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Part II. Data Collection, Parameter Estimation, and Stochastic Disturbance Identification

A state space model, developed for multivariable control studies on a pilot plant packed-bed reactor for the hydrogenolysis of butane, is fitted to experimental temperature and concentration data collected under unsteady state conditions. The parameters estimated are the fundamental transport parameters of the packed-bed reactor and a catalyst activity parameter. A discrete stochastic model for the process disturbances is also identified, and a principle component type of procedure is used to reduce its dimensionality and to gain insight into the nature of these disturbances.

SCOPE

Considerable work has been done on the steady state modeling of nonisothermal packed-bed tubular reactors and the estimation of the transport properties in these reactors. Some of the difficulties associated with this estimation problem have been discussed by Beek (1962), Froment (1967, 1974), Hlavacek (1970), and Carberry and White (1969).

For reactor control purposes, an unsteady state or dynamic model of the reactor is required. While a detailed description of the reactor dynamics can be obtained in terms of partial differential equations derived from unsteady state material and energy balances, such a model, used directly, is certainly impractical and unnecessarily complex for process control. Empirical models, such as

transfer function models or state variable models in canonical form, identified directly from plant data, are often sufficient for regulatory control purposes if all the controlled variables are being measured. However, the number of parameters to be estimated in these black box models increases rapidly with the dimensionality of the multivariable process. Furthermore, if some of the variables to be controlled are not measured directly, then some type of inferential control is necessary, and a model incorporating some of the major mechanistic features of the process would appear to be necessary in order to estimate these unmeasured states.

In part I of this paper (Jutan et al., 1977*a*), such a dynamic state space model was developed for highly exothermic packed-bed catalytic reactor carrying out the hydrogenolysis of butane. A simplified, linearized, seven-dimensional model was developed directly from the three-dimensional nonlinear partial differential equations describing the system. The measured states of the system were the temperatures through the center of the reactor bed, but the model provided estimates of the unmeasured radial temperatures and the concentrations of the various species at the output. The ultimate objective of the model was to provide control over these exit concentrations. The numerous kinetic parameters of the reaction system were already well determined in other studies (Shaw, 1974; Orlikas, 1970), but the transport properties and a catalyst activity parameter were to be estimated from operating data from the reactor. No previous studies have been reported which attempt to estimate reactor transport and catalyst parameters from multivariate, unsteady state data. This paper reports on the on-line collection of the data, the use of multivariate statistical procedures to estimate the parameters, and an assessment of the fitted model.

Multivariate time series methods are also used to develop a model for the stochastic disturbances in the reactor system. Such a model must be fitted simultaneously with the reactor model for efficient estimation of the reactor model parameters from dynamic data. A principle component procedure is applied to this multivariate time series model in order to reduce its dimensionality for later use in control and to give some insight into the type and sources of the inherent disturbances in the reactor.

CONCLUSIONS AND SIGNIFICANCE

Multivariate statistical estimation methods were used to successfully fit a state space model for a packed-bed catalytic reactor to dynamic data collected from the reactor. The predicted dynamic behavior of the temperature profile and the exit concentrations was quite satisfactory, particularly for the control purposes for which the model was developed.

A multivariable stochastic model was identified for the reactor disturbances for use in the fitting and later in designing stochastic controllers. A principle component type of analysis on the collected disturbance data was used to significantly reduce the dimensionality of the stochastic model, to reveal the locations of the most significant disturbances, and to locate the source of one such disturbance.

Estimation of the parameters in process dynamic models from actual process data is an important step in the development of control systems. That this step is often ignored can largely be attributed to the fact that most such studies have been control simulations. Very few real applications of modern multivariable control procedures to complex processes have been reported, but those of which the authors are aware, parameter estimation has often been one of the major difficulties.

PROCESS MEASUREMENTS

A description of the experimental reactor setup and computer interfacing, illustrated schematically in Figure 1, has been given (Jutan et al., 1977*a*). Butane and excess hydrogen are fed to the reactor at feed rates controlled by the process minicomputer. These inlet flows are measured, and digital PI controllers are used to maintain them at their set points. The reactor wall temperature is maintained constant at approximately 520°K by regulating the temperature of the cooling oil flowing through the annulus of a cooling jacket, and the inlet gases are preheated to the wall temperature by an electrical resistance preheater.

The main measurements taken on the system are temperature readings taken using thermocouples positioned at nine locations along the central axis of the reactor, at a few selected radial positions, in the feed and exit gas streams. These were available once every 12 s but were utilized for modeling and control only every 60 s. As previously mentioned (Jutan et al., 1977*a*), modeling and control of the reactor were based on the temperature measurements only, although the control objective function was to be expressed in terms of exit concentrations. These exit concentrations could be predicted from the temperature measurements using the reactor model. However, towards the end of this work, an on-line process gas chromatograph was interfaced to the system, and measurements of the exit concentrations of the five components

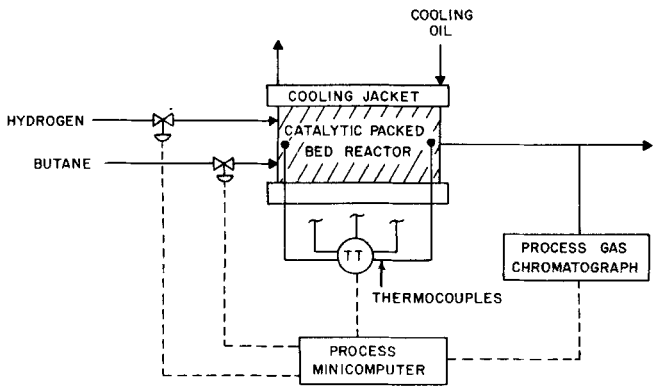

Fig. 1. Reactor control configuration.

(hydrogen, butane, propane, ethane, and methane) were available once every 6 min.

The noise level in the thermocouple measurements was quite high ($\sigma_T^2 \doteq 4\ K^2$) as determined from a constant temperature run with inactive catalyst. This preliminary run also enabled individual thermocouple biases to be detected and corrected for in all later control and data collection runs.

