CHAPTER 185

DISCRETE-TIME MODELLING OF DISPERSION IN ESTURARIES

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1 INTRODUCTION

This paper aims to put forward a case in favour of a simple discrete-time model describing mixing in an estuary. The model derives from the remarkably simple concepts developed by Ketchum (1951 a,b) which describe mixing in terms of tidal prism exchanges between segments. The author's view is that Ketchum's ideas were abandoned before they were fully explored. A major factor was the advent of the high-speed computer which opened up the possibility of using an approach based on the space-time formulation of the problem in terms of the partial differential equations of transport theory.

Intrinsically this approach, based on a continuum description, is more attractive than a gross description based on relatively large segments: one obvious reason is the possibility of providing a comprehensive space-time prediction of the spread of a pollutant. In practice, though, significant problems arise in its use: in particular, the following can be mentioned -

a) substantial computing costs relating to computer program development and machine time

b) specification of transport parameters inherent in the partial differential equations of transport: for example, dispersion coefficients

c) model validation and state/parameter estimation.

The last of these is the primary concern of this paper. It is probably true to say that, to date, too little attention has been given to these topics, in the context of estuarine modelling. The point to be made is that there is small justification in using a sophisticated description of a system if the resulting predictions of the model cannot be effectively validated.

The ideas used in this paper stem from those put forward by Beck and Young (1975) in studies on non-tidal river pollution. The subsequent discussion suggests an extension to estuarine systems.

2 BASIS OF THE PROPOSED MODEL

A complete description of the proposed model can be found in the published paper by Wood (1979). Only the essentials relevant to the subsequent discussion in this paper are presented here, namely, the segmentation procedure and the exchanges between segments.

2.1 Segmentation

The estuary is segmented sequentially from the fresh water end. Segment (1) is always fresh; thereafter a progressive increase in salinity takes place through segments (2), (3), ...,(n). The high tide volumes H_i, and the low-tide volumes L_i, are determined from the fresh water input R per tidal cycle (assumed known) and the hydrography of the estuary, as follows -

$$L_i = R \tag{1a}$$

$$L_i = H_{i-1} \tag{1b}$$

Thus, except for segment (1), the low-tide volume of any segment is equal to the high-tide volume of its upstream neighbour.

2.2 Exchanges Between Segments

As a consequence of the chosen segmentation procedure, water is exchanged over a tidal cycle between a segment and its nearest neighbours. Thus the high-tide volume, H_i, of segment (i) is distributed over a tidal cycle, as follows -

$v_{i-1,i}$: the volume transferred to segment (i-1) from segment (i)

$v_{i,i}$: the volume returned to segment (i)

$v_{i+1,i}$: the volume transferred to segment (i+1) from segment (i)

Each volume of water carries with it the salinity, s_i, of its origin. Therefore, from one high-tide to the next, the discrete-time model describing salinity distribution changes is as follows -

$$H_i\, s_i(k)=v_{i,i-1}s_{i-1}(k-1) + v_{i,i}\, s_i(k-1) + v_{i,i+1}s_{i+1}(k-1) \tag{2}$$

where i = 2 to n - 1
and k is a time index based on a tidal cycle.

3 STATE/PARAMETER ESTIMATION

The principal point to be made in this paper is that the discrete-time model proposed in the previous section is directly amenable to the techniques of state and parameter estimation formulated by Kalman (1960). The mathematical background is too extensive to be discussed here and, indeed, the main purpose is to demonstrate what can be achieved by using these techniques, rather than to put forward an exposition of the mathematics per se. Excellent accounts are available in texts by Eykhoff (1974) and Jazwinski (1970).

