Estimation of Flows and Temperatures in Process Networks

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It is shown that temperatures and flows in a process network can be estimated from a quasi steady state model and a discrete Kalman filter. The data needed for such an application are readily available in many operating plants, and the computational requirements are within the capabilities of available process computers.

SCOPE

In the course of daily operation of a petroleum refinery or chemical complex, many thousands of items of information are generated, gathered, and recorded. These data are, in turn, used to plan, schedule, control, and evaluate process operations. Because of the highly integrated nature of modern processes, inaccurate data taken from one part of the process can easily lead to poor decisions that affect other parts of the processes. For instance, if inventory and production data on one product are inaccurate, the manufacturer may be forced to substitute a premium grade product to meet his delivery, thereby incurring a quality giveaway and creating an additional demand for the substitute product. Or, he may have to procure the supply from some other sources at additional costs. Or, he may accumulate unnecessarily large inventory, thereby tying up production and storage facilities needed for other products. Because of the immense scale of operations, even a small percentage change in inventory or flow may make a substantial difference in revenues or profits. The availability of accurate and consistent process data is therefore crucial to all process analyses.

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In a previous paper (Mah et al., 1976), we have shown how the constraints imposed by an integrated process could be turned to advantage in enhancing the information content of the raw process data. Specifically, we showed how the overall data enhancement problem involving redundant but inconsistent data on the one hand and missing measurements on the other hand can always be resolved into two disjoint subproblems which can then be readily solved. We also showed how gross errors such as leaks and measurement biases may be detected and identified. These results were derived for flow and inventory data in a process network and based on the availability of a single set of measurements.

In this paper the treatment is extended to cover estimation of temperatures and energy flows as well as material flows in a process network. Even more importantly, the proposed estimator takes advantage of continual updates of measurements as well as the aforementioned redundancy. The estimator is designed to possess functional attributes that are judged desirable on the basis of process data collected from the atmospheric crude distillation unit of an operating refinery. The performance characteristics and computational requirements of such an estimator were investigated by simulation experiments.

CONCLUSIONS AND SIGNIFICANCE

A quasi steady state model of the process network was developed on the basis of the process data logged over a 2 mo period. The model lends itself to the application of the discrete Kalman filter. It was found that by adjusting the relative weights of process noise and measurement noise covariances, the filter could be tuned to give significant error reduction (up to 70%) and respond rapidly and stably to sudden changes of process conditions. Redundant measurements contributed significantly to the overall error reduction. Further experiments showed that the filter functioned reasonably well with isolated biases. However, indiscriminant inclusion of biases and parameters as estimation variables is not recommended.

The computer program that we have implemented will generate estimators for different process networks and filter parameters. The computational requirements of a typical application can easily be accommodated on a process computer. With process data now available in abundance as a result of process computerization, the implementation of the proposed technique for on-line estimation of temperatures and flows in process networks appears to be a realistic possibility.

In a previous paper (Mah, Stanley, and Downing 1976), we pointed out the pervasive role of process data in all aspects of process control and performance evaluation and formulated three specific problems associated with enhancement of data gathered from an operating process. They are, respectively, the problems of data reconciliation, coaptation, and fault detection and rectification. The underlying information utilized in the treatment of these problems is the data redundancy in the sense that there are more measurements (or data) available than needed if the measurements were not subject to errors. This redundancy, which is brought about as a result of the interconnectedness of a process network, will be referred to as spatial redundancy.

In the investigations reported so far (Kuehn and Davidson, 1961; Ripps, 1965; Vaclavek 1969a, 1969b; Umeda, Nishio, and Komatsu, 1971; Mah, Stanley, and Downing, 1976) the data enhancement problems are analyzed on the assumptions that only a single set of measurements is available and that the process operates under steady state conditions. In reality, neither of these simplifications always applies. At a given instant, a "snapshot' of the conditions of a continuously operated process may appear to be steady state, but over a longer period the successive "snapshots" of conditions will almost certainly reveal changing process conditions. Moreover, with the data sampling and recording techniques now available, it is not uncommon to find process data being sampled continually at regular time intervals of 1 to 5 min. There is, therefore, also a data redundancy in the sense that more measurements are available than needed, if the process conditions were truly at a steady state. We shall refer to this as temporal redundancy.

With reference to Figure 1, the state variables and the measurements associated with a process at time t_k are denoted by $\mathbf{x}_k$ and $\mathbf{z}_k$, respectively, and the estimates of the state variables by $\hat{\mathbf{x}}_k$. If a steady state estimator is used, the state estimates at times t_k and t_{k+1} are obtained independently, no information is carried over from t_k to t_{k+1}. In other words, no relationship between the present and past conditions is exploited; all historical information is discarded.

In the other extreme, spatial redundancy is ignored, and measurements are simply averaged over time. Under the steady state assumption, the averaging procedure may be viewed as a method of exploiting temporal redundancy. A slightly more esoteric alternative to time averaging is the so-called exponential filter. For a measurement z_{ik} of a scalar variable x_{ik}, this filter give the estimate

$$\hat{x}_{ik} = \hat{x}_{i,\,k-1} + \xi_i\,(z_{ik} - \hat{x}_{i,\,k-1}),\ 0 < \xi_i < 1 \qquad (1)$$

Both time averaging and exponential smoothing make no use of spatial redundancy. Nor do they guarantee that the estimates obtained will be consistent with material and enthalpy balances.

In this paper we shall consider the problem of data enhancement in applications in which the time framework is sufficiently long that short-term variations of process conditions can be safely ignored but in which the long-term process trends such as fouling of heat transfer surfaces must be accounted for. Supervisory control and production scheduling are two examples of such applications. To be specific, we shall describe the observed characteristics of an important class of processes and show how this information can be used to specify an estimator with the desired characteristics. We shall explore the behavior of such an estimator under different simulated conditions, and, finally, we shall report our experience on the computational requirements of such an estimator.

