_w||\ \mathcal{E}(U) \qquad (4.10)$$

where $\Gamma_w \equiv G\Gamma =$ the distortion matrix for $w_e(t)$.

From (4.9) and (4.10) it is clear that the estimation error will be small if the global transient error and the norm of the distortion matrix are small. The distortion matrix is fixed by the set of measurement which are chosen for use in the estimator. Thus, the size of the distortion matrix norm is another factor which can be brought in to distinguish between measurements. The global transient error can, at least conceptually, be made as small as desired by suitably restricting the class of allowable inputs. Thus, for any process there exists a class of inputs for which the static estimator will yield satisfactory dynamic estimates. Unfortunately, for all but the most trivial problems, it will be prohibitively expensive to compute $\mathcal{E}(U)$ given U or vice-versa. A more practical approach is to design the best static estimator possible and then test this estimator on a simulation of the process. If the dynamic performance of the estimator is unsatisfactory then some form of dynamic compensation can be added to improve performance. A fruitful area for future research would be the development of rational methods for adding dynamic compensation to the static estimator.

APPLICATION OF THE STATIC ESTIMATOR TO A MULTICOMPONENT DISTILLATION COLUMN

As a test of the validity of the concepts presented in the previous sections, the static estimator was used to estimate the product compositions of a simulated 16 stage distillation column taken from the literature (*1*). The column operating conditions are given in Table 1. The following assumptions were used in constructing the process model: 1. no heat loss from the column, 2. perfect mixing on the trays, 3. constant molar overflow, and 4. no hydraulic lags.

The model matrix R and the P and Q matrices needed for estimating the overhead and bottoms composition from temperature, reflux ratio, and steam flow measurements were obtained from perturbation tests on the simulated process. The complexity of the model precluded the possibility of obtaining these matrices algebraically from the process model.

Temperature measurements for the estimator were selected by finding that set of measurements having the minimax row dot product. The set of five temperatures picked using this method are the 1st, 3rd, 8th, 14th, and 16th. The reduced model matrix associated with these measurements has a minimax row dot product of 0.97 and a condition number of 85.0 (*2*). This means that the matrix chosen by the minimax row dot product heuristic is not very well conditioned. However, the smallest condition number for all 5×5 square submatrices of R is 58, which is not that much better. Further, when the minimum condition number estimator (which uses measurements 1, 2, 7, 9 and 12) was compared with the estimator chosen by the minimax row dot technique, it was found that the latter yielded better estimates. This is not surprising since as mentioned previously the condition number of the model matrix is not the only factor affecting estimator performance.

Lest one get the impression that any reasonable set of temperature measurements yields a good estimator, we point out that the condition number of the reduced model matrix using measurements 1, 3, 10, 11, and 12 is 2,300

Table 1. Distillation Column Operating Conditions

Component	Feed composition	Overhead product composition	Bottoms product composition
Ethane	0.03	0.125	0.000
Propane	0.20	0.782	0.021
Butane	0.37	0.093	0.456
Pentane	0.35	0.000	0.458
Hexane	0.05	0.000	0.065

Feed enters as a liquid on the eighth stage from the bottom.
Reflux Ratio = .75.
Vapor Flow Rate = 16 moles/min.
Feed Flow Rate = 17 moles/min.
Column Pressure = 250 lb./sq.in.abs.

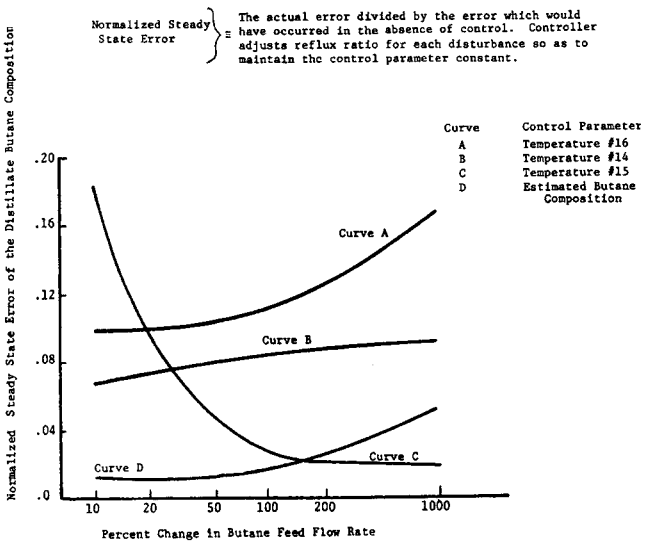


Fig. 2. Normalized steady state error of the distillate butane composition.

