F = pressure deviation function = $P_{calc} - P$
P = pressure
T = temperature
x = independent variable
y = dependent variable
Δ = deviation
ρ = density

Subscripts

calc = calculated quantity
min = minimum quantity
max = maximum quantity

Superscripts

* = special variation of the dependent variable, y
' = first derivative
" = second derivative

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Optimal Sensor Location with an Application to a Packed Bed Tubular Reactor

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A number of approaches to the optimal selection of sensor locations are presented, and some of these are applied to determine optimal thermocouple positions in a packed bed tubular reactor. As expected, the optimal locations were found to be those surrounding the hot spot location. The theory also revealed that for good state estimation and for goodlinear quadratic control of the reactor, only one or two well located temperature measurements are necessary rather than the entire temperature profile.

SCOPE

In most processes, it is not feasible to measure all the process variables of interest. This may be due to economic constraints, lack of on-line detectors, or the hostile environment in which the sensors are located. Therefore, only a certain subset of these variables, or variables related to these process or state variables are measured. If all the states are to be inferred from such measurements, the precision of the state estimates will depend on which subset of the states, or auxiliary variables are measured, and on the precision of the measurements. Assum-

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ing that one has chosen the type of measurements and the measurements to be used, thereby fixing their precision, it would be desirable to select the location of these sensors in some optimal manner.

If the purpose is to obtain the best estimate of the state vector, this problem is just the dual of that which arises in the optimal design of regression experiments. In that problem, one is interested in choosing the settings of the independent variables in a number of experiments to maximize the amount of information that will be obtained on the parameters in the regression equation. The statistical literature contains an abundance of theory on this subject and this provides a basis for the sensor location problem. Some of the theoretical aspects of these techniques and their potential applications to sensor location problems have been examined by Mehra (1976).

Previous studies on sensor locations in tubular reactors, Colantuoni and Padmanabhan (1977), and Kumar and Seinfeld (1978), looked at the state estimation problem, using a chosen optimality criterion, by retaining the continuous time models for simple reaction systems. This study reviews a number of different design criteria, and applies some of them to the discrete time model of a highly exothermic-packed bed tubular reactor carrying out the multiple reactions of the hydrogenolysis of n-butane.

CONCLUSIONS AND SIGNIFICANCE

Theory for the optimal location of sensors closely parallels theory on the optimal design of regression experiments in the statistical literature. This theory was applied to the optimal location of thermocouples along a packed bed tubular reactor carrying out a highly exothermic series-parallel reaction. The proposed methods, by contrast with other published work, are simple to apply and lead to sensible results which agree with engineering intuition. In particular, the results of this analysis revealed that very efficient state estimation can be accomplished using only one or two thermocouples located in the region of the hot spot. The effect of sensor location on the performance of a linear quadratic controller was also studied. The variation in the temperature profile using linear quadratic control based on only one or two optimally located thermocouples was shown to be almost identical to that obtained using complete state measurements. This was not true for nonoptimally located thermocouples.

Consider a process which can be described by the discrete linear (linearized) state variable equation:

$$\mathbf{x}_{t+1} = \mathbf{A}\,\mathbf{x}_t + \mathbf{B}\,\mathbf{u}_t + \mathbf{w}_t \tag{1}$$

where $\mathbf{x}_t$ is an $n \times 1$ vector of state variables, $\mathbf{u}$ is an $r \times 1$ vector of manipulated inputs, and $\mathbf{w}_t$ is a vector of Gaussian white nosie disturbances with covariance matrix, $\mathbf{R}_w$.

The process variables that are measured, $\mathbf{y}_t$, an $m \times 1$ vector are related to the state vector $\mathbf{x}_t$ by the measurement equation:

$$y_t = H\,x_t + v_t \tag{2}$$

where $\mathbf{v}_t$ is an $m \times 1$ vector of measurement noise with covariance matrix, $\mathbf{R}_v$. Provided that Equations (1) and (2) are observable, the entire state vector $\mathbf{x}_t$ can be estimated from the measurements of $\mathbf{y}_t$ by the use of a filter equation. Obviously, the precision of the state will depend on the precision of the measurements, $\mathbf{R}_v$, as well as on the location of these measurements, that is, on $\mathbf{H}$. Assuming that one has chosen the number and type of measurements to be used ($\mathbf{R}_v$ is therefore fixed), it may be desirable to select in some optimal manner which variables should be measured (that is, to specify $\mathbf{H}$).

THEORY ON THE OPTIMAL LOCATION OF SENSORS

The placement of sensors must obviously depend on one's optimality criterion, and there have been a number of different approaches in the literature.

Optimizing an Observability Index

One of the earliest approaches to the sensor location problem was suggested by Johnson (1969) for the nonstochastic state reconstruction problem ($\mathbf{w}_t = 0$, $\mathbf{v}_t = 0$). He suggested that as a measure of the observability of the system, one use the determinant of the generalized observability matrix:

$$\mathbf{W} = \sum_{j=0}^{n-1} (\mathbf{H}\mathbf{A}^j)^T(\mathbf{H}\mathbf{A}^j) \tag{3}$$

Johnson (1969), and Muller and Weber (1972) then suggested maximizing $|\mathbf{W}|$ through a choice of the sensor locations to improve the degree of complete observability.