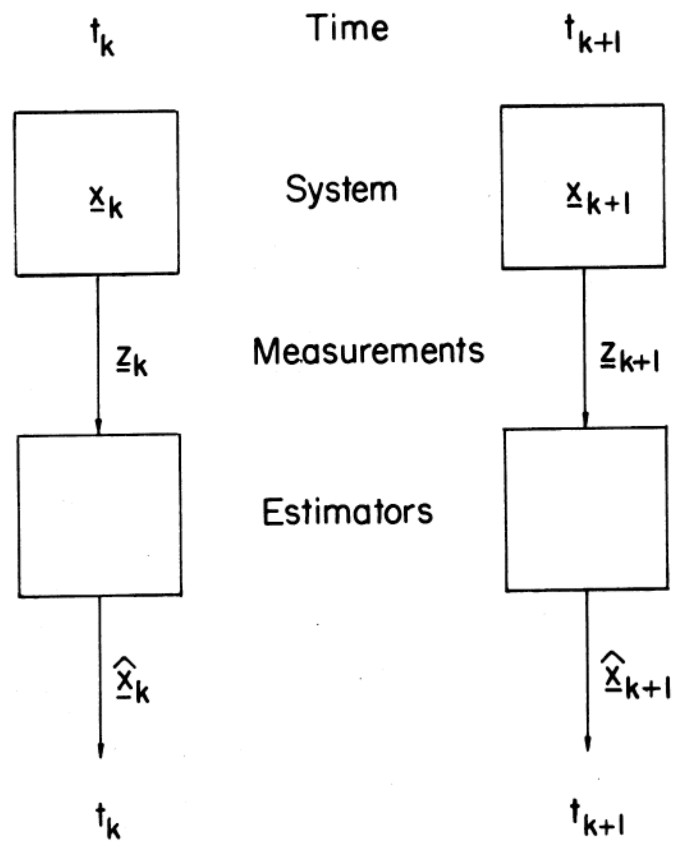

Fig. 1. Steady state reconciliation.

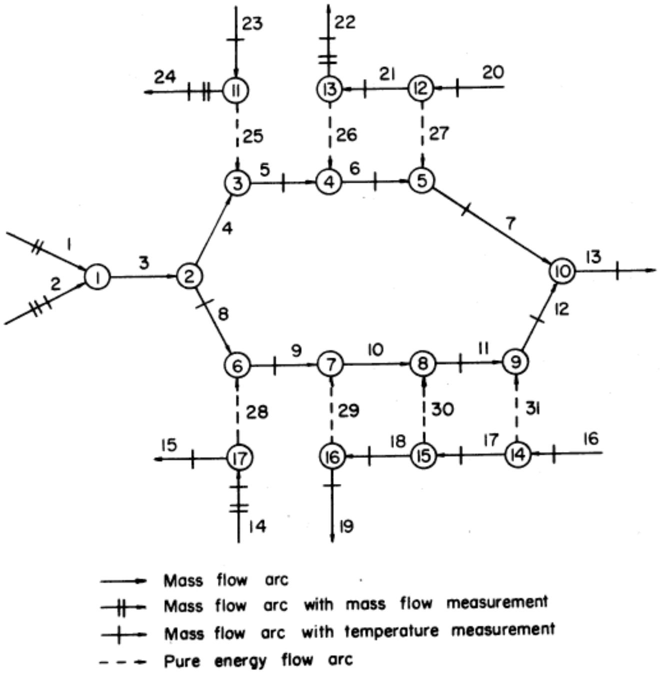

Fig. 2. The crude preheat heat exchanger network.

PROCESS CHARACTERISTICS

For the purpose of this study a 140 000 bbl/day crude oil distillation unit at the Amoco refinery at Whiting, Indiana, was selected as an example of an important class of process units. A dominant feature of this unit is the presence of a large number of heat exchangers. Process data from approximately 250 sensors were scanned every minute, and once every 2 hr the averages were transmitted and logged. These data were in turn automatically transcribed on a magnetic tape every 24 hr and used as a basis of our analysis.

The following conclusions were reached after discussions with refinery personnel and examination of data logged during a 2 mo period. Steady state conditions are typically maintained for 8 hr to 8 days, with 2 hr transitions between steady states. Steady state mass and energy balances hold in almost any time period in the extensive heat exchanger network, with the high flow rates of incompressible fluids precluding significant mass or energy accumulation. However, efficient operation requires a close monitoring of the heat transfer coefficients, which can decay slowly over a period of months due to fouling. This type of process, which is essentially at steady state except for slow drift or occasional sharp transition between steady states, will be referred to as a quasi steady state (QSS) process.

Our goal is to construct a practical on-line estimator for a QSS process that will substantially improve flow and temperature estimates at steady state conditions, yet quickly follow plant upsets, say, within an hour. Furthermore, the estimates should be consistent, that is, satisfy the steady state mass and energy balances.

In this study we shall be concerned with flow and temperature estimates only, and only the following information will be assumed to be available: flow and temperature measurements, process network configuration, and enthalpy correlations relating temperature to enthalpy. No assumption is made that the flow and temperature of every stream are measured. We note that these requirements are satisfied by the refinery unit in which the volumetric flow measurements are converted to mass flows using assumed densities, and the enthalpy correlations are also developed using assumed densities.

A concise representation of the network characteristics of the process is given by the process graph (Mah, Stanley, and Downing, 1976). In this representation, the nodes indicate process units, tanks, or junctions and the directed arcs the flows of material and energy streams. A single node is used to represent the environment from which the process receives its feeds and to which it delivers its products. Parallel arcs between a pair of nodes are also allowed.

The process graph for the crude preheat heat exchanger network (a section of the Whiting crude oil distillation unit) is shown in Figure 2 as an illustration. The environment node is omitted in this process graph for typographical clarity. Note that in addition to the connections between units, the locations of measurements and the types of flows may also be indicated on the process graph. Temperature and mass flow measurements are indicated by single and double slashes, respectively, on the arcs. Solid lines and broken lines are used to differentiate between mass flow arcs and pure energy flow arcs. Examples of the latter are heat transfer in a heat exchanger, heat loss through radiation, and electrical inputs to pumps and compressors.

