Principles of Dynamic Balancing

The principles of static balancing, also called measurement error reconciliation (MER), have been generalized to transient conditions. An exactly linear dynamic balance model has been stated where flow variables are assumed to be stochastic processes with independent increments. With this model the residual error of static MER due to dynamic effects can be estimated. Dynamic balancing is proposed as the estimation of flow and inventory variables by Kalman filtering applied to the balance model. The error of estimates obtained in this way is significantly less than that for the static MER estimates, even if the process is nearly in steady state. The main problem of dynamic balancing is that it requires not only the redundant observation of flow variables but also the observation of inventory variables. Compatibility of MER and dynamic balancing has been shown.

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Introduction

Measurement error reconciliation (MER) is a mathematical technique to test and improve the accuracy of process measurement data. It utilizes some *a priori* information about processes, and provides estimates that are more exact than the measurements themselves. The *a priori* information is given mainly in the form of linear relationships between process variables. If these relationships are formulated on the basis of rules of conservation, such as those of total mass, chemical elements, chemical invariants, nonreacting compounds in separation processes, or energy, this technique is called also balancing.

The first publications on this topic appeared in the early 1960s (Kuehn and Davidson, 1961; Swenker, 1964). Several subsequent papers have been published refining the basic idea and proposing some mathematical methods for gross error identification. Because there are good survey papers on the state of the art (Mah, 1987; Crowe, 1988), a detailed overview is not presented here. The common basic condition of almost all of the contributions is the steady state of the process concerned.

Only a few papers deal with balancing unsteady-state processes. Vaclavek (1974) applied correct dynamic balance equations to compute limits for static balancing. Stanley and Mah (1977) applied Kalman filtering to measurement error reconciliation of linear systems with flow and inventory variables. Rooney et al. (1978) used Kalman filtering similarly but without really considering the rules of conservation. Darouach et al. (1988) proposed taking into consideration the time correlation of flow variables but without considering inventory variables. This topic was discussed recently at the AIPAC' 89 Symposium (Almasy, 1989). Up to now there has not been a sound theoretical basis for the problem of balancing unsteady state processes comparable to that of MER for steady-state balancing.

On the other hand, a very popular topic is the so-called analytical redundancy, utilizing filtering, observers, or parity equations, and its application to monitoring, mostly called sensor validation and fault detection and isolation in the control literature. The relevant literature includes a survey paper by Frank (1989), various papers presented at the AIPAC '89 Symposium, and papers by Willsky and Jones (1976), Gertler (1988), and Narasimhan and Mah (1988). Although these methods are closely related in their aims to use MER and gross error identification, in essence they cannot be regarded as extensions of MER to unsteady-state processes because they are not on a balance equation basis.

There are essential differences between the above two approaches. Static balancing applies, at least in its strict sense, only exact and unquestionable knowledge about the process (apart from that of measurement error distribution) but does not take into consideration the time correlation of data or any other information on process behavior, either static or dynamic. Thus, the verification of measurements is not complete by balancing; only errors influencing the balance can be detected in this way. On the other hand, dynamic filtering supposes full knowledge of process dynamics and works sufficiently quickly only if the model is linear. Neglecting nonlinearities is dangerous and can mislead estimation greatly. Even if the process model is correctly linearized locally and filtered by the so-called extended Kalman filter, sufficiently simple nonlinear models themselves are of questionable accuracy in many situations in chemical engineering. Sometimes their accuracy is less than

that of the measurements, so that filtering on this basis would cause higher error than unfiltered measurement data are subject to.

The aim of this paper is to extend the principles of static balancing to the unsteady state. The basic principles, possibilities, advantages, and limitations of dynamic balancing are discussed. The application of dynamic balancing to other than measurement error reconciliation, such as to fault detection, extreme event detection, and others, has been left to further contributions.

Balance Equations as Linear Submodels

Almost without exception, chemical engineering processes are nonlinear. The main feature of static balancing is the application of strictly linear balance equations of physics for validity tests even if the process itself is nonlinear. Balance equations can be regarded as exactly linear submodels of the process.

We say that a dynamic mathematical model contains a linear submodel if, after appropriate transformation of the variables, it can be decomposed into two submodels so that one of them describes the behavior of a subset of state variables and is linear. Formal mathematical treatment, such as definition and conditions of existence, is not given here. According to the following, the existence of a linear submodel in a well-posed model, describing all environmental effects, is evident if the system contains components that are subject to laws or rules of conservation.

It is easy to see that laws of conservation of physics or other rules of conservation can be expressed as linear submodels. These submodels express the fact that the amounts of components present in the system that obey these rules change only due to environmental effects. These environmental effects are essentially those called flow variables (FV) in the relevant literature. These submodels are usually called balance equations. In this sense balance equations do not express knowledge about the detailed dynamics of the process. Components subject to independent rules of conservation in the actual system are essentially the same as what are called inventory variables (IV) in the literature.

All physical effects influencing the process, either observed or unobserved, including inlets (physical inputs), outlets (physical outputs), losses, or others, are considered as FVs in the following. These FVs, regardless of their physical direction, will be considered as random information inputs, and measurements as outputs (information outputs). Thus the words "input" and "output" will be used according to their sense in system and control theory. Inputs and physical inlets, outputs and physical outlets shall be carefully distinguished. It is very important in the following that balance equations in this framework do not contain so-called source terms describing time dependence of the amounts of components inside the system (i.e., that of chemical compounds or energy, depending on chemical reaction rate). This means that the concept of a balance equation is used in a more narrow sense than is often the practice in chemical engineering science. In principle, the very same interpretation of balance equations is applied here as in MER, considered as static balancing.

It is fundamental in this work that FVs are considered as multidimensional self-correlated stochastic processes with independent zero mean white Gaussian stationary increments where the increments represent in practice the process noises or disturbances. This assumption corresponds to the very general fact that both inlets and outlets of real processing plants are self-correlated and their significant jumps are to be regarded as extraordinary events. Moreover, signaling such events is regarded as one of the main functions of monitoring systems. The above process model and its critique will be discussed in the section on noise distribution.