THE REACTOR MODEL

In part I of this paper (Jutan et al., 1977*a*), a low-order state space dynamic model, suitable for use in multivariable control studies, was developed starting from the basic three-dimensional partial differential equations describing the material and energy balances:

Material balances

$$\frac{-G_o}{\epsilon L}\frac{\partial C^i}{\partial z} + \frac{D_{er}}{\epsilon R^2 r}\frac{\partial}{\partial r}\left(r\frac{\partial C^i}{\partial r}\right) - \frac{\rho_B R^i}{\epsilon} = \frac{\partial C^i}{\partial t} \tag{1}$$

where $i = 1, 2, 3$ is the component number.

Energy balance: solid/gas

$$\frac{-G_o C_{pg}\rho_g}{L\,\overline{C}}\frac{\partial T}{\partial z} + \frac{\lambda_{er}}{R^2\,\overline{Cr}}\frac{\partial}{\partial r}\left(r\frac{\partial T}{\partial r}\right) + \frac{\sum_{i=1}^{3}\Delta h_i R_i \rho_B}{\overline{C}} = \frac{\partial T}{\partial t} \tag{2}$$

where

$$\overline{C} = [C_{ps}\rho_B - C_{pg}\rho_g\epsilon] \tag{3}$$

and T represents a homogeneous gas/solid temperature.

An examination of these differential equations and their boundary conditions shows that there are only a few transport parameters which could be estimated: D_{er} (effective radial diffusivity), λ_{er} (effective radial thermal conductivity), and Bi [the Biot number appearing in the boundary condition $\partial T/\partial r = Bi(T_w - T)$ at the reactor wall]. There are, of course, a large number of parameters associated with the kinetics of the reaction system (implicit in the reaction rate terms R^i). However, these have been precisely estimated for this butane hydrogenolysis system in other studies (Shaw, 1974; Orlikas, 1970) and are considered to be known here. The kinetic models for R^i and their parameters are reported in the Appendix of Part I of this paper (Jutan et al., 1977*a*). One important kinetic parameter which cannot be ignored, however, is the catalyst activity (k/k_o) which is specific to the particular catalyst batch being used.

Parametric Sensitivity

From simulation studies on the reactor model (Jutan, 1976), the catalyst activity (k/k_o) and the effective radial conductivity (λ_{er}) were found to be the most sensitive parameters. The effective radial diffusivity (D_{er}) was shown to have little effect on the central axis temperature profile over a rather wide range of values but was found to influence the exit concentration behavior quite significantly. The Biot number (Bi) was found to have little effect on either the concentration or temperature behavior in the range of values applicable to this system. The value estimated from the literature for our reactor was $Bi = 43.5$ (Beek, 1962). Such a large value implies that most of the resistance to heat transfer is in the bed itself rather than being lumped at the wall. The insensitivity of the reactor differential equations to variations in the Biot number in this range can be seen clearly from the reduced energy balance equation, obtained after using orthogonal collocation approximations to eliminate the radial derivatives (Jutan et al., 1977*a*), in which the Biot number appears in a term of the form

$$\frac{\lambda_{er}^4}{R^2\,\overline{C}} \cdot \frac{B_i}{(B_i + 2)}$$

Clearly, for large values ($Bi > 20$) a precise estimate of the Biot number is not required.

Therefore, in the actual estimation studies which follow, the catalyst activity parameter (k/k_o) and the effective radial thermal conductivity (λ_{er}) were the only two parameters estimated from the dynamic data collected on reactor temperatures. However, during one final run, when an on-line gas chromatograph provided concentration data as well, it was found necessary to estimate a third parameter D_{er}. The λ_{er} parameter was also fitted in the form $\lambda_{er} = \lambda_o + \alpha(T^4 - T_w^4)$ which allowed for a pseudo radiation effect (Beek, 1962) and gave somewhat more flexibility in the fitting of the data. Experience gained from a few preliminary estimation runs showed that the value of α was necessary but insensitive. As a result, in all the final fits α was held constant and only λ_o was estimated.

The Simplified State Space Model

In part I of this paper (Jutan et al., 1977*a*) the partial differential Equations (1) and (2) were reduced to seven ordinary first-order linear differential equations using methods of orthogonal collocation to approximate the spatial derivatives, linearizing about an historical operating temperature profile, and applying a quasi steady state approximation to the concentration dynamics. The steps can be briefly summarized as follows:

1. Apply collocation to the radial derivatives.
2. Solve the steady state equations corresponding to a desired temperature profile to obtain the corresponding concentration profiles.
3. Apply quasi steady state assumption to the concentration dynamics.
4. Apply collocation to the axial derivatives.
5. Linearize the collocated equation about the operating profiles.
6. Eliminate the concentration variables to obtain a state space model in the axial temperatures only by using the algebraic equations which result from the quasi steady state assumption.
7. Integrate the continuous model over the sampling interval (60 s) to obtain a discrete state space model of the form

$$\mathbf{x}(t+1) = \mathbf{A}\mathbf{x}(t) + \mathbf{B}\mathbf{u}(t) \tag{4}$$

The seven-dimensional state vector $\mathbf{x}$ corresponds to the axial temperature deviations from the operating profile at seven collocation points along the central axis of the reactor, and $\mathbf{u}$ is the (2×1) vector of deviation manipulated variables: hydrogen and butane feed rates. The coefficient matrices $\mathbf{A}$ and $\mathbf{B}$ are automatically determined for a given choice of the parameters $(k/k_o, \lambda_{er}, D_{er})$ in Equations (1) and (2) by the application of steps 1 to 7. The nine temperature measurements made along the central axis of the computer were used to interpolate the temperatures at these seven collocation points by using a quadratic interpolation formula on the measurements immediately around each collocation point. The measurement equation is, therefore

$$\mathbf{y}(t) = \mathbf{I}_7\,\mathbf{x}(t) + \mathbf{N}(t) \tag{5}$$

where $\mathbf{y}(t)$ is the vector of interpolated deviation temperature measurements, and $\mathbf{N}(t)$ is a vector of residuals or deviations between the measured axial temperatures deviations and those predicted by the model. A predictive relationship for the three independent concentration deviations at the reactor exit in terms of the temperature and inlet flow deviations could also be obtained as an eighth step in the above modeling sequence:

$$\mathbf{C}(t) = \mathbf{Z}\,\mathbf{x}(t) + \mathbf{P}\,\mathbf{u}(t-1) \tag{6}$$

This relationship was used for fitting the concentration data when the on-line process chromatograph was interfaced and is used in part III of this paper (Jutan et al., 1977*b*) for designing a multivariable control scheme.

