ON-LINE ESTIMATION OF NITRIFICATION DYNAMICS

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PREFACE

A previous paper (IIASA Professional Paper PP-78-70) has reported the preliminary results of a small collaborative project investigating the modeling and control of the activated sludge process in wastewater treatment. This paper provides a more detailed description of the identification of a dynamic model for nitrification. The results are also discussed from the perspective of on-line state estimation and state reconstruction as features of operational control. The identified model for nitrification has subsequently been incorporated in a simulation study of a fuzzy controller for the activated sludge process.

ABSTRACT

Results from a small collaborative project on modeling and control of the activated sludge process are presented. The identification of a dynamic model for nitrification is discussed using time-series field data from the Norwich Sewage Works in eastern England. This analysis of the field data is also used for examination of the feasibility and benefits of on-line (or real-time) state estimation in the context of activated sludge process control. A recursive estimation algorithm -- the extended Kalman filter -- is applied both for system identification and state estimation. The results illustrate an unstable nitrification condition associated with a period in which new plant was being commissioned. It is found that both oxygen limitation of nitrification and the compaction of solids in the clarifier are important factors affecting process dynamics. For real-time operation of the process it is argued that models and forecasting algorithms may be best utilized as a support service for the plant management in their day-to-day decision-making role.

On-Line Estimation of Nitrification Dynamics

1. Introduction

There is currently considerable interest in the automation and control of wastewater treatment plant operations (2), (34), (39). In particular, the activated sludge process is regularly cited as the one unit process most amenable to operational control, for example (12), (15), (25), (26), (30), (37), (40). Even though interest in such subjects is already well established, it is still useful to question the objectives of wastewater treatment plant automation and control. Indeed, one might ask what is meant by the terms "automation" and "control". For this paper we shall use the following definitions. Automation is understood as the automation of information retrieval about process conditions, e.g. on-line sensors, and the automation of implementing control actions, e.g. turning on and off pumps, blowers, and scrapers. Control is the activity that links together these two automated functions: it is the use of the information retrieved for determination of the control actions to be implemented. As indicated in a recent appraisal by Hegg et al (20), the incentive to automate and control wastewater treatment facilities lies with the desire to achieve "design performance", or better, through adequate day-to-day operation. Water quality management does not consist only of building for a better future; what has been built also has to be operated effectively. But such effective operation does not depend entirely on "automation"; it depends also upon the application of "control" as defined above.

Early work by Briggs (11) demonstrated the feasibility of controlling dissolved oxygen (DO) concentration in the aerator basin of an activated sludge unit. Closed-coop control of both the DO profile and the volume of recycled sludge are now relatively commonplace. However, these individual control loops by no means imply complete process control. In fact, it is debatable whether unit treatment processes can or should be placed under totally closed-loop control. Suppose, as would be pragmatic, that the human element -- the plant manager or operator -- is retained in the control loop. How much more effective would his control decisions be if the information retrieved from the on-line sensors were restructured in useful ways? For example, assuming the availability of a computing facility, what is the potential for using on-line mathematical models and information processing algorithms in:

(i) rapid evaluation of the short-term future consequences of various control actions;

(ii) prediction of future events, typically the expected variations in quality and flow-rate of the settled sewage influent to the aerator;

(iii) statistical estimation of process performance from error-corrupted measurements; and the reconstruction of information about process variables that may be important for the control function but which are not directly measured by instruments, e.g. the concentrations of nitrifying bacteria.

These kinds of question provide the motivation for this paper. In terms of Figure 1, therefore, we shall be concerned principally with the use of models as information processing mechanisms. The use of models in evaluating and determining suitable control actions will be of lesser importance.

In 1977 a small collaborative project was initiated by the Anglian Water Authority (U.K.) and the University of Cambridge. The project was to undertake a study of dynamic modelling and operational control of the activated sludge unit at the Norwich Sewage Works in eastern England. Preliminary results of the project are reported in Beck et al (8). The present paper gives a more detailed discussion of the identification and verification of a dynamic model for nitrification in the activated sludge process. The presentation of these results, however, will emphasise aspects of (on-line, real-time) state estimation and state reconstruction as they might relate to an operational control situation. The algorithm used for this purpose is the extended Kalman filter (EKF), see for example Jazwinski (21). The modelling results are restricted to the process of nitrification simply because the poor quality of the field data did not permit any effective identification of models for the dynamics of biochemical oxygen demand (BOD) and suspended solids (SS) removal. Further details of the historical operating records for the Norwich plant are given in Beck et al (8). The identified nitrification model has subsequently been used in a simulation study of a fuzzy control approach to day-to-day operation of the activated sludge process (8), (9), (44).

2. A Model for Nitrification Dynamics

One reason why models for the nitrification of waste materials are easier to verify than corresponding models for carbonaceous BOD and SS removal is that in nitrification fairly specific substrates and equally specific groups of micro-organisms can be identified. Moreover, observations of ammonium-, nitrite-, and nitrate-nitrogen concentrations are both less ambiguous and much closer to the "microscopic" kinetic behaviour of interest than are the somewhat "macroscopic" and crude measurements of BOD and SS concentrations. Thus several models for nitrification have been proposed, all notably constructed around the assumption of Monod Kinetics (32), and have been verified with considerable success against various types of experimental observations.

Qualitatively the basic biochemical model for nitrification shows that ammonium-N is oxidised in two stages to nitrate-N,

$$\text{ammonium-N} \xrightarrow{\text{Nitrosomonas}} \text{nitrite-N} \xrightarrow{\text{Nitrobacter}} \text{nitrate-N} \qquad (1)$$

where Nitrosomonas and Nitrobacter are the mediating species of micro-organism. Under the assumption that the conversion step from ammonium-N to nitrite-N occurs more slowly, and is therefore rate-limiting for the overall process, Downing et al (14) obtained a simple model which they verified with daily observations from laboratory-scale activated sludge units treating domestic sewage. More recently Gujer (17), (18) has presented equally good results for a similar model. He demonstrated the ability of his model to simulate diurnal variations characterised by a sequence of 2-hourly measurements from a pilot plant treating sewage from the city of Zürich. Gujer's model, however, while it also assumes a single-step conversion from ammonium-N to total oxidised nitrogen, contains a modified kinetic expression. This modification permits the modulation of Nitrosomonas activity according to: (i) the difference in growth-rates of the Nitrosomonas and the sludge as a whole; and (ii) the balance of the distribution of sludge between the aerator and the rest of the unit (17). Lijklema (29) also bases his model for nitrification on a single conversion stage, with again ammonium-N to nitrite-N being the rate-limiting step, but he includes the possibility of predation of the nitrifiers by populations of protozoa and rotifers. Harleman (19) and Leonov (27) consider nitrification as only a part of the complete aerobic nitrogen cycle. They propose models that include in addition: particulate organic nitrogen, dissolved organic nitrogen, heterotrophic bacterial conversion of dissolved organic nitrogen to ammonium-N, and uptake and release of nitrogen compounds by phytoplankton and zooplankton. Both authors have tested their various models with laboratory chemostat data.

The model used for this study is one of intermediate complexity and is identical (in all but two minor respects) with the model of Poduska and Andrews (38). Figure 2 gives a schematic diagram of the activated sludge process together with a definition of some of the notation. The major assumptions of the model are listed as follows:

(i) all biochemical reactions take place in the aerator;

(ii) the aerator mixing regime is approximated by a continuously stirred tank reactor (CSTR);

(iii) the species <u>Nitrosomonas</u> and <u>Nitrobacter</u> grow according to a Monod function;

(iv) there is no generation of ammonium-N by heterotrophic bacteria acting upon organically bound nitrogen in the aerator;

(v) no denitrification takes place;

(vi) the only component of interest entering the aerator with the settled sewage is the ammonium-N component;

(vii) the clarifier has no dynamic properties and thus all components are returned instantaneously from the aerator effluent to the aerator recycle influent;

(viii) only the <u>Nitrosomonas</u> and <u>Nitrobacter</u> concentrations are increased by compaction in the settler;

(ix) the rate of nitrification is essentially independent of ambient DO and temperature conditions.

Assumptions (vii) and (ix) are clearly strong assumptions. They can only be reasonably justified first by pointing out that any hydraulic transients associated with the clarifier appear virtually as "instantaneous" dynamics when compared with the low sampling frequency of the data (once per day). Second, no data were available regarding the daily averages of the mixed liquor DO concentration and temperature.

