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MATHEMATICAL MODELLING OF ESTUARIES AND COASTAL WATERS

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1. INTRODUCTION

Mathematical modelling has contributed significantly to our ability to handle pollution problems in estuaries and coastal water. The complexities of the hydraulics and biogeochemical cycles preclude the use of simple empirical approaches which are satisfactory in rivers and lakes. Although physical modelling is an alternative not all the phenomena concerned may be simulated physically; there are problems of scaling and the cost is very high. (Novak and Cabelka, 1981) In these circumstances mathematical models are an essential tool in the control of pollution.

Estuaries and coastal waters are physically contiguous and share many hydraulic characteristics but there are important differences which have made the modelling approaches to the two environments fundamentally different. The two most important differences are as follows:-

a) The common pollution problems in the two situations are different. In estuaries the water quality is concerned with the level of dissolved oxygen, with acute toxins as a secondary parameter. The greater dilution in coastal waters usually obviates any problems of deoxygenation or acute toxicity so visual amenity and microbiological quality are the primary concerns.

b) The mechanisms responsible for dilution are somewhat different. In the case of coastal waters the initial mixing of the waste is due to the entrainment of seawater in the buoyant jet and subsequently to advection and turbulent diffusion at the surface in a relatively unconfined area. Discharges to estuaries occur usually at or near the surface so dispersion by advection and turbulent diffusion takes place in a confined area where differences vertically and laterally may often be neglected.

Because of these and other differences, modelling of estuaries and coastal waters has proceeded on divergent lines and are therefore discussed separately.

2. MODELLING OF ESTUARIES

In considering the state-of-the-art in estuarine modelling it is important to remember that nearly all models have been produced for planning purposes. Operational models have not yet been required. Models of estuarine water quality therefore need to be judged not only in terms of their contemporary validity but their prodictive ability under future conditions.

Several reviews of estuarine models have been published notably those by Hinwood and Wallis 1975; McDowell and O'Connor 1977; Kinsman 1978. Most of the models have used dissolved oxygen as their primary quality criterion, although some also attempt to predict water quality in terms of other parameters, mainly sediment (e.g. Festa and Hansen 1978), metals (Burton 1976; De Groot, Solomons and Allersma 1976) or hot water (USF&WL 1978). The models vary considerably in their degree of sophistication in representing the biochemical processes for sources and sinks of oxygen. The simplest models use Streeter Phelps kinetics (Ratasuk 1971). More elaborate models take into account other processes such as nitrification (Hobbs and Fawcett 1973) and photosynthesis (Orlob 1969; Thomann 1972). It is difficult to judge the level of sophistication required to model future conditions although it is apparent from experience in the River Thames (Thames W.A. 1977) that nitrification may become much more important as the water quality improves.

One other refinement that may be required is the partition of the oxygen demand into benthal and planktonic since it has been shown that a significant proportion of the uptake is associated with the bottom muds (James 1980; Moniwa 1978).

2.1 Hydraulic Classification

The majority of water quality models are based upon a representation of the estuarine hydraulics together with sources and sink terms. Within the general framework of hydraulic models there is such a wide variety of approach that it has become difficult to classify the models. Hinwood and Wallis (1975) in their comprehensive review suggested three bases for classifying models and gave examples of some of the models (Table 1):

a) Number of spatial dimensions - zero, 1, 2 or 3.
b) Type of reference framework - Eulerian, Lagrangian or Constant Upstream Volume.
c) Degree to which hydrodynamic processes are included:
   Hydrodynamic - Velocities computed from equations of motion
   Kinematic - Velocities computed from conservation of mass
   Transport - Velocities supplied

As can be seen from Table 1 there are a wide variety of models available. The choice is determined mainly by the users requirements but there are some general considerations, notably:

a) The data requirement for increasing by one dimension is an order of magnitude greater, so choice is the minimum dimension to give a realistic representation.

b) Non-Eulerian models suffer much less numerical dispersion (Mollowney 1973; O'Kane 1980) and are a distinct improvement on Eulerian models.

c) The data requirements of hydrodynamic, kinematic and transport models are not significantly different. The choice between these 3 is determined by whether the interest is solely concerned with pollutant distribution or whether there is a wider interest in predicting other features such as water level.

