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Modelling water quality in the upper Klip river

Arnold, Roderick William

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will have to consider the dispersion aspect carefully and in some cases 'dead zone' models or cellular models may be more suitable than the bulk diffusion model.

10.2.6 Self-purification in the Klip River

The general decrease in oxygen demand with distance downstream indicates that self-purification does in fact take place in the Klip River. Although the oxygen demands are not high when compared to many rivers overseas, the dissolved oxygen does drop to the critical level required for fish life. Despite the fact that the DO recovers rapidly to acceptable levels within the comparitively short length of the study reach, making use of the river's self-purification properties should only be considered with caution. In this regard modelling, as was attempted in this study, is essential.

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APPENDIX A

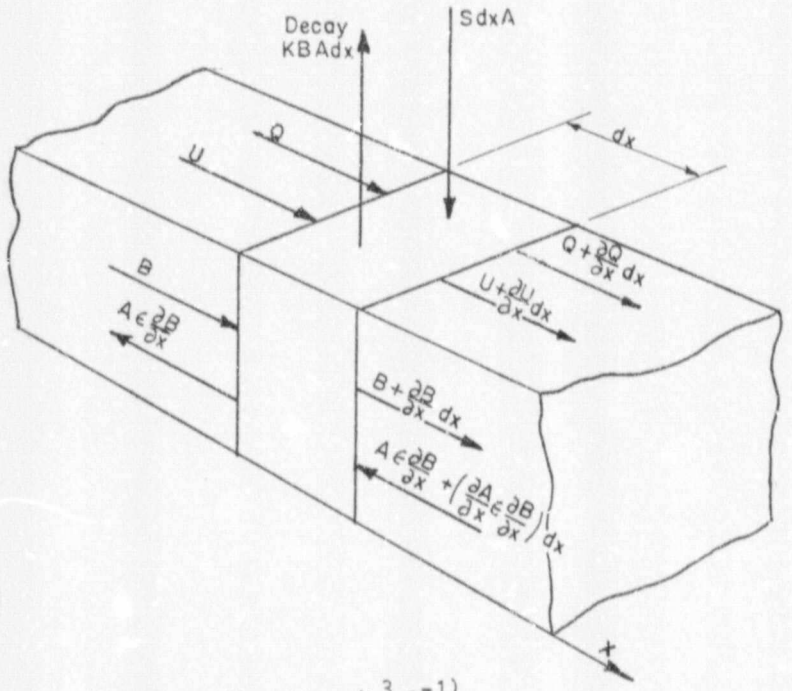
DERIVATIONS

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APPENDIX A

DERIVATIONS

A1 DERIVATION OF BOD-DO COUPLED EQUATIONS



Q = flow in x direction ($L^3 T^{-1}$)
U = velocity in x direction ($L T^{-1}$)
B = concentration of pollutant ($M L^{-3}$)
A = cross-sectional area of element (L^2)
dx = length of element (L)
ϵ = longitudinal disperson coefficient ($L^2 T^{-1}$)
K = decay coefficient (T^{-1})
S = source/sink of pollutant ($ML^{-3} T^{-1}$)

The net increase of pollutant in the element is given by:

$$A\,dx\,dB = dt\,(S\,A\,dx + B\,Q - (B + \frac{\partial B}{\partial x}\,dx)\,(Q + \frac{\partial Q}{\partial x}\,dx) - K\,B\,A\,dx - A \epsilon \frac{\partial B}{\partial x} + A \epsilon \frac{\partial B}{\partial x} + (\frac{\partial A}{\partial x} \epsilon \frac{\partial B}{\partial x})\,dx)$$

Simplifying and ignoring second order differentials,

$$A\,dx\,dB = dt\left[(S\,A\,dx - (B\frac{\partial Q}{\partial x}\,dx + Q\frac{\partial B}{\partial x}\,dx) - K\,B\,A\,dx + \frac{\partial A}{\partial x}\in\frac{\partial B}{\partial x}\,dx)\right]$$

Dividing throughout by A dx dt and rearranging,

$$\frac{\partial B}{\partial t} + KB + \frac{B}{A}\frac{\partial Q}{\partial x} + \frac{Q}{A}\frac{\partial B}{\partial x} - \frac{1}{A}\frac{\partial}{\partial x}(A\in\frac{\partial B}{\partial x}) - S = 0$$