In Figure 2 the crude oil enters at arc 1, and water is added at arc 2 for later desalting. The flow is split into two streams at node 2 and recombined at node 10. In between these two junctions the crude oil is heated in seven countercurrent heat exchangers by different intermediate and product streams. Each heat exchanger is represented by a pair of nodes connected by a pure energy flow arc to emphasize that only heat exchange but no material exchange takes place between the two streams. Arcs 16 to 19 and 20 to 22 represent distillation column pump-around streams, while arcs 14 to 15 and 23 to 24 represent hot product streams. Flow rates range from 19 to 380 kg/s with temperatures between 292.6 and 460.9^{0}K. The amount of water added in arc 2 is small, and the flows in all other arcs can be treated as single-phase hydrocarbon liquids. Figure 2 exemplifies many features of a typical process graph and will be referred to again in subsequent discussions.

THE QUASI STEADY STATE ESTIMATOR

We shall now turn to the development of QSS estimators. In recent years, the Kalman filter has been evaluated for on-line estimation in several chemical engineering applications, brief reviews of which may be found in papers by Hamilton, Seborg, and Fisher (1973) and Jo and Bankoff (1976). The motivation behind these investigations is improved process control for which the dynamic models of the process system are needed. These models are generally quite complex, and a very recent study by Jo and Bankoff (1976) provided substantial evidence to suggest that the utility of the Kalman filter might be severely limited by the model uncertainties in certain applications.

In supervisory control, the set points of controllers are manipulated on the basis of long-term trends; the full complexity of dynamic models is therefore not required (Smith, 1972). A suboptimal filter for QSS systems was developed by Masiello and Schweppe (1971). The use of steady state estimators was suggested by Goldmann and Sargent (1971). The development of QSS estimators for a process network is given below.

Since Kalman filter theory is fully documented in several books (Bryson and Ho, 1968; Jazwinski, 1970; Gelb, 1974), we shall only recapitulate the relevant results in our development. For a sampled data system, let the (l x 1) measurement vector $\mathbf{z}$ be related to the (n x 1) state vector $\mathbf{x}$ through the equation

$$z_k = H_k\, x_k + v_k \tag{2}$$

Then the Kalman filter equations fall into two groups. First, the measurements are used to update the prior estimates of x_k and of the error covariance matrix P_k for x_k in the equations

$$\hat{x}_k(+) = \hat{x}_k(-) + K_k\,[z_k - H_k\,\hat{x}_k(-)] \tag{3}$$

$$K_k = P_k(-)\,H_k^T\,[H_k\,P_k(-)\,H_k^T + R_k]^{-1} \tag{4}$$

$$P_k(+) = (I - K_k\,H_k)\,P_k(-) \tag{5}$$

Next, these estimates are extrapolated to time t_{k+1}. The extrapolations (or predictions) are based on the system model postulated. In a QSS process, flow rates and temperatures are assumed to be held constant over short time periods, say 5 min, with slow drifts which may persist for days or weeks and occasional sharp changes on a time scale of several hours. Hence, the prediction for the immediate future is that there will be no change in the values of the state variables. This prediction will be accurate if the process is actually at a steady state or drifting slowly. However, during periods of rapid change, the prediction will not be as good, and the estimator will use the measured values to correct for the prediction error. Mathematically, the QSS model is described by the equation

$$x_{k+1} = x_k + w_k \tag{6}$$

where the process noise vector has an expected value of zero and a covariance matrix Q. The process noises and the measurement noises are assumed to be uncorrelated. Summarizing mathematically, we have

$$E\{w_k\} = 0 \tag{7}$$

$$E\{w_j w_k^T\} = Q \tag{8}$$

$$E\{v_k\} = 0 \tag{9}$$

$$E\{v_j v_k^T\} = R \tag{10}$$

$$E\{w_j v_k^T\} = 0 \quad \text{for all } j \text{ and } k \tag{11}$$

$$E\{x_o\} = \hat{x}_o \tag{12}$$

$$E\{(x_o - \hat{x}_o)(x_o - \hat{x}_o)^T\} = P_o = P_o(-) \tag{13}$$

The prior estimates $\hat{x}_o$ and $P_o(-)$ are assumed to be available. With this model, the prediction equations are

$$\hat{x}_{k+1}(-) = \hat{x}_k(+) \tag{14}$$

$$P_{k+1}(-) = P_k(+) + Q_k \tag{15}$$

Equations (3), (4), (5), (14), and (15) constitute the QSS estimator.

Let us now introduce the special features of a process network. First consider material flows only. The constraining equations are

$$A\,x = 0 \tag{16}$$

where x takes on the special significance of material flow rates. Following a similar development reported earlier (Mah et al., 1976) we now partition A and x such that A_1 and x^1 are the incidence matrix of and materiai flows in the tree arcs of the process graph, and A_2 and x^2 are their counterparts in the chords of the process graph. Then, A_1^{-1} always exists (Mah and Shacham, 1977), and

$$x^1 = -\,A_1^{-1} A_2\, x^2 \tag{17}$$

Hence, Equations (6) and (2) may be modified to read

$$x^2_{k+1} = x^2_k + w_k \tag{18}$$

and

$$Z_k = H_k^*\, x_k^2 + v_k \tag{19}$$

where

$$H_k^* = H\begin{bmatrix} -A_1^{-1}A_2 \\ I \end{bmatrix} \tag{20}$$

For material and energy flows in a process network, we have the additional constraints

$$A\,y = 0 \tag{21}^*$$

where the column vector of energy flow rates is related to x through the enthalpies h_i according to the equation

$$y_i = h_i x_i \tag{22}$$

In this case, the constraints will be nonlinear, and a process of linearization must be applied. Let the generalized nonlinear constraints be

$$g(x) = 0 \tag{23}$$

and let

$$G = \frac{\partial g}{\partial x} \tag{24}$$

Then, the linearized constraints based on estimates $\hat{x}$ are

$$G(\hat{x})x = G(\hat{x})\,\hat{x} - g(\hat{x}) \tag{25}$$

As before, we partition G and x so that G_1 is a regular square matrix, and we obtain in place of Equations (17), (19), and (20)