Table 1 : Classification of models for tidal waters (modified from HINWOOD & WALLIS, 1975)

Reference Framework	Dimension								
	Zero	One		Two (Plan View)		Two (Elevation)		Three	
	Eulerian	Eulerian	Other	Eulerian	Other	Eulerian	Other	Eulerian	Other
Hydrodynamic		1,8,9,20, 27,28,36, 47,52,58, 59,60,79, 83,101, 102,118, 124,126	66	2,3,10,12, 22,23,25, 28,29,30, 34,38,43, 44,54,61, 62,63,64, 70,73,83, 91,92,93, 95,101, 103,105, 109,110, 113,114, 115,125		13,14,15 68,113, 114,115,118		38,57	
Kinematic		121	36,74 100,116			46			
Transport	17,26,41, 67,90,108, 111,119	27,89,96	36,74, 80,81, 100,117	12,35,63, 77,84,85, 105,107	44,92	27,42,44, 94,118	117		

McDowell and O'Connor (1977) used a bivariate system of classification based on the following:

i) Analytical or numerical solutions to equations.

ii) Time-scale - Time varying, tidal-averaged or steady-state.

The constraints on analytical solutions are so severe that almost all models use numerical techniques. The choice of time-scale is a balance between the need for detailed information on variations in dissolved levels and the extra data requirement. Some approximations are involved in extending the time-scale as can be seen from equation (1) time-varying, equation (2) tidal-averaged and equation (3) steady-state:

$$(1) \quad \frac{\partial C}{\partial t} + \frac{\partial}{\partial x}(V_x C) + \frac{\partial}{\partial y}(V_y C) + \frac{\partial}{\partial z}(V_z C) = \frac{\partial}{\partial x}\left(D_x \frac{\partial C}{\partial x}\right) + \frac{\partial}{\partial y}\left(D_y \frac{\partial C}{\partial y}\right) + \frac{\partial}{\partial z}\left(D_z \frac{\partial C}{\partial z}\right) + S$$

$$(2) \quad \frac{\partial \bar{C}}{\partial \bar{t}} + \frac{\partial}{\partial x}(\bar{V}_x \bar{C}) + \frac{\partial}{\partial y}(V_y C) + \frac{\partial}{\partial z}(\bar{V}_z \bar{C}) = \frac{\partial}{\partial x}\left(\bar{E}_x \frac{\partial \bar{C}}{\partial x}\right) + \frac{\partial}{\partial y}\left(\bar{E}_y \frac{\partial \bar{C}}{\partial y}\right) + \frac{\partial}{\partial z}\left(\bar{E}_z \frac{\partial \bar{C}}{\partial z}\right) + \bar{S}$$

$$(3) \quad \frac{\partial}{\partial x}(\bar{\bar{V}}_x \bar{\bar{C}}) + \frac{\partial}{\partial y}(\bar{\bar{V}}_y \bar{\bar{C}}) + \frac{\partial}{\partial z}(\bar{\bar{V}}_z \bar{\bar{C}}) = \frac{\partial}{\partial x}\left(\bar{\bar{E}}_x \frac{\bar{\bar{C}}}{x}\right) + \frac{\partial}{\partial y}\left(\bar{\bar{E}}_y \frac{\bar{\bar{C}}}{y}\right) + \frac{\partial}{\partial z}\left(\bar{\bar{E}}_z \frac{\bar{\bar{C}}}{z}\right) + \bar{\bar{S}}$$

Where C = concentration
t = time
x, y and z are three spatial dimensions
V_x, V_y and V_z are velocities in the three dimensions
D_x, D_y and D_z are turbulent diffusion coefficients
E_x, E_y and E_z are effective dispersion coefficients
The single overbar indicates tidal-average
The double overbar indicates steady-state
(Fischer 1979; Pollock 1973)

