A ONE-DIMENSIONAL WATER QUALITY MODEL BASED UPON FINITE DIFFERENCE METHODS

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A non-stationary one-dimensional water quality model and its operational uses are described. The main applications of the model have been in estuaries, where a place dependent longitudinal mixing coefficient and a non-stationary approach are necessities and where the phenomenon of salt intrusion provides a tool for determining the exchange coefficients.

1. INTRODUCTION

A one-dimensional model of the type under consideration first came into use at Rijkswaterstaat in 1964. Since that time, the model has been improved and extended. Below, the present form as it is in operational use, is briefly described. Differential equations and finite difference schemes as applied are presented and some of the limitations and problems in this connection are discussed.
A survey is given of applications in the past, in addition to more recent ones; in the latter context the approach will be linked to the two-dimensional approach wich makes use of the superposition model presented in paper 11 of this conference (Van Dam, 1976) (1).
The differential equations and difference schemes are equal or analogous to what is found in the reports of several authors. Some specific points with regard to the work reported here are the iterative determination of mixing coefficients from the salt water movement over long periods, the reliable prediction of concentration distributions of other substances based thereon, and the simultaneous solution of the equations for BOD and DO, thus taking into account the horizontal exchange transport of oxygen.

2. THE EQUATIONS

For computing one-dimensional distributions of single pollutants, salt, heat etc., one equation is solved i.e.

$$A(x)\frac{\partial C(x,t)}{\partial t} = -\frac{\partial}{\partial x}\{R(x,t)C(x,t) - A(x)\ K(x)\frac{\partial C(x,t)}{\partial x}\} - A(x)\ \frac{C(x,t)}{\tau} + q(x,t) \qquad \text{(I)}$$

A = cross sectional area
x = (longitudinal) distance
t = time
R = (net) water flow
K = longitudinal exchange coefficient
τ = time constant of decay
q = sources of pollutant or substance under consideration
C = concentrations of pollutant etc.

For computing one-dimensional distributions of heat, the same equation is applied with the exception that τ is replaced by

$$\tau(x) = \frac{\rho\ c\ h(x)}{A_W} \qquad \text{(II)}$$

with h = average water depth in a cross section, ρ = mass density, c = specific heat, and A_w = heat dissipation coefficient at the surface.
For computing BOD-DO-distributions two differential equations are solved simultaneously, i.e. equation (1) for the oxidizable pollutant and

$$A(x)\ \frac{\partial G(x,t)}{\partial t} = -\frac{\partial}{\partial x}\{R(x,t)\ G(x,t) - A(x)\ K(x)\ \frac{\partial G(x,t)}{\partial x}\} - \beta\ A(x)\ C(x,t) + \alpha(x)\ \frac{A(x)}{h(x)}\ \{G_v - (G(x,t)\} +$$

$$+\ q_{O_2}(x,t) \qquad \text{(III)}$$

for the oxygen.

G = oxygen concentration

G_v= saturation value

β = rate of oxygen consumption per unit of pollutant

$\alpha(x)$ = reaeration coefficient

q_{O_2} = possible sources of O_2

The fact that A(x) and h(x) appear instead of A(x,t) and h(x,t) indicates that water levels are considered constant or are inserted as time averages. For example, in an estuary or a tidal river, level variations due to the tide are not taken into account. (Longitudinal) horizontal displacements due to tidal flow can be inserted, if desired, by means of R(x,t), as a given input function. However, the water level changes being neglected, this refinement, in general, makes little sense and will even cause errors if K(x) is derived on the basis of tidal averages. Reasonable estimates of conditions at tidal phases deviating from the average can be obtained by adding an extra amount to R(x,t) just for the last few hours of the simulated period of time. On most occasions, the tidal phase is not considered at all, which means that in general R(x,t) simply represents the river discharge. The dependency of R on x makes it possible to account for water discharges from tributaries, drain channels etc. Tributaries and channels that also withdraw water and pollutants from the main channel or river would require an extension of the model to a network. This would give no particular problems. In one of the previous programmes a provision was made for a maximum of two side branches; it is now the intention to provide for branching in a more general way.

