VIII.- Numerical methods

The equation which governs the evolution of a passive pollutant (e.g. a dye tracer) in a shallow sea has been established by Nihoul (1971).

In axes moving with the center of the patch, this equation may be written, neglecting eddy diffusivity as compared to shear effect diffusivity

$$\frac{\partial r}{\partial t} = \frac{\alpha}{H} \nabla \left[\frac{H^2}{U} \mathbf{u}(\mathbf{u}.\nabla r)\right] . \tag{1}$$

Three groups of methods (double discretization, simple discretization, pseudo-analytical) have been tested on this equations in the case of Talbot's experiment of dye release at point B .

As boundary condition, it is assumed that $r = 0$ for all time outside some large domain Ω (Ω must be large enough to contain the patch of pollutant for all time of interest). As initial condition, it is assumed that the tracer is spread initially over some small domain Ω' ($\Omega' \ll \Omega$).

In view of the rather crude approximation made by using currents and depth data given by current atlas and bathygraphic maps, it is satisfactory to consider the velocity vector $\mathbf{u}$ as a function of time only and H a constant over the region of interest. This approximation saves core memory storage in the computer and this is an advantage in the preliminary work of perfecting the method.

Eq. (1) can now be written in cartesian coordinates

$$\frac{\partial r}{\partial t} = \frac{\alpha H}{U} \left(u_1^2 \frac{\partial^2 r}{\partial x_1^2} + 2\, u_1 u_2 \frac{\partial^2 r}{\partial x_1 \partial x_2} + u_2^2 \frac{\partial^2 r}{\partial x_2^2}\right) \tag{2}$$

where u_1 and u_2 are the components of the velocity vector $\mathbf{u}$.

1.- Double discretization method

1.1.- Time discretization

The operator $\frac{\partial}{\partial t}$ is approximated by a time-forward finite difference expression

$$\frac{\partial r}{\partial t} \sim \frac{1}{\Delta t} [r(\mathbf{x}, t+\Delta t) - r(\mathbf{x},t)] + O(\Delta t) . \tag{3}$$

With symmetric differences, the truncation error would have been $0(\Delta t^2)$. However the numerical stability analysis shows that in this case the difference scheme is *always* unstable. This is the consequence of the fact that time appears in a non-symmetric way in equation (2). Δt must be chosen in order to minimize the truncation error without increasing unreasonably the computation time. In most of our applications

$$\Delta t \sim 600 \text{ s} .$$

1.2.- Space discretization

We superpose a net-grid R_ℓ upon the (x_1,x_2) plane. This net-grid is square-shaped and the mesh-size is $\ell = \Delta x_1 = \Delta x_2$; Ω_ℓ is the subset of R_ℓ representing the inner points of Ω .

The space derivatives are then approximated by the finite differences

$$\frac{\partial^2}{\partial x_1^2} r_{i,j} = \frac{1}{\ell^2} (r_{i+1,j} - 2\, r_{i,j} + r_{i-1,j}) + 0(\ell^2)$$

$$\frac{\partial^2}{\partial x_2^2} r_{i,j} = \frac{1}{\ell^2} (r_{i,j+1} - 2\, r_{i,j} + r_{i,j-1}) + 0(\ell^2) \qquad (4)$$

$$\frac{\partial^2}{\partial x_1 \partial x_2} r_{i,j} = \frac{1}{4\ell^2} (r_{i+1,j+1} + r_{i-1,j-1} - r_{i+1,j-1} - r_{i-1,j+1}) + 0(\ell^2)$$

First, an explicit scheme was tried. In this case, all values $r_{m,n}$ in (4) are taken at time t . This scheme however did not conserve mass and negative concentrations were found. Gorenflo (1970) has shown that, under certain conditions, which are sometimes fulfilled in our problems, there exist no explicit method giving non negative results everywhere and preserving conservation of mass.

