# THE PROPAGATION OF ERRORS AND UNCERTAINTY IN FORECASTING WATER QUALITY
-- PART I: METHOD

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## PREFACE

In recent years there has been a considerable interest in the development of models for river and lake ecological systems. Much of this interest has been directed towards the development of progressively larger and more complex simulation models. In contrast, relatively little attention has been devoted to the problems of uncertainty and errors in the field data, of inadequate numbers of field data, of uncertainty in the relationships between the important system variables, and of uncertainty in the model parameter estimates. IIASA's Resources and Environment Area's Task on "Models for Environmental Quality Control and Management" addresses problems such as these.

This paper examines how the uncertainties of the model calibration exercise -- essentially uncertainties associated with the estimated model parameter values -- will affect the confidence that can be placed in any predictions of future behaviour obtained from the model. Earlier papers (WP-79-27 and WP-79-63) have examined similar topics with different approaches. The purpose of this paper is to present a method of analysis suitable for use with relatively large, complex models, an area in which it is particularly difficult to make any rigorous and systematic studies of the effects of uncertainty and errors. For the time being, therefore, our concern is with model development and with methods of analysis; in the future we intend to consider the implications that these analyses have for the problems of environmental management.

SUMMARY

A method is proposed for recursive computation of the propagation of forecasting error covariances where the forecast is derived from a nonlinear state space model of water quality dynamics. This particular method, based on the idea of an extended Kalman filtering algorithm, is more commonly applied to the problem of real-time state and parameter estimation and to the problem of model calibration. This paper exploits that connection in order to stress the close relationship between model calibration and the use of models for forecasting the future behaviour of a system. It is argued that the analyst is frequently unaware of the levels of uncertainty in a calibrated water quality model; nor is it obvious how this uncertainty is distributed among the individual relationships that make up the model. Such uncertainty in the model, i.e., the model parameter estimation errors, has a significant effect on the confidence that can be assigned to model-based forecasts. A partitioned form of the algorithm is presented. This not only permits a considerable saving in computational effort but it also provides useful insight into the way in which the various sources of uncertainty propagate forward in time with the forecast.

# THE PROPAGATION OF ERRORS AND UNCERTAINTY IN FORECASTING WATER QUALITY - PART I: METHOD

## 1. Introduction

When forecasting the future behavior of water quality in a lake or river, the customary practice is to use a deterministic simulation; a simulation, in fact, that provides an apparently unique trajectory for future variations in the state of the system. In spite of all the qualifications that may be openly attached to such a forecast, the forecast is by its very appearance deceptive: a single line drawn across the page is unavoidably a confident statement. In this paper we question the confidence that can be placed in predictions about the future long-term behavior of lake water quality. Indeed, rather than being interested in the prediction or forecast itself, we shall be more concerned with the propagation of forecasting errors.

Other than as a concise representation of existing knowledge about a system's behavior, mathematical models are intended for forecasting. Frequently this application to forecasting will be embedded in the solution of a management problem. If decisions are to be made on the basis of the model's forecast, how certain can one be that this forecast is correct, and what is the risk of making a wrong decision? We would argue that it is not possible to answer such questions without stepping back from the subject of model application and examining the prior stage of model development. Model development ideally includes the process of model calibration, in which the model is evaluated by reference to experimental

observations of historical patterns of the lake's behavior (henceforth, the use of dynamic models and time-series field data is assumed). Since all field data are subject to measurement error (noise) a primary objective of model calibration -- or system identification -- is to discriminate against this kind of uncertainty, and thus to discern the underlying deterministic phenomena governing system behavior. Calibration is not exactly a matter of "filtering out" the uncertainty from the field data, although this may be a useful way of visualizing system identification for the following discussion. The important point is that the model, even when calibrated, remains an uncertain approximation of reality. Consequently, when the calibrated model is applied to the forecasting problem such uncertainty ought somehow to be visible in the plotted future trajectories of lake water quality.

In this paper we present an algorithm for computing the propagation of uncertainty and errors in water quality model forecasts. Part I of the paper describes the method and its origins. Part II of the paper will illustrate the capabilities of the algorithm using both simple examples and also a more complex model of water quality variations in Lake Ontario (see also Di Toro and van Straten, 1979). Further results of the application of the algorithm with an alternative model of Lake Ontario are given in Halfon and Beck (1979). There are two main reasons for using the proposed algorithm, the extended Kalman filter (e.g., Jazwinski, 1970). First, the extended Kalman filter (EKF) is more usually associated with the problem of system identification, as in Beck and Young (1976) and Beck (1979a). Hence we shall be able to emphasize

the crucial and intimate connection between model calibration and model-based prediction. Second, a principal target of this analysis is an ability for relatively rapid evaluation of the errors of predictions from large complex models, without excessive computational requirements. We suggest that the EKF is capable of fulfilling that role.

## 2. Calibration and Prediction - Inseparable Problems.

### 2.1 Deterministic and Uncertain Predictions.

The problem we wish to address is the computation of a (long-term) forecasting error covariance matrix. This can be stated as follows. Suppose the model of lake water quality behavior is defined by a set of nonlinear ordinary differential equations, i.e., in vector notation,

$$\dot{\underline{x}}(t) = \underline{f}\{\underline{x}(t), \underline{u}(t), \underline{\alpha}(t)\} + \underline{\xi}(t) \quad , \tag{1}$$

together with an accompanying set of nonlinearly related output observations,

$$\underline{y}(t_k) = \underline{h}\{\underline{x}(t_k)\} + \underline{\eta}(t_k) \quad . \tag{2}$$

In equations (1) and (2) $\underline{u}$, $\underline{x}$, and $\underline{y}$ are respectively vectors representing the measured input (forcing) disturbances, the state variables, and the measured output (response) variables; $\underline{\xi}$ and $\underline{\eta}$ are respectively vectors of random unmeasured input disturbances, i.e., system noise, and random output measurement errors, i.e., measurement noise; $\underline{f}$ and $\underline{h}$ are nonlinear vector functions; $\underline{\alpha}$ is a vector of model parameters, which may possibly be time-varying; and t is the independent variable of time, where $t_k$ is the kth discrete sampling instant. The dot

notation in (1) denotes differentiation with respect to t, and the discrete-time formulation of (2) indicates the assumption that sampled measurements of water quality are available.

It is necessary to distinguish between a deterministic prediction and an uncertain prediction. A deterministic prediction of lake water quality behavior at a future time $(t_o + \tau)$ may be defined from equation (1) as:

$$\dot{\underline{x}}(t_o + \tau) = \underline{f}\{\underline{x}(t_o + \tau), \underline{u}(t_o + \tau), \underline{\alpha}(t_o + \tau)\} \quad , \qquad (3)$$

given the initial conditions at the (current) time $t_o$, i.e., $\underline{x}(t_o)$, and assuming that $\underline{u}(t)$ and $\underline{\alpha}(t)$ are known functions of time for $t_o \leq t \leq t_o + \tau$. It is further assumed that there are no unknown disturbances of the system behavior between times $t_o$ and $t_o + \tau$ since a comparison of equation (3) with equation (1) shows that $\underline{\xi}(t) = \underline{0}$ has been substituted in equation (3).

Let us now dismantle these assumptions one by one. First, we are not certain about the present state $(\underline{x}(t_o))$ of water quality in the lake. Neither can it be assumed that there are no unknown disturbances $(\underline{\xi}(t))$ of the lake's behavior in the future, and clearly one cannot have knowledge of a completely determined pattern of future measured input disturbances $(\underline{u}(t))$, such as incident solar radiation and nutrient loadings. But most significantly for our argument here, it is highly unlikely that one can be completely confident about the accuracy of the model and hence, by implication, about the accuracy of the parameter values $(\underline{\alpha}(t))$. In view of these sources of error and uncertainty, let us thus state the desired form of an uncertain prediction, i.e.,

$$\dot{\underline{\hat{x}}}(t_o+\tau|t_o) = \underline{f}\{\underline{\hat{x}}(t_o+\tau|t_o), \underline{\hat{u}}(t_o+\tau|t_o), \underline{\hat{\alpha}}(t_o+\tau|t_o)\} + \underline{\hat{\xi}}(t_o+\tau) \quad (4a)$$

$$P^s(t_o+\tau|t_o) = E\{(\underline{x}(t_o+\tau) - \underline{\hat{x}}(t_o+\tau|t_o))(\underline{x}(t_o+\tau) - \underline{\hat{x}}(t_o+\tau|t_o))^T\} \quad (4b)$$

where $E\{\cdot\}$ is the expectation operator and superscript T denotes the transpose of a vector or matrix. According to equation (4a) we shall refer to $\underline{\hat{x}}(t_o + \tau|t_o)$ as a best estimate of the future state of water quality, given all measured information from the past and up to the current time $t_o$. The matrix $P^s(t_o + \tau|t_o)$ therefore represents the variance-covariance matrix of the errors of prediction between the future state $\underline{x}(t_o + \tau)$ and this best estimate $\underline{\hat{x}}(t_o + \tau|t_o)$ of that future state. $P^s$ and $\underline{\hat{x}}$ jointly characterize the uncertain prediction.

For the case where Gaussian distributions are assumed for the random processes $\underline{\xi}$ and $\underline{\eta}$ -- the system and measurement noises respectively -- $\underline{\hat{x}}$ and $P^s$ are likewise the mean and variance of a Gaussian probability distribution for the future state of the lake. The uncertain prediction thus seeks to specify the time-evolution of a probability distribution; Figure 1 shows a simple scalar interpretation of such a prediction. The notable assumptions required for an uncertain prediction are that:

(i) We have available average estimated trajectories (patterns) for future variations in the inputs, parameters, and noisy disturbances of the system, that is $\underline{\hat{u}}(t), \underline{\hat{\alpha}}(t)$, and $\underline{\hat{\xi}}(t)$, respectively, where $t_o \leq t \leq t_o + \tau$;

(ii) A mean value can be specified for the current state of the lake, i.e., $\underline{\hat{x}}(t_o|t_o)$;

(iii) And, although not explicitly indicated in equation (4), it will be required that variance-covariance matrices can be specified for the expected uncertainty (i.e., errors, or confidence bounds) in the estimates of $\underline{u}$, $\underline{\alpha}$, $\underline{\xi}$, and $\underline{x}(t_0)$.

In the following it will be apparent that the deterministic prediction can usefully be viewed as a scenario forecast, whereas the uncertain prediction more closely resembles an a posteriori sensitivity analysis of such a scenario forecast. Here "a posteriori" is used in the sense of "after having calibrated the model against experimental field data," (a priori sensitivity analysis would be a sensitivity analysis carried out without calibration of the model).

There is nothing radically novel about our definition of an uncertain prediction, though it is not a common feature of studies in ecological modeling. An earlier examination of the same kind of problem is reported by Mankin et al. (1976). They use a Monte Carlo simulation method to analyze the responses of a restricted class of linear dynamic models that are subject to uncertainty in the estimated values for the model parameters. This work has since been extended to cover a much more comprehensive investigation (O'Neill and Gardner, 1979) of sources of uncertainty in ecological models, for example, the uncertainty arising from model structure inadequacy, parameter errors, and natural variability of population attributes (e.g., genetic variability) and meteorological conditions. For models of limited size and complexity theoretical analysis can yield closed-form solutions for the effects of natural variability on model predictions (O'Neill, 1978). In general, however,

it is extremely difficult to obtain exact analytical solutions for an uncertain prediction. The customary numerical solution is to generate a sample of random realizations of future behavior using Monte Carlo simulation (for example, Whitehead, 1979, Tiwari et al., 1978), although somewhat more sophisticated simulation algorithms are available (Harris, 1977). From the sample distributions generated by the simulations the means and covariances of equations (4a) and (4b) may thus be calculated.

In a recent and closely parallel study Di Toro and van Straten (1979) have analyzed the prediction errors resulting from parameter uncertainty in a phytoplankton model for Lake Ontario. Their method of computing the prediction error variances, which derives from linear regression analysis, shows a clear link with the notion of sensitivity analysis. Essentially, the prediction error variance is a function of sensitivity coefficients -- in our terms the sensitivity of the nominal predicted state trajectory to changes in the parameter values -- and the covariance of estimation errors for pairwise combinations of the parameters. Since we also treat the case of Lake Ontario, although with a different model in the companion paper by Halfon and Beck (1979), we shall have more to say about the results of Di Toro and van Straten in Part II of the paper.

## 2.2. State and Parameter Estimation

The key feature of the method we shall propose for an uncertain predictor is its intimate connection with the problem

of model calibration, i.e., with system identification and parameter estimation. Let us now, therefore, digress from the subject of prediction in order to consider the essential purposes and properties of calibration procedures.

The main concern of model calibration and verification is one of obtaining estimates $\hat{\underline{\alpha}}$ for the model parameter values, and of comparing estimates $\hat{\underline{y}}$ of the model outputs with the actually observed historical patterns of behavior $\underline{y}$. Formally, the problem can be defined as:

> Given - a set of experimental field data comprising time-series of the measured inputs $\underline{u}(t)$ and measured outputs $\underline{y}(t)$;
>
> Determine - values for the parameters $\underline{\alpha}$ and the states $\underline{x}$ of the model chosen to characterize the system's behavior.