A Stochastic Disturbance Model

The complete input-output model for the reactor as shown in Equation (5) is made up of two parts: the deterministic state variable model given in Equation (4) for the effect of the inlet feedrates on the temperature profile and a stochastic model for the noise vector $\mathbf{N}(t)$. Briefly, $\mathbf{N}(t)$ can be thought of as representing the total effect, in the measurements, of all the disturbances or noises in the process not accounted for by the deterministic model. Such disturbance might be due, among other things, to uncontrolled fluctuations in feed rates, in wall temperature, in catalyst activity; to local hot spots; and to measurement noise. These stochastic disturbances are of major importance in that they cause the reaction to run away or to die out if the reactor is left uncontrolled.

A class of linear stochastic models capable of representing such disturbances are the multivariable autoregressive-integrated-moving-average (ARIMA) time series models (Box and Jenkins, 1970; Wilson, 1970; Quenouille, 1957) of the general form

$$\varphi(z^{-1})\ \nabla^d \mathbf{N}(t) = \theta(z^{-1})\,\mathbf{a}(t) \tag{7}$$

where $\mathbf{a}(t)$ is a multivariate white noise sequence with covariance matrix $\boldsymbol{\Sigma}$, and $\varphi(z^{-1})$ and $\theta(z^{-1})$ are low-order matrix polynomials in the backward shift operator z^{-1}. One of the simplest of this general class of models is the autogressive model of order 1:

$$\mathbf{N}(t) = \varphi\,\mathbf{N}(t-1) + \mathbf{a}(t) \tag{8}$$

This particular model is used extensively in later fitting of the data.

MULTIVARIATE ESTIMATION

Least-squares parameter estimation in systems where a single response is measured is a well-known procedure whose justification relies on the assumption that the residuals are independent random variables with zero mean and constant variance. If the residuals are not independent but highly autocorrelated, as is usually the case with the time series type of data taken in process dynamic and control studies, then the estimation procedure based on a Bayesian or a Maximum Likelihood approach is to minimize the sum of squares of the computed white noise sequence $[a(t)]$ from the stochastic model for the noise $N(t)$ (Box and Jenkins, 1970).

When we deal with multivariate data, a Bayesian approach which maximizes the posterior density function of the parameters (Box and Draper, 1965; Wilson, 1970) is to minimize the determinant J with respect to the unknown parameters, where

$$J = \left| \sum_{t=1}^{N} \mathbf{a}(t)\ \mathbf{a}'(t) \right| \tag{9}$$

The $\mathbf{a}(t)$'s can be computed recursively from the identified stochastic model for the noise (7). This criterion (9) represents a multivariate generalization of the least-squares criterion. The determinant J may be minimized by any available optimization routine. An iterative approach to minimizing this determinant (Wilson, 1970, 1973) was used in this study. By iterating between the conditional estimate of the covariance matrix of the innovations $\mathbf{a}(t)$

$$\hat{\boldsymbol{\Sigma}}(\hat{\boldsymbol{\beta}}) = \frac{1}{n-m-1} \sum_{t=1}^{n} \mathbf{a}(t)\ \mathbf{a}'(t) \tag{10}$$

(conditional of the current estimates of the parameters $\hat{\boldsymbol{\beta}}$) and the conditional estimate of the parameter vector $\hat{\boldsymbol{\beta}}$ (conditional on $\hat{\boldsymbol{\Sigma}}$), convergence to the unconditional estimates of the parameters which minimize J can be shown to result. A multivariate generalization of the Gauss-Newton algorithm modified by Marquardt (1963) was used to accomplish this (Jutan 1976; Wilson, 1973). This was found in most cases to be superior to using general minimization routines (Simplex, Powell) to minimize J directly.

Data Collection

In classical linear systems identification techniques, data are collected under open-loop conditions. However, in this situation the reactor is open-loop unstable. Furthermore, the linearized state space model (4) is an approximation to the highly nonlinear system only in the region around the desired operating profile. Therefore, all data collections were performed under closed-loop conditions in which a univariate digital proportional-integral feedback controller on the hydrogen flow was used to maintain the hot spot temperature of the reactor reasonably near the desired value throughout the run. Because of possible system identifiability problems or poor conditioning of the estimation space when data are collected under closed-loop conditions (Box and MacGregor, 1974, 1976; Soderstrom et al., 1975, 1976; Ljung et al., 1974), an externally generated white noise (dither) signal was superimposed on the feedback signal to the hydrogen flow rate.

An independent autoregressive disturbance of order 1 was also programmed into the butane flow rate using a random number generator on the minicomputer. The variances of these signals were selected to give as much variation as possible without causing reactor instability. These variances generally had to be kept small because of the inability of the univariate controller to maintain the reactor near the desired conditions. Data were collected on temperatures over a period of several hours with a 60 s sampling interval. Usually about 100 multivariate data points were obtained for the parameter estimation.

Estimation Algorithm

The actual procedure by which the models and the estimation methods were combined in order to obtain estimates of the parameters is detailed in this section.

For a given choice of the parameters λ_{er}, k/k_o, D_{er} in the partial differential Equations (1) and (2), by application of the seven steps previously described, the **A** and **B** matrices in the discrete state space model (4) can be determined. Conditional on these parameters, the residuals sequence $\mathbf{N}(t)$ then can be evaluated from Equation (5). Preliminary estimates of these transport and catalyst parameters were therefore used to evaluate $\mathbf{N}(t)$, and from the autocorrelation and partial autocorrelation matrices of this residual sequence, the multivariate autoregressive process of order 1 shown in Equation (8) was identified as being an adequate model structure for the stochastic disturbance.

