ONLINE DATA RECONCILIATION FOR PROCESS CONTROL

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ABSTRACT

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Combined data reconciliation with estimation of slowly changing parameters has been implemented for closed-loop control in a Chemical Plant. Goals include streamlining use of redundant measurements for backing up failed instruments, filtering noise, and, in some cases, reducing steady state estimation errors. Special considerations include bumpless transfer from failed instruments and automatic equipment up/down classification. Parameters are calculated and filtered, then held fixed during each data reconciliation.

INTRODUCTION

The purposes of this paper are to clarify the nature of the online estimation problem, and provide a “tool kit” for practical online data reconciliation applications. In this paper, “online” data reconciliation implies use in closed-loop control or optimization. It will be seen that there are different considerations in using data reconciliation in a process control environment than when doing typical offline applications like adjusting pilot plant or lab data. The necessary tools presented here include new techniques, extensions of previous work, ideas adapted from process control, and different philosophies for applying existing algorithms. It is also hoped that this paper will demonstrate some common ground for practitioners of process control and data reconciliation. It is written from the standpoint of the practicing process control engineer. As a result, there is an emphasis on small applications of data reconciliation, easy to use techniques, practical problems, and a heavy use of ideas from process control.

This paper was written following the implementation of online data reconciliation in a process plant. It was recognized that the existing literature did not address all the concerns adequately, and that some new tools had been developed. The new tools include equipment up/down indicators, dynamic reconciliation, cascade estimation, and a new approach to bias estimation. Also, it was difficult to find a summary of other existing tools that might be relevant. This paper is an attempt to fill the gap by summarizing both new and existing tools.

A brief summary of the contents of this paper follows.

Following a brief review of data reconciliation, the paper starts with a discussion of the special needs for process control and online optimization. The needs discussed include forcing flows to zero for equipment that is shut down, handling instrument failure and out-of-range problems, recognition that noise at different frequencies should be handled differently (including estimation of slowly-changing process parameters and handling instrument bias), dealing with process dynamics, and recognition that in some cases steady state estimation errors are acceptable.

One of the first needs addressed in this paper is forcing flow estimates to zero when a part of a unit is shut down. The new technique of using up/down status indicators, and classifying this status automatically, is introduced to solve this problem.

Next, some practical details of implementing online data reconciliation are discussed. After some general comments on the selection of model equations, specification of measurement variances, propagation of variance, and processing interval for data reconciliation, the section discusses preprocessing of data, the actual data reconciliation, and some comments on how the reconciled data is used. Preprocessing of the data includes filtering and checking for instrument failure. In discussing the data reconciliation, several examples are introduced, and the sequential estimation approach is demonstrated. In using the data, potential pitfalls such as loss of true process feedback are brought out.

For online estimation, process dynamics are a major consideration. This is examined next. Three approaches are considered: Smoothing over a multiple time period model, ignoring process dynamics in the estimator, and the new technique called dynamic reconciliation.

Finally, the paper considers the problem of quasi-steady state variables. These are slowly changing variables such as instrument bias. The paper reviews the random walk model for these variables, and introduces the new technique called “cascade estimation” for these variables.

The appendix provides summaries of existing concepts needed for online data reconciliation. This includes a review of data reconciliation, the concepts of observability and redundancy, some simple extensions of data reconciliation to dynamic systems, and concepts from Kalman filtering and the related topics of random walk and quasi-steady state systems.

The remainder of this introduction is a brief overview of data reconciliation.

Data reconciliation is used to obtain the “best” estimates of variables in a system, given a set of noisy measurements and a set of constraints (equations) that apply to that system. The constraints do not need to be a complete simulation model; frequently they are simple overall mass and energy balances.

The usual data reconciliation approach is constrained least-squares estimation, resulting in a linear estimator, with direct extensions to nonlinear problems by linearization. The first chemical engineering application was reported by Kuehn and Davidson (1961). For some extensions and other references, see, for example, Stanley and Mah (1976, 1977), and the survey by Mah (1981).

A review of data reconciliation is given in Appendix I. This includes comments on the types of noise usually found in chemical processes, the fundamental statistical property of variance, the general least-squares estimation problem and some solutions, some very simple special cases, and a simple example with two measurements. The behavior of the estimate assuming continuous application of data reconciliation is shown for some assumed measurement values over time.

The usual benefits cited for data reconciliation are that better steady state estimates can be obtained, and that these estimates are consistent with the steady state constraints which model the system. It will turn out that for online data reconciliation we sometimes sacrifice these objectives for others. Online objectives include formalizing and simplifying the handling of instrument failure or saturation, attenuating noise at certain frequencies, and detecting changes in variables rather than estimating absolute values. These goals are different than those for accounting, pilot plant work, and other conventional applications.

There are always some “byproduct” benefits associated with using data reconciliation. These include a forced formalization of judgment on instrument quality, and an improved understanding of the process. Associated with the data reconciliation effort, there is usually a concurrent checking of mass and energy balances to detect instrument problems and plant problems or losses.

Several other important topics are associated with the literature on data reconciliation. These topics, which are observability, redundancy, and gross error handling, are reviewed next. Methods for dealing with these topics should be part of the engineer's "tool kit".

In analyzing the behavior of a data reconciliation scheme, the concepts of observability and redundancy are useful. Loosely speaking, a variable is observable if it can be estimated using available measurements and the process model. A measurement is redundant if it could be deleted, but the variable would still be observable; that is, it could still be calculated using other measurements and the process model. Both observability and redundancy are properties related to the information available in a system (model and measurements), independent of any estimation technique. These properties depend only on the measurements available and the model chosen. Some common examples in process plants are given in Appendix II. As is shown in several of the examples, even within one system some measurements might be redundant while others are not.

An in-depth study of redundancy (and the related property of observability) and its impact on estimation is available (Stanley and Mah, 1981A). For the special case of flow networks with mass and energy balances, redundancy (and observability) can be determined directly from the process structure (Stanley and Mah, 1981B).

Observability and redundancy are crucial to practical least-squares estimation due to the presence of instrument failure. If a variable is unobservable, no meaningful estimate will be obtained, and also numerical difficulties may arise. Redundancy is needed for data reconciliation to provide better estimates, and is also essential if variables must remain observable even in the case of instrument failure. It will be seen later that data reconciliation automatically exploits redundancy, using backup instrumentation when primary instruments fail.

Another problem has been addressed in the data reconciliation literature: the "gross error" problem, usually due to instrument failure. Instrument failure is a major problem for closed loop control, optimization and estimation. The larger the number of measurements involved, the more likely it is that at least one of them will fail. This has been an inhibiting factor in the practical application of multivariable control schemes and online optimization.

There are two aspects to the gross error problem: detecting the error and correcting for it. A variety of procedures available for detecting gross errors are summarized in the survey paper by Mah (1981). Detection and subsequent correction are important because a gross error completely violates the normal statistical assumptions. If an attempt is made to use the measurement, the gross error is "smeared" over all the estimates. Thus, contrary to a popular misconception, it is impossible to determine the original source of the error by simply examining the magnitudes of measurement "adjustments" (Merrill and Schweppe, 1971; Ripps, 1965).

SPECIAL NEEDS FOR PROCESS CONTROL AND ONLINE OPTIMIZATION

When would it be desirable to implement data reconciliation and related tools online for process control and optimization? How do these tools need to be modified? To answer these questions, it is necessary to review data reconciliation and review special needs encountered in online applications. It will be seen that data reconciliation provides a convenient tool for addressing some process control problems. In this section of the paper, we discuss online considerations such as forcing flow estimates to zero for equipment that is shut down, handling instrument failure and out-of-range problems, recognizing that noise at different frequencies should be handled differently (including estimation of slowly-changing process parameters and handling instrument bias), dealing with process dynamics, and recognizing the cases where steady state estimation errors are acceptable.

One of the first problems encountered in our application of online data reconciliation occurred when a piece of equipment was shut down--one of two parallel towers. The problem was that the associated flow meters did not read zero. In these cases, since the flow is known to be zero, it is undesirable to either use the erroneous measurement or allow any adjustment away from zero. This problem is less likely to occur with offline reconciliation, where the true plant structure is fixed or at least well documented. This problem will be resolved for online systems using automatic equipment up/down indicators (to be described).

Instrument failure is a major problem for closed loop estimation, control and optimization. This “gross error” problem is more severe in online than offline cases, since bad estimates in a control or optimization scheme may drive the plant to an unsafe condition. Correct, timely human intervention is more likely in the offline case than the online case.

A closely related problem is the case of an instrument going out-of-range, that is, when an instrument reaches its maximum or minimum value. In addition to being caused by unusual operating conditions, this can also occur by design. For instance, sometimes two flow meters are installed in the same line, one to accurately measure low flow rates, and one for high flow rates. At high flow rates, the low-range meter cannot be used. For all practical purposes, an out-of-range instrument can be considered “failed”.

Ideally, when an instrument is declared invalid (due to failure or going out of range), we would like to continue control or optimization using other instruments to calculate a value for the failed instrument. This can very quickly become cumbersome when using ad-hoc procedures for each possible single or multiple failure. The complex logic becomes difficult to correctly determine, and results in computer code which is difficult to write, debug, or update when there are changes. It will be seen that data reconciliation provides an ideal, systematic procedure for accommodating instrument failure. In fact, this is a major incentive for data reconciliation.

Another problem with an instrument failing or going out of range is “bumpless transfer” to the backup instrumentation. Since measurements never agree, suddenly substituting an alternate or calculated value for a measured one frequently results in a large jump in the estimate of that variable. This causes an undesirable plant upset when the controller or optimizer responds to the apparent change. As will be discussed later, data reconciliation cannot be directly applied because of this problem. However, a modified algorithm will allow bumpless transfer.

In addition to instrument failure, the next major topic we address is the importance of frequency domain considerations. Full consideration should be given to the source and impact of noise at all frequencies. This approach is generally ignored in the data reconciliation literature. A summary of some noise sources is given in Appendix I, mainly characterized in terms of frequencies. Some analog and simple digital filtering is usually useful to handle the higher frequency noise prior to using techniques such as data reconciliation. Consideration must be given to aliasing (high frequency noise appearing as low frequency noise due to inadequate sampling rate).

The estimator needs to pass through frequencies at which the process is truly changing, and block out the others as much as possible. Also, phase lag or lead introduced by any estimator must be consistent with the needs of the controller or optimizer. A large lag in the input to a controller is equivalent to a large lag in the process, slowing down the overall response of the system. Excessive lead can also be a problem. In the examples later, it will be seen that estimators based on steady state models for plants with dynamics have a "feedforward" effect on some variables. Feedforward acting too early can be worse than none at all.

Gross errors are mainly a problem only at lower frequencies, in terms of their causes in the plant and their impacts on control schemes. In a properly designed system, there are relatively few failure modes that cause "spike" noises, for instance. More often, an instrument failure is permanent when it is abrupt, or it is a slow drift. One notable exception is in analyzers, where startling errors sometimes appear and disappear, sometimes due to sampling problems. These problems can sometimes be caught with rate-of-change detection schemes.

High frequency gross errors are simply filtered out by exponential filters. "One-time" gross errors rarely cause severe problems--a control scheme will typically "bump" the process once, then recover on the next control action. The process itself will filter out most of the effect. Also, most computer controls limit the rate of change of the manipulated variables, again limiting the impact of these noise spikes.

The low frequency errors such as instrument bias are difficult to deal with. Unfortunately, instrument bias is a very common problem. This can be constant, or there may be a slow drift. Simultaneous estimation of both process variables and some measurement biases requires special treatment (described later). Single "snapshots" of the process taken for standard data reconciliation do not provide adequate information for this--a recursive updating procedure is required.

In general, slowly-changing process parameters must be handled specially. Standard data reconciliation, working with variables averaged over a period long enough to handle the most slowly-changing parameters, is frequently not useful for online purposes. For example, some variables such as compositions in large tanks or other vessels may change only very slowly. Similarly, one flow may split into two flows based on unknown manual valve positions and piping geometry. The ratio of the flows may change only rarely, but cannot just be assumed at some fixed value. Estimates of variables affected by these slowly-changing variables may be needed very frequently for control purposes. These systems are called "quasi-steady state", and are discussed later.

One of the most obvious concerns in online systems is dealing with process dynamics. Why do we need to consider process dynamics? In a typical process, data reconciliation will involve inputs and outputs to a process unit. While the steady state balances do not reflect it, there is at least a lag and/or deadtime between the input and output, even in the simplest case. Some of these will be significant in the time scale chosen for control or optimization, raising questions about the validity of reconciliation.