If we recall the form of equations (1) and (2), it is clear that computation of both state estimates $\hat{\underline{x}}$ and parameter estimates $\hat{\underline{\alpha}}$ is required. This is because (usually) calibration seeks the minimization of the errors between observed and computed outputs, i.e.,

$$\underline{e}(t_k) = \underline{y}(t_k) - \hat{\underline{y}}(t_k) = \underline{y}(t_k) - \underline{h}\{\hat{\underline{x}}(t_k)\} \quad , \tag{5}$$

where $\hat{\underline{x}}(t_k)$ may be computed from $u(t)$ -- given $\hat{\underline{\alpha}}(t)$ -- by solving

$$\dot{\hat{\underline{x}}}(t) = \underline{f}\{\hat{\underline{x}}(t), \underline{u}(t), \hat{\underline{\alpha}}(t)\} \quad . \tag{6}$$

It is helpful to visualize the procedure of calibration as a process of restructuring measured information: information about the "external" description of the system, $\underline{u}$ and $\underline{y}$, is

translated into information about the model-related "internal" description of the system, $\underline{\hat{\alpha}}$ and $\underline{\hat{x}}$. We may note in passing that there is no unique choice of variables and coefficients to be included in the state and parameter vectors of the model. On the other hand, the historical field data imply that the external description of the system's behavior is the fixed, immutable basis for calibration.

Assuming that the structure of the model, i.e., the form of the functional relationships $\underline{f}$ and $\underline{h}$ in equations (5) and (6), is known or has been identified -- this may in fact be quite a strong assumption (Beck, 1979a) -- the calibration procedure is intended to improve the accuracy of the parameter estimates. At the beginning of the procedure the accuracy of the a priori parameter estimates may range between the accuracies of guesses, of values quoted in the literature, of values determined from laboratory chemostat experiments, and of values estimated from previous in situ field experiments. Though it is rarely acknowledged, it is desirable, and it ought to be possible, to specify confidence bounds for these a priori estimates. A simple measure of this kind would be the variance-covariance matrix of a priori estimation errors for the parameters, i.e.,

$$P^{p}(0|0) = E\{(\underline{\alpha}(0) - \underline{\hat{\alpha}}(0|0))(\underline{\alpha}(0) - \underline{\hat{\alpha}}(0|0))^{T}\} \quad , \qquad (7)$$

in which $\underline{\alpha}(0)$ is the vector of "true" parameter values at time $t = 0$, the beginning of the experiment, and superscript p denotes a matrix associated with the parameters. The calibration procedure would thus, in principle, use the observed input/output information not only to provide improved estimates $\underline{\hat{\alpha}}$ of the

parameters, but also to reduce the levels of uncertainty in the a priori estimates. In other words, for the ideal case where the experiment continues until the current time $t_o$ (the beginning of the forecasting period), we could expect that

$$p^p_{ii}(t_o|t_o) < p^p_{ii}(0|0) \tag{8}$$

where the subscript ii indicates the ith diagonal element of the matrix $P^p$. Equation (8) states simply that the a posteriori error variance for parameter $\alpha_i$, $p^p_{ii}(t_o|t_o)$, is less than the a priori parameter estimation error variance.

So the calibration procedure increases our confidence in the accuracy of the model parameter estimates. But can we accept such a statement without qualification? Suppose there is a method that allows the changes in $p^p_{ii}$ to be followed as the experimental data for the period $0 \leq t \leq t_o$ are processed sequentially by an estimation algorithm, as in Figure 2. There are two illustrative examples to be considered. First, for the trajectory of $p^p_{11}$ in Figure 2 a significant reduction in the uncertainty of the parameter estimate $\hat{\alpha}_1$ is achieved, and the rate at which this uncertainty is reduced is especially rapid during the period $\Delta t$. We might suggest here that such an accelerated rate of decrease in error variance is due to the existence of a substantial amount of information in the data that refers to the system behavior associated with parameter $\alpha_1$. Second, the trajectory of $p^p_{22}$ displays a negligible decrease in the uncertainty of the related parameter estimate, $\hat{\alpha}_2$. Assuming the opposite of the argument for the $p^p_{11}$ trajectory it might be concluded that there is virtually no information in the data that con-

firms the type of behavior simulated by $\alpha_2$ and its associated sector of the model.

If the examples of Figure 2 are now seen from the different prospective of a Venn diagram, a useful generalization can be made about the calibration problem. This same device has been used elsewhere in order to sketch the features of the model validation problem, Mankin, et al. (1977). Thus in Figure 3 P represents the set of all possible behavior patterns exhibited by the system; A denotes the somewhat more restricted sample behavior observed in the historical field data; and M characterizes the set of behavior patterns simulated by the model. It is not difficult to imagine that actual (A) and simulated (M) behavior do not correspond exactly so that there is only a partial overlap between A and M. From the example of Figure 2 let us say that parameter $\alpha_1$ is associated with a part of the behavior covered by the shaded area of Figure 3, while $\alpha_2$ is related to that part of M that does not intersect with A. When the model is calibrated against the field data one would expect the uncertainty of parameter estimates associated with the intersection of A and M to decrease significantly. But for parameters associated with the non-intersecting remainder of M estimation error variances should not decrease because there is no information in the historically observed data with which to evaluate the existence of such behavior.

## 2.3 Uncertainty Transactions.

We see therefore that calibration serves the purpose of reducing the uncertainty in the model parameter estimates. At the same time, any procedure used for this purpose must be

capable of discriminating against the unwanted effects of error and uncertainty in the field data (i.e., uncertainty associated with $\underline{\xi}$ and $\underline{\eta}$ in equations (1) and (2)). The reduction in the uncertainty of the parameter estimates will also be approximately inversely related to the number of historical field observations. The variances of the a posteriori parameter estimation errors represent, therefore, a kind of "fingerprint" of the calibration process; they indicate, among other things, the relative degrees of uncertainty in the various sectors of the model relationships.

In order to discuss the notion of "uncertainty transactions" let us consider Figure 4. For this figure, uncertainty transactions are understood as the transactions of uncertainty between the activities of model calibration and subsequent forecasting with the model. It is clear that the matrix of a posteriori parameter estimation errors is the key factor that connects calibration with prediction. How, then, might one expect to see the influence of the a posteriori parameter estimation errors on the error bounds of forecasts about the future? Again, a Venn diagram is a useful starting point. Figure 5 shows a possible situation in which, for example, the future behavior of the system lies within the set of patterns represented by F. The sets P, A, and M have the same interpretations as previously, although the definition of M may be further qualified by stating that M represents simulated behavior of both the past and the future. Let us consider, in particular, what happens when at initial time $t_0$ the model simulates behavior that is characteristic of the set $\beta$ $(M \cap A \cap F)$ and

then at time $t_0 + \tau$ it simulated behavior characteristic of the set marked $\gamma$ $(M \cap F)$ in Figure 5. In other words, a well calibrated sector of the model is initially dominant in the simulated behavior, i.e., a pattern of behavior observed in the past, although subsequently a poorly identified sector of the model becomes dominant in the simulated behavior. With a nonlinear model such a transition could be easily brought about, for example, by a slightly modified combination of commonplace input disturbances that force the state of the model into a quite different region of the state space. Figure 6 illustrates the associated, hypothetical trajectory of one of the state variable forecasts, $\hat{x}$, and its error bounds, which here are simply denoted by $\hat{x} \pm \sigma$, where $\sigma$ is the standard deviation of the forecasting error (compare with Figure 1). Thus, as the state variable trajectory crosses the "boundary" between "past" and "future" behavior patterns the error bounds on the forecast expand rapidly. This occurs because the response of the model is becoming very sensitive to relatively uncertain parameter estimates and their respective sectors of the model. Of course, it might also be that the future forcing functions are also unlikely events, in which case the sudden loss of confidence in the model forecasts arises both from the uncertainty of these functions and from the parameter estimation errors.

A second example of uncertainty transactions -- this time transactions <u>within</u> the model -- due to the relative errors of the parameter estimates can be demonstrated with a prey-predator model. Suppose that the behavior of the prey is well known,

whereas the behavior of the predator is highly uncertain. An uncertain quantity of predator preying upon an initially certain quantity of prey leads to an increasingly uncertain quantity of remaining prey. This sort of situation is reflected in Figure 6.

To summarize, let us note that a most important feature, from the forecaster's point of view, is that when forecast-error bounds are computed it is possible to deduce where the model is making predictions for which there is very little historical empirical justification. Likewise, when calibrating large models against (probably inadequate) field data it will not be at all obvious which sectors of the model are properly calibrated, if the a posteriori parameter estimation errors are not calculated.

## 3. The Algorithm.

We mentioned already in the introduction of the paper that the extended Kalman filter (EKF) will be used to compute the uncertain prediction defined by equation (4). The argument supporting such an application of this algorithm requires first a discussion of state estimation and then introduction of the problem of combined state and parameter estimation. The idea of the (linear) Kalman filter (Kalman, 1960, Kalman and Bucy, 1961) originated in the field of control theory at a time when stochastic process control was a topic of increasing importance. Although its origins are in control theory, the Kalman filter has come to enjoy considerable application in non-technical fields, and particularly so in hydraulics, hydrology, and water resources, Chiu (1978), Wood and Szöllösi-Nagy (1979).

The linear filter was designed to compute the state estimates for a system whose behavior could be described by linear dynamic equations. The filter provides estimates $\underline{\hat{x}}(t_k|t_k)$ where, according to the notation introduced previously for equation (4), this denotes an estimate at time $t_k$ given all measured input/output information, $\underline{u}$ and $\underline{y}$ up to and including that available at time $t_k$.

However, our general description of lake water quality behavior, equations (1) and (2), is nonlinear and in principle requires a nonlinear filtering algorithm for computation of the state estimates. The extended Kalman filter (see, for example, Jazwinski, 1970, or Gelb, 1974) is a linear filter that gives a first-order approximation to the non-linear filter that would ideally be required. Our present interest lies not so much in the computation of state estimates for nonlinear systems, but more in the problem of combined state and parameter estimation.

## 3.1 Combined State and Parameter Estimation

A conceptual picture of the extended Kalman filter is given in Figure 7. As stated in section 2.2, calibration is a procedure whereby measured information $(\underline{u},\underline{y})$ about the external description of the system is restructured to provide information $(\underline{\hat{x}},\underline{\hat{\alpha}})$ about the internal nature of the system's behavior. Figure 7 bears out this statement. In this rather simplified picture of the filter the block labeled "estimation algorithms" carries out two functions. In part it compares the predicted model response with the observations $\underline{y}$ and

uses this error for revising the state and parameter estimates, which in turn are to be used for prediction at the next time step. It also weights the errors in this feedback correction mechanism according to a suitably defined balance between the respective levels of uncertainty in the model (i.e., the parameter estimates), in the input disturbances, and in the input measurements.

We shall not deal with the derivation of the linear or the extended Kalman filter. The reader previously unacquainted with these techniques will find suitable derivations in Gelb (1974), Young (1974), and Beck (1979b). Briefly, the problem of combined state and parameter estimation, in the context of calibration, can be set up by reformulating the dynamic system description of equations (1) and (2) as follows. Suppose we begin by defining the vector $\underline{x}^*$,

$$\underline{x}^* \triangleq \begin{bmatrix} \underline{x} \\ \hline \underline{\alpha} \end{bmatrix} ,$$

in which the state vector has been augmented with the parameter vector; and then let us assume that the parameters either do not vary with time, i.e.,

$$\dot{\underline{\alpha}}(t) = \underline{0} \tag{9}$$

or else they vary in an unknown "random walk" fashion, i.e.,

$$\dot{\underline{\alpha}}(t) = \underline{\zeta}(t) \tag{10}$$

where $\underline{\zeta}(t)$ is a vector of white noise disturbances (we shall

define a white noise sequence below). The basic system description of equations (1) and (2) may now be rewritten as,

$$\dot{\underline{x}}^*(t) = \begin{bmatrix} \dot{\underline{x}}(t) \\ \hline \dot{\underline{\alpha}}(t) \end{bmatrix} = \begin{bmatrix} \underline{f}\{\underline{x}^*(t), \underline{u}(t)\} \\ \hline \underline{0} \end{bmatrix} + \begin{bmatrix} \underline{\xi}(t) \\ \hline \underline{\zeta}(t) \end{bmatrix} \tag{11a}$$

$$\underline{y}(t_k) = \underline{h}^*\{\underline{x}^*(t_k)\} + \underline{\eta}(t_k) \quad . \tag{11b}$$

Or, more concisely,

$$\dot{\underline{x}}^*(t) = \underline{f}^*\{\underline{x}^*(t), \underline{u}(t)\} + \underline{\xi}^*(t) \tag{12a}$$

$$\underline{y}(t_k) = \underline{h}^*\{\underline{x}^*(t_k)\} + \underline{\eta}(t_k) \tag{12b}$$

in which $\underline{f}^*$ and $\underline{\xi}^*(t)$ have the obvious definitions.