$$x^1 = a(\hat{x}) + B(\hat{x})x^2 \tag{26}$$

$$z = H^*(\hat{x})x^2 + b(\hat{x}) + v \tag{27}$$

$$H^*(\hat{x}) = H\begin{bmatrix} B(\hat{x}) \\ I \end{bmatrix} \tag{28}$$

where

$$a(\hat{x}) = G_1^{-1}(\hat{x})[G(\hat{x})\hat{x} - (\hat{x})] \tag{29}$$

$$b(\hat{x}) = H\begin{bmatrix} a(\hat{x}) \\ 0 \end{bmatrix} \tag{30}$$

$$B(\hat{x}) = -\,G_1^{-1}(\hat{x})G_2(\hat{x}) \tag{31}$$

With the additional simplifications of constant R and Q, the equations for the QSS estimator now becomes

$$P_k(-) = P_{k-1}(+) + Q \tag{32}$$

$$K_k = P_k(-)H^{*T}_{k-1}\,[H^*_{k-1}P_k(-)H^{*T}_{k-1} + R]^{-1} \tag{33}$$

$$P_k(+) = (I - K_k H^*_{k-1})P_k(-) \tag{34}$$

$$\hat{x}^2_k(-) = \hat{x}^2_{k-1}(-) + K_k(z_k - H^*_{k-1}\hat{x}^2_{k-1}(-) - b_{k-1}) \tag{35}$$

$$\hat{x}_k^1(-) = a_{k-1} + B_{k-1}\hat{x}_k^2(-) \tag{36}$$

SIMULATION EXPERIMENTS

The estimator described by Equations (32) to (36) was implemented on a computer, and its behavior was studied by means of computer simulation to answer the following questions: What magnitude can we expect of the error re-

* If pure energy flows are present, the incidence matrix A in Equation (21) should be augmented to include these arcs.

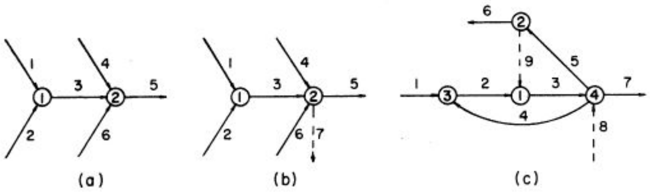

Fig. 3. Typical segments of process networks.

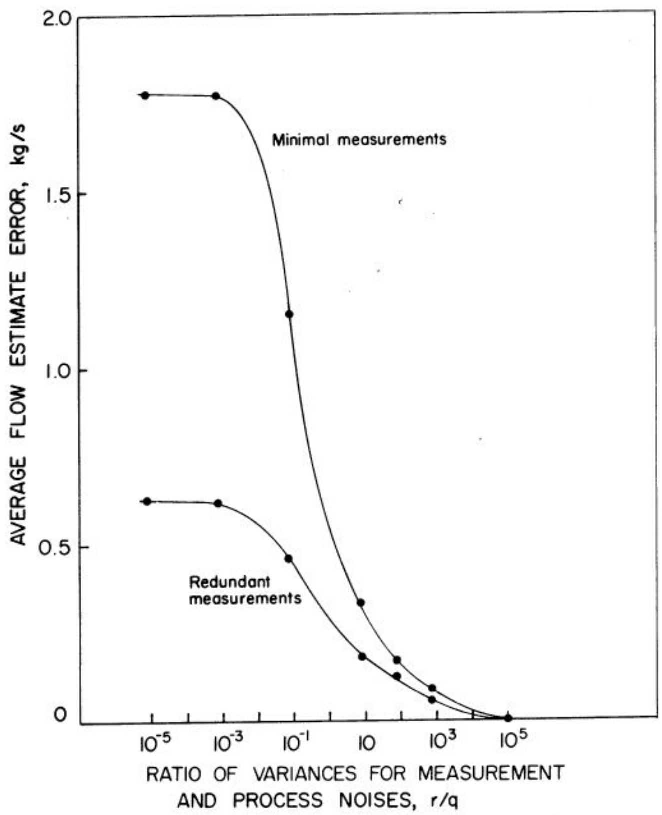

Fig. 4. Errors in flow estimates for blending network.

TABLE 1. TRUE FLOW RATES FOR THE BLENDING NETWORK

Ars	1	2	3	4	5	6
Flow, kg/s	10	10	20	30	70	20

duction? What is the relative importance of spatial and temporal redundancies? Can the estimator be tuned to respond satisfactorily to sudden changes without being unstable? What are the effects of systematic errors? Can we obtain meaningful estimates of parameters such as heat transfer coefficients and measurement bias in addition to the state variables using the same process data? The results of these experiments will now be presented and discussed.

Tuning for Steady State Error and Step Change

In all our experiments, the process noise covariance matrix **Q** was treated as a filter design parameter and chosen to be diagonal for simplicity and ease of computation. The measurement noise covariance matrix **R** was assumed to be diagonal, since it seemed reasonable to assume that measurement noises due to different instruments were uncorrelated. The variances of temperature measurements were each taken as a constant fraction of the true temperature, and the variances of flow measurements were each taken as a constant fraction (0.05) of the true flow rate. That is, if the flow rate were 10 kg/s, the variance would be 0.5 kg^2/s^2 and the standard deviation $\sqrt{0.5}$ kg/s. Preliminary experiments indicated negligible differences in filter performance with the ratio of these two fractions varying between 1 and 10. For each simulation, the same ratio of measurement variance to process variance was maintained for all temperatures and flows. This ratio *r/q* was used to tune the filter, as in Hamilton et al. (1973).

The parameter *r/q* may be thought of as a memory length for the filter. A large value of *r/q* indicates a high level of measurement noise, and hence past data are weighted heavily. A low *r/q* ratio, on the other hand, is an indication that the measurement noise is low and that past data are ignored. Alternatively, *r/q* may be interpreted as a measure of the contribution of temporal redundancy to data enhancement. More belief is placed on past data and temporal redundancy when a high value of *r/q* is selected.

The impact of this ratio on estimator behavior was investigated in the experiments performed on the blending network shown in Figure 3a. The results are summarized as a plot of the average error vs. the *r/q* ratio shown in Figure 4 with the true conditions shown in Table 1. It should be noted that in this and all subsequent discussions the errors reported are root-mean-squares averages over all streams, averaged over time. Usually the averages smooth out after twenty time steps.