Given these models for both the process dynamics and the stochastic disturbances, all their parameters could be estimated simultaneously by minimization of the multivariate Bayesian estimation criterion in Equation (9). However, considerable computational effort can be saved by noting that the matrix of stochastic parameters φ enters the regression in a linear manner. Therefore, conditional on the nonlinear reactor model parameters, φ can be estimated very easily by a linear regression

$$\hat{\varphi}\,(\lambda_{er}, k/k_o, D_{er}) = \hat{\mathbf{\Gamma}}_1' \hat{\mathbf{\Gamma}}_o^{-1} \qquad (11)$$

where $\hat{\mathbf{\Gamma}}_1$ and $\hat{\mathbf{\Gamma}}_o$ are the estimated autocovariance matrices of the residual sequence $\mathbf{N}(t)$ at lags 1 and 0, respectively. This segregation of the linear and nonlinear parameters in difficult regression problems and then iterating between the conditional estimates of each has been suggested by Lawton and Sylvestre (1971) and Watts and Broekhoven (1972).

Our estimation algorithm consisted of the following steps:

1. Select starting estimates of the reactor model parameters λ_o, k/k_o (and possibly D_{er}).
2. Generate the **A** and **B** matrices of the discrete state variable model by the application of steps 1 through 7.
3. Generate the residual sequence $\mathbf{N}(t)$ from Equation (5).
4. Compute the conditional estimate $\varphi(\lambda_o, k/k_o)$ of the stochastic model parameter matrix using (11).
5. Calculate the innovation sequence $\mathbf{a}(t)$ recursively using (8).
6. Use these innovations in the multivariate Gauss-Newton estimation routine to obtain new estimates of the reactor parameters and return to step 2.

Obviously, step 2 is the time consuming one, and since within each iteration of the Gauss-Newton algorithm, numerical evaluation of the derivatives of the innovation vector $\mathbf{a}(t)$ with respect to each reactor parameter is necessary, steps 2 through 5 had to be repeated $p + 1$ times each iteration (where p is the number of parameters estimated, usually two). Each iteration typically took approximately 60 s on a CDC 6400.

The bulk of the fitting was performed using temperature data only. Towards the end of the study, a process gas chromatograph was interfaced, and concentration data on hydrogen, butane, propane, and ethane in the reactor effluent became available once every 361.3 s. These concentration data, although not synchronized with the temperature data, were incorporated into the estimation scheme in order to eliminate biases between the observed concentrations and those predicted using Equation (6). (Only interpolated predictions were available, since the concentration data fell between sampling instants.) To do this, a simple sum of squares of the deviations between the predicted and observed concentrations was appended to the estimation criterion J and weighted in such a way that the parameter estimates obtained eliminated any major biases in the concentration predictions, yet still placed most emphasis on the more numerous temperature data. With the concentration data, a third parameter D_{er} was also estimated, and as observed in the simulation studies, it had very little effect on the fit of the temperature profile but did improve the concentration fit.

Estimation Difficulties

Some of the estimation difficulties encountered, particularly in the early stages of this problem, are discussed below.

The estimation space was found to contain local minima. However, these were immediately recognizable because it was known that at the global minimum, the diagonal elements of the dispersion matrix $\hat{\mathbf{\Sigma}}$ in (10) should be very close to $\sigma^2 = 4.0$, the measurement error variance in the thermocouples.

Discontinuities were occasionally encountered at parameter values which gave rise to an **A** matrix in the discrete state space model which had one or more eigenvalues outside the unit circle.

Extreme parameter correlation existed between the estimates of the two important parameters k/k_o and λ_{er}. Examination of the steady state energy balance differential equations, after collocating in the radial direction (Jutan et al., 1977*a*), shows that these parameters feature prominently in the subtraction of two large almost equal terms. This can be demonstrated by writing this steady state energy balance as

$$\frac{dT}{dz} = \frac{\lambda_{er}\,(\text{heat removal term}) - (k/k_o)\,(\text{heat generation term})}{v_T}$$

Because of the highly exothermic nature of this reaction and the small temperature wave velocity ($v_T \approx 10^{-4}$), a very small change in λ_{er} without a compensating change in (k/k_o) could cause a large change in the model predictions. When the concentration data were incorporated into the estimation procedure, the correlation between these parameter estimates was reduced considerably, since these parameters enter into the material balance equation in a different manner.

To aid in overcoming these difficulties, a certain amount of preliminary fitting was done (Jutan, 1976) using steady state data in order to provide reasonable initial estimates for fitting the complete set of dynamic data.

RESULTS

Two alternative procedures were used in the linearization steps 2 and 5 in the development of the state space model: linearization about the steady state temperature profile of the reactor model and linearization about an average operating profile obtained from reactor data records. Usually the two profiles were similar, but in general the average profile was better centered in the data and gave better fits, and so this approach was adopted.

Several data collection runs were performed, and in all cases very good fits to the data were obtained. Only the final run for which concentrations are available will be discussed here. Results from the other runs appear in Jutan (1976). Some of the results from this run are summarized

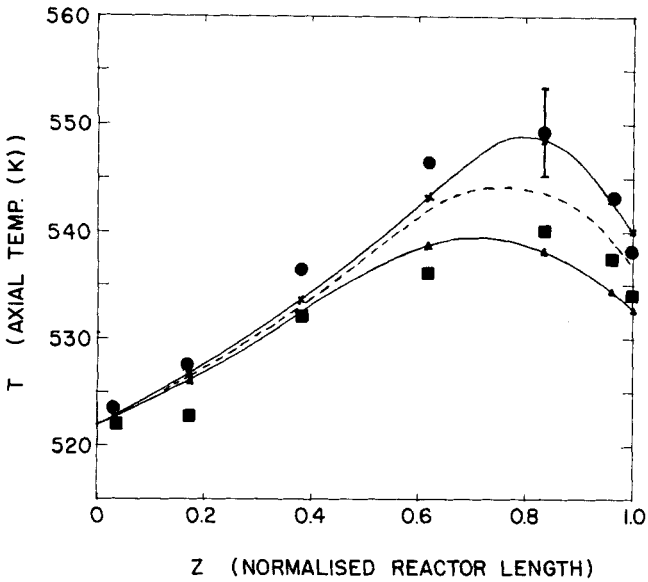

Fig. 2. Axial temperature profiles:
× Model, ● Data, at 36 min
▲ Model, ■ Data, at 82 min
---- Average operating profile.