Obtaining "Best" State Estimates

When stochastic disturbances are present, unmeasured states can be estimated with the Kalman Filter:

$$\hat{\mathbf{x}}_{t+1/t} = \mathbf{A}\,\hat{\mathbf{x}}_{t/t} + \mathbf{B}\,\mathbf{u}_t \tag{4}$$

$$\hat{\mathbf{x}}_{t/t} = \hat{\mathbf{x}}_{t/t-1} + \mathbf{K}_t(\mathbf{y}_t - \mathbf{H}\,\hat{\mathbf{x}}_{t/t-1}) \tag{5}$$

$$\mathbf{K}_t = \mathbf{P}_{t/t-1}\,\mathbf{H}^T(\mathbf{H}\,\mathbf{P}_{t/t-1}\,\mathbf{H}^T + \mathbf{R}_v)^{-1} \tag{6}$$

$$\mathbf{P}_{t+1/t} = \mathbf{A}\,\mathbf{P}_{t/t}\,\mathbf{A}^T + \mathbf{R}_w \tag{7}$$

$$\mathbf{P}_{t/t} = \mathbf{P}_{t/t-1} - \mathbf{P}_{t/t-1}\,\mathbf{H}^T(\mathbf{H}\,\mathbf{P}_{t/t-1}\,\mathbf{H}^T + \mathbf{R}_v)^{-1}\,\mathbf{H}\,\mathbf{P}_{t/t-1} \tag{8}$$

with $\mathbf{P}_{o/o} = \mathbf{P}_o$.

$\mathbf{P}_{t/t-1}$ is the covariance matrix of the state prediction error $(\mathbf{x}_t - \hat{\mathbf{x}}_{t/t-1})$ and $\mathbf{P}_{t/t}$ is the covariance matrix of the filter error $(\mathbf{x}_t - \hat{\mathbf{x}}_{t/t})$. These covariance matrices provide a direct measure of the precision of the state estimates $(\hat{\mathbf{x}}_{t/t-1}, \hat{\mathbf{x}}_{t/t})$ and their dependence on the sensor location matrix $\mathbf{H}$ is given explicitly in Equations (6), (7), and (8). Since these matrices are independent of the observations ($\mathbf{y}_t$, $t = 1, 2, \ldots N$), they can be evaluated for $t = 1, 2, \ldots N$ and examined for any given choice of the sensor locations. However, the number of elements in these covariance matrices makes it difficult to assess the precision of the state estimates in each case, and therefore a single scalar function of one of these is usually chosen.

One such overall criterion is to minimize, by the choice of $\mathbf{H}$, the function:

$$v_1 = \frac{1}{N} \sum_{t=1}^{N} \text{trace } \mathbf{P}_{t/t-1} \tag{9}$$

This is an extension of the usual A-optimality criterion in the statistical literature in which the average variance of the state estimates over the first N observation periods is minimized. This criterion was suggested by Mier (1967). Athans (1972) used this criterion to determine the selection of one measurement from a number of possible measurements. Herring and Melsa (1974) extended this to the optimal selection of a set of measurements. Both methods require finding switching functions to determine the best time at which to change to a different sensor or set of sensors. One drawback of this criterion is that it is not invariant

with respect to linear transformations and its minimum will therefore depend on the units in which the states are expressed. This becomes a problem when the states are of mixed units, say temperatures and concentrations.

Another overall criterion is to minimize, by choice of $\mathbf{H}$, the quantity:

$$v_2 = \frac{1}{N} \sum_{t=1}^{N} |\mathbf{P}_{t/t-1}| \tag{10}$$

This is an extension of the commonly used D-optimality criterion in the statistical literature. It can be shown that, by minimizing this, one is minimizing the average volume of the joint confidence region of the states over the first N steps. Since the determinant is invariant for linear transformations, the minimum of this criterion is independent of the units used for the various states.

In many instances, one is interested in the steady-state solutions to the Kalman filter Equations (7) and (8). These equations will converge to unique positive definite solutions $\mathbf{P}^{\infty}_{t/t-1}$ and $\mathbf{P}^{\infty}_{t/t}$, if the pair $(\mathbf{A}, \mathbf{H})$ is observable, $(\mathbf{A}, \mathbf{R}_w)$ is controllable, and $|\mathbf{P}_0| > 0$ (Kushner, 1971). The A-optimality criterion for sensor location then becomes that of minimizing:

$$v_3 = \text{trace } \mathbf{P}^{\infty}_{t/t-1} \tag{11}$$

and D-optimality involves minimizing:

$$v_4 = |\mathbf{P}^{\infty}_{t/t-1}| \tag{12}$$

Although we have used $\mathbf{P}_{t/t-1}$ throughout in these criteria, one could use the covariance matrix $\mathbf{P}_{t/t}$ of the filter estimates if that was of most interest. Furthermore, if only a subset of the state vector (say the first n_1 elements) is of interest, Equations (11) and (12) can be applied to the upper left $(n_1 \times n_1)$ submatrix of $\mathbf{P}_{t/t-1}$.