3.1 The Defining Equations

The following equations describe the change in the state vector of salinity, $\underline{s}$, at discrete-time intervals and the relationship between the vector of salinity measurements, $\underline{z}$, and the salinity vector -

Model Equation: $$\underline{s}\,(k+1) = T.\underline{s}(k) + \underline{n}(k) \qquad (3a)$$

Measurement Equation: $$\underline{z}(k) = M.\underline{s}(k) + \underline{e}(k) \qquad (3b)$$

$\underline{s}$: (nx1) vector describing salinity distribution
T: (nxn) matrix describing exchanges between segments
$\underline{n}$: (nx1) vector of model error (Gaussian)
$\underline{z}$: (mx1) vector of measured salinities
M: (mxn) matrix relating measurement to salinity
$\underline{e}$: (mx1) vector of measurement error (Gaussian)
k: an index of discrete-time

3.2 The Kalman Filter: State Estimation

The Kalman Filter provides an estimate of the salinity vector at each time interval, based upon the measurements received up to that time. The procedure is recursive in that an updated estimate can readily be made each time new measurement information is received, based on the previous estimate and the new information. This scheme of sequential updating of estimates is particularly well suited to a system which is monitored in a regular way.

Kalman's solution to the problem of recursive state estimation assumes that the statistical properties of the vectors $\underline{n}(k)$ and $\underline{e}(k)$, representing system and measurement noise respectively, are known and described by -

$$\begin{aligned} &E[\,\underline{n}(k)\,] = E\,[\underline{e}(k)] = 0 \\ &E[\,\underline{n}(k)\ \underline{n}(j)^{1}] = Q\ \delta_{kj} \\ &E[\,\underline{e}(k)\ \underline{e}(j)^{1}] = R\ \delta_{kj} \\ &E[\,\underline{n}(k)\ \underline{e}(j)^{1}] = 0 \text{ for all } k,j \end{aligned} \qquad (3c)$$

The following two-stage filter estimation algorithm can now be deduced -

<u>Stage 1</u> - Prediction

$$\hat{\underline{s}}(k,k-1) = T\ \hat{\underline{s}}(k)$$

$$P(k,k-1) = T\ P(k-1)\ T + Q$$

Stage 2 - Correction

$$\hat{\underline{s}}(k) = \hat{\underline{s}}(k,k-1) + P(k,k-1)\, M' \,[M\, P(k,k-1)\, M' + R]^{-1}\, [\underline{z}(k) - M\, \hat{\underline{s}}(k,k-1)]$$

$$P(k) = P(k,k-1) - P(k,k-1)\, M' \,[M\, P(k,k-1)\, M' + R]^{-1}\, M\, P(k,k-1)$$

(3c)

where $\hat{\underline{s}}(k,k-1)$ is the first-stage estimate of the salinity distribution, previous estimate $\hat{\underline{s}}(k-1)$

$P(k,k-1)$ is the covariance matrix of the estimation error with $\hat{\underline{s}}(k,k-1)$

$\hat{\underline{s}}(k)$ is the second-stage estimate, based on the first-stage estimate $\hat{\underline{s}}(k,k-1)$ and the latest measurement information $\underline{z}(k)$

$P(k)$ is the covariance matrix of the estimation error associated with $\hat{\underline{s}}(k)$

The second-stage estimates $\hat{\underline{s}}(k)$, $P(k)$ for the kth time instant are therefore based on the complete data set collected between instants 1 and k.

3.3 The Extended Kalman Filter: State-Parameter Estimation

In many practical problems, the matrix appearing in the model equation cannot be specified because some of its elements are unknown. In the context of the dispersion model, the T matrix describing the exchanges between segments contains unknowns which have to be estimated from salinity measurements. The estimation problem then extends to the unknown parameters of the T matrix as well as the state vector of salinities mentioned in the previous section. The approach adopted essentially involves reformulating the defining equations (3a) and (3b) in terms of an augmented vector which contains as its elements the salinity vector elements and the unknown parameters. A simple example in the next section demonstrates the principle but for a comprehensive account of the technique the reader should consult the references previously mentioned, Eykhoff (1974) and Jazwinski (1970).

4 SIMPLE EXAMPLE OF THE APPLICATION OF STATE/PARAMETER ESTIMATION

A simple 4-segment example is used to demonstrate the use of the proposed discrete-time model and the application of the Kalman filter. Segment (1) is completely fresh at all times and segment (4) is completely saline at all times ($s_1 = 0$, $s_4 = 1$ all values of k). The transition matrix, T, in equation (3a) is -

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ t_{21} & t_{22} & t_{23} & 0 \\ 0 & t_{32} & t_{33} & t_{34} \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

where $t_{ij} = v_{ij}/H_i$

Various categories of problem can be analysed, as described below.