For this system, equations (12), the extended Kalman filter for combined state and parameter estimation is given by the following set of algorithms,

Prediction: between the sampling instants $t_k$ and $t_{k+1}$,

$$\hat{\underline{x}}^*(t_{k+1}|t_k) = \hat{\underline{x}}^*(t_k|t_k) + \int_{t_k}^{t_{k+1}} \underline{f}^*\{\hat{\underline{x}}^*(t|t_k), \underline{u}(t)\}dt \tag{13a}$$

$$P^*(t_{k+1}|t_k) = \Phi\{t_{k+1}, t_k\}P^*(t_k|t_k)\Phi^T\{t_{k+1}, t_k\} + Q^* \tag{13b}$$

Correction: at time $t_{k+1}$ when the most recent observations $\underline{y}(t_{k+1})$ become available,

$$\hat{\underline{x}}^*(t_{k+1}|t_{k+1}) = \hat{\underline{x}}^*(t_{k+1}|t_k) + K(t_{k+1})[\underline{y}(t_{k+1}) - \underline{h}^*\{\hat{\underline{x}}^*(t_{k+1}|t_k)\}] \tag{13c}$$

$$P^*(t_{k+1}|t_{k+1}) = [I-K(t_{k+1})H(t_{k+1})]P^*(t_{k+1}|t_k)[I-K(t_{k+1})H(t_{k+1})]^T + K(t_{k+1})RK^T(t_{k+1}) \tag{13d}$$

where $K(t_{k+1})$, the Kalman gain matrix, is given by,

$$K(t_{k+1}) = P^*(t_{k+1}|t_k)H^T(t_{k+1})$$
$$[H(t_{k+1})P^*(t_{k+1}|t_k)H^T(t_{k+1}) + R]^{-1} \quad . \tag{13e}$$

In equations (13) I denotes the unit identity matrix. After our summary statement of the EKF it is necessary to make some additional definitions:

(i) The matrix $\Phi\{t_{k+1},t_k\}$ is the <u>state transition matrix</u> (see, for example, Dorf, 1965) and is defined thus,

$$\Phi\{t_{k+1},t_k\} \triangleq \exp\left[F\{\underline{\hat{x}}^*(t_k|t_k),\underline{u}(t_k)\}(t_{k+1}-t_k)\right] \tag{14}$$

where the matrix $F\{\underline{\hat{x}}^*(t_k|t_k),\underline{u}(t_k)\}$ has elements $f_{ij}$,

$$f_{ij} \triangleq \left[\frac{\partial f_i^*\{\underline{x}^*(t),\underline{u}(t)\}}{\partial x_j^*}\right]_{\substack{\underline{x}^*(t) = \underline{\hat{x}}^*(t_k|t_k) \\ \underline{u}(t) = \underline{u}(t_k)}} \tag{15}$$

and is derived in the procedure of linearizing the state vector dynamics of equation (12a).

(ii) The matrix $H(t_{k+1})$ derives from the linearization of the observations, equations (12b), and has elements $h_{ij}$,

$$h_{ij} \triangleq \left[\frac{\partial h_i^*\{\underline{x}^*(t_{k+1})\}}{\partial x_j^*}\right]_{\underline{x}^*(t_{k+1}) = \underline{\hat{x}}^*(t_{k+1}|t_k)} \tag{16}$$

(iii) The matrices Q* and R are defined under the assumptions that $\underline{\xi}^*$ and $\underline{\eta}$ are zero-mean, Gaussian, white-noise sequences, i.e.,

$$E\{\underline{\xi}^*(t_k)\} = E\{\underline{\eta}(t_k)\} = \underline{0} \tag{17}$$

$$E\{\underline{\xi}^*(t_k)\underline{\xi}^{*T}(t_j)\} = Q^*\delta_{kj} \tag{18}$$

$$E\{\underline{\eta}(t_k)\underline{\eta}^T(t_j)\} = R\delta_{kj} \tag{19}$$

with $\delta_{kj}$, the Kronecker delta function defined as,

$$\delta_{kj} = \begin{cases} 0 \text{ for } k \neq j \\ 1 \text{ for } k = j \end{cases} \tag{20}$$

and with $E\{\cdot\}$ being the expectation operator.

(iv) The matrix $P^*$ is the variance-covariance matrix of state and parameter estimation errors, i.e.,

$$P^*(t|t_k) = E\{(\underline{x}^*(t)-\underline{\hat{x}}^*(t|t_k))(\underline{x}^*(t)-\hat{x}^*(t|t_k))^T\} \ ,$$

$$= \left[\begin{array}{c|c} P^S(t|t_k) & P^C(t|t_k) \\ \hline [P^C(t|t_k)]^T & P^P(t|t_k) \end{array}\right] \tag{21}$$

in which $P^S$ is the state estimation error covariance matrix, $P^P$ is the parameter estimation error covariance matrix, and $P^C$ is a matrix representing error covariances between states and parameters (compare with equations (4b) and (7)).

(v) The initial conditions of the filter at time $t = 0$ -- the beginning of the experiment -- are specified as,

$$\underline{\hat{x}}^*(0|0) = \left[\begin{array}{c} \underline{\hat{x}}(0|0) \\ \hline \underline{\hat{\alpha}}(0|0) \end{array}\right] \text{ and } P^*(0|0) = \left[\begin{array}{c|c} P^S(0|0) & 0 \\ \hline 0 & P^P(0|0) \end{array}\right] \tag{22}$$

assuming that there are no a priori correlations between the state and parameter estimation errors. Finally, note that for the use of algorithms (13) in a calibration procedure, time t varies between the bounds $0 \leq t \leq t_o$, i.e., the period of the experiment.

A detailed block diagram of the EKF algorithms, equations (13), is shown in Figure 8. We may note first the parallel functions of the estimate and error covariance computations. Notice also how the matrix H is dependent upon the one-step ahead state-parameter predictions, $\underline{\hat{x}}^*(t_{k+1}|t_k)$, and how $\Phi$ depends upon the corrected estimates $\underline{\hat{x}}^*(t_{k+1}|t_{k+1})$. Figure 8 and equation (13) demonstrate the recursive nature of the EKF: for each increment of time $t_k \rightarrow t_{k+1}$ one pass is made through the two main feedback loops of the block diagram. Not only does this recursive nature of the algorithm permit the estimation of time-varying parameters, but it also implies that it would in fact be possible to compute the changes in $P^p(t_k|t_k)$ over the calibration period, as indicated earlier in Figure 2. However, in view of the linearization approximation of the EKF one should be cautious in interpreting $P^p(t_k|t_k)$ from equation (21) as the true parameter estimation error covariance matrix.

## 3.2 The Uncertain Prediction Algorithm.

Had we thus calibrated the model we should ideally be at the start, $t_0$, of the current forecasting period. Since from this time onwards no measurements are available, it is not possible to suppose that the filtering algorithms can be used in exactly the same fashion as they have been used in the calibration procedure. Inspection of equation (13) shows that the uncertain prediction of equation (4) might be obtained by extrapolation of equations (13a) and (13b) to some future time $t_{j+1}$, say, i.e., by computing $\underline{\hat{x}}^*(t_{j+1}|t_0)$ and $P^*(t_{j+1}|t_0)$. And since no future measurements are available, it is evident

that the "correcting" part of the EKF algorithms, i.e., equations (13c), (13d), and (13e), becomes redundant. In other words, the feedback loop of the filter (in Figure 7) is "opened," and the filter is being used as if it were anticipating measurements to be available at some time in the future. This is almost as though the act of prediction is an extension of the act of calibration; we have deliberately used a form of notation in the paper that emphasizes this point.

There are two very important features about such a use of the filter. First, because the model parameters are included in the augmented state-parameter vector, this enables us to account for the effects of (a posteriori) parameter uncertainty on the state variable predictions. Second, in view of the likelihood of nonlinearities in the original state-vector dynamics, equation (1), the inevitable nonlinearities of combined state-parameter prediction appear as only a marginal increase in the difficulties of solving the general nonlinear filter/prediction problem. Indeed, if we were to suggest that there is no conceptual distinction between "states" and "parameters" -- that parameters are merely variables that behave as if they were at steady state -- this may provide insight into the reasons why the EKF is being used in the present context.

From Appendix 1 the uncertain predictor can now be stated as follows (see also Figure 9):

$$\underline{\hat{x}}^*(t_{j+1}|t_0) = \underline{\hat{x}}^*(t_j|t_0) + \int_{t_j}^{t_{j+1}} \underline{f}^*\{\underline{\hat{x}}^*(t|t_0), \underline{\hat{u}}(t)\}dt \; ; \; t_j \leq t \leq t_{j+1} \qquad (23a)$$

$$P^*(t_{j+1}|t_o) = \Phi\{t_{j+1},t_j\}P^*(t_j|t_o)\Phi^T\{t_{j+1},t_j\}$$

$$+ \Gamma\{t_{j+1},t_j\}S(t_j)\Gamma^T\{t_{j+1},t_j\} + Q^* \qquad (23b)$$

The matrix $S(t_j)$ is defined as the covariance of errors in the estimated future variations of the input (forcing) disturbances ($\underline{\hat{u}}$), i.e.,

$$S(t_j) \triangleq E\{\underline{\tilde{u}}(t_j)\underline{\tilde{u}}^T(t_j)\} \qquad (24)$$

with

$$\underline{\tilde{u}}(t_j) \triangleq \underline{u}(t_j) - \underline{\hat{u}}(t_j) \qquad (25)$$

Hence, $\underline{\tilde{u}}$ is the vector of errors between actual and estimated input disturbances. The matrix $\Gamma$ in equation (23b) is defined in Appendix 1; it derives from the linearized relationship between states $\underline{x}^*(t_{j+1})$ and inputs $\underline{u}(t_j)$.

Given the particular form of the state-parameter dynamics of equation (11a), the predictor of equation (23) can be simplified by matrix partitioning to the following (see Appendix 2), in which some of the functional arguments have been omitted for clarity,

$$\underline{\hat{x}}(t_{j+1}|t_o) = \underline{\hat{x}}(t_j|t_o)$$

$$+ \int_{t_j}^{t_{j+1}} \underline{f}\{\underline{\hat{x}}(t|t_o),\underline{\hat{u}}(t),\hat{\underline{\eta}}\}dt \ ;$$

$$t_j \leq t \leq t_{j+1} \qquad (26a)$$

$$P^s(t_{j+1}|t_o) = \Phi_{11}P^s(t_j|t_o)\Phi_{11}^T + \Phi_{11}P^c(t_j|t_o)\Phi_{12}^T + \Phi_{12}[P^c(t_j|t_o)]^T\Phi^T{}_{11} + \Phi_{12}P^p(t_j|t_o)\Phi_{12}^T + \Gamma^s S(t_j)[\Gamma^s]^T + Q^s \quad (26b)$$

where in equation (26b),

$$P^c(t_{j+1}|t_o) = \Phi_{11}P^c(t_j|t_o) + \Phi_{12}P^p(t_j|t_o) \quad (26c)$$

$$P^p(t_{j+1}|t_o) = P^p(t_j|t_o) \quad (26d)$$

Equations (26) are equivalent to those of equations (23) by virtue of the matrix indentities,

$$\Phi\{t_{j+1},t_j\} \equiv \left[\begin{array}{c|c} \Phi_{11}\{t_{j+1},t_j\} & \Phi_{12}\{t_{j+1},t_j\} \\ \hline 0 & I \end{array}\right] ;$$

$$\Gamma\{t_{j+1},t_j\} \equiv \left[\begin{array}{c} \Gamma^s\{t_{j+1},t_j\} \\ \hline 0 \end{array}\right] ;$$

$$Q^* \equiv \left[\begin{array}{c|c} Q^s & 0 \\ \hline 0 & 0 \end{array}\right] ;$$

$$P^*(t_{j+1}|t_o) \equiv \left[\begin{array}{c|c} P^s(t_{j+1}|t_o) & P^c(t_{j+1}|t_o) \\ \hline [P^c(t_{j+1}|t_o)]^T & P^p(t_{j+1}|t_o) \end{array}\right] .$$

The dimensions of $\Phi_{11}$, $\Phi_{12}$, and $\Gamma^s$ are $n_s \times n_s$, $n_s \times n_p$, and $n_s \times m$ respectively, where $n_s$, $n_p$, and m are respectively the dimensions of the state, parameter, and input vectors. Precise

definitions of the matrices are given in Appendix 2. Further, in equations (26) it is assumed that the parameters $\underline{\alpha}$ are invariant with time so that $\underline{\zeta}(t) = \underline{0}$ for all $t > t_0$. Hence, in the above identity for $Q^*$,

$$Q^s \triangleq E\{\underline{\xi}(t_j)\underline{\xi}^T(t_j)\} \quad . \tag{27}$$

In both equations (23) and (26) the matrices $\Phi$ and $\Gamma$ are evaluated on the basis of the estimated trajectories $\underline{\hat{x}}$, $\underline{\hat{u}}$, and $\underline{\hat{\alpha}}$.

## 3.3 Comments on the Algorithm

Let us examine the computational aspects of the algorithm, equation (26); this will reveal a number of key features about the method. In order to run the algorithm the user must specify:

(i) the estimate of the current state of water quality in the lake or river, $\underline{\hat{x}}(t_0|t_0)$, i.e., the initial conditions of equation (26a);

(ii) the a posteriori parameter estimates derived from the preceding calibration exercise, i.e., $\underline{\hat{\alpha}} = \underline{\hat{\alpha}}(t_0|t_0)$ in equation (26a);

(iii) the estimated future trajectories of the input (forcing) disturbances, $\underline{\hat{u}}(t)$, for $t > t_0$;

(iv) the error variance-covariance matrix $P^s(t_0|t_0)$ associated with the estimates of the current state of water quality, i.e., the initial conditions of equation (26b);

(v) the error covariance matrix $(P^c(t_0|t_0)$ of correlated errors between the current state and parameter estimates; i.e.,

the initial conditions of equation (26c);

(vi) the a posteriori parameter estimation error variance-covariance matrix $P^p(t_o|t_o)$, which according to equation (26d) does not change over future time (this depends on the assumption of time-invariant parameters);

(vii) the covariance matrices $S(t_j)$ and $Q^s$ for both the measured and unmeasured input disturbances respectively.

The component computational steps of the uncertain predictor are given in Appendix 3. A primary reason for partitioning the matrix manipulations of equation (23b) which leads to equations (26b), (26c), and (26d), is the considerable economy it affords in computational effort. For example, when there are two state variables, two parameters, and two inputs, equation (23b) requires 160 multiplication operations, where as equations (26b) and (26c) require only 96 such operations. In addition, the particularly burdensome operation of matrix exponentiation can be much reduced by partitioning the transition matrix $\Phi$ of equation (23b) -- see Appendix 3. It is also worth noting that the solution of equation (26a) can be carried out independently of the remainder of the algorithm.