Detection of Load Disturbances

Attention has been focussed on the placement of sensors to detect load disturbances acting on the system. Jorgensen and Clement (1977) considered the placement of temperature and concentration sensors in a tubular reactor to best detect inlet flow, temperature and concentration disturbances as well as estimating the states of the original system. These inlet disturbances were assumed to be modelled by the autoregressive model:

$$\mathbf{x}^*_{t+1} = \mathbf{\Phi}\, \mathbf{x}^*_t + \mathbf{a}_t \tag{13}$$

These authors used a simulation approach to evaluate the reactor concentration and temperature profile responses to such load disturbances by considering one disturbance at a time. A qualitative analysis of these results led them to their choice of sensor locations. When many load disturbances are simultaneously operating on the system such an intuitive approach may be difficult. However, the optimality Equations (11) and (12) can easily be applied to this situation. Defining the augmented state model,

$$\begin{bmatrix} \mathbf{x}_{t+1} \\ \mathbf{x}^*_{t+1} \end{bmatrix} = \begin{bmatrix} \mathbf{A} & \mathbf{F} \\ \mathbf{0} & \mathbf{\Phi} \end{bmatrix} \begin{bmatrix} \mathbf{x}_t \\ \mathbf{x}^*_t \end{bmatrix} + \begin{bmatrix} \mathbf{B} \\ \mathbf{0} \end{bmatrix} \mathbf{u}_t + \begin{bmatrix} \mathbf{w}_t \\ \mathbf{a}_t \end{bmatrix} \tag{14}$$

the D-optimal design would be to choose the sensor locations to minimize the determinant of the augmented covariance matrix:

$$\begin{vmatrix} \mathbf{P}^{\infty}_{11\ t/t-1} & \mathbf{P}^{\infty}_{12\ t/t-1} \\ \mathbf{P}^{\infty}_{21\ t/t-1} & \mathbf{P}^{\infty}_{22 t/t-1} \end{vmatrix}$$

If only the detection of load disturbances was of interest, one would minimize $|\mathbf{P}^{\infty}_{22\ t/t-1}|$.

Location for Optimal Control

Since control of a process is often the objective behind the installation of sensors, it is logical that one try to improve the control as much as possible by selecting the location of the sensors. Mier (1967), and Mellefont and Sargent (1977, 1978) considered such an approach for the case of linear quadratic (L.Q.) control. The control strategy minimizing the objective function

$$v_5 = E\left\{\mathbf{x}^T_N \mathbf{Q}_1 \mathbf{x}_N + \sum_{t=1}^{N-1} \mathbf{x}^T_t \mathbf{Q}_1 \mathbf{x}_t + \mathbf{u}^T_{t-1} \mathbf{Q}_2 \mathbf{u}_{t-1}\right\} \tag{15}$$

is given by

$$\mathbf{u}_t = -\mathbf{L}_t \hat{\mathbf{x}}_{t/t} \tag{16}$$

where $\mathbf{L}_t$ satisfies the equation:

$$\mathbf{L}_t = (\mathbf{Q}_2 + \mathbf{B}^T \mathbf{S}_{t+1} \mathbf{B})^{-1}\, \mathbf{B}^T \mathbf{S}_{t+1}\, \mathbf{A} \tag{17}$$

$$\mathbf{S}_t = \mathbf{A}^T \mathbf{S}_{t+1} \mathbf{A} + \mathbf{Q}_1 - \mathbf{A}^T \mathbf{S}_{t+1} \mathbf{B} (\mathbf{Q}_2 + \mathbf{B}^T \mathbf{S}_{t+1} \mathbf{B})^{-1} \mathbf{B}^T \mathbf{S}_{t+1} \mathbf{A} \tag{18}$$

with initial conditions $\mathbf{S}_N = \mathbf{Q}_1$, (Astrom 1970). If this control law is substituted into the objective function, one obtains

$$v_5 = \mathbf{m}^T \mathbf{S}_1 \mathbf{m} + \text{trace } (\mathbf{S}_1 \mathbf{R}_0) + \sum_{t=1}^{N-1} \text{trace}(\mathbf{S}_{t+1} \mathbf{R}_w) + \sum_{t=1}^{N-1} \text{trace}(\mathbf{P}_{t/t-1}) \mathbf{L}^T_t (\mathbf{B}^T \mathbf{S}_{t+1} \mathbf{B} + \mathbf{Q}_2) \mathbf{L}_t \tag{19}$$

where $\mathbf{R}_0$ is the initial covariance of the state, and $\mathbf{m}$ is the initial state estimate. The only contribution to the objective function v_5 that arises from the state estimator is through the last term in Equation (19). Mellefont and Sargent (1977) found switching functions which determined how sensor location should be changed to minimize Equation (19). However, such an analysis assumes that the matrices $\mathbf{Q}_1$ and $\mathbf{Q}_2$ in the quadratic cost functions Equation (15) would be the same for all sensor arrangements and are known in advance. This usually is not the case. In fact, they may be considered as design parameters which are to be varied until the variances of $\mathbf{x}$ and $\mathbf{u}$ are jointly acceptable.