Naturally, in the case of composite systems, corresponding physical outlets of a subsystem are identical with the physical inlets of others, just as in the case of static balancing.

Dynamic Balance Model

According to the above concepts, rules of conservation are state space models where inventory variables $\boldsymbol{x}$ are the state variables and flow variables $\boldsymbol{e}$ are the formal process inputs:

$$\boldsymbol{x}_k = \boldsymbol{x}_{k-1} + \boldsymbol{G} * \boldsymbol{e}_{k-1} \tag{1}$$

It will be shown later that matrix $\boldsymbol{G}$ is essentially the same as the coefficient matrix used in static balancing where the change of IVs within the system is assumed to be zero. Note that matrix $\boldsymbol{G}$ is generally not square, that is, the number of elements of $\boldsymbol{e}$ is not necessarily equal to that of $\boldsymbol{x}$.

The flow variables are assumed to be self-correlated stochastic processes, with dynamics

$$\boldsymbol{e}_k = \boldsymbol{e}_{k-1} + \boldsymbol{w}_{k-1} \tag{2}$$

Thus $\boldsymbol{e}$ is a process with independent random increments $\boldsymbol{w}$, of incremental variance $\boldsymbol{W}$. The pair of Eqs. 1 and 2 is referred to as the balance model.

The most important feature of the above balance model is that $\boldsymbol{G}$ does not depend on the detailed dynamics of the process and usually can be specified on *a priori* knowledge (graphs describing networks, stoichiometric coefficients in chemical, Kirchhoff equations in electrical problems, etc.).

It should be noted that, in practice, the amounts of IVs present possibly bias FVs either by regulator action, manual control, or due to equipment construction and layout. If such state feedback exists and is not observed, it disturbs the simplicity and exactness of the above model. This is discussed further in the section on state feedback. First we discuss the state feedback free case.

The above balance model can easily be reduced into standard linear state space model form, composing Eqs. 1 and 2 into a common state space model. With

$$\boldsymbol{z} = \begin{pmatrix} \boldsymbol{x} \\ \boldsymbol{e} \end{pmatrix}$$

the $n(\boldsymbol{x}) + n(\boldsymbol{e})$ dimensional composite state variable of the balance model

$$\boldsymbol{z}_k = \begin{pmatrix} \boldsymbol{I} & \boldsymbol{G} \\ \boldsymbol{O} & \boldsymbol{I} \end{pmatrix} * \boldsymbol{z}_{k-1} + \begin{pmatrix} \boldsymbol{O} \\ \boldsymbol{I} \end{pmatrix} * \boldsymbol{w}_{k-1}$$

is obtained. Introducing new notation, Eqs. 1 and 2 become

$$\boldsymbol{z}_k = \Phi * \boldsymbol{z}_{k-1} + \Gamma * \boldsymbol{w}_{k-1} \tag{3}$$

Equation 3 is an autonomous stochastic state space model. Naturally, Φ with its minor G does not depend on the detailed dynamics of the process either.

It should be noted for readers familiar with control theory concepts that all modes of this state space model are unity, that is, all eigenvalues of the coefficient matrix Φ are 1, in accordance with Almasy and Virag (1986). A consequence of this fact is that balance models are not suitable for design of control.

Observation

Sometimes the state variables of the balance model differ from those that are directly measured in chemical engineering systems. Their dependence on each other, however, must be known for any state estimation. The mathematical description of these dependencies is the so-called observation model or observation equations. Not only state transition equations but also observation equations are often nonlinear in chemical engineering practice.

The treatment here is restricted to the direct observation case. The reason for this is its relative simplicity. But it can be assumed that smooth nonlinear relations between measured and state variables do not cause serious troubles or estimation errors if the former can be expressed as a function of the latter. In such cases the calculated values may be regarded as measured. This is discussed later, in the noise distribution section.

Let us assume that the state variables of the composite balance model are directly observed, that is, measured, subject to an additive zero mean, state-independent, uncorrelated measurement error, as is also assumed in the static balancing case for FVs. This is expressed by the observation equations

$$\tilde{\boldsymbol{x}}_k = \boldsymbol{x}_k + \boldsymbol{q}_k \tag{4}$$

$$\tilde{\boldsymbol{e}}_k = \boldsymbol{e}_k + \boldsymbol{r}_k \tag{5}$$

or the same for the composite model as

$$\tilde{\boldsymbol{z}}_k = \boldsymbol{z}_k + \boldsymbol{s}_k \tag{6}$$

with $\boldsymbol{q}$, $\boldsymbol{r}$, and $\boldsymbol{s}$ independent time-correlated measurement noises of variances $\boldsymbol{Q}$, $\boldsymbol{R}$, and $\boldsymbol{S}$.

A precondition for stable estimation is the observability of the system concerned. The question of observability is of high importance with respect to dynamic balancing. It can be stated generally that there are more measured variables necessary to dynamic than to static balancing of the same process: not only flow variables but also the quantities of inventory variables present must be observable. In the static balancing case these latter are postulated as time independent and their values are irrelevant.

The related concept of observability in control theory is controllability. Its role in balancing means that the coefficient G must be of full row–rank in order to have the system controllable, to allow any changes in each IV.

Note that if the state variables are measured indirectly, there is no reason not to incorporate the functional relationship between measured and state variables into the model, as is usual in state space modeling.

Noise Distribution

Introducing the concept of process noise needs a somewhat unusual way of looking at chemical processes. As discussed earlier, flow variables are considered as unknown representations of stochastic processes. In principle their value at a given time instance can be estimated if there is sufficient information about them. Indeed, the magnitude of any FV in a plant is never exactly constant and never exactly known. Its changes are random and unknown to the operator unless it has been observed either directly or in some indirect way. Even a handle position, in the absence of a measuring instrument, must be observed.

