

Solving hydrodynamics and dispersion

5.1 Introduction

In the previous chapter the hydrodynamic equations have been presented and a finite difference method to solve them has also been described. The dispersion equation was treated in a simple one dimensional form in chapter 3. Now, the solution of the hydrodynamic equations together with dispersion will be discussed. Also, the dispersion equation is generalized to a 2D depth-averaged form with variable water depth and to an arbitrary direction of the flow. Some discussion on boundary conditions for the dispersion equation is finally included.

5.2 Hydrodynamics on-line and off-line

As has already been pointed out, modelling radioactivity dispersion in the marine environment involves two models: a hydrodynamic model and a transport model. The hydrodynamic model calculates the water flows required by the transport model to calculate tracer dispersion according to such flows. Both models can be linked in a way that they run simultaneously, using the same time step. This coupling is called the *on-line* mode. However, it is also possible to run the models separately. The transport model uses in this case time series of flows that have been previously calculated by the hydrodynamic model and stored in files. This coupling is called the *off-line* mode. A scheme showing both approaches can be seen in figure 5.1, taken from [154].

The off-line mode has a clear advantage over the on-line mode: the stability conditions imposed by the transport equation are much less restrictive than the CFL condition due to the hydrodynamic equations. Thus, a larger time step can be used. This, together with the fact that hydrodynamic calculations have all been carried out in advance, and thus only the transport equation is solved each time step, implies that computation is much faster. An off-line dispersion model can use flows derived from different hydrodynamic

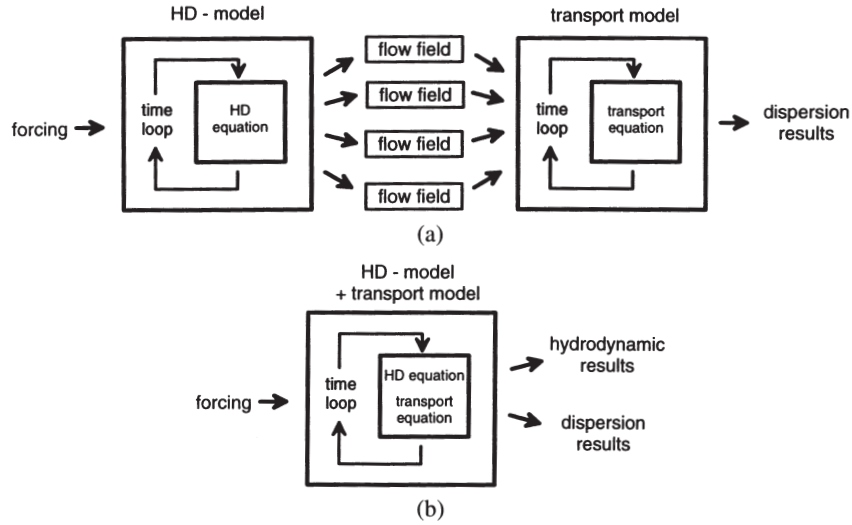


Fig. 5.1. Coupling of the hydrodynamic and dispersion models in the off-line (a) and on-line (b) modes (from [154])

models, or use the same flow field for different source terms, radionuclides or parameters in a much faster way. It is also possible to combine tidal residuals with wind induced flows, as has been done by Breton and Salomon [24]. The drawback is that currents fields are stored at time intervals much larger than the hydrodynamic model time step. Time interpolation between these flow fields cuts off variability at short temporal scale.

In the on-line mode the transport equations are integrated with the hydrodynamic equations, and thus are solved with the same time step. This approach is computationally much more expensive, but the transport equation is receiving flow fields with the highest possible temporal resolution.

Both methods have strengths and weaknesses, but anyway, the flow fields have to be provided to the transport equation in time intervals that allows the reproduction of the dominant flow variability. This time resolution depends on the model area and objective of the work. Studying tidal dispersion in a coastal area requires solving tidal cycles. This will require a much higher resolution than studying long term dispersion in a whole sea or ocean basin.