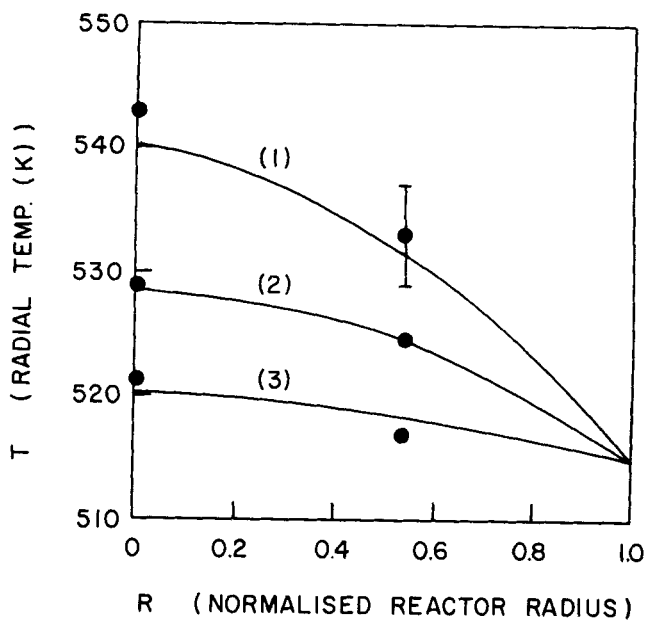

Fig. 3. Radial temperature profiles at $t = 41$ min for different axial positions: (1) $z = 0.904$, (2) $z = 0.531$, (3) $z = 0.282$ (a 2σ measurement error interval is indicated).

in Figures 2, 3, and 4, and the estimated parameters and the resulting state space model matrices obtained are given in the Appendix. Figure 2 shows the average temperature operating profile about which the linearization was performed and illustrates the temperature dynamics predicted from the model by comparing predicted profiles at two randomly selected times ($t = 36$ and 82 min into the run) with the corresponding measured temperatures. Also indicated in this figure are the 2σ limits for the thermocouple error. The predicted profiles can be seen to provide a reasonable fit to the data.

Statistical lack of fit tests on the innovation residuals $\mathbf{a}(t)$ revealed no significant lack of fit in the model. Autocorrelation checks on the $\mathbf{a}(t)$'s showed them to be white noise, and the diagonal elements of the estimated dispersion matrix $\hat{\boldsymbol{\Sigma}}$ (10) were all very close to 4.0, the estimated measurement error of the thermocouples.

Thermocouple measurements were available at the radial collocation points ($r = 0.577$) at three different axial positions along the catalyst bed. In Figure 3, the three radial profiles predicted by the model at an arbitrary time are compared with the measured temperatures. The reasonable agreement tends to confirm that the model assumption of quadratic radial profiles was adequate and that radial gradients were significant.

Figure 4 shows the reactor exit mole fraction data from the on-line chromatograph and the model predictions over the course of the run. If we take into account that the data and predictions in this plot were not well synchronized the figure indicates that both the level and the dynamic trends in the mole fractions of the various species have been well matched by the model. Conversion of butane is also plotted, but the mole fraction of ethane was usually quite small and is not shown.

CANONICAL REDUCTION OF THE DISTURBANCE MODEL

A multivariate autoregressive model of order 1 was identified and used in the estimation procedure to model the stochastic disturbances as they appear in the seven temperature measurements along the central axis of the reactor. However, it is quite unreasonable to expect that the stochastic disturbances in the system (due perhaps to wall or inlet temperature fluctuations, feed rate fluctuations, etc.) would affect all these seven temperatures along the profile in an independent manner. At best, one might expect that the disturbances might cause the whole profile to move up or down, shift along the reactor, etc., in other words, that the stochastic disturbance model has less than seven dimensions. In this section we look into a procedure for reducing the disturbance model down into a few canonical variates which contain all the activity and a remaining subset of variates which are simply white noise. This reduced model was used (Jutan, 1976) to design a stochastic controller for the reactor, and it is used here to give some insight into the nature and sources of the inherent disturbances in the reactor.

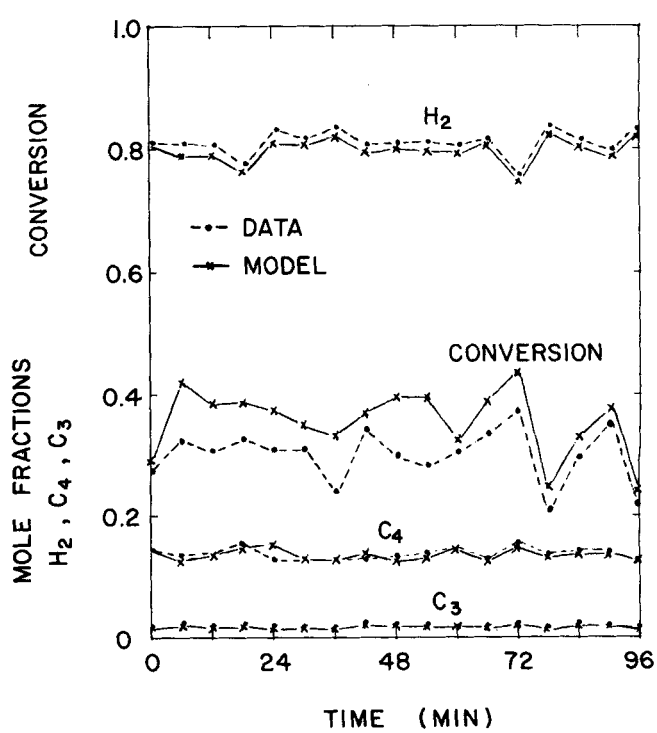

Fig. 4. Reactor exit mole fractions, model vs. data.