An especially useful advantage of the uncertain predictor of equation (26) is its flexibility and the insight it provides in appreciating the notion of "uncertainty transactions." Flexibility is demonstrated by the ease with which different prediction trajectories can be obtained for different nominal estimates $\underline{\hat{u}}(t)$, $\underline{\hat{\alpha}}(t_o|t_o)$, and $\underline{\hat{x}}(t_o|t_o)$. In effect, these nominal estimates allow us to make different scenario forecasts, for instance, "dry" or "wet" years, "sunny" or "dull" years, for each of which different assumptions about the co-

variance properties ($P^s(t_o|t_o)$, $P^p(t_o|t_o)$, $P^c(t_o|t_o)$) can be rapidly evaluated. Recall that with Monte Carlo simulation any change in the means and variances of the assumed probability distributions entails, in principle, a complete regeneration of the distributions for the state predictions. Insight is provided by separating equation (26b) into <u>additive</u> component parts, i.e.,

$$P^s(t_{j+1}|t_o) = \Phi_{11}P^s(t_j|t_o)\Phi_{11}^T$$

{Uncertainty in the state variable predictions}

{Uncertainty propagated from the current state of water quality}

$$+ (\Phi_{11}P^c(t_j|t_o)\Phi_{12}^T + \Phi_{12}[P^c(t_j|t_o)]^T\Phi_{11}^T)$$

{Uncertainty deriving from correlated state-parameter errors}

$$+ \Phi_{12}P^p(t_j|t_o)\Phi_{12}^T$$

{Uncertainty propagated from the a posteriori parameter estimation errors}

$$+ \Gamma^s S(t_j)[\Gamma^s]^T$$

{Uncertainty contributed by future input disturbance estimation errors}

$$+ Q^s$$

{Uncertainty arising from other factors e.g., residual errors of model calibration}

(28)

Since, by equation (28) it is possible to trace the source of the uncertainty, it appears that an "envelope" of uncertainty could be constructed within the total error (uncertainty) associated with the prediction. Figure 10 illustrates such a predic-

tion. The interesting point here is the information that can be inferred from the prediction when it is placed in the context of a management problem. Useful questions to ask might then be: if the objective is to regulate the occurrence of a peak event at a certain time, how sensitive is the prediction of the peak event to uncertainty in the parameter estimates, uncertainty in the current water quality state, and uncertainty in the estimated future input disturbances. Problems such as that, however, have yet to be explored.

Some numerical aspects of the proposed method should also be considered. For example, when the original description of the state vector dynamics, equation (7), is linear with constant parameters, the matrix $\Phi_{11}$ of equation (26b) is time-invariant. Hence, only a once-and-for-all computation of this matrix exponential is required (see Appendix 3). In the more general case, however, where $\Phi_{11}$, $\Phi_{12}$, and $\Gamma^s$ are all time-varying, the accuracy of the matrix exponentiation routine will be an important factor in determining the overall accuracy of the algorithm (see also Halfon and Beck, 1979). To some extent, since $\Phi_{11}$ is re-evaluated at each step in time, and since it is assumed that $\Phi_{11}$, $\Phi_{12}$, and $\Gamma^s$ can be approximated as constant matrices over the interval $t_j \rightarrow t_{j+1}$, numerical inaccuracies can be compensated by decreasing the magnitude of the time-step.

## 4. Concluding Remarks

It must be admitted that the algorithm of equations (26) has limitations of a technical and an analytical nature. A key assumption of the extended Kalman filter is that the

perturbations of the true state of the system about the nominal reference trajectory used for linearization are small (see Appendix 3 and Beck, 1979b). This implies for the uncertain predictor that the errors of prediction should be small, if the linearization procedure inherent in the covariance equations is to be a valid approximation. How then should one interpret a large prediction error covariance? The answer to that question is not very satisfactory: it seems that one can only be reasonably assured that the prediction errors are indeed large. A second key assumption of the algorithms is their use of Gaussian distributions for the system variables; clearly, in many cases skewed distributions would be more realistic.

Both of the above "problems" will be apparent in the examples chosen for illustration and discussion in Part II of the paper. Nevertheless, we would assert that uncertain predictions derived using the extended Kalman filter are good, first-order approximations. They can be obtained relatively rapidly in computational terms; moreover, it is argued that the algorithm can accomodate the analysis of relatively large-scale models (Halfon and Beck, 1979); and the predictions can easily account for cross-correlated parameter estimation errors, a feature that is not always easy to treat with other methods.

## Appendix 1 - The Uncertain Prediction Algorithm

In this Appendix a brief derivation is provided for the uncertain predictor, equation (23). This derivation of the predictor does not differ substantially from the derivation of the EKF algorithms as used in the procedure of calibration. Further details of the derivation, therefore, are available in Beck (1979b).

We start from the nonlinear representation of state-parameter dynamics given in equation (12),

$$\dot{\underline{x}}^*(t) = \underline{f}^*\{\underline{x}^*(t), \underline{u}(t)\} + \underline{\xi}^*(t) \quad . \tag{A1.1}$$

Let us define a nominal reference trajectory for the future input disturbances $\bar{\underline{u}}(t)$, and hence define a nominal (deterministic) reference trajectory, $\bar{\underline{x}}^*$, for the augmented state-parameter vector, i.e.,

$$\dot{\bar{\underline{x}}}^*(t) \triangleq \underline{f}^*\{\bar{\underline{x}}^*(t), \bar{\underline{u}}(t)\} \quad ;$$

with

$$\bar{\underline{x}}^*(t) = \bar{\underline{x}}^*(t_0) \text{ for } t = t_0 \quad . \tag{A1.2}$$

The reference trajectory thereby defined does not necessarily have to be identical with the deterministic prediction defined by equation (3) in the text, although there are obvious similarities between these two definitions. We thus have small perturbations $\delta\underline{u}$ and $\delta\underline{x}^*$ about the reference trajectories $\bar{\underline{u}}$ and $\bar{\underline{x}}^*$ defined by,

$$\delta\underline{u}(t) \triangleq \underline{u}(t) - \bar{\underline{u}}(t) \tag{A1.3a}$$

$$\delta\underline{x}^*(t) \triangleq \underline{x}^*(t) - \bar{\underline{x}}^*(t) \tag{A1.3b}$$

If the nonlinear function $\underline{f}^*\{\cdot\}$ in equation (A1.1) is expanded about the reference trajectories and approximated by a first-order Taylor series, then

$$\begin{aligned}\underline{f}^*\{\underline{x}^*(t),\underline{u}(t)\} = {} & \underline{f}^*\{\bar{\underline{x}}^*(t),\bar{\underline{u}}(t)\} \\ & + F\{\bar{\underline{x}}^*(t),\bar{\underline{u}}(t)\}\delta\underline{x}^*(t) \\ & + G\{\bar{\underline{x}}^*(t),\bar{\underline{u}}(t)\}\delta\underline{u}(t) \quad ,\end{aligned} \tag{A1.4}$$

where the matrix F has elements $f_{ij}$, defined by (compare with equation (15) in the text),

$$f_{ij} \triangleq \left[\frac{\partial f_i^*\{\underline{x}^*(t),\underline{u}(t)\}}{\partial x_j^*}\right]_{\substack{\underline{x}^*(t) = \bar{\underline{x}}^*(t) \\ \underline{u}(t) = \bar{\underline{u}}(t)}} \quad , \tag{A1.5}$$

and the matrix G has elements $g_{ij}$ defined by,

$$g_{ij} \triangleq \left[\frac{\partial f_i^*\{\underline{x}^*(t),\underline{u}(t)\}}{\partial u_j}\right]_{\substack{\underline{x}^*(t) = \bar{\underline{x}}^*(t) \\ \underline{u}(t) = \bar{\underline{u}}(t)}} \quad . \tag{A1.6}$$

Hence, noting that

$$\begin{aligned}\frac{d(\delta\underline{x}^*(t))}{dt} = \dot{\underline{x}}^*(t) - \dot{\bar{\underline{x}}}(t) = {} & \underline{f}^*\{\underline{x}^*(t),\underline{u}(t)\} \\ & - f^*\{\bar{\underline{x}}^*(t),\bar{\underline{u}}(t)\} + \underline{\xi}^*(t)\end{aligned} \tag{A1.7}$$

we obtain a set of <u>linear equations for the small perturbations</u> by substituting from equation (A1.4), i.e.,

$$\delta\dot{\underline{x}}^*(t) = F\{\bar{\underline{x}}^*(t),\bar{\underline{u}}(t)\}\delta\underline{x}^*(t)$$

$$+ G\{\bar{\underline{x}}^*(t),\bar{\underline{u}}(t)\}\delta\underline{u}(t) + \underline{\xi}^*(t) \quad . \qquad \text{(A1.8)}$$

Integration of the differential equation (A1.8) over the interval $t_j \rightarrow t_{j+1}$ gives (see, for example, Dorf, 1965),

$$\delta\underline{x}^*(t_{j+1}) = \Phi\{t_{j+1},t_j\}\delta\underline{x}^*(t_j)$$

$$+ \Gamma\{t_{j+1},t_j\}\delta\underline{u}(t_j) + \underline{\xi}^*(t_j) \qquad \text{(A1.9)}$$

in which,

$$\Phi\{t_{j+1},t_j\} \triangleq \exp\left[F\{\bar{\underline{x}}^*(t_j),\bar{\underline{u}}(t_j)\}(t_{j+1} - t_j)\right] \qquad \text{(A1.10)}$$

$$\Gamma\{t_{j+1},t_j\} \triangleq \int_{t_j}^{t_{j+1}}\left[\Phi\{t_{j+1},t\}G\{\bar{\underline{x}}^*(t_j)\bar{\underline{u}}(t_j)\}\right]dt \qquad \text{(A1.11)}$$

$$\underline{\xi}^*(t_j) \triangleq \int_{t_j}^{t_{j+1}}\left[\Phi\{t_{j+1},t\}\underline{\xi}^*(t)\right]dt \qquad \text{(A1.12)}$$

Equations (A1.1) and (A1.9) are the important equations of the development (A1.1) → (A1.12). Equation (A1.9) will subsequently be used to derive the error covariance equation of the uncertain predictor, while equation (A1.1) determines the structure of the equations for the state-parameter prediction trajectory. In order to obtain equation (13a) of the original EKF algorithm (as used for calibration), the expected value of the stochastic disturbances $\underline{\xi}^*(t)$, i.e., $E\{\underline{\xi}^*(t)\} = \underline{0}$, was substituted in equation (12a). We may likewise make the same substitution in (A1.1). In addition, however, since the future variations in $\underline{u}(t)$ are not known beyond the present time $t_0$, it is necessary to substitute the estimated input trajectory

$\underline{\hat{u}}(t)$ for $\underline{u}(t)$ in (A1.1). Hence,

$$\underline{\hat{x}}^*(t_{j+1}|t_o) = \underline{\hat{x}}^*(t_j|t_o) + \int_{t_j}^{t_{j+1}} \underline{f}^*\{\underline{\hat{x}}^*(t|t_o), \underline{\hat{u}}(t)\}dt \quad ;$$

$$t_o \leq t \leq t_o + \tau \quad . \tag{A1.13}$$

Given $\underline{\hat{x}}^*(t_o|t_o)$ and $\underline{\hat{u}}(t)$ equation (A1.13) can be repeatedly solved over consecutive intervals $t_j \rightarrow t_{j+1}$ until the predicted mean value of the state and parameter estimates, $\underline{\hat{x}}^*(t_o + \tau|t_o)$, is obtained. Equation (A1.13) is the first half of the required uncertain predictor, i.e., equation (23a) in the main body of the text.