The supposition that the FVs are self-correlated, as described by Eq. 2, is essential as well. Indeed, self-correlation of FVs is general in chemical processes and uncorrelated FVs must be very rare. It is reasonable therefore to consider uncorrelated sudden jumps of FVs as extraordinary events that are to be signaled.

Almost nothing is known about the adequate stochastic model of process noise in chemical processes. For their increments we consider first the Gaussian distribution for practical reasons, namely, this results in linear estimation formulas in the case of linear systems. It can be assumed to be more or less adequate in many cases; however, it is never exactly correct because all FVs are limited while processes defined by Eq. 2 are not. As an example, consider a buffer tank of limited capacity between two streams. Near the capacity limits, either upper or lower, the distribution of the change in the corresponding flow rates is certainly asymmetrical and bounded, contradicting the Gaussian model. It is a challenge for systems engineers to find appropriate models that are more adequate to several practical cases and are simple enough to result in useful algorithms for estimation.

The self-correlation of outlet increments due to the process is not taken into consideration.

The problem of a random measurement error model seems to be much simpler and is the same as in the case of static balancing. Measurement errors are usually supposed to be multidimensional zero mean Gaussian white noise, and this is adequate in many cases. Problems arise when the state variables are nonlinear functions of the observed quantities. It can be assumed that the observed values can be transformed into state variables easily, even if this transformation is nonlinear. The problem is that these transformations distort the distribution of measurement errors so that if they were Gaussian, that of the transformed observation is not any more. In the case of strong nonlinearities there is also a danger of biasing. Again, studies are necessary to decide in each actual case if the use of a Gaussian model for the transformed error is allowed or not. It should be noted that state estimation by Kalman filter keeps its minimum variance property even if the distributions are non-Gaussian. The only thing that gets lost in this way is the maximum likelihood (ML) property of the estimate.

State Feedback

Flow variables can be influenced by the present values of inventory variables. This influence is called state feedback. The problem is treated here according to whether state feedback is observed or not and is linear or not.

Observed state feedback

An observed state feedback, depending either linearly or nonlinearly on the state variables, can be regarded as an FV and handled exactly in the same manner as any other FV. If its dependence is exactly known in the form of one or more model equations, this knowledge is additional information about the process, enhancing the quality of estimation. But if there is any doubt about the model adequacy, it seems to be more advantageous to discard it, in order to avoid biased estimation.

Linear state feedback

State feedback, either observed or unobserved, can be included in the balance model if the feedback rule is known and linear. It may be represented by additional linear terms in the state transition and FV models. Thus they become

$$x_k = x_{k-1} + \Psi_P * (x_{k-1} - x^s) + G * e_{k-1} \tag{7}$$

$$e_k = e_{k-1} + \Psi_I * (x_{k-1} - x^s) + w_{k-1} \tag{8}$$

with constant setpoint vector x^s. Note that now in Eq. 7 the term $G * e_{k-1}$ represents only those FVs that are not included in the state feedback term.

The standard state space model form can be obtained by combining Eqs. 7 and 8 into the single state space model

$$z_k = \left(\begin{pmatrix} I & G \\ O & I \end{pmatrix} + \begin{pmatrix} \Psi_P & O \\ \Psi_I & O \end{pmatrix}\right) * z_{k-1} + \begin{pmatrix} O \\ I \end{pmatrix} * w_{k-1} - \begin{pmatrix} \Psi_P \\ \Psi_I \end{pmatrix} * x^s$$

With

$$z^s = \begin{pmatrix} x^s \\ O \end{pmatrix}$$

and $\zeta = z - z^s$, Eqs. 7 and 8 become

$$\zeta_k = \Phi * \zeta_{k-1} + \Gamma * w_{k-1} \tag{9}$$

This corresponds formally to Eq. 3 but with an altered meaning of notation.

Matrix coefficients Ψ_P and Ψ_I are assumed to be known. But this is not a serious restriction provided that they can be estimated on the basis of measurements. Ψ_P is the matrix of proportional control coefficients (diagonal in the case of independent control), and Ψ_I the same for integral control. Equation 9 is no longer as exact as the state feedback free balance equation, Eq. 3, and the modes of this model are no longer unity.

The above state feedback model can be included in the balance model whether the feedback is measured or not.

Unobserved nonlinear state feedback

This problem cannot be handled by a linear model and seems to be of similar complexity as any other nonlinear filtering problem. Therefore this case cannot be handled as simply as other balancing problems and is not treated in this paper. If balancing is of high importance, additional instrumentation is recommended in order to make all nonlinear state feedback effects observed. This situation is represented later in example 4.

Estimation

The primary application of the dynamic balance model is the estimation of measured variables. This corresponds in its function to MER in the static case. The evident way is maximum likelihood estimation on the basis of the balance model. For the sake of comparison the error due to process changes, using the MER estimator is treated first.

Estimation error of MER

With the notation of the balance model, Eqs. 3 and 6, the usual MER estimator with the static condition $G * e_k = 0$ is

$$\hat{e}_{\mathrm{MER},k} = [I - R * G' * (G * R * G')^{-1} * G] * \tilde{e}_k \tag{10}$$

The residual estimation error, involving unsteady state effects, can be obtained on the basis of the dynamic balance model. According to the results of Appendix 1, supplied in the supplementary material, it is

$$E_{\mathrm{MER|\,unsteady}} = R - R * G' * (G * R * G')^{-1} * G * R + R * G' * (G * R * G')^{-1} * (G * W * G') * (G * R * G')^{-1} * G * R \tag{11}$$

The last term of this formula is the increment of estimation error due to the dynamic effects. Since it is positive definite, the estimation error variance of MER increases if FVs are not exactly time independent. MER is useful only when $G * W * G'$ is significantly less than $G * R * G'$ (e.g., according to the maximum eigenvalue norm). A good basis to estimate the efficiency of MER is the fact that the estimation error variance $E_{\mathrm{MER|\,unsteady}}$ is exactly equal to R when $W = R$, as can be seen directly from Eq. 11.