In regulatory control where one is usually interested in the steady-state solution $\mathbf{L}_\infty$ of Equation (17), the following approach could be used to evaluate the effect of sensor locations on L.Q. control. The covariance matrices of the state and control variable vectors under optimal steady-state L.Q. control are given by MacGregor (1973):

$$\text{Var}(\mathbf{x}) = \mathbf{V}_x = (\mathbf{A} - \mathbf{B}\mathbf{L}_\infty)\mathbf{V}_x\, (\mathbf{A} - \mathbf{B}\mathbf{L}_\infty)^T + (\mathbf{A} - \mathbf{B}\mathbf{L}_\infty)\mathbf{P}^{\infty}_{t/t}\, \mathbf{L}^T_\infty\, \mathbf{B}^T + \mathbf{B}\mathbf{L}_\infty\, \mathbf{P}^{\infty}_{t/t} (\mathbf{A} - \mathbf{B}\mathbf{L}_\infty)^T + \mathbf{B}\mathbf{L}_\infty\, \mathbf{P}^{\infty}_{t/t}\, \mathbf{L}^T_\infty\, \mathbf{B}^T + \mathbf{R}_w \tag{20}$$

$$\text{Var}(\mathbf{u}) = \mathbf{V}_u = \mathbf{L}_\infty (\mathbf{V}_x - \mathbf{P}^{\infty}_{t/t}) \mathbf{L}^T_\infty \tag{21}$$

For a given choice of $\mathbf{Q}_1$ in the objective function and any choice of the sensor location, one can evaluate the trace or the determinant of the state covariance matrix Equation (20). $\mathbf{Q}_2$ is then used as a design matrix to find the control which yields acceptable variances for the manipulated variables, $\mathbf{u}$.

Thus, for any choice of the sensor locations, one can evaluate the performance of the linear quadratic controller as indicated by the elements of the covariance matrix of the state vector, $\mathbf{x}$. This provides a means of either selecting sensor locations directly or of evaluating the performance of the controller for sensor locations chosen by other means. This is applied to the catalytic reactor in the present work.

Note that since the optimal control Equation (16) is a linear function of the state estimate, $\hat{\mathbf{x}}_{t/t}$, the D-optimal design procedure discussed earlier should provide good control since it selects sensor locations which provide the best estimate of the entire state vector. However, since only a reduced m-dimensional subspace of the state estimates $(\mathbf{L}_\infty \mathbf{x}_{t/t})$ is used in control, it would seem preferable to use the D-optimality criterion directly on this subspace, that is, minimize by the choice of the sensor locations, the determinant

$$v_6 = |\mathbf{L}_\infty\, \mathbf{P}^{\infty}_{t/t}\, \mathbf{L}^T_\infty| \tag{22}$$

This would directly provide the best sensor locations for evaluating the linear quadratic control action. However, again since this subspace determined by $\mathbf{L}_\infty$ depends on the choice of $\mathbf{Q}_1$ and $\mathbf{Q}_2$ in the performance index, this probably should involve some iteration on $\mathbf{Q}_2$ (as discussed above) to compare under conditions for the same Var(u).

Distributed Parameter Systems and Tubular Reactors

Sensor location for linear distributed parameter systems has been studied by Yu and Seinfeld (1973), Kumar and Seinfeld (1978a), Aidarous et al. (1975), and Omatu et al. (1978). No attention is directed towards the use of the estimated states for control purposes. Due to the nonlinear nature of the distributed parameter Riccati equation, a function of the upper bound on the error covariance matrix is minimized. Most of these methods require knowledge of the Green's function for the system and approximate the solution of the differential equation by some orthogonal function. Tubular reactors are usually described by coupled nonlinear partial differential equations in several spatial coordinates, if significant temperature and concentration gradients exist. The above methods are difficult to apply to such processes.

Sensor allocation in tubular reactor systems has been studied by Kumar and Seinfeld (1978b), Jorgensen and Clement (1977), and Colantuoni and Padmanabhan (1977) for a single reaction. In the first two cases, orthogonal collocation was used to obtain a lumped approximation to the original distributed parameter system. The process models were not discretized. Measurements of concentrations and temperatures were assumed to be available continuously. Kumar and Seinfeld (1978b) consider placement of concentration and/or temperature sensors by minimizing the continuous equivalent criterion v_1 using an algorithm suggested by Athans (1972). Their conclusion as to the optimal location of the temperature sensors using this criterion are seen to correspond to that obtained in this paper for the infinite time estimation problem.