In this series of experiments, only material flows are measured and estimated. The upper curve in Figure 4 corresponds to a system with no spatial redundancy: Flows 1, 2, 5 and 6 are measured. The measured values are smoothed over time, and the unmeasured values are computed by the estimator. By contrast, all six flows are measured, and both spatial and temporal redundancies are present in the lower curve. The limiting case as *r/q* approaches zero corresponds to repeated application of steady state reconciliation with no carry-over of information from one time instant to the next. Comparison of the two curves shows that spatial redundancy reduces the average error by approximately 66%. As *r/q* increases, temporal redundancy plays a more important role in error reduction. When the ratio is very large, the absolute magnitude of improvement due to spatial redundancy becomes less significant. However, there is always a relative improvement of at least 30 % between the two cases.

Unfortunately, *r/q* cannot be chosen arbitrarily large because the filter would then be far too sluggish to respond to any process changes, and the assumption of steady state conditions does not hold over long time periods. To obtain greater accuracy at constant conditions, this ratio should be chosen as large as possible subject to the requirement that the filter response to a step change in process conditions be completed in some given time. Based on the observed refinery behavior, it was decided that the step response should be completed in 1 hr. Assuming that the filter would be applied once every 5 min on time averaged data, it was tuned to complete its step response in approximately twelve time steps. This behavior was obtained using an *r/q* ratio of 10 which is the value used in all subsequent experiments.

To determine whether the filter would track all reasonable changes in process conditions without diverging, the filter was subject to more than twenty extremely severe step tests with flow rate changes of up to 400% and temperature changes up to 105^0K. No instability was observed for filters estimating flows and temperatures. Instability was occasionally observed when parameter estimation was also attempted. As these step changes are far more severe than one might expect to encounter in a real system, the results give every indication that the filter will be stable.

Table 2. True Process Conditions for the Blending Network

Case 1

Arc	Enthalpy $h \times 10^{-5}$, J/kg	Temperature T, °K	Energy flow $y \times 10^{-6}$, W
1	2.3239	329	2.3239
2	6.9717	440	6.9717
3	4.6478	384	9.2956
4	2.3239	329	6.9717
5	3.0211	345	2.1148
6	2.4401	331	4.8802
7	—	—	—

Case 2

Arc	Enthalpy $h \times 10^{-5}$, J/kg	Temperature T, °K	Energy flow $y \times 10^{-6}$, W
1	2.3239	329	2.3239
2	6.9717	440	6.9717
3	4.6478	384	9.2956
4	2.3239	329	6.9717
5	2.9049	340	20.3342
6	2.4401	331	4.8802
7	—	—	0.8137

Case 3

Arc	Enthalpy $h \times 10^{-5}$, J/kg	Temperature T, °K	Energy flow $y \times 10^{-6}$, W
1	2.3239	329	2.3239
2	6.9717	440	6.9717
3	4.6478	384	9.2956
4	2.3239	329	6.9717
5	2.7887	340	19.5208
6	2.4401	331	4.8802
7	—	—	1.6267

Case 4

Arc	Enthalpy $h \times 10^{-5}$, J/kg	Temperature T, °K	Energy flow $y \times 10^{-6}$, W
1	2.3239	329	2.3239
2	6.9717	440	6.9717
3	4.6478	384	9.2956
4	2.3239	329	6.9717
5	2.5563	334	17.8941
6	2.4401	331	4.8802
7	—	—	3.2535

One modification to the filter for nonlinear constraints may be noted here. During rapid transitions it was found that the constraints were not always satisfied by the estimates. To decrease the error caused by linearization about incorrect estimates, extra iterations were performed using the most recent set of measurements with relinearization after each step. The modified procedure was found to work satisfactorily.

The conclusions drawn from the above experiments were confirmed on the more extensive crude preheat network. As shown in Figure 2, there are twenty state variables and twenty-five measurements in this problem. Flow and temperature measurement errors were generated from rectangular distributions with maximum errors of ±10% and ±0.5% (of the absolute temperature), respectively. The average estimation errors in temperature, mass, and energy flows were 0.94°K, 6.75 kg/s, and 151 kW, respectively. If T_1, T_4, and T_{10} and x_6, x_{10}, x_{13}, and x_{16} were also measured, these errors could be further reduced to 0.61°K, 3.28 kg/s, and 136 kW.

Effects of Systematic Errors

The performance of QSS estimator in the presence of systematic errors was investigated in the next set of experiments. Systematic errors in this context include unsuspected material and energy leaks, measurement biases, and errors in enthalpy correlations. In order to make the effects more apparent, measurement noise was reduced to very low levels (maximum errors of ±0.5% for flows and ±0.025% for absolute temperatures). In practice such reductions may be achieved by "prefiltering" or averaging measurements over time between filter iterations.

To study the effects of an unsuspected leak, we applied a QSS estimator based on the process graph shown in Figure 3a to the process graph shown in Figure *3b*. The extra arc (arc 7) in the latter represents a heat leak to the environment. The true conditions for this problem are given in Tables 1 and 2. The resulting errors in temperature estimates are plotted against heat loss in Figure *5*. As before, the upper curve represents estimation with no spatial redundancy, while the lower curve corresponds to full measurements and redundancy. Substantial error reduction is again obtained with the exploitation of spatial redundancy.

The effects of measurement biases were studied using the recycle network shown in Figure 3c. The presence of measurement bias was simulated by adding a bias vector to the simulated measurement vector **z**. The bias vector was chosen to be either a multiple of the alternating sign vector (1, -1, 1, -1, …) or the one sign vector (1, 1, 1, 1, …). These bias distributions were purposely chosen to exhibit the contrast in filter behavior. The true conditions for the recycle network are given in Table 3.