ML estimator

Equations 3 and 6 are of the form of the generally used discrete time, time invariant, linear state space models. The maximum likelihood state estimation of such systems is the well-known and widely used Kalman filter. Thus, the dynamic balancing problem is reduced to the usual Kalman filtering with the model consisting of Eqs. 3 and 6. Details of filtering are not treated here, but are available in several textbooks (Gelb et al., 1974; Anderson and Moore, 1979; Brown, 1983).

Making use of the special assumption that all state variables are directly observed in the balance model, the formulas are as follows (see Appendix 2 in the supplementary material). The estimator for dynamic balancing is

$$\hat{z}_k = (\Phi - K_{k-1}) * \hat{z}_{k-1} + K_{k-1} * \tilde{z}_{k-1} \tag{12}$$

with the so-called Kalman gain

$$K_{k-1} = \Phi * Z_{k-1} * (S + Z_{k-1})^{-1} \tag{13}$$

Z is the matrix of estimation error variance and is time dependent. It can be computed recursively with the formula

$$Z_k = \Gamma * W * \Gamma' + \Phi * [Z_{k-1} - Z_{k-1} * (S + Z_{k-1})^{-1} * Z_{k-1}] * \Phi' \quad (14)$$

Knowledge of W, the incremental variance of FVs as stochastic processes, is additional information about the process, compared to the static treatment, that is necessary to handle the problem also in unsteady state. However, if W is specified more or less correctly, it enhances the quality of estimation, as can be seen later in comparative numerical examples.

Under very general conditions the estimation error variance Z_k tends to a limit for $k \rightarrow \infty$. This limit can be computed either recursively or through solving a nonlinear matrix equation, the so-called matrix Riccati equation (Laub, 1985).

Compatibility of Dynamic and Static Balancing

It is a natural requirement that dynamic balancing should include the usual MER algorithm as the limit for steady state conditions.

It can be stated by inspection that balance Eq. 1 together with observation Eq. 5 reduces to the problem of linear MER if x_k is independent of time. Thus, the constrained ML state estimation must give the same result under steady-state conditions with either steady-state or dynamic estimation formulas.

It is lengthier to show compatibility by algebraic means. The balance model given in Eqs. 1 to 5 offers the possibility of showing how compatibility can be understood. But the original Kalman filter is unable to provide this as a limit because it inherently supposes the self-correlated property of state variables and becomes meaningless in the static limit case.

In order to obtain the formula of static balancing, ML estimation of e_k on the basis of the dynamic balance model and on measurements up to time instance k is necessary, specifying the static condition as

$$x_k - x_{k-1} = 0$$

The estimator, according to Appendix 3 in the supplementary material, results in

$$\hat{e}_k = [I - R * G' * (G * R * G')^{-1} * G] * \tilde{e}_k = \hat{e}_{\mathrm{MER},k} \quad (15)$$

which is identical with the usual formula for static balancing or MER. As can be seen, the incremental variance W of FVs does not play any role now in the estimation, as is obvious in the case of static balancing.

Examples

1. Container with several inlets and outlets

Let us consider a container, and a fluid as IV. Let the amount of fluid contained be denoted by the scalar x, that is, $n(x) = 1$. Several fluid inlets and outlets are connected to the container and an element of vector e is associated with each inlet and outlet. Thus the change of the IV is the algebraic sum of all e_i (inflow positive, outflow negative), so that the balance model can be written as

$$x_k = x_{k-1} + \mathbf{1}' * e_{k-1}$$

This means that in this case matrix coefficient G is a row vector of elements 1:

$$G = \mathbf{1}' = (1, 1, \ldots, 1)$$

A paper by Griffin et al. (1988) reports on an application resembling this type of balancing if only the amount of fluid is considered.

Numerical Examples. Let us investigate the case of a container with two connected flows. Assume for both flows equal incremental variances and equal measurement error variances. Results with

$$Q = I, \quad W = \alpha * I, \quad R = \beta * I,$$
$$\alpha = 1/4, 1, 4, 16, \quad \text{and} \quad \beta = 1/8, 1/4, 1/2, 1, 2, 4, 8$$

are presented in Table 1. It can be concluded from the data in Table 1 that:

- The trace of the dynamic balancing estimation error variance is always less than that of MER. This is necessarily so and is good to verify the correctness of the theoretical result.
- The gain that can be obtained by MER is never higher than reducing the trace of measurement error variance to a limit. In this example the values $\mathrm{tr}(R)/\mathrm{tr}(E_{\mathrm{MER}})$ never reach 2. The ratio $\mathrm{tr}(E_{\mathrm{MER}})/\mathrm{tr}(E)$ is very high if the incremental variance of changes of FVs is high and measurement error variance is low. But in this case the gain that can be achieved compared to the measurement error, that is, $\mathrm{tr}(R)/\mathrm{tr}(E)$, is very near to 1 (row 22, 23, Table 1).
- The best results have been obtained in cases when the trace of incremental variance is small compared to that of the measurement errors of present amounts of IVs; see the case of $\mathrm{tr}(W) = 0.25$, $\mathrm{tr}(R) = 8$ in row 7, where the error variance of the estimated values is more than 8 times less than that of the measurement error.

Note that these conclusions are true for the simplest possible case. The qualitative statements, however, seem to be valid in general, as it can be seen from the next examples.

2. Network of flows

Consider a complex network of flows of some component subject to a rule of conservation (gas, water, total mass irrespective of its composition, energy, electrical current, etc. Then matrix G, specifying the balances in each node, is the node–arch incidence matrix of the directed graph describing the arrangement. Let us regard the network according to the scheme given in Figure 1, where each node represents a container. Matrix G is given in Table 2 in tabular form describing the balances.