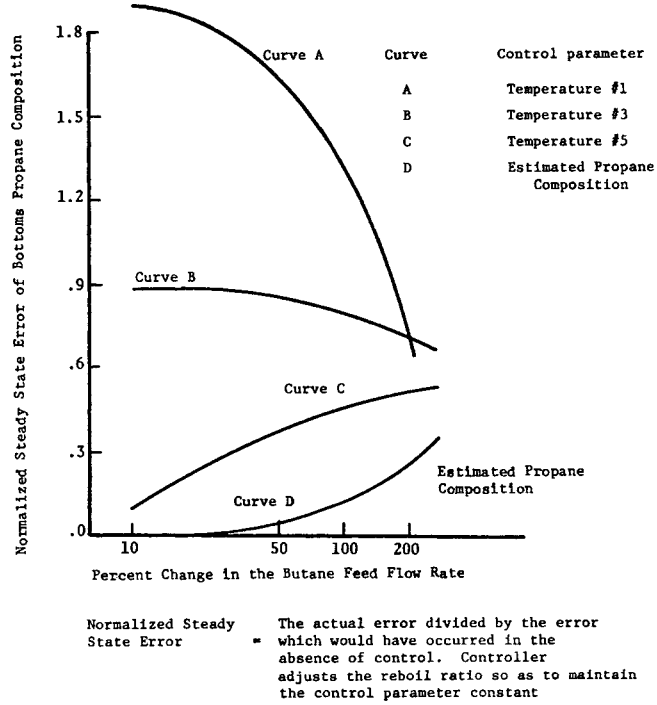


Fig. 3. Normalized steady state error of the bottoms propane composition.

and the minimax row dot product is 0.9999. This very high condition number reflects the strong coupling between the temperatures on neighboring trays in certain areas of the column.

To determine whether the use of an additional measurement would improve the estimator, a set of six measurements was picked using the minimax row dot product technique. The reduced model matrix condition number associated with the enlarged measurement vector was 84.5 —no real improvement. Also simulation studies showed that there was no significant difference between the performance of the two estimators. Therefore, only five temperature measurements were used in the static estimator.

The coefficient matrices used by the estimator to map the temperature perturbations into composition perturbations (that is, the matrices equivalent to $K\hat{R}^{-1}$ in 2.4) are found in Table 2. Examination of the overhead composition estimation matrix shows that the temperature of the 14th stage is weighted much more than any of the other measurements. This result indicates that a control system which maintains a constant tray temperature will also do a reasonable job of maintaining the desired overhead composition. Results presented in Figure 2 do indeed bear this out. However, these same results also show that the small corrections which arise from the use of all five temperature measurements lead to a significant improvement in control system performance. Examination of the estimation matrix for the bottom composition shows that there is no one temperature which is weighted much more heavily than any other. Therefore one could not reasonably expect to maintain a desired bottoms composition by maintaining a constant temperature on any of the stages

TABLE 2. ESTIMATION MATRICES ($K\hat{R}^{-1}$)

Overhead Composition Estimation Matrix
(All elements have been multiplied by 10^4)

	Temperature measurement	1	3	8	14	16
Output Compositions	Ethane	2.047	−2.093	−1.133	85.267	−119.963
	Propane	−3.323	3.397	1.820	−130.482	119.973
	Butane	1.331	−1.361	−0.715	45.213	−0.027
	Pentane	−0.054	0.054	0.031	0.030	0.016
	Hexane	0.000	0.000	0.000	0.000	0.000

Bottoms Composition Estimation Matrix
(All elements have been multiplied by 10^8)

	Temperature measurement	1	3	8	14	16
Output Compositions	Ethane	00.0001	−00.0004	00.0003	00.0002	−00.0003
	Propane	−00.0936	−01.7637	01.8243	−00.7976	00.0684
	Butane	05.5984	−09.6118	−06.8750	07.6177	−03.0396
	Pentane	−42.1540	47.8277	08.1812	−19.3935	09.8505
	Hexane	36.6496	−36.4523	−03.1308	12.5735	−06.8791

listed. This, too, is borne out by results presented in Figure 3. Thus, it appears that the estimation matrix can be used as a guide to whether or not a single temperature control system will perform satisfactorily.