For this reason, an attempt was made to use an implicit scheme. In this case, values of $r_{m,n}$ at $t + \Delta t$ also occur in (4). Hence simultaneous *coupled* linear equations (~ 400) must be solved to compute the concentrations at time $t + \Delta t$.

The scheme had however to be abandonned because of non conservation(1)

(1) Note that eq. (2) is actually parabolic in space (due to the neglecting of eddy diffusivity). Gauss-Seidel method is suitable for elliptic spatial operators describing phenomenons such that each point influences all its neighbours. Now, in parabolic case,

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and prohibitive computation time.

As the solution of the diffusion equation in the one-dimensional case is the sum of error functions, it would seen that a grid with meshes enlarging from the origin to the boundary is particularly adapted to diffusion problems.

If we choose ℓ_i-steps following

$$\ell_1 = \ell$$

$$\ell_i = \ell_{i-1}\left(1 + \frac{\beta\,\ell_{i-1}}{L}\right) \qquad L = \Sigma\,\ell_i$$

we get a net shown in figure 12.

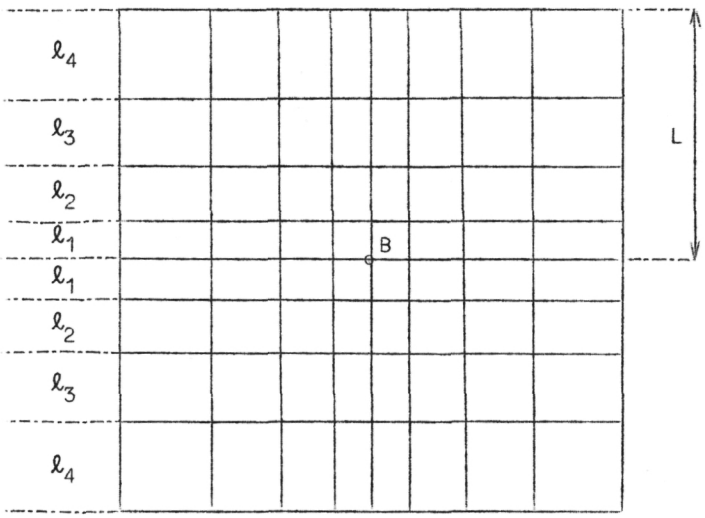

fig. 12.

Finite difference expressions established by Sundquist and Veroins (1969) for one-dimensional problems make it possible to approximate the spatial operator with a truncation error of $0(\ell^2)$, and to reduce in a significant way the number of net-points for the same precision as constant-step net-grids. But in the two-dimensional case, this reduction of memory storage is counterbalanced by an increasing computation time due to sophisticated formulas.

On the other hand, this scheme is not conservative, because there is no symmetry, neither in x_1, nor in x_2, in the expressions of the coefficients.

2.- Simple discretization method (Galerkin method)

The method consists in a conventional time discretization and a decomposition of $r(x_1,x_2,t)$ into series of orthonormed functions $\zeta_j(x_k)$, i.e.

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each point influences its neighbours only in a definite direction (**u** direction), therefore the Gauss-Seidel method is ill-adapted (no conservation, lateral diffusion).

functions such that :

$$(6) \qquad \int_{\Omega_k} \zeta_i(x_k)\ \zeta_j(x_k)\ dx_k = \delta_{ij} \ .$$

We write $r(x_1,x_2,t)$ in the following discrete form :

$$(7) \qquad r(x_1,x_2,t) = \sum_{i,j=1}^{N} a_{ij}(t)\ \zeta_i(x_1)\ \zeta_i(x_2) \ ,$$

N being the maximum number of approximation functions for each independent variable.

$$(8) \qquad \dot{r} = \frac{\partial r}{\partial t} = \sum_{i,j=1}^{N} \dot{a}_{ij}(t)\ \zeta_i(x_1)\ \zeta_j(x_2)$$

$$(9) \qquad Lr = \sum_{i,j=1}^{N} a_{ij}(t)\ \ L[\zeta_i(x_1)\ \zeta_j(x_2)]$$

where L is the spatial operator.