Table 1. Results for Example 1

Row No.	tr(W)	tr(R)	tr(E)	tr(E_{MER})	$\frac{tr(R)}{tr(E)}$	$\frac{tr(R)}{tr(E_{MER})}$	$\frac{tr(E_{MER})}{tr(E)}$
1	0.2500	0.1250	0.0896	0.1875	1.3954	0.6667	2.0931
2	0.2500	0.2500	0.1477	0.2500	1.6930	1.0000	1.6930
3	0.2500	0.5000	0.2304	0.3750	2.1706	1.3333	1.6279
4	0.2500	1.0000	0.3431	0.6250	2.9143	1.6000	1.8214
5	0.2500	2.0000	0.4941	1.1250	4.0481	1.7778	2.2770
6	0.2500	4.0000	0.6955	2.1250	5.7513	1.8824	3.0554
7	0.2500	8.0000	0.9658	4.1250	8.2830	1.9394	4.2709
8	1.0000	0.1250	0.1121	0.5625	1.1155	0.2222	5.0199
9	1.0000	0.2500	0.2054	0.6250	1.2173	0.4000	3.0433
10	1.0000	0.5000	0.3583	0.7500	1.3954	0.6667	2.0931
11	1.0000	1.0000	0.5907	1.0000	1.6930	1.0000	1.6930
12	1.0000	2.0000	0.9214	1.5000	2.1706	1.3333	1.6279
13	1.0000	4.0000	1.3726	2.5000	2.9143	1.6000	1.8214
14	1.0000	8.0000	1.9763	4.5000	4.0481	1.7778	2.2770
15	4.0000	0.1250	0.1213	2.0625	1.0306	0.0606	17.0044
16	4.0000	0.2500	0.2359	2.1250	1.0599	0.1176	9.0093
17	4.0000	0.5000	0.4482	2.2500	1.1155	0.2222	5.0199
18	4.0000	1.0000	0.8215	2.5000	1.2173	0.4000	3.0433
19	4.0000	2.0000	1.4333	3.0000	1.3954	0.6667	2.0931
20	4.0000	4.0000	2.3627	4.0000	1.6930	1.0000	1.6930
21	4.0000	8.0000	3.6856	6.0000	2.1706	1.3333	1.6279
22	16.0000	0.1250	0.1240	8.0625	1.0078	0.0155	65.0011
23	16.0000	0.2500	0.2462	8.1250	1.0155	0.0308	33.0022
24	16.0000	0.5000	0.4852	8.2500	1.0306	0.0606	17.0044
25	16.0000	1.0000	0.9435	8.5000	1.0599	0.1176	9.0093
26	16.0000	2.0000	1.7929	9.0000	1.1155	0.2222	5.0199
27	16.0000	4.0000	3.2860	10.0000	1.2173	0.4000	3.0433
28	16.0000	8.0000	5.7331	12.0000	1.3954	0.6667	2.0931

Numerical Examples. Let:

$$\begin{pmatrix} 10.1 & -0.1 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ -0.1 & 10.3 & -0.1 & -0.1 & 0.0 & -10.0 & -0.1 & 0.0 & -0.1 & 0.0 \\ 0.0 & -0.1 & 0.3 & 0.0 & -0.1 & -0.1 & 0.1 & -0.1 & 0.0 & 0.0 \\ 0.0 & -0.1 & 0.0 & 0.2 & -0.1 & 0.0 & 0.0 & 0.0 & 0.1 & 0.0 \\ 0.0 & 0.0 & -0.1 & -0.1 & 10.2 & -10.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & -10.0 & -0.1 & 0.0 & -10.0 & 30.1 & 0.0 & 0.1 & 0.0 & -10.0 \\ 0.0 & -0.1 & 0.1 & 0.0 & 0.0 & 0.0 & 0.1 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & -0.1 & 0.0 & 0.0 & 0.1 & 0.0 & 0.1 & 0.0 & 0.0 \\ 0.0 & -0.1 & 0.0 & 0.1 & 0.0 & 0.0 & 0.0 & 0.0 & 0.1 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & -10.0 & 0.0 & 0.0 & 0.0 & 10.0 \end{pmatrix}$$

$$Q = 5.0 * I, W = \alpha * 10^{-3}, R = \beta * I$$

varying the values of scalar α and $\beta = 1/16$, 1, 16. Results are tabulated in Table 3.

In general, the conclusions are the same as those drawn from example 1. The extremely high values of tr(R)/tr(E) and tr(E_{MER})/tr(E) are due to the low variance of increments compared to that of measurement errors. Note that these high values can be obtained only after long periods of trouble-free operation.

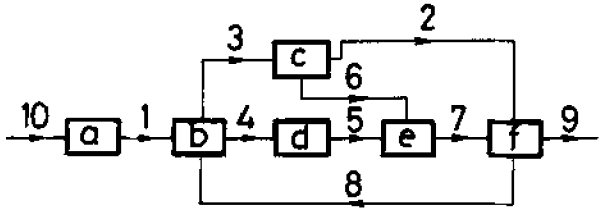

Figure 1. Network of fluid flows.

3. Complex chemical reaction

Let us consider a perfectly stirred tank reactor where a mixture of nitrogen oxides reacts with oxygen and water, producing nitrous and nitric acids.

