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Part III. On-line Linear Quadratic Stochastic Control Studies

A linear low-order state space dynamic model for a catalytic butane hydrogenolysis reactor which has been fitted to reactor dynamic data is used to develop a multivariable linear quadratic feedback control algorithm for regulatory control of the reactor exit concentrations using temperature measurements only. Kalman filter theory is used to obtain state estimates for the system. The control algorithm developed is implemented on the pilot plant reactor in a series of DDC control studies. The controller is shown to perform very well and considerably better than a single loop PI controller with a feedback on the hot spot temperature. Performance is evaluated both under the normal stochastic disturbances in the system and under a severe deterministic load disturbance. Exit concentrations predicted by the model and used in the performance index are shown to compare very favorably with actual concentrations obtained from a process gas chromatograph.

SCOPE

Multivariable control studies in the chemical engineering literature have concentrated almost entirely on distillation columns, adsorbers, and evaporators (Fisher and Seborg, 1973, 1976; Shinskey, 1971). The lack of control studies on the fixed-bed reactor appears to be directly attributable to modeling complexities. Whereas the processes described above are often quite adequately described by sets of ordinary differential equations and hence are amenable to relatively direct application of state space control theory, many fixed-bed catalytic reactors, in particular the one in this study, require a set of partial differential equations to fully describe their complex dynamics. A first attempt at this problem (Michelsen et al., 1973) considered an exothermic noncatalytic reaction occurring in a liquid phase. For the system studied there, an effective method for representing fixed-bed reactor dynamics in a state space form, that is, by a set of linearized ordinary differential equations, was presented. In a sequential paper (Vakil et al., 1973), the state space model was used to derive a feed forward control scheme through simulation of the reactor, and various configurations were evaluated numerically. The simulation was subjected to random feed disturbances in temperature and concentration, and random measurement error was added. Use was made of a Kalman filter to estimate states of the system, although under the measurement configuration used, state estimation became a severe problem.

The present work uses a low-order state space model for a highly exothermic, catalytic packed-bed reactor, having three independent species, to derive an optimal stochastic controller. Kalman filter theory is used for state estimation. The control scheme is then implemented by an on-line computer to test its performance on the reactor under plant operating conditions. Controller performance is compared with that of a well-tuned proportional integral controller for both the stochastic disturbances which are present in the plant and for induced deterministic load disturbances. Part I of this paper derived the model, and in part II its parameters were estimated from dynamic data collected from the reactor (Jutan et al., 1977*a*, *b*).

CONCLUSIONS AND SIGNIFICANCE

An optimal multivariable stochastic controller for regulation of the output concentrations of a catalytic reactor for the hydrogenolysis of butane was successfully implemented using a minicomputer.The reactor model parameters and noise model covariances were estimated from plant operating data, and Kalman filter theory was used for state estimation. Control was based on temperature measurements only, and outlet concentrations were inferred from process models. Predicted concentration values compared well with measured values in final control runs. The stochastic controller performed very well compared with a univariate PI controller and gave significant reductions in the variances of the reactor exit concentrations. The stochastic controller also performed well under the influence of severe deterministic load changes in reactor wall temperatures and was quite robust to process parameter changes (for example, in catalyst activity) and to deviations in the operating conditions from those about which the models had been linearized. . .

This work represents one of the first multivariable control studies to be published on a heterogeneous exothermic reactor with several independent reacting species. We do not necessarily feel that the stochastic control algorithm developed and implemented in this paper is the best or the only approach to multivariable control of reactors. This study is part of an ongoing project to evaluate many different techniques. Other approaches being investigated include model reference adaptive control and self-tuning controllers. The emphasis has been on applied control studies in the hope that the implications of these studies may be extended to include industrial process control problems.

In part I of this paper (Jutan et al., 1977*a*) a description of the hydrogenolysis of butane over nickel on silica gel catalyst was described. For reference, the dynamic partial differential equations describing that system are repeated here.

Mass balance

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

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

Energy balance: solid/gas

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

where

$$\overline{C} = [C_{ps}\rho_B + C_{ps}\rho_g\epsilon]$$

The system consists of three independent reactions producing propane, ethane, and methane from a butane and excess hydrogen feed. A low-order state space model of the dominant temperature dynamics of the system was derived in conjunction with a prediction equation for concentrations in terms of temperatures and control inputs. The form of these equations is shown below

$$\frac{d\mathbf{T}_0}{dt}=\underline{\bar{\mathbf{A}}}\,\mathbf{T}_o+\underline{\bar{\mathbf{B}}}\,\mathbf{u} \tag{3}$$

where $\mathbf{T}_o$ is a (7×1) state vector of reactor center line temperature deviations and

$$\mathbf{C}(t)=\underline{\mathbf{M}}\,\mathbf{T}_o(t)+\underline{\mathbf{N}}\,\mathbf{u}(t-1) \tag{4}$$

where $\underline{\mathbf{C}}(t)$ is a (3×1) vector of radially averaged reactor effluent species compositions. The control problem considered here is to regulate the selectivity of the reaction in favor of one or other of the intermediate components in the face of stochastic disturbances which upset the system. In part II of this paper, the nature of some of these stochastic disturbances was identified, and the parameters of the model were estimated from reactor operating data.

DIRECT DIGITAL CONTROL (DDC) CONFIGURATION

A description of the experimental setup as well as the process control configuration has been given (Jutan et al., 1977*a*). An equation relating temperature measurements to concentrations was also derived and is repeated here (4) for convenience. This equation enables one to develop a control scheme based on an objective function expressed in terms of concentrations. Actual concentration measurements from the process gas chromatograph were not used as part of the control algorithms.