McDowell and O'Connor (1977) also draw attention to three other categories of models namely simulation, statistical and stochastic. The construction and use of these models may be briefly summarised as follows:-

a) Simulation models are those in which the convective - diffusion equation is replaced by a single mixing operation between segments in an estuary (e.g. Pearson and Pearson 1965; Downing 1971; Bella and Dobbins 1968). Such models provide a satisfactory engineering solution provided that steep gradient concentrations are not involved and required. As the size of segment tends to zero so the simulation models become almost equivalent to those based on mass continuity.

b) Statistical models are based on the use of multiple regression to correlate the level of the dependent parameter such as dissolved oxygen with various independent environmental variables such as freshwater flow, temperature, tidal amplitude, etc (e.g. Mackay and Fleming 1969). Regression equations are produced for various sections along the estuary and may incorporate refinements such as non-linear correlations and use of composite antecedent flows.

   Statistical models have the merits of simplicity and minimal data requirements but suffer the serious disadvantages that they may only be used for interpolation within the observed ranges of flow, temperature, etc. Since the data rarely cover a period of low BOD loadings, such models cannot be used to predict the effect of reduced loadings.

c) Stochastic models take account of the random fluctuations that occur in pollutant concentration due to variations in environmental variables and measurement errors. The output from such models (e.g. Custer and Kruthkoff 1969) gives a more realistic pattern of dissolved oxygen fluctuations but is perhaps better suited to operational requirements rather than those of a planning model.

2.2 Validation and Sensitivity Analysis

Kinwood and Wallis in 1975 pointed out that there had been no systematic study of the consequences of errors in calibration data and that of the few models which had been verified, dissolved oxygen improvements were predicted to within 20-100% of their measured values. In the intervening six years very little has been published on model verification but one useful study has been made of the accuracy of the data required (Lin 1981). Table 2 summarises his findings and shows that data collection is still the major weakness in water quality modelling in estuaries. In particular this study reveals the importance and difficulties in evaluating the dispersion coefficient (see also Thatcher and Harleman 1972).

2.3 Economic Models

In the past five years there has been some interest in combining the output from water quality models with optimisation models to obtain the least cost solution to pollution abatement. This field has been recently reviewed by O'Kane (1980).

One example is a study of pollution of the River Tees. Rowley (1979) argued that considerable savings in pollution control may be obtained by use of these models plus pollution taxation.

	INPUR VARIABLES	Ranges of Variation	C_{NH} (mg/1)	C_{NO} (mg/1)	C_{DO} (% saturation)	max. C_{DO} change due to probable error
Boundary concentrations	C_{FC} & C_{SC}	-40%	-0.1	+0.1	+3.0	<1.0 γ
		+40%	+0.1	-0.3	-2.8	
	C_{FN} & C_{SN}	-40%	0.0	-0.2	+0.5	<1.0 γ
		+40%	+0.1	0.0	-0.4	
	C_{NH}	-40%	-2.6	+0.6	+7.0	2.0 γ
		+40%	+3.4	-0.6	-7.0	
	C_{DO}	-40%	+0.2	-0.8	-30.0	8.0 β
		+40%	-0.2	+0.9	+30.0	
Rate coefficients	R_{FC} & R_{SC}	-100%	-0.9	+2.1	+47.0	11.0 β
		+100%	+0.3	-2.0	-6.0	
	R_{FN} & R_{SN}	-100%	-0.2	+0.6	+4.0	2.0 γ
		+100%	+0.2	-0.1	-1.0	
	R_{NH}	-100%	+2.2	-0.9	+31.0	10.0 β
		+100%	-0.5	+0.3	-15.0	
	R_{EA}	-10%	+0.1	-1.3	-4.0	∿40.0 α
		+50%	-0.3	+1.0	+22.5	
Effluent Solute Inputs	C_{FC} & C_{SC}	-100%	-0.8	+1.7	+40.5	18.0 α
		+25%	+0.2	-2.1	-6.5	
	C_{FN} & C_{SN}	-100%	-0.3	+0.05	+4.0	2.0 γ
		+100%	+0.2	-0.2	-3.0	
	C_{NH}	-100%	-2.4	+0.4	+13.0	6.0 β
		+50%	+1.3	-2.0	-4.0	
	Temperature	-4°C	+0.1	+0.7	+8.0	4.0 γ
		+4°C	-0.2	-1.0	-8.0	
	Computed D*	-40%	+1.4	-2.0	-6.0	6.6 β
		+40%	-1.0	+0.1	+6.6	
	Q_H & river solute inputs	-50%	-0.7	+0.1	-21.0	11.0 β
		+100%	+0.7	-2.3	+13.0	
	Q_H coupled with D*	-50%	+0.7	-0.6	-22.0	11.0 β
		+100%	-0.5	+0.6	+11.0	