4.1 State Estimation Only (all elements of T known).

4.1.1 Segments (2) and (3) monitored.

The Kalman filter provides estimates $\hat{s}_2(k)$, $\hat{s}_3$ (k) of the salinities in segments (2) and (3) from a sequence of monitored salinities z_2 (p), z_3 (p), for p = 1 to k. The measurement matrix, M, is

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

4.1.2 Either segment (2) or segment (3) monitored.

The Kalman filter provides estimates $\hat{s}_2(k)$, $\hat{s}_3(k)$ from a sequence of monitored salinities: either z_2 (p) or z_3 (p), for p = 1 to k. The measurement matrix, M, is -

either $\begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$ or $\begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$

Segment (2) monitored Segment (3) monitored

4.1.3 A numerical example of state estimation

Consider a system with a T matrix specified as -

$$T = \begin{vmatrix} 1 & 0 & 0 & 0 \\ 0.5 & 0.3 & 0.2 & 0 \\ 0 & 0.35 & 0.45 & 0.2 \\ 0 & 0 & 0 & 1 \end{vmatrix}$$

Let the covariance matrices Q, R representing the system noise and the measurement noise, respectively, be -

$$Q = R = \begin{vmatrix} 0 & 0 & 0 & 0 \\ 0 & 4x10^{-4} & 0 & 0 \\ 0 & 0 & 4x10^{-4} & 0 \\ 0 & 0 & 0 & 0 \end{vmatrix}$$

Then, given a set of monitored salinities at successive sampling instants k = 1,2.......10, for segments (2) and (3), the recursive estimates for the true salinities s_2, s_3 can be obtained using the Kalman Filter algorithm. Table 1 summarizes the results.

TABLE 1

k	z_2	$\hat{s}_2$	$P_{22}x10^3$	z_3	$\hat{s}_2$	$P_{33}x10^3$
1	0.526	0.499	3.94	1.02	1.02	0.398
2	0.358	0.326	0.626	0.753	0.775	0.289
3	0.254	0.252	0.470	0.660	0.661	0.237
4	0.197	0.209	0.451	0.594	0.590	0.226
5	0.225	0.183	0.448	0.561	0.551	0.225
6	0.179	0.162	0.447	0.480	0.494	0.224
7	0.162	0.150	0.447	0.504	0.493	0.224
8	0.134	0.146	0.447	0.503	0.491	0.224
9	0.073	0.138	0.447	0.426	0.446	0.224
10	0.130	0.134	0.447	0.476	0.470	0.224

k — is the discrete sampling time index, based on an interval of a tidal cycle

z_2, z_3 — are the monitored salinities in segments (2),(3) (relative to sea water as unity).

$\hat{s}_2, \hat{s}_3$ — are the filtered estimates of the relative salinities in segments (2),(3).

P_{22}, P_{33} — are the variances associated with the filtered estimates.

4.2 State/Parameter Estimation (some elements of T unknown)

4.2.1 Dimension of the problem

Although it would appear that there are six nonzero elements to be specified in the T matrix, only two need, in fact, to be estimated. The element t_{21} is fixed by the fresh water flow from segment (1) to segment (2). Also the following relationship for the exchanges between neighbouring segments leaves only two elements unknown -

$$H_i = v_{i,i-1} + v_{i,i} + v_{i,i+1} = v_{i-1,i} + v_{i,i} + v_{i+1,i} \qquad (4)$$

where $i = 2$ to $n - 1$

Therefore in the 4-segment example there are two states and two parameters to be estimated: $\hat{s}_2, \hat{s}_3, t_{22}, t_{33}$.