In order to derive the second half of the predictor, that is the prediction error covariance matrix equation (23b), let us first define $\underline{\tilde{u}}(t)$ as the error (difference) between the estimated future input variations, $\underline{\hat{u}}(t)$, and the actual future inputs, $\underline{u}(t)$,

$$\underline{\tilde{u}}(t) \triangleq \underline{u}(t) - \underline{\hat{u}}(t) \quad . \tag{A1.14}$$

A corresponding estimation error $\underline{\tilde{x}}^*(t)$ may also be defined by,

$$\underline{\tilde{x}}^*(t|t_o) \triangleq \underline{x}^*(t) - \underline{\hat{x}}^*(t|t_o) \quad . \tag{A1.15}$$

Now observe that the state estimate equation (A1.13) is identical with the nominal reference trajectory of equation (A1.2) if $\underline{\hat{u}}(t)$ is substituted for $\underline{\bar{u}}(t)$ and if $\underline{\hat{x}}^*(t_o|t_o)$ is substituted for $\underline{\bar{x}}^*(t_o)$. In fact, by this particular substitution the Taylor series expansion, which is used for the linearization procedure, is always taken about the most recent state estimates

-- a key feature of the EKF algorithms when used for combined (on-line) state and parameter estimation (Peck, 1979b). On the basis of such a substitution, i.e., $\underline{\bar{x}}^*(t_o) = \underline{\hat{x}}^*(t_o|t_o)$ and $\underline{\bar{u}}(t) = \underline{\hat{u}}(t)$, then (compare equations (A1.14), (A1.15) with equations (A1.3)),

$$\underline{\tilde{x}}^*(t|t_o) = \delta\underline{x}^*(t) \quad \text{and} \quad \underline{\tilde{u}}(t) = \delta\underline{u}(t) \quad .$$

Hence, from equation (A1.9), by substitution of the above, it is found that the state-parameter prediction errors $\underline{\tilde{x}}(t|t_o)$ propagate (approximately) according to,

$$\underline{\tilde{x}}^*(t_{j+1}|t_o) = \Phi\{t_{j+1},t_j\}\underline{\tilde{x}}^*(t_j|t_o) + \Gamma\{t_{j+1},t_j\}\underline{\tilde{u}}(t_j) + \underline{\xi}^*(t_j) \quad . \qquad \text{(A1.16)}$$

This in turn gives the desired state-parameter prediction error covariance,

$$P^*(t_{j+1}|t_o) \triangleq E\{\underline{\tilde{x}}^*(t_{j+1}|t_o)\underline{\tilde{x}}^{*T}(t_{j+1}|t_o)\}$$

which, when expanded using equation (A1.16), yields,

$$\begin{aligned} P^*(t_{j+1}|t_o) = E\{ & \Phi\underline{\tilde{x}}^*(t_j|t_o)\underline{\tilde{x}}^{*T}(t_j|t_o)\Phi^T \\ & + \Gamma\underline{\tilde{u}}(t_j)\underline{\tilde{u}}^T(t_j)\Gamma^T + \underline{\xi}^*(t_j)\underline{\xi}^{*T}(t_j) \\ & + \Phi\underline{\tilde{x}}^*(t_j|t_o)\underline{\tilde{u}}^T(t_j)\Gamma^T \\ & + \Gamma\underline{\tilde{u}}(t_j)\underline{\tilde{x}}^{*T}(t_j|t_o)\Phi^T \\ & + \Phi\underline{\tilde{x}}^*(t_j|t_o)\underline{\xi}^{*T}(t_j) \\ & + \underline{\xi}^*(t_j)\underline{\tilde{x}}^{*T}(t_j|t_o)\Phi^T \end{aligned}$$

$$+ \Gamma\underline{\tilde{u}}(t_j)\underline{\xi}^{*T}(t_j)$$

$$+ \underline{\xi}^{*}(t_j)\underline{\tilde{u}}^{T}(t_j)\Gamma^{T}\} \quad . \tag{A1.17}$$

Under the assumptions that there are no cross-correlations among $\underline{\tilde{x}}^{*}(t_j|t_0)$, $\underline{\tilde{u}}(t_j)$, and $\underline{\xi}^{*}(t_j)$, which assumptions are not too restrictive since they merely state that there is no instantaneous transmission of input disturbances to the state variables and that the measured and unmeasured input disturbances are independent, equation (A1.17) simplifies to,

$$P^{*}(t_{j+1}|t_0) = \Phi\{t_{j+1},t_j\}P^{*}(t_j|t_0)\Phi^{T}\{t_{j+1},t_j\}$$

$$+ \Gamma\{t_{j+1},t_j\}S(t_j)\Gamma^{T}\{t_{j+1},t_j\} + Q^{*} \tag{A1.18}$$

In equation (A1.18) $S(t_j)$ is defined as the variance-covariance matrix of errors in the estimated future variations of measurable input disturbances, i.e.,

$$S(t_j) \triangleq E\{\underline{\tilde{u}}(t_j)\underline{\tilde{u}}^{T}(t_j)\} \quad . \tag{A1.19}$$

The matrices $\Phi$ and $\Gamma$ are evaluated by substituting $\underline{\hat{x}}(t_j|t_0)$ for $\underline{\bar{x}}^{*}(t)$ and $\underline{\hat{u}}(t_j)$ for $\underline{\bar{u}}(t)$ in the matrices F and G defined by equations (A1.5) and (A1.6).

Since equation (A1.18) is the desired covariance equation for the uncertain predictor, i.e., equation (23b), our derivation is thus completed.

## Appendix 2 - Matrix Partitioning in the Uncertain Prediction Algorithm

The computational requirements of the uncertain predictor given by equation (23) in the text can be reduced by exploiting the specific form of the augmented state-parameter vector dynamics. Our primary concern is that of reducing the amount of matrix manipulation in the covariance propagation equation (23b). We shall proceed in the same fashion as previously with Appendix 1, although in places somewhat more briefly.

The augmented state-parameter dynamics, equation (11a) in the text, has the form,

$$\dot{\underline{x}}^*(t) = \begin{bmatrix} \dot{\underline{x}}(t) \\ \hline \dot{\underline{\alpha}}(t) \end{bmatrix} = \begin{bmatrix} \underline{f}\{\underline{x}^*(t), \underline{u}(t)\} \\ \hline \underline{0} \end{bmatrix} + \begin{bmatrix} \underline{\xi}(t) \\ \hline \underline{\zeta}(t) \end{bmatrix} \tag{A2.1}$$

Thus, for the nominal reference trajectory defined by $\bar{\underline{u}}$ and $\bar{\underline{x}}^*$ we have the linearized small perturbation equations,

$$\begin{aligned} \delta\dot{\underline{x}}(t) = {} & F_{11}\{\bar{\underline{x}}^*(t), \bar{\underline{u}}(t)\}\delta\underline{x}(t) \\ & + F_{12}\{\bar{\underline{x}}^*(t), \bar{\underline{u}}(t)\}\delta\underline{\alpha}(t) \\ & + G^s\{\bar{\underline{x}}^*(t)\bar{\underline{u}}(t)\}\delta\underline{u}(t) + \underline{\xi}(t) \end{aligned} \tag{A2.2a}$$

$$\delta\dot{\underline{\alpha}}(t) = \underline{0} + \underline{\zeta}(t) \quad , \tag{A2.2b}$$

in which small perturbations $\delta\underline{\alpha}$ in the parameters are defined by reference to a set of nominal parameter values $\bar{\underline{\alpha}}$ as

$$\delta\underline{\alpha}(t) \triangleq \underline{\alpha}(t) - \bar{\underline{\alpha}}(t) \quad . \tag{A2.3}$$

The matrices $F_{11}$, $F_{12}$, and $G^s$ are defined as,

$$F_{11} \triangleq \left[\frac{\partial f_i\{\underline{x}^*(t),\underline{u}(t)\}}{\partial x_j}\right]_{\substack{\underline{x}^*(t)=\bar{\underline{x}}^*(t)\\ \underline{u}(t)=\bar{\underline{u}}(t)}} \tag{A2.4}$$

$$F_{12} \triangleq \left[\frac{\partial f_i\{\underline{x}^*(t),\underline{u}(t)\}}{\partial \alpha_j}\right]_{\substack{\underline{x}^*(t)=\bar{\underline{x}}^*(t)\\ \underline{u}(t)=\bar{\underline{u}}(t)}} \tag{A2.5}$$

$$G^s \triangleq \left[\frac{\partial f_i\{\underline{x}^*(t),\underline{u}(t)\}}{\partial u_j}\right]_{\substack{\underline{x}^*(t)=\bar{\underline{x}}^*(t)\\ \underline{u}(t)=\bar{\underline{u}}(t)}} . \tag{A2.6}$$

In line with the development of Appendix 1 we obtain the discrete-time difference equations for the interval $t_j \rightarrow t_{j+1}$,

$$\begin{aligned}\delta\underline{x}(t_{j+1}) = {} & \Phi_{11}\{t_{j+1},t_j\}\delta\underline{x}(t_j) \\ & + \Phi_{12}\{t_{j+1},t_j\}\delta\underline{\alpha}(t_j) \\ & + \Gamma^s\{t_{j+1},t_j\}\delta\underline{u}(t_j) + \underline{\xi}(t_j)\end{aligned} \tag{A2.7a}$$

$$\delta\underline{\alpha}(t_{j+1}) = \delta\underline{\alpha}(t_j) + \underline{\zeta}(t_j) \tag{A2.7b}$$

where

$$\Phi_{11}\{t_{j+1},t_j\} \triangleq \exp\left[F_{11}(t_{j+1} - t_j)\right] \tag{A2.8}$$

$$\Phi_{12} \triangleq \int_{t_j}^{t_{j+1}} \left[\Phi_{11}\{t_{j+1},t\}F_{12}\right]dt \tag{A2.9}$$

$$\Gamma^s \triangleq \int_{t_j}^{t_{j+1}} \left[\Phi_{11}\{t_{j+1},t\}G^s\right]dt \tag{A2.10}$$

$$\underline{\xi}(t_j) \triangleq \int_{t_j}^{t_{j+1}} \left[\Phi_{11}\{t_{j+1},t\}\underline{\xi}(t)\right]dt \tag{A2.11}$$

$$\underline{\zeta}(t_j) \triangleq \int_{t_j}^{t_{j+1}} \underline{\zeta}(t)dt \qquad \text{(A2.12)}$$

In equations (A2.8) → (A2.12) some of the arguments have been omitted for convenience. We may also note that the dimensions of $\Phi_{11}$, $\Phi_{12}$, and $\Gamma^s$ are $n_s \times n_s$, $n_s \times n_p$, and $n_s \times m$ respectively, where $n_s$, $n_p$, and m are respectively the number of state variables, parameters, and inputs.

Hence, substituting the estimates $\hat{\underline{u}}(t)$, $\hat{\underline{x}}(t_o|t_o)$, and $\hat{\underline{\alpha}}(t_o|t_o)$ -- where $\hat{\underline{\alpha}}(t_o|t_o)$ is the vector of a posteriori parameter estimates obtained during calibration -- for the corresponding variables defining the nominal reference trajectory, $\bar{\underline{x}}(t)$, the equations for the state-parameter prediction errors $\tilde{\underline{x}}(t|t_o)$ and $\tilde{\underline{\alpha}}(t|t_o)$ propagate (approximately) according to,

$$\begin{aligned}\tilde{\underline{x}}(t_{j+1}|t_o) = {} & \Phi_{11}\{t_{j+1},t_j\}\tilde{\underline{x}}(t_j|t_o) \\ & + \Phi_{12}\{t_{j+1},t_j\}\tilde{\underline{\alpha}}(t_j|t_o) \\ & + \Gamma^s\{t_{j+1},t_j\}\tilde{\underline{u}}(t_j) \\ & + \underline{\xi}(t_j)\end{aligned} \qquad \text{(A2.13a)}$$

$$\tilde{\underline{\alpha}}(t_{j+1}|t_o) = \tilde{\underline{\alpha}}(t_j|t_o) + \underline{\zeta}(t_j) \qquad \text{(A2.13b)}$$

If the state and parameter prediction error variance-covariance matrices are now defined respectively by,

$$P^s(t_{j+1}|t_o) \triangleq E\{\tilde{\underline{x}}(t_{j+1}|t_o)\tilde{\underline{x}}^T(t_{j+1}|t_o)\}$$

and

$$P^{P}(t_{j+1}|t_o) \triangleq E\{\underline{\tilde{\alpha}}(t_{j+1}|t_o)\underline{\tilde{\alpha}}^{T}(t_{j+1}|t_o)\}$$

and if the cross-covariances between state and parameter prediction errors are defined by

$$P^{C}(t_{j+1}|t_o) \triangleq E\{\underline{\tilde{x}}(t_{j+1}|t_o)\underline{\tilde{\alpha}}^{T}(t_{j+1}|t_o)\}$$

and

$$[P^{C}(t_{j+1}|t_o)]^{T} \triangleq E\{\underline{\tilde{\alpha}}(t_{j+1}|t_o)\underline{\tilde{x}}^{T}(t_{j+1}|t_o)\}$$

it would be possible to formulate the desired partitioned covariance evolution equations by generating $P^{S}$, $P^{P}$, and $P^{C}$ from equations (A2.13). However, let us instead combine the two equations (A2.13a) and (A2.13b) to give,

$$\underline{\tilde{x}}^{*}(t_{j+1}|t_o) = \left[\begin{array}{c|c} \Phi_{11} & \Phi_{12} \\ \hline 0 & I \end{array}\right]\left[\begin{array}{c} \underline{\tilde{x}}(t_j|t_o) \\ \hline \underline{\hat{\alpha}}(t_j|t_o) \end{array}\right] + \left[\begin{array}{c} \Gamma^{S} \\ \hline 0 \end{array}\right]\underline{\tilde{u}}(t_j) + \left[\begin{array}{c} \underline{\xi}(t_j) \\ \hline \underline{\zeta}(t_j) \end{array}\right] . \qquad \text{(A2.14)}$$

Comparison of equation (A2.14) with equation (A1.16) from Appendix 1 shows that the following identities hold,

$$\Phi \equiv \left[\begin{array}{c|c} \Phi_{11} & \Phi_{12} \\ \hline 0 & I \end{array}\right] \qquad \text{(A2.15a)}$$

$$\Gamma \equiv \left[\begin{array}{c} \Gamma^{S} \\ \hline 0 \end{array}\right] \qquad \text{(A2.15b)}$$

After substituting for $\Phi$ and $\Gamma$ from equations (A2.15) in equation (A1.18) from Appendix 1 we have (under the same assumptions as those made previously),

$$P^*(t_{j+1}|t_O) = \left[\begin{array}{c|c} \Phi_{11} & \Phi_{12} \\ \hline 0 & I \end{array}\right]\left[\begin{array}{c|c} P^s(t_j|t_O) & P^c(t_j|t_O) \\ \hline [P^c(t_j|t_O)]^T & P^p(t_j|t_O) \end{array}\right]\left[\begin{array}{c|c} \Phi_{11}^T & 0 \\ \hline \Phi_{12}^T & I \end{array}\right]$$

$$+\left[\begin{array}{c} \Gamma^s \\ \hline 0 \end{array}\right] S(t_j)\left[[\Gamma^s]^T \,\middle|\, 0\right] + \left[\begin{array}{c|c} Q^s & 0 \\ \hline 0 & Q^p \end{array}\right] \qquad \text{(A2.16)}$$

in which

$$Q^s \triangleq E\{\underline{\xi}(t_j)\underline{\xi}^T(t_j)\} \qquad \text{(A2.17)}$$

and

$$Q^p \triangleq E\{\underline{\zeta}(t_j)\underline{\zeta}^T(t_j)\} \qquad \text{(A2.18)}$$

Finally, from equation (A2.16) we obtain,

$$\begin{aligned} P^s(t_{j+1}|t_O) = {} & \Phi_{11}P^s(t_j|t_O)\Phi_{11}^T \\ & + \Phi_{11}P^c(t_j|t_O)\Phi_{12}^T \\ & + \Phi_{12}[P^c(t_j|t_O)]^T\Phi_{11}^T \\ & + \Phi_{12}P^p(t_j|t_O)\Phi_{12}^T \\ & + \Gamma^s S(t_j)[\Gamma^s]^T + Q^s \end{aligned} \qquad \text{(A2.19a)}$$

$$P^c(t_{j+1}|t_O) = \Phi_{11}P^c(t_j|t_O) + \Phi_{12}P^p(t_j|t_O) \qquad \text{(A2.19b)}$$

$$\begin{aligned} [P^c(t_{j+1}|t_O)]^T = {} & [P^c(t_j|t_O)]^T\Phi_{11}^T \\ & + P^p(t_j|t_O)\Phi_{12}^T \end{aligned} \qquad \text{(A2.19c)}$$

$$P^p(t_{j+1}|t_O) = P^p(t_j|t_O) + Q^p \qquad \text{(A2.19d)}$$

If one further assumption is made, that the parameters are truly constant and not subject to the random disturbances $\underline{\zeta}$, i.e., assuming $\underline{\zeta}(t) = 0$ for all t and therefore $Q^p = 0$ in equation (A2.19d), we have the desired partitioned covariance algorithms of equations (26) in the text.