Given the above assumptions, component mass balances across the aerator yield the following five nonlinear ordinary differential equations for the dynamic nitrification model,

Ammonium-N:

$$\dot{x}_1(t) = Q_I(t)(u_1(t)/V_A - \mu_1(t)x_4(t)/Y_1 + \xi_1(t) \tag{2a}$$

Nitrite-N:

$$\dot{x}_2(t) = -Q_I(t)x_2(t)/V_A + \mu_1(t)x_4(t)/Y_1 - \mu_2(t)x_5(t)/Y_2 + \xi_2(t) \tag{2b}$$

Nitrate-N:

$$\dot{x}_3(t) = -Q_I(t)x_3(t)/V_A + \mu_2(t)x_5(t)/Y_2 + \xi_3(t) \tag{2c}$$

Nitrosomonas:

$$\dot{x}_4(t) = (Q_R(t)C(t) - Q_I(t)-Q_R(t))x_4(t)/V_A + \mu_1(t)x_4(t) - k_1x_4(t) + \xi_4(t) \tag{2d}$$

Nitrobacter:

$$\dot{x}_5(t) = (Q_R(t)C(t) - Q_I(t) - Q_R(t))x_5(t)/V_A + \mu_2(t)x_5(t) - k_2x_5(t) + \xi_5(t) \tag{2e}$$

where the dot notation refers to differentiation with respect to time t. In equation (2) the growth-rate expressions for Nitrosomonas and Nitrobacter are given respectively by,

$$\mu_1(t) = \hat{\mu}_1 x_1(t)/(K_1 + x_1(t)) \quad (3a)$$

$$\mu_2(t) = \hat{\mu}_2 x_2(t)/(K_2 + x_2(t)) \quad (3b)$$

and the other notation is defined by,

$x_i(t)$ = component concentration in the aerator: i=1, ammonium-N; i=2, nitrite-N; i=3, nitrate-N; i=4, Nitrosomonas bacteria; i=5, Nitrobacter bacteria (all in gm^{-3})

$u_1(t)$ = concentration of ammonium-N in the settled sewage influent (gm^{-3})

$Q_I(t), Q_R(t)$ = respectively the influent and recycle flow-rates ($m^3 day^{-1}$)

V_A = volume of sewage in the aerator (m^3)

$\hat{\mu}_1, \hat{\mu}_2$ = maximum specific growth-rate constants for Nitrosomonas and Nitrobacter respectively (day^{-1})

Y_1, Y_2 = yield coefficients for Nitrosomonas and Nitrobacter respectively (g organism produced/g substrate consumed)

K_1, K_2 = saturation concentrations for Nitrosomonas and Nitrobacter respectively (gm^{-3})

k_1, k_2 = specific decay-rate constants for Nitrosomonas and Nitrobacter respectively (day^{-1})

$\xi_i(t)$ = random input unknown disturbance for each state variable ($gm^{-3}\ day^{-1}$).

Finally, C(t) is defined as being the equivalent of a compaction ratio for the Nitrosomonas and Nitrobacter. C(t) can be obtained by taking a component mass balance across the clarifier for either species, i.e.

$$(Q_I(t) + Q_R(t))x_4(t) = (Q_I(t) - Q_W(t))(1-p)x_4(t) + (Q_R(t) + Q_W(t))x_{4R}(t) \qquad (4)$$

in which p is defined as a coefficient of solids-liquids separation efficiency, $Q_W(t)$ is the sludge wastage rate ($m^3 day^{-1}$), and $x_{4R}(t)$ is the concentration of Nitrosomonas in the recycle sludge stream (gm^{-3}). Rearranging equation (4) gives the recycle Nitrosomonas concentration in terms of the aerator Nitrosomonas concentration,

$$x_{4R}(t) = \left\{ \frac{Q_R(t) + pQ_I(t) + (1-p)Q_W(t)}{Q_R(t) + Q_W(t)} \right\} x_4(t) \qquad (5)$$

from which we define

$$C(t) \triangleq \left\{ \frac{Q_R(t) + pQ_I(t) + (1-p)Q_W(t)}{Q_R(t) + Q_W(t)} \right\} \qquad (6)$$

The above balance for compaction of bacterial species in the clarifier is accounted for respectively by the terms $[Q_R(t)C(t)x_4(t)/V_A]$ and $[Q_R(t)C(t)x_5(t)/V_A]$ in equations (2d) and (2e).

Further qualification of the model of equation (2) may be provided by noting that the argument t is retained for all variables that are not assumed to be invariant with time. The two major differences between the present model and the model of Poduska and Andrews are that here the sludge wastage rate (Q_W) is not zero and that we have accounted for unknown disturbances (ξ_i) of the process dynamics (this latter therefore places our model in a probabilistic setting).

If we make the following vector definitions,

$$\underline{x}^T(t) \triangleq [x_1(t), x_2(t), x_3(t), x_4(t) x_5(t)]$$

$$\underline{\Theta}^T(t) \triangleq [Q_I(t), Q_R(t), Q_W(t), V_A]$$

$$\underline{\alpha} \quad \triangleq [\hat{\mu}_1, \hat{\mu}_2, Y_1, Y_2, K_1, K_2, k_1, k_2]$$

$$\underline{\xi}^T(t) \triangleq [\xi_1(t), \xi_2(t), \xi_3(t), \xi_4(t), \xi_5(t)]$$

the model of equation (2) can be rewritten concisely, and in general terms, as

$$\dot{\underline{x}}(t) = \underline{f}\{\underline{x}(t), u_1(t), \underline{\Theta}(t), \underline{\alpha}\} + \underline{\xi}(t) \qquad (7a)$$

The superscript T denotes the transpose of a vector or matrix. We shall refer to $\underline{x}$ as the state vector, to $\underline{\xi}$ as the unmeasured system disturbance vector, to $\underline{x}$ as the (time-invariant) model parameter vector, and to $\underline{\Theta}$ as a vector of known "internal" variables. A distinction is drawn between $\underline{\Theta}$ and u_1 so that we can refer to u_1, the influent ammonium-N concentration, as the measured input disturbance. The vector function $\underline{f}\{\cdot\}$ has elements that represent each of the expressions on the RHS of equation (2).

For state estimation purposes the system description is completed by noting that discretely-sampled, error-corrupted measurements $y_1(t_k)$, $y_2(t_k)$, $y_3(t_k)$ are available at the kth day for the ammonium-N, nitrite-N, and nitrate-N concentrations of the aerator (i.e. clarifier) effluent,

$$\underline{y}(t_k) = H\,\underline{x}(t_k) + \underline{\eta}(t_k) \tag{7b}$$

The additional vector and matrix definitions are given by

$$\underline{y}^T(t_k) \triangleq [y_1(t_k), y_2(t_k), y_3(t_k)]$$

$$\underline{\eta}^T(t_k) \triangleq [\eta_1(t_k), \eta_2(t_k), \eta_3(t_k)]$$

$$H \triangleq \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \end{bmatrix}$$

$\underline{y}(t_k)$ is referred to as the measured output vector, and $\underline{\eta}(t_k)$ is a vector of random measurement errors.

3. On-Line Estimation

We have said that the key feature of the current study is concerned with restructuring measured information. Moreover, if this information processing is to be carried out in an on-line (real-time) fashion the basis of the processing mechanism will most probably be a recursive estimation algorithm (see, for example, (16), (46)). The linear Kalman filter (22), (23) and the extended Kalman filter (21), which is of particular interest here, are two examples of recursive estimators. The recent literature indicates that applications of recursive estimation in water-related fields are becoming increasingly widespread, for example: in water resources, hydrology, and hydraulic systems, (13), (43); in stream quality modelling, (10), (45), (47); in lake water quality modelling, (42); in water quality monitoring network design, (28), (33); in sewage flow prediction (3); and in fermentation and biological waste treatment processes, (1), (41).

A simplified conceptual picture of the EKF is shown in Figure 3. Inspection of the information flows into and out of the block labelled "Extended Kalman Filter" reveals that the measured input/output information $\underline{u}$ and $\underline{y}$ is translated into statistically based estimates of the measurable state variables $(\hat{\underline{x}}_m)$, of the state variables that are not easily measured $(\hat{\underline{x}}_u)$, and of the model parameters $(\hat{\underline{\alpha}})$. A number of problems of potential interest, and potentially capable of solution with an EKF algorithm, can now be listed as follows:

(i) determination of the structure of the dynamic relationships between inputs $\underline{u}$, state variables $\underline{x}$, and outputs $\underline{y}$ (model structure identification);

(ii) computation of values for the parameters $\underline{\alpha}$ that appear in the identified model structure (parameter estimation);

(iii) determination of the current and future values of the state variables (state estimation and prediction);

(iv) estimation of the inaccessible state variables that are not measured (state reconstruction);

(v) simultaneous determination of the values of $\underline{x}$ and $\underline{\alpha}$ (combined state and parameter estimation, or adaptive estimation and prediction).

Problems (i) and (ii) are clearly directed towards system identification, model calibration, and model varification. Problems (iii) and (v) are identical when, as here, the state vector dynamics are nonlinear; both problems can be solved using an EKF algorithm in the sense that the EKF is a first-order linear approximation to the ideal nonlinear filtering algorithms that such situations require. With respect to (v) it is worth noting that for adaptive control part of the function of the controller might be to choose values for the controlling inputs, $\underline{u}(t)$, that enhance the possibilities for system identification and parameter value updating, i.e. on-line experimentation with the plant.

A derivation of the EKF algorithms will not concern us here. Sufficient details of this derivation are given elsewhere, for example (6), (16), (21), (46). It is important, however, to discuss why the present application of the EKF is different from its earlier application in stream quality modelling (5), (7). The previous study addressed the problem of model structure identification. The solution of that problem depended strongly upon the proposition that any mismatch between the true structure of the system's dynamics and the structure of the model results in time-varying estimates for parameters that are assumed to be time-variant. It is not possible to rely upon this proposition for identifying the structure of the nitrification model because the model contains unobserved state variables, $\underline{x}_u^T = [x_4, x_5]$, i.e. the concentrations of Nitrosomonas and Nitrobacter bacteria. Any discrepancy between model and reality in this case would result in adaptation of the estimates $\hat{\underline{x}}_u$ in preference to adaptation of the parameters $\underline{\alpha}$. To put this in straightforward curve-fitting terms, one may make the following remark. If the number of model parameters is equivalent to the degrees of freedom available for fitting the curve to the data, then inaccessible state variables add proportionately many more degrees of freedom. In fact there are other features of the nitrification model that make parameter estimation technically very difficult. We shall return to them later.