Table 2: Summary of the orders of magnitude of the changes in C_{HN}, C_{NO} and C_{DO} concentrations w.r.t. the various input variables FC and SC are fast and slow carbon; EA is reaeration. (N.N.α, β and γ in the last column denote respectively that the input variable is either very significant, significant or negligible).

The model takes the form:-

$$\text{Minimise } D = \sum_{i=1}^{n} \sum_{ki=1}^{mi} \sum_{t=3}^{g} D^{t}_{ki} \; X^{t}_{ki}$$

subject to the constraints that

$$-X^{t}_{hi} + X^{t}_{ki} \quad 0 \text{ for some } k \text{ and } h, \quad h \neq k$$

$$X^{t}_{ki} + X^{t}_{ji} \quad 1 \text{ for some } k \text{ and } j, \quad j \neq k$$

Their conclusion has been challenged by Elliott (1981) who considers that the data requirements for an efficient taxation scheme are no less than those for efficient regulation by consent conditions. As with water quality models it appears that further advances depend mainly on more extensive data collection.

3. MODELS OF COASTAL WATERS

Waste materials arrive in coastal waters in a variety of ways - through submarine pipelines, via estuaries and by discharge from ships. Although there has been considerable interest in the fate of material such as sludges discharged from ships it has produced little modelling activity (see Palmer and Cross 1977). Similarly discharge from estuaries has not aroused much interest by modellers. The basic hydraulics of the situation have been described by 1975 and this theoretical framework was used for modelling nutrient discharges from the estuaries (Dahl-Madsen 1978; James 1979).

The majority of modelling of the water quality in coastal areas has therefore been concerned with discharges from submarine pipelines and this is discussed in the next sections under its various aspects:-

a) Modelling of initial dilution
b) Modelling of surface dispersion
c) Modelling of bacterial die-off.

3.1 Modelling of Initial Dilution

This subject has received intensive study by a number of workers notably by Rawn and Palmer 1929; Abraham 1965; Rawn, Bowerman and Brooks 1960. (For a full bibliography see Agg 1978)

There is unanimity in the approach adopted to modelling the initial dilution. This is based on two dimensionless ratios:

$$\text{Froude Number} = \frac{\text{Inertial Velocity}}{\text{Gravitational Velocity}}$$

and Depth/Jet diameter

White & Agg (1974) added a correction factor for increased dilution due to movement of the ambient fluid to produce the dimensionless groups

$$\frac{Co}{Cm} = f\left(\frac{D}{Y},\ \frac{Ua}{\left(gy\,\frac{Pa - Po}{Po}\right)^{\frac{1}{2}}},\ \frac{Q}{\left(g\,\frac{Pa - Po}{Po}\right)^{\frac{1}{2}}}\right)$$

where C_o = Initial concentration

C_m = concentration at surface

D = Diameter of jet

Y = Depth of sea water

Ua = Velocity of sea water

g = Gravitational constant

Po and Pa = Densities of effluent and sea water

which has then been transformed into design charts. White & Agg (1975) pointed out that the initial dilution required is a function of amenity and distance from the shoreline.