Using the orthogonality property (6), we get a linear system of $N \times N$ differential equations of first order which can be solved by a classical Runge-Kutta or predictor-corrector method, of which well-adapted versions exists.

We have tested this method with two very different sets of basis functions.

1st set

$$(10) \qquad \zeta_n(x_k) = \cos\ (n\kappa x_k) \qquad n = 1,2,3 \ ; \ k = 1,2$$

κ is choosen such that $\cos\ (\kappa \times 10\ km) = 0$ to satisfy boundary conditions on Γ . Orthogonality of trigonometric functions is well-known.

2nd set

$$(11) \qquad \zeta_n(x_k) = c_n \exp\ (-\frac{x_k^2}{2})\ \ H_n(x_k) \qquad n = 1,\ldots,6 \ ; \ k = 1,2$$

where $H_n(x_k)$ is the Hermite polynomial of order n , with the orthogonality relation

$$(12) \qquad \int_{-\infty}^{+\infty} c_i c_j \exp\ (-x_k^2)\ \ H_i(x_k)\ H_j(x_k)\ dx_k = \delta_{ij} \ .$$

The length scale for x_1 and x_2 is choosen so that $\exp(-x_k^2)$ practically vanishes outside a circle with a diameter of 2 km .

In both cases, properties of approximation functions are such that, while integrating, terms corresponding to

$$\frac{\partial^2 r}{\partial x_1 \partial x_2}$$

vanish and then do not influence evolution. Thus, this representation is not perfectly consistent.

The Galerkin method diverges in both cases after computations corresponding to a couple hours in actual time.

In the first case, it can be admitted that the total number of basis functions is insufficient to represent the initial concentration distribution, which is very sharp. Moreover, on the boundary Γ , the concentration may actually vanish, but not its spatial derivatives, and this fact is physically not true.

In the second case, the initial distribution is well-represented by the $\zeta_n(x_k)$, the spatial derivatives of which vanish at boundary.

But because the ζ_k's do not vary with time, it is impossible to approximate, with any accuracy, the smoothing of the function $r(x_1,x_2,t)$ in time.

We have had in mind to change the length-scale at each time step, to take smoothing into account, but this technique leads to very sophisticated problems of connexion between consecutive solutions and is of no practical interest.

3.- Analytical methods

3.1.- Pseudo-analytical method

If we choose the time-step Δt small enough, we may admit that $\mathbf{u}(t)$ is constant. We choose the x-axis in the $\mathbf{u}$-direction. So eq. (2) becomes one-dimensional, with constant coefficients.

$$\frac{\partial r}{\partial t} = D \frac{\partial^2 r}{\partial x^2} \qquad D = \alpha H u \ . \tag{13}$$

If we assume that the initial concentration is r_0 within a range $(-d,+d)$, the analytical solution is (Crank) :

$$(14) \qquad r(x,t) = \frac{1}{2} r_0 \left[\operatorname{erf}\left(\frac{d - x}{2\sqrt{Dt}}\right) + \operatorname{erf}\left(\frac{d + x}{2\sqrt{Dt}}\right)\right]$$

drawn in figure 13.