For the results of the analysis in the next section it is more appropriate to consider the following. Let us assume in equation (7) that $u_1(t)$ and $\underline{\Theta}(t)$ are known functions of time -- in practice measurements are substituted -- and that estimates $\hat{\underline{\alpha}}$ can be substituted for $\underline{\alpha}$. Hence, given $y(t_k)$ we shall determine estimates for both the measured states $\hat{\underline{x}}_m(t_k|t_k)$ and the inaccessible states $\hat{\underline{x}}_u(t_k|t_k)$. In other words, we imagine the situation in which (from Figure 1) the measured information is being processed in real-time for operational control purposes; further, the provision of information about the status of the nitrifying bacteria is assumed to be of special importance. The notation $\hat{\underline{x}}(t_k|t_k)$ signifies estimates at time t_k based upon all the information available up to and including the measurements at time t_k. As a diagnostic check on the performance of the algorithm and on the approximate accuracy of the parameter estimates $\hat{\underline{\alpha}}$, it is helpful to compute the innovations process residual errors of the filter, i.e.

$$\underline{\varepsilon}(t_k|t_{k-1}) = \underline{y}(t_k) - \hat{\underline{x}}_m(t_k|t_{k-1}) \tag{8}$$

where $\hat{\underline{x}}_m(t_k|t_{k-1})$ are the one-step ahead predictions of the measurable state variables.

4. Results for the Norwich Sewage Works

Daily measurements have been taken from the activated sludge plant at the Norwich Sewage Works for the period January 1st to April 30th, 1976, a possible total of 121 sampled values for each variable. The salient operating conditions reflected by these data are discussed fully in (8). This period was chosen particularly for the reason that it was a time of commissioning new plant, during which the plant manager was assessing alternative strategies for recycle control. Consequently, longer-term "steady" operation had not been achieved and, in the absence of suitably planned experimentation (such as that reported by Olsson and Hansson (37)), the expectation was that these historical records would contain significant perturbations in process performance. In fact there was a gradual increase of aeration rate over these winter months, yet for a substantial portion of the time maximum aeration maintained only low DO concentrations. Some of these problems of commissioning undoubtedly relate to the phases in gain and loss of nitrification that are evident in the following results.

4.1 State Estimation and State Reconstruction

Figures 4(a), 4(b), and 4(c) respectively show the observations $\underline{y}(t_k)$ and state estimates $\hat{\underline{x}}_m(t_k|t_k)$ for the aerator concentrations of ammonium-N, nitrite-N, and nitrate-N. Figures 4(d) and 4(e) show the reconstructed state estimates $\hat{\underline{x}}_u(t_k|t_k)$ for the Nitrosomonas and Nitrobacter -- the dashed lines indicate corresponding estimates when C(t), the clarifier compaction ratio, is assumed to be constant, say C(t) = C*. Based on the details of these last two diagrams the total period of observation can be divided approximately into three distinct intervals of interest, i.e. the periods $t_4 \rightarrow t_{33}$, $t_{36} \rightarrow t_{58}$, and $t_{67} \rightarrow t_{111}$. First, however, let us discuss the initial conditions of the plant. During the Christmas holiday period, i.e. just prior to day t_0, an underloaded plant condition allowed a high level of nitrification to become established, which led subsequently to problems of denitrification and rising sludge in the clarifier. At the beginning of the year, therefore, the plant was deliberately being overloaded (the plant manager's response to the denitrification situation, whereby he hoped to suppress nitrification) and was again receiving normal strength sewage. The ammonium-N concentration of the settled sewage influent is given in Figure 5. The sudden drop in nitrification at day t_4 actually resulted from a faulty recycle pump that was operating at less than half its desired capacity.

Between t_4 and t_{33} both groups of nitrifying organisms are able to recover from the upset caused by the loss of recycled sludge; their population concentrations increase at virtually identical rates. For the same period Figure 4(b) shows the model (in the filter) to be estimating a consistently higher level of aerator effluent nitrite-N concentration than was observed in practice. If anything, this suggests that the model's estimated rate of nitrite-N production is here relatively too high in comparison with the corresponding estimated rate of consumption of nitrite-N.

At about t_{34} the process of re-establishing nitrification is temporarily halted, with an accompanying drop in the levels of Nitrosomonas and Nitrobacter. It is possible to attribute this effect to the following cause. Towards the end of January (t_{30}) the aeration rate had reached its maximum allowable limit. Since at the Norwich plant aeration rate is operated under closed loop control in relation to DO levels, this suggests that for some unknown reason aeration was not meeting the true oxygen demand. Consequently, from t_{34} onwards an increasing loss of fine solids over the clarifier weir was observed, which was probably due to the dispersion of the biological floc by excessive aeration, and by t_{39} a DO level of $1 gm^{-3}$ could not be maintained in the aerator. Both the loss of solids and the insufficient oxygen conditions are reasonable "causes" for the unstable nitrification conditions estimated over the period $t_{34} \rightarrow t_{58}$. Moreover, given the higher residual levels of nitrite-N over this period, it appears that the Nitrosomonas are relatively better at surviving under these unstable conditions -- compare the "slopes" in the curves of Figures 4(d) and 4(e).

The rapid loss of nitrification between t_{58} (about 97% nitrification) and t_{67} (about 30% nitrification) is not easily understood. Most probably it results from a combination of a high carbonaceous oxygen demand, which was particularly high over this interval, and an under-aeration of the mixed liquors -- the aeration rate was inexplicably low on day t_{63}. The apparent change of recycle control policy from a fixed recycle rate to a fixed ratio control which was effected at about day t_{56}, could be an additional coincidental factor of significance. Nevertheless, once again the nitrifying organisms slowly re-establish themselves from t_{67} onwards to t_{111}. Although it is only a marginal difference, the Nitrobacter population maintains a more stable growth pattern during this period.

By t_{112}, however, conditions have been reversed such that at the end of the experimental period both species of organism have been reduced to very low concentrations and nitrification has more or less ceased (approximately 20% nitrification). It is possible to speculate, with some accuracy, on the causes underlying this loss of nitrification. The dominant operating conditions over the interval prior to t_{112} were a combination of: unsatisfactory DO levels (less than $1gm^{-3}$, with maximum aeration); a poor sludge condition with the absence of ciliates; a steadily decreasing mixed liquor SS concentration, with a loss of solids over the clarifier weir; and hence the decision of the plant manager to reduce recycle sludge rate and to stop sludge wastage altogether. The Easter holiday period -- with missing observations for $t_{105} \rightarrow t_{108}$ (incl.) -- is marked by a drop in the influent ammonium-N concentration (see Figure 5). Then, with a higher recycle rate resumed on t_{106}, $350m^3$ sludge was wasted on day t_{112}. The error of this action, which probably precipitated the collapse of the nitrifier populations, is substantiated by the fact that on day t_{113} no sludge was wasted. This situation certainly could not have been improved by a suspected spillage of toxic material into the sewer network on the same day.

4.2 Parameter Estimates and Residual Errors

It would be unjustified to claim that the results of Figure 4 are an unqualified success in model verification. And in any case these results are intended to illustrate the potential of state estimation and state reconstruction in the context of on-line operational management. Nevertheless, it is important to give an approximate check on the performance of the model by assessing its parameter estimates and the residual error sequences. Indeed, in this particular modelling exercise the level of accuracy is such that a judgement like "the model did not give demonstrably unreasonable results" is more appropriate than saying that "the model performed well with only small residual errors". We can apply the former judgement, for example, to the period $t_{69} \rightarrow t_{80}$ (see Figure 4) when the model manages to predict effluent ammonium-N, nitrite-N, and nitrate-N concentrations across an interval of missing observations without excessive deviations from "reasonable" values (-a subjective judge--ment).

Table 1 gives the set of parameter values used for the results of Figure 4. The manner in which these estimates were obtained is not at all sophisticated. As we have said in section 3, because there is a need to reconstruct state estimates for the unobserved state variables, $\hat{\underline{x}}_u$, the effectiveness of combined

Table 1 Parameter estimates for the model of equation (2) and parameter estimates from two sources in the literature

Parameter	Estimate $C(t)$[1]	Estimate C^*[2]	Estimate Poduska and Andrews (38)	Estimate Harleman (19)[3]
$\hat{\mu}_1$ (day^{-1})	0.72	0.82	1.08	1.20
$\hat{\mu}_2$ (day^{-1})	0.93	1.03	1.44	1.80
Y_1	0.041	0.044	0.05	0.05
Y_2	0.033	0.034	0.02	0.02
K_1 (gm^{-3})	2.5	2.5	0.063	0.6
K_2 (gm^{-3})	1.2	1.2	0.160	1.7
k_1 (day^{-1})	0.2	0.2	0.12	0.2
k_2 (day^{-1})	0.17	0.17	0.12	0.2
p (%)	88	-	94	-
C^*	-	1.81	-	-

[1] Time-varying compaction ratio $C(t)$ assumed

[2] Time-invariant compaction ratio C^* assumed (value quoted is a mean value computed from the ratio of mixed liquor to recycle sludge SS concentrations.)

[3] These estimates obtained using the data of Knowles et al (24)

Volume of aerator at Norwich Sewage Works = 8320m^3; mean settled sewage influent flow = 2×10^4 m^{3}day^{-1}

Table 2 Statistics of the residual error sequences of Fig.6

ariable	Standard deviation of output time-series, σ_y (gm^{-3})	Time-varying $C(t)$: Standard deviation of residual errors, σ_ε (gm^{-3})	Time-varying $C(t)$: $(\sigma_\varepsilon^2/\sigma_y^2)$%	Time-invariant C^*: Standard deviation of residual errors σ_ε (gm^{-3})	Time-invariant C^*: $(\sigma_\varepsilon^2/\sigma_y^2)$%
H_4-N	8.3	5.2	39	7.8	88
O_2-N	1.8	2.1	>100	2.0	91
O_3-N	10.8	7.5	48	9.5	78

state-parameter estimation as in (5) becomes particularly problematic. In terms of information restructuring it is highly likely that the useful information content of the measured input/output sequences (refer to Figure 3) is being "translated" into information about $\hat{\underline{x}}_u$ and not into efficient estimates $\hat{\underline{\alpha}}$ of the parameters. It is doubtful, therefore, whether one could carry out meaningful checks on the model and its parameters in any way other than by hypothesising estimates $\hat{\underline{\alpha}}$, processing the field data to obtain $\hat{\underline{x}}$, and thence computing the residual errors $\underline{\varepsilon}(t_k|t_{k-1})$ of equation (8). Following such a procedure, the three sequences $\varepsilon(t_k|t_{k-1})$ for ammonium-N, nitrite-N, and nitrate-N in Figure 6 thus correspond to the results of Figure 4 given the parameter estimates of Table 1. Some statistics of the residual sequences are provided by Table 2.