Let vector x_k be the amount of chemical elements contained at time instance k. Chemical elements to be considered are

x_1 = N, nitrogen
x_2 = H, hydrogen
x_3 = O, oxygen

There are several inlets and outlets of reacting components:

e_j = NO in, moles of entering nitrogen monoxide

Table 2. Matrix G for Example 2

	Arcs									
Nodes	1	2	3	4	5	6	7	8	9	10
a	−1	0	0	0	0	0	0	0	0	1
b	1	−1	0	−1	0	0	0	1	0	0
c	0	1	−1	0	0	−1	0	0	0	0
d	0	0	0	1	−1	0	0	0	0	0
e	0	0	0	0	1	1	−1	0	0	0
f	0	0	1	0	0	0	1	−1	−1	0

Table 3. Results for Example 2

Row No.	tr(W)	tr(R)	tr(E)	tr(E_{MER})	$\frac{tr(R)}{tr(E)}$	$\frac{tr(R)}{tr(E_{MER})}$	$\frac{tr(E_{MER})}{tr(E)}$
1	0.00446	0.625	0.020	0.252	30.109	2.472	12.178
2	0.00446	10.000	0.054	4.002	183.489	2.498	73.446
3	0.00446	160.000	0.137	64.00	1164.09	2.499	465.656
4	0.07150	0.625	0.095	0.294	6.552	2.121	3.087
5	0.07150	10.000	0.332	4.044	30.109	2.472	12.178
6	0.07150	160.000	0.871	64.04	183.489	2.498	73.446
7	1.14400	0.625	0.246	0.962	2.531	0.649	3.899
8	1.14400	10.000	1.526	4.712	6.552	2.121	3.087
9	1.14400	160.000	5.313	64.712	30.109	2.472	12.178

e_2 = NO_2 in, moles of entering nitrogen dioxide
e_3 = HNO_2 in, moles of entering nitrous acid
e_4 = HNO_3 in, moles of entering nitric acid
e_5 = O_2 in, moles of entering oxygen
e_6 = H_2O in, moles of entering water
e_7 = NO out, moles of exiting nitrogen monoxide
e_8 = NO_2 out, moles of exiting nitrogen dioxide
e_9 = HNO_2 out, moles of exiting nitrous acid
e_{10} = HNO_3 out, moles of exiting nitric acid
e_{11} = O_2 out, moles of exiting oxygen
e_{12} = H_2O out, moles of exiting water
e_{13} = N_2O_4 out, moles of exiting dinitrogen oxide

Coefficient matrix G of the balances of chemical elements is composed from the appropriate stoichiometric coefficients, with positive sign for entering and negative for exiting flows, as shown in Table 4.

Numerical Examples. Let

$$Q = \text{diag}(0.1,0.01,0.1), \quad W = \alpha * 0.01 * I$$

$$R = \beta * \text{diag}(0.1,0.05,0.1,0.1,0.2,0.01,0.2,0.1,$$
$$0.1,0.1,0.1,0.1,0.1)$$

varying the values of scalar α and $\beta = 1/16$, 1, 16. Results are tabulated in Table 5.

The conclusions are in general the same as those drawn from examples 1 and 2.

4. Two-tank or double-integrator example

Consider a system consisting of two tanks as shown in Figure 2. If linearization is permissible, this leads to the typical control engineering example of a double integrator (Astrom and Wittenmark, 1984).

The first tank is fed by an inlet liquid flow e_o. The liquid level therein is denoted by x_1. The second tank is fed by an inlet liquid flow e_1 originating from tank 1 and depending on liquid level x_1. The level therein is denoted by x_2. The outlet of the system is the flow leaving tank 2, denoted by e_2. It depends on the level x_2. Each variable, inlets, outlets, and liquid levels are assumed to be observed.

A Nonlinear Model. The system can be described by the nonlinear state space model

$$\begin{aligned} x_{1,k} &= x_{1,k-1} - f_1(x_{1,k-1}) + e_{0,k-1} \\ x_{2,k} &= x_{2,k-1} + f_1(x_{1,k-1}) - f_2(x_{2,k-1}) \end{aligned} \tag{E4.1}$$

and

$$\begin{aligned} \tilde{x}_{1,k} &= x_{1,k} + s_{x,1,k} \\ \tilde{x}_{2,k} &= x_{2,k} + s_{x,2,k} \\ \tilde{e}_{1,k} &= f_1(x_{1,k-1}) + s_{e,1,k} \\ \tilde{e}_{2,k} &= f_2(x_{2,k-1}) + s_{e,2,k} \end{aligned} \tag{E4.2}$$

with

$$f_j(x) = a_j * x^{0.55}, \quad j = 1, 2 \tag{E4.3}$$

where s_x and s_e are the measurement errors. The model is nonlinear because the flow leaving a tank depends nonlinearly on the inventory variable, as expressed by functions $f_j(.)$, $j = 1, 2$. It is an adequate model if liquid levels are always high enough so that the flows are turbulent.

A possible approach to filtering the measurement errors would be to apply Eq. E4. 3, the relationship between liquid level and flow rate, in some kind of nonlinear filtering scheme. However, the high computational efforts involved are not justified unless the problem is of extreme technical importance. Note that the system would also be observable without measuring $\tilde{e}_{1,k}$.

Notice that, contrary to MER, this model is unsuitable for handling measurement errors uniformly. There is an essential asymmetry in handling the inlet and outlet flow measurement errors: $e_{o,k}$ is regarded here as exactly known and is unobservable while e_1 and e_2 are observable.

A Linearized Model. The conventional linear state space model is formulated as

$$\begin{aligned} \xi_{1,k} &= \xi_{1,k-1} - \alpha_1 * \xi_{1,k-1} + e_{0,k-1} \\ \xi_{2,k} &= \xi_{2,k-1} + \alpha_1 * \xi_{1,k-1} - \alpha_2 * \xi_{2,k-1} \end{aligned} \tag{E4.4}$$

and

$$\begin{aligned} \tilde{\xi}_{1,k} &= \xi_{1,k} + s_{x,1,k} \\ \tilde{\xi}_{2,k} &= \xi_{2,k} + s_{x,2,k} \\ \tilde{e}_{1,k} &= \alpha_1 * \xi_{1,k-1} + s_{e,1,k} \\ \tilde{e}_{2,k} &= \alpha_2 * \xi_{2,k-1} + s_{e,2,k} \end{aligned} \tag{E4.5}$$

Table 4. Matrix G for Example 3

Chemical Elements	Compound Flows												
	1	2	3	4	5	6	7	8	9	10	11	12	13
Nitrogen	1	1	1	1	0	0	−1	−1	−1	−1	0	0	−2
Hydrogen	0	0	1	1	0	2	0	0	−1	−1	0	−2	0
Oxygen	1	2	2	3	2	1	−1	−2	−2	−3	−2	−1	−4

Here

$$\alpha_j * \xi_j \quad \text{with} \quad \xi_j = x_j - \bar{x}_j, \quad j = 1, 2$$

is the linear approximation of $f_j(\xi_j)$, around suitably chosen operating points $\bar{x}_j$.