As before, comparisons were made for the minimal and redundant measurement cases. The measurement vectors

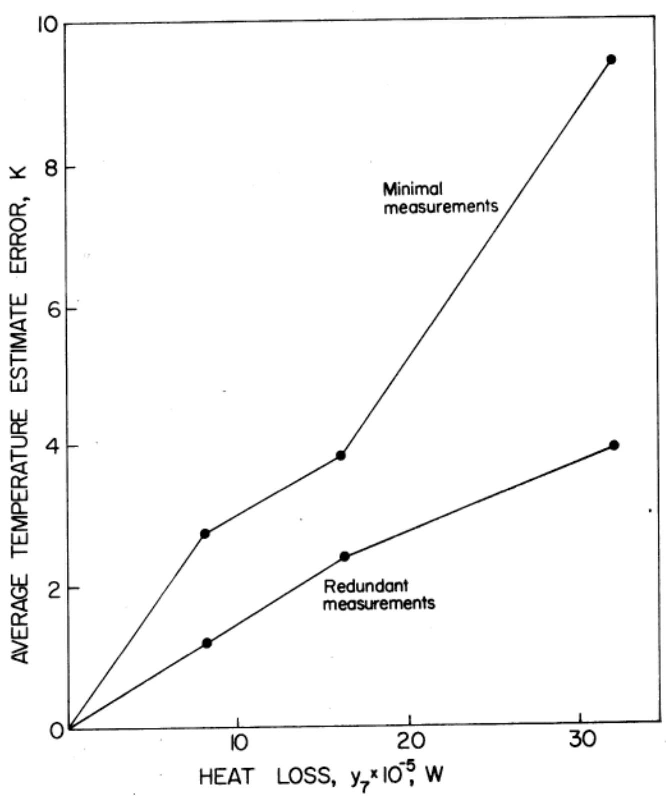

Fig. 5. Errors in temperature estimates for blending network with heat leak.

Table 3. True Process Conditions for the Recycle Network

Arc	1	2	3	4	5	6	7	8	9
Material flow, kg/s	99.982	149.97	149.97	49.99	60.03	60.03	39.95	—	—
Energy flow × 10^{-6}, W	—	—		—	—	—	—	13.0349	5.2793
Temperature, °K	328.58	356.72	373.06	409.27	427.34	389.34	389.94	—	—

for these two cases were (x_1, T_1, x_2, T_2, T_3, x_5, T_5, T_7) and (x_1, T_1, x_2, T_2, x_3, T_3, x_4, T_4, x_5, T_5, x_6, T_6, x_7, T_7), and the alternating sign bias vectors were taken to be multiples of (1, 1, -1, -1, 1, -1, -1, 1) and (1, 1, -1, -1, 1,1, -1, -1, 1, 1, -1, -1, 1, 1), respectively, the basic unit of bias perturbation being 7.94 kg/s for a flow measurement and 1.8^0K for a temperature measurement. The errors in temperature and flow estimates are plotted against the maximum bias errors in Figures 6 and 7, respectively.

For the alternating sign biases, the estimation errors were reduced substantially in both cases with the introduction of spatial redundancy. For the one sign biases, improvement was obtained only in temperature estimates; the flow estimates were actually degraded. In interpreting this apparent anomaly, it should be remembered that the filter attempts to minimize all forms of errors. In this case, the temperature estimates were apparently improved at the expense of flow estimates when spatial redundancy was introduced.

Further analysis of results revealed that the error reduction in the case of alternating sign biases was, to a large measure, attributable to cancellations (Stanley, 1977). The improvement obtainable with spatial redundancy depends strongly on the distribution of the biases. For linear or linearized constraints, Equation (16), the biases are corrected only if the bias vector is not orthogonal to the row space of **A**.

Systematic errors can also be introduced into the estimation procedure through biases in the measurement matrix. This situation was simulated in our analysis by errors in enthalpy correlations. For petroleum liquids, the enthalpy h is correlated with temperature T and density ρ as follows:

$$h = (c_1 + c_2T + c_3T^2)/\sqrt{\rho} \qquad (37)$$

Alternating sign biases or one sign biases were introduced into the densities, and the filter behavior was studied. The results are summarized in Figure 8.

With the alternating sign biases, large errors are incurred in the temperature estimates, but redundant measurements offer a very significant improvement. When the enthalpy errors are one sided, all energy flows are scaled in the same direction [see Equations (21) and (22)]. Consequently, the errors in temperature estimates are small regardless of the number of measurements. But even in this case, filter with spatial redundancy gives superior performance.

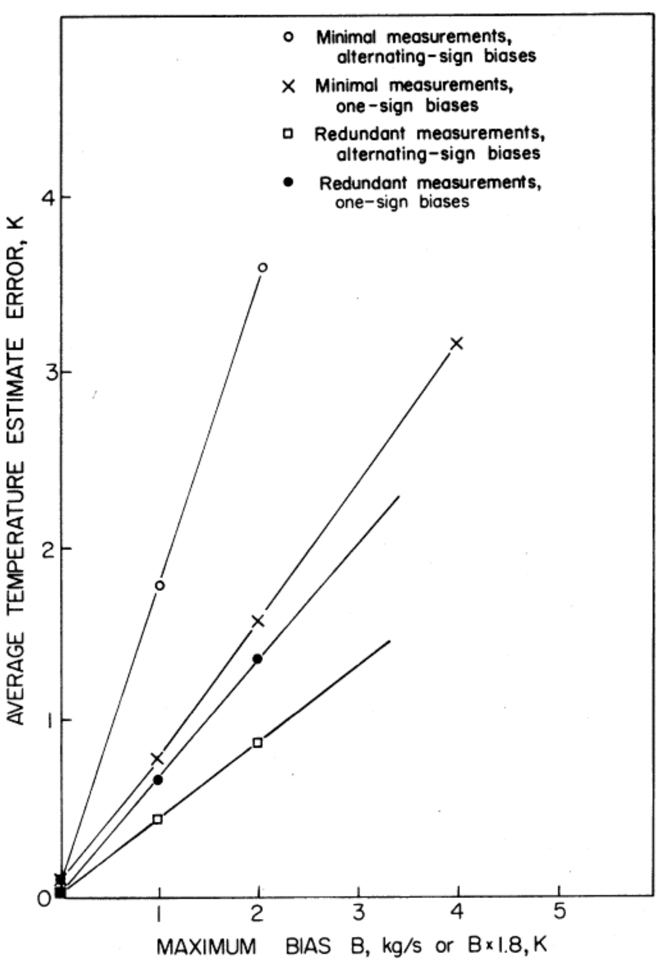

Fig. 6. Errors in temperature estimates for recycle network with measurement bias.