Figures 2 and 3 allow a comparison of the steady state performance of various single temperature control systems versus the performance of a control system using the estimated concentrations of the butane (heavy key) in the overhead and the propane (light key) in the bottoms products. The static estimator equations in this case reduce to:

$$x_{D3} = 10^{-4}\,[1.33\,T_1 - 1.36\,T_3 - 0.72\,T_8 + 45.2\,T_{14} + 2.6\,u + 45\,u_2] \quad (5.1)$$

$$x_{B2} = 10^{-3}\,[5.60\,T_1 - 9.61\,T_3 - 6.88\,T_8 + 7.62\,T_{14} - 3.06\,T_{16} + 0.041\,u_1 - 21.6\,u_2] \quad (5.2)$$

where x_{D3} = estimated change in overhead butane concentration
x_{B2} = estimated change in bottoms propane concentration
T_i = measured change in the temperature on stage i
u_1 = measured change in the reflux ratio
u_2 = measured change in the steam flow, steam pressure = 100 lb./sq.in.abs.

Equations (5.1) and (5.2) are accurate to within a few % for feed flow and composition changes of between ± 20%. This range might be considered the range of validity of the linear model from which (5.1) and (5.2) were derived. However, as evidenced by Figures 2 and 3 the range of validity of the combined estimator and feedback control system is much larger than that of the estimator alone, and extends to disturbances of the order of ± 100%. This is due to the fact that the controller adjusts the reflux or steam flow so as to compensate for the disturbance and thus the column never really gets very far from its original steady state operating point. Figure 4 shows the uncontrolled transient response of the top butane composition of the multicomponent distillation column to a step change of 15% in the input butane flow rate. It demonstrates that the estimate is within 1% of

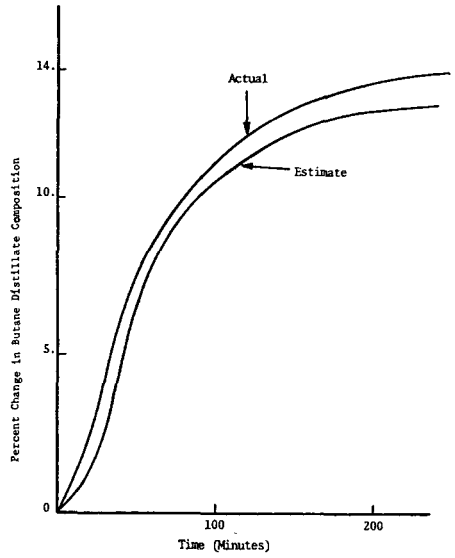


Fig. 4. Comparison of actual and estimated dynamic response of distillate butane composition for a step change of 10% in the butane feed flow rate.

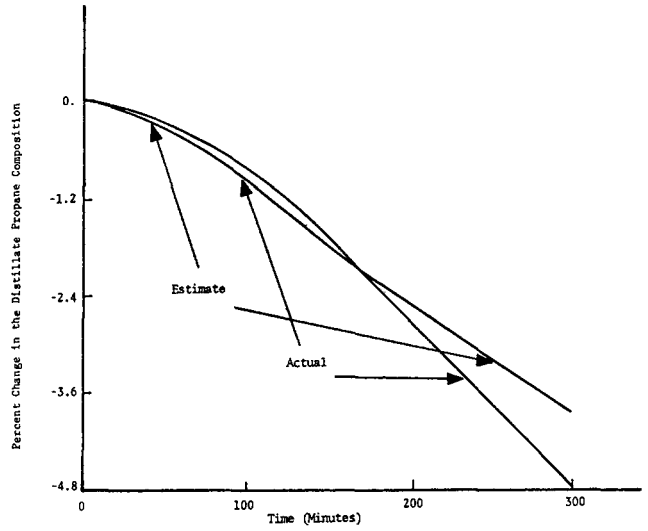


Fig. 5. Dynamic response of the distillate propane composition for a ramp change of 10% per 95 minutes in the feed flow rate of butane