Another possibility for running a dispersion model off-line and, at the same time, maintaining temporal resolution high enough to solve tidal mixing consists of using standard tidal analysis. As was explained in chapter 4, tides can be represented as a number of harmonics in the form of equation 4.28. Tidal analysis consists of determining, by a standard fitting algorithm, the amplitude and phase (tidal constants) for each constituent included in the model

and for each grid cell. These tidal constants have to be calculated for both components of the flow, u and v , and for water elevation z . Tidal constants, for each tide constituent, are calculated by the same hydrodynamic code and are stored in files that will be read by the dispersion model. Once that tidal constants are known, computation of flow and water elevation at any cell and time just involves the evaluation and addition of a few cosine terms. This is very fast, and simultaneously, the dispersion model is not limited by the CFL condition. The net residual current has to be evaluated by the hydrodynamic model and added to the current obtained from tidal analysis since a net transport cannot be obtained from the pure harmonic currents provided by the tidal analysis. It has to be clearly pointed out that tidal analysis is carried out running the hydrodynamic model for each constituent separately. This technique is usually applied in rapid response Lagrangian models (see chapter 7), although has also been used in finite difference dispersion models [127]. It has the clear advantage of joining the strengths of the off-line mode with a temporal resolution that is high enough to solve tidal processes.

5.3 The transport equation in non constant water flows and depths

The transport equation, in a 2D depth averaged form and for a constant diffusion coefficient and a constant water depth, has already been presented in chapter 2:

$$\frac{\partial C}{\partial t} + \frac{\partial uC}{\partial x} + \frac{\partial vC}{\partial y} = K_h \left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} \right) \quad (5.1)$$

However, depth will not be constant over the model domain due to changes in bed topography. These changes in depth have to be considered in the transport equation in order that tracer mass is conserved. The transport equation can be generalized to the case in which depth is constant in time for each point but changes from one point in the domain to another. Also, a variable diffusion coefficient can be considered. The new form of the equation would be:

$$\begin{aligned} & \frac{\partial C}{\partial t} + \frac{1}{H} \left\{ \frac{\partial(uHC)}{\partial x} + \frac{\partial(vHC)}{\partial y} \right\} \\ &= \frac{1}{H} \left\{ \frac{\partial}{\partial x} \left(K_x H \frac{\partial C}{\partial x} \right) + \frac{\partial}{\partial y} \left(K_y H \frac{\partial C}{\partial y} \right) \right\} \end{aligned} \quad (5.2)$$

where K_x and K_y are the diffusion coefficients in the directions of x and y respectively, although in practical applications they are generally assumed to be equal and constant.

If water depths also change in time due to tidal oscillations, the transport equation would be written in the following form:

$$\begin{aligned} & \frac{\partial(HC)}{\partial t} + \frac{\partial(uHC)}{\partial x} + \frac{\partial(vHC)}{\partial y} \\ &= \frac{\partial}{\partial x} \left(K_x H \frac{\partial C}{\partial x} \right) + \frac{\partial}{\partial y} \left(K_y H \frac{\partial C}{\partial y} \right) \end{aligned} \quad (5.3)$$

This is the most general case, and a numerical scheme to solve it will be discussed. The advection terms will be initially treated with the upstream method already presented in chapter 3. The treatment of diffusion is essentially the same as in equation 3.17. The equation will be solved in the same computational grid as the hydrodynamic equations (figure 4.1). Concentration C is defined at the centre of the cell and the diffusion coefficients at the same points as the velocities.