4.2.2 The augmented state vector

The state vector $(0\ s_1\ s_2\ 1)^T$ is augmented with the two unknown parameters t_{22}, t_{33} to yield $(0\ s_1\ s_2\ 1\ t_{22}\ t_{33})^T$. Let the augmented vector be designated $\underline{x}$. The defining equations can then be reformulated as follows -

Model Equation: $\underline{x}(k+1) = T'\underline{x}(k)+\underline{n}'(k)$ (5a)

Measurement Equation: $\underline{z}(k) = C'\underline{x}(k)+\underline{e}'(k)$ (5b)

The problem now becomes non-linear because some of the elements of T' contain elements of the augmented vector $\underline{x}$. After each estimate of the augmented vector $\hat{\underline{x}}$ the matrix T' is accordingly updated. Apart from this the Extended Kalman Filter follows the same algorithms as before, so that monitored salinities in segment (2) and/or segment (3) can provide recursive estimates of $\hat{s}_2$, $\hat{s}_3$, $\hat{t}_{22}$ and $\hat{t}_{33}$.

4.2.3 A numerical example of state/parameter estimation

As explained above, the T matrix contains effectively two unknown elements, and these are to be estimated in addition to the salinity values in segments (2),(3). The T matrix itself must therefore be updated at the beginning of each cycle of the Kalman Filtering process, using the best available estimates for $\hat{t}_{22}$, $\hat{t}_{33}$. At the beginning of the calculation, the initial values for the elements of the augmented vector $\underline{x}$ and its associated error cavariance matrix P must be guessed.

Consider a system with noise covariance matrices Q, R (for the model and measurements respectively), as follows -

Q Matrix (diagonal terms): 0 $9\text{x}10^{-4}$ $9\text{x}10^{-4}$ 0 0 0

R Matrix (diagonal terms): 0 $4\text{x}10^{-4}$ $4\text{x}10^{-4}$ 0 0 0

(all off-diagonal terms are zero).

Let the initial guesses for the augmented vector $\underline{x}$ and its associated error covariance matrix P, be as follows -

$\underline{x}(0)$:	0	0.5	0.5	1	0.5	0.5
P(0):	0	10	10	0	10	10

(diagonal terms only; off-diagonal terms zero)

Table 2 summarizes the filtered estimates from a sequence of monitored salinity values z_2, z_3 in segments (2), (3).

TABLE 2

k	z_2	$\hat{s}_2$	$\hat{t}_{22}$	z_3	$\hat{s}_3$	$\hat{t}_{33}$
1	0.483	0.483	0.316	0.961	0.961	0.368
2	0.376	0.375	0.226	0.831	0.830	-0.287
3	0.274	0.278	0.273	0.671	0.672	0.631
4	0.188	0.199	0.292	0.609	0.603	0.495
5	0.185	0.186	0.290	0.554	0.550	0.450
6	0.166	0.168	0.290	0.567	0.557	0.401
7	0.174	0.172	0.287	0.525	0.526	0.400
8	0.190	0.183	0.278	0.518	0.518	0.393
9	0.096	0.114	0.295	0.457	0.472	0.436
10	0.142	0.139	0.292	0.458	0.457	0.432

5 DISCUSSION

The potential advantage to be gained from using a discrete-time modelling approach to dispersion studies in estuaries would appear to lie in the area of model validation, and in particular in state/parameter estimation. The principal disadvantage is the trade-off of model accuracy, whereby the less rigorous, spatially segmented, discrete-time description is adopted in place of a continuum model in continuous time, in favour of a well-proven approach to system identification in the form of Kalman filtering. Clearly, the issue is far from proven either way, and only a series of thorough assessments based on actual case studies will indicate which is the more fruitful approach.

The principal merits of the discrete-time model are related to the principal features of the Kalman Filter, as follows -

a) The procedure is recursive whereby the latest estimates are obtained from the most recent estimates and the latest available measurement information.

b) The Kalman Filter algorithms incorporate measures of the uncertainties inherent in the model equations and the measured data.

c) The method can be applied to a partially monitored system which is an important factor when resources of manpower and money are limited.

d) The method provides a continuous updating of estimates and the errors associated with the estimates.

e) The method offers a consistent approach to parameter estimation which is undoubtedly the key problem in modelling studies.

5 REFERENCES

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