However, their comment that for nonoptimally located sensors, the trace $\mathbf{P}_{t|t}$ is in general not a monotonically decreasing function of time deserves some qualifications. If the system (**A**, **H**) is observable and (**A**, $\mathbf{R}_w$) controllable, the trace $\mathbf{P}_{t|t}$ indeed may not converge monotonically to its steady state value. Using an expression developed in Bucy and Joseph (1968), it can be shown that **P** is monotone nonincreasing if $|\mathbf{P}_o - \mathbf{P}^\infty| > 0$. When $\mathbf{P}_o$ is chosen as $c\mathbf{I}$, this condition is satisfied if c is greater than the largest eigenvalue of $\mathbf{P}^\infty$. Depending on the initial choice of the covariance matrix $\mathbf{P}_o$, it is possible for $\mathbf{P}_{t|t}$ to converge in a nonmonotonic fashion to its steady state value for any choice of sensor locations.

Colantuoni and Padmanabhan (1977) retained the partial differential equations (linearized) in time and axial distance, and minimized the integral trace of the prediction error covariance matrix over the spatial domain and over the time elapsing between discrete measurements. However, their procedure is very complicated, and it is difficult to imagine employing it for the case of multiple reactions or when radial gradients exist.

The present work considers the placement of temperature sensors in a catalytic-packed bed tubular reactor involving the multiple reactions of the hydrogenolysis of n-butane. The criterion used here for sensor location is that of D-optimality on the steady-state filter Equation (12). A simple method is used to check the sensitivity of the criterion to the order of the lumped model approximation. The effect of the sensor locations on the performance of linear quadratic control strategies is examined

DESCRIPTION OF THE TUBULAR REACTOR SYSTEM AND MODEL

The hydrogenolysis of n-butane over a nickel on silica gel catalyst is a series-parallel reaction involving five chemical species and three stoichiometrically independent reactions. A schematic diagram of the system is shown in Figure 1. The mass

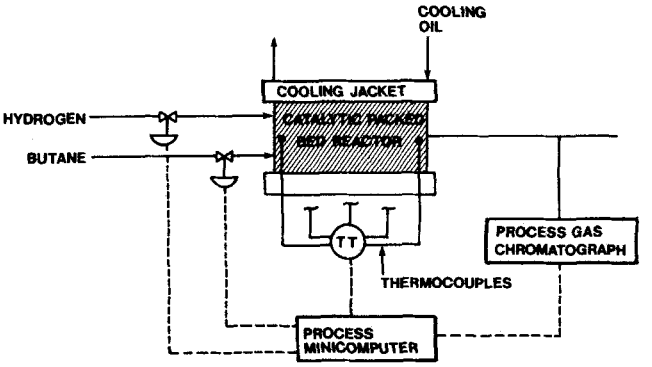

Figure 1. Reactor control configuration.

and energy balances describing this hydrogenolysis in a packed bed tubular reactor are a set of four-coupled, highly nonlinear partial differential equations in time and two spatial coordinates.

Orthogonal collocation was used to approximate temperature and concentration profiles in both the axial and radial directions (Jutan et al., 1977a, 1977b, 1977c). The enlarged set of nonlinear ordinary differential equations were then linearized about a steady state operating profile. These equations were further simplified by assuming a quasisteady state relationship for the concentration dynamics. This was justified because the concentration wave was approximately 500 times as fast as the thermal wave and, therefore, the time derivative of concentration could be eliminated. As a final step, the enlarged set of differential equations were discretized over a 60-second control interval.

The temperature dynamics were represented by the state equations:

$$\mathbf{x}_{t+1} = \mathbf{A}\mathbf{x}_t + \mathbf{B}\mathbf{u}_t \tag{23}$$

The states, $\mathbf{x}_t$, represent the temperatures at the interior collocation points used in obtaining the lumped approximation to the partial differential equations. Jutan et al. (1977a, 1977b, 1977c) found that seven interior collocation points adequately described the axial temperature profile. The manipulated input $\mathbf{u}_t$ comprises the hydrogen and butane feedrate to the reactor. The **A** and **B** matrices for Equation (23) are given in the Appendix. An experimental operating profile is shown in Figure 2. The concentrations at the exit are given by an algebraic relationship (resulting from the quasisteady state assumption):

$$\mathbf{z} = \mathbf{C}\mathbf{x}_t + \mathbf{D}\mathbf{u}_{t-1} \tag{24}$$

The model [Equation (23)] does not exactly describe the dynamic behavior of the reactor. Disturbances due in part to fluctuations in flow rates, catalyst activity and packing, wall temperature, and local hot spots, were modelled as additive Gaussian white noise with mean zero and covariance, $\mathbf{R}_W$.

$$\mathbf{x}_{t+1} = \mathbf{A}\mathbf{x}_t + \mathbf{B}\mathbf{u}_t + \mathbf{w}_t \tag{25}$$

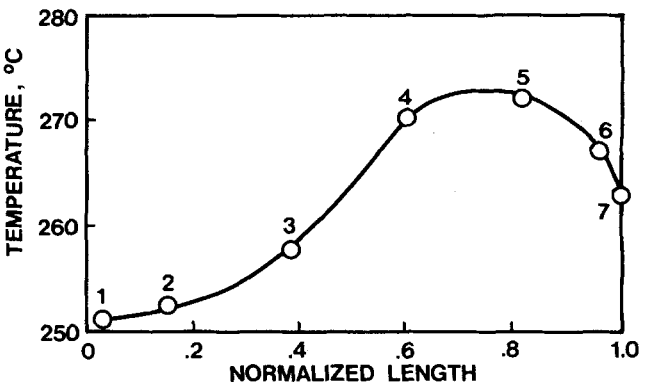

Figure 2. Typical temperature profile. (Circles denote collocation points by number.)