## Appendix 3 - Computational Steps in the Uncertain Predictor

This appendix outlines the sequence of computations in the uncertain predictor of equation (26).

(1) At time $t = t_j$ substitute $\underline{x}^*(t) = \underline{\hat{x}}^*(t_j|t_0)$ and $\underline{u}(t) = \underline{\hat{u}}(t_j)$ for evaluation of the matrices,

$$F_{11} = \left[\frac{\partial f_i\{\underline{x}^*(t),\underline{u}(t)\}}{\partial x_j}\right] ;$$

$$F_{12} = \left[\frac{\partial f_i\{\underline{x}^*(t),\underline{u}(t)\}}{\partial \alpha_j}\right] ;$$

$$G^s = \left[\frac{\partial f_i\{\underline{x}^*(t),\underline{u}(t)\}}{\partial u_j}\right] .$$

(2) Compute the matrix exponential, or state transition matrix $\Phi_{11}$, i.e.,

$$\Phi_{11} = \exp\,(F_{11}\Delta t) \quad , \tag{A3.1}$$

where $\Delta t = t_{j+1} - t_j$. There are numerous ways of calculating $\Phi_{11}$, see for example, Moler and Van Loan (1977). The particular method used here, proposed by Shah (1971) is to exploit the identity,

$$\exp(F_{11}\Delta t) \equiv \left[\exp(F_{11}[\Delta t/2^{\lambda}])\right]^{2^{\lambda}} \quad , \tag{A3.2}$$

and then to approximate $\exp(F_{11}[\Delta t/2^{\lambda}])$, denoted $\Phi_{11}(\delta t)$ for convenience, by the series expansion,

$$\Phi_{11}(\delta t) = I + F_{11}\delta t + F_{11}^2(\delta t^2/2!) + F_{11}^3(\delta t^3/3!) + \ldots\ldots \tag{A3.3}$$

in which $\delta t = \Delta t/2^{\lambda}$. The evaluation of $\Phi_{11}(\delta t)$ from equation (A3.3), as opposed to similarly evaluating $\Phi_{11}(\Delta t)$, gives a more rapidly convergent series, which thus saves computational effort. Equally so, the partitioning of matrices (see Appendix 2) means that operations such as equation (A3.3) need only be carried out on an $n_s \times n_s$ matrix ($F_{11}$) instead of an $(n_s + n_p) \times (n_s + n_p)$ matrix (F).

(3) Compute the integral $\Phi'_{11}$ of the matrix exponential, i.e.,

$$\Phi'_{11} = \int_{t_j}^{t_{j+1}} \Phi_{11} dt = I\Delta t + F_{11}(\Delta t^2/2!) + F_{11}^2(\Delta t^3/3!) + \ldots . \qquad \text{(A3.4)}$$

Again, matrix partitioning provides a significant computational economy at this step.

(4) Using $\Phi'_{11}$ derive the matrices $\Phi_{12}$ and $\Gamma^s$ as,

$$\Phi_{12} = \Phi'_{11}F_{12} \quad ; \qquad \Gamma^s = \Phi'_{11}G^s \quad . \qquad \text{(A3.5)}$$

Implicit in the computations of equations (A3.4) and (A3.5), when compared with the definitions of $\Phi_{12}$ and $\Gamma^s$ in equations (A2.9) and (A2.10) of Appendix 2, is the assumption that $F_{12}$ and $G^s$ are constant over the interval $t_j \rightarrow t_{j+1}$.

(5) Now obtain $P^s(t_{j+1}|t_0)$, $P^c(t_{j+1}|t_0)$, and $P^p(t_{j+1}|t_0)$ according to equations (26b), (26c), and (26d) in the main body of the text.

(6) Solve for $\underline{\hat{x}}(t_{j+1}|t_0)$ from equation (26a) and return to step (1).

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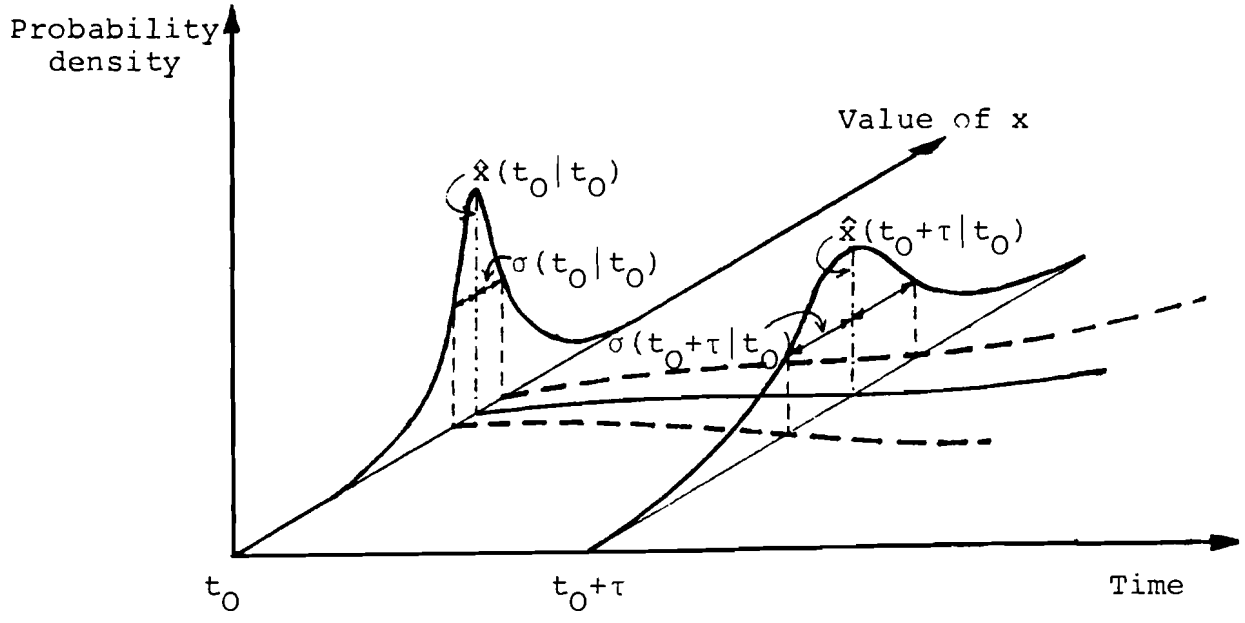


Figure 1. Pictorial representation of an uncertain prediction. $p^s = \sigma^2$ is the variance of the probability density function, i.e. the variance of the prediction error.

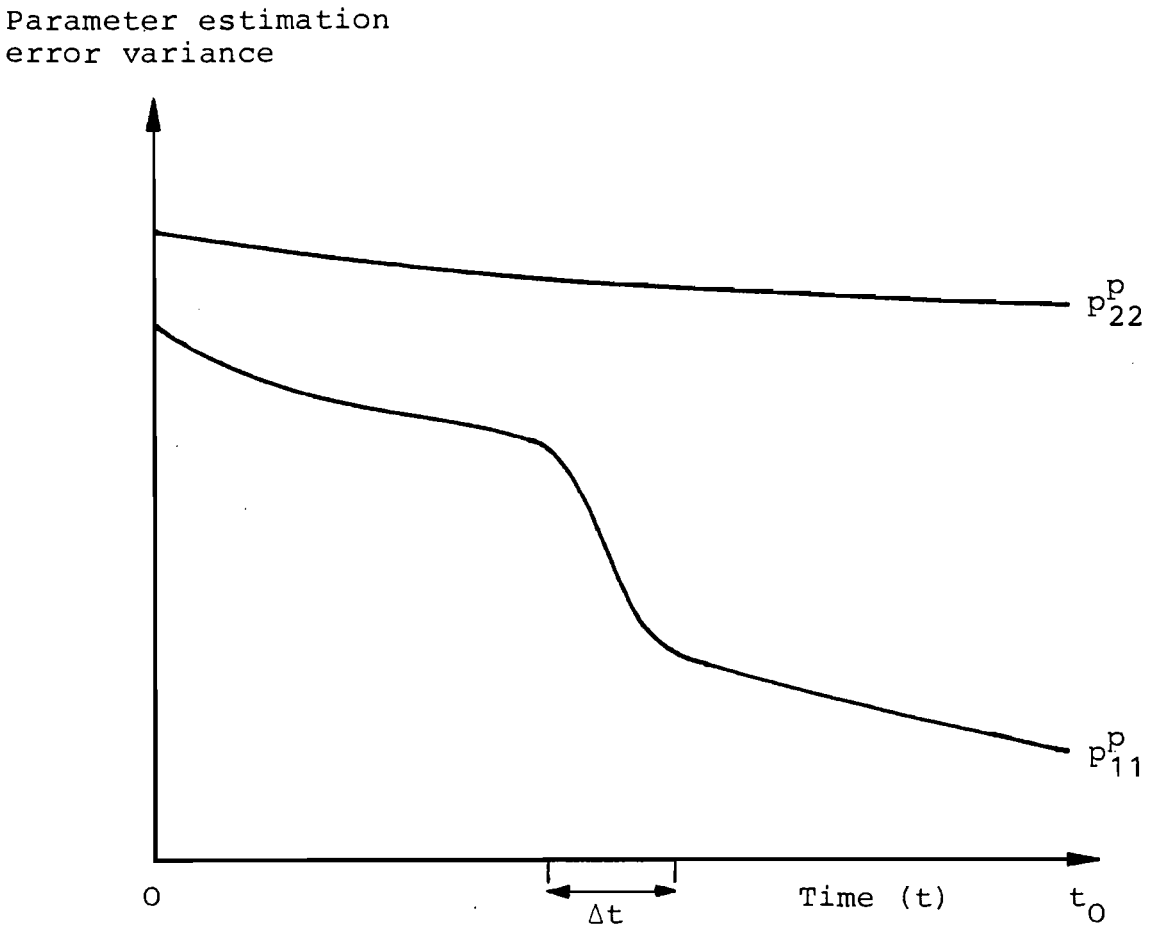


Figure 2. Examples of changes in parameter estimation error variances during calibration (calibration is assumed to refer to the period of observations from time $t = 0$ to time $t_0$).

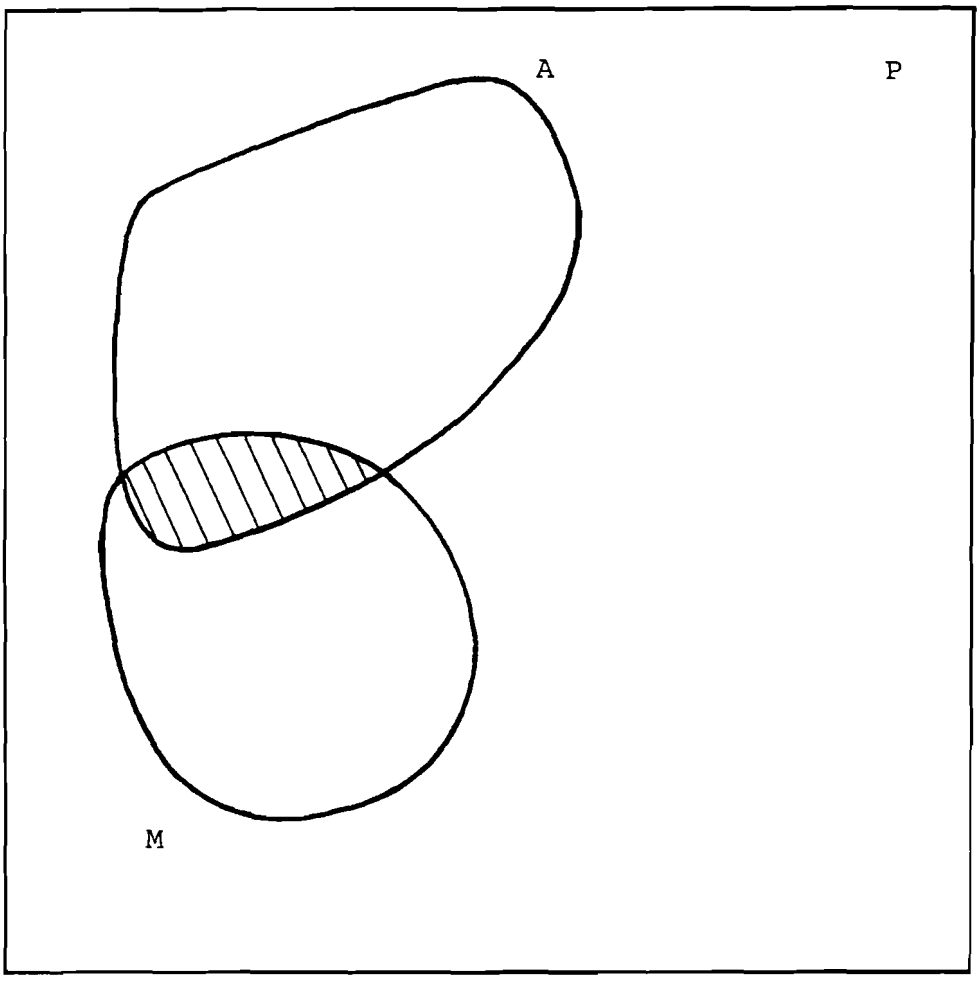


Figure 3. Calibration: A represents the set of system behaviour patterns observed in the past; M represents the set of behaviour patterns simulated by the model; the shaded area represents the overlap between A and M.