What arguments can be advanced to justify the model and its parameter estimates? First, we may note from Figure 6 that again -- as in Figure 4 -- the total interval of observation divides into three qualitatively distinct phases, i.e. approximately $t_1 \rightarrow t_{30}$, $t_{31} \rightarrow t_{68}$, and $t_{81} \rightarrow t_{104}$. In the first and last of these phases all three residual sequences display significantly smaller amplitudes of variation than the errors of prediction over the second period. On the basis of the earlier discussion this probably reflects the model's ability to perform better under conditions of steady growth in the nitrifier populations than under unstable growth/collapse situations. This is consistent with the fact that the model contains no account of oxygen limitation of growth-rates.

Second, merely by inspection the residual error sequences are seen not to exhibit any strong tendency to be significantly biased. That is to say, if the model persistently underestimates, or overestimates, the observed substance concentrations, one would suspect that the model is substantially in error. The relatively unbiased performance of the model and filtering algorithms is also reflected in the step-by-step corrections applied to the reconstructed state estimates $\hat{\underline{x}}_u$, where the corrections $\upsilon(t_k|t_{k-1})$ are defined form the relationship,

$$\hat{\underline{x}}(t_k|t_k) = \hat{\underline{x}}(t_k|t_{k-1}) + K(t_k)\{\underline{y}(t_k)-\hat{\underline{x}}_m(t_k|t_{k-1})\} \tag{9}$$

in which $K(t_k)$ is (here) a 5 x 3 matrix, known as the Kalman gain matrix, so that,

$$\underline{\nu}(t_k|t_{k-1}) = \begin{bmatrix} \underline{\nu}_m(t_k|t_{k-1}) \\ \hline \underline{\nu}_u(t_k \;\; t_{k-1}) \end{bmatrix} \triangleq K(t_k)\underline{\varepsilon}(t_k|t_{k-1}) \tag{10}$$

The method of computing $K(t_k)$ will not concern us further, except to note that it acts as an error-weighting factor in the procedure of updating the one-step ahead predictions as new measurements $\underline{y}(t_k)$ are received, i.e. equation (9). $K(t_k)$ is in fact derived from algorithms in the filter that provide the time-evolution of the state estimation error covariance matrix in parallel with the state estimates themselves. It is in this latter context that the filtering algorithms (Figure 3) require specification of the relative levels of uncertainty in the model, the process disturbances, and the measurements (see, for example, (6)). Figure 7 shows thus the corrections $\nu_u(t_k|t_{k-1})$ for the estimates of Nitrosomonas and Nitrobacter concentrations. In general, these corrections oscillate randomly about the zero level with no predominant, or persistent tendency to be positive of negative. There is little in these results to suggest how the model is inadequate, if indeed it is inadequate, although that is not a positive statement of the model's adequacy.

Third, the observation that the model's performance remains stable is a point in favour of the model. To see why this is so, let us rewrite either of equations (2d) or (2e) in an alternative form, i.e.

$$\dot{x}_4(t) = \alpha'(t)x_4(t) \tag{11}$$

where now α' is a time-variable parameter dependent upon the relevant elements from the previously defined vectors $\underline{\theta}(t)$, $\underline{x}(t)$, and $\underline{\alpha}$ (stating equation (11) in deterministic form, i.e. $\xi_4(t) = 0$, does not alter the substance of the following). For any $x_4(t+\tau) > x_4(t), \tau > 0$, that is Nitrosomonas population growth, it is required that equation (11) exhibits temporary, marginal instability -- exponential growth instead of exponential decay. Consequently, a small inaccuracy in the substituted values for $\underline{\alpha}$, or errors in the state estimates $\hat{\underline{x}}$, may lead to significant instability in the model. Such instability occured frequently, even for small changes in the estimated parameter values of Table 1. The model assuming a constant compaction ratio, C*, was more sensitive to the problem of instability than the model with a time-varying compaction ratio C(t). The high level of Nitrobacter concentration just after day t_{30}

(the dashed line in Figure 2(e)) is evidence of a potential gross instability. A model assuming C(t) computed from measured MLSS and recycle sludge SS concentrations proved to be a completely unworkable hypothesis because of instability problems. So by our criterion of "not unreasonable" behaviour the performance of the model given in Figures 4,6, and 7 is perhaps the best that could be expected.

Set against the three arguments supporting the adequacy of the model, Table 2 indicates that the model accounts for between 50% and 60% of the variance of the original time-series for two of the variables. In other comparable studies it has been possible to approach a figure of 60-70% for this statistic (4). Furthermore, the sampling frequency of the data (once per day) precludes identification of any fast transient effects that may be significant for the nitrifier population dynamics, for example, hydraulic variations, and intermittent oxygen limitation of growth. The model can therefore be expected to be seriously deficient in these latter respects.

From Table 2 one would conclude that the performance of the model when the compaction ratio is assumed to be constant ($C^*=1.81$) is inferior to that of the model with a time-varying compaction ratio, C(t). An average value for C(t), where C(t) is computed according to equation (6), is given as 1.98, i.e. a value approximately 10% higher than C^*. The effect of assuming C^* constant is clearly one of reduced levels of nitrifying organisms in the aerator -- See Figures 4(d) and 4(e). This is consistent with the implication that on average for $C^*=1.81$ fewer organisms are recycled to the aerator. However, during periods of relatively stable growth in the nitrifier populations, the effect appears to be particularly pronounced. The suggestion that the higher estimated concentrations of organisms are "more correct" is supported by the sequence of corrections $\nu(t_k|t_{k-1})$ for the <u>Nitrosomonas</u> population in Figure 8. These corrections are, on balance, positive corrections, which would indicate that the model persistently under-estimates the size of the population. The same is true with respect to the estimated <u>Nitrobacter</u> concentrations.

Lastly, a comparison of the parameter estimates obtained from this analysis with the parameter estimates quoted from Poduska and Andrews (38) in Table 1 shows one dominant feature. The slower specific growth-rates, higher decay-rates, and higher saturation concentrations in the present study all imply a smaller capability for growing the nitrifying organisms. This could result from the fact that no sludge was wasted in the Poduska-Andrews system. The lower separation efficiency (here) associated with the clarifier performance is not unreasonable because Poduska and Andrews deliberately over-designed the clarifier in their laboratory experiment in order to avoid the potentially complex features of a description of the clarifier dynamics. Our results tend to confirm, through the limited comparative analysis of the effects of C(t) and C*, that any model of activated sludge dynamics would be improved by a better knowledge of the behaviour of the clarifier.

5. Further Considerations

Let us recall Figure 1. Section 4.1. has assessed the performance of an EKF algorithm in the context of on-line information processing for operational control purposes. There are at least four factors that would determine the usefulness of applying such ideas in practice:

(i) the ability to make on-line measurements of process performance;

(ii) the requirements of the plant manager for additional and restructured operating information;

(iii) the accuracy of the process dynamic model used in the algorithm (see also Figure 3);

(iv) the computational requirements of the algorithm.

We shall deal with each of these factors in turn.

The availability of reliable, but not necessarily highly accurate, instrumentation is a key assumption underlying this study. Why should that be so? First, reliable instrumentation suggests that reliable control can be effected, whereas accurate instrumentation would be consistent with accurate control. The fact that for wastewater treatment processes the capacity to act, i.e. the capacity to implement control actions, is clearly quite restricted leads one to view the costs and high sensitivity of accurate instruments as arguably unjustified at present. Second, it is thus more appropriate to establish which measurements can be made reliably, examine the kind of information that can be reconstructed from these measurements, and then to account (and compensate) for both random and systematic measurement errors as part of the information processing function. The results presented here for on-line estimation of nitrification dynamics are one example of restructuring operating information. The information that can be derived from dissolved oxygen profile measurements is another example (35), (36), and one which might usefully be combined with the first example in order to achieve nitrification and denitrification in biological treatment.

The requirements of the plant manager for pertinent information about operating performance is possibly an area in which more questions need to be asked. For instance, is it necessary to know the biological activity of the sludge, or its susceptibility to bulking, or the amount of unmetabolized substrate attached to the biological floc? And what would the plant manager do with this information if it were available? A useful comparison can be drawn between the pilot of an aircraft and the manager of a wastewater treatment plant. A large volume of information on performance indicators is accessible by the aircraft pilot. What is in short supply is the pilot's ability to attend to this vast array of information; he requires therefore an information processing system that calls his attention only to the abnormal events in the behaviour of the aircraft. While the same might be true of the wastewater treatment plant manager, it is more probable that he would appreciate increased amounts of (pertinent) information on plant behaviour.

Just as the performance of the EKF algorithms is limited by the quality of the available measurements, so too is this performance limited by the quality of the model embedded in the filter. That is partly the reason why the discussion of the model in section 4.2 has been so detailed. There is nothing unique or absolute about the reconstructed state estimates ($\hat{\underline{x}}_u$) of

Figures 4(d) and 4(e). They reflect the results of processing the field data with the given model and would be different had a different model been assumed. Since the model, or equation (2), has only been verified for slow, low-frequency variations there is clearly scope for further application of recursive estimation techniques in model identification studies.