For a uniform channel A and $\in$ = constant and if Q = constant

$$\frac{\partial B}{\partial t} + KB + U\frac{\partial B}{\partial x} - \in\frac{\partial^2 B}{\partial x^2} - S = 0 \qquad \text{A-1}$$

For BOD the equation becomes:

$$\frac{\partial L}{\partial t} = \in\frac{\partial^2 L}{\partial x^2} - U\frac{\partial L}{\partial x} - K_1 L + S \qquad \text{A-2}$$

Where L = concentration of BOD (ML^{-3})
K_1 = deoxygenation coefficient (T^{-1})
S = source /sink term for BOD ($ML^{-3}T^{-1}$)

If a reaeration term is included and with the biodegradable oxygen demand governed by the BOD concentration a simiiar equation can be written for the dissolved oxygen:

$$\frac{\partial C}{\partial t} = \in\frac{\partial^2 D}{\partial x^2} - U\frac{\partial C}{\partial x} - K_1 L + K_2\,(C_s - C) + P \qquad \text{A-3}$$

Where C = concentration of dissolved oxygen (ML^{-3})
K_2 = reaeration coefficient (T^{-1})
C_s = saturation concentration of dissolved oxygen (ML^{-3})
P = dissolved oxygen sources and sinks ($ML^{-3}T^{-1}$)
$K_1 L$ = decxygenation term from equation A-2

For describing the dissolved oxygen sag curve, it is often preferable to express equation A-3 in terms of the dissolved oxygen deficit:

$$\frac{\partial D}{\partial t} = \epsilon \frac{\partial^2 D}{\partial x^2} - U\frac{\partial D}{\partial x} + K_1 L - K_2 D - P \qquad \text{A-4}$$

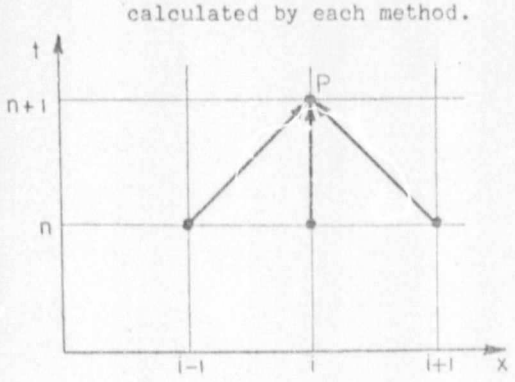
Where $D = C_s - C$ = dissolved oxygen deficit (ML^{-3})

A2 DERIVATION OF THE FINITE DIFFERENCE APPROXIMATION TO THE COUPLED EQUATIONS

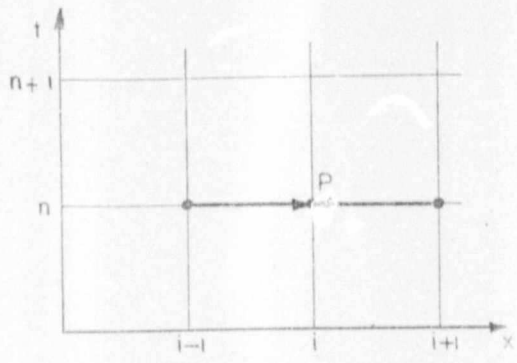
A2.1 Finite difference methods

Finite difference methods are used to solve problems involving partial differential equations, such as the BOD-DO coupled equations, where analytical solutions are either not available or too restricted in their use. The method involves making use of finite differences to approximate the partial differentials. The smaller the differences used in the computation, the closer the finite difference solution will be to the true solution; but a balance has to be struck here between the additional computational effort required when using smaller differences and the degree of accuracy required.

Finite difference procedures may be either *explicit* or *implicit* or a combination of both. In explicit computations, the value at a certain time step is calculated explicitly from values calculated at the previous time step. The procedure calculates values from one time step to the next. In implicit computations, each value is calculated implicitly from adjacent values which are not yet known and all values are solved for simultaneously. The x-t diagram below show how a point P may be calculated by each method.



Explicit



Implicit

The implicit method has the advantage that it is unconditionally stable (see section A2.2(b)) whereas the explicit is not.

However the implicit system of simultaneous equations may become very cumbersome for large problems, requiring large amounts of storage on the computer, and does not have the flexibility of explicit methods. Explicit methods were employed for this study and therefore no further consideration will be given to implicit methods.