The control configuration, as indicated in Figure 1, used computer algorithms for control of the hydrogen and butane flow rates. These were sampled once per second by the system, and well-tuned digital proportional-integral control algorithms were implemented once per second by the software. The set points to these PI controllers were adjusted by the algorithms derived in the following sections once every 60 s, which was found to be an adequate sample period in other studies (Tremblay, 1973). One interesting feature of the control software was that checks were made to insure that the ratio of hydrogen to butane molal flow rates never dropped below the stoichiometric ratio of 3.0 even briefly during flow transients resulting from control action. Catastrophic deposition of carbon would result should this condition be violated.

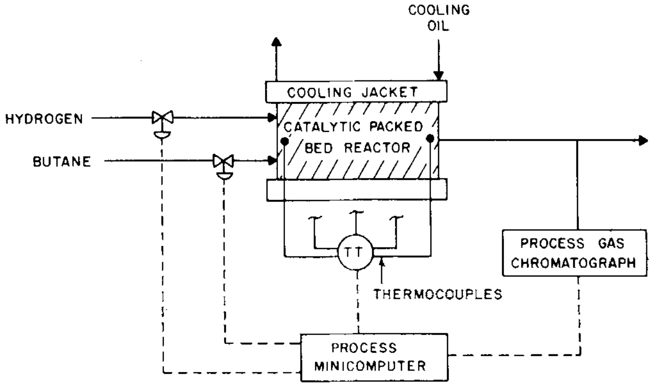

Fig. 1. Reactor control configuration.

The on-line process gas chromatograph was not interfaced during the early part of this work but was available for checking of final control runs. All control strategies were based upon temperature measurements only, with concentrations being inferred and ultimately compared with actual measurements. Use of the concentration measurements for control was not feasible, as the 6 min sample time of the chromatograph was too slow. Combinations of these measurements with faster temperature measurements will form the basis for some future studies on the system.

The cooling oil temperature was controlled independently by the computer. For this small reactor system, the dynamics of the coolant system were too slow to allow effective use of wall temperature as a manipulated variable. However, it was used to adjust the steady state operating conditions in the reactor and also as a load disturbance in the present study.

Some control simulations were performed with arbitrary noise characteristics to obtain some experience with the multivariable control algorithms (Jutan, 1976). Real time control software was developed using a Data General Nova 2/10 minicomputer operating under a real time disk operating system (RDOS). Data General's real time Fortran language was used to write a multivariable, linear quadratic control task as a module program which formed part of a general data acquisition and control package (Tremblay, 1977).

OPTIMAL STOCHASTIC CONTROL THEORY

Linear-Quadratic Stochastic Feedback Control

The design of constrained feedback controllers for linear, discrete, state space systems is well known (Noton, 1965; Astrom, 1970; Sage and Melsa, 1971). Analytical solutions to the general problem are available for systems which can be formulated with a quadratic performance criterion or objective function.

Consider the linear discrete state space equations

$$\mathbf{x}(t+1)=\underline{\mathbf{A}}\mathbf{x}(t)+\underline{\mathbf{B}}\mathbf{u}(t)+\mathbf{w}(t) \tag{5}$$

$$\mathbf{y}(t)=\underline{\mathbf{H}}\mathbf{x}(t)+\mathbf{v}(t) \tag{6}$$

where $\mathbf{x}(t)$ is an $n \times 1$ state vector, $\mathbf{y}(t)$ is an $m \times 1$ vector of observed outputs (temperature in our case),

$\mathbf{u}(t)$ is $r \times 1$ vector input variables (butane and hydrogen feed rates), and $\mathbf{w}(t)$ and $\mathbf{v}(t)$ are independent white noise vectors with covariance matrices:

$$\begin{aligned} E[\mathbf{w}(t)\mathbf{w}'(t)] &= \underline{\mathbf{R}}_w \\ E[\mathbf{w}(t)\mathbf{v}'(t+k)] &= 0 \quad \text{for all } k \\ E[\mathbf{v}(t)\mathbf{v}'(t)] &= \underline{\mathbf{R}}_v \end{aligned} \tag{7}$$

$\mathbf{w}(t)$ is usually thought of as representing the process noise or disturbances and modeling error, and $\mathbf{v}(t)$ represents the measurement noise. For convenience, all variables are in deviation form.

Suppose it is desired to find the sequence of discrete control policies $\mathbf{u}(t), \mathbf{u}(t+1), \ldots \mathbf{u}(N)$ which will optimize the quadratic performance criterion

$$\begin{aligned} \underset{\substack{u(t) \\ 0 \le t < N}}{\text{Min}} \; E \Big[\sum_{t=0}^{N-1} \{ & \mathbf{x}'(t)\underline{\mathbf{Q}}_1\mathbf{x}(t) + \mathbf{u}'(t)\underline{\mathbf{Q}}_2\mathbf{u}(t) \\ & + \mathbf{u}'(t)\underline{\mathbf{V}}\mathbf{x}(t) + \mathbf{x}'(t)\underline{\mathbf{V}}'\mathbf{u}(t)\} \Big] \end{aligned} \tag{8}$$

where $E[x]$ is the expectation of x. $\underline{\mathbf{Q}}_1$ and $\underline{\mathbf{Q}}_2$ are symmetric positive semidefinite matrices. This quadratic performance criterion is quite general and includes the case of minimum mean-square error control on the exit deviation concentrations, subject to constraints on the variances of the manipulated flow rates, that is

$$\underset{u(t)}{\text{Min}} \; E \Big[\sum_{t=0}^{N-1} \{ \mathbf{C}'(t)\mathbf{C}(t) + \mathbf{u}'(t)\underline{\mathbf{Q}}\mathbf{u}(t)\} \Big] \tag{9}$$

Remembering that the exit (deviation) concentrations $\mathbf{C}(t)$ may be expressed as a linear combination of the states $\mathbf{x}(t)$ and (deviation) controls $\mathbf{u}(t)$, in the present notation we can write Equation (4) as

$$\mathbf{C}(t) = \underline{\mathbf{Q}}_3\mathbf{x}(t) + \underline{\mathbf{Q}}_4\mathbf{u}(t-1) \tag{10}$$