A related factor for online data reconciliation applications is that the goals for an estimator for control and optimization purposes are sometimes different than in steady state cases. In many cases, a bias (low frequency) error may be acceptable. Instead of absolute accuracy, it may only be trend information ("middle" frequency) that is needed. For instance, consider online optimization by various direct search techniques. Using the values of the objective function obtained from recent "experiments", the optimizer estimates a gradient and continually moves the process toward an optimum. (The optimum point is probably also shifting slowly). As long as an estimator sees the incremental results from each experiment, the process can be optimized. More generally, any secondary controller in a cascade control system needs to respond to moderate-to-high frequency disturbances. A bias or other low-frequency error causes no harm to the control. For example, in a distillation tower with a product purity controlled by manipulating steam flow, purity will be maintained regardless of any bias error in the flow meter. The primary controller simply adjusts the steam control setpoint to the necessary, biased value. Suppose the purity target is in turn set by an overall plant optimizer. The bias error will cause no problem for optimization, as long as there is some form of feedback from the plant to the optimizer.

This contrasts with typical offline estimation applications, such as reconciling conflicting data for accounting purposes, or analyzing lab or pilot plant data. In those cases, only the steady state or low frequency information is useful. The higher frequencies are filtered out by averaging.

There are a host of practical concerns for online data reconciliation. For instance, there must be a straightforward operator and engineer interface that is easy to understand and troubleshoot. Furthermore, it must be easy for the operator to manually intervene and override any particular instrument. The operator will usually know when an instrument is about to be calibrated, and may wish to have the controls ignore that instrument.

There is an incentive to keep online estimation (and optimization) applications small. Operators and engineers alike are generally not comfortable with computer applications employing dozens of variables, because they are hard to understand and troubleshoot, and there is always something not working right in the plant. Many opportunities for small-scale applications (less than a dozen variables) are being missed because they are not “dramatic” enough. One advantage of small applications is that an undetected gross error will not be propagated very far. Another advantage is that process control computer capacity will not be overtaxed. Another advantage of small applications is their flexibility. Plant configuration changes will have a more limited impact on many small estimators, keeping maintenance easy. Small applications are “suboptimal” since they don’t use all possible measurements. However, this is usually a minor sacrifice. To keep things in perspective, remember that almost all process control is suboptimal also, relying mainly on single-loop and cascade controllers for feedback control.

Starting with the next section, we will demonstrate the impact of these process needs in applying and developing data reconciliation tools.

EQUIPMENT UP/DOWN INDICATORS

When pieces of equipment are shut down (e.g., one of two parallel towers), their flow meters frequently have nonzero readings. Since the flow is known to be zero, it is undesirable to either use the erroneous measurement or allow any adjustment away from zero. To accomplish this, the “measurement” should be forced to zero and its variance set to zero (or a very small number) in the usual data reconciliation. Using this method, no further specialized logic is required for various shutdown cases.

For equipment likely to be taken in and out of service, an equipment “up/down” indicator keeps track of the status (in or out of service). Prior to data reconciliation, these statuses are checked, and the inputs for data reconciliation are modified if necessary.

This indicator could be set as a manual entry by the plant operator, but that is usually impractical. Humans tend to either forget to make these entries (unless such an entry is a necessity for safe plant operation), or get mad when they are forced to do it. After all, computers should make their lives easier! There may be other more urgent tasks at hand. Any operator could deduce that the equipment was out of service, based on checking some key variables to see if they are in a normal range. The computer can do the same, using a very simple procedure.

To determine the up/down status, key variables are examined. Each is assigned “reasonableness” limits. If a variable is outside these limits, that is considered a “vote” for a shut down unit. Each variable generates one “vote” based on a comparison to its reasonableness limits, and the majority vote classifies whether the equipment is “ up “ or “ down

The more instruments that can fail, the more measurements that must be examined to avoid misclassification due to faulty instruments. In the case of Figure 1, T-1 and T-2 are two parallel reactor/towers. Each tower up/down classifier uses 6 variables: feed, steam, one of two water (reactant) flows, pressure, and two temperatures. The indicator, used to modify inputs to data reconciliation, avoids errors in a unit constraint control based on a calculated variable. In this case, several instruments could malfunction, but the correct up/down status would still be determined.

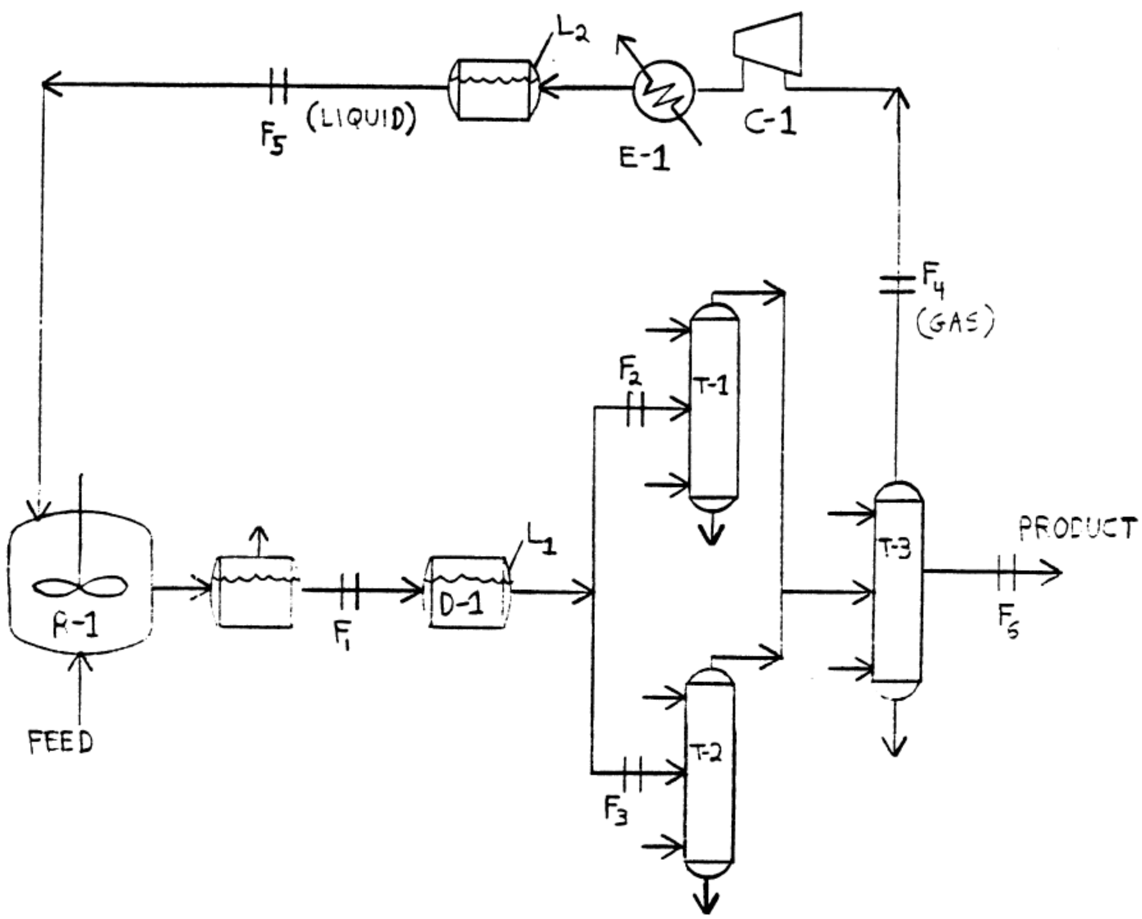


Figure 1. Simplified portion of Exxon Bayway Chemical Plant

Note that frequently the up/down indicator is based on instruments that are not involved in the data reconciliation, e.g., tower tray temperatures. By using this extra information available from the process (in a very nonlinear way), we are at times improving the accuracy of our standard linear estimator.

A common pitfall to be avoided in designing up/down classifiers is using multiple instruments with common failure modes. For instance, temperatures tied into a multiplexer may all read too high or too low due to a faulty A/D conversion or multiplexer chip, or a faulty cold reference junction. In this case, one hardware failure may cause many incorrect votes. In general, it is desirable to have the variables be as "independent" as possible. Also, calculated variables should be avoided, since they frequently go "bad" when the primary instruments fail.

SOME DETAILS OF PRACTICAL DATA RECONCILIATION IMPLEMENTATION

This section reviews some practical considerations in applying data reconciliation at Exxon's Bayway Chemical Plant in Linden, New Jersey. The emphasis in this section is on steady state reconciliation. After some general comments on the selection of model equations, specification of measurement variances, propagation of variance, and processing interval for data reconciliation, the section discusses preprocessing of data, the actual data reconciliation, and some comments on how the reconciled data is used. Preprocessing of the data includes filtering and checking for instrument failure. In discussing the data reconciliation, several examples are introduced, and the sequential estimation approach is demonstrated. In using the data, potential pitfalls such as loss of true process feedback are brought out.

Applications at Bayway use as few as two measurements to as many as 11 (plus variables for up/down indicators). All applications use only overall mass balances, along with the QSS equations to be discussed later. In general, it is recommended that only the simple mass, energy, and component balances be used, to avoid force-fitting to inaccurate models. These models are "parameter-free" and "non-predictive". Other models will frequently require parameter updating.

The data base includes not only each raw measurement and its adjusted, best estimate, but also its measurement noise variance and the variance of the estimated value. The measurement variance is specified by the engineer, and is regarded as a rough tuning parameter. "Rules of thumb" based on a percentage of instrument range are usually good enough, and no attempt is made to fine-tune these values (such an attempt is rarely worth the time spent). The variance of the estimates (adjusted values) is a byproduct of the data reconciliation. When calculated variables are used in place of actual measurements as inputs to data reconciliation, their variances are calculated using the standard propagation of variance equations (see Appendix I). Nonlinear equations are linearized whenever necessary.

The data reconciliations are done as often as required for the control or optimization programs which use the adjusted data as inputs. The cases that have arisen so far have been in control schemes that run once every minute, as in the process shown in Figure 1. A slower optimization scheme is also run on that process every two hours, using a search technique. It averages the same once-per-minute reconciled variables (using a least-squares curve fit) over a period prior to the end of the second hour.

The measurements go through several preprocessing steps prior to data reconciliation. They are filtered, for reasons such as eliminating as much high-frequency noise as possible. Checks are made for instruments out of service or in gross error, and equipment up/down statuses are checked. Measurements and their variances are modified as a result of these checks before being used in data reconciliation. Details of these preprocessing steps will now be described.

Filtering of the measurements is an important preprocessing step in online data reconciliation for two reasons: noise reduction and dealing with process dynamics. Simple analog and exponential or averaging filters are applied to measurements prior to data reconciliation. We approach the filtering problem from a frequency response viewpoint.

Higher-frequency noise is easily reduced in magnitude by simple analog and digital filters. The highest frequencies must be treated with analog filters prior to sampling, to eliminate aliasing errors. Aliasing, caused by inadequate sampling rate, makes high-frequency noise appear as low-frequency noise. For further information, see Goff (1966). A rule of thumb to minimize aliasing without excessive phase lag is to set the analog filter time constant equal to half the sampling interval time. For instance, this analog filter is a standard feature of the Honeywell TDC-2000 digital instrument system in use at the Bayway Chemical Plant. The input is sampled every 1/3 of a second, with an analog filter time constant of 1/6 of a second.

Similar considerations apply in the process control computer. The TDC-2000 user-settable digital filter looks like an analog filter to the computer. When the variable is in a flow control loop, this requires fast (once per second) computer sampling to allow minimum phase lag in the flow control loop. One additional source of aliasing errors is easily overlooked--the processing interval for data reconciliation. For example, the data reconciliation is done every minute for the process of Figure 2, and this interval can easily be much longer in other applications. An additional filter is used on the rapidly-scanned computer tags before use in the data reconciliation. First order (exponential) digital filters are used in almost all cases. The only exception is for levels, because their derivative is used in material balances. For levels, after initial first-order filtering, a least-squares fit is done on a set of recent values and the slope of that line is used as the derivative.

Anti-aliasing protection establishes minimal filtering guidelines, but there may be other concerns. For instance, it may be desirable to filter out the dynamic behavior of some fast-responding process. Some measurements or processes may be exceptionally noisy, or controller cycling may affect some variables. If these variations are not related to the final control or optimization scheme, then heavier filtering is needed for the offending variables. It is possible that some measurements will be much more heavily filtered than others, but the “dynamic reconciliation” viewpoint described later should be kept in mind.

Input filtering will significantly attenuate higher frequency noise and other disturbances. On the other hand, data reconciliation is useful for all frequencies where the constraints apply, typically the lower frequencies. Thus, filtering complements data reconciliation, rather than competing with it as a technique. Filtering exploits redundancy of information available over a period of time--a steady signal is presumed to be masked by noise. Data reconciliation exploits redundancy available in one “snapshot” because of steady state model information. This has been called “spatial redundancy” by Stanley and Mah (1977) in the flow network context.

The second major preprocessing step in a practical system is detection and the subsequent processing of gross errors. In our system, we attempt to detect and then correct for gross errors before any data reconciliation is done. For detection, all that is done automatically at this time is a simple check against minimum and maximum limits for each variable. However, another type of test that has proven useful for detecting both gross errors and bias errors is the equation imbalance test for the material balance constraints (Mah, Stanley, and Downing, 1976).