A2.2 The standard finite difference approximation

The partial differential equations for the BOD-DO balance are given by equations 4.8:

$$\frac{\partial L}{\partial t} = \epsilon \frac{\partial^2 L}{\partial x^2} - U\frac{\partial L}{\partial x} - K_1 L \pm S \qquad 4.8a$$

$$\frac{\partial D}{\partial t} = \epsilon \frac{\partial^2 D}{\partial x^2} - U\frac{\partial D}{\partial x} - K_2 D + K_1 L \pm P \qquad 4.8b$$

If we consider the finite different grid with the two independent variables distance x and time t forming the axes as shown in figure A2.1, then the BOD concentration at x = i and time n can be estimated from equation 4.8a, using the concentrations at time n - 1, by means of finite difference approximations to the partial differential terms.

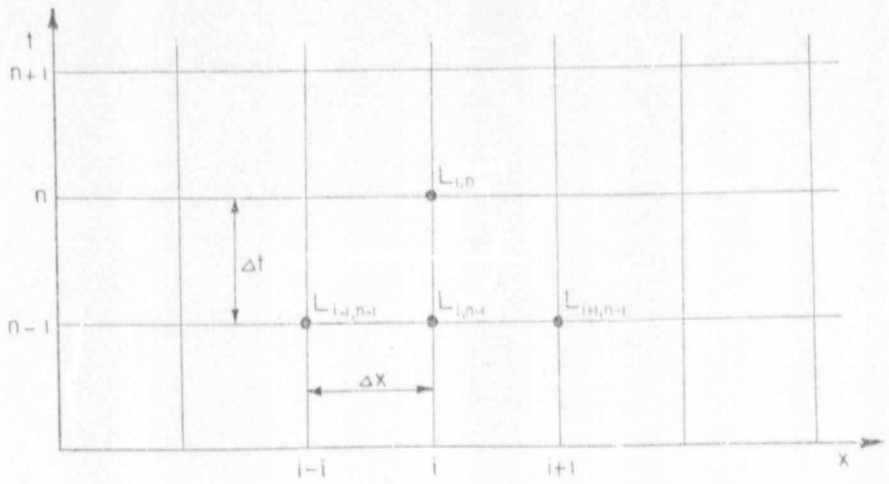


Fig. A2.1 Finite difference grid for solution of the BOD-DO partial differential equations

Using backward differences, the standard finite difference approximations to the BOD partial differentials are as follows:

$$\frac{\partial L}{\partial x} = \frac{L_{i,n} - L_{i-1,n}}{\Delta x}$$

$$\frac{\partial^2 L}{\partial x^2} = \frac{(L_{i+1,n} - L_{i,n}) - (L_{i,n} - L_{i-1,n})}{\Delta x^2}$$

$$= \frac{L_{i+1,n} - 2L_{i,n} + L_{i-1,n}}{\Delta x^2}$$

$$\frac{\partial L}{\partial t} = \frac{L_{i,n+1} - L_{i,n}}{\Delta t}$$

Thus equation 4.8a in terms of finite differences becomes:

$$\frac{L_{i,n+1} - L_{i,n}}{\Delta t} = \epsilon \frac{(L_{i+1,n} - 2L_{i,n} + L_{i-1,n})}{\Delta x^2} - U \frac{(L_{i,n} - L_{i-1,n})}{\Delta x} - K_1 L_{i,n} \pm S$$

Solving for $L_{i,n+1}$ this becomes

$$L_{i,n+1} = \Delta t \frac{(\epsilon + U\Delta x)}{\Delta x^2} L_{i-1,n} + (1 - 2\epsilon \frac{\Delta t}{\Delta x^2} - \frac{U\Delta t}{\Delta x} - K_1 \Delta t) L_{i,n}$$

$$+ \frac{\epsilon \Delta t}{\Delta x^2} L_{i+1,n} \pm S\Delta t$$

$$\text{or } L_{i,n+1} = A1\, L_{i-1,n} + A2\, L_{i,n} + A3\, L_{i+1,n} \pm \Delta t S \qquad \text{A2.1a}$$

$$\text{Where } A1 = (\frac{\epsilon + U\Delta x}{\Delta x^2}) \Delta t$$

$$A2 = (1 - \frac{2\epsilon \Delta t}{\Delta x^2} - \frac{U\Delta t}{\Delta x} - K_1 \Delta t)$$

$$A3 = \frac{\epsilon \Delta t}{\Delta x^2}$$

Similarly equation 4.8b can be approximated by:

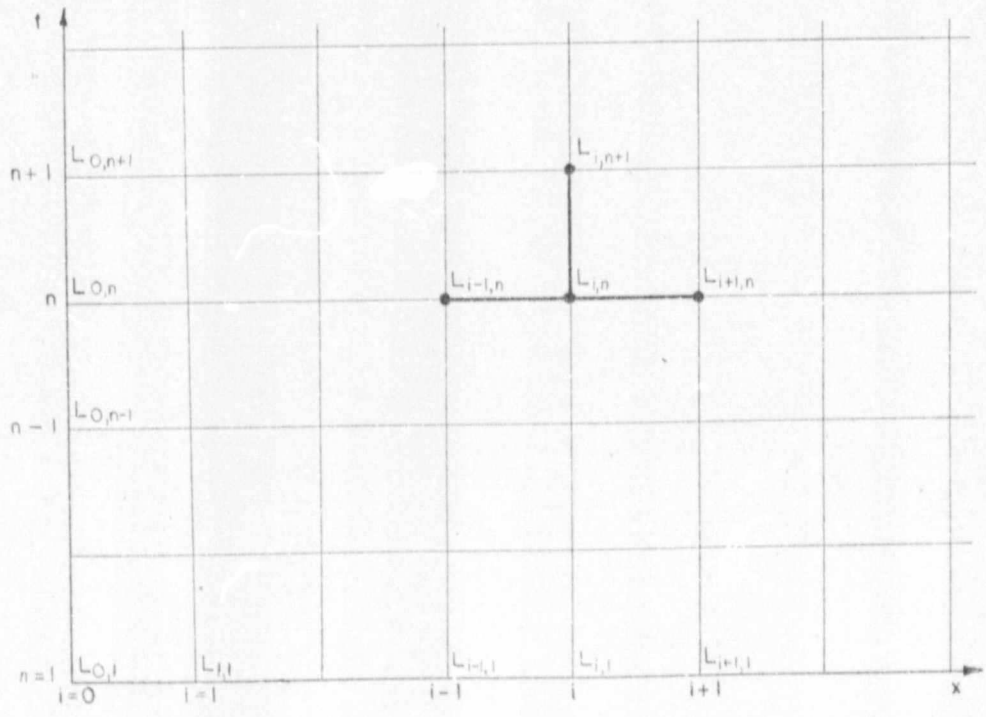
$$D_{i,n+1} = B1\ D_{i-1,n} + B2\ D_{i,n} + B3\ D_{i+1,n} + \Delta t\ K_1\ L_{i,n} \pm \Delta tP \qquad A2.1b$$

Where $B1 = \left(\frac{\epsilon + U\Delta x}{\Delta x^2}\right)\Delta t$

$$B2 = \left(1 - \frac{2\epsilon\Delta t}{\Delta x^2} - \frac{U\Delta t}{\Delta x} - K_2\,\Delta t\right)$$

$$B3 = \frac{\epsilon\Delta t}{\Delta x^2}$$

Computational procedure



Initial conditions

The initial conditions, $L_{i,1}$, at all points along the x axis must be specified. These conditions do not have to be known accurately as, provided a sufficient number of time steps are used before a result is obtained, any inaccuracies in the initial conditions will disappear from the computation.

Upstream boundary conditions

The upstream boundary conditions, $L_{o,n}$, are specified by the input at the upstream end.

Computation

For each successive time step, the BOD values of the previous time step, $L_{i,n}$, starting with the initial values, are used to calculate the next row of BOD concentrations, $L_{i,n+1}$, from equation A2.1a. After the BOD's for a time step have been calculated, the values obtained are used in the dissolved oxygen computation which proceeds parallel to the BOD computation in a similar manner, using equation A2.1b.

Downstream boundary conditions

At the end of each time step, an additional pseudo - BOD and DO value must be calculated beyond the furthermost downstream point of interest for use in the next time step computation. Such points may be either assigned a zero value (Dresnack and Dobbins (1968)), or put equal to the preceding point, or extrapolated from the preceding two points. For this study extrapolation was used.