It is important to note here that this equation is not being used as a measurement equation in the sense of Equation (6), which represents temperatures. If we take the performance criterion (9) as being reasonable, then upon substitution of Equation (10), it can be expressed in the general form of (8) with

$$\begin{aligned} \underline{\mathbf{Q}}_1 &= \underline{\mathbf{Q}}_3'\underline{\mathbf{Q}}_3 \\ \underline{\mathbf{Q}}_2 &= \underline{\mathbf{Q}} + \underline{\mathbf{Q}}_4'\underline{\mathbf{Q}}_4 \\ \underline{\mathbf{V}} &= \underline{\mathbf{Q}}_4'\underline{\mathbf{Q}}_3 \end{aligned} \tag{11}$$

$\underline{\mathbf{Q}}$ is usually chosen as a diagonal matrix of the form

$$\underline{\mathbf{Q}} = \begin{bmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{bmatrix} \tag{12}$$

where λ_i are Lagrange multipliers or simply cost parameters to be adjusted to obtain a desired level of constraint on the inputs $\mathbf{u}(t)$.

The steady state solution (as final time $N \to \infty$) to the optimal control problem is given by

$$\mathbf{u}(t) = -\underline{\mathbf{L}}_\infty\hat{\mathbf{x}}(t \mid \tau) \tag{13}$$

where $\mathbf{u}(t)$ is the optimal control setting to be applied at time t, $\hat{\mathbf{x}}(t \mid \tau)$ is the conditional expectation of the state vector $E[\mathbf{x}(t) \mid \mathbf{Y}(\tau)]$, and where $\mathbf{Y}'(\tau) = [\mathbf{y}(\tau), \mathbf{y}(\tau - 1) \ldots]$ represents the data available (up to time τ) for computing the control action at time t. This conditional state expectation is obtained from the Kalman filter. $\mathbf{L}_\infty$ is a constant feedback gain matrix obtained as the steady state solution to the matrix Riccati equations

$$\begin{aligned} \underline{\mathbf{L}}(t) &= [\underline{\mathbf{Q}}_2 + \underline{\mathbf{B}}'\underline{\mathbf{S}}(t+1)\underline{\mathbf{B}}]^{-1}[\underline{\mathbf{V}} + \underline{\mathbf{B}}'\underline{\mathbf{S}}(t+1)\underline{\mathbf{A}}] \\ \underline{\mathbf{S}}(t) &= \underline{\mathbf{A}}'\underline{\mathbf{S}}(t+1)[\underline{\mathbf{A}} - \underline{\mathbf{B}}\underline{\mathbf{L}}(t)] - \underline{\mathbf{V}}'\underline{\mathbf{L}}(t) + \underline{\mathbf{Q}}_1 \end{aligned} \tag{14}$$

with initial condition $\mathbf{S}(t) = \mathbf{Q}_1$.

The Kalman Filter

The discrete Kalman filter has been derived in several ways (Sage and Melsa, 1971; Jazwinski, 1970) and only the final equations will be given here.

For the general dynamic-stochastic model (5), (6), and (7), the conditional simultaneous and delayed state estimates are given by

$$\hat{\mathbf{x}}(t \mid t) = \hat{\mathbf{x}}(t \mid t-1) + \underline{\mathbf{K}}(t)[\mathbf{y}(t) - \underline{\mathbf{H}}\hat{\mathbf{x}}(t \mid t-1)] \tag{15}$$

$$\hat{\mathbf{x}}(t \mid t-1) = \underline{\mathbf{A}}\hat{\mathbf{x}}(t-1 \mid t-1) + \underline{\mathbf{B}}\mathbf{u}(t-1) \tag{16}$$

$\underline{\mathbf{K}}(t)$ is the Kalman gain, and, in general, one is interested in the steady state gain $\underline{\mathbf{K}}_\infty$ which is obtained as the steady state solution to the following matrix Riccati equations:

$$\underline{\mathbf{K}}(t) = \underline{\mathbf{P}}(t \mid t-1)\underline{\mathbf{H}}'[\underline{\mathbf{H}}\underline{\mathbf{P}}(t \mid t-1)\underline{\mathbf{H}}' + \underline{\mathbf{R}}_v]^{-1} \tag{17}$$

$$\underline{\mathbf{P}}(t \mid t) = \underline{\mathbf{P}}(t \mid t-1) - \underline{\mathbf{K}}(t)\underline{\mathbf{H}}\underline{\mathbf{P}}(t \mid t-1) \tag{18}$$

$$\underline{\mathbf{P}}(t+1 \mid t) = \underline{\mathbf{A}}\underline{\mathbf{P}}(t \mid t)A' + \underline{\mathbf{R}}_w \tag{19}$$

where $\underline{\mathbf{P}}(\cdot)$ is the conditional covariance matrix for the state estimate $\hat{x}(\cdot)$ in (15) and (16) and $\underline{\mathbf{P}}_\infty(\cdot)$ the corresponding steady state value.

In the reactor system, there is no appreciable time lag or transport delay, and a change in the input $\mathbf{u}$ is registered at the output before the next sampling interval 60 s later. The simultaneous states estimates $\hat{\mathbf{x}}(t \mid t)$ in (15) are therefore required, and the optimal control algorithm (13) becomes

$$\mathbf{u}(t) = -\underline{\mathbf{L}}_\infty\hat{\mathbf{x}}(t \mid t) \tag{20}$$

VARIANCE FORMULAS

Variance formulas for the closed loop system (5), (6), and (20) are easily derived (MacGregor, 1973). These formulas are useful for calculating, a priori, the covariance matrices of inputs $\mathbf{u}$ and outputs $\mathbf{y}$ for a given constrained feedback control matrix $\underline{\mathbf{L}}_\infty$ derived from a constraint matrix $\underline{\mathbf{Q}}$. The constraint matrix $\underline{\mathbf{Q}}$ is varied until the variances of the inputs and the outputs are jointly acceptable. It would be unacceptable for the input flow control valves to bang open and closed frequently, and some level of constraint on $\mathbf{u}$ (introduced through $\underline{\mathbf{Q}}$) usually provides smoother control action without appreciably increasing the variances of the output.