For instance, at each drum where data reconciliation is done, a variable with a title like “material lost at drum” is calculated and is available for display or historical recall. It is the difference between inlet and outlet flow, corrected for level changes, and exponentially filtered with a time constant of typically 4-8 hours in our plant. (Further discussion is in the QSS section of this paper.) This is done because higher frequency or onetime gross errors are rarely a problem, as discussed earlier. This is currently only done "open loop" in our system. Engineers use this more than operators, since they tend to be more concerned about steady-state instrument errors.

Operator intervention is a factor that should not be overlooked in gross error detection. The operator will generally know when an instrument will be out of service for repairs, calibration, etc. The operators also usually remember which instruments are involved in control schemes. The simple rule used in our system is to take a variable "off scan" whenever the instrument is known to be bad and it is part of a control or optimization scheme ("Off scan" means that the measurement is declared useless and the computer data base is no longer updated by periodic scans of the measurement.) The computer system then automatically considers the value "bad".

Whenever a measurement is recognized as being "bad", due to limit checking or manual intervention, its measurement variance for data reconciliation is set to "infinity". In practice, a large number such as 99999 is used. With this input, the usual data reconciliation can then be done, without any further special logic. The measurement is effectively ignored due to the large variance, and it has no effect on the associated control or optimization scheme.

There is one exception to the standard procedure of checking a measurement against its limits and declaring it bad. This is the case of dual range flow meters on the same stream. If the low-range meter is reading full-scale, but the high-range meter has a lower reading, the low range meter is still presumed good. In that case, the two meters are still reconciled. This is done in several places (flare metering, and also in a flow between the Chemical Plant and the Refinery), for accounting purposes rather than for control.

We now discuss the actual data reconciliation implementation. A general-purpose data reconciliation program (to handle the matrix inversion, etc.) was not written, mainly due to time pressures and clumsiness of our major computer applications language (BICEPS) and its interface to FORTRAN programs. A general solution was not needed, since all the problems encountered could be decomposed into a series of sequential, single-constraint problems that are trivial to solve. This decomposition and sequential estimation approach will now be illustrated in several examples.

A simplified flow plan for one application area at the Bayway plant is shown in Figure 1. (Instruments and other flows not involved in the data reconciliation are not shown.) Flows and levels that are used are indicated. Towers T-1 and T-2 perform chemical reactions as well as distillation.

Several needs are addressed in the data reconciliation. First, for a constraint control scheme on the reactor-towers T-1 and T-2, a reliable, non-noisy estimate of overall reaction extent in the two towers was required. This variable was also needed for a scheme to optimize T-1 and T-2. The reaction extent is indicated reasonably well by the ratio $F_6/(F_4 + F_6)$, after some adjustments for assumed compositions of those flows. Second, it was desirable to have a composition estimate for the key component in the feed to T-1 and T-2. This could be inferred reasonably well by the ratio $(F_4 + F_6)/F_1$ after adjustment for the assumed compositions in F_4 and F_6. This is a useful indicator, and it will later be used in another optimization scheme. Third, Operations desired a calculated level in D-2 when the level instrument failed. Instrument reliability is a major problem in this unit, mainly due to the presence of sulfuric acid.

For the case of Figure 1, the solution could proceed as follows. Data reconciliation could be done around D-2, using measurements F_4, F_5, and the derivative of the L_2 measurement. The derivative is estimated as the slope of the line that is the least-squares curve fit to recent level readings. The single constraint would be the mass balance around D-3. Similarly, data reconciliation with a single mass balance constraint could be done around 0-4, using F_1, F_2, F_3, and the derivative of L_1. The desired reaction extent and composition indicators could now be calculated using the reconciled flows.

The approach actually taken is similar, except that there is a single additional variable at each drum resulting from instrument biases, and there is one additional reconciliation. This will be explained following the review of QSS systems. Also, up/down indicators are used for T-1 and T-2, as already discussed. Also, F_6 is actually a calculated variable. Its variance is calculated from the variances of the measurements that determine it.

Note that there are two completely independent reconciliation problems in the plant example, due to lack of redundancy. The constraints and measurements around each drum have no variables in common. However, even in cases where there are common variables, it is frequently possible to solve a series of sequential problems.

Consider, for example, the figure in Appendix III. (A volume measurement is considered equivalent to a flow measurement for simplicity.) Data reconciliation can be done around the first (top) node, and revised estimates obtained. The estimate of V(1) and its variance can then be used as input to data reconciliation around the second node, and the process repeated on the third node. The results after the last reconciliation will still be optimal for $X_1(3)$, $X_2(3)$, V(2), and V(3). The results for the other variables will be suboptimal, and may not even meet the constraints. If we are only interested in the last results, there is no problem. That would be the case in this example--this is a recursive estimator to give the optimal results for the most recent time period. In many process examples, a similar situation may arise. For instance, in the example of Figure 2, all the measurements are needed just to obtain a few key ratios that matter in the control and optimization schemes. When the estimate of F_4 is further adjusted following its initial reconciliation around D-2, the controls do not notice that F_5 is not updated.

This combining of estimates sequentially is only simple if a single variable from one reconciliation is used in the next reconciliation. The complication is that reconciled estimates are correlated, so that we are forced back to using the general, matrix-oriented solution to account for the correlation. In general, estimates can be combined to allow a problem decomposition. See, for example, Schweppe (1973).

Now that we have discussed some details of implementing the data reconciliation, the next step is using the reconciled estimates in a control or optimization scheme. There are a few potential pitfalls here, related to the input/output relationships ignored by data reconciliation, and loss of observability due to multiple instrument failures. These topics will now be discussed.

When using an estimate from data reconciliation in a feedback control or optimization scheme, care should be taken that true process feedback is reflected in the estimate. Lack of feedback usually occurs due to instrument failure. For instance, consider the case of a surge drum with measured inlet and outlet flow, but with an out-of-service level instrument. Data reconciliation can calculate level changes, and hence a level estimate can be obtained given some initial value. However, true feedback level control cannot be achieved. A level control using this estimate is actually a feed-forward control. Any inaccuracy in the level-volume relationship, or any flow meter bias, will result in the wrong level estimates. The control will eventually either empty or fill the drum. Feedforward control cannot be relied on in an unstable process, although it may do better than no control at all. The fundamental problem is that the steady state equations used in data reconciliation do not recognize the difference between inputs and outputs.

In many cases this will not be a severe problem, for instance when fully predictive models are used in a stable system. As an example, suppose a distillation column has all inputs measured, but no outputs measured. With a predictive model, control can be done, but it is open loop. Without true feedback, there can be steady state offset error due to model error, instrument bias, etc.

To avoid potential problems when feedback control is needed, the simplest check is to set a maximum allowable variance for control. If a variable estimate has a higher variance than the limit, do not use it. This will detect at least some of the problems with inadequate measurements, but the check does not distinguish inputs from outputs. Further guidelines need to be developed.

In all systems there will be the possibility that too many instruments will be out of service. It may then be impossible to calculate a reasonable estimate for some variables--they lose observability. With the failed instrument variances set to a large number, this will result in a similarly large number for the unobservable variable's variance. Any optimization or control scheme using data reconciliation should check the variance of each variable to ensure that it is reasonable. If not, control action should stop and a warning message should be sent to the operator. This is an automatic check for observability.

PROCESS DYNAMICS AND DYNAMIC RECONCILIATION

Up to this point, we have focused mainly on steady-state estimation. However, process dynamics play a role in all of our processes. This section of the paper addresses the problem of data reconciliation when process dynamics are present. Three approaches are considered. The first is smoothing data over a multiple time period model. This is mentioned briefly, mainly for the sake of completeness of the "tool kit". The second approach, simply ignoring the dynamics (but understanding the impact), is examined in more detail. The third approach, called "dynamic reconciliation", is introduced here and is new to the data reconciliation literature.

The first approach of applying data reconciliation to a multiple time period model is described in Appendix III. By looking at a fixed number of recent time periods, and generating a set of variables and measurements for each time period, it is always possible to convert discrete time dynamic equations to a large set of algebraic equations for data reconciliation. While it may seem slightly cumbersome, the corresponding control technique is beginning to be used--direct optimization of control action over a limited number of future time periods. An example is "Dynamic Matrix Control" (Cutler and Ramaker, 1980). In practice at the plant, our models have not been good enough to justify this approach.

We now consider a second approach--simply ignoring the dynamics. This may sound counterintuitive, because in many cases the steady state constraints become poorer models as frequency increases. For instance, consider the case of a process unit with measured inlet and outlet flow, but with no measurement of holdup. At steady state, the inlet flow must be equal to the outlet flow. During normal operation, the steady state mass balance is satisfied "on the average". As the averaging period becomes shorter (we look at higher frequency changes), the steady state constraint becomes less and less relevant. Short-term input variations do not match short-term output variations, due to changes in internal holdup. Forcing compliance with a steady state model can obviously lead to some large errors. On the other hand, it is also obvious in this example that the random measurement errors will still tend to partially cancel each other out in data reconciliation, so that most of the estimator error is due to the model. In many cases this tradeoff of model-induced error for random error reduction may be acceptable.

In some processes, fast dynamics can easily be neglected in comparison to the dynamics of interest; those fast dynamics can be filtered out. Examples of “fast” processes, such as heat exchangers, are given in Appendix III. With the filtering, steady state equations are adequate for these processes.

It should be remembered that some “steady-state” algebraic models are actually good dynamic models. For instance, a mass balance around a process with no variable holdup (such as a pipe junction for blending or flow splitting, or a liquid-liquid heat exchanger) is good under steady state or transient conditions. The dynamic equation for drum level is simple enough that we trend it as an algebraic equation by using a calculated level derivative (Appendix II) or by using the discrete time formulation directly in terms of levels (Appendix III).

Even when dealing with processes that are only approximately steady state, there is an incentive for using steady state techniques. The steady state estimator (the matrix derived from data reconciliation that transforms measurements into adjusted measurements) has the advantage of simplicity. It is a constant matrix, with no dynamic elements. This would appear useful for all frequencies, because there is constant gain for all frequencies, and no phase lag.

One feature that should be recognized is the “feedforward” effect when applied to a process. For instance, suppose the process in the previous example experiences a step increase at its input. To balance the input with the output, the data reconciliation will tend to adjust the input measurement downward, and adjust the output measurement upward. This limited feed-forward has a low gain, set by the relative sizes of the variances for each measurement.

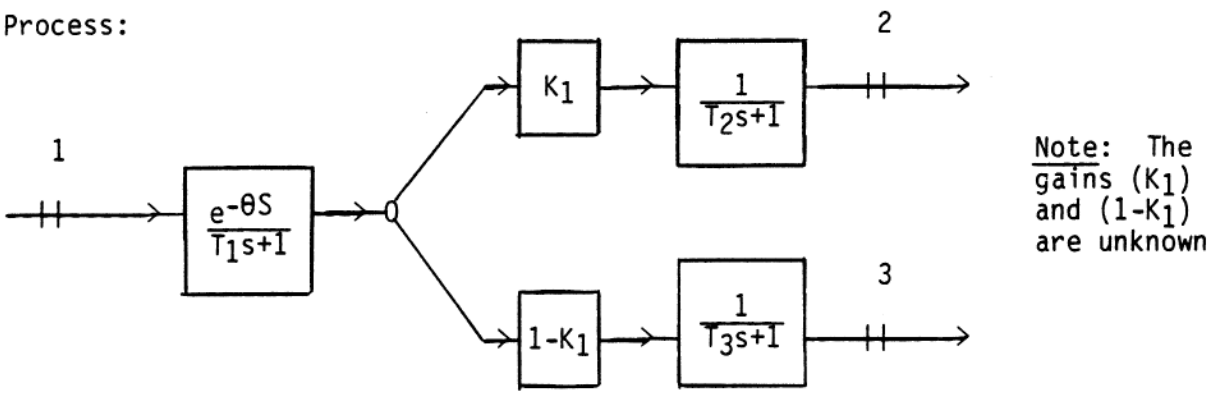
A closing comment on the approach of simply ignoring the dynamics is that it would not shock any practitioner in the process control area. “Steady-state decoupling” is frequently done in multivariable control schemes. This only treats the steady-state interactions between variables. Similarly, static estimators have been used in dynamic systems (Weber and Brosilow, 1972), (Joseph and Brosilow, 1978). In those two papers, redundant measurements were discarded. The approach here is more general; all measurements can be used (instead of a selected subset), and no distinction is made between inputs, outputs, disturbances, and “secondary measurements”.

A more systematic approach to handling dynamics is “dynamic reconciliation”. This term was used in a different context by Bartman (1981), but the idea developed independently here follows the same philosophy of accounting for unequal dynamic responses. The concept behind “dynamic reconciliation” is fairly simple. Consider again the example of a process unit with measurements on the single input and single output. Suppose further that the response of the outlet flow to an inlet flow upset can be modeled as a first-order lag plus deadtime system. Then if the inlet flow measurement is filtered and delayed using the same model parameters, it should match the outlet flow measurement, except for measurement error. In other words, we can use data reconciliation, applying the steady state equation on what Bartman calls the “dynamically synchronized” values.