3. METHODS OF SOLUTION

Analytical solutions to (I) and (III) are only possible in a very lmited number of cases such as stationary conditions; for example if q(x,t) represents a number of constant sources at discrete points and if at the same time $\tau = \infty$. In such a case, A(x) and K(x) may be arbitrary functions in so far that for each source a definite integral in the formula remains, e.g. for the case of one source at $x = x_B$ with constant release P, the concentration for $x > x_B$ (x increasing in the direction of flow) can be written

$$C(x) = \frac{P}{R}\ (1 - e^{-R\int_x^{\infty} \frac{d\xi}{A(\xi)K(\xi)}}) \qquad \text{(IV)}$$

This notation implies that A(x)K(x) tends to infinity for $x \longrightarrow \infty$ at such a rate that the integral converges. For a river mouth, this is a realistic supposition; it would otherwise mean that everywhere downstream the concentration will become P/R. Anyhow, (IV) determines the concentration near the source

$$C(x_B) \leqq \frac{P}{R} \qquad \text{(V)}$$

This provides the boundary condition for $x < x_B$.
For this section

$$C(x) = C(x_B)\,e^{-R\int_x^{x_B} \frac{d\xi}{A(\xi)K(\xi)}} \qquad \text{(VI)}$$

The latter case is similar to that for salt, for which the boundary condition $C(x_B)$ = constant has moved to "infinity":

$$S(x) = S_{riv} + (S_{sea} - S_{riv}) e^{-R \int_x^\infty \frac{d\xi}{A(\xi)K(\xi)}} \qquad \text{(VII)}$$

In the latter case the solution for $R = R(x)$ can also be given, provided that the salt content S_o of all tributaries and other sources is identical or neglegible:

$$S(x) = S_o + (S_{sea} - S_o) e^{-\int_x^\infty \frac{R(\xi)d\xi}{A(\xi)K(\xi)}} \qquad \text{(VIII)}$$

Of course various other sub-cases and refinements can be distinguished. In the case of several sources, the individual solutions can be superimposed. It would be interesting if analytical solutions could be given for instantaneous point sources. In that case, all other solutions could be obtained by superposition, including the influence of a finite τ. Unfortunately however, the analytical solution for the instantaneous point source is basically dependent upon homogenous conditions in a uniform field and therefore cannot be given for the case that K and/or A depend upon x. For this reason, the choice of solving the equations by finite difference methods was not a free one. In the case of K and A independent of x, analytical solutions can also be given for finite τ. For one constant continuous source at x_B, the solution is

$$C(x) = p\, e^{q(x-x_B)} \qquad \text{(IX)}$$

and additionally in the case of BOD/DO:

$$G(x) = m\, e^{n(x-x_B)} + r\, e^{q(x-x_B)} + G_V \qquad \text{(X)}$$

In these expressions (IX) and (X)

$$p = \frac{P/A}{\sqrt{v^2 + 4K/\tau}} \qquad \left(\text{with } v = \frac{R}{A}\right) \qquad \text{(XI)}$$

$q = q_1$, $n = n_1$ for $x \leqq x_B$

$q = q_2$, $n = n_2$ for $x \geqq x_B$

$$q_{1,2} = \frac{v \pm \sqrt{v^2 + 4K/\tau}}{2K} \quad \text{(XII)} \qquad m = \frac{r(q_2 - q_1)}{n_1 - n_2} \quad \text{(XIII)} \qquad n_{1,2} = \frac{v \pm \sqrt{v^2 + 4\alpha K/h}}{2K} \quad \text{(XIV)}$$

Again, in the case of several sources, the individual solutions, G(x) as well as C(x), can be obtained by superposition.

The importance of the analytic solutions and the variety of cases therein, as demonstrated in this section, is the possibility of checking results of the numerical computations and the computer programme concerned, by results which are obtained completely independent of the numerical procedure. The above stationary solutions are obtained in the general, non-stationary model, by simulation of the constant source for an "infinite" time, i.e. as long as appears necessary for obtaining a stationary distribution. One might object that in that case the "dynamic" part of the calculation is only checked indirectly. If for this reason one insists on an explicit dynamic test, the solution for an instantaneous point source can be used if A and K are taken independent of x and the channel is taken sufficiently long. Then the analytic solution for a release of M kg

$$C(x,t) = \frac{M}{2A\sqrt{\pi K t}} e^{-\frac{x^2}{4Kt}} \qquad \text{(XV)}$$

can be compared with the numerical computation as a function of time and space as well.