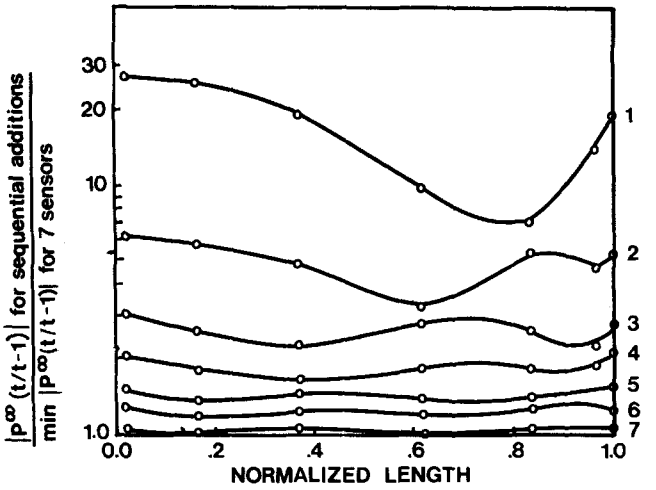

Figure 3. Objective function v_4 evaluated at different sensor locations: $R_v = 4I$, $R_W = \sigma^2(\rho)$.

$\mathbf{R}_W$ and a set of transport parameters were estimated from operating data (Jutan et al., 1977b). Rather than try to identify a full matrix $\mathbf{R}_W$, the following two parameter covariance structure was used.

$$\mathbf{R}_W = \sigma^2 \begin{bmatrix} 1 & \rho & \rho^2 & \cdots & \rho^{n-1} \\ & 1 & \rho & \cdots & \\ & & \cdots & & \rho \\ & \text{sym} & & 1 & 1 \end{bmatrix} \tag{26}$$

The values $\hat{\sigma} = 3$ and $\rho = 0.1$ gave the best fit. The low value of the correlation coefficient implies that the disturbances are of a very local nature.

Temperatures were measured by thermocouples at nine points along the reactor central axis. Since these positions did not adequately coincide with the collocation points, quadratic interpolation was used to estimate the temperature at the seven collocation points. The measurement equation was:

$$\mathbf{y}_t = \mathbf{x}_t + \mathbf{v}_t \tag{27}$$

where $\mathbf{H} = \mathbf{I}$ implies that the full state vector was measured. The measurement error vector $\mathbf{v}_t$ was a mean zero Gaussian process with covariance matrix $\mathbf{R}_v = \sigma^2\mathbf{I}$, $\sigma = 2°C$. The variance σ^2 was independent of the frequency at which the measurements were taken.

THE OPTIMAL LOCATION OF REACTOR THERMOCOUPLES

Although our ultimate objective for reactor control studies was to maintain the exit concentrations at specified levels some practical problems precluded this. The effluent chromatographic analysis was available only infrequently (every 6 min.) which is inadequate for control of this reactor. Therefore, control decisions were based on temperatures measured along the axis of the reactor. The interesting problems in looking at optimal thermocouple locations were: (1) to see which locations provided the greatest amount of information on the temperature profile, and (2) to see how much the optimal stochastic control scheme studied by Jutan et al. (1977a, 1977b, 1977c) could be expected to degrade if only one or two thermocouples had been used instead of the full set as in Equation (27).

Therefore, consider the measurement equation to be of the form:

$$\mathbf{y}_t = \mathbf{H}\,\mathbf{x}_t + \mathbf{v}_t \tag{28}$$

where each of the m rows of $\mathbf{H}$ consists only of one nonzero element whose value is 1.0. To determine the sensor locations which best estimate the temperatures given by Equation (23), we use the D-optimality criterion and minimize with respect to the choice of the thermocouple locations, the determinant, v_4. When there are a finite number of time invariant sensor locations the minimization of v_4 is straightforward. One method is to simply evaluate v_4 for all seven possible combination of locating m ($m \leq 7$) sensors.

Alternatively, a less time-consuming approach is to proceed sequentially and to choose the second sensor to minimize the objective function conditional on the location of the first sensor and so on. This latter approach does not insure that the sensors' locations will be optimal as in the simultaneous approach, although this approximation may often be adequate in practice. When the number of possible locations is large, one should resort to using any of a number of efficient algorithms that exist in the statistical literature for adding and dropping locations in order to arrive at a globally D-optimum design. [For example, see Wynn (1970) and Mitchell (1974)].