Let us start with the advective terms. In the upstream method the spatial derivative is shifted to the direction where the current comes from, as was explained in chapter 3. Thus, the form of the derivative depends on the current direction. The upstream scheme given by equations 3.2 and 3.5 can be extended to an arbitrary current direction and changing depth. The finite difference form of the transport equation would result as follows:

$$\begin{aligned} & \frac{H_{i,j}^* C_{i,j}^* - H_{i,j} C_{i,j}}{\Delta t} \\ &= \frac{-n_1 u_{i,j} H_1 C_{i,j} - (1 - n_1) u_{i,j} H_1 C_{i+1,j}}{\Delta x} \\ &+ \frac{n_2 u_{i-1,j} H_2 C_{i-1,j} + (1 - n_2) u_{i-1,j} H_2 C_{i,j}}{\Delta x} \\ &+ \text{y derivative} + \text{diffusion terms} \end{aligned} \quad (5.4)$$

In this equation H_1 and H_2 are water depths at the right and left sides of cell i, j respectively, as described in chapter 4, and numbers n are defined in the following way:

$$n_1 = \begin{cases} 1 & \text{if } u_{i,j} > 0 \\ 0 & \text{if } u_{i,j} < 0 \end{cases} \quad (5.5)$$

and

$$n_2 = \begin{cases} 1 & \text{if } u_{i-1,j} > 0 \\ 0 & \text{if } u_{i-1,j} < 0 \end{cases} \quad (5.6)$$

From this equation $C_{i,j}^*$ is obtained since depth at the new time level, $H_{i,j}^*$, is known from the previous solution (either on- or off-line) of the hydrodynamic equations. It can be noted that the advective flux through a land boundary is automatically zero since the current component normal to the boundary is defined as zero when solving hydrodynamics. The treatment of the y derivative is the same.

The diffusion terms will be written now using the numerical scheme for non constant K given by equation 3.17:

$$\begin{aligned}
& \text{diffusion terms} \\
& = \frac{1}{\Delta x} \left\{ n_5 K_{i,j} H_1 \frac{C_{i+1,j} - C_{i,j}}{\Delta x} - n_6 K_{i-1,j} H_2 \frac{C_{i,j} - C_{i-1,j}}{\Delta x} \right\} \\
& + \text{y derivative}
\end{aligned} \tag{5.7}$$

Here $n_5 = 0$ if $H_{i+1,j} = 0$ to avoid diffusion through a land boundary. Else, $n_5 = 1$. Similarly, $n_6 = 0$ if $H_{i-1,j} = 0$. The treatment for the y derivative is exactly the same. These boundary conditions are mathematically expressed as

$$\frac{\partial C}{\partial n} = 0 \tag{5.8}$$

where n is the direction normal to the land boundary. From these schemes it is easy to obtain the finite difference form of the dispersion equation when depths are constant in time (equation 5.2).

The stability condition due to diffusion terms is different to the one dimensional case (equation 3.18): the factor 2 appearing at the denominator must be 4. In a three dimensional case it would be 6.

The application of the MSOU scheme in the case of flow in arbitrary direction is more tedious. The advective part of the dispersion equation is now written as:

$$\begin{aligned}
& \frac{H_{i,j}^* C_{i,j}^* - H_{i,j} C_{i,j}}{\Delta t} \\
& = \frac{-n_1 u_{i,j} H_1 F_1 - (1 - n_1) u_{i,j} H_1 F_2}{\Delta x} \\
& + \frac{n_2 u_{i-1,j} H_2 F_3 + (1 - n_2) u_{i-1,j} H_2 F_4}{\Delta x} \\
& + \text{y derivative}
\end{aligned} \tag{5.9}$$

where factors F include the second order correction to the upstream scheme:

$$F_1 = C_{i,j} + \frac{1}{2} \psi (C_{i,j} - C_{i-1,j}) \tag{5.10}$$

with

$$\psi = \max(0, \min(2r, 1), \min(r, 2)) \tag{5.11}$$

where

$$r = \frac{C_{i+1,j} - C_{i,j}}{C_{i,j} - C_{i-1,j}} \tag{5.12}$$

$$F_2 = C_{i+1,j} - \frac{1}{2} \psi (C_{i+1,j} - C_{i,j}) \tag{5.13}$$

but now

$$r = \frac{C_{i+2,j} - C_{i+1,j}}{C_{i+1,j} - C_{i,j}} \tag{5.14}$$

$$F_3 = C_{i-1,j} + \frac{1}{2} \psi (C_{i-1,j} - C_{i-2,j}) \tag{5.15}$$

$$r = \frac{C_{i,j} - C_{i-1,j}}{C_{i-1,j} - C_{i-2,j}} \quad (5.16)$$

and finally,

$$F_4 = C_{i,j} - \frac{1}{2}\psi(C_{i,j} - C_{i-1,j}) \quad (5.17)$$

$$r = \frac{C_{i+1,j} - C_{i,j}}{C_{i,j} - C_{i-1,j}} \quad (5.18)$$

In all F factors ψ is defined as in equation 5.11. It must be taken into account that r may diverge if the denominator tends to zero. This has always to be checked and, if occurs, an arbitrary large value is given to r (for instance 10). Thus ψ would be 2 automatically and overflow errors are not generated.

Some additional control is required in the vicinity of land boundaries since it may be necessary to remove the second order correction. The following conditions are included in the code:

$$F_1 = C_{i,j} \quad \text{if} \quad H_{i-1,j} = 0 \quad (5.19)$$

$$F_2 = C_{i+1,j} \quad \text{if} \quad H_{i+2,j} = 0 \quad (5.20)$$

$$F_3 = C_{i-1,j} \quad \text{if} \quad H_{i-2,j} = 0 \quad (5.21)$$

$$F_4 = C_{i,j} \quad \text{if} \quad H_{i+1,j} = 0 \quad (5.22)$$

It can be easily realized that the inclusion of a second order scheme is more complicated and computationally expensive than the simple upstream scheme. However, it is worth making such effort given the results obtained with both methods: an example of the solution of a 2D advection problem with both the upstream and MSOU methods is presented in figure 5.2. Water depths are considered as constants, equal to 5 m, as well as velocities, $u = 0.5$ and $v = 0.15$ m/s. Temporal and spatial resolution are $\Delta t = 180$ s and $\Delta x = \Delta y = 5000$ m. The advection equation has been integrated for 100 hours, that means 2000 time steps. An initial concentration equal to 1.0×10^5 units/m³ is assumed at cell (5,10). It can be seen that the upstream scheme produces a very high numerical diffusion. Indeed, concentrations obtained with this method are an order of magnitude smaller than those obtained by the MSOU scheme, which reflects much better the advective transport process. Nevertheless, as expected, the position of the center of the patch is the same with both numerical schemes.

5.4 Open boundary conditions

As for the case of the hydrodynamic equations, open boundary conditions have to be prescribed to solve the transport equation. A review of boundary conditions for the transport equation may be seen in [35]; a brief summary is included here.