The size of the model determines the computational effect required for executing the EKF algorithms. Since this computational effort, which in the EKF is essentially the effort of matrix addition, exponentiation, multiplication, and inversion, is particularly sensitive to the size of the model, there may well be good reasons for seeking compact model forms. The objective of obtaining micro-processor realisations of similar algorithms has recently led Marsili-Libelli (31) to propose a reduced-order dynamic model for carbonaceous BOD removal in an activated sludge unit. Indeed, it is the advent of relatively cheap, small-scale, and personalised computing services that makes the application of recursive, on-line estimation techniques substanitally more realistic and attractive.

6. Conclusions

The results presented in this paper are part of a larger study on modelling and operational control of the activated sludge process (8). An on-line, or recursive, estimation algorithm, the extended Kalman filter, has been applied to the two problems of: (i) identifying a dynamic model for nitrification; and (ii) examining the feasibility of state estimation and state reconstruction as features of operational control. For the first problem the analysis shows that a model proposed by Poduska and Andrews (38) can be approximately verified against time-series data from the Norwich Sewage Works in England. The most serious constraints on the model are its lack of characterisation of oxygen limitation of nitrifier growth, and its inadequate description of the clarifier dynamics. The analysis also emphasises the intractable difficulties of model identification in the presence of unobserved state variables, i.e. the concentrations of *Nitrosomonas* and *Nitrobacter* bacteria. For real-time control purposes it may be argued that less computationally expensive algorithms than the EKF would be desirable. Nevertheless, the EKF serves well the purpose of illustrating the range of possibilites for on-line estimation algorithms.

A major point is that this study views models and information processing algorithms as a support service in the day-to-day decision-making of operational management of wastewater treatment plants. Plant automation and computerisation should neither merely assume the passive role of recording plant performance, nor aim for elimination of the human element from the control function. Rather, these technological innovations should be designed to meet and encourage an active interaction of man and computer in operational management.

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APPENDIX II - Notation

The following symbols are used in this paper:

$C(t)$ = time-variable compaction ratio for solids passing through clarifier;

C^* = time-invariant compaction ratio for solids passing through clarifier;

$\underline{f}$ = nonlinear vector function;

$\underline{H}$ = matrix relating state variables to output observations;

k_1, k_2 = specific decay-rate constants for *Nitrosomonas* and *Nitrobacter* respectively (day^{-1});

K_1, K_2 = saturation concentrations for *Nitrosomonas* and *Nitrobacter* respectively (gm^{-3});

p = coefficient of solids-liquids separation efficiency in clarifier (%);

Q_I, Q_R, Q_W = influent settled sewage, recycle sludge, and waste sludge flow-rates, respectively ($m^3 day^{-1}$);

t = time (days);

u_1 = concentration of ammonium-N in influent settled sewage (gm^{-3});

V_A = volume of aerator (m^3);

x_i = component concentration in the aerator: $i=1$, ammonium-N; $i=2$, nitrite-N; $i=3$, nitrate-N; $i=4$, *Nitrosomonas* bacteria; $i=5$, *Nitrobacter* bacteria (all in gm^{-3});

$\underline{x}$ = vector of state variables;

x_{4R}, x_{5R} = concentrations of *Nitrosomonas* and *Nitrobacter* bacteria in recycle sludge, respectively (gm^{-3});

Y_1, Y_2 = yield coefficients for *Nitrosomonas* and *Nitrobacter* respectively (g organism produced/g substrate consumed);

$\underline{y}$ = vector of measured output variables;

$\underline{\alpha}$ = vector of model parameters;

$\underline{\varepsilon}$ = vector of innovations process residual errors (one-step ahead prediction errors) from the EKF;

$\underline{\xi}$ = vector of unknown (stochastic) disturbances of process dynamics;

$\underline{\eta}$ = vector of random measurement errors associated with output measurements;

$\underline{\nu}$ = vector of state estimate corrections generated by the EKF;

$\underline{\theta}$ = vector of known "internal" variables used in the model;

$\hat{\mu}_1, \hat{\mu}_2$ = maximum specific growth-rate constants for *Nitrosomonas* and *Nitrobacter* respectively (day^{-1}).

Subscripts

k = kth sampling instant of time;

m = measured state variables;

u = unmeasured state variables;

Superscripts

^ = estimated variable or parameter.

LIST OF FIGURE CAPTIONS

Figure 1: The basic features of process control; on-line measurements are available for some of the input disturbances and for some of the output responses.

Figure 2: Schematic diagram of the activated sludge process; all notation is defined in the text and in Appendix II.

Figure 3: Conceptual picture of the (extended) Kalman filter.

Figure 4: Observations $y(t_k)$ and state estimates $\hat{\underline{x}}_m(t_k|t_k)$ for the aerator concentrations of (a) ammonium-N, (b) nitrite-N, and (c) nitrate-N; reconstructed state estimates $\hat{\underline{x}}_u(t_k|t_k)$ for (d) aerator Nitrosomonas concentration and (e) aerator Nitrobacter concentration. The dashed lines in (d) and (e) denote corresponding results when a time-invariant compaction ratio C* is used in the model.

Figure 5: Concentration of ammonium-N in influent settled sewage.

Figure 6: One-day ahead prediction errors (residual errors) for the model when a time-varying compaction ratio C(t) is assumed, and given the associated parameter estimates of Table 1.

Figure 7: Corrections (as defined in equation (10)) obtained from the filter when a time-varying compaction ratio C(t) is assumed, and given the associated parameter estimates of Table 1.

Figure 8: Corrections obtained from the filter (for *Nitrosomonas* concentration) when a time-invariant compaction ratio C* is assumed, and given the associated parameter estimates of Table 1.

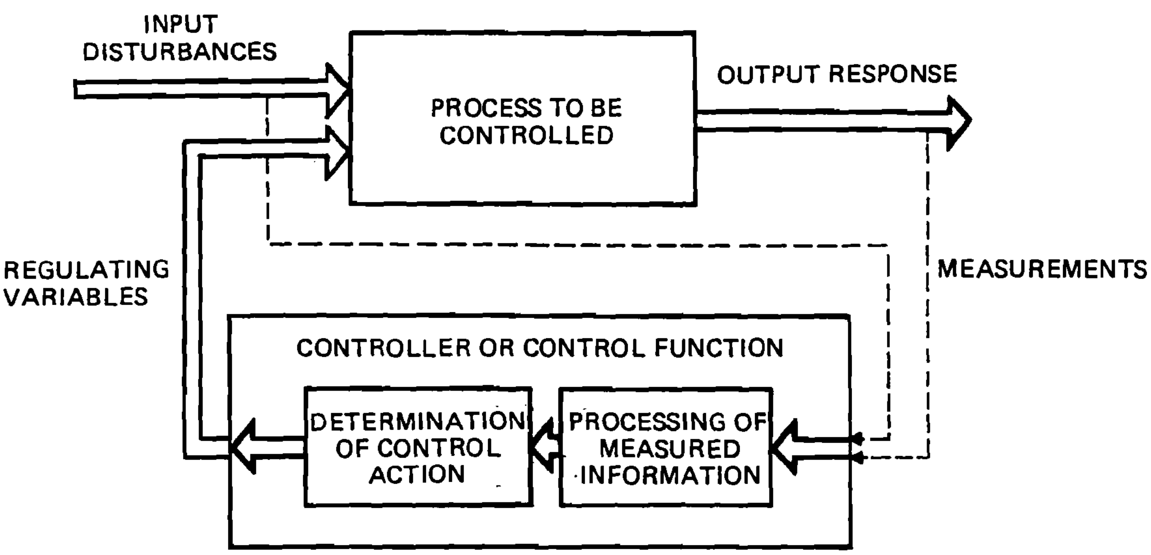

INPUT
DISTURBANCES
PROCESS TO BE
CONTROLLED
OUTPUT RESPONSE
REGULATING
VARIABLES
MEASUREMENTS
CONTROLLER OR CONTROL FUNCTION
DETERMINATION
OF CONTROL
ACTION
PROCESSING OF
MEASURED
INFORMATION

Figure 1.

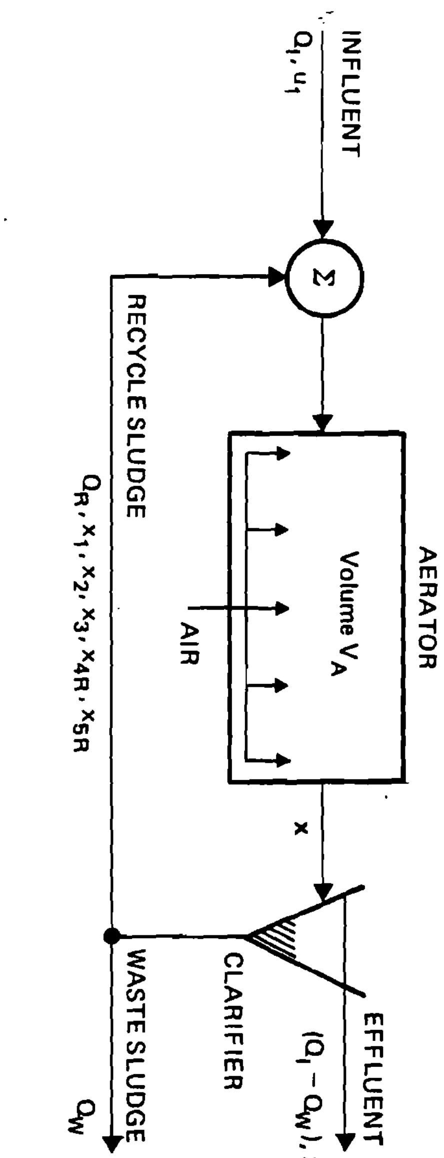

INFLUENT
Q_I, u_I
Σ
RECYCLE SLUDGE
$Q_R, x_1, x_2, x_3, x_{4R}, x_{5R}$
AERATOR
Volume V_A
AIR
x
EFFLUENT
$(Q_I - Q_W), x$
CLARIFIER
WASTE SLUDGE
Q_W

Figure 2.