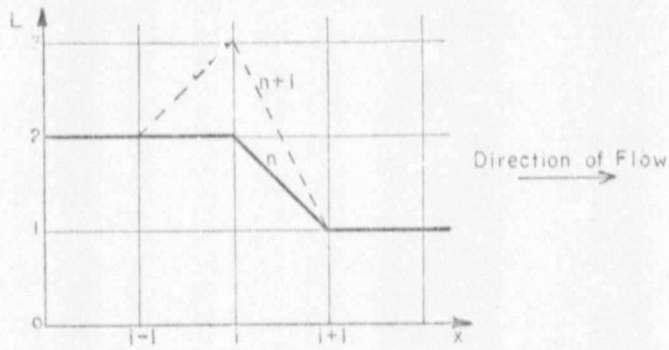
Some problems associated with the standard finite difference approximation

(a) Backward, central and forward differences

In the above finite difference approximations, backward differences were used for the first order differential. An alternative would have been to use forward differences as shown below:

$$\frac{\partial L}{\partial x} = \frac{L_{i+1,n} - L_{i,n}}{\Delta x}$$

This however leads to problems when the numerical technique is applied.



Considering advection only in the example shown by the solid line above, and putting $\Delta x = U\Delta t$, we get

$$L_{i,n+1} - L_{i,n} = -\left(\frac{\Delta t U}{\Delta x}\right)(L_{i+1,n} - L_{i,n})$$

or $$L_{i,n+1} = 2L_{i,n} - L_{i+1,n}$$

This is shown by the dashed line in the above figure. The reason for this inaccuracy in the method lies in the direction of flow being in the same forward direction as the differences.

The use of central differences will lead to similar problems

$$\frac{\partial L}{\partial x} = \frac{L_{i+1,n} - L_{i-1,n}}{\Delta x}$$

$$L_{i,n+1} - L_{i,n} = -\left(\frac{\Delta t U}{\Delta x}\right)(L_{i+1,n} - L_{i-1,n})$$

$$L_{i,n+1} = -\left(\frac{\Delta t U}{\Delta x}\right)(L_{i+1,n} - L_{i-1,n}) + L_{i,n}$$

$$= L_{i-1,n} + L_{i,n} - L_{i+1,n}$$

which also gives incorrect results.

Using backward differences however yields:

$$L_{i,n+1} = L_{i,n} - \left(\frac{\Delta t U}{\Delta x}\right)(L_{i,n} - L_{i-1,n})$$

$$= L_{i-1,n}$$

which is correct.

In the finite difference approximation to the second-order term, both forward and backward differences must be used:

$$\frac{\partial^2 L}{\partial x^2} = \frac{L_{i+1,n} - 2L_{i,n} + L_{i-1,n}}{\Delta x^2}$$

and from equation A2.1a for dispersion only we have

$$L_{i,n+1} = \frac{\Delta t}{\Delta x^2}(L_{i+1,n} - 2L_{i,n} + L_{i-1,n}) + L_{i,n}$$

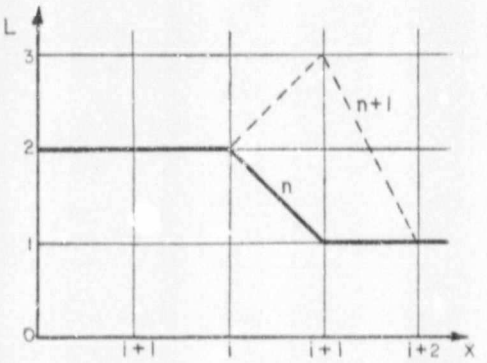
This however does not lead to problems in the numerical solution provided that the stability criteria set out in the following section are satisfied.

(b) Stability of the solution

Successful numerical solution also depends on the ratio $\frac{\Delta x}{\Delta t}$. For example, considering our simple convective model, using backward differences and putting $\Delta x = \frac{U\Delta t}{2}$ we get

$$L_{i,n+1} = -L_{i,n} + 2L_{i-1,n}$$

In this case we get numerical instability as shown by the broken line in the figure below. The condition gets progressively worse for increasing time steps and is not dependent on the direction of flow.



The general criteria for numerical stability in the solution of the standard finite difference equations A2.1 are derived below.