The covariance matrices of $\mathbf{u}$ and $\mathbf{y}$ are calculated from (MacGregor, 1973)

$$E[\mathbf{y}(t)\mathbf{y}'(t)] = \underline{\mathbf{H}}\,\underline{\mathbf{\Gamma}}_x(0)\underline{\mathbf{H}}' + \underline{\mathbf{R}}_v \tag{21}$$

$$E[\mathbf{u}(t)\mathbf{u}'(t)] = \underline{\mathbf{L}}_\infty[\underline{\mathbf{\Gamma}}_x(0) - \underline{\mathbf{P}}_\infty(t \mid t)]\underline{\mathbf{L}}_\infty' \tag{22}$$

where $\underline{\mathbf{\Gamma}}_x(0)$ is the covariance matrix of the state vector $\mathbf{x}(t)$ and can be obtained by solving the matrix Riccati equation

$$\mathbf{\Gamma}_x(0) = E[\mathbf{x}(t)\mathbf{x}'(t)] = \underline{\mathbf{D}}\underline{\mathbf{\Gamma}}_x(0)\underline{\mathbf{D}}' + \underline{\mathbf{D}}\underline{\mathbf{P}}_\infty(t \mid t)\underline{\mathbf{L}}_\infty'\underline{\mathbf{B}}'$$

$$+ \underline{\mathbf{B}}\underline{\mathbf{L}}_{\infty}\underline{\mathbf{P}}_{\infty}(t \mid t)\underline{\mathbf{D}}' + \underline{\mathbf{B}}\underline{\mathbf{L}}_{\infty}\underline{\mathbf{P}}_{\infty}(t \mid t)\underline{\mathbf{L}}_{\infty}'\underline{\mathbf{B}}' + \underline{\mathbf{R}}_w \qquad (23)$$

where $\underline{\mathbf{D}} = (\underline{\mathbf{A}} - \underline{\mathbf{B}}\underline{\mathbf{L}}_{\infty})$. These matrix Riccati equations are most conveniently solved numerically using an iterative approach.

CONTROL SYNTHESIS USING THE REACTOR MODEL WITH ADDITIVE WHITE NOISE

The measurement matrix $\underline{\mathbf{H}}$ in (6) is the unit matrix $\underline{\mathbf{I}}_7$ (Jutan et al., 1977*a*). The measurement error $\mathbf{v}(t)$ in (6) can be approximated by a white noise sequence with covariance matrix given by

$$\underline{\mathbf{R}}_v = \text{diagonal} <4.0> \qquad (24)$$

where the measurement error variance in the thermocouples was estimated to be $\sigma^2 = 4.0$ (Jutan et al., 1977*b*).

Determination of the Covariance Matrix $\mathbf{R}_w$

In order to determine $\underline{\mathbf{K}}_{\infty}$ from (17) to (19), both $\underline{\mathbf{R}}_v$ and $\underline{\mathbf{R}}_w$ are required. $\mathbf{w}(t)$ is often referred to as the generation noise and is difficult to interpret physically in the way in which $\mathbf{v}(t)$ can. For simplicity then, it is assumed that $\mathbf{w}(t)$ can be approximated by specifying a covariance matrix $\underline{\mathbf{R}}_w$ as

$$\underline{\mathbf{R}}_w = \text{diagonal} <\beta> \qquad (25)$$

where β is a single parameter to be chosen. A similar idea was proposed by Hamilton et al. (1973) where the ratio between the diagonals of $\underline{\mathbf{R}}_v$ and $\underline{\mathbf{R}}_w$ was used to weight the state estimate. A large ratio of $\mathbf{R}_v$ to $\underline{\mathbf{R}}_w$ caused the model's contribution to be emphasized in the state estimate, while a small ratio caused the data to be emphasized.

In this study, β and the corresponding $\underline{\mathbf{K}}_{\infty}(\beta)$ were chosen by minimizing the following objective function:

$$J_{K_\infty} = \sum_{t=0}^{N} [\mathbf{y}(t) - \hat{\mathbf{x}}(t \mid t-1)]' [\mathbf{y}(t) - \hat{\mathbf{x}}(t \mid t-1)] \qquad (26)$$

Equation (26) is minimized off-line based on a set of collected data $[\mathbf{y}(t)]$, and $\hat{\mathbf{x}}(t \mid t-1)$ is calculated from (15) and (16).

The sum of squares surface was not very sensitive to the value of β as indicated below:

$\mathbf{R}_w$ diagonal $<\beta>$	J_{K_∞}
$\beta = 1.0$	2 765
$\beta = 2.5$	2 752
$\beta = 4.0$	2 770

A value for $\beta = 2.5$ was selected as being satisfactory.

Another approach for accounting for the stochastic disturbances when synthesizing the stochastic controller is to use the identified structure of the colored noise $[N(t)]$ in the measured temperatures (Jutan et al., 1977*b*) and augment a state space model for it to the seven-dimensional state space reactor model. This approach is discussed in Jutan (1976) and is not presented here for the sake of brevity and because it led to essentially the same controller performance on exit concentrations as that obtained with the additive white noise model approach described above.

Determination of the Input Constraint Matrix, Q

A satisfactory constraint matrix $\underline{\mathbf{Q}}$ may be chosen by calculating the variances of the outputs $\mathbf{y}$ and inputs $\mathbf{u}$ from the variance formulas (21) and (22) and searching for a value of $\underline{\mathbf{Q}}$ which yields jointly acceptable values of these variances. For simplicity, $\underline{\mathbf{Q}}$ was chosen to be

$$\underline{\mathbf{Q}} = \lambda \underline{\mathbf{I}}_2 \qquad (27)$$

and the single parameter λ was varied until a satisfactory combination of input-output variances was obtained.