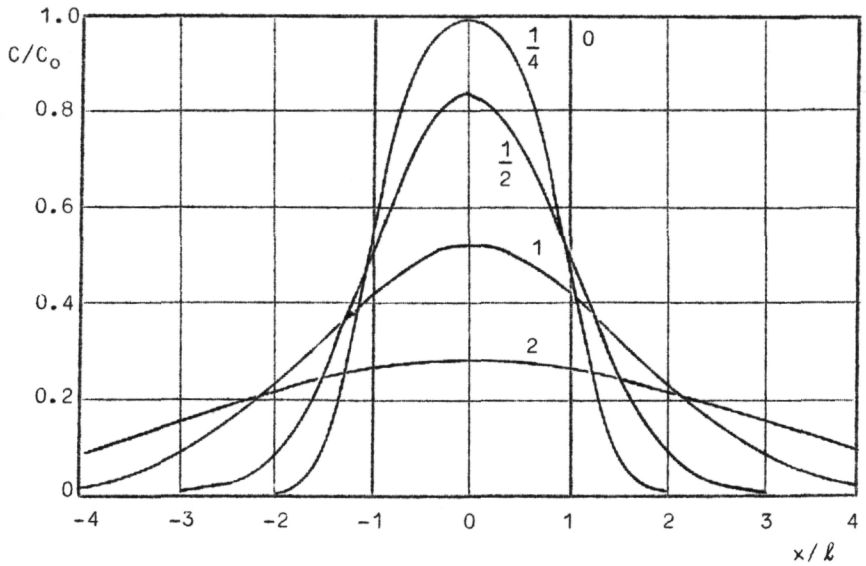
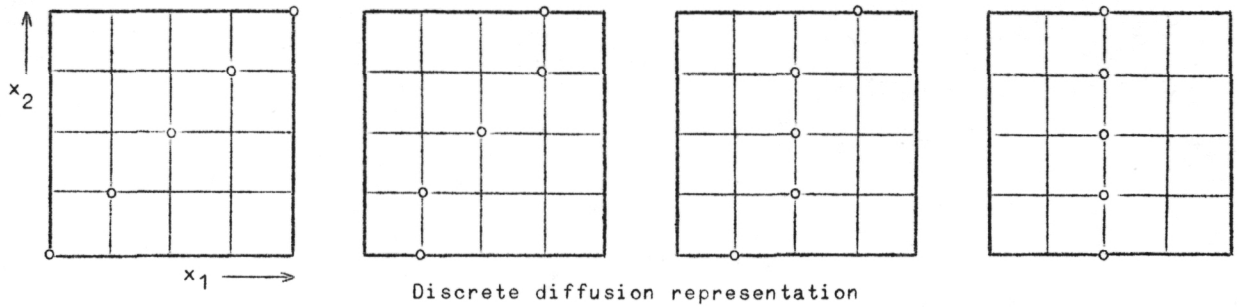


fig. 13.- Concentration-distance curves for an extended source of limited extent. Numbers on curves are values of $(Dt/\ell^2)^{\frac{1}{2}}$.

With the former assumptions we can use this solution locally, at each point of a net-grid (x_1,x_2) if we consider at each instant, the concentration $r(x_1,x_2,t)$ as an initial concentration to compute $r(x_{1_i},x_{2_i},t+\Delta t)$. The problem is now to determine for each point (x_1,x_2) , the points (x_{1_i},x_{2_i}) of the net, which are sufficiently near to (x_1,x_2) in the **u**-direction, to be influenced by $r(x_1,x_2,t)$.

The number of these points is determined by $\left(\frac{D\,\Delta t}{\ell^2}\right)^{\frac{1}{2}}$ [see figure 13]. Figure 14 shows the choice of these points depending upon the direction of vector **u** in the case where $u_1u_2 > 0$ and $\frac{u_2}{u_1} > 1$

a) $$1 \leq \frac{u_2}{u_1} < \frac{4}{3} ,$$



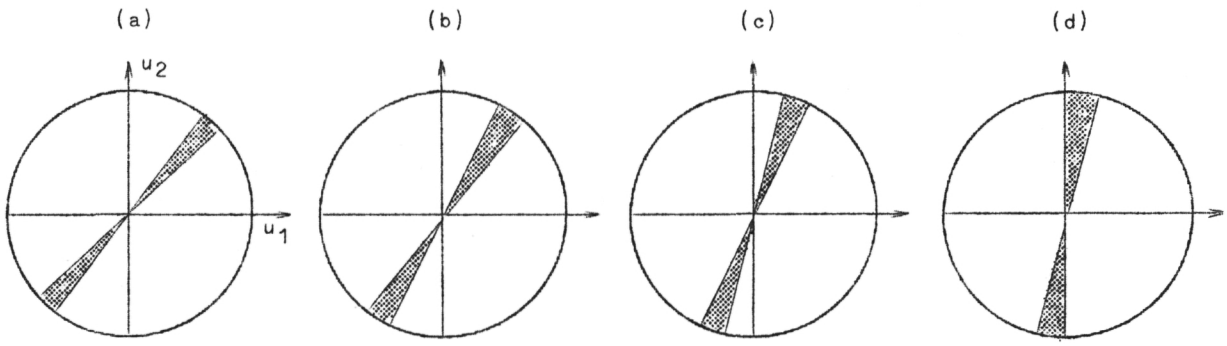


fig. 14.