Consider again the autoregressive model

$$\mathbf{N}(t) = \boldsymbol{\varphi}\,\mathbf{N}(t-1) + \mathbf{a}(t) \tag{12}$$

Defining the autocovariance matrix at lag k as

$$\boldsymbol{\Gamma}_k = E[\mathbf{N}(t)\ \mathbf{N}'(t+k)] \quad k = 0, 1, 2, 3 \ldots \tag{13}$$

we can express the parameter matrix $\boldsymbol{\varphi}$ as

$$\boldsymbol{\varphi} = \boldsymbol{\Gamma}_1'\boldsymbol{\Gamma}_o^{-1} \tag{14}$$

and an analysis of variance breakdown is given by

$$\boldsymbol{\Gamma}_o = \boldsymbol{\Gamma}_1'\,\boldsymbol{\Gamma}_o^{-1}\,\boldsymbol{\Gamma}_1 + \boldsymbol{\Sigma} \tag{15}$$

where $\boldsymbol{\Gamma}_o$, $\boldsymbol{\Gamma}_1'\,\boldsymbol{\Gamma}_o^{-1}\,\boldsymbol{\Gamma}_1$, and $\boldsymbol{\Sigma}$ are, respectively, the covariance matrices of $\mathbf{N}(t)$, of the one-step ahead forecast $\hat{N}(t/t-1) = \boldsymbol{\varphi}\,\mathbf{N}(t-1)$, and of the white noise innovation sequence $\mathbf{a}(t)$.

Following Box and Tiao (1976) and MacGregor (1972) we suppose that there exists some canonical form for $\mathbf{N}(t)$ such that most of its activity can be represented by a few linear combinations of $N(t)$'s, say $\dot{N}_1(t) = \mathbf{l}_1'\,\mathbf{N}(t)$, $\dot{N}_2(t) = \mathbf{l}_2'\,\mathbf{N}(t)$, etc., Box and Tiao (1976) have suggested as a scale free measure of activity, the idea of the most forecastable variation. If we use this idea, the first principal component

$$\dot{N}_1(t) = \mathbf{l}_1'\,\mathbf{N}(t) = \mathbf{l}_1'\,\boldsymbol{\varphi}\,\mathbf{N}(t-1) + \mathbf{l}_1'\,\mathbf{a}(t)$$

$$= \hat{\dot{N}}_1(t/t-1) + \dot{a}_1(t) \tag{16}$$

is obtained by finding that linear combination $\mathbf{l}_1$ which maximizes the ratio of the variance of the one-step ahead forecast $\hat{\dot{N}}_1(t/t-1)$ to the variance of the forecast error $\dot{a}_1(t)$ That is

$$\underset{\mathbf{l}_1}{\text{Max}}\ \frac{V[\hat{\dot{N}}_1(t/t-1)]}{V[\dot{a}_1(t)]} = \frac{\mathbf{l}_1'\,\boldsymbol{\Gamma}_1'\,\boldsymbol{\Gamma}_o^{-1}\boldsymbol{\Gamma}_1\,\mathbf{l}_1}{\mathbf{l}_1'\,\boldsymbol{\Sigma}\,\mathbf{l}_1} \tag{17}$$

where $V[x]$ denotes the variance of x. Equation (17) is known as the Rayleigh quotient (Noble, 1969), and the solution can be obtained by solving the generalized eigenvalue problem

$$[\boldsymbol{\Gamma}'_1\,\boldsymbol{\Gamma}_o^{-1}\boldsymbol{\Gamma}_1 - \lambda\boldsymbol{\Sigma}]\,\mathbf{l}_1 = 0 \tag{18}$$

The maximum value of (17) is equal to λ_1, the largest eigenvalue of (18), and the corresponding eigenvector $\mathbf{l}_1$ gives that linear combination of the $\dot{N}(t)$'s which maximizes (17). Alternatively, because of the identity (15), one could obtain the same solution $\mathbf{l}_1$ by maximizing the ratio

$$\underset{\mathbf{l}_1}{\text{Max}}\ \frac{V[\hat{\dot{N}}_1(t/t-1)]}{V[\dot{N}_1(t)]} = \underset{\mathbf{l}_1}{\text{Max}}\ \frac{\mathbf{l}_1'\,\boldsymbol{\Gamma}_1'\,\boldsymbol{\Gamma}_o^{-1}\,\boldsymbol{\Gamma}_1\,\mathbf{l}_1}{\mathbf{l}_1'\,\boldsymbol{\Gamma}_o\,\mathbf{l}_1} = \mu_1 \tag{19}$$

Since all the covariance matrices in (15) are positive definite, there will be m real positive roots $\mu_1 > \mu_2 > \ldots$.

TABLE 1. EIGENVALUES OF THE CANONICAL TRANSFORMATION

λ	μ
3.361	0.7707
1.040	0.5098
0.2706	0.2130
0.1130	0.1051
0.0318	0.0308
0.0156	0.0154
0.0057	0.0057

TABLE 2. SIGNIFICANCE TEST FOR THE HYPOTHESIS THAT LAST r μ'S ARE ZERO

Ho: last r μ's $= 0$	$-[(n-m)-\frac{1}{2}(2m+1)]\ln\Lambda$	$x^2_{2r}(0.05)$
$r = 4$	7.25	15.5
$r = 5$	18.16	18.3

μ_m. Taking the matrix $\mathbf{L}$ to be that formed by letting the $\mathbf{l}_j$'s form its rows (and normalizing such that $\mathbf{L}\,\boldsymbol{\Sigma}\,\mathbf{L}' = \mathbf{I}_7$), one can make a nonsingular transformation of the AR(1) model in (12) to give

$$\dot{\mathbf{N}}(t) = \mathbf{L}\,\mathbf{N}(t) = (\mathbf{L}\,\boldsymbol{\varphi}\,\mathbf{L}^{-1})\,\mathbf{L}\,\mathbf{N}(t-1) + \mathbf{L}\,\mathbf{a}(t)$$

$$= \dot{\boldsymbol{\varphi}}\,\dot{\mathbf{N}}(t-1) + \dot{\mathbf{a}}(t) \tag{20}$$

such that the new canonical variables $\dot{N}_1(t)$, $\dot{N}_2(t)$, etc., are the most forecastable, the next most forecastable, and so forth.