4. NUMERICAL SOLUTION BY FINITE DIFFERENCE METHODS

Essential for the numerical solution of (I) and (II) are only the terms with partial derivatives which have, of course, the same form in both equations, so that only

$$A(x)\,\frac{\partial C(x,t)}{\partial t} = -\frac{\partial}{\partial x}\left\{R(x,t)C(x,t) - A(x)K(x)\,\frac{\partial C(x,t)}{\partial x}\right\} \qquad \text{(XVI)}$$

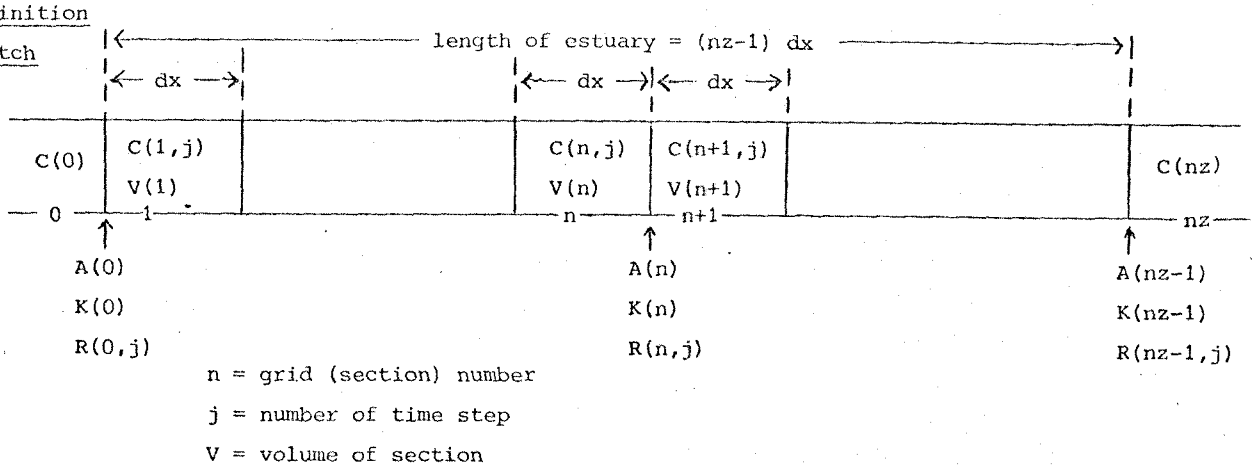
needs to be considered. The extra terms for decay, release and reaeration have no influence on the essential problems: numerical diffusion, and stability in time and space. These problems have in common that they can be suppressed by reducing the length of time steps and grid size. For reasons of computation time and extent of input (x-dependency of A(x) and K(x)) it is desirable to restrict the reduction of dt and dx to only what is necessary. Therefore, criteria for making a proper choice are needed. These criteria have in part been built into the computer programme; and, in part, decisions have to be made before a computation is started, especially with regard to the division of the channel in sections dx. The main problems arise from the advective term,

$$\frac{\partial}{\partial x}\{R(x,t)C(x,t)\} \qquad \text{(XVII)}$$

so that these problems tend to vanish as R approaches zero. This pertains especially to instabilities ("oscillations") in space, which are stable in time, and to numerical diffusion. The first can be suppressed by reduction of dx, but, for maintaining stability and suppressing numerical diffusion, this can only be done by lowering dt sufficiently at the same time.
Instabilities with respect to x, stable with respect to t, occur especially where C(x) exhibits a jump; an example is given in figure 1a. Such a jump is caused by a local release of the substance concerned; its asymmetry and therefore its steepness on one side, increase when the local value of $v = R/A$ becomes larger. Figure 1b illustrates an improvement obtained by decreasing dx. It should be borne in mind that a smaller dx implies a smaller dt for the sake of stability in time.

The present computer programme allows for two different finite difference schemes, as given below.

Definition sketch



The symmetric difference scheme (Dorrestein and Otto (2))

$$C(n,j+1) = dt\,E_1(n,j)\,C(n-1,j) + (1-dt\,E_2(n,j))\,C(n,j) + dt\,E_3(n,j)\,C(n+1,j) \qquad \text{(XVIII)}$$

with

$$E_1(n,j) = \frac{A(n-1)K(n-1)}{V(n)\ dx} + \frac{R(n-1,j)}{2\ V(n)} \tag{XIX}$$

$$E_2(n,j) = \frac{A(n)K(n) + A(n-1)K(n-1)}{V(n)\ dx} + \frac{R(n,j) - R(n-1,j)}{2\ V(n)} \tag{XX}$$