From the table below it can be seen that increasing the value of λ from 0 to 10^{-4} greatly reduces the variances of the input flow rates $\mathbf{u}$ necessary to accomplish the control while increasing the variance of the outputs y only slightly. The variances of $\mathbf{u}$ were unacceptably large for λ less than 10^{-4} but were satisfactory at or above this value. Therefore, 10^{-4} was selected for the control studies.

λ	Var u_{C_4}	Var u_{H_2}	Σ Var$[y_i]$	Var$[y_{\text{av}}]$
10^{-2}	0.510	0.048	68.92	9.85
10^{-3}	0.639	0.049	68.34	9.76
10^{-4}	0.973	1.372	66.90	9.56
10^{-5}	4.034	26.02	65.58	9.37

DDC CONTROL OF THE REACTOR

As mentioned previously, the control algorithms are based solely on temperature measurements, although the objective function is expressed as a function of the concentrations. The control algorithm developed in the previous sections was implemented on the reactor. A single loop control scheme based on control of the hot spot temperature by regulating the hydrogen flow was also tested to provide a comparison. Without the availability of concentration data, the basis used for comparison was the ability of the control algorithms to hold the mole fractions of the various species (as predicted by the model) steady, at their target values, in the presence of stochastic process disturbances. The ability of the algorithms to control the reactor (that is, to prevent reactor runaway) for step disturbances in the major load variable (the wall temperature) was also tested.

When concentration data became available at a later stage in the study, the state model was refitted using both concentration and temperature data. The control algorithm derived from this model was implemented and the controller evaluated in terms of the variations in the measured concentrations in the exit gases. A comparison could also be made between the measured concentrations and those predicted by the model.

Catalyst Deactivation

One of the most important parameters as far as reactor performance is concerned is the catalyst activity. This parameter cannot be directly measured and was estimated, a posteriori, in conjunction with several other parameters (Jutan et al., 1977*b*). No provision was made for a time varying catalyst activity since, from experience gained with this catalyst in previous years (Orlikas, 1970; Shaw, 1974), no significant loss of activity was expected during the period of an experimental run (~ 10 hr). This fact was confirmed in the present experimental work. However, after a run, the reactor was shut down and the catalyst stored inside the reactor under a blanket of carbon dioxide. Some loss of activity was evident after each shutdown period. This was detected by the fact that a lower temperature profile was obtained for the same wall temperature and gas flow rates previously used. A higher reactor wall temperature was therefore used to compensate for this loss in activity from run to run. This, of course, was not entirely satisfactory, since an increase in wall temperature cannot exactly compensate for a loss in catalyst activity. From the control standpoint, this problem presented a good test of the robustness of the control algorithms developed. These algorithms were obtained directly from the state models which were fitted (off-line) to the reactor data obtained several days or months earlier.

The problem is primarily due to the laboratory nature of the experiments. An industrial process reactor of this type is not often shut down, and if catalyst activity is approximately constant during operation, the off-line parameter estimates would be valid. If necessary, they could be updated from time to time.

Practically the problem had been solved in the isothermal packed-bed reactors used to study the reaction kinetics for this system by reconditioning the catalyst in the reactor at temperatures 150°C or more above the operating conditions prior to a run. This was tried by Tremblay (1973) for the present packed-bed reactor but led to severe leakages of hot oil. For the reactor used in this study, catalyst was conditioned externally and transferred to the reactor under a blanket of carbon dioxide.

Multivariable Stochastic Control Run with Concentration Data

A multivariable stochastic control run was implemented on the reactor a few days after fresh catalyst (different from that used during the data collection run used for parameter estimation) had been installed. Since actual concentration measurements were not available in these early runs, all evaluation had to be made on the basis of the reactor exit concentrations predicted by the model. These predicted concentrations were shown to compare quite favorably with actual concentration data in part II of this paper (Jutan et al., 1977*b*) and will again be shown to be quite good in a later control run. The controller was designed to minimize the variances of the exit concentration deviations from their set points, subject to constraints on the variances of the manipulated inlet flow rates [Equation (9)]. The predicted exit concentrations and the manipulated flow rates of hydrogen and butane from this run are shown in Figure 2 together with a plot of the performance index

$$J = \sum_t \mathbf{C}(t)'\mathbf{C}(t)$$

For the first 30 min, during which time the reactor is subject to only the inherent stochastic disturbances, the controller is able to hold (with fairly smooth control action) all the mole fractions as well as the conversion reasonably constant. The performance index (J) rises by less than 0.1 over this period. Previous attempts at steady state open loop runs indicated that removal of the control during this period would cause the conversion to drop to zero (reaction quenched) or soar to 100% (reactor runaway). (The reactor is open loop unstable.) The stochastic control algorithms developed here are designed specifically to compensate for the stochastic disturbances present in the process. Nevertheless, a good test of the robustness of the algorithm is to examine its response to a deterministic load disturbance. The most severe load disturbance in this system would be to step up the wall coolant temperature by even a few degrees. Without control, the highly exothermic nature of the reactions would cause a reactor temperature runaway, giving rise to near 100% conversions and hot spot temperatures in excess of 400°C.

After approximately 30 min under control, a 5°C step in the wall coolant temperature was made. The controller promptly responded (see Figure 2) by reducing the butane flow rate, thus cutting off the potential supply of heat (through the exothermic reaction) and preventing reactor runaway. The flow rate of hydrogen is increased slightly, which tends to decrease the reaction rate (Jutan et al., 1977*a*), but the controller obviously sees the butane flow as the more important manipulated variable. The reactor exit concentrations are stabilized very quickly at new levels which represent offsets due to the fact that the stochastic controller is of a proportional state feedback form and contains no integral action; although, if this type of disturbance were common, integral action could be incorporated through the use of additional states. After the process had stabilized at its new level, the wall temperature was stepped back down by 5°C and the flow controls returned to their original levels. The rate of increase of the (cumulative) performance index is reduced accordingly, rising to just under 2.0 for the total 77 min control run.