Stability criteria

The stability of the solution of a system of finite difference equations given in matrix form by $L_{n+1} = ML_n$; where M is the matrix

$$M = \begin{bmatrix} & & & & 0 \\ 0 & a_1 & a_2 & a_3 & 0 \\ 0 & & & & \end{bmatrix}$$

can be determined from the following two theorems (Fried, 1975, chp. 9):

Theorem 1: The general convergence theorem

An iterative process $X_m = MX_{m-1} + B$ converges for any initial vector X_o if and only if all the eigenvalues of the matrix M are strictly less than one in absolute value.

Theorem 2: Gerschgoren's theorem

The eigenvalues of a matrix $M = (a_{i,j})$ are in the domain D defined as the union of all circles of centres $a_{i,i}$ and of respective radii $\sum_{j \neq i} a_{i,j}$

By theorem 2 it is possible to determine the upper and lower bounds of the eigenvalues of matrix M and hence theorem 1 can be applied to determine the conditions for convergence.

For the system of equations A2.1a the matrix coefficients are given by

$$a_1 = A1 = (\epsilon \frac{\Delta t}{\Delta x^2} + \frac{U \Delta t}{\Delta x})$$

$$a_2 = A2 = (1 - 2\epsilon \frac{\Delta t}{\Delta x^2} - \eta \frac{\Delta t}{\Delta x} - K_1 \Delta t)$$

$$a_3 = A3 = \epsilon \frac{\Delta t}{\Delta x^2}$$

By theorem 2 the upper bound of the eigenvalues of M is given by

$$a_2 + (a_1 + a_3)$$

For stability this must be less than one in absolute value (by theorem 1), i.e.

$$(1-2\epsilon\frac{\Delta t}{\Delta x^2} - U\frac{\Delta t}{\Delta x} - K_1\Delta t) + (\epsilon\frac{\Delta t}{\Delta x^2} + U\frac{\Delta t}{\Delta x}) + \epsilon\frac{\Delta t}{\Delta x^2} \quad < \quad 1$$

or $\quad 1 - K_1\Delta t \quad < \quad 1$

Since K_1 is always positive this is always true

The lower bound, by theorem 2, is given by

$$a_2 - (a_1 + a_3)$$

Hence for stability

$$1 - 4\epsilon\frac{\Delta t}{\Delta x^2} - 2U\frac{\Delta t}{\Delta x} - K_1\Delta t \quad > \quad -1$$

This is true for $\Delta t < \Delta t_c = \dfrac{\Delta x}{(2\frac{\epsilon}{\Delta x} + U + \frac{K_1}{2}\Delta x)}$ A2.2a

The solution of the system of equations A2.1a is therefore conditionally stable.

Similarly it can be shown for the system of equation A2.1b that the solution is stable if

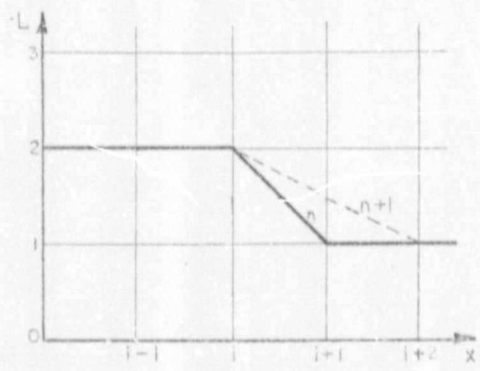
$$\Delta t < \Delta t_c = \frac{\Delta x}{(2\frac{\epsilon}{\Delta x} + U + \frac{K_2}{2}\Delta x)}$$ A2.2b

(c) Numerical dispersion

A problem also arises if $\frac{\Delta x}{\Delta t}$ is chosen to be greater than U; for example, considering once again the simple

convection equation, and taking $\Delta x = 2U\Delta t$ we get:

$$L_{i,n+1} = \frac{1}{2}(L_{i,n} + L_{i-1,n})$$



As indicated by the dotted line above, this leads to a dispersion taking place due solely to the numerical process. Chevereau (1973) has pointed out that if the partial differential equations 4.8 are expanded in a Taylor series to the second order it can be shown that the numerical dispersion coefficient ϵ_n so obtained has a maximum value when:

$$\epsilon_n = \frac{\Delta x^2}{8\Delta t}$$

In order to minimise this effect, it is necessary to choose Δx as small as possible and Δt as large as possible. However this is limited by stability criteria given by equation A2.2, which, for convection only, reduces to

$$\Delta t \leq \frac{\Delta x}{U}$$

A2.3 The Two-step explicit finite difference method

It is evident from the above discussion that in order to model pure convection by finite differences, it is necessary that backward differences be used, i.e.

$$L_{i,n+1} = L_{i,n} - (\frac{\Delta t U}{\Delta x})(L_{i,n} - L_{i-1,n})$$

In addition, for stability we require that $\frac{\Delta x}{\Delta t}$ U and to minimise numerical dispersion the ratio $\frac{\Delta x^2}{\Delta t}$ should be as small as possible The best means of satisfying both these conditions would be to take $\frac{\Delta x}{\Delta t} = U$

The approximation now becomes

$$L_{i,n+1} = L_{i-1,n}$$

which, as shown above is completely representative of the pure convection process.