$$E_3(n,j) = \frac{A(n)K(n)}{V(n)\ dx} - \frac{R(n,j)}{2\ V(n)} \tag{XXI}$$

The computation is stable if all coefficients of C in (XVIII) are ≥ 0, i.e. if

$$dx \leq \text{Minimum}\left\{\frac{2\ A(n)K(n)}{R(n,j)}\right\} \tag{XXII}$$

$$dt \leq \text{Minimum}\left\{\frac{1}{E_2(n,j)}\right\} \tag{XXIII}$$

The asymmetric difference scheme

$$C(n,j+1) = dt\ F_1(n,j)\ C(n-1,j) + (1-dt\ F_2(n,j))C(n,j) + dt\ F_3(n)\ C(n+1,j) \tag{XXIV}$$

with

$$F_1(n,j) = \frac{A(n-1)K(n-1)}{V\ (n)\ dx} + \frac{R(n-1,j)}{V(n)} \tag{XXV}$$

$$F_2(n,j) = \frac{A(n-1)K(n-1) + A(n)K(n)}{V(n)\ dx} + \frac{R(n,j)}{V(n)} \tag{XXVI}$$

$$F_3(n,j) = \frac{A(n)K(n)}{V(n)\ dx} \tag{XXVII}$$

stable if

$$dt \leq \text{Minimum}\left\{\frac{1}{F_2(n,j)}\right\} \qquad \text{(any dx)} \tag{XXVIII}$$

Discussion

The asymmetric scheme behaves better in the case of a jump in C, but introduces a numerical diffusion of the order vdx/2. For practical purposes the model generated diffusion can be compensated for by means of the diffusion coefficient K. Preference for a particular difference scheme for the computation under specific conditions is sometimes a matter of taste. Restrictions as given for dx and dt in (XXII),(XXIII) and (XXVIII) can determine the choice. Comparison of the accuracy of both schemes for a variety of cases is still under investigation.

5. DETERMINATION OF K(x) IN ESTUARIES

The function K(x) has to be determined with the help of empirical data. If no natural tracer or existing pollution patterns are available for the area in concern, experiments with artificial tracers will be necessary.

In estuaries, a natural tracer, the sea salt, usually covers the entire area of interest and does so the better if river discharges exhibit more variations. The salt is a representative tracer for other substances as long as no important stratification occurs, which is the case in The Netherlands in the Ems- and Scheldt-estuaries. If there is a rather pronounced salt wedge, as in the Rotterdam Waterway, the salinity distribution, also as a function of time (with varying river discharge), does not provide adequate information on the behaviour of other substances, especially when released in the (relatively) fresh upper layer of the wedge system.

For Ems and Scheldt, a rather extensive analysis has been made of salt distributions as functions of time, for periods of several years. Such a long period reduces the influence of accidental errors such as those caused by variations in sampling time or position in relation to the tide, influences of meteorological effects upon the tide and so on. By using the non-stationary simulation of the model for the entire period, and comparing it with all salt concentration data available in that period, not only is the advantage gained that all data are used and equally weighted, but the method itself is also entirely independent of assumptions of stationary conditions, which, because of the large time constant of the estuary and the relatively rapid discharge variations, hardly ever occur (figure 2). Large variations in river discharges however are a welcome instrument for obtaining gradients of sufficient steepness in all relevant parts of the estuary and tidal river. In periods of substantial discharges, the part of the river that becomes fresh is not sensitive to changes in the value of K in that area.

Approximations of a few stationary or nearly stationary situations are useful for obtaining first estimates for the sets of K. For the case of salt (C(x) = S(x), no sources q within the boundaries of the model area, no decay) under stationary conditions, (I) reduces to

$$0 = \frac{d}{dx}\left\{ R(x)S(x) - A(x)K(x)\frac{dS(x)}{dx} \right\} \qquad \text{(XXIX)}$$

or

$$R(x)S(x) - A(x)K(x)\frac{dS(x)}{dx} = P \qquad \text{(XXX)}$$

in which P = net transport of salt from river to sea, which can often be neglected. In any case, for a stationary situation with given (measured) distribution S(x), K(x) is the only unknown in (XXX) and can be resolved. The first estimate thus obtained is then used in the non-stationary model for simulation over an adequate period of several years. Adjustments are made to K(x) until the best possible fit to the data has been obtained. The underlying supposition of this procedure is that for fixed x, K(x) is reasonably constant. This supposition was confirmed by the result for Ems and Western Scheldt in so far that a fair approximation of the data could be obtained using a fixed set K(x), but a considerable improvement was found when two different sets were permitted, one for "wet" and one for "dry" conditions (high and low river flow). This concerns differences of 10 to 30%. The two sets found for the Ems estuary are pictured in figure 3; they were published earlier by Eggink (3). One may speculate about the mechanism influencing K(x); rougher and less stable weather conditions in wet periods, as well as weak density currents may play a part; the latter however would only affect K in a limited stretch of the entire region concerned.