The concept can be applied to a general process network, filtering and delaying all measurements, generally to the slowest-responding variable. For instance, consider the process shown in Figure 2, drawn in block diagram form using Laplace transforms. This might represent, for example, a distillation column.

DYNAMIC RECONCILIATION EXAMPLE IN CONTINUOUS TIME

Process:



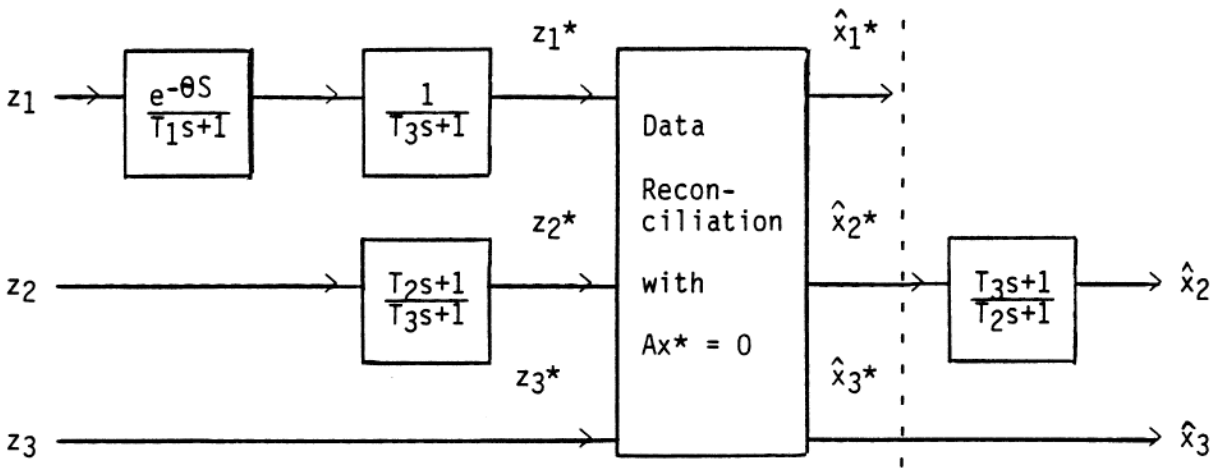
—||—→ = flow measurements z_1, z_2, z_3, of flows x_1, x_2, x_3

Measurements: $z = x + v$ v is noise with covariance matrix R

Constraints: $Ax^* = 0$ where the "*" superscript indicates the "dynamically synchronized" values.

where $A = [1, -1, -1]$

Overall reconciliation process, synchronizing dynamics to match x_3:



(Dynamic) Data Reconciliation Block solves:

$$\hat{x}^* = z^* - RA^T (ARA^T)^{-1} Az^*$$

Optional attempt to translate back to "real time"

Figure 2. Dynamic reconciliation example in continuous time

Note the flexibility possible in this type of model; the split between x_2 and x_3 is not specified. This is not a simulation model that can predict the outputs x_2 and x_3 given x_1. Instead, there is only the requirement that the overall material balance be satisfied, combined with some knowledge of the process dynamics. This is a departure from the standard Kalman filter approach for dynamic systems, which requires a full dynamic model (see Appendix IV). These constraint-oriented formulations allow “partial” models. The flexibility arises from treating the steady state and dynamic models separately, and allowing non-predictive steady state constraints that are parameter-free.

In the example of Figure 2, the measurements are dynamically synchronized to match z_3. For now, we will assume for illustrative purposes that the data reconciliation is performed continuously. Following the path from z_1 to z_3, two first-order filter blocks and a delay are needed to synchronize z_1 to z_3. Following the path from z_2 to z_3 requires a lead/lag block. The lead term arises from inverting the lag model when going “backwards” from z_2. The z_3 measurement is used without modification. The dynamically synchronized estimates are then fed into a standard data reconciliation scheme. The remaining task is to translate the synchronized estimates back into current time if desired. In the case of flow 3, no translation is required. For measurement 2, the input lead/lag is simply inverted. In the case of z_1, this translation would result in two pure lead blocks in series with a pure prediction. A difficulty of this sort (non-realizable transfer function) should not be surprising. In effect, for current time estimates, there is no real redundancy of information about x_1. It takes time for a change in x_l, to have any effect on x_2 and x_3. Of course, there is no problem if only the best estimates of x_2 and x_3 are desired. The best real-time estimate for x_1 is simply z_1.

In a practical system, the data reconciliation is done on a sampled-data basis. The synchronized estimates are usually used directly with no harm, since there is already a built-in deadtime associated with the interval between data reconciliations. That sampling interval should be set long enough for every possible input step change of interest to have had a noticeable effect on every output of interest. The input filters, delays, and lead/lags are also digital, but they are run at a much shorter sample period.

The dynamic reconciliation approach can frequently be implemented easily, because the required filters, lead/lag blocks, and delay tables are standard features of process control computer software. Unfortunately, processes with many recycle loops or large numbers of measurements can result in complicated filter networks if exact solutions are required. Breaking the problem into subproblems will reduce the overall complexity. Developing a systematic, suboptimal method of dynamic reconciliation is a promising research area.

In practice, the dynamic reconciliation viewpoint has been taken, without elaborate computations. Inputs are filtered more heavily than outputs, roughly consistent with process time constants. Fast-responding outputs are filtered moderately to “slow them down” to match other outputs that receive little filtering. In effect, lead/lag elements are replaced with pure lags with the time constant set at the difference between the theoretical lead and lag.

The general approach of solving a steady state estimation problem and then separately accounting for dynamics using simple lead/lag networks has also been proposed by Brosilow and Tong (1978). As in the pure steady state case, the approach here is more general, because all measurements can be used, not just a selected subset.

CASCADE ESTIMATION FOR QUASI-STEADY STATE (QSS) VARIABLES

The previous discussions have dealt with steady state and dynamic systems, and described appropriate estimation procedures. However, there is another class of variables, called quasi-steady state (QSS), which fit "in between" the steady state and dynamic variables. A variable is called quasi-steady state if it can change only very slowly, or have occasional sharp transitions between steady state values. Some examples are given in Appendix IV, including instrument bias, heat transfer coefficients, and others. Data reconciliation at the Bayway Chemical Plant has involved two types of QSS variables: instrument bias and a slowly-changing composition.

Estimation with QSS variables requires a technique different from those discussed so far. This section examines the random walk model as a good representation for a QSS variable, and the resulting Kalman filter. To reduce the complexity of this approach, a new technique called "cascade estimation" is introduced. It is a suboptimal approximation to the full Kalman filter. An example with a slowly-changing composition or split fraction is examined. The new technique uses exponential filters; two approaches to designing the filters are given. A final example of instrument bias estimation is then presented.

Why are we concerned about QSS variables? If it is known that a variable can only change very slowly, it seems reasonable that we should be able to use that information to improve our estimates--this is a type of model. Unfortunately, the standard data reconciliation algorithm offers no help--it focuses on a "snapshot" of the process. To develop an appropriate algorithm, a model of a "slowly-changing variable" is needed.

The random walk model provides a convenient representation of a QSS variable (see Appendix IV). From one time period to the next it predicts that no change occurs in the variable, based on expected value. However, there is "process noise" with a variance that allows deviations from the expected value. Larger deviations can occur from one time period to the next when the variance is larger. Measurements will be used to correct the random walk model prediction, with a filter combining model and measurement information based on process noise variance vs. measurement noise variance.

Since random walk is a dynamic model, it would seem logical to apply the Kalman filter for optimal estimation (see Appendix IV). This in fact was done in Stanley and Mah (1977). The steady state constraints were used to eliminate dependent variables, leaving a set of independent variables with no constraints. In effect, the reconciliation problem was transferred into the filter's measurement matrix. The random walk model was applied to all variables, with process noise variances set very small for the QSS variables, and large for the others. The model was linearized as necessary, and the Kalman filter was used to combine the model information and measurement information. This approach worked, and provided useful insight into the estimation of plant parameters.

The Kalman filter for random walk processes behaves like a first-order (exponential) filter. This is most clearly seen in the single-variable, single-measurement case described in Appendix IV. In the multivariable case, complexity is introduced due to the interactions through the steady state constraints. However, the response to a step input still looks like a first-order lag. (Deviations from this pattern occur when the constraints are nonlinear.) This filter performance for linear systems is desirable, but unfortunately, the Kalman filter is relatively complicated to implement.

A simple alternative estimation technique has been developed which guarantees the desired lagged response for QSS variables, even with nonlinearity. The "cascade" method completely separates the slowly-changing parameter estimation from the data reconciliation. The algorithm is described in Figure 3. It first directly calculates the QSS variables based on current measurements, then in effect exponentially filters the result. (The modification will be described later.) These filters are given long time constants, consistent with the designer's feelings on the possible rates of change of the QSS variables. Finally, the QSS parameters are considered to be constant for data reconciliation using the defining equations for the QSS variables, along with any other balance equations.

This approach is suboptimal because it neglects the correlation between the QSS variable estimate and the current measurement. However, this is a good approximation. Even in the optimal estimator, the current measurement adds little new information to the QSS variable estimate due to the heavy weighting of old measurements.

CASCADE ESTIMATION:
DATA RECONCILIATION WITH A SLOWLY CHANGING PARAMETER IN PROCESS MODEL

- MODEL

  Let c be the parameter vector

Constraints:	$f(x, c) = 0$ is the equation defining c $g(x) = 0$ (other constraints)
Measurements:	$z = x +$ noise
Random Walk:	$c(k+1) = c(k) +$ process noise (small) diagonal covariance matrix $= Q$

- ALGORITHM

  At each time step k:

  (1) calculate c_{new} by solving $f[z(k),c] = 0$

  (2) exponentially filter c: $\hat{c}(k) = \alpha\hat{c}(k-1) + (1-\alpha)\, c_{new}$

  (3) hold c(k) fixed, and do data reconciliation with $f[x, c(k)] = 0$ and any other "balance" equations.

- IMPLIED STATISTICAL ASSUMPTION: $Q << R_z$

  - The parameter is well-known before data reconciliation, and further adjustment would make no sense.

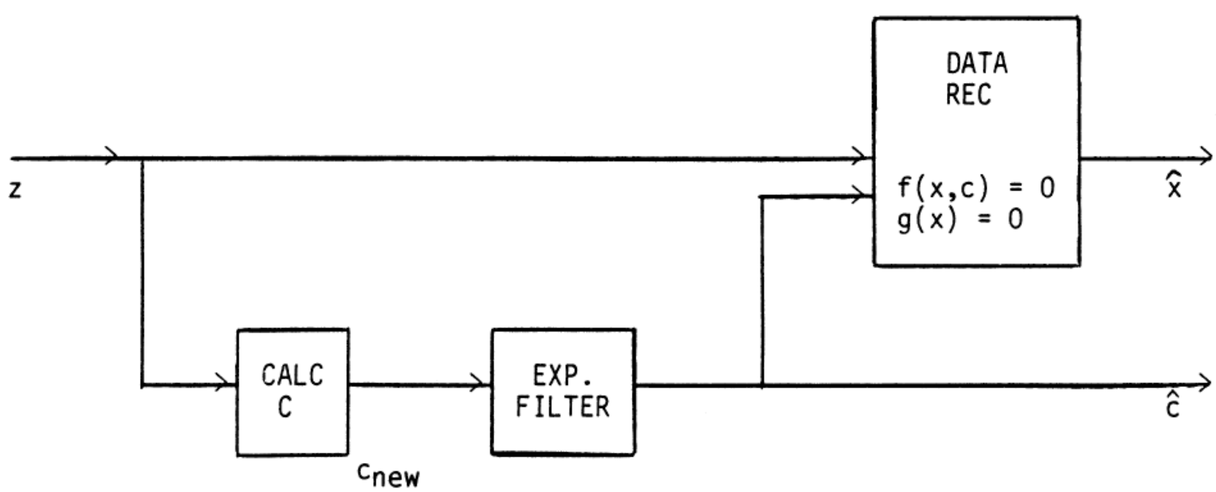


Figure 3. Cascade estimation: data reconciliation with a slowly changing parameter in process model

This strategy is loosely analogous to cascade control. The highest frequencies are eliminated by simple filtering. The moderate frequencies are dealt with at a low, data reconciliation level, and the low frequencies are handled at a higher QSS level. Like this "cascade estimation", cascade control is a suboptimal approximation of an optimal, multivariable control. The suboptimal, cascade approach is easy to understand, easy to tune, and works well in either control or estimation.

In most cases, the QSS variables will not be used directly in a control or optimization scheme, unless the scheme is extremely slow. The time scale for control will usually be fast, relying on the data reconciliation for error reduction. The QSS estimator provides parameter estimation for models on a slow time scale; error reduction in current estimates is achieved using those models.