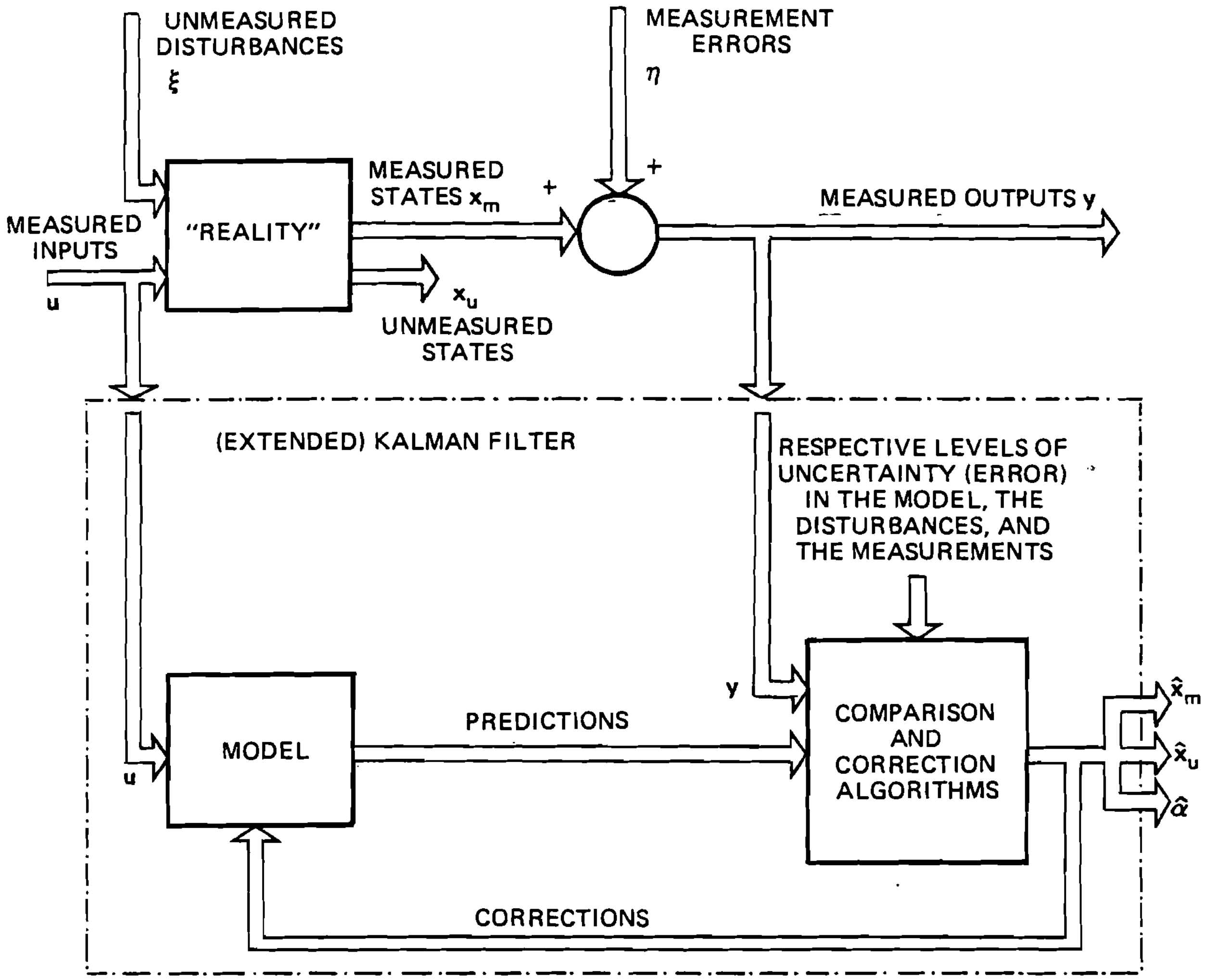

UNMEASURED DISTURBANCES
ξ
MEASUREMENT ERRORS
η
MEASURED INPUTS
u
"REALITY"
MEASURED STATES x_m
+
+
-
MEASURED OUTPUTS y
x_u
UNMEASURED STATES
(EXTENDED) KALMAN FILTER
RESPECTIVE LEVELS OF UNCERTAINTY (ERROR) IN THE MODEL, THE DISTURBANCES, AND THE MEASUREMENTS
y
MODEL
u
PREDICTIONS
COMPARISON AND CORRECTION ALGORITHMS
$\hat{x}_m$
$\hat{x}_u$
$\hat{\alpha}$
CORRECTIONS

Figure 3.

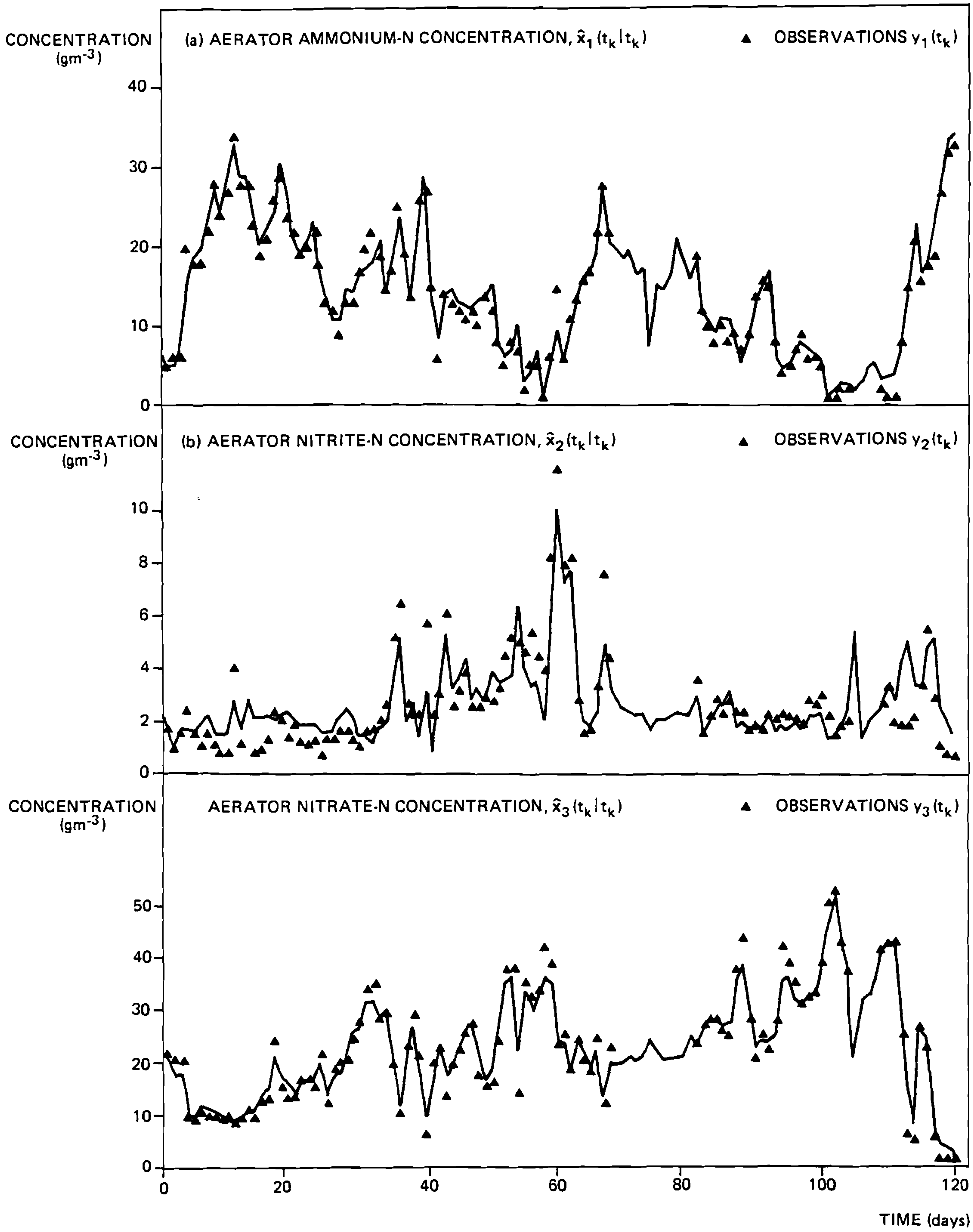

CONCENTRATION (gm-3)
(a) AERATOR AMMONIUM-N CONCENTRATION, x̂1 (tk|tk)
OBSERVATIONS y1 (tk)
40
30
20
10
0
CONCENTRATION (gm-3)
(b) AERATOR NITRITE-N CONCENTRATION, x̂2 (tk|tk)
OBSERVATIONS y2 (tk)
10
8
6
4
2
0
CONCENTRATION (gm-3)
AERATOR NITRATE-N CONCENTRATION, x̂3 (tk|tk)
OBSERVATIONS y3 (tk)
50
40
30
20
10
0
0
20
40
60
80
100
120
TIME (days)

Figure 4.