For a reliable determination of K(x), it is highly essential that accurate data on river discharge are available for the entire period analysed. For the Scheldt this has been a problem until recently, leading to an initial underestimation of K. When better data became available, K(x) could be corrected and the simulation of salinity distributions as a whole improved at the same time, as could be expected. By that time a similar trend with respect to wet and dry conditions as found for the Ems came to the fore in the Scheldt. Details are still being studied. A further improvement can be obtained by moving the boundary at the sea side further seaward. The earlier position of the boundary appeared to show a distinct influence of river flow while the boundaries are kept constant in the model. A seaward displacement of the boundary is considered a more satisfactory solution than introduction of a variable salt concentration at the boundary on the basis of measurements. Of course, if significant variations do occur due to sources other than the internal contributions of the estuary itself, the latter solution would be unavoidable.

6. APPLICATION TO POLLUTION PROBLEMS

K(x) being derived from the salt behaviour, or in some other way (for rivers or channels without salt intrusion), the result can be used for computation of distributions of pollutants and other

substances if two conditions are fulfilled:
1. the material or property concerned behaves as a dissolvable substance.
This excludes coarse particles; it may include finely dispersed matter.
2. a one-dimensional description is adequate.

An example whereby this second condition holds completely, is the case of a substance released at a fair distance upstream from the area of interest, especially if the release takes place in a relatively narrow section of the water course.

An example whereby this condition is not met at all, is the case of a short-lived substance, injected from a small source at one of the banks of a relatively wide section. In such a case the substance will have decayed even before it has reached a somewhat even distribution in the cross section. All material present in the body of water is distributed in a distinct two-dimensional pattern. The one-dimensional model is not of any use for obtaining information on this pattern. The two-dimensional model described in paper 11 (1) may be a good instrument; there is no problem involved in spreading on a large scale of time and distance.

In practice, there is an important category of problems lying in between the two extremes mentioned. For these problems, profitable use can be made of the one-dimensional model as far as somewhat larger distances are concerned; in the section where the source is located a rough estimate may be made as to the cross-sectional average. Details of cross-sectional differences and more reliable cross-sectional averages in the region where such differences are significant can only be obtained by using two-dimensional models or similar approaches but not by means of a one-dimensional model. The total amount of matter present, say in a stationary stage, can be divided into two parts. First there is the part "older" than a certain age (after release), which can be properly described one-dimensionally. The second part, consisting of the rest of the material, is relatively young and shows a clearly two-dimensional pattern. The two-dimensional component of the total distribution becomes more important as the local width of the water course becomes larger (compared to the size of the source) and as the lifetime of the substance concerned decreases. This component may, however, be of no importance if it is located outside the area of interest (e.g. when it lies abroad) even though it might contain a large fraction of the dispersed substance.

In practice, a combined approach with both the two-dimensional model described in paper 11 (1) and the one-dimensional model under consideration, has been applied on several occasions. An interesting aspect here has been the possibility (in one case) of adjusting parameters in the two-dimensional model by means of the one-dimensional model. The procedure was followed because of a gap in the empirical data expressed as a function of time and distance scales. Dye experiments had provided data up to a scale of a few kilometers, corresponding to a time range of about two days. For the wider part of the estuary this was still too small to switch directly to the one-dimensional desdription. Some extrapolation of the two-dimensional behaviour in time was necessary. Because of inaccuracies in the experimental results and uncertainties about the constancy of the trend, an extrapolation would be rather speculative. The necessity that the extrapolation should connect to the behaviour that is reliably described by the one-dimensional approach however, gives a firm basis to the extrapolation thus providing a reliable covering of the entire range of interest.

Some examples will now be given of purely one-dimensional approximations of particular problems.

Most applications have been in the Ems and Scheldt estuaries, which can both be considered well-mixed estuaries, although locally (where horizontal salinity gradients are at a maximum) some slight stratification may occur.

One of the most interesting applications in the Scheldt-estuary has been the computation of the influence on water quality of the future B a a l h o e k k a n a a l, a canal to be dug parallel to the Scheldt near the Belgian-Dutch border. This canal would have a water intake about 15 km downstream from the border and an outlet at about 15 km upstream from the border. The flushing flow that would be added to the river flow in the 30 km track concerned, might be several times as large as the river discharge in the summer months. A considerable influence upon the river water quality at the frontier could be the consequence.