For systems with linear parameter estimation, the new estimator performance should be similar to its optimal Kalman filter counterpart developed by Stanley and Mah (1977). With nonlinear parameter estimation, the new estimator sometimes offers an improvement. For instance, in the case of a split fraction (ratio) as a QSS variable, the full Kalman filter must be linearized at each time step. With the cascade estimator, the data reconciliation is linear. The nonlinearity only appears in calculating the input to the exponential filter. Thus, none of the stability problems observed in the Kalman filter with parameter estimation can occur (for the split fraction case).

In the 1977 paper by Stanley and Mah, it was concluded that QSS parameter estimation was never helpful for the systems studied. There are several reasons why that conclusion does not apply for the current applications. The major reasons are due to different process needs and design goals. The previous work required that QSS parameters have relatively fast step response, so the error figures reported included the complete step response. That approach weighted the long-term steady state error very heavily. The current approach does not design for step response of QSS variables--it is assumed that QSS variables change so slowly so that a step change is irrelevant. As a result, there is much heavier use of historical data, a source of redundancy. The current approach concentrates on attenuating error at the middle and higher frequencies which are of concern for process control. In the case of instrument bias estimation, multiple steady state solutions were recognized as a problem. It will be seen later that this problem can be overcome by estimating QSS variables related to bias, and sacrificing long-term steady state estimation accuracy to obtain higher frequency noise attenuation. This possibility was not considered in the earlier work.

Another difference resulted from different types of problems. In the 1977 paper, it was assumed that there was one overall reconciliation problem, with all variables observable. In the example of Figure 1 in the current work, the entire network contains many unobservable variables. The flow F_6 would not have been involved in any problem considered in the previous work. Only with a QSS variable was there any hope of tying F_6 to any data reconciliation. This technique attenuates high frequency noise, and allows control even if F_6 fails. The importance of control with instruments out of service, even if normal accuracy must be sacrificed, was not considered in the previous work.

One facet of the cascade estimation technique has not yet been mentioned: designing the required exponential filters. Several approaches can be taken to designing the filters for the QSS estimator. The simplest is to directly specify the required exponential filters. The designer uses intuition about the process and how the estimates will be used to decide on an appropriate time constant for the QSS variable based on step response, phase lag, etc. The formula to convert that time constant into the exponential filter constant is given in Appendix IV. For this design method, no direct reference is made to the random walk model and process noise variance. Control engineers will probably be comfortable with this approach, due to their experience in tuning.

A second approach to the QSS estimator is taken for the plant application. The filters are specified indirectly by specifying the process noise variances. (The measurement noise variances are already specified for data reconciliation.) This approach is summarized in Figure 4. It is essentially a derivation of the Kalman filter for a single random walk variable with a single measurement, except that the measurement is actually a calculated variable.

FILTERING BASED ON PROCESS NOISE SPECIFICATION

- MODEL

QSS Calculation:	c = f(x)	c is a single variable, x is vector
Random Walk:	c(k+1) = c(k) + w(k)	E[w(k)] = 0 variance [w(k)] = q
Measurements:	z(k) = x(k) + v(k)	E[v(k)] = 0 covariance matrix of v(k) = R

- LINEARIZATION

Define c_{meas} = f [z(k)] and let $F = f'(x) = \begin{bmatrix} \frac{\partial f}{\partial x_1} & \frac{\partial f}{\partial x_2} & \ldots \end{bmatrix}$ (matrix F has one row)

Approximate variance of c_{meas} = $r_c = FRF^T$

$= \sum_k F_{1k}^2 R_{kk}$ for diagonal R

- FILTER

Let p(k) = variance in estimate ĉ(k) of c(k)

Prediction: $c_{pred}(k) = \hat{c}(k-1)$

Variance in prediction: p(k-1) + q (previous variance + random walk noise variance)

The prediction ĉ(k-1) and its variance p(k-1) + q are then combined with the calculated "measurement" c_{meas} and its variance r_c using the standard formula in Appendix I for combining estimates.

$$\hat{c}(k) = \left[\frac{r_c}{p(k-1)+q+r_c}\right] \hat{c}(k-1) + \left[\frac{p(k-1)+q}{p(k-1)+q+r_c}\right] c_{meas}$$

$$p(k) = \left[\frac{p(k-1)+q}{p(k-1)+q+r_c}\right] r_c$$

Figure 4. Filtering based on process noise specification

The resulting filter is of the same form as an exponential filter, except that the filter parameter changes over time. When the process noise and measurement noise variances are held constant, the sequence of p(k) will always converge. After a period of time, the filter then matches an exponential filter exactly.

The main advantage of this more complex approach is the built-in error analysis given by the sequence of p(k). This eliminates the need for special logic to handle cases of instrument failure or unit shutdowns. As discussed in the steady-state case, measurement variances are already set to 0 by unit up/down detectors, or a large number when an instrument fails. These changes simply propagate through the system and the filter adjusts accordingly.

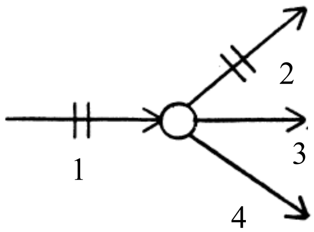
For instance, in Figure 1, F_4 is reconciled against F_5. The reconciled result and its variance are then used to calculate the slowly-changing QSS composition variable. If either F_4 or F_5 fails, the variance of the F_4 estimate from the data reconciliation will increase. The filter will then adjust by weighting the new measurements less heavily, thus increasing the equivalent lag time (relying more heavily on the old information). The p(k) values will also get larger, indicating less confidence in the estimate of the QSS variable. In the extreme case where both F_4 and F_5 are out of service, there is no new information available for the QSS variable. The lag time goes infinite, so the current QSS variable estimate remains fixed as the best possible estimate. The variance sequence increases at the constant rate q, indicating the gradual loss of confidence in the quality of the QSS variable estimate. When either F_4 or F_5 finally become good again, the variance p(k) will be large compared to the variance for the new calculated QSS variable. As a result, the new measurement will be weighted heavily at first, which is desirable as a form of initialization. In the case where a measurement is declared "perfectly known" due to a shutdown, its variance is set to zero. This also propagates through the variance equations, and the filter ignores all past history when it should. The lag time goes to zero.

In general, the approach described here retains most of the advantages of a full-scale Kalman filter, without the complexity. It provides a sophisticated, automatic form of estimation, with adjustment for any event affecting the measurement variances. The tuning of the process noise variances is reasonably intuitive, since it represents a noise, just as the measurement variances do.

An example of the cascade estimation strategy is given in Figure 5, where it is applied to a split fraction or slowly-changing composition. This approach of treating composition as a slowly changing variable is being used successfully in the plant example of Figure 1. The feed flow (at measurement F_1) is downstream of a large drum and the equivalent of a large stirred-tank reactor. As a result, the feed composition can only change slowly. The key component, n-butene absorbed in sulfuric acid either leaves the unit as product at F_6, or is recycled by F_4. The feed butene composition can be calculated essentially as $c = (F_4 + F_6)/F_1$. (The flows F_4 and F_6 are actually converted to component flows using assumed compositions.) This composition is filtered heavily, as is done in the example of Figure 4. When c is held fixed, the data reconciliation on the defining equation is still linear (after multiplication by F_1). As indicated earlier, F_4 is the result of a separate data reconciliation with F_5. The reconciled value of F_4 is used as input to the calculation of c and subsequent reconciliation. Similarly, F_1 is itself the result of another reconciliation.

The data reconciliation with a slowly-changing composition achieves several goals. First, it ties together all the measurements in Figure 1 to provide better estimates of F_4 and F_6, needed for the reaction extent control. More importantly, it allows meaningful estimates of reaction extent [essentially $F_6/(F_4 + F_6)$] despite multiple instrument failures. For instance, even with F_4 and F_6 out of service, they both will still be calculated automatically by the procedure. Another important feature is that there is no "bump" to any

COMPOSITION (OR SPLIT FRACTION) AS SLOWLY-CHANGING PARAMETER



$c = x_2 / x_1$
or
$cx_1 - x_2 = 0$

- EXAMPLES
  - The node is a simple pipe split, with unknown, fixed valve position.
  - Stream 1 is coming from a large, well mixed reactor or tank and hence its composition can only change slowly. The node is a perfect separator for the pure component in stream 2 (e.g., lighter-than-light key in distillation).

- MODEL

  Constraints: $cx_1 - x_2 = 0$

  Measurements: $z_1 = x_1$ + noise; $z_2 = x_2$ + noise

  Random Walk: $c(k+1) = c(k)$ + process noise (small)

- ALGORITHM

  At each time step k:

  (1) Calculate $c_{new} = z_2(k) / z_1(k)$

  (2) Exponentially filter c_{new}: $\hat{c}(k) = \alpha\hat{c}(k-1) + (1-\alpha)c_{new}$

  (3) Hold c(k) fixed and do standard linear data reconciliation on $\hat{c}(k)x_1 - x_2 = 0$

- STATISTICAL EFFECT
  - Similar to bias estimation.
  - Reconciles higher-frequencies, passes lower frequencies.

Figure 5. Composition (or split fraction) as slowly-changing parameter

estimate when an instrument fails, because the filtering technique of Figure 4 is used. When instruments fail, there is inadequate information to update parameter estimates so they "freeze" at their last value. In effect, the model is used to back-calculate a missing measurement; there is no bump because the model is up-to-date. This applies to the composition and to the instrument biases described next.

As a final example of QSS variable estimation, we consider the common case of instrument bias. There are several approaches to dealing with this problem. The first is to ignore it in the estimation problem formulation. Data reconciliation will then do a good job of reducing error due to most systematic errors, including bias (Stanley and Mah, 1977). Unfortunately, severe "bumps" to variable estimates can occur upon instrument failure in this case. The second approach is to try to include instrument biases in the system model and attempt to estimate them.

Instrument bias can usually be considered as a slowly-changing variable. Unfortunately, each bias variable added to an existing process model increases the number of variables to be estimated without adding any constraints or measurements. This reduces the overall level of redundancy present. In general (with some mild restrictions), the number of "steady-state" constraints plus the number of measurements must be greater than or equal to the number of variables to be estimated in a system. This includes the QSS variables as well as the "steady state" variables. (The random walk model does not count as a constraint.) If the criterion is not met, there are an infinite number of solutions to the estimation problem, as was confirmed by Stanley and Mah (1977). For the theoretical basis for determining whether or not estimation will be successful in either steady-state or QSS systems, see Stanley and Mah (1981a).

Based on the above comments, it will not be possible to estimate all the instrument biases in the usual systems with more variables than constraints. It is possible to estimate biases for a subset of measurements, but there will rarely be reasonable criteria declaring bias possible in some instruments but not others. A new approach is needed.

For simplicity, we assume that every variable is measured (with noise), and every measurement has a bias. However, no attempt will be made to estimate all the biases. Instead, an overall bias term is associated with each constraint, rather than each measurement. (We assume that the constraints, or their linearized versions, are linearly independent.) Each of these biases are estimated as QSS variables. The algorithm is described in Figure 6.

If these biases were estimated along with the other variables on a purely steady state basis, this would result in the constraints effectively being ignored. To minimize the least-squares objective function, each of the normal "x" variables would be estimated as its measurement value. These values would be plugged into the constraint equation to calculate the corresponding bias terms.

In the QSS case, higher frequency noise is reduced by the data reconciliation procedure. The lowest frequencies, down to steady state, are passed on through the estimator. These errors are absorbed in the bias term. Operation with this estimator can been seen in the Figure 7 example. Here there are two flow measurements, with one material balance constraint. Its physical meaning is "constraint imbalance"--in this case "material lost at node" since it is the difference between flow into the node and out of the node. Step response plots are shown, for changes in either instrument bias. The plots for $\hat{x}$ and $\hat{z}$ match, except for the dashed lines. The bias estimate has the expected exponential response. Note that since measurement 2 has twice the variance of measurement 1, a step change in z_1 has double the initial impact of a step change in z_2.

DATA RECONCILIATION WITH A SLOWLY CHANGING BIAS

- MODEL

  Constraints: $Ax = 0$ without bias, $Ax = b$ with bias

  Measurements: $z = x + \text{noise}$

  Random Walk: $b(k+1) = b(k) + \text{process noise (small)}$

  Note: Adding biases adds one variable for each constraint, but no new equations. This reduces the overall "amount" of redundancy for low frequencies.

- ALGORITHM

  At each time step k:

  (1) Calculate $b_{new} = Az(k)$

  (2) Exponentially filter b: $b(k) = \alpha \hat{b}(k-1) + (1-\alpha)\, b_{new}$

  (3) Hold $\hat{b}(k)$ fixed, do data reconciliation for $Ax = \hat{b}(k)$

- IMPLIED STATISTICAL ASSUMPTION: $R_b << R_z$

  - Bias is well-known before data reconciliation. Adjustment would make no sense.