Excluding, for the moment, the possibility of having multiple, independent measurements at the same position, the locations of sensors were picked sequentially using the D-optimality criterion [Equation (12)] for three ranges of the covariance matrices ($\mathbf{R}_W, \mathbf{R}_v$). The results of this optimal selection are shown in Table 1. The first thermocouple appears in location 5 for all cases. The second thermocouple, given the first, is located at position 4 and so on. The preferential selection of sensors at location 5, 4, and 6 which bracket the hot spot location of the profile was not surprising. This is what any chemical engineer would have guessed a priori. However, it does show that the sensor location procedures do lead to sensible results. In other situations where the optimal locations are not at all obvious, the procedures will provide a logical basis for their selection. The insensitivity of the choice of $\mathbf{R}_W, \mathbf{R}_v$ indicates that the reactor dynamics, not the stochastic disturbances, influence the optimal location of the sensors.

Figure 3 shows the effect that sequentially adding sensors in the optimal manner has on the determinant $|\mathbf{P}^{\infty}_{t/t-1}|$ for the case with the identified reactor stochastics $\mathbf{R}_v = 4\mathbf{I}$ and $\mathbf{R}_W = \sigma^2(\rho)$.

TABLE 1. SEQUENTIAL SENSOR LOCATION

Sequential Additions	Thermocouple Location Conditional on Preceding Selection		
Number of Sensors	$R_v = 10I$ $R_W = I$	$R_v = 4I$ $R_W = \sigma^2(\rho)$ (Eq. 26)	$R_v = I$ $R_W = 10I$
1	5	5	5
2	4	4	4
3	6	6	6
4	3	3	3
5	2	2	2
6	1	7	7
7	7	1	1

Refer to Figure 2 for thermocouple positions.

TABLE 2. SEQUENTIAL SENSOR LOCATION MULTIPLE SENSORS AT THE SAME POSITION PERMITTED

Sequential Additions	Thermocouple Location Conditional on Preceding Selection		
Number of Sensors	$R_v = 10I$ $R_W = I$	$R_v = 4I$ $R_W = \sigma^2(\rho)$ (Eq. 26)	$R_v = I$ $R_W = 10I$
1	5	5	5
2	4	4	4
3	5	6	6
4	4	3	3
5	5	5	2
6	6	2	7
7	5	4	1

Refer to Figure 2 for thermocouple positions.

TABLE 3. EFFECT OF THERMOCOUPLE POSITION ON CONTROLLER PERFORMANCE
($R_v = 4$, $R_W = \sigma^2(\rho)$ (EQ. 26), $Q_1 = 1$)

Thermocouples Used	trace Var (x), Var(u) constant
None (open loop)	59.6
5	44.0
4, 5	42.9
4, 5, 6	42.8
all	42.6
1, 4 (non-optimal)	51.9*

For thermocouple locations, refer to Figure 2.

* When thermocouples 1, 4 were used, it was impossible to reduce the trace Var(x) below this value no matter what Var(u) was used.

For successive sensors the dotted lines indicate the value of the determinant across the reactor. The minimum on each curve gives the optimum sensor location (as shown in Table 1). As we increase the number of thermocouples the determinant, $|\mathbf{P}^{\infty}_{t/t-1}|$, will decrease continually. However, one can see that most of the information about the temperatures is obtained after the first few thermocouples have been chosen.

The simultaneous location of three sensors was investigated. The thermocouple locations were identical to those placed in the sequential fashion for the covariance matrices considered.

The reactor model [Equation (25)] is discrete and expresses the temperatures at the collocation points only. Having placed the first thermocouple near the hot spot, we cannot decide how close the next thermocouple should be placed since we have restricted our thermocouple locations to the collocation points. A laborious approach would be to increase the number of collocation points and examine the sensor location for this new model. An easier approach is to allow multiple independent sensors at the same collocation point. Although this may not be appealing from an operating viewpoint, it does allow us to examine the sensitivity of sensor locations to the number of collocation points.

Table 2 shows the results allowing for multiple sensors at the same collocation point. Only when the signal to noise ratio is low do we find clustering of sensors.

To assess the extent to which the optimal stochastic control scheme of Jutan et al. (1977a, 1977b, 1977c) might be expected to degrade if fewer thermocouples were used, the procedure outlined in Equations (20) and (21) and following was applied. Using the optimal one sensor, two sensor, and three sensor locations obtained by minimizing v_4 for $m = 1$, 2, and 3. The trace of the state variable covariance matrix trace Var(x) was evaluated for each of these cases under the linear quadratic control using $\mathbf{Q}_1 = \mathbf{I}$ in the performance index [Equation (15)] and using a $\mathbf{Q}_2$ which gave essentially the same Var(u) in each case. The results are shown in Table 3 together with those obtained for one nonoptimal placement of the thermocouples, for complete measurement (all seven positions), and for the predicted open-loop process. (The open-loop variance predicted is only entered here for comparitive purposes and it is not accurate since the extreme nonlinearities in the reaction system lead to reactor instability in this situation. The predicted results under the closed-loop conditions, however, agree well with experimental results.)