First, an attempt was made to simulate measured BOD-DO-distributions for the existing situation. For this purpose, it appeared to be necessary to add a facility to the programme which had not been needed earlier. This became mandatory because the BOD-load in the present situation was so large, that if the differential equations (I) and (III) were used with an ordinary constant oxidation rate β, oxygen concentrations would become negative in several sections. What happens in practice is that β decreases when the oxygen content approaches zero. This process was simulated by writing

$$\beta = \beta(x,t) = \beta_{max} \tanh \left\{ \zeta \frac{G(x,t)}{G_v} \right\} \qquad \text{where } \zeta > 0 \qquad \text{(XXXI)}$$

For example, if $\zeta = 20$, $0.95\,\beta_{max} \lesssim \beta < \beta_{max}$ for $G(x,t) > 0.1\,G_v$, but $\beta \simeq 0.5\,\beta_{max}$ for $G(x,t) = 0.025\,G_v$ and $\beta \simeq 0.1\,\beta_{max}$ for $G(x,t) = 0.005\,G_v$ and $\beta \longrightarrow 0$ as $G \longrightarrow 0$ for any ζ. Of course, at the same time, τ has to be varied accordingly since

$$\tau = \frac{d}{\beta} \qquad \text{(XXXII)}$$

in which d = the (total) demand of oxygen (kg) per kg of oxidizable matter. By employing this method, a quite satisfactory approximation of the measured BOD-DO-distributions could be obtained, although initially only a rough estimate of the BOD-load could be made. BOD-DO-data being available for various river discharges, a better estimate could be achieved using an iterative approach. After these activities had been completed, computations were made to determine the influence of the future canal on the water quality near the border.

Another interesting application for the same area was the forecasting of excess temperatures caused by projected electricity plants. A good agreement with the results obtained from a similar model used by Belgian colleagues was obtained.

For the Ems-estuary, computations were made for conservative substances and organic matter. For the latter, the one dimensional approximation proved less satisfactory than in the above case for the Scheldt, since, for the Ems, much wider sections of the estuary were concerned. Therefore, additional computations were performed with the help of the two-dimensional model (1).

The first important non-estuarine application will be a number of computations for the river Rhine, now in preparation.

7. PRESENT ACTIVITIES

Presently, aside from operational use for urgent problems, the following activities are in progress. A first approximation of K(x) for the Eastern Scheldt is being made on the basis of a limited set of salinity data. The very low freshwater discharge of this estuary restricts the accuracy of the results. The purpose of the investigation is, together with other techniques, to obtain more insight into silt movement.

The new set of K(x) values for the Western Scheldt is being extended in seaward direction in connection with the displacement of the sea boundary to a point at which salinity variations are smaller. Errors caused by the finite grid size, such as numerical diffusion and oscillations in space, are under further study. For the grid size of 5000 m which was used in most cases so far, certain differences in the optimal set of K(x) values are found, dependent on the difference scheme that is used. Because of the very short computing times that have been attained by improving the efficiency of the programme and by the use of a faster computer, the best solution may be a substantial decrease in dx, with the acceptance of the concomitant increase in computing time.

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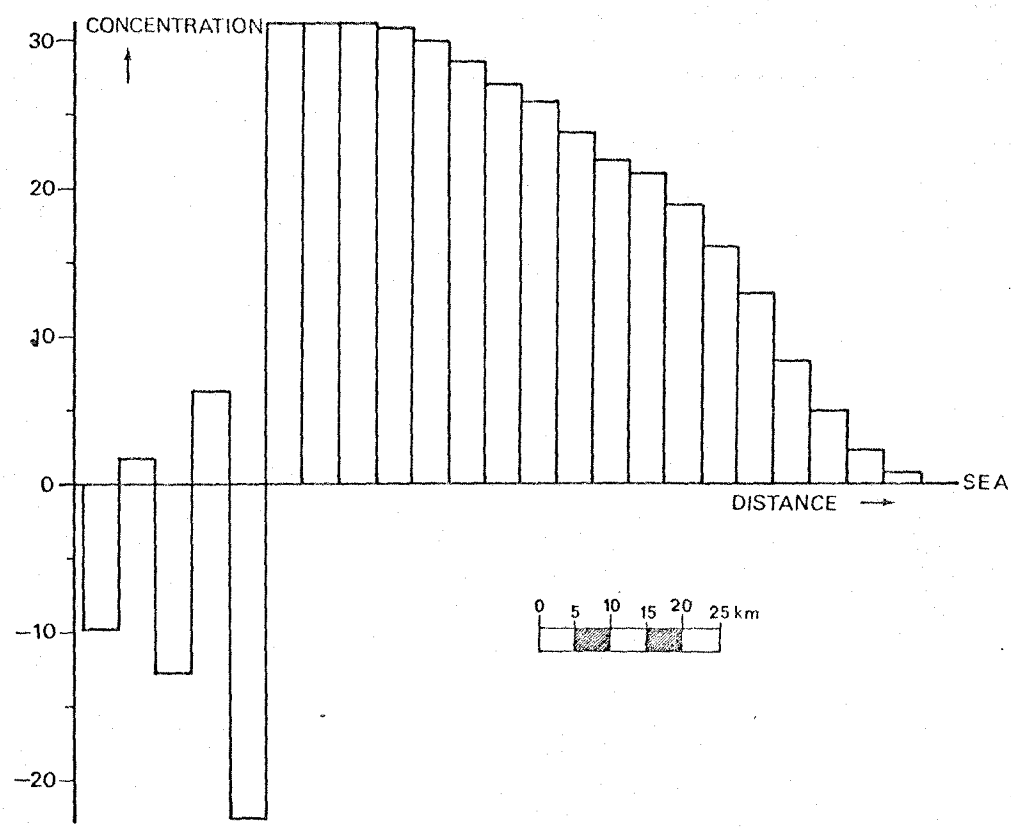