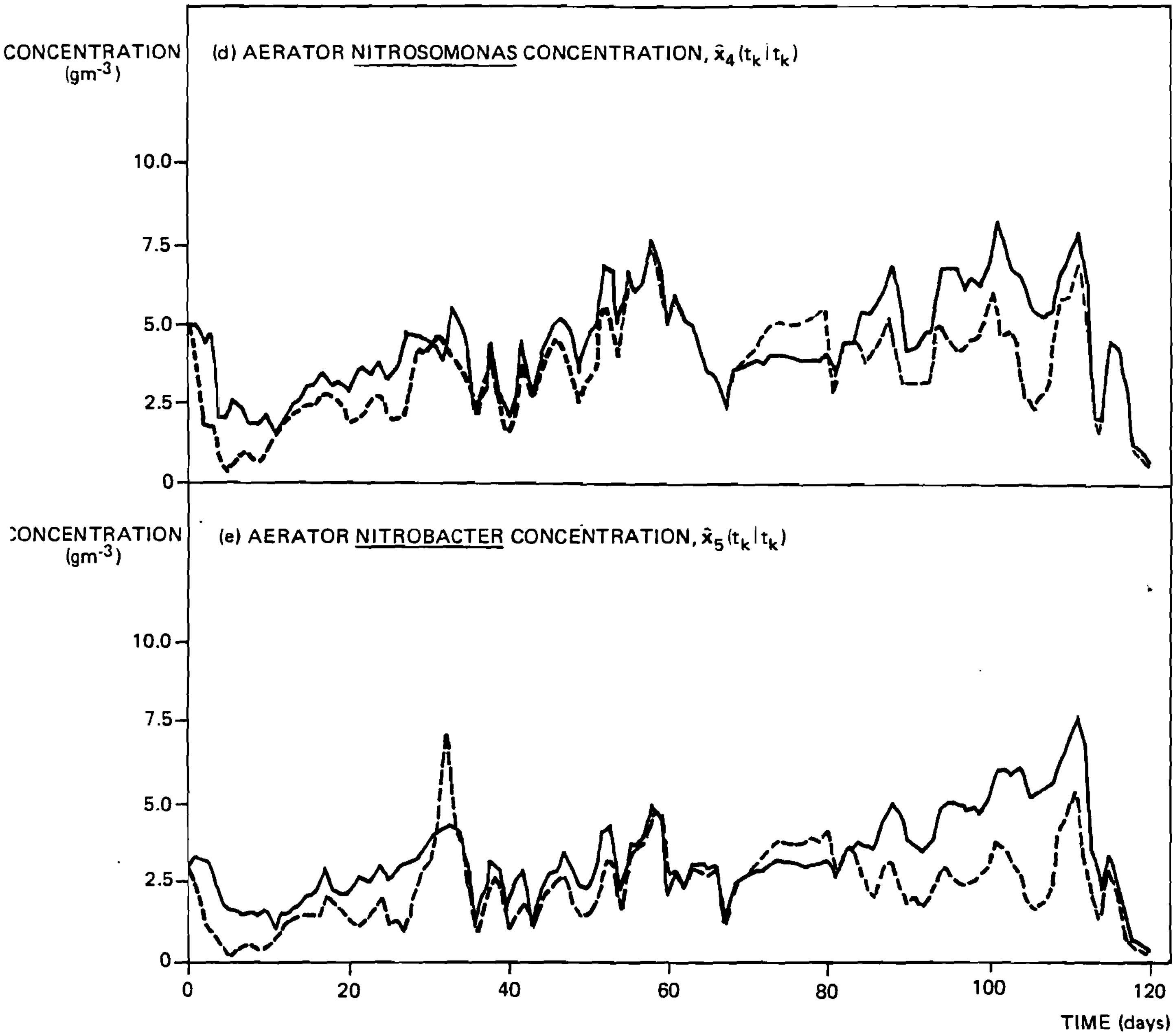


Figure 4. (cont.)

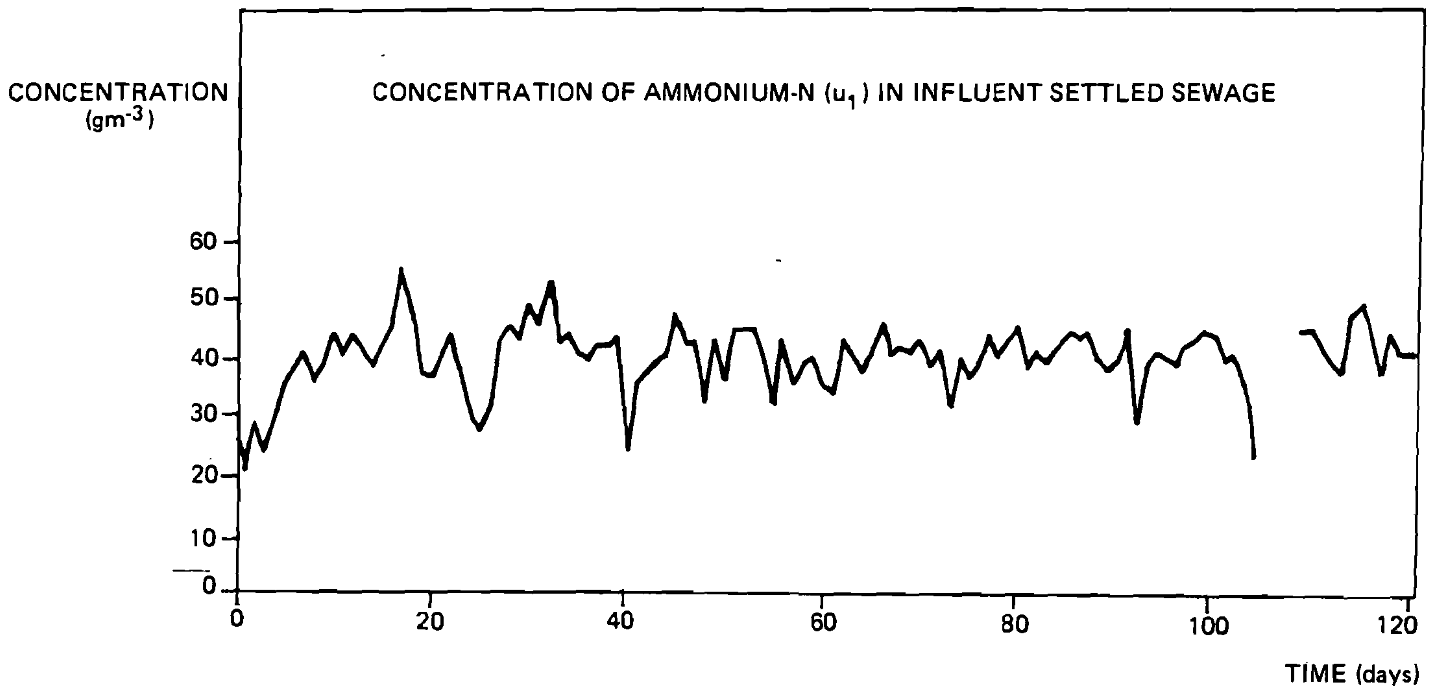
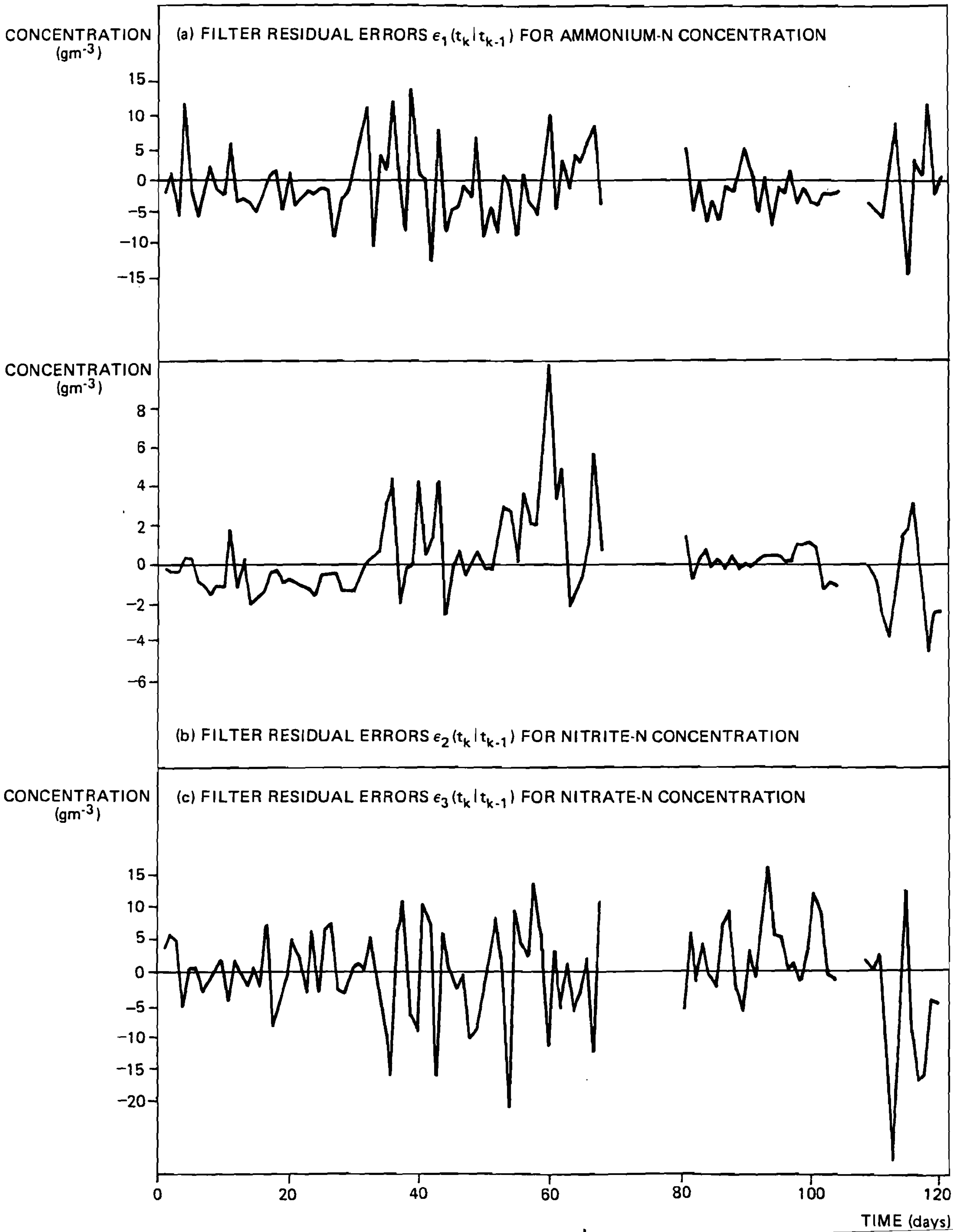

CONCENTRATION
(gm-3)
CONCENTRATION OF AMMONIUM-N (u1) IN INFLUENT SETTLED SEWAGE
60
50
40
30
20
10
0
0
20
40
60
80
100
120
TIME (days)

Figure 5.