The eigenvalues $\mu_j (0 < \mu_j < 1)$ are equal to the proportion of the variance of the canonical variate series which is forecastable (19). A multivariate statistical test for the hypothesis that the r smallest roots μ_{m-r+1}, μ_{m-r+2}, ..., μ_m are zero, given that the first $m-r$ roots are nonzero (Bartlett, 1947; MacGregor, 1972), is to compare the statistic

$$-\{(n-m) - \tfrac{1}{2}(2m+1)\}\ln\Lambda \tag{21}$$

with a chi squared distribution with $2r$ degrees of freedom [where $\Lambda = \prod_{j=m-r+1}^{m}(1-\mu_j)$]. The implication to be attached to r roots that are not significantly different from zero is that the disturbance model (12) is not fully m dimensional but rather $(m-r)$ dimensional. The corresponding r canonical variates $\dot{N}_j(t) = \mathbf{l}_j'\mathbf{N}(t)$ $(j = m-r+1, \ldots, m)$ are simply white noise sequences $[=\dot{a}_j(t)]$ with no forecastable variation. The structure of the canonical autoregressive disturbance model in (20) can be written as a reduced $(m-r)$ dimensional autoregressive model plus an r-dimensional white noise vector:

$$\dot{\mathbf{N}}_{m-r}(t) = \dot{\boldsymbol{\varphi}}_{m-r}\,\dot{\mathbf{N}}_{m-r}(t-1) + \dot{\boldsymbol{\alpha}}_{m-r}(t)$$

$$\dot{\mathbf{N}}_r(t) = \dot{\mathbf{a}}_r(t) \tag{22}$$

where $\dot{\boldsymbol{\varphi}}_{m-r}$ is the upper left-hand corner of $\dot{\boldsymbol{\varphi}} = \mathbf{L}\,\boldsymbol{\varphi}\,\mathbf{L}^{-1}$, and $\dot{\boldsymbol{\alpha}}_{m-r}(t)$ is a white noise sequence.

TABLE 3. EIGENVECTORS l' OF THE CANONICAL TRANSFORMATION (18) ASSOCIATED WITH THE THREE LARGEST EIGENVALUES

	Temperature location						
Eigenvector	1	2	3	4	5	6	7
l_1'	0.0996	0.0353	0.1647	−0.0635	−0.1940	0.5982	0.1494
l_2'	−0.5721	0.0683	0.1260	0.1409	−0.1807	0.2650	−0.3134
l_3'	0.0007	0.3305	−0.3280	−0.3220	−0.2457	0.2444	0.1183

Application to the Reactor Data

Applying the canonical reduction analysis to the disturbance sequence $\mathbf{N}(t)$ from one experimental data set collected on the reactor ($n = 60$ observations), the eigenvalues listed in Table 1 were obtained. Looking at these values one might suspect that perhaps only the first two or perhaps the first three are significant. Bartlett's statistic (21) can be applied to test the hypothesis that the smallest r eigenvalues are zero. The results of this test are shown in Table 2 for $r = 4$ and $r = 5$. One can see that there is no reason to doubt that the last four eigenvalues are different from zero, and that a test on the last five eigenvalues falls just at the critical 5% level of the chi squared distribution with 10 deg of freedom. This implies that at most the canonical disturbance model is of order 3 and possibly only 2. If we take its order as 3, then only the first three linear combinations of the temperatures defined by the first three eigenvectors shown in Table 3 can be said to exhibit any significant amount of forecastable stochastic variation. Therefore, the seven-dimensional stochastic disturbance model was reduced to a three-dimensional one in these first three canonical variates. This reduced model, given in the Appendix, was used (Jutan 1976) to form an augmented state space dynamic-stochastic model which is used in designing a stochastic controller for the reactor.

It is of considerable interest to try to place physical interpretations on the linear combinations of the temperatures which exhibit the most disturbance activity in order to gain an understanding of the nature of the major stochastic disturbances in the reactor and possibly to be able to pinpoint their sources. From Table 3 the linear combination which contains the greatest amount of disturbance activity (l_1') places by far the largest weight (0.5982) on the sixth temperature location. This is associated with hot spot in the reactor (see Figure 2). This confirms the intuitive feeling that the hot spot temperature is the most important single temperature measurement in the bed and that any disturbances in the reactor will show up most strongly at this point. The second linear combination (l_2') surprisingly places the greatest weight (-0.5721) on the first temperature position, a position which, because it is just at the entrance to the reactor bed, was not expected to exhibit any significant disturbance activity other than white measurement noise. A recheck of the physical reactor equipment revealed that this was due to an improperly designed temperature preheater which was designed to provide a constant heat flux rather than a constant temperature output and so could not keep up with the gas flow rate fluctuations. Therefore, a redesign of this preheater would eliminate the second most significant stochastic disturbance in the reactor system. The third linear combination is associated with only a very minor disturbance and appears to weight all the interior thermocouples almost equally. No physical significance was able to be associated with this combination.

One interesting implication of this reduction (which is being pursued now in other studies) is that the stochastic control problem, if it were the temperatures (rather than the concentrations) that were the variables to be controlled, would be only two or three dimensional rather than seven dimensional. For if one controlled only those linear combinations of the temperatures given by the eigenvectors associated with the nonzero eigenvalues, then one would remove all the forecastable stochastic variation in the system.