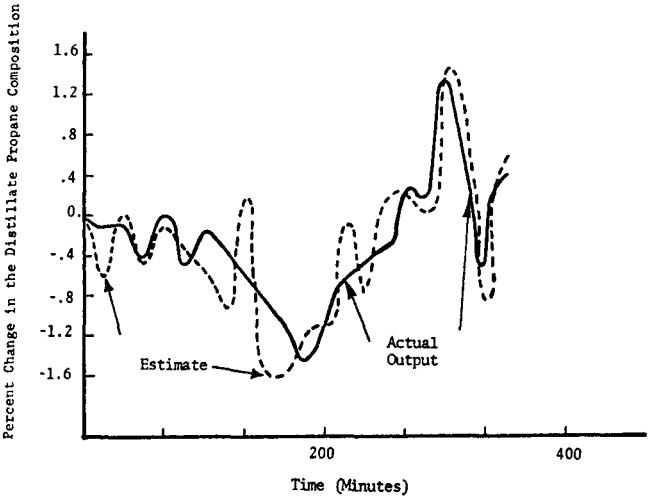


Fig. 6. Dynamic response of the distillate propane composition for random disturbances in the feed composition and flow rate.

the true composition over the entire range of operation. Similar results were obtained for the other output compositions. As additional evidence of the quality of the static estimator, Figure 5 shows the case where a ramp disturbance in the butane flow has entered the distillation column. The estimated composition was obtained using the estimation matrix given in Table 2. As can be seen, the estimate is nearly exact over the first 200 minutes, which corresponds to a 20% input disturbance. The estimate only begins to show significant error when the disturbance is so large as to cause the linear model to lose its validity. Finally, Figure 6 shows the behavior of the estimator when Gaussian, zero mean disturbances were applied to all of the input flow rates simultaneously. The standard deviation of each disturbance was set at 10% of the respective steady state input flow rates. Comparing the estimate to the actual composition, one sees that the estimator does a reasonably good job of tracking the outputs.

In order to gauge the effect of noisy measurements on the estimator performance, all temperature measurements were corrupted with zero mean Gaussian noise. The standard deviation of the noise on all but the top tray was ± 0.1 °F. The top tray measurement was taken to have a

larger standard deviation of ± 0.15 °F. so as to simulate the effect of imperfect mixing of the cold reflux entering the top tray. The autocorrelation function of the noise was taken to drop off to 0 for correlation times greater than 3 seconds.

Before use in the estimator, the noisy temperature measurements were passed through a two-stage filter. The first stage of the filter averages 9 samples, collected at the rate of 1 sample every 6 seconds. Since at the sampling rate selected the samples are statistically independent, the effect of the first stage of the filter is to reduce the standard deviation of the noise component of the signal by a factor of three (3). The decision to average over nine samples represents a compromise between noise reduction which is enhanced by longer averages, and controller performance which is degraded by longer averages. The second stage of the filter was a simple digital lag described

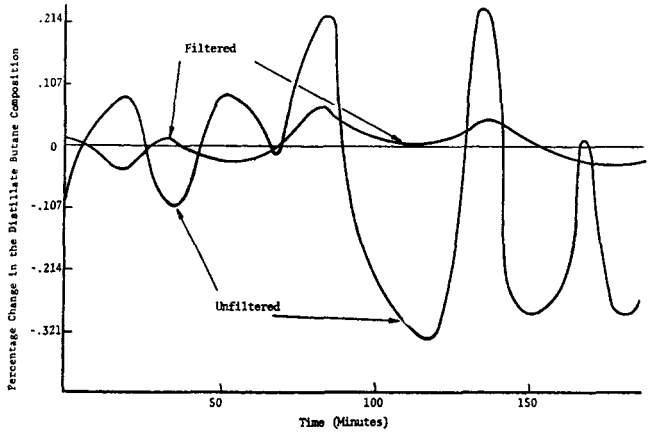


Fig. 7. Effect of noise on filtered and unfiltered estimates. Uncontrolled system.