- THIS IS AN EXAMPLE OF "CASCADE" ESTIMATION

- BLOCK DIAGRAM:

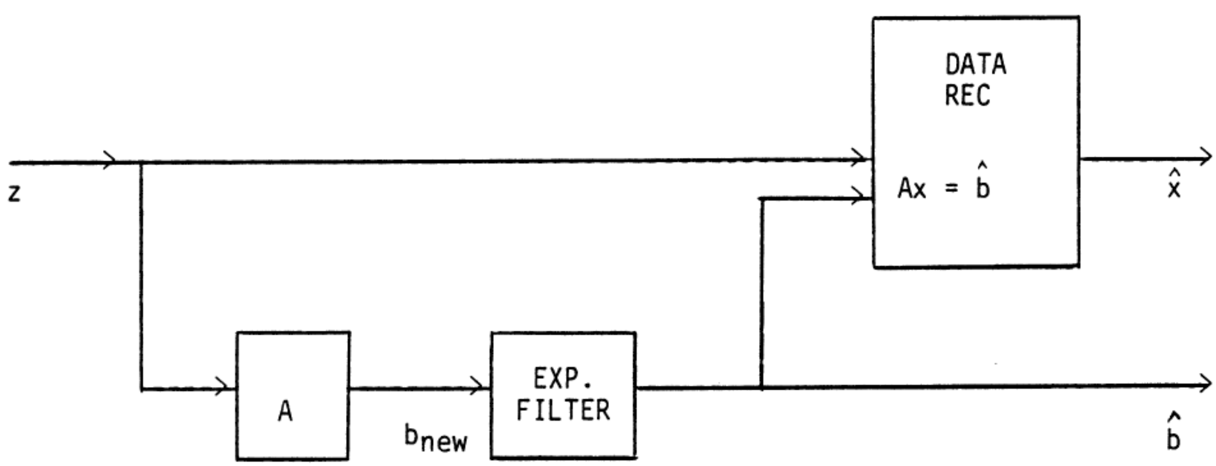


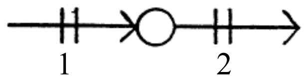
Figure 6. Data Reconciliation with a slowly changing bias

What are the criteria for choosing this approach? In cases where long-term steady state estimation accuracy is important, or an estimate consistent with the long-term steady state constraints is needed, this technique would not be used. However, in cases where the measurement noise is moderate frequency to high frequency, significant error reduction will result. The constraints are only honored on a moderate to high-frequency basis. When using the estimates in closed loop control and instrument failure is a major concern, this approach to bias is very useful. The main reason is that when an instrument fails, and its variance is set to a large number, there is no "bump" in the estimate. In the example of Figure 7, suppose no bias estimation were done, and suppose x_2 is used in a control scheme. When both measurements are present, the x_2 estimate would be between z_1 and z_2 (closer to z_1). If z_1 fails, the estimate would immediately jump to z_2. Conversely, if zi fails, the estimate would immediately jump to z_2. Feeding these jumps to a control scheme would upset the process. On the other hand with the constraint imbalance as a QSS variable, there is no bump on instrument failure. The bias estimate is no longer updated and control continues using one measurement. When both measurements are in service, moderate to high frequency noise is attenuated.

For the plant problem shown in Figure 1, constraint imbalances (including level changes) were calculated as QSS variables at drums D_1 and D_2. The main concern was providing an automatic switch to "backup" instrumentation upon instrument failure. The redundancy was used more for reliability than for estimation accuracy.

The optimal estimation of instrument bias in dynamic systems was considered by Friedland (1969), with biases treated as state variables in a Kalman filter. The overall problem was decomposed into separate bias and state estimation problems. His general approach differed in several ways. First, bias was treated as a fixed parameter, not a random walk variable with process noise as used here. This means that different problems were addressed. Second, Friedland maintained optimality by recognizing correlation between the bias estimate and the current state estimate. The optimality was dropped here to simplify the estimation.

EXAMPLE OF DATA RECONCILIATION WITH BIAS ESTIMATION



A = [1, -1]
b = "material lost at node 1"

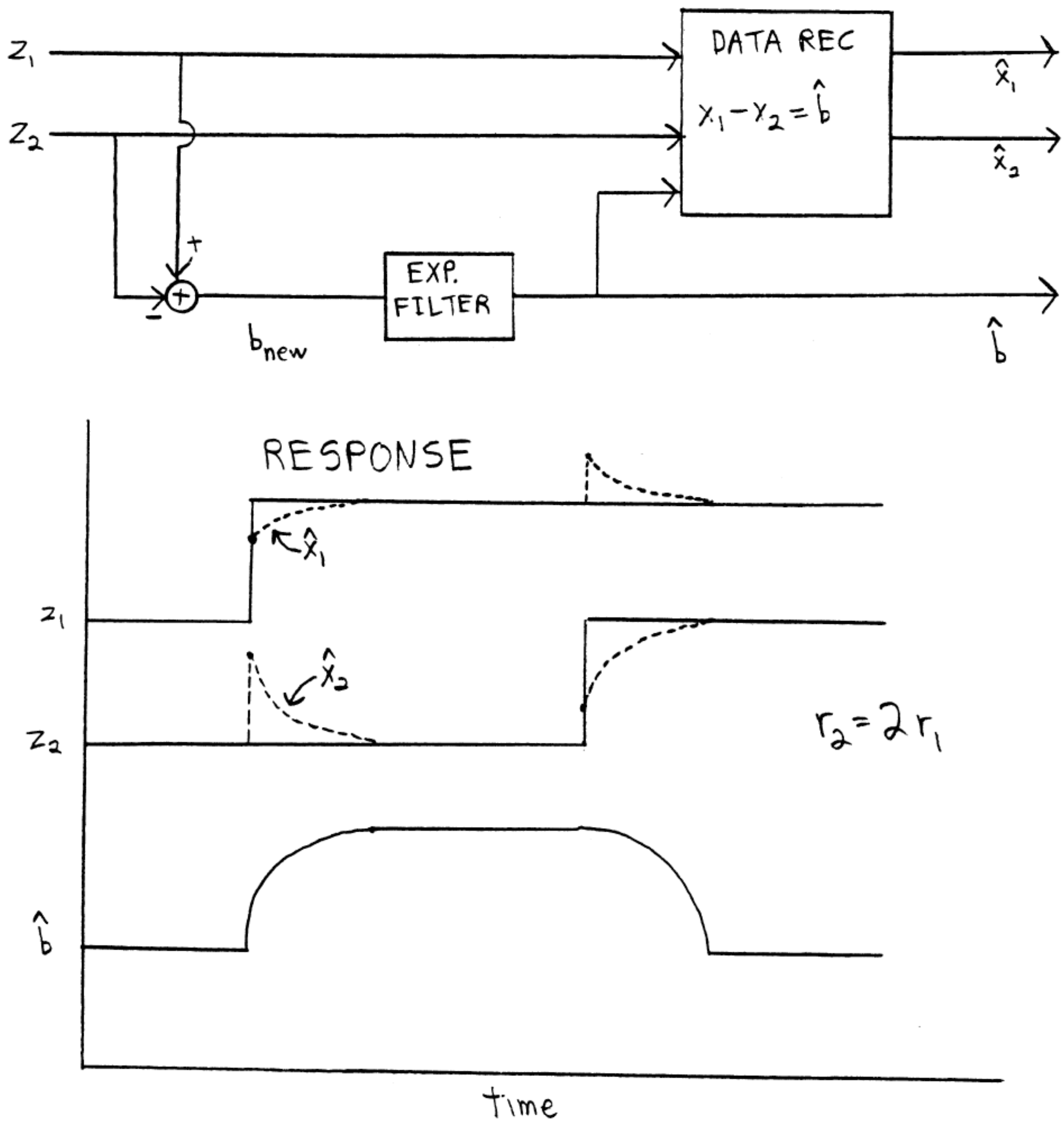


Figure 7. Example of data reconciliation with bias estimation

CONCLUSIONS

Data reconciliation is recognized as a tool for obtaining improved estimates of process variables. Assuming that a steady state model is correct, and assuming that measurement error can be approximated by a normal distribution, the estimates are in fact “optimal”. This tool can be easily extended into the process control environment, despite what appear to be overly restrictive assumptions. However, some modifications must be introduced, because the solution of data reconciliation does not exactly match the problems arising in process control and online optimization. In fact, data reconciliation provides a convenient tool for addressing some process control problems only loosely related to the original purpose of data reconciliation. An example is using it as a convenient method to back-calculate failed instrument readings, rather than emphasizing normal error reduction. This is easy because of the flexibility in specifying variances--numerical values which at times are used to indicate structural changes like instrument failure.

The paper has provided a tool kit, showing how to use data reconciliation in online applications such as process control and optimization. These applications were shown to different from other offline applications, especially in the areas of instrument failure, frequency response, and process dynamics considerations. New tools had to be developed, such as equipment up/down indicators, dynamic reconciliation, and cascade estimation. A new approach to bias estimation that does not lead to multiple solutions was developed.

Existing tools from the process control area were integrated with data reconciliation. For instance, filtering is a key feature for online applications. Unified approaches to filtering both the measurements and the slowly-changing parameters were presented. Another example is separation of dynamic behavior from steady state behavior in solving problems. This general concept is extended from process control to develop dynamic reconciliation. The sequential estimation approach, and a general tendency toward suboptimal solutions has been far more common in the control and filtering literature than in the data reconciliation literature. It is hoped that this paper will stimulate further efforts in online data reconciliation, and help narrow the gap between the practitioners of process control and those of data reconciliation.

APPENDIX

I. REVIEW OF DATA RECONCILIATION (STEADY-STATE LEAST SQUARES ESTIMATION)

- Noise
- Variance
- Least squares estimation (steady state)
- Some special data reconciliation cases
- Simple example of data reconciliation

II. EXAMPLES OF SYSTEMS WITH REDUNDANCY

- Simplest example of system with redundancy
- Another sample of a system with redundancy
- Classifying measurements as redundant or non-redundant
- Redundancy examples with material and energy balance
- Redundancy example with material and energy balance
- Other examples of systems with redundant measurements

III. SIMPLE EXTENSIONS OF DATA RECONCILIATION TO DYNAMIC SYSTEMS

- "Steady state" estimation isn't just for steady state systems
- Data smoothing approach on a surge drum
- Data smoothing in a first order linear system

IV. QSS SYSTEMS, KALMAN FILTER, AND RANDOM WALK

- Examples of systems with quasi-steady state variables
- Kalman filter overview
- Exponential filter as special case of Kalman filter for "random walk"

NOISE

- "HIGH" FREQUENCY
  - APPEARS RANDOM
  - GAS FLOW
  - INDUCED ELECTRICAL NOISE (e.g., 60 HZ AC, WELDING, PUMP STARTS, ETC.)

- QUANTIZATION ERRORS (e.g., ONE-DEGREE RESOLUTION FROM DTI SYSTEM INTERFACE)

- "MODERATE" FREQUENCY
  - FLOW, PRESSURE, OR LEVEL CYCLING DUE TO TIGHT CONTROLLER TUNING, BAD VALVE POSITIONERS, ETC.
  - ALIASING (DUE TO SAMPLING DATA TOO INFREQUENTLY, eg., IN A SLOW PRIMARY OF A DDC CASCADE LOOP)

- "LOW" FREQUENCY
  - INSTRUMENT BIAS (TRANSMITTER ERROR, WRONG FLUID IN FLOWMETER LINES, GROUND LOOPS)
  - SYSTEMATIC ERRORS (THERMOCOUPLE INSULATED FROM PROCESS BY COKING)
  - STICKING BALL FLOAT IN LARGE TANK

- "GROSS" ERRORS (e.g., INSTRUMENT OUT OF SERVICE)

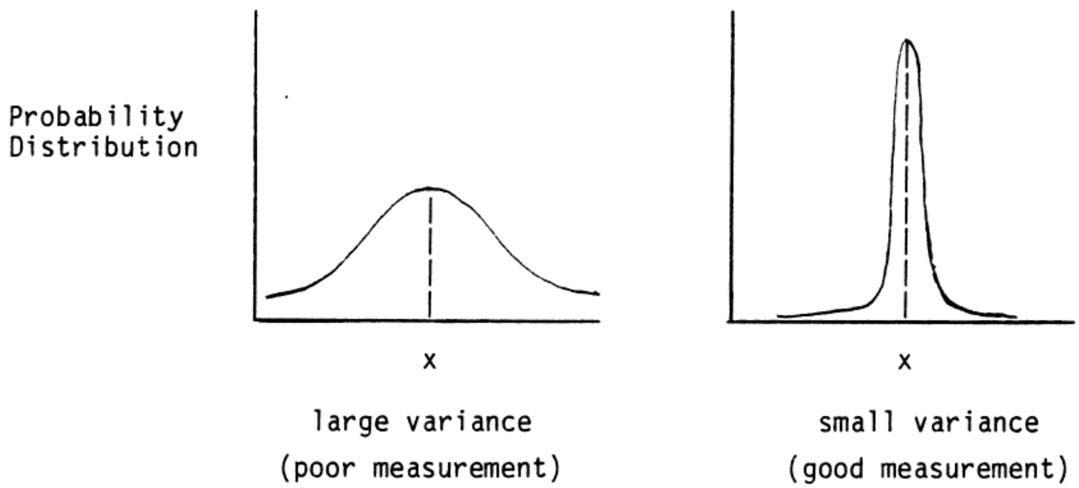
- SIMPLE DIGITAL FILTERS (EXPONENTIAL, LEAST-SQUARES) ARE MAINLY USEFUL FOR REDUCING HIGH FREQUENCIES, AND ARE USELESS FOR "LOW" FREQUENCIES OR ALIASING.