This modelling approach has been tested extensively in practice in a number of parts of the world and has been found to give acceptable engineering answers. The largest remaining source of error is in the dilution required to avoid slick formation which varies depending upon surface conditions and the grease content of the sewage. But there seems to be little need for much further modelling work on initial dilution.

3.2 Modelling of Surface Spreading

The modelling of the subsequent dispersion of the waste field at the surface has received almost as much attention as the modelling of the initial dilution (e.g. Bowden 1965; Carter and Okubo 1965; Gameson 1975). This interest has been intensified by the widespread adoption of microbial standards for bathing waters.

Calaway (1975) pointed out that there seemed to be general agreement that the surface spreading is due to two different processes, namely:

a) The near-field situation which is dominated by buoyancy and momentum flux. This is usually represented by

$$B_o = \frac{K^2\ \Delta gQ}{2U_o^{\ 3}} \qquad \text{(Hyden and Larsen 1975)}$$

where B_o = Half width of patch

K = A constant

g = gravitational constant

U_o = Velocity of current

Q = Waste flow

= Specific gravity difference between patch and sea water

b) The far-field situation where dispersion is due to eddy diffusion which is represented by a two dimensional convective - diffusion equation:

$$C(x,y,t) = \frac{M}{\pi W^2 D t^2} \exp\left(\frac{-(x-Ut)^2 - y^2}{W^2\, t^2}\right)$$

Where $C(x,y,t)$ = Concentration of waste at a distance x from the source and a distance y from the centreline at time t since the instantaneous release of mass M which is uniformly distributed through depth D

U = Ambient velocity

W = Diffusion velocity

There has been general agreement on the modelling of dispersion of surface patches (see Joseph and Sendner 1958 for background). However Lewis (1980) has criticised the assumption made by Carter and Okubo (1965) that the process takes place in unbounded space. He considers that the effect of the sea surface is to give a semi-bounded situation and the shear term is reduced by a factor of 4.7 times. Since Carter and Okubo's dispersion formulation has been widely used, it is important that this difference of opinion be resolved.

The main problems with modelling of surface dispersion are not theoretical but relate to validation. Talbot (1975) published a useful summary of dispersion measurements which showed a wide range of values.
Some standardisation of technique would obviously help to improve this situation but field conditions must cause a wide range of variation so it is doubtful whether these models can achieve the same accuracy as models of initial dilution.

3.3 Modelling of Bacterial Die-off

Modelling the die-off of micro-organisms in sea water has not yet reached a stage where completely reliable and accurate predictions can be ontained. The difficulty is due to poor understanding of the mechanism of die-off. Despite extensive studies in both field and laboratory the variable remains uncertain. Gameson and Gould 1975 concluded from their studies that although shore-based experiments demonstrated the large effect of solar radiation on the mortality of coliform bacteria in sea water, that in-situ studies failed to demonstrate a consistent quantitative relation between mortality rate and solar radiation. Further studies have similarly failed to produce a quantitative bases for modelling of die-off.

In the absence of a good descriptive model various empirical relationships have been used. Munro 1975 used a simple experimental death rate -

$$C_x = C_o\, e^{-kt}$$

where C_x = coliform concentration at time t

C_o = initial coliform concentration

K = death rate

K does not vary with light or other external conditions. Mancini 1978 assembled a large data base of over 100 measurements on coliform die-off and concluded that the rate was best expressed as follows:-

$$K = \left[0.8 + 0.006(\%\ \text{sea water})\right] \times 1.07^{(t-20)}$$

$$+ \frac{I_A}{K_a H}\left[1 - e^{-K_a H}\right]$$

but pointed out that there was a wide scatter around the predicted values.

Much more experimental work is obviously required before satisfactory die-off models can be obtained. This is especially true for viruses since even less is known about the die-off than coliforms (see Mitchell 1968).

From a modelling viewpoint there is no intrinsic difficulty in model construction and many models already exist but are still to be validated.

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