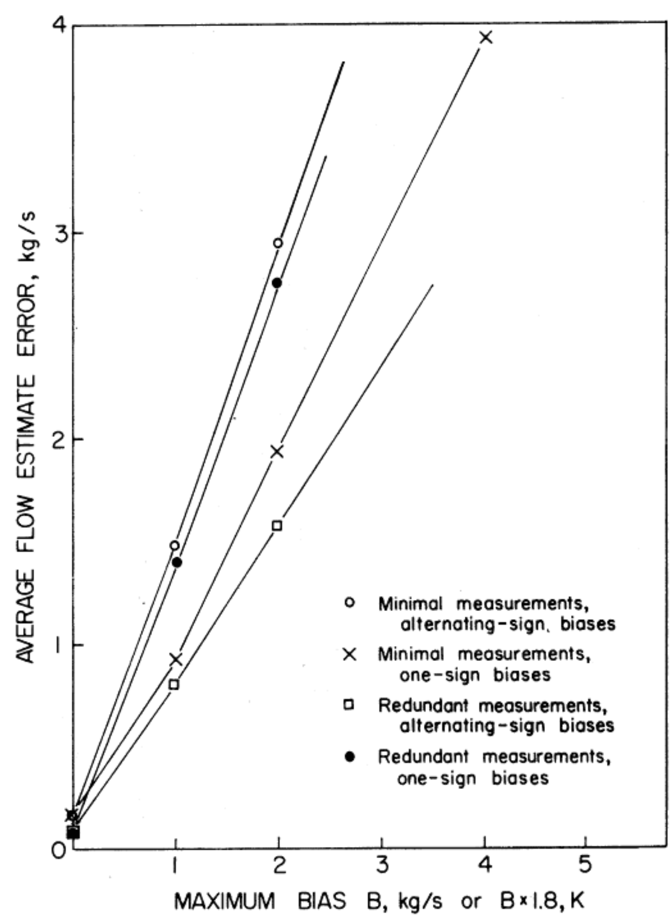

Fig. 7. Errors in flow estimates for recycle network with measurement bias.

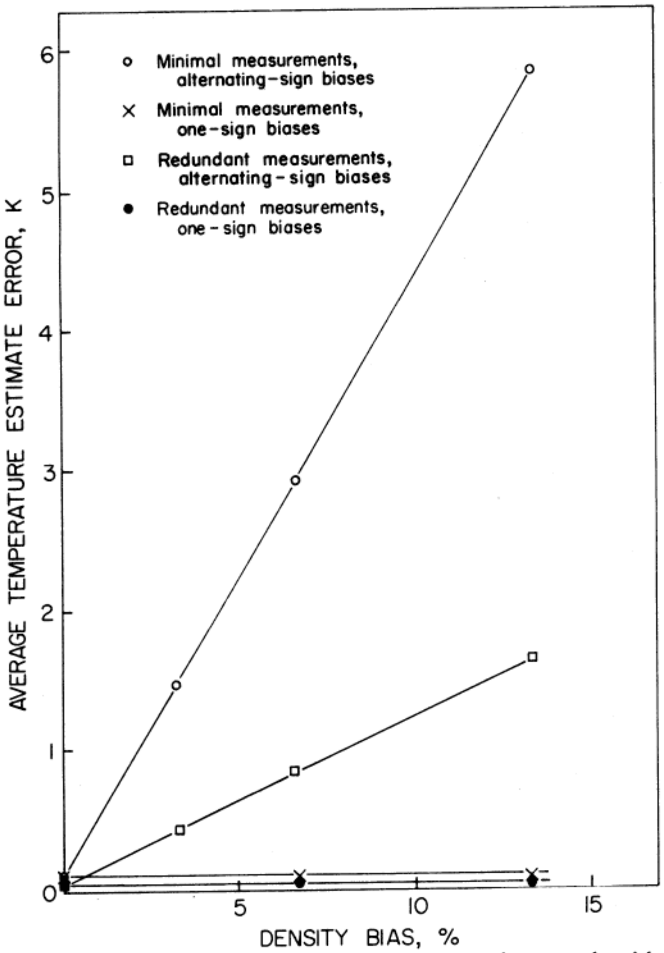

Fig. 8. Errors in temperature estimates for recycle network with density bias.

Simultaneous Estimation of States and Parameters

The utility of adaptive parameter estimation was explored in the final set of experiments. The parameters studied were split fractions (valve positions), heat transfer coefficients, and measurement biases. These parameters were incorporated as new state variables, and their process noise variances were set at one to seven orders of magnitude smaller than the variances for flows and temperatures, constraining the parameter values to change much more gradually than the flows and temperatures.

It should be noted that the introduction of the parameters does not always lead to an increase in the number of state variables. Consider the subnetwork involving nodes 1 and 2 in Figure 2. Normally, mass flows x_1, x_2, x_8 would be chosen as state variables by the filter. But when the split fraction α at node 2 is included as a state variable, x_8 is dropped as a state variable, since it may be computed in terms of measured variables $x_8 = \alpha(x_1 + x_2)$. Similarly, when heat transfer coefficients are estimated, there is no change in the number of state variables. Only in the case of bias estimation is the state vector augmented by the additional parameters.

The first simulation experiments in this series were performed on the recycle network in Figure 3c. The heat transfer coefficient for the exchanger (nodes 1 and 2) was estimated along with the two split fractions at node 4. It was found that the best parameter estimates were obtained with process noise variances set to 10^{-7} for split fractions and 5.27×10^{-5} for heat transfer coefficients. For the same runs, the process noise variances for flows and temperatures were set to 0.5% of their initial values. Our results show that the average flow estimates were degraded by 12% and the average temperature estimates by 3% as a result of incorporating these three parameters in the estimation schemes. Despite repeated attempts with different flow networks, no filter with parameter estimation was ever found to yield superior estimates than a filter without parameter estimation and, at the same time, to respond satisfactorily to step changes.