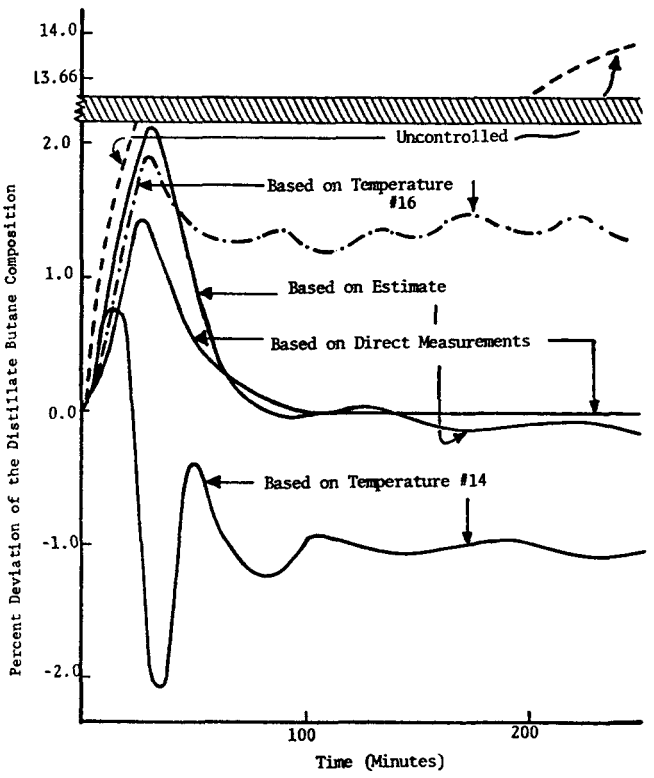


Fig. 8. Comparison of various control systems for maintaining a constant distillate butane composition.

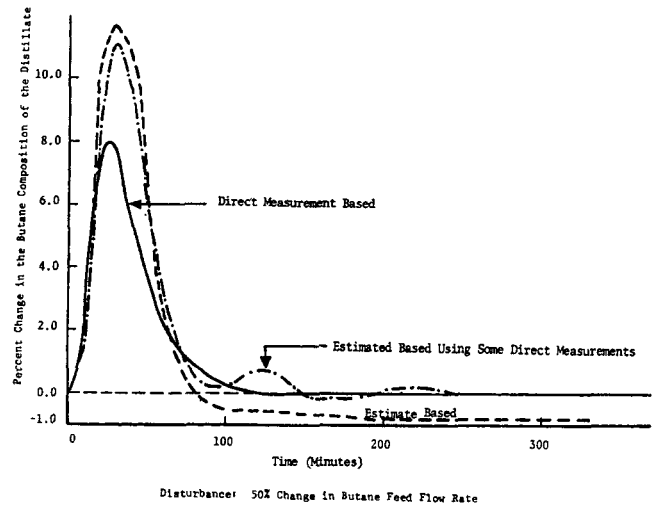


Fig. 9. Use of periodic composition measurements to correct for modeling errors.

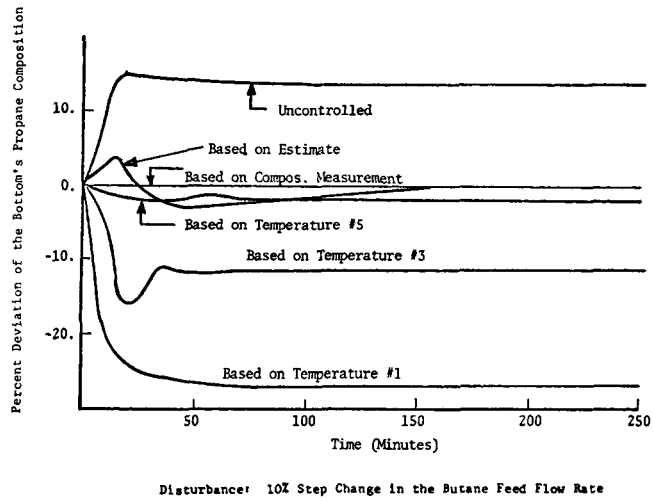


Fig. 10. Comparison of various control systems for maintaining a constant bottom's propane composition.

by the following equation:

$$y^*(t_{n+1}) = 0.1\ y(t_{n+1}) + 0.9\ y^*(t_n) \qquad (5.3)$$

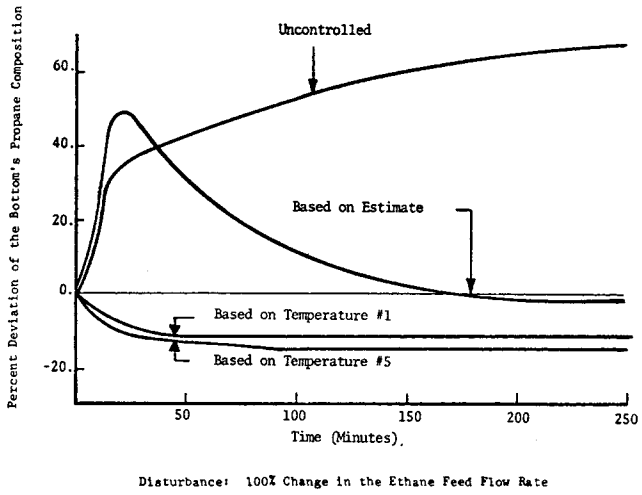
where $y^*(t_n)$ = the filtered measurement of time t_n
$y(t_n)$ = the averaged measurement at time t_n