Figure 6.


CONCENTRATION (gm-3)
(a) FILTER RESIDUAL ERRORS ε1 (tk | tk-1) FOR AMMONIUM-N CONCENTRATION
15
10
5
0
-5
-10
-15
CONCENTRATION (gm-3)
8
6
4
2
0
-2
-4
-6
(b) FILTER RESIDUAL ERRORS ε2 (tk | tk-1) FOR NITRITE-N CONCENTRATION
CONCENTRATION (gm-3)
(c) FILTER RESIDUAL ERRORS ε3 (tk | tk-1) FOR NITRATE-N CONCENTRATION
15
10
5
0
-5
-10
-15
-20
0
20
40
60
80
100
120
TIME (days)

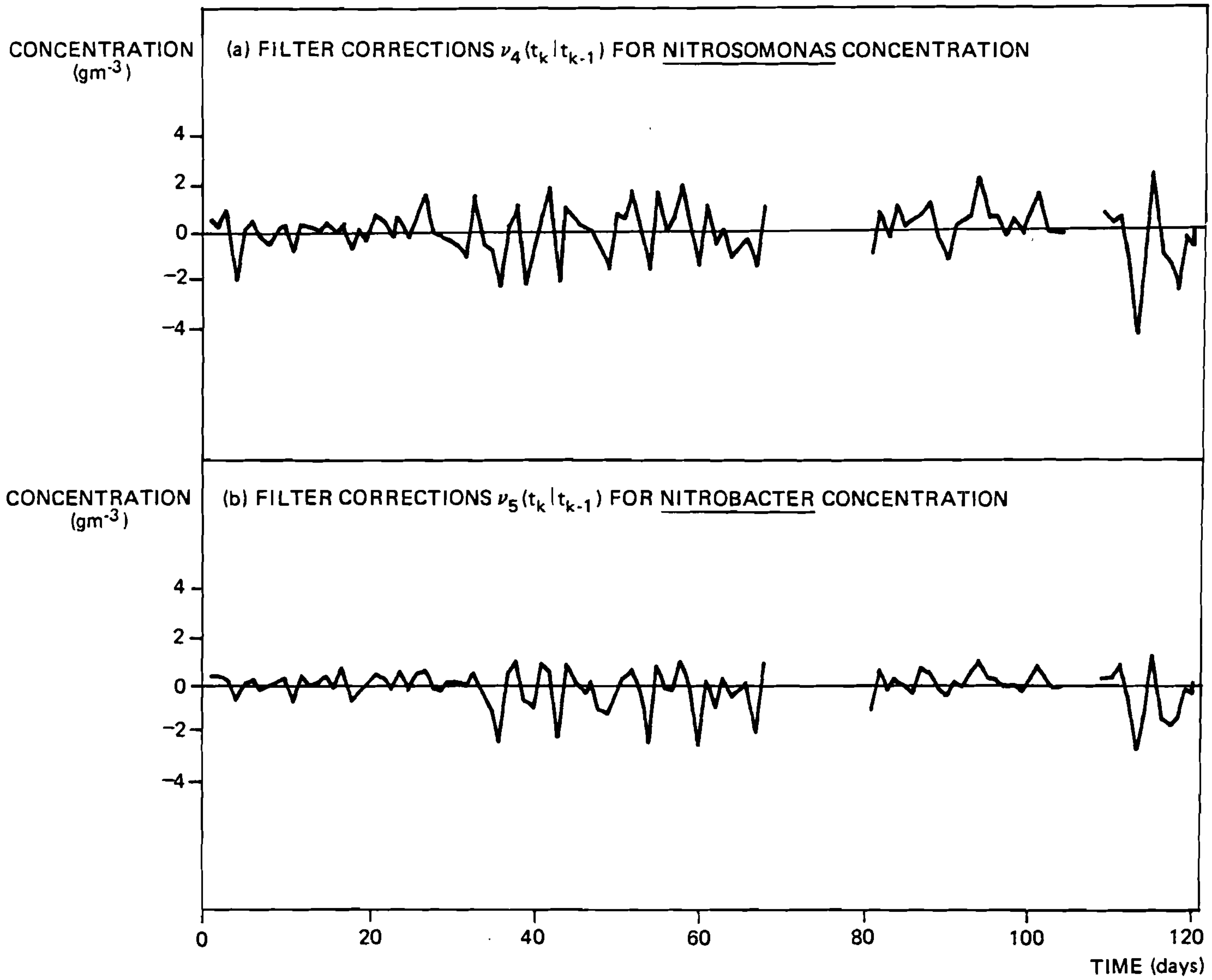

CONCENTRATION (gm-3)
(a) FILTER CORRECTIONS ν4(tk|tk-1) FOR NITROSOMONAS CONCENTRATION
4
2
0
−2
−4
CONCENTRATION (gm-3)
(b) FILTER CORRECTIONS ν5(tk|tk-1) FOR NITROBACTER CONCENTRATION
4
2
0
−2
−4
0
20
40
60
80
100
120
TIME (days)

Figure 7.

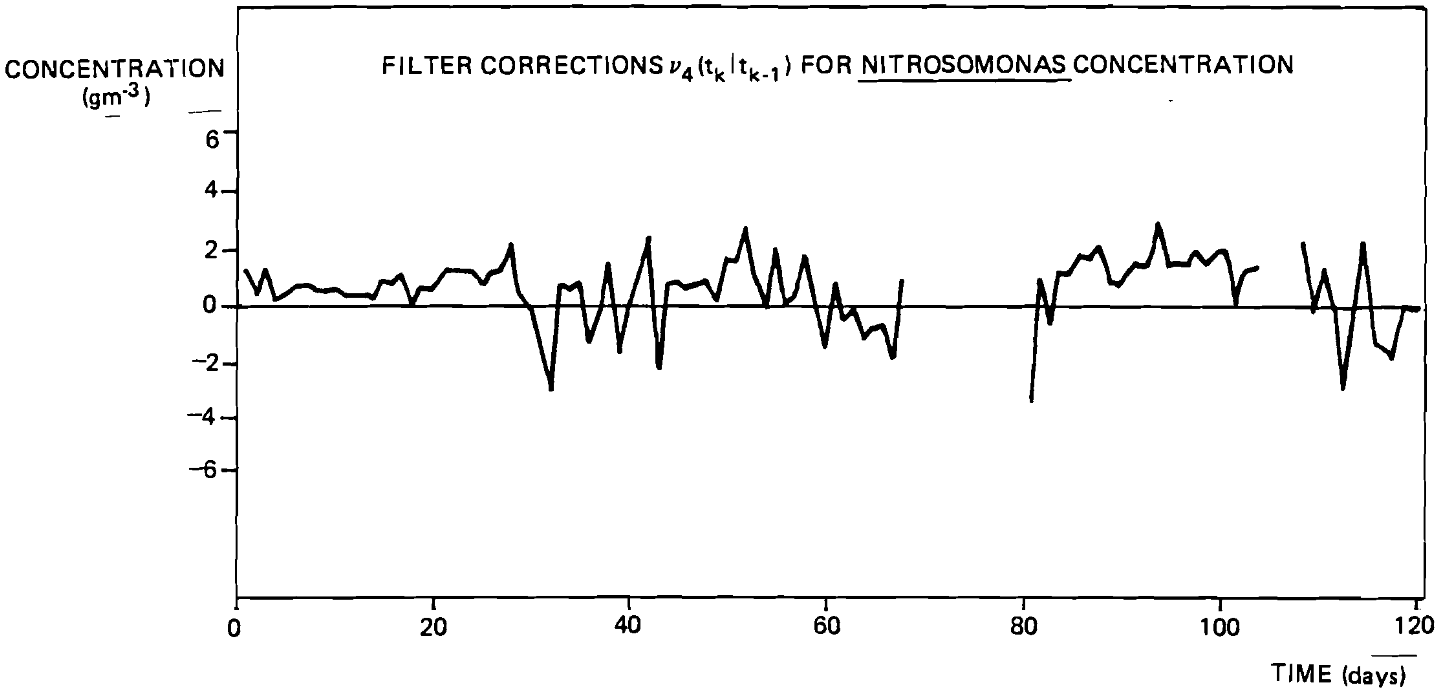

CONCENTRATION
(gm-3)
FILTER CORRECTIONS $\nu_4(t_k|t_{k-1})$ FOR NITROSOMONAS CONCENTRATION
6
4
2
0
-2
-4
-6
0
20
40
60
80
100
120
TIME (days)

Figure 8.