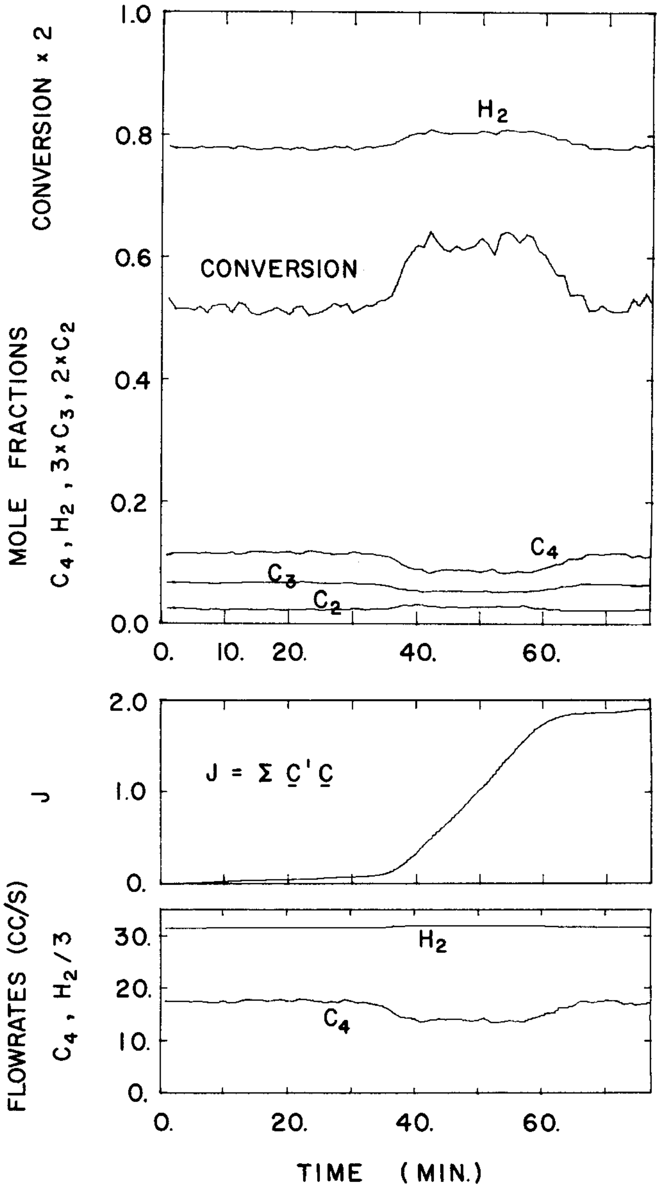

Fig. 2. Multivariable stochastic control run on the reactor.

Single Loop Control

Historically, the reactor was controlled by fixing the butane flow and implementing a single loop PI controller on the hydrogen flow (Tremblay and Wright, 1974). It was evident, from an examination of the data from a control run, that if a controller could regulate both the position and height of the hot spot, the product distribution too would be well controlled (given that the catalyst activity was constant). An attempt was made therefore to regulate the hot spot temperature about a desired value by manipulating the hydrogen flow. This PI controller was

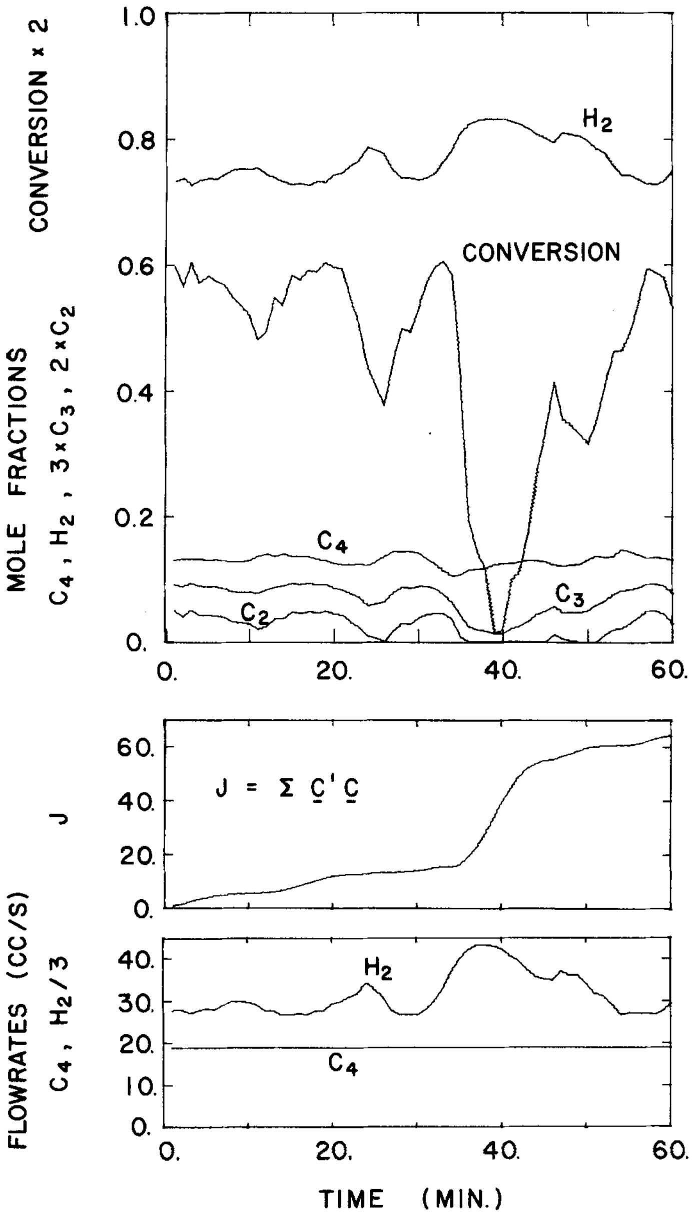

Fig. 3. Single loop PI control run.