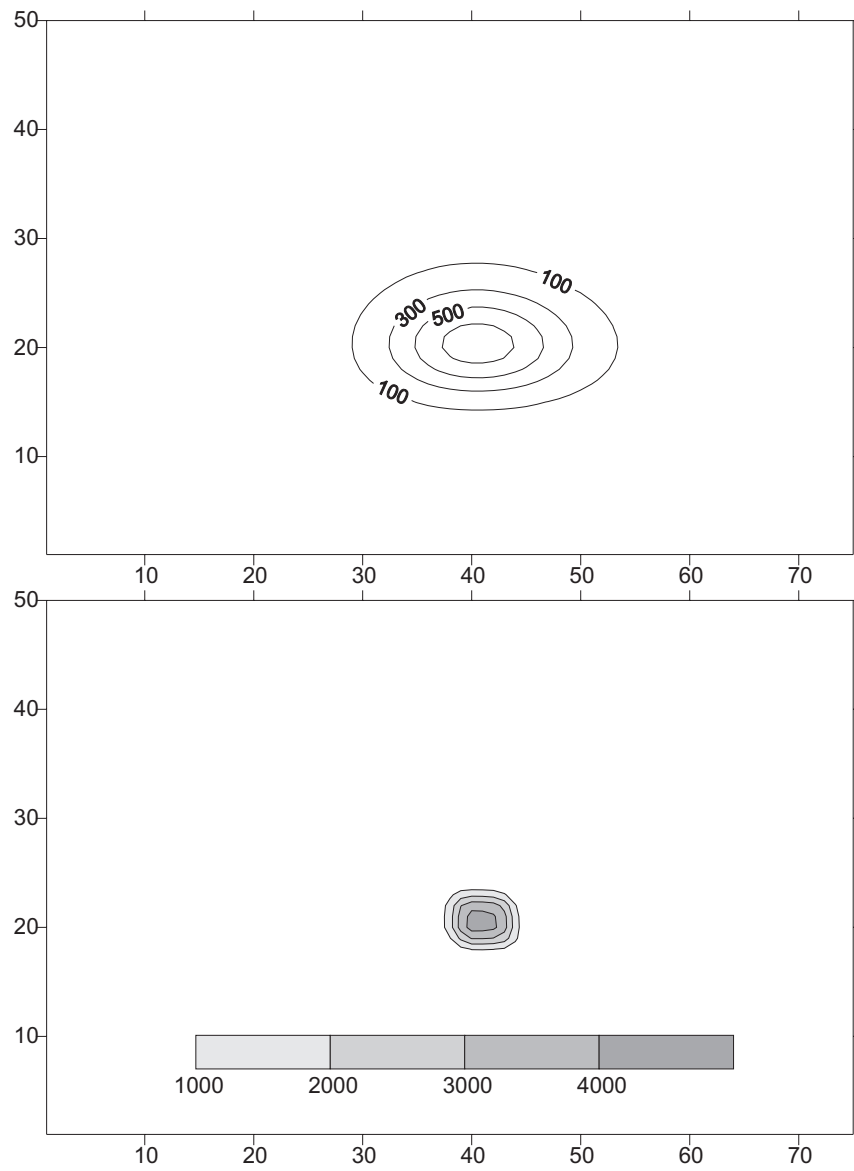


Fig. 5.2. Solution of a 2D advection problem with the upstream scheme (up) and MSOU scheme (down). Contour line units are concentrations, given in arbitrary units per m^3 , and numbers in the axis indicate grid cell number

The Dirichlet boundary condition is applied when the concentration at the boundary is given at each time step:

$$C_b(t) = A(t) \quad (5.23)$$

where C_b is concentration at the boundary and A is a function giving the time evolution of such concentration. Of course, as a particular case, A may be a constant.

The Cauchy condition is applied when the total incoming flux of material is prescribed as a function of time at the boundary:

$$-q_n H C + K_n H \frac{\partial C}{\partial n} = f_b(t) \quad (5.24)$$

where n is the direction normal to the boundary, q_n is the current component normal to the boundary and f_b is the prescribed flux per unit length along the boundary.

A variable boundary condition can also be used. It consists of checking if the flow is coming into the domain from outside or if it is going out from inside. This condition may be interesting when tides are the dominant effect in controlling dispersion. It has been used in [114, 115]. If the flow is going out a decay in concentrations can be specified to account for the decrease in concentrations with increasing distance from the source:

$$C_b = \Gamma C_{b-1} \quad (5.25)$$

where C_{b-1} is concentration just inside the domain and Γ is a non dimensional number obtained from calibration. A value that can be used is, for instance, $\Gamma = 0.99$.

If flow is incoming, it can be specified as in the Cauchy condition or, alternatively, a Dirichlet condition can be applied, specifying concentration at the boundary.

In the tidal models of the Irish Sea and English Channels [121, 122], where the distance traveled by radionuclides during a single flood or ebb period is very small compared with the model domain and open boundaries are far from the radioactive source, condition given by equation 5.25 is always applied with $\Gamma < 1$. This simulates the observed general decrease in concentrations with increasing distance from the source. Equation 5.25 has also been used in the long-term model of the English Channel [130] and in the Irish Sea model described in [65].

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