One can conclude from these results that by using only one or at most two optimally located thermocouples one should be able to achieve essentially the same quality of control as with the entire temperature profile (all seven measurements). However, the same conclusion cannot be said for the situation where the thermocouples are poorly located. For this reactor we know from operating experience that a variance as large as 51.9 appears to preclude stable operation.

If one is interested in concentrations rather than temperatures one can locate thermocouples to obtain good estimates of the effluent concentration. In this case we minimize, by the choice of $\mathbf{H}$, the objective function.

$$v_7 = |\mathbf{C}\mathbf{P}^{\infty}_{t/t-1}\mathbf{C}^T| \tag{29}$$

For the covariances of $\mathbf{R}_W$, and $\mathbf{R}_v$ previously considered, the first optimally located sensor was always at position 5. Additional sensors located in a sequential fashion using v_7 did not coincide with those positions found by minimizing v_4. However, most of the information about the effluent concentrations was obtained from the first thermocouple and additional thermocouples had only a small effect on the value of the objective function.

APPENDIX: state transition and control matrices for reactor system (Eq. 23).

State Transition Matrix A

.18710	−.09739	.05139	−.04127	.03884	−.04325	.02504
.25590	.4330	−.11100	.7539	−.06659	.07236	−.04169
−.07925	.23460	.56390	−.15280	.11210	−.11460	.06527
.05104	−.11200	.24120	.81500	−.23800	.20720	−.11490
−.03824	.04680	−.13130	.28570	.91440	−.38970	.20020
.00525	−.03535	.01342	−.13570	.46390	.64700	−.25420
.01604	−.03182	.00816	−.09017	.17230	.83338	−.24640

Control Matrix B

.01957	−.00998
.05133	−.02440
.12920	−.04145
.43210	−.09468
.67550	−.10450
.49000	−.04814
.42120	−.31510

NOTATION

$\mathbf{A}$ = state transition matrix
$\mathbf{a}_t$ = vector of inlet disturbances
$\mathbf{B}$ = state control matrix
$\mathbf{C}$ = matrix of parameters
$\mathbf{D}$ = matrix of parameters
$\mathbf{F}$ = matrix defining coupling between process and disturbances
$\mathbf{H}$ = measurement matrix
$\mathbf{K}_t$ = kalman filter gain
$\mathbf{L}_t$ = state feedback controller gain
$\mathbf{P}_{t/t}$ = covariance of filtered state estimate
$\mathbf{P}_{t/t-1}$ = covariance of state prediction error
$\mathbf{Q}_1$ = state weighting matrix
$\mathbf{Q}_2$ = control weighting matrix
$\mathbf{R}_W$ = covariance of process noise
$\mathbf{R}_v$ = covariance of measurement noise
$\mathbf{u}$ = vector of manipulated variables
$\mathbf{v}_t$ = vector of measurement disturbances
$\hat{\mathbf{x}}_{t/t}$ = filtered state estimate
$\hat{\mathbf{x}}_{t/t-1}$ = predicted state estimate
$\mathbf{w}_t$ = vector of process disturbances
$\mathbf{y}_t$ = vector of measured outputs
$\mathbf{z}_t$ = vector of concentrations at reactor exit

Subscripts

o = value at $t = 0$

Superscripts

∞ = steady state value
T = transpose

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The Synthesis of Distillation Trains with Heat Integration

Due to rising energy costs, there is an increasing need to include the goal of energy conservation as an integral part of process synthesis. This paper discusses the problem of finding the optimum sequence of distillation columns for separating a multicomponent mixture, when heat exchange is permitted between the columns. The major difficulties are associated with the nonserial nature of the problem, the large combinatorial variety and the size of the optimization task. The synthesis strategy presented here overcomes these problems by the use of a bounding technique together with the Lagrangian theory from nonlinear programming. Accurate lower bounds on the optimal costs permit the elimination of nonoptimal sequences with minimal computational effort.

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SCOPE

Distillation is probably the most widely used method of separation in industry. U.S. distillation energy consumption for 1976 is conservatively estimated as two quads (1 quad = 10^{15} Btu), which is nearly 3% of the entire national energy consumption (Mix et al., 1978). In a recent study, the energy usage of 45 refineries and 226 chemical plants was surveyed (Prengle et al., 1974) and almost everywhere distillation was a major energy consumer. In petroleum refineries, crude and vacuum distillation was found to account for 22.5 to 51% of the total energy consumption. Thus, it is obvious that any small enhancement of efficiency can have a major impact on the national energy situation.

The techniques of vapor recompression and using the heat of condensation of an overhead stream in the reboiler of a neighboring column have been known for almost a century. However, systematic design methods which make maximum use of these ideas of heat integration or thermal coupling are still lacking. The problem of synthesizing optimal separation trains for multicomponent mixtures has attracted much attention recently. A survey is given by Hlavacek (1978). Heat integration between separators or with other streams in the plant has not been considered in these publications. Very elegant results on the so-called heat exchanger network synthesis problem have appeared recently (Linnhoff and Flower, 1978). Much of the earlier work in this area has been reviewed by Nishida et al. (1977).

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