- DATA RECONCILIATION IS USEFUL AT ALL FREQUENCIES WHERE CONSTRAINTS APPLY, SO IT BECOMES MOST IMPORTANT AT MODERATE TO LOW FREQUENCIES.

- GROSS ERRORS SHOULD BE DETECTED SEPARATELY (eg., LIMIT CHECKING, CHECKING CONSTRAINTS DIRECTLY) BEFORE DATA RECONCILIATION.

VARIANCE

- MEASURE OF "UNCERTAINTY" OR "SPREAD": VARIABILITY FROM MEAN
- SQUARE OF STANDARD DEVIATION
- DENOTED BY r FOR ONE VARIABLE, COVARIANCE MATRIX R FOR MULTIPLE VARIABLES
- EXAMPLES:



PERFECT MEASUREMENT:	r	=	0
GOOD MEASURMENT:	r	=	small
POOR MEASUREMENT:	r	=	large
WORTHLESS MEASUREMENT:	r	=	INFINITY

- PROPAGATION OF VARIANCE:

IF $y = Ax + b$ with covariance matrix of $x = R$

THEN covariance matrix of $y = ARA^T$ (= A^2R for single variable)

LEAST SQUARES ESTIMATION (STEADY STATE)

General System:

measurements: $z = h(x) + v$ — v is noise with covariance matrix R; usually R is taken as diagonal

constraints (model): $g(x) = 0$

General Least squares estimation

Find the estimate $\hat{x}$ as the solution to the problem:

$$\underset{\text{over } x}{\text{minimize}} \quad (z - h(x))^T R^{-1} (z - h(x))$$

$$\text{subject to} \quad g(x) = 0$$

Common cases

- Linear, unconstrained
  measurements: $z = Hx + b + v$ where b is fixed (a "bias")
  (no constraints)

  The solution to the estimation problem is: $\hat{x} = (H^T R^{-1} H)^{-1} H^T R^{-1} (z - b)$

  $$\text{cov}(\hat{x}) = (H^T R^{-1} H)^{-1}$$

- Linear, constrained, direct measurements
  measurements: $z = x + v$
  constraints: $Ax = c$

  The solution to the estimation problem is: $\hat{x} = z - RA^T (ARA^T)^{-1} (Az - c)$

  $$\text{cov}(\hat{x}) = R - RA^T (ARA^T)^{-1} AR$$

- Linear problems can be put in either form, for instance, to minimize the order of the matrix inversion (number of variables in first case, number of constraints in second case.)

- Matrix inversion can be avoided if variance of estimate is not needed (but a system of linear equations still must be solved

SOME SPECIAL DATA RECONCILIATION CASES

- SINGLE CONSTRAINT, MANY VARIABLES:

MEASUREMENTS: $z_i = x_i + \text{noise}_i$ (variances r_i)

ONE CONSTRAINT: $\sum_i a_i x_i = 0$

SOLUTION: $$\hat{x}_i = z_i - \frac{a_i r_i}{\sum_j a_j^2 r_j} \sum_j a_j x_j$$

$$\text{var}(\hat{x}_i) = r_i - \frac{a_i^2 r_i^2}{\sum_j a_j^2 r_j}$$

- NO CONSTRAINT, ONE VARIABLE:

MEASUREMENTS: $z_i = h_i x + \text{noise}_i$ (variances r_i)

SOLUTION: $$\hat{x} = \frac{\sum_i \frac{h_i z_i}{r_i}}{\sum_i \frac{h_i^2}{r_i}}$$

$$\text{var}(\hat{x}) = \frac{1}{\sum_i \frac{h_i^2}{r_i}}$$

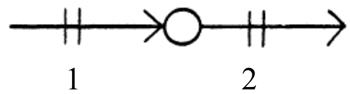
- SPECIAL CASE OF ABOVE: $h_i = 1$, 2 measurements:

(Combining two estimates)

$$\hat{x} = \frac{r_2}{r_1 + r_2} z_1 + \frac{r_1}{r_1 + r_2} z_2$$

$$\text{variance}(\hat{x}) = \frac{r_1 r_2}{r_1 + r_2}$$

SIMPLE EXAMPLE OF DATA RECONCILIATION



- MEASUREMENTS: z_1 and z_2

  $z_1 = x_1 + \text{noise}$ (variance = r_1)

  $z_2 = x_2 + \text{noise}$ (variance = r_2)

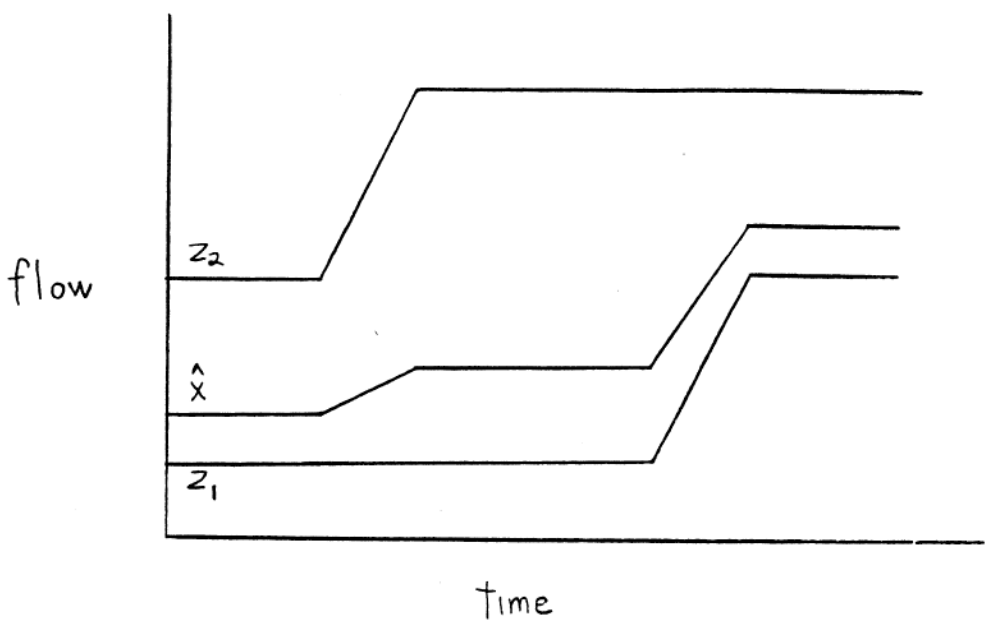
- CONSTRAINT: $x_1 - x_2 = 0$

- WE ESTIMATE: $\hat{x} = \hat{x}_1 = \hat{x}_2$

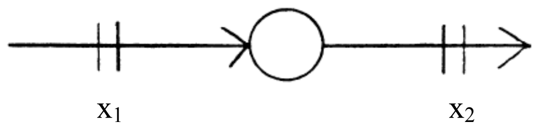
- SOLUTION: $\hat{x} = \dfrac{r_2}{r_1 + r_2} z_1 + \dfrac{r_1}{r_1 + r_2} z_2 = z_1 - \dfrac{r_1}{r_1 + r_2}(z_1 - z_2)$

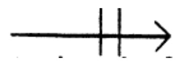
- NOTE THAT EXTREME CASES ($r_i = 0$ or $r_i = \infty$) MAKE SENSE

- EXAMPLE: $r_2 = 3r_1$ Then $\hat{x} = .75z_1 + .25z_2$



SIMPLEST EXAMPLE OF A SYSTEM WITH REDUNDANCY



Note  = meter in line.

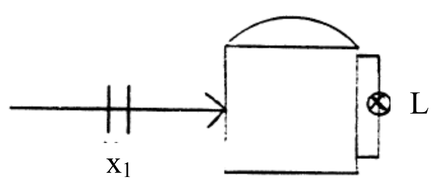
The above "node" is simply a point around which a material balance is taken

<u>CONSTRAINT</u> $x_1 - x_2 = 0$

(or more generally $a_1x_1 + a_2x_2 = 0$)

<u>COMMON EXAMPLES</u>:

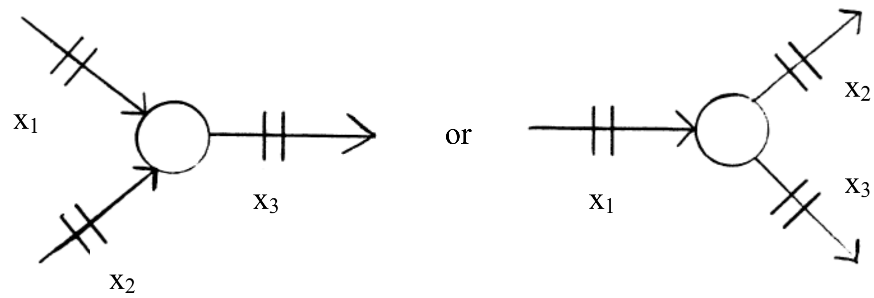
- DUAL FLOW METERS, FREQUENTLY WITH DIFFERENT RANGES (FLARE, STREAMS THAT CROSS UNIT BOUNDARIES)
- GAS FLOW BEFORE COMPRESSOR + CONDENSOR, LIQUID FLOW AFTER THAT
- FILLING A TANK:



CONSTRAINT IS $x_1 - A\dfrac{dL}{dT} = 0$

WHERE $x_2 = \dfrac{dL}{dT}$ AND A = CROSS-SECTIONAL AREA OF TANK

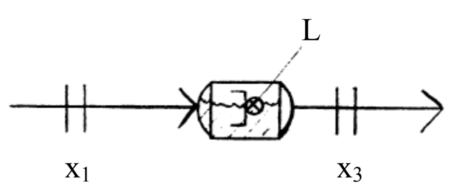
ANOTHER SAMPLE OF A SYSTEM WITH REDUNDANCY



CONSTRAINT $a_1x_1 + a_2x_2 + a_3x_3 = 0$

COMMON EXAMPLES:

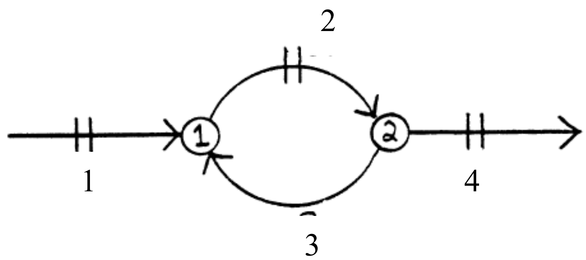
- ON-LINE BLENDING
- SPLITTING OR COMBINING FEEDS AT FURNACE PASSES, PARALLEL TOWERS, HEAT EXCHANGER BYPASSES WITH THREE-WAY VALVES
- SURGE DRUM WITH MEASURED LEVEL, INPUT FLOW, OUTPUT FLOW



CONSTRAINT IS $x1 - A\frac{dL}{dT} - x3 = 0$

WHERE $x_2 = \frac{dL}{dT}$ AND A = CROSS-SECTIONAL AREA OF DRUM

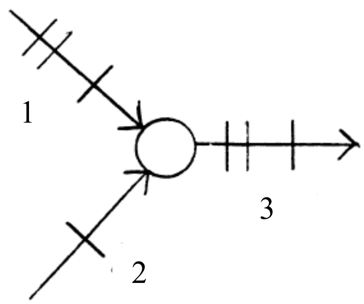
CLASSIFYING MEASUREMENTS AS REDUNDANT OR NON-REDUNDANT



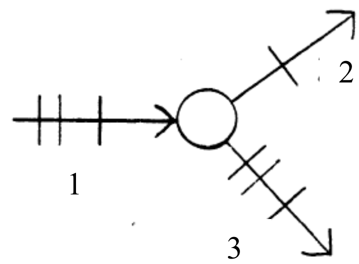
- IN THIS EXAMPLE, FLOW MEASUREMENTS 1 AND 4 ARE REDUNDANT, BUT FLOW MEASUREMENT 2 IS NOT.
- IF FLOW 2 WERE NOT MEASURED, IT COULD NOT BE CALCULATED.
- CANNOT JUST COUNT EQUATIONS AND MEASUREMENTS VS. VARIABLES. IN A LARGER SYSTEM, FINDING REDUNDANT VARIABLES MIGHT NOT BE OBVIOUS.
- A MEASUREMENT MUST BE REDUNDANT FOR “ADJUSTMENT” IN DATA REC.
- A VARIABLE MUST BE “OBSERVABLE” TO EVEN GET CALCULATED BY DATA REC.
- IMPACT OF OBSERVABILITY / REDUNDANCY ON ESTIMATORS, AND CLASSIFICATION ALGORITHMS ARE AVAILABLE.