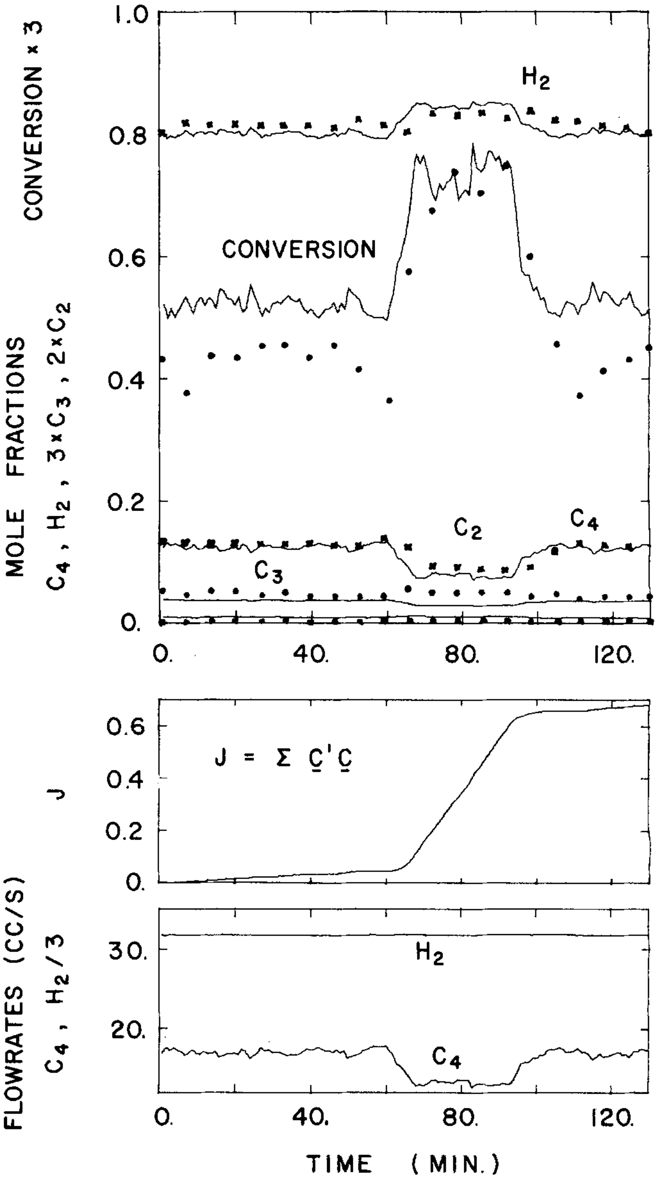

Fig. 4. A multivariable stochastic control run showing measured reactor exit mole fractions.

usually tuned on-line. The bases for tuning were stability of the reactor and speed of response to step disturbances in wall temperature and flows (see also Tremblay, 1973). The proportional gain was obtained by trial and error (in the absence of integral action), and then sufficient integral action was introduced to remove any observed offset. The controller gains usually took several hours to obtain and depended on many factors including wall temperature, catalyst activity, and upper and lower constraints imposed upon the flow rates. This control run (shown in Figure 3) was performed 1 day before the multivariable control run in Figure 2. The flow rate of butane, u_{C_4}, is shown as a constant next to the hydrogen flow control which exhibits a wandering cyclic behavior. This occurs even over the first 30 min, where the PI controller is attempting to regulate the hot spot temperature in the presence of inherent stochastic disturbances. The cumulative objective function rises up to 20.0 over this period (about 200 times that for the multivariable scheme). The mole fractions and conversion (as predicted by the model) are seen to oscillate considerably about their mean values. A 5°C step in the wall temperature introduced after 30 min causes the hydrogen to increase to its upper limit. An upper and lower constraint of 120 and 80 cm^3/s (101.3 kPa, 25°C) was imposed by means of the control software to stabilize the control action. The rapid drop to almost zero conversion (due to increased hydrogen flow) predicted by the model is probably not very accurate, but it does indicate that the control action resulted in a temporary quenching of the reaction. The mole fractions and conversion never really recover to their original values in spite of the presence of integral action until after the wall temperature is lowered back down by 5°C to its original position some 15 min later. The (cumulative) objective rises to about 65 over a 60 min control run, a considerable increase over the multivariable scheme.

The multivariable control schemes (which followed this run) indicated that butane was the preferred manipulated variable, in contrast to hydrogen flow which historically was used for control. On this basis, a single loop butane PI controller was later implemented by Tremblay (1977). He found that using butane flow as the controller for a data collection run allowed him to obtain higher hot spot temperatures (up to 300°C) with less danger of reactor temperature runaway. The behavior of this controller was otherwise similar to that shown in Figure 3. However, the large manipulations in the butane flow (the limiting reactant) which were required on Tremblay's runs had the effect of upsetting the production rates of the various products, thereby making its usefulness limited in an industrial environment.

A Multivariable Control Run with Concentration Data

The concentrations predicted by the model in the previous runs used only temperature measurements. At the very end of this study, the gas chromatograph was successfully interfaced, and concentration data could be obtained. The multivariable controller's ability to regulate the actual concentrations (measured by the gas chromatograph) could therefore be evaluated. An exact comparison between predicted mole fractions and the data was not possible owing to a lack of proper synchronization between temperature and concentration data (Jutan, 1976). Nevertheless, the comparisons (shown in Figure 4) generated considerable confidence in the model and the control algorithm. The state space reactor model had been fitted to both concentration and temperature data (Jutan et al., 1977*b*) and used to derive the control algorithm. The data for fitting this state space model were collected 10 days before the control run, and some loss of catalyst activity was observed when the control run was performed. To offset this, the wall temperature was raised by 3°C, and thus some change in the product distribution could be expected. In spite of this, the model predicted the mole fractions and conversion remarkably well, as shown in Figure 4. The controller is seen to hold the mole fractions fairly constant and close to the values measured by the chromatograph, over the initial period of control (60 min) where only stochastic disturbances were present. Over this period, the cumulative performance index rose to only 0.07.