b) $$\frac{4}{3} \leq \frac{u_2}{u_1} < 2 \ ,$$

c) $$2 \leq \frac{u_2}{u_1} < 4 \ ,$$

d) $$\frac{u_2}{u_1} \geq 4 \ .$$

It is easy to see that all situations are analogous to one of the formers.

3.2.- Local analytical solution

If

(15) $$\frac{\partial u}{\partial t} = 0 \quad , \quad \frac{\partial v}{\partial t} = 0 \ ,$$

it can easily be shown that equation (2) has a solution

(16) $$r = r_0 \, t^{-\frac{1}{2}} \exp \left[- \frac{U}{16 \, \alpha H t} \left(\frac{x_1}{u_1} + \frac{x_2}{u_2} \right)^2 \right]$$

u_1 and u_2 being neither constant nor uniform, we could try to write the solution $r(x_1,x_2,t)$ in the form

(17) $$r = \tilde{r}\, K(x_1,x_2,t)$$

or

(18) $$r = \tilde{r} + K(x_1,x_2,t)$$

where K is a continuous and continuously differentiable function of t, x_1, x_2, which satisfies a partial differential equation with given boundary conditions

(19) $$\frac{\partial K}{\partial t} = N(K,x_1,x_2,t) \ .$$

In this way, we get rid of the part of the solution that is the most difficult to treat by numerical methods (because of its exponential form), and we may admit that (19) has a smoother solution than (2), more accessible numerically.

This method is now being investigated.

3.3.- Isoconcentration curves drawing

We have worked out a routine to draw isoconcentration curves. This routine needs, as input data, the values of the concentration at all the points of a net-grid with constant step.

By means of these data (and interpolation) the routine :

1) computes all the points belonging to the segments of the net, where the concentration is equal to a given value (for instance, one tenth of the maximum concentration) ;
2) stores the coordinates of these points (initial point is the origin) ;
3) classifies and brings together all the points, mesh after mesh, taking into account that the concentration inside a curve is always greater than the given value on the curve (the curves are assumed to have a general convex shape) ;
4) draws a smooth curve joining all the points.

The program allows to draw several curves for one net, with different graphical representation (see fig. 6-8, pp. 42-44).

4.- Results of the tests

A.1.- Explicit scheme

- conservative method
- existence of negative concentration ($7 . 10^{-2}$ of the total mass)
- the Gorenflo corrections are little effective
- very rapid computation
- resulting curves can be compared to Talbot's experiments for $\alpha \sim 0.5$

A.2.- Implicit scheme

- non conservative scheme
- lateral diffusion (physically inexistent)
- existence of small negative values
- little effective corrections
- computation time rather large

A.3.- Variable steps

- non conservative scheme
- rather large negative concentrations
- rather rapid computation

B.- Galerkin method

- rapid divergence in both tests

C.- Pseudo-analytical method

- no negative concentrations
- lateral diffusion
- very rapid computation
- seems to be difficult to use for non-uniform **u** and H

5.- Conclusion

At the present time, the best methods are the simplest ones. Most of the well-known discrete methods for spatial elliptic operator failed to solve our problems. It seems that the pseudo-analytical methods are, at present

and for very simplified problems, the most effective. Let us note finally that a research engineer of EAI Inc. is now working to solve our problem by means of hybrid (analog-digital) computers, but unfortunately, he has no results yet. We emphasize more the lack of accurate experimental data.

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