The constants in (5.3) were obtained by tuning the second stage of the filter.

Figure 7 shows the improvement in estimation performance obtained using the above filter. (The curves in Figure 8 should be compared only as regards their statistical properties since they were obtained for different inputs with the same statistics.) It is noteworthy that while the filtered temperature measurements have a standard deviation from their mean of only 0.02%, the estimated overhead composition has a standard deviation of about 0.15%. This noise amplification is actually somewhat less than might be expected from an estimator obtained from a model matrix whose condition number is 85.

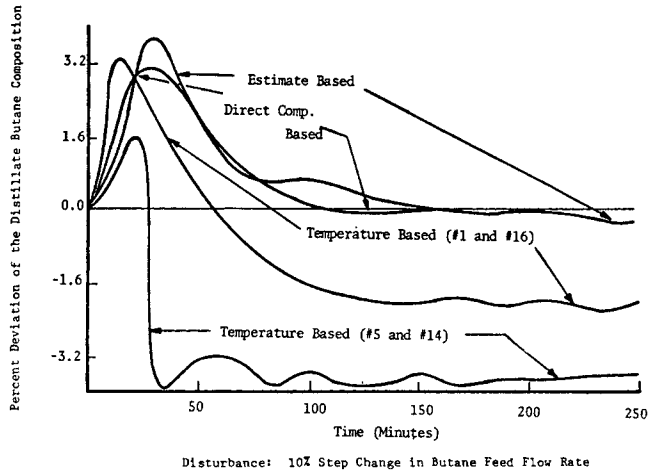
The ultimate test of estimator performance is how well it performs in conjunction with a control system in meeting control objectives. Figure 2 compares the steady state performance of the estimator, used in conjunction with a P-I (proportional plus integral) controller, with the performance of three other P-I controllers which use a single temperature measurement. The control objective was taken

to be the maintenance of a constant overhead butane composition. The manipulated variable was the reflux ratio. Figure 8 compares the dynamic performance of the three control systems. Each control system was tuned separately to get the best possible performance. Also shown in Figure 8 for the purpose of comparison is the response of a P-I controller which uses instantaneous noise-free measurements of the butane composition. Notice that there is little difference between the response obtained with either the exact or the estimated compositions. Figure 9 shows how the steady state error of the estimator based controller is reduced through the use of periodic composition measurements, such as those described earlier. The measurements were assumed to arrive once every 45 minutes. Figures 3, 10, and 11 compare the response of various P-I control systems when the control objective is to maintain a constant bottoms product propane composition. The manipulated variable in this case is the heat input to the reboiler. Again, each control system was separately tuned to give the best possible response to the various disturbances. In this case the estimator based controller is clearly superior to any of the controllers based on a single temperature measurement. Also notice that when the type of disturbance is changed, as from Figure 10 to Figure 11, the "best" single temperature controller changes from one which uses temperature #5 to one which uses temperature #1. Finally, Figures 12 and 13 compare the response



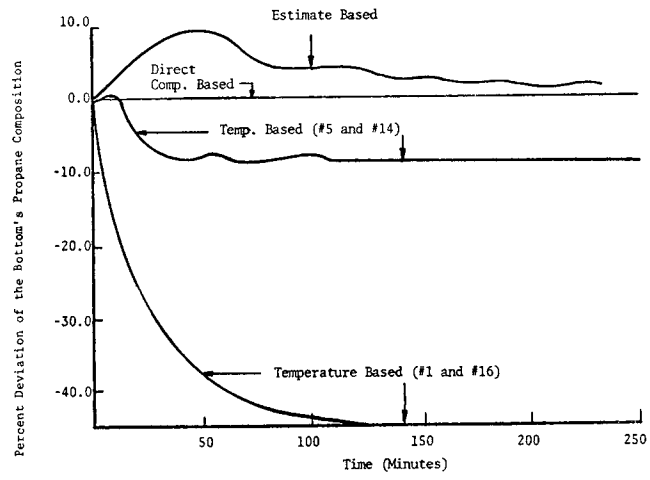
Disturbance: 100% Change in the Ethane Feed Flow Rate

Fig. 11. Comparison of various control systems for maintaining a constant bottom's propane composition.