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NOTATION

$\mathbf{A}$ = $n \times n$ dynamic state matrix (4)
$\mathbf{a}(t)$ = white noise sequence (7)
$\dot{\mathbf{a}}(t)$ = canonical white noise sequence (16)
B_i = Biot number ($h_w R/\lambda_{er}$)
$\mathbf{B}$ = coefficient matrix (4)
C^i = concentration of species i, mole/cm^3
$\mathbf{C}(t)$ = vector of exit concentrations (6)
C_{ps} = specific heat of solid, J/(kg · °K)
C_{pg} = specific heat of gas, J/(kg · °K)
$\overline{C}$ = specific heat term $[C_{ps}\rho_B + C_{pg}\rho_g\epsilon]$, Equations (3) to (6)
D_{er} = effective radial diffusivity (based on empty reactor volume), m^2/s
$E[\cdot]$ = expectation operator (13)
G_o = superficial gas velocity, m^3 gas/(m^2 reactor · s)
h_w = heat transfer coefficient at reactor wall, W/(m^2 · °K)
$\mathbf{I}_m$ = m^{th} order unity matrix
k = discrete time lag
$\mathbf{L}$ = $m \times m$ matrix for canonical nonsingular transformation (20)
m = dimension of y vector
n = number of observations
$\mathbf{N}(t)$ = residual noise vector (5)
$\mathbf{N}(t)$ = canonical noise vector (16)
$\hat{\mathbf{N}}(t/t-1)$ = one-step ahead forecast for canonical noise vector (16)
r = radial distance in reactor (normalized)
r = number of zero eigenvalues
R = radius of reactor bed, m
R^i = net reaction rate for species i, mole/(kg catalyst · s)
R_i = reaction rate for reaction i, mole/(kg catalyst · s)
T = homogeneous gas/solid temperature, °K
T_w = temperature of reactor wall, °K
t = time
$\mathbf{u}$ = vector of manipulated variables (hydrogen and butane feed rates)
v_T = thermal wave velocity $\dfrac{G_o C_{pg}\rho_g}{L\overline{C}}$, m/(s · m)
$V[\cdot]$ = variance operator
$\mathbf{x}(t)$ = state vector at sample time t
$\mathbf{y}$ = vector of output variables (axial temperatures)
z = axial distance along reactor (normalized)

Greek Letters

$\dot{\boldsymbol{\alpha}}(t)$ = white noise vector (22)
λ_{er} = effective radial thermal conductivity, W/(m · °K)
λ_o = parameter in expression for λ_{er}
α = parameter in expression for λ_{er}
ρ_B = bulk density of catalyst, kg/m^3
ρ_g = gas density, kg/m^3
Δh_i = heat of reaction for reaction i, J/mole
ϵ = void fraction, m^3 gas in voids/m^3 empty reactor
∇^d = d^{th} backward difference operator
$\boldsymbol{\varphi}$ = $m \times m$ autoregressive matrix of parameters (8)
$\boldsymbol{\Sigma}$ = $m \times m$ variance-covariance matrix of $\mathbf{a}(t)$
$\boldsymbol{\Gamma}_k$ = auto covariance matrix at lag k (13)
λ = generalized eigenvalue (18)
μ = generalized eigenvalue (19)
Λ = function of eigenvalue defined in (21)
χ^2_{2m} = chi squared distribution with $2m$ deg of freedom
σ = standard deviation of temperature measurements

Special Symbols

$'$ = transpose of matrix or vector, for example, $\mathbf{a}'(t)$

$\wedge$ = estimate, for example, $\hat{\boldsymbol{\beta}}$

$\cdot$ = canonical variate, for example, $\dot{\mathbf{N}}(t)$

Subscripts

i = species number

o = center axial conditions

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APPENDIX

The reactor parameter values obtained upon fitting the data set discussed in the Results section were the following:

$$
\begin{aligned}
(k/k_o) &= 1.09 \\
\lambda_o &= 1.888 \times 10^{-3}\ \text{cal/(cm} \cdot {}^\circ\text{K} \cdot \text{s)} \\
\alpha &= 3.0 \times 10^{-14}\ \text{(fixed)} \\
D_{er} &= 5.0 \times 10^{-5}\ (\text{cm}^2/\text{s}) \\
T_w &= 522^\circ\text{K}
\end{aligned}
$$

These estimates in turn give rise to the following A and B matrices of the discrete state space model (4) (states T in degrees Kelvin and flow rates u in cubic centimeters per second):

$$
A = \begin{bmatrix}
0.187 & -0.097 & 0.051 & -0.041 & 0.039 & -0.043 & 0.025 \\
0.256 & 0.433 & -0.111 & 0.075 & -0.067 & 0.072 & -0.042 \\
-0.079 & 0.235 & 0.564 & -0.153 & 0.112 & -0.115 & 0.065 \\
0.051 & -0.112 & 0.241 & 0.815 & -0.238 & 0.207 & -0.115 \\
-0.038 & 0.047 & -0.131 & 0.286 & 0.914 & -0.390 & 0.200 \\
0.005 & -0.035 & 0.013 & -0.136 & 0.464 & 0.647 & -0.254 \\
0.016 & -0.032 & 0.008 & -0.090 & 0.172 & 0.834 & -0.246
\end{bmatrix}
$$

$$
B' = \begin{bmatrix}
0.020 & 0.051 & 0.129 & 0.432 & 0.676 & 0.490 & 0.421 \\
-0.101 & -0.024 & -0.041 & -0.095 & -0.105 & -0.048 & -0.032
\end{bmatrix}
$$

A three-dimensional stochastic disturbance model obtained by applying the canonical reduction precedure in the last section is

$$
\begin{bmatrix} \dot{N}_1(t) \\ \dot{N}_2(t) \\ \dot{N}_3(t) \end{bmatrix} = \begin{bmatrix} 0.862 & -0.127 & -0.061 \\ -0.045 & 0.681 & 0.027 \\ -0.008 & -0.018 & 0.432 \end{bmatrix} \begin{bmatrix} \dot{N}_1(t-1) \\ \dot{N}_2(t-1) \\ \dot{N}_3(t-1) \end{bmatrix} + \begin{bmatrix} \dot{a}_1(t) \\ \dot{a}_2(t) \\ \dot{a}_3(t) \end{bmatrix}
$$

where the variance matrix of the innovation sequence $\dot{a}(t)$ is given by $V[\dot{a}(t)] = I_3$.

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