Figure 1a Spatial oscillations (stable in time) generated near a strong concentration gradient.

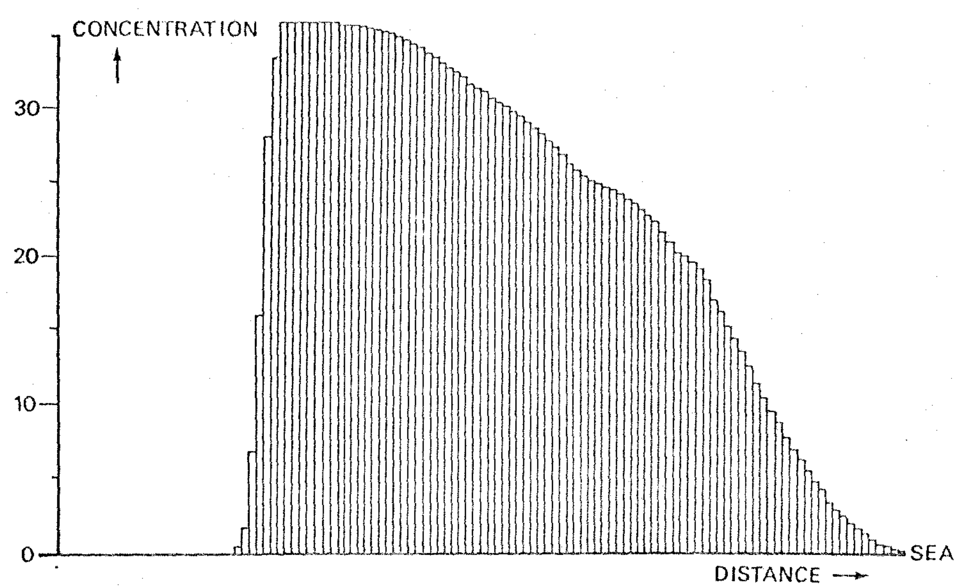

Figure 1b Result of a computation under precisely the same conditions as above but performed on a five times smaller grid size