Again, a 5°C step in the wall temperature was introduced (at 60 min), and, as before, the controller prevented reactor runaway and stabilized the exit concentration levels very quickly by dropping the butane flow significantly and raising the hydrogen flow slightly (the hydrogen flow scale is divided by a factor of 3 in Figure 3). The offset in the levels is again due to the absence of integral action in the control algorithm. Even at the new level, the model is able to predict the mole fractions well. After approximately 35 min at the offset levels, the wall temperature was stepped back down by 5°C, and the mole fractions and conversion returned to their previous levels. Note the smooth behavior of the manipulated input flows over the entire run. The total rise in the objective function over the 130 min control run was 0.68.

Robustness of the Controllers

An interesting feature of the multivariable stochastic controller implemented in this study was its robustness, or ability to perform well even under conditions moderately different from those for which it was derived. It appeared to be robust to changes in process parameters (in particular, catalyst activity) and to deviations in the operating temperature profile from that about which the original highly nonlinear model had been linearized. This was demonstrated very clearly in an early control run in which the catalyst had become very deactivated during a shutdown. In spite of this deactivation and a shift in the temperature profile, the resulting control was quite satisfactory. The control was also able to stabilize the reactor very quickly under severe step load disturbances in wall temperature for which it was not specifically designed. Finally, it accomplished the control using extremely noisy temperature measurements ($\sigma_T^2 = 4°K$ as compared with a maximum temperature rise through the bed of approximately 30°K) and using a reasonable sampling interval (60 s).

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NOTATION

$\underline{A}$ = $n \times n$ dynamic state matrix (5)
C^i = concentration of species *i*, mole/cm^3
$\bar{C}^i$ = radial average concentration of species *i*, mole/cm^3
C_{ps} = specific heat of solid, J/(kg · °K)
C_{pg} = specific heat of gas, J/(kg · °K)
$\bar{C}$ = specific heat term $[C_{ps}\rho_B + C_{pg}\rho_g\epsilon]$ (3)
D_{er} = effective radial diffusivity (based on empty reactor volume, m^2/s
$E[\cdot]$ = expectation operator (7)
G_o = superficial gas velocity, m^3 gas/(m^2 reactor · s)
$\underline{H}$ = $m \times n$ measurement matrix (27)
$\underline{I}_m$ = m^{th} order unity matrix
$\underline{K}_\infty$ = steady state Kalman gain matrix (16)
k = discrete time lag
L = reactor length, m
$\underline{L}_\infty$ = optimal steady state feedback gain matrix (12)
$N(t)$ = residual noise vector
r = radial distance in reactor (normalized)
R^i = net reaction rate for species *i*, mole/(kg catalyst · s)
R_i = reaction rate for reaction *i*, mole/(kg catalyst · s)
$\underline{R}_w$ = variance covariance matrix for $w(t)$ (7)
$\underline{R}_v$ = variance covariance matrix for $v(t)$ (7)
T = homogeneous gas/solid temperature, Equation (2), °K
T_o = temperature along centre axis of reactor, °K
t = time: continuous (s); discrete (min)
u = vector of manipulated variables
$v(t)$ = white measurement noise sequence (6)
$w(t)$ = white generating noise sequence (5)
$x(t)$ = state vector at sample time t
$\dot{x}$ = time derivative of state vector (continuous)
$\hat{x}(t \mid t)$ = state estimate (simultaneous of x
y = vector of output variables
z = axial distance along reactor (normalized)

Greek Letters

λ_{er} = effective radial thermal conductivity, W/(m · °K)
ρ_B = bulk density of catalyst, kg/m^3
ρ_g = gas density, kg/m^3
Δh_i = heat of reactor for reaction *i*, J/mole
ϵ = void fraction, m^3 gas in voids/m^3 empty reactor
σ = standard deviation

Special Symbols

$'$ = transpose of matrix or vector
$\wedge$ = estimate

Subscripts

ex = exit conditions for reactor
i = species number
o = center axial conditions
∞ = steady state value

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Calculation of Phase Equilibria for Ethylene/Low-Density Polyethylene Mixtures

We have used recent ethylene/low-density polyethylene gas sorption data to calculate phase equilibria for ethylene/polyethylene mixtures from 0 to 30.3 MN/m^2 (0 to 300 atm), the pressure range normally used in the flash separation step in low-density polyethylene manufacture. The computations show significant differences from results obtained by extrapolation of the results of a previous study to the relatively low pressure range considered here.

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SCOPE

The purpose of our study of ethylene/low-density polyethylene phase equilibrium was to calculate phase equilibrium between ethylene and polyethylene using corresponding states analysis applicable to low-density gases as well as to dense liquids and gases. Our emphasis is primarily on the pressure range in which ethylene is removed from polyethylene in industrial production after the reaction to produce polyethylene. Estimates of ethylene/low-density polyethylene phase equilibria have been published previously. However, the present analysis uses an improved statistical mechanical model of gas/polymer equilibrium. The parameters used in the model are obtained from recently published ethylene/polyethylene phase equilibrium data.

CONCLUSION AND SIGNIFICANCE

We have used an improved model for phase equilibria in gas/polymer solutions to calculate phase equilibria for ethylene/low-density polyethylene mixtures, taking into account polymer molecular weight distribution. The calculations indicated differences in phase compositions at less than 30.3 MN/m^2 (300 atm) from those of a previous study of such a magnitude that design of the flash separation and ethylene recycle steps in a low-density polyethylene process could be affected. Further, the new model predicts ethylene partial pressures in polyethylene solutions well at low pressures characteristics of devolatilization conditions in low-density polyethylene manufacture.

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