If we now include the dispersion term we get

$$L_{i,n+1} = L_{i-1,n} + \frac{\Delta t \epsilon}{\Delta x^2} (L_{i-1,n} - 2 L_{i,n} + L_{i+1,n}) \quad A2.3$$

The stability criterion for convection plus dispersion from condition A2.2, is:

$$\Delta t \leq \frac{1}{\frac{2\epsilon}{\Delta x^2} + \frac{U}{\Delta x}} \quad A2.4$$

Rearranging gives

$$1 \geq \frac{2\Delta t}{\Delta x^2} + \frac{U \Delta t}{\Delta x}$$

Clearly for $\frac{\Delta x}{\Delta t} = U$ this condition can only be satisfied if $\epsilon = 0$.

Dresnack and Dobbins (1968) have suggested a two-step explicit procedure, which overcomes the above problem. In this method

the convection process is carried out separately from the other processes as follows:

Step 1: $L_{i,n} = L_{i-1,n}$
and $L_{o,n} = L_{o,n+1}$

Step 2: $L_{i,n+1} = A1\ L_{i-1,n} + A2\ L_{i,n} + A1\ L_{i+1,n} \pm S\Delta t$

Where $A1 = \frac{\epsilon \Delta t}{\Delta x^2}$

$A2 = (1-2\ \frac{\epsilon \Delta t}{\Delta x^2} - K_1 \Delta t)$

A similar procedure can be used for the dissolved oxygen calculation

Step 1: $D_{i,n} = D_{i-1,n}$
and $D_{o,n} = D_{o,n+1}$

Step 2: $D_{i,n+1} = B1\ D_{i-1,n} + B2\ D_{i,n} + B1\ D_{i+1,n} + K_1 L_{i,n} \pm P\Delta t$

Where $B1 = \frac{\epsilon \Delta t}{\Delta x^2}$

$B2 = (1-2\ \frac{\epsilon \Delta t}{\Delta x^2} - K_2 \Delta t)$

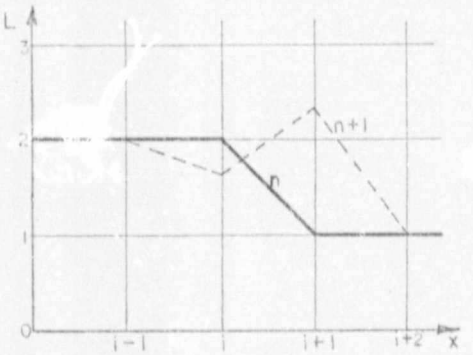
It is convenient to compute the BOD values for a time step and then use these to compute the DO values for that time step before moving on to the next time step.

Dresnack and Dobbins proposed this method to overcome the type

of problem depicted in the figure below, which arises from the use of equation A2.3.

In this example $\Delta t = \frac{\Delta x^2}{3}$

$$L_{i,n+1} = \frac{1}{3}\left(4L_{i-1,n} - 2L_{i,n} + L_{i+1,n}\right)$$



Obviously the concentration L should not increase and this effect shown by the broken line becomes progressively greater for increasing n. Although Dresnack and Dobbins failed to point out that this was due to the fact that the full criteria for stability according to condition A2.2 could not be fulfilled, the two-step method does provide a satisfactory solution to the problem.

In their paper the example used to show the method of computation works satisfactorily with the same time interval Δt for both steps. However, this is not necessarily the case and it was found in this study that the time step had to be decreased in the second computational step for larger values of the dispersion coefficient. This is to be expected considering the fact that the stability of the second step requires, from conditions A2.2, that

$$\Delta t \leq \frac{1}{\frac{2\epsilon}{\Delta x^2} + \frac{K_1}{2}}$$

Author Arnold Roderick William
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