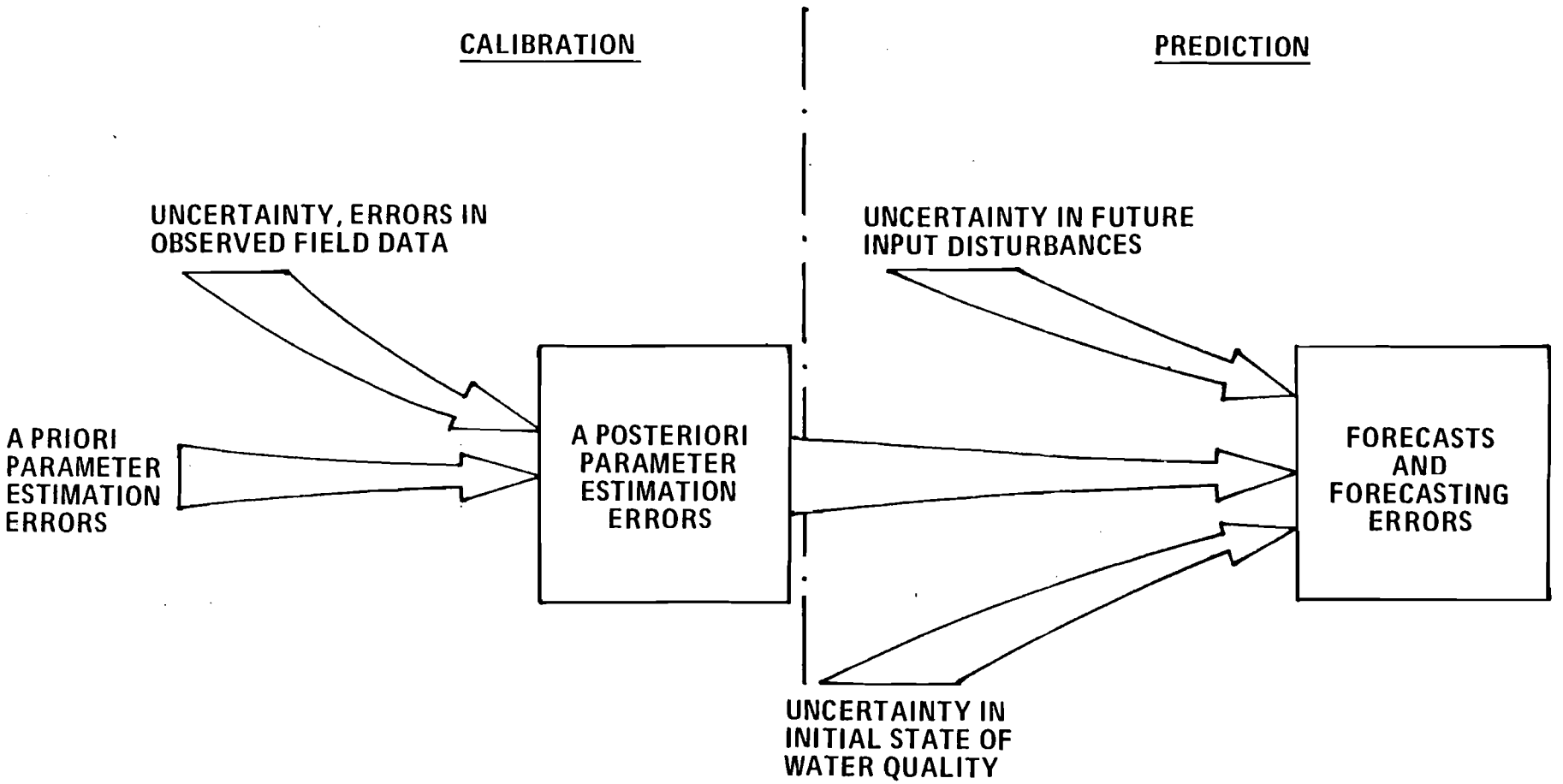


Figure 4. Uncertainty transactions between calibration and prediction.

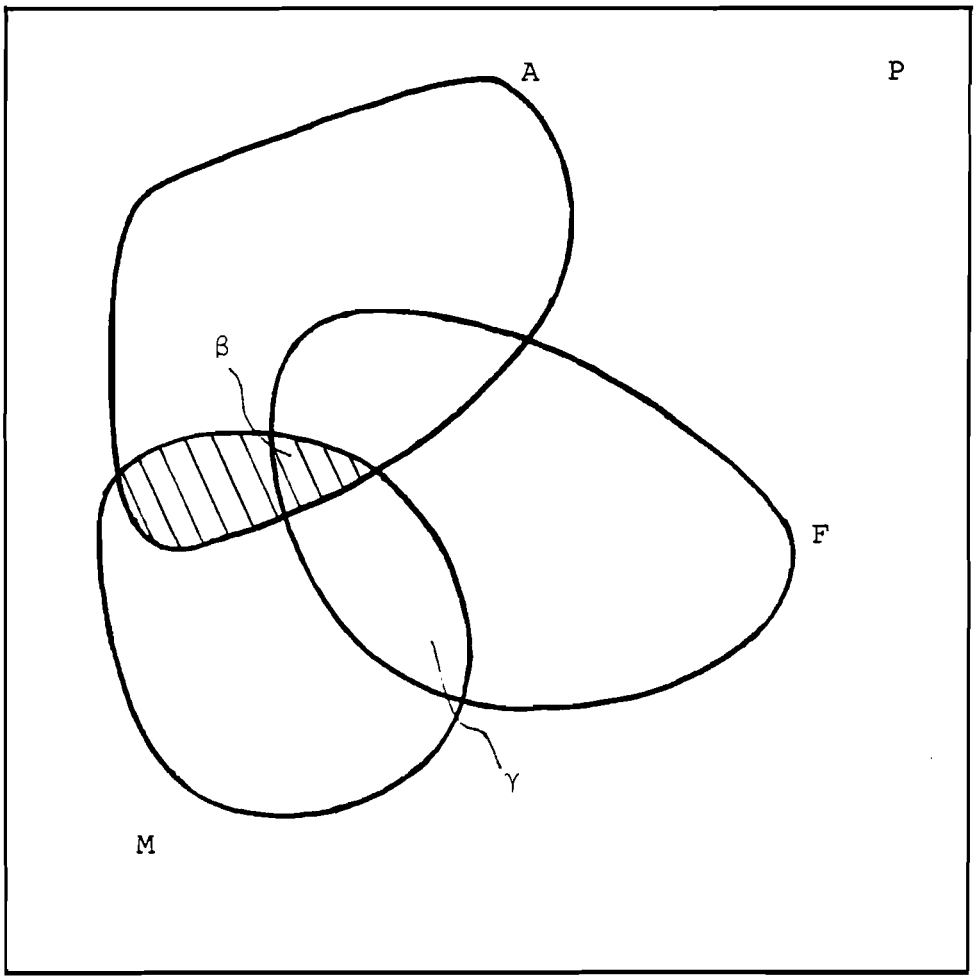


Figure 5. Prediction with the calibrated model: A and M are as defined for Figure 3 (see also text); F represents the set of future system behaviour patterns; β represents behaviour patterns associated with a well-calibrated part of the model; γ represents behaviour patterns associated with a poorly-calibrated part of the model.

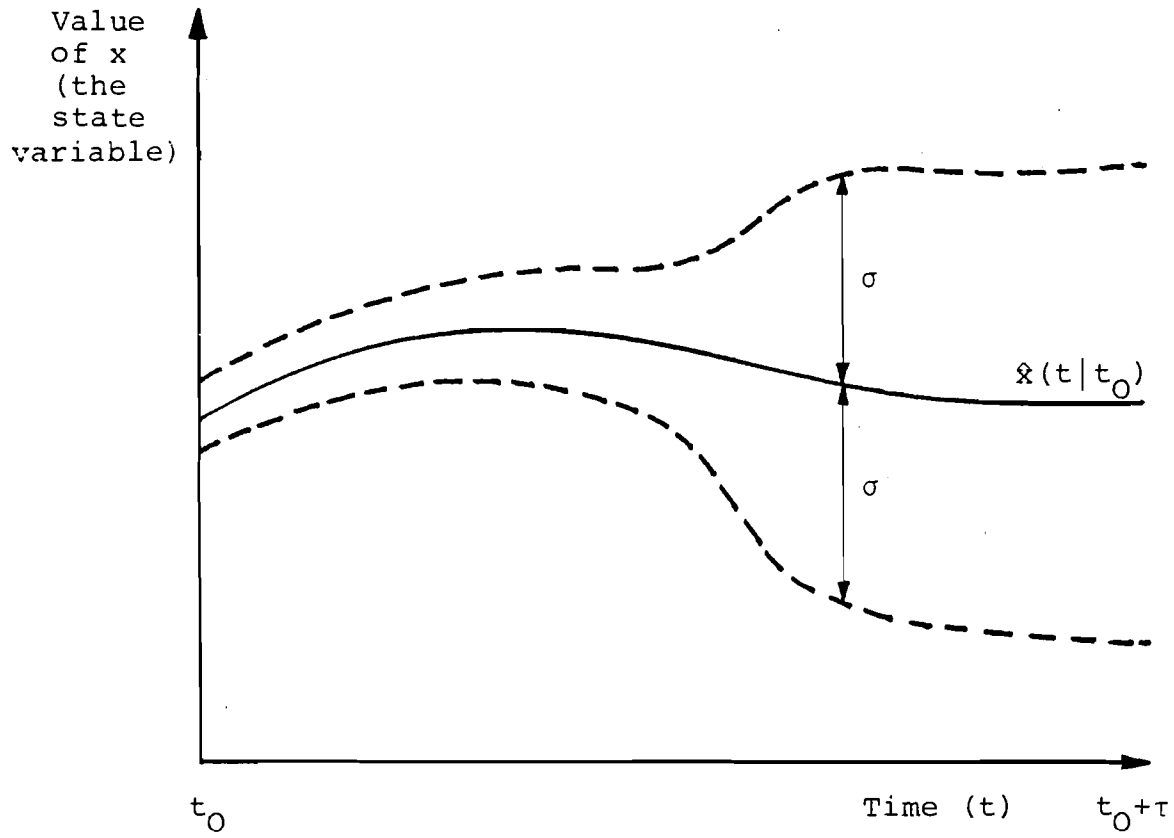


Figure 6. An example of the effects of uncertainty transactions (within the model) on the forecasting error. σ is the standard deviation of the forecasting error.