REDUNDANCY EXAMPLES WITH MATERIAL AND ENERGY BALANCE

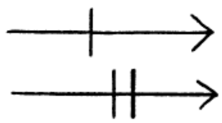
BLENDING



SPLITTING



KEY



Measured temperature

Measured flow

- MATERIAL BALANCE

  $f_1 + f_2 - f_3 = 0$ $\qquad$ $f_1 - f_2 - f_3 = 0$

- ENERGY BALANCE

  $f_1H_1 + f_2H_2 - f_3H_3 = 0$ $\qquad$ $f_1H_1 - f_2H_2 - f_3H_3 = 0$

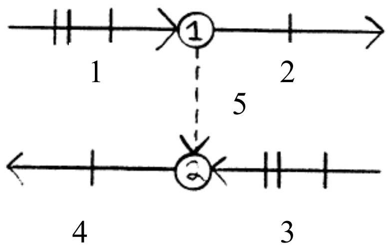
  where $H_i = H_i(T_i)$ = enthalpy of stream i
  f_i = mass flow of stream i
  T_i = temperature of stream i

- BLENDING CASE
  - Normally every measurement is redundant. For instance, if the f_3 measurements were deleted, f_3 could still be calculated using the material and energy balances.
  - However, if all temperatures (enthalpies) are equal, the flow measurements are not redundant, because the energy balance degenerates to the material balance (factor out enthalpy).

- SPLITTING CASE
  - Flow measurements are not redundant. As above, the energy balance always degenerates. Due to the additional constraints $T_1 = T_2 = T_3$, the temperature measurements are more redundant.

REDUNDANCY EXAMPLE WITH MATERIAL AND ENERGY BALANCES

HEAT EXCHANGER



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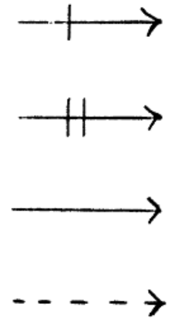


Measured temperature

Measured flow

Mass flow

Energy flow only

- MATERIAL BALANCES

$$f_1 - f_2 = 0$$
$$f_3 - f_4 = 0$$

- ENERGY BALANCES

$$f_1H_1 - f_2H_2 - e_5 = 0$$
$$f_3H_3 - f_4H_4 + e_5 = 0$$

where $H_i = H_i(T_i)$ = enthalpy of stream i
f_i = mass flow of stream i
T_i = temperature of stream i
e_i = energy flow of stream I

- CASE 1 - HEAT EXCHANGE IS OCCURRING ($e_5 \neq 0$)
  - Then f_3 is a redundant measurement. Even if it were deleted, f_3 could be calculated (by calculating e_5, then using energy balance around node 2)
  - Similarly, all other measurements are redundant

- CASE 2 - NO HEAT EXCHANGE IS OCCURRING ($e_5 = 0$)
  - Then f_1 and f_3 are not redundant, because the energy balance degenerates
  - Temperatures are still redundant

OTHER EXAMPLES OF SYSTEMS WITH REDUNDANT MEASUREMENTS

- DISTILLATION TOWERS WITH TOP AND BOTTOM PRESSURE MEASUREMENTS, AND ΔP MEASUREMENT

- ESTIMATION OF COMPOSITION USING PRESSURE-TEMPERATURE CURVES AND MEASUREMENTS vs. AN ANALYZER

  (e.g., BOILING ACID P, T vs. DENSITY ANALYZER)

"STEADY STATE" ESTIMATION ISN'T JUST FOR STEADY-STATE SYSTEMS

- DEPENDS ON TIME SCALE OF INTEREST
- "NETWORK" BALANCES HAVE BROAD APPLICABILITY
- MANY "FAST" DYNAMICS CAN BE NEGLECTED FOR ESTIMATION AND CONTROL OF SLOW PROCESSES
  - -- Heat Exchangers
  - -- Valve Dynamics
- OVERALL MASS BALANCES ARE ALWAYS GOOD IF HOLDUP CHANGES CAN BE NEGLECTED
  - -- Tower Levels
  - -- Tray Holdup
- INCLUDE LEVEL (VOLUME) DERIVATIVE OR DIFFERENCE TERMS IF HOLDUP IS SIGNIFICANT
  - -- Surge Drums
  - -- Reflux Drums, Flooded Condensers
- WITH SMALL HOLDUP, CAN NEGLECT DYNAMICS OF ENERGY OR COMPONENT MASS BALANCES
  - -- Note that sometimes holdup for some components can be very small, such as heavier-than-heavy key with feed near bottom.
- CAN USE DATA "SMOOTHING" APPROACH ON ANY DYNAMIC SYSTEM
  - -- Formulate as Discrete-Time Model
  - -- Use Model, Data Only for N Time Steps
  - -- Model Gets Built Into Measurement Matrix or Constraint Matrix, depending on Choice of Variables
  - -- "Least Squares" Filter Can be Derived This Way
- EXTREMELY SLOWLY CHANGING VARIABLES DISCUSSED LATER

DATA SMOOTHING APPROACH ON SURGE DRUM

MODEL:

$V(k) = V(k-1) + x_1(k) - x_2(k)$

$x_1(k)$ = FLOW IN AT TIME k

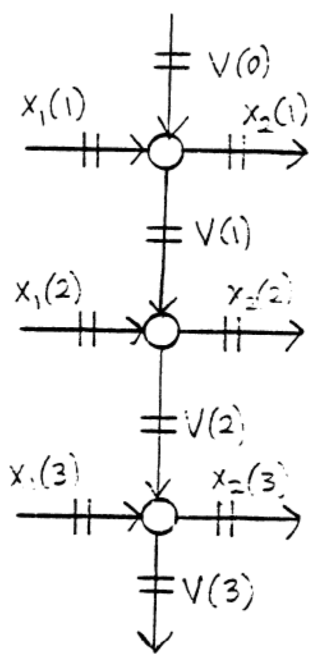
$x_2(k)$ = FLOW OUT AT TIME k

$V(k)$ = VOLUME (FROM LEVEL) AT TIME k

ALL VARIABLES MEASURED

AS AN EXAMPLE, SMOOTH DATA OVER 3 TIME PERIODS

This is equivalent to SS estimation on the following network:



DATA SMOOTHING IN A FIRST-ORDER LINEAR SYSTEM

MODEL: $x(k) = ax(k-1) + bu(k-1)$

MEASUREMENTS: All x(k) and u(k) measured

To smooth data over 3 time periods, use SS Technique on:

$$z = Hx + \text{noise}$$

$$z = \begin{bmatrix} x(0) \\ x(1) \\ x(2) \\ x(3) \\ u(0) \\ u(1) \\ u(2) \end{bmatrix} + \text{noise} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ a & b & 0 & 0 \\ a^2 & ab & b & 0 \\ a^3 & a^2b & ab & b \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x(0) \\ u(0) \\ u(1) \\ u(2) \end{bmatrix} + \text{noise}$$

Because

$$\begin{aligned} x(1) &= ax(0) + bu(0) \\ x(2) &= a^2 x(0) + abu(0) + bu(1) \\ x(3) &= a^3 x(0) + a^2bu(0) + abu(1) + bu(2) \end{aligned}$$

Once x(0) is estimated, x(3) can be calculated using the model. In a practical application, x(3) would be chosen as the independent variable, not x(0).

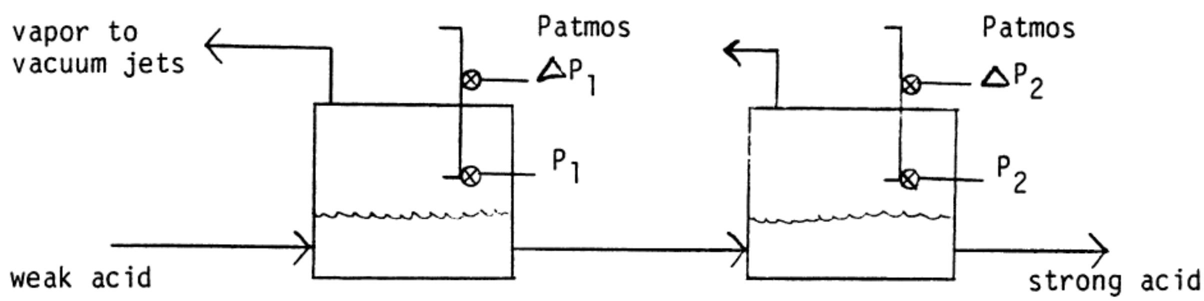
The "Least-Squares Filter" can be derived similarly, with a = b = 1, and deleting u(1) - u(k). u(0) is the unmeasured slope, and x(k) is the current estimate.

EXAMPLES OF SYSTEMS WITH QSS VARIABLES
("QUASI-STEADY STATE")

- ATMOSPHERIC PRESSURE (VACUUM SYSTEMS)

  Dual Acid Concentrators. Due to the "shared" variable (atmospheric pressure), there are already redundant measurements. In addition, atmospheric pressure only changes slowly, so its estimate is forced to change only slowly.

  (A barometer was not available online!)



- SLOWLY CHANGING COMPOSITIONS (EXAMPLE LATER)

- HEAT TRANSFER COEFFICIENTS

  Use the heat-transfer coefficient definition as an additional constraint and force the heat transfer coefficient to change very slowly

- CATALYST ACTIVITY

- INSTRUMENT BIAS

  e.g., transmitter zero error, wrong fluid on one side of delta-P cell, wrong specific gravity fluid for flows or levels, thermocouple coking.

- RATIO OF UNCONTROLLED FLOWS MAY BE CONSTANT DUE TO PIPING GEOMETRY (e.g., "SPLITTER, FURNACE PASSES)

  - even though individual flows change quickly, ratio does not

KALMAN FILTER OVERVIEW

- GENERATES BEST ESTIMATES OF VARIABLES IN A SYSTEM WITH MEASUREMENTS AND PROCESS MODEL (DYNAMIC)
- SOLUTION TO A GENERAL LEAST-SQUARES ESTIMATION PROBLEM
- "PREDICTOR - CORRECTOR" APPROACH:
  - PREDICTION BASED ON MODEL, PREVIOUS ESTIMATE
  - CORRECTION BASED ON MEASUREMENTS - PROVIDES FEEDBACK
- IN EFFECT, BALANCES MEASUREMENT INFORMATION vs. MODEL INFORMATION
- WEIGHTING FACTORS (VARIANCES) INDICATE QUALITY OF MEASUREMENTS AND MODELS
- CAN BE "TUNED" IN FAIRLY INTUITIVE WAY BY CHOOSING VARIANCES
- EXPONENTIAL FILTER IS AN EXAMPLE OF A KALMAN FILTER!
- A DISCRETE TIME MODEL AND FILTER EQUATIONS:
  - SYSTEM MODEL: $x(k) = \Phi x(k-1) + Bu(k-1)$ + process noise (variance Q)
  - MEASUREMENTS: $z(k) = Hx(k)$ + measurement noise (variance R)
  - KALMAN FILTER: $\hat{x}_{pred} = \Phi \hat{x}(k-1) + Bu(k-1)$ prediction

    $\hat{x}(k) = \hat{x}_{pred} + K(z(k) - H\hat{x}_{pred})$ correction

    (Gain matrix K requires calculations, based on Q, R, H, and Φ)

    (MORE GENERAL VERSIONS ARE AVAILABLE)

EXPONENTIAL FILTER AS A SPECIAL CASE OF KALMAN FILTER "RANDOM WALK"

- MODEL = RANDOM WALK MODEL ("DRUNK AROUND LAMPOST")

  $x(k) = x(k-1)$ + process noise (noise has variance q)

- MEASUREMENT:

  $z(k) = x(k)$ + noise (noise has variance r)

- FILTER:

$$\begin{aligned}\hat{x}(k) &= x_{pred} + K\,[z(k) - H\,x_{pred}] \\ &= \hat{x}(k-1) + K[z(k) - \hat{x}(k-1)] \\ &= (1-K)\,\hat{x}(k-1) + Kz(k)\end{aligned}$$

- FOR A LONG LAG: $q \to 0$ and $K \to 0$ (model so good, no measurements needed)
- FOR A SHORT LAG: $q \to \infty$ and $K \to 1$ (model so bad, it is ignored)
- RELATION TO CONTINUOUS-TIME FIRST ORDER LAG:

  For a first order lag with time constant τ, the equivalent exponential filter has

  $K = 1 - e^{-\Delta T/\tau}$

  where T is the sample interval

LITERATURE CITED

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