Disturbance: 10% Step Change in Butane Feed Flow Rate

Fig. 12. Comparison of various dual control systems.



Disturbance: 10% Step Change in the Butane Feed Flow Rate

Fig. 13. Comparison of various dual control systems.

of control systems designed to maintain both the overhead butane and bottoms propane compositions constant. Two single loop P-I controllers (simultaneously manipulating the reflux ratio and heat input to the reboiler) were used to accomplish this objective. Each control loop was tuned separately for the best single loop response, and no effort was made to compensate for control loop interactions. Clearly, the estimator based controllers are much superior to the temperature based controllers.

CONCLUSIONS

A technique has been presented for designing an inexpensive estimator which predicts product quality from selected process output and input measurements. An important feature of the design algorithm is the method of selecting a subset of the available process output measurements which insures that the resulting estimator will be relatively insensitive to modeling errors and measurement noise. Once the appropriate measurements have been selected the estimator design can deviate from that presented to include important process nonlinearities and dynamic lags. Following the suggested design method leads to a static estimator which forms the estimate from a linear combination of measurements. This estimator is shown to give acceptable dynamic estimates for the class of processes which when viewed only from the process outputs *appears* to move from one steady state to another through a sequence of steady states. Experiments with a dynamic simulation of a multicomponent distillation column suggests that multicomponent distillation processes fall into the above class. It was found that the composition control achieved using the estimated product composition is comparable to that achieved with an instantaneous composition measurement and is markedly superior to the composition control achieved by maintaining a constant tray temperature.

ACKNOWLEDGMENT

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NOTATION

x = process state perturbation vector
y = measurable process output perturbation vector
w = product quality perturbation vector
v = process input perturbation vector

u = unmeasured components of v
m = measured components of v
F, G, H, J, K, M, P, R = matrices defined by (2.1) to (2.3)
R^+ = generalized inverse of R
$\Re$ = error free (actual) model matrix, R
E = error matrix ($R = \Re + E$)
b = $y - Qm$
$\sup_x$ = supremum over all x
S = diagonal matrix of reciprocal standard deviations of ϵ
ϵ = noise component of b
$DP(i, j)$ = normalized dot product of vectors r_i, r_j defined by (2.9)
Γ = distortion matrix given by (4.4)
$\mathcal{E}^\circ(t)$ = local transient error = $x(t) - Jd^\circ(t)$
$\mathcal{E}(u)$ = global transient error given by (4.9)

Superscripts

$\wedge$ = denotes vector or matrix which has been reduced by selecting certain elements from the original quantity
-1 = inverse
$+$ = generalized inverse

Subscripts

c = denotes estimated quantity
m = denotes measured quantity

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A Mathematical Model for Heat Transfer in a Packed Bed and a Simplified Solution Thereof

Heat transfer in packed beds can be mathematically modeled to account for the heat transfer between the particles and the gas phase, the conduction through the solid phase of particles, and the mixing or dispersion within the gas phase in the void structure of the porous media. To solve the resulting differential equations numerically is not easy. The solution for sinusoidal gas temperature input assumes linearity of the logarithm of the temperature with time. If, in addition, linearity with distance can be assumed, then the solution can be vastly simplified to finding the real root of a fourth-order algebraic equation.

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SCOPE

Our research in porous media was originally directed toward the elucidation of the heat transfer between the gas phase and the particles in a fluidized bed system; this was to be accomplished by frequency response methods. In order to understand the fluidized bed system it was first necessary to investigate the heat transfer characteristics of the packed bed system and to consider all the effective modes of transfer of heat that are known or suspected to occur. It is well known that the heat transfer coefficient from the particle to the gas phase cannot be established without assuming some mathematical model for the process. The coefficient depends upon the model assumed. In any adequate model there will usually be several adjustable parameters that describe the pysical attributes of the system. Unfortunately, models that are

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