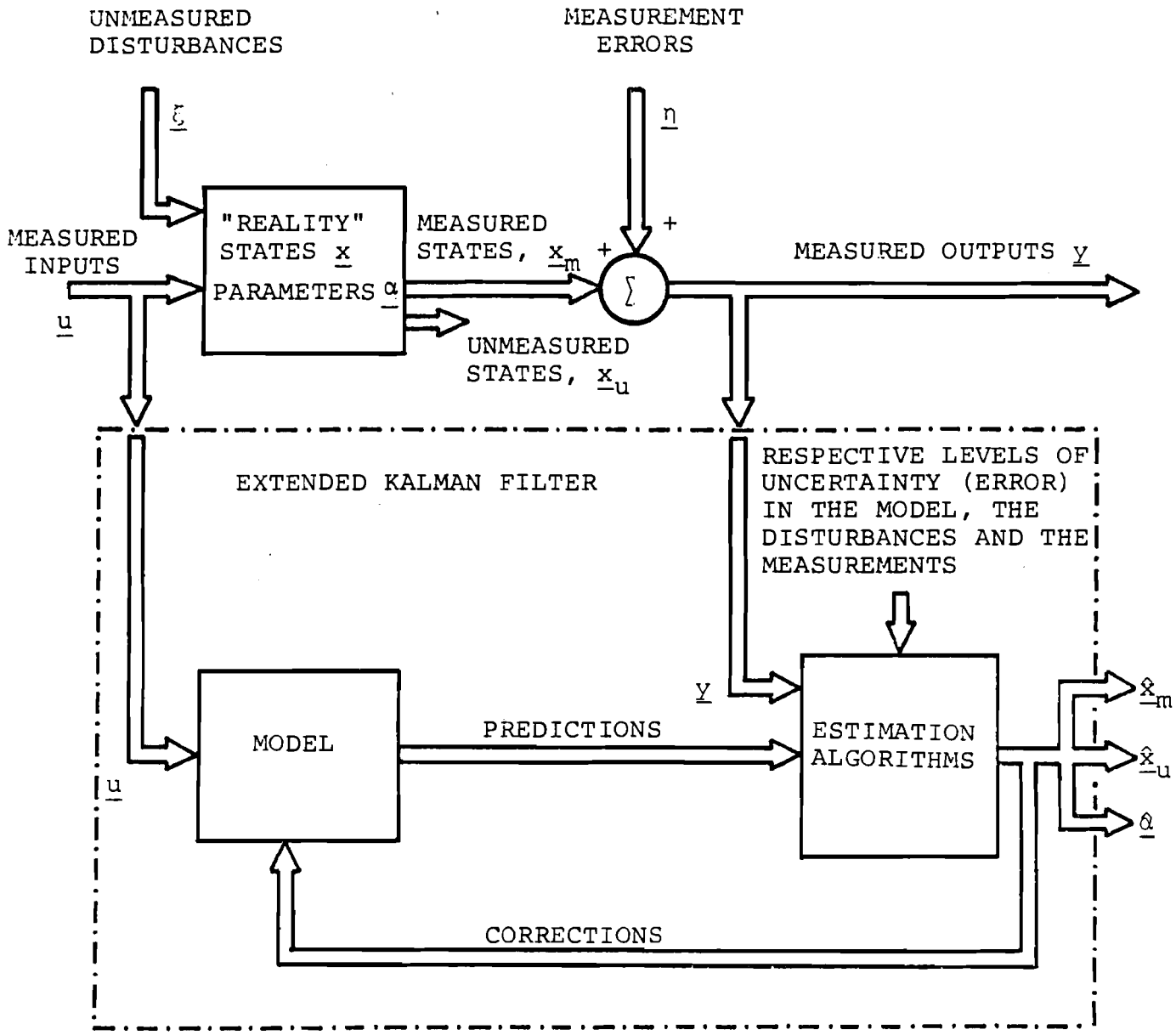


Figure 7. The extended Kalman filter, an algorithm for estimation and forecasting; $\hat{x}_m$, $\hat{x}_u$, and $\alpha$ are respectively estimates of the measured state variables, the unmeasured state variables, and the model parameters. (Estimation of $\hat{x}_u$ will not be of further concern in this discussion.)

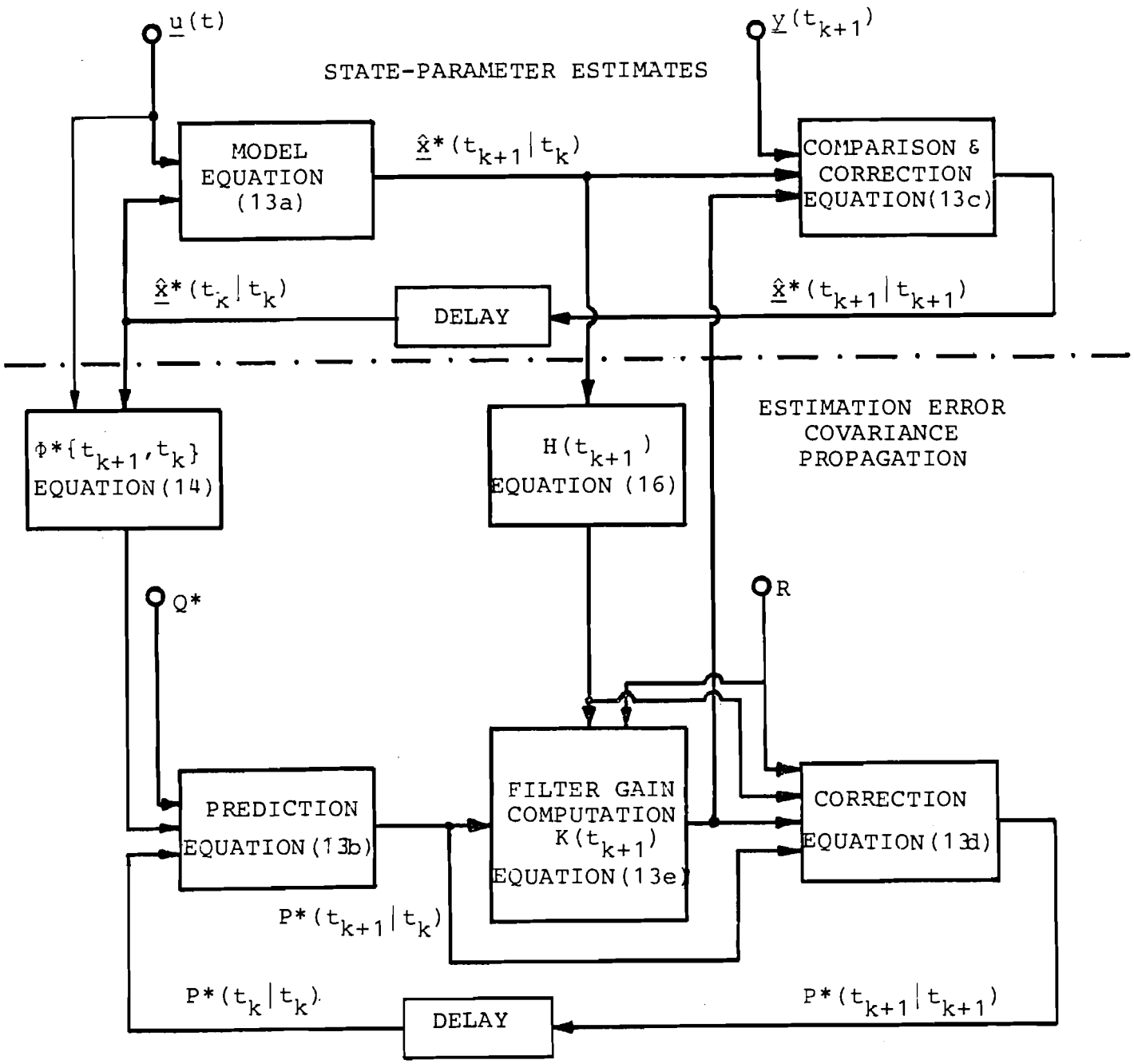


Figure 8. Block diagram of the extended Kalman filter showing both the computation of the state-parameter estimates and the computation of the covariance matrix. The block labelled "Delay" indicates that the estimates and covariances are propagated from one recursion through the algorithm to the next recursion.

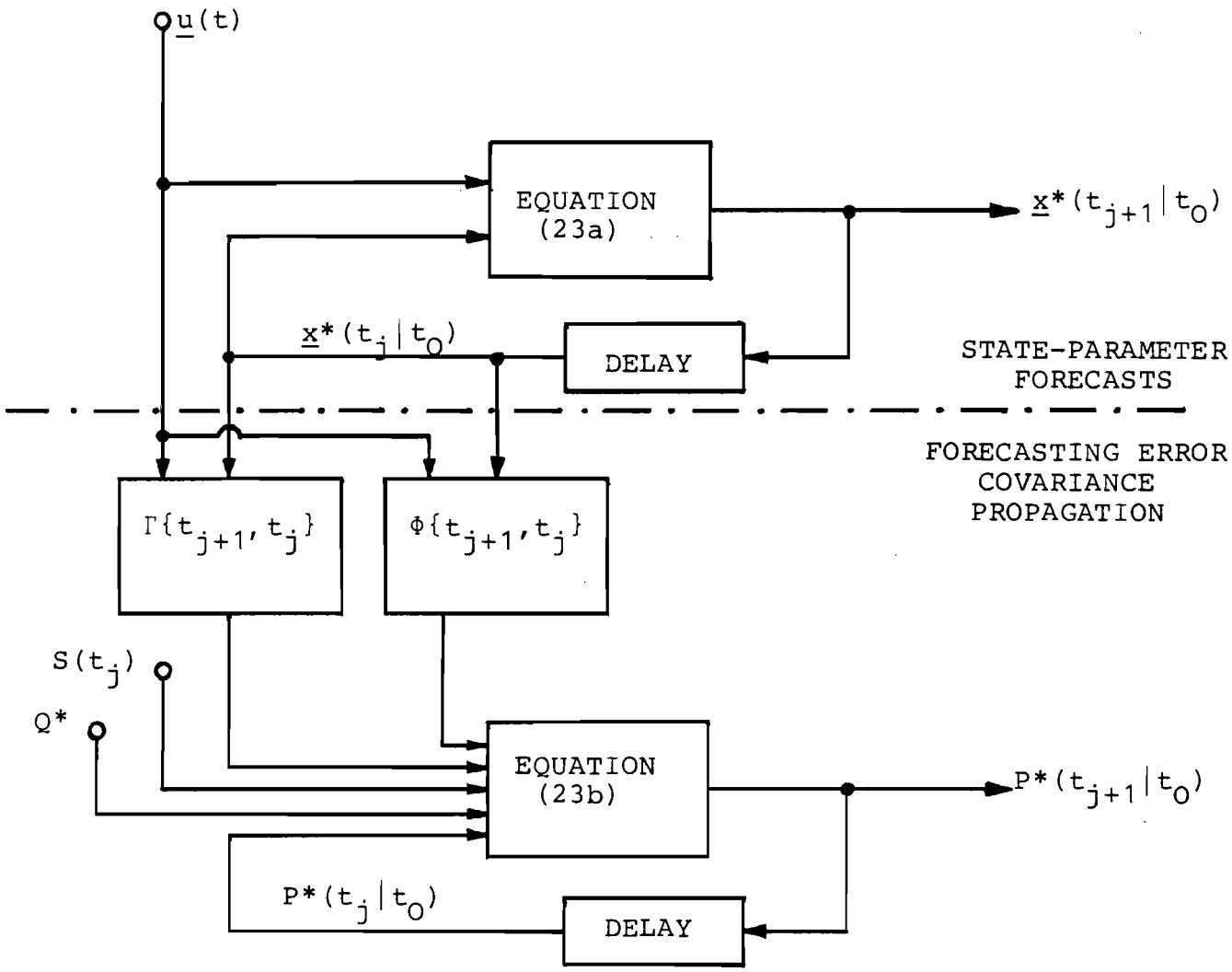


Figure 9. Block diagram of the uncertain prediction algorithm.

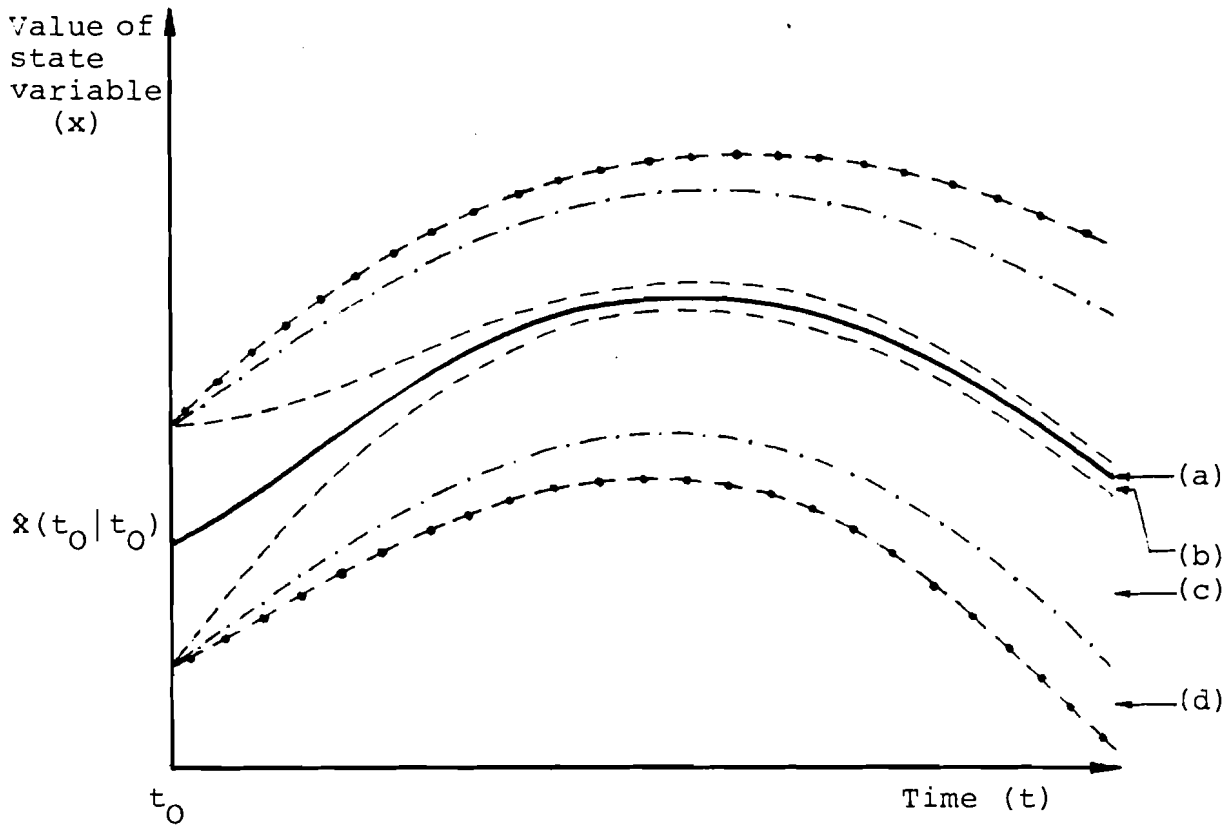


Figure 10: Envelope of uncertainty associated with state variable forecast: (a) represents the forecast; (b) represents the uncertainty propagated from current state of water quality; (c) represents uncertainty propagated from a posteriori parameter estimation errors; (d) represents uncertainty contributed from future input disturbances.