The above model can be written in the usual linear state space model form

$$z_k = \Phi * z_{k-1} + e_{k-1} \tag{E4.4}$$

$$\tilde{y}_k = \Theta * z_k + q_k \tag{E4.5}$$

Note that this is not a balance but a general linear state space model. Thus, the notation is inconsistent with Eqs. 1 to 6. The special notation of this example is as follows:

$$z = \begin{pmatrix} \xi_1 \\ \xi_2 \end{pmatrix} \tilde{y} = \begin{pmatrix} \tilde{\xi}_1 \\ \tilde{\xi}_2 \\ \tilde{e}_1 \\ \tilde{e}_2 \end{pmatrix} \quad e = \begin{pmatrix} e_0 \\ 0 \end{pmatrix}$$

$$\Phi = \begin{pmatrix} 1-\alpha_1 & 0 \\ \alpha_1 & 1-\alpha_2 \end{pmatrix} \quad \Theta = \begin{pmatrix} 1 & 0 \\ 0 & 1 \\ \alpha_1 & 0 \\ 0 & \alpha_2 \end{pmatrix}$$

with deterministic input e_0.

This model formally describes the process dynamics, but is valid only in a narrow range of ξ. Out of its validity range it leads to biased estimation.

The above model does not reflect the conservation property of liquid. In order to obtain such a balanced state transition matrix, Φ should have been decomposed into two terms, one expressing the balance, the other the state feedback. Note that state feedback is not due to any control device but to the system itself.

As for the asymmetry of handling flow measurements, the same is true here as in the former nonlinear case.

Balance Model. There are two ways of constructing balance models. The system can be regarded as composed of two tanks with distinct balances for both, or as a simple one with a global balance for the sum of total liquid contained in both tanks. The composite balance model is discussed first.

In order to obtain a balance model, a modification of the original nonlinear model is necessary. The essence of this modification is that flows leaving the tanks are now only observed and not computed from the liquid levels. Regarding them as stochastic processes with independent increments, model Eqs. E4.1 and E4.2 becomes

$$\begin{aligned} x_{1,k} &= x_{1,k-1} + e_{0,k-1} - e_{1,k-1} \\ x_{2,k} &= x_{2,k-1} + e_{1,k-1} - e_{2,k-1} \\ e_{0,k} &= e_{0,k-1} + w_{0,k-1} \\ e_{1,k} &= e_{1,k-1} + w_{1,k-1} \\ e_{2,k} &= e_{2,k-1} + w_{2,k-1} \end{aligned} \tag{E4.6}$$

and

$$\begin{aligned} \tilde{x}_{1,k} &= x_{1,k} + s_{x,1,k} \\ \tilde{x}_{2,k} &= x_{2,k} + s_{x,2,k} \\ \tilde{e}_{0,k} &= e_{0,k} + s_{e,0,k} \\ \tilde{e}_{1,k} &= e_{1,k} + s_{e,1,k} \\ \tilde{e}_{2,k} &= e_{2,k} + s_{e,2,k} \end{aligned} \tag{E4.7}$$

As seen, the nonlinear state feedback has been formally eliminated by considering the state-dependent flows as measured FV quantities.

The above is a linear balance model with state vector

$$z = \begin{pmatrix} x_1 \\ x_2 \\ e_0 \\ e_1 \\ e_2 \end{pmatrix}$$

Table 5. Results for Example 3

Row No.	tr(W)	tr(R)	tr(E)	tr(E_{MER})	$\frac{\text{tr}(R)}{\text{tr}(E)}$	$\frac{\text{tr}(R)}{\text{tr}(E_{MER})}$	$\frac{\text{tr}(E_{MER})}{\text{tr}(E)}$
1	0.0081	0.0850	0.0187	0.0641	4.5522	1.3259	3.4334
2	0.0081	1.3600	0.0780	0.9914	17.4301	1.3718	12.7063
3	0.0081	21.7600	0.3114	15.8283	69.8811	1.3747	50.8318
4	0.1300	0.0850	0.0551	0.0984	1.5438	0.8635	1.7880
5	0.1300	1.3600	0.2988	1.0257	4.5522	1.3259	3.4334
6	0.1300	21.7600	1.2484	15.8627	17.4301	1.3718	12.7063
7	2.0800	0.0850	0.0812	0.6477	1.0474	0.1312	7.9814
8	2.0800	1.3600	0.8809	1.5750	1.5438	0.8635	1.7880
9	2.0800	21.7600	4.7801	16.4120	4.5522	1.3259	3.4334

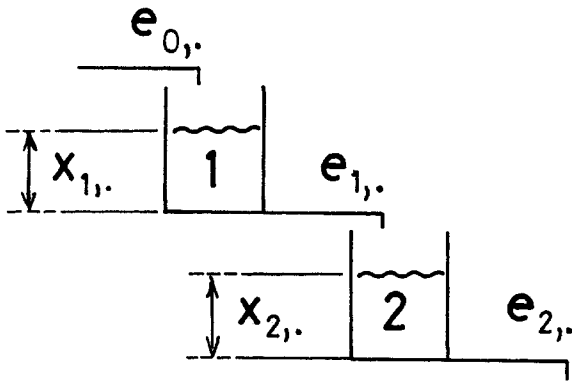

Figure 2. Two-tank system.

and with

$$G = \begin{pmatrix} 1 & -1 & 0 \\ 0 & 1 & -1 \end{pmatrix}$$

The above model satisfies the formal requirements formulated for the balance models. It does not comprise detailed process dynamics nor coefficients α_1 or α_2, as does the linearized process model. It is symmetrical in e_0, e_1, and e_2, corresponding to the fact that their function in the balance model is equivalent.