Finally, we shall consider the estimation of measurement biases. In the absence of any prior information, there is no rational basis for predesignating any subset of measurements with biases. When all biases were estimated, flow estimate error was increased by 17 to 67% and temperature estimate error by up to 46% as compared with the base case of no bias estimation. Significantly, the worst errors with bias estimation occurred when a measurement bias was actually present. The basic difficulty with bias estimation is that with the increase in the number of variables, multiple solutions are possible. In every case that we have tested, the filter converged to incorrect steady state estimates. The problem of multiple solution was also noted by Goldmann and Sargent (1971).

Computational Requirements

The simulation experiments described above were carried out on a CDC 6400 computer. The program consists of an estimator generator and a process simulator. The former constructs a QSS estimator based on the process network structure, assigned values of filter parameters, and initial guesses of variables, and the latter supplies the simulated process measurements, including the prescribed noise and bias.

As an indication of computational requirements, the crude preheat network (shown in Figure 2) required 1.35 CP (central processor) s/filter iteration, of which approximately 1 s was taken up by the filter gain matrix calculation (inversion and linearization). Thus, discounting the time required for input, output, and initialization and assuming that the filter is applied once every s mm, a total of 16 CP s/hr are needed for on-line estimation of temperatures and flows in such a network.

The filter and data storage occupied approximately 15 000 words. Of these, 1 500 words were required for initialization, 3 600 words for the filter, 3 000 words for library subroutines, and the remainder for variable storage. The process simulator which took up an additional 13 000 words will, of course, be replaced by data sensor input in a real process application. Thus, even allowing for the shorter word length of a typical process computer, the computing time and storage requirements are well within the capabilities of such computers.

Further details of the simulation experiments and their implementation may be found elsewhere (Stanley, 1977).

CLOSING REMARKS

Hitherto, one of the major limitations of applying Kalman filters to industrial processes is the uncertainty in process models. Flow and temperature estimation in a process network appears to be one application of major industrial significance, in which the model validity is not in question, since only conservation relationships are invoked. Our investigation has shown how the Kalman filter may be adapted to take advantage of both spatial and temporal redundancies in a QSS process. The estimator can be tuned to follow sudden changes in process conditions in a satisfactory manner and, at the same time, reduce estimation errors by up to 70%. In almost all instances studied, spatial redundancy contributes significantly to the overall error reduction. The estimator is reasonably effective with isolated systematic errors, but indiscriminant inclusion of bias estimation is not recommended. Simultaneous estimation of split fractions, heat transfer coefficients, and state variables appears to offer no special advantage in improving the estimates. Of great practical significance are the computational requirements of the QSS estimator. For a typical process network, these requirements can easily be accommodated on a current process computer.

In this paper we have assumed that a one-to-one functional relationship exists between the temperature and the enthalpy of a fluid stream, although the functional relationship need not be limited to the form shown in Equation (37). This assumption is generally not very restrictive, since it allows streams to be gas, liquid, or two-phase mixtures of two or more components. However, it does preclude the two-phase stream of a single component. One way of bypassing this difficulty is to eliminate such a stream from the estimation scheme by merging its two adjacent nodes. But to remove this restriction otherwise will clearly require an extension of state and measurement vectors.

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NOTATION

$\mathbf{A}$ = a node-arc incidence matrix
$\mathbf{A}_1, \mathbf{A}_2$ = partitions of incidence matrix $\mathbf{A}$ corresponding to tree arcs and chords of a process graph
$\mathbf{a}(\hat{\mathbf{x}})$ = vector defined by Equation (29)
$\mathbf{B}(\hat{\mathbf{x}})$ = matrix defined by Equation (31)
$\mathbf{b}(\hat{\mathbf{x}})$ = vector defined by Equation (30)
c_1, c_2, c_3 = constants in the enthalpy correlation given by Equation (37)
$\mathbf{G}$ = $\partial \mathbf{g}/\partial \mathbf{x}$
$\mathbf{G}_1, \mathbf{G}_2$ = partitions of $\mathbf{G}$ such that $\mathbf{G}_1$ is a regular square matrix
$\mathbf{g}(\mathbf{x})$ = nonlinear constraints
$\mathbf{H}$ = measurement matrix
$\mathbf{H}_k$ = measurement matrix at time t_k
h_i = enthalpy per unit mass for stream i, J/kg
$\mathbf{I}$ = identity matrix
$\mathbf{K}$ = gain matrix for Kalman filter
$\mathbf{K}_k$ = gain matrix for Kalman filter at time t_k
l = number of measured variables
n = number of state variables
$\mathbf{P}_k(+)$ = the error covariance matrix immediately after a discrete measurement at time t_k
$\mathbf{P}_k(-)$ = the error covariance matrix immediately before a discrete measurement at time t_k
$\mathbf{Q}$ = process noise covariance matrix
$\mathbf{R}$ = measurement noise covariance matrix
r/q = numerical ratio of variances for measurement and process noises, i.e. ratio of the diagonal elements r_i of $\mathbf{R}$ and q_i of $\mathbf{Q}$. Since the same ratio applies to all corresponding elements in each simulation $r_i/q_i = r/q$
T = temperature, °K
t_k = time at which the k^{th} measurement is taken, s
$\mathbf{v}$ = measurement noise vector
$\mathbf{v}_k$ = measurement noise vector at time t_k
$\mathbf{w}_k$ = process noise vector at time t_k
$\mathbf{x}$ = vector of true values of state variables at steady state
$\mathbf{x}^1, \mathbf{x}^2$ = partitions of state vector $\mathbf{x}$ corresponding to the tree arcs and chords of a process graph, respectively
$\mathbf{x}_k$ = vector of state variables at time t_k
$\hat{\mathbf{x}}_k$ = estimates of state variables at time t_k
$\hat{\mathbf{x}}_k(+)$ = estimates of state variables immediately after a discrete measurement at time t_k
$\hat{\mathbf{x}}_k(-)$ = estimates of state variables immediately before a discrete measurement at time t_k
$\mathbf{y}$ = vector of true values of energy flows y_i at steady state, W
y_i = energy flow in stream (arc) i, W
$\mathbf{z}_k$ = vector of measurements taken at time t_k
α = split fraction
ρ = density
ξ_i = the weighting factor in exponential filter

Subscripts

o = prior estimate

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