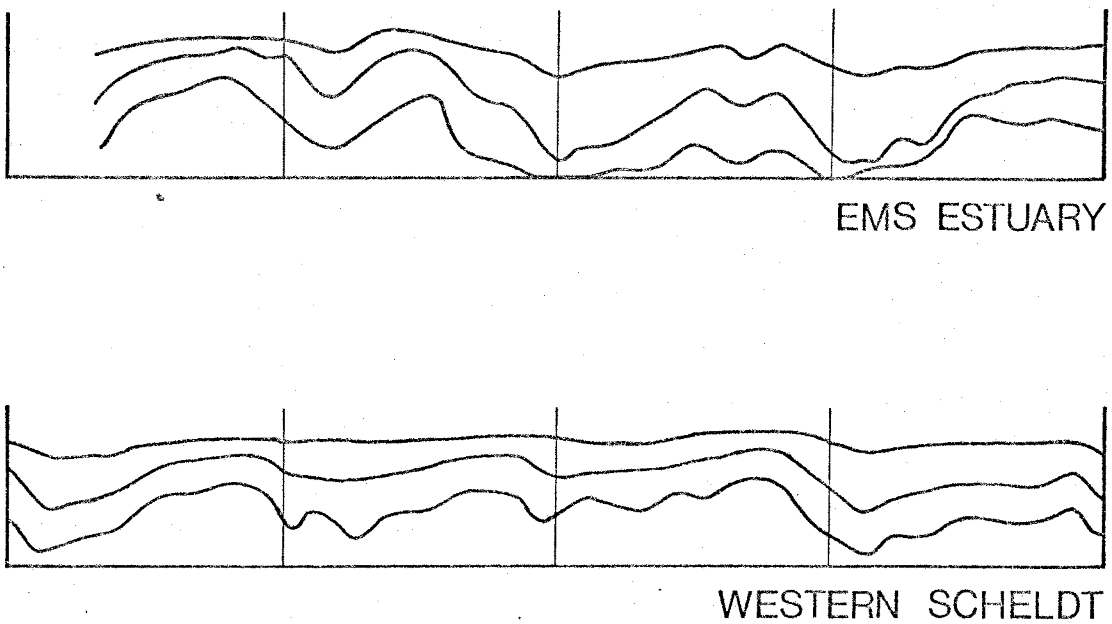

Figure 2 Salt concentrations taken over 3½ and 4 year periods respectively, at three different points in Ems and Scheldt estuaries.

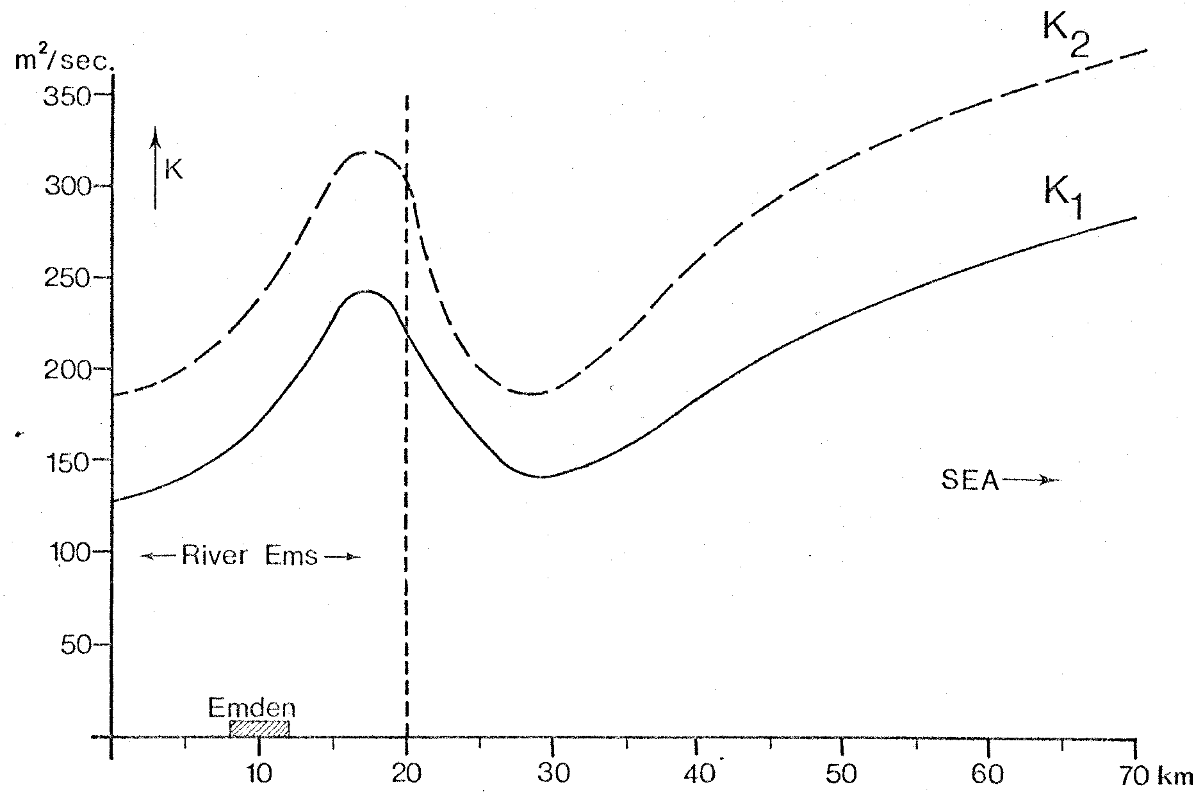

Figure 3 Longitudinal mixing coefficients for dry (K_1) and wet (K_2) periods in the Ems estuary.