Global Balance Model. In this case the whole system is considered as a single unit with a single balance for the sum of all liquid contained in both tanks. The flow between the two tanks is not taken into consideration. The essence of this balance is that instead of liquid contents x_1 and x_2 of the two tanks, the sum

$$x_t = x_1 + x_2 \tag{E4.8}$$

is regarded as a state variable. Thus the global balance model from Eqs. E4.7 and E4.8 becomes

$$\begin{aligned} x_{t,k} &= x_{t,k-1} + e_{0,k-1} - e_{2,k-1} \\ e_{0,k} &= e_{0,k-1} + w_{0,k-1} \\ e_{2,k} &= e_{2,k-1} + w_{2,k-1} \end{aligned} \tag{E4.9}$$

and

$$\begin{aligned} \tilde{x}_{t,k} &= x_{t,k} + s_{x,t,k} \\ \tilde{e}_{0,k} &= e_{0,k} + s_{e,0,k} \\ \tilde{e}_{2,k} &= e_{2,k} + s_{e,2,k} \end{aligned} \tag{E4.10}$$

Also this is a linear balance model, with the state vector

$$z = \begin{pmatrix} x_t \\ e_0 \\ e_2 \end{pmatrix}$$

and with

$$G = (1 \quad -1)$$

This model belongs to the category of example 1. Having defined the sum of the two liquid contents as the only inventory variable, the problem becomes identical with the system of a single tank with two connected flows.

Conclusions

On the basis of rules of conservation applying to the process, a dynamic balance model describing the inventory and flow variables has been set. This is a submodel of the full model, and is always linear, even if the process itself is not. Formally it corresponds to the state space models generally applied in control theory.

Flow variables have been postulated to be stochastic processes with independent increments under regular operating conditions. Beside the redundancy in space, exhausted in static MER, this assumption also utilizes redundancy in time. This enhances the quality of estimation, compared to the static case.

An attractive feature of the balance model is that its structure and coefficients are exact and can be specified on *a priori* information, without cumbersome identification. State feedback does not obstruct dynamic balancing if all flows, including those due to the feedback, are measured. If there is, however, a linear model describing the feedback, it is possible to include it in the model. Unmeasured, nonlinear state feedback cannot be handled in this way.

Since the dynamic balance model has the form of the usual discrete-time, linear, state space model, in general it is possible to apply practically all known methods to sensor validation, fault detection and isolation, and so on, for such models.

The drawback of applying the balance instead of the full model to monitoring is that only those faults that influence balances in some way can be detected. Further, application of linear submodels to fault detection is possible only if the measuring apparatus has enough redundancy. For economy, often this is not the case and the number of measuring instruments is as little as possible. The dynamic balancing method described in this paper also needs the measurement of present storage amounts in the apparatus, increasing investment costs. In turn, this information, if it is accurate enough, reduces the estimation error of flow variables considerably. This fact can be seen from the numeric examples. Thus, application of dynamic balancing should be considered even from the point of view of economy. Note that present amounts of inventory variables are especially problematic if there is significant spatial inhomogeneity in the distribution of the IVs.

Estimation formulas look lengthy and complicated. But after certain preparatory computation, real-time dynamic balancing needs practically no more than two matrix-vector multiplications and addition of the size of the state vector. Thus, computational demand does not hinder the real-time application of dynamic balancing to monitoring.

How the variances and covariances of the increments of FVs shall be estimated, has not been treated here.

The solution has been formulated and solved with the assumption of a discrete time model. The balance model is also correct when flow variables vary continuously. In this case the vectors of integrated amounts of IVs entering or leaving the system during the time interval $[k-1, k)$ have to be considered as discrete time FVs. The theoretical treatment of continuous time balancing is possible if necessary, but has not yet been done.

Notation

e = vector of flow variables
E = variance matrix of estimation error of $\hat{e}$
G = matrix of coefficients, transforming e into the vector of increments of inventory variables
k = subscript for discrete time instance
$n(\cdot)$ = dimension of vector in the argument
q = vector of zero mean measurement error of inventory variables
Q = variance matrix of vector q (nonsingular)
r = vector of zero mean measurement error of flow variables
R = variance matrix of vector r (nonsingular)
s = vector of zero mean measurement error of state variables
S = variance matrix of vector s (nonsingular)
$\mathrm{tr}(\cdot)$ = trace of the matrix in its argument
w = time-uncorrelated, zero mean incremental variance vector of flow variables
W = variance matrix of vector w (nonsingular)
x = vector of amounts of inventory variables
$z = \begin{pmatrix} x \\ e \end{pmatrix}$, $n(x) + n(e)$ dimensional composite state variable of the balance model
Z = variance of estimation error of $\hat{z}$

Greek letters

$\Gamma = \begin{pmatrix} 0 \\ I \end{pmatrix}$, coefficient matrix for process disturbances
$\zeta = z - z^s$
$\Phi = \begin{pmatrix} I & G \\ O & I \end{pmatrix} + \begin{pmatrix} \Psi_P & O \\ \Psi_I & O \end{pmatrix}$, state transition matrix
$\Psi = \begin{pmatrix} \Psi_P & O \\ \Psi_I & O \end{pmatrix}$, state feedback coefficient matrix

Superscripts

^{s} = setpoint value
$\tilde{}$ = observed value
$\hat{}$ = estimate
$\bar{}$ = operating point

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