

## Stochastic modelling of dispersion in shallow water

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**Abstract:** A random walk model to describe the dispersion of pollutants in shallow water is developed. By deriving the Fokker-Planck equation, the model is shown to be consistent with the two-dimensional advection-diffusion equation with space-varying dispersion coefficient and water depth. To improve the behaviour of the model shortly after the deployment of the pollutant, a random flight model is developed too. It is shown that over long simulation periods, this model is again consistent with the advection-diffusion equation. The various numerical aspects of the implementation of the stochastic models are discussed and finally a realistic application to predict the dispersion of a pollutant in the Eastern Scheldt estuary is described.

**Key words:** advection-diffusion equation, random walk model, random flight model, stochastic differential equation, Fokker-Planck equation

### 1 Introduction

The last few years we have been confronted several times with serious water pollution problems due to ship accidents in coastal waters. In such cases accurate predictions of the dispersion of pollutant are required. There are two basic approaches to describe and predict dispersion processes in shallow waters. One might adopt an Eulerian point of view and solve the well-known two-dimensional advection-diffusion equation numerically. This is, however, not an easy task. Finite difference schemes for approximating the advection-diffusion equation are often not mass conserving or may introduce negative concentrations of pollutants in case of high concentration gradients. Since in practice the initial concentration of the prediction problem is usually a delta-like function, we may expect serious difficulties using a numerical procedure (Van Stijn et al., 1987).

Another approach to describe dispersion processes is by means of random walk models. By interpreting the advection-diffusion equation as a Fokker-Planck equation, it is possible to derive a stochastic model for the position of one particle of the pollutant. In this way, the resulting particle model can be made consistent with the advection-diffusion equation. By simulating the position of many different particles using a random generator, it is possible to describe the dispersion process (De Jong, 1979). This stochastic approach is mass conserving. Furthermore, concentrations can never become negative. Another important advantage of particle models compared to the numerical approach is that relevant subgrid details of the particle distribution can be obtained. A disadvantage of random walk models is that for long simulation periods in which case the particles are spread over a large area, many particles are required to obtain acceptable

results.

To combine the best of the two approaches we developed particle models to describe the dispersion process during the period shortly after the deployment of the pollutant. From a certain time, when the particles are spread over a large area and concentration gradient are small, we determine the concentration by solving the advection-diffusion equation numerically.

An advantage of stochastic modelling of dispersion in turbulent fluid flow not yet mentioned lies in its simplicity. It is a well-known fact that the advection-diffusion equation does only describe dispersion accurately if the diffusing particles have been in the flow longer than a Lagrangian time scale and they have spread to cover a distance that is a size larger than the largest scales of the turbulent fluid flow (Fisher et al., 1979). Using the particle concept, it is a relatively easy task to improve the particle model and to take into account more accurately certain characteristics of the turbulent motion. Within the Eulerian framework this tends to be very complicated and in general results in an additional set of partial-differential equations that has to be solved simultaneously with the advection-diffusion equation.

Random walk models have seldom been used for water pollution prediction problems. In the literature attention has been concentrated on the modelling of relative diffusion, i.e. the spreading of a single cloud of particles with respect to its center of mass (Van Dam, 1981; Dyke and Robertson, 1985; Jenkins, 1985). This provides us with important insight into the spreading of individual clouds of particles and into the variations between different realisations. It, however, does not directly produce the ensemble mean concentration, which is, for predictive purposes, the most important quantity.

Unlike in environmental hydraulics, particle models describing ensemble mean concentrations are often used to predict the dispersion of pollutants in the atmosphere. Van Dop et al. (1985) developed a one-dimensional random flight model to describe the particle displacements in inhomogeneous unsteady turbulent flows. More recently, an application of this model to predict dispersion in a convective boundary layer is discussed by De Baas et al. (1986). Our work is inspired by the ideas of Van Dop, Nieuwstadt, Hunt and De Baas and in this paper we generalize some of their one-dimensional vertical results to two horizontal dimensions. Furthermore, we introduce depth variations into the model to describe the dispersion in shallow water and discuss the various numerical aspects of the implementation. In section 2 we develop a random walk model that is consistent with the two-dimensional advection-diffusion equation. Here both the depth of the water as well as the dispersion coefficient is allowed to vary in space. To improve the behaviour of the model shortly after the deployment of the pollutant, we introduce in section 3 a random flight model. Furthermore, we show that our model has the correct asymptotic behaviour and for long simulation periods it is again consistent with the advection-diffusion equation. In section 4 the various numerical aspects of the implementation of the stochastic models are discussed. Finally in the sections 5 and 6 some numerical experiments and a realistic application to predict the dispersion of a pollutant in the Eastern-Scheldt estuary are discussed.

## 2 Random walk models

Consider a shallow water area with a depth  $H(x,y,t)$  and horizontal water velocities  $U(x,y,t)$  and  $V(x,y,t)$  in respectively the  $x$ - and  $y$ -directions. It is also assumed that  $H(x,y,t)$ ,  $U(x,y,t)$  and  $V(x,y,t)$  satisfy the continuity equation:

$$\frac{\partial H}{\partial t} + \frac{\partial(UH)}{\partial x} + \frac{\partial(VH)}{\partial y} = 0 \quad (1)$$

The deterministic background flow field  $[U(x,y,t) \ V(x,y,t)]^T$  and the water depth  $H(x,y,t)$  are usually determined by running a numerical hydrodynamic model.

To model dispersion in a shallow water area, we have developed a random walk model that is exactly consistent with the well-known depth integrated advection-diffusion equation (Fisher et al., 1979). In the following we first formulate the particle model and then we show that this model is indeed consistent with the advection-diffusion equation. Consider that the position  $(X_t, Y_t)$  of a particle injected in the water at time  $t=t_0$  at  $(X_{t_0}, Y_{t_0})$  is described by means of the following Itô stochastic differential equations:

$$dX_t = \left[ U + \left( \frac{\partial H}{\partial x} D \right) / H + \frac{\partial D}{\partial x} \right] dt + \sqrt{2D} d\alpha_t \quad (2)$$

$$dY_t = \left[ V + \left( \frac{\partial H}{\partial y} D \right) / H + \frac{\partial D}{\partial y} \right] dt + \sqrt{2D} d\beta_t \quad (3)$$

Here, as we will see,  $D(x, y)$  turns out to be the well-known dispersion coefficient and  $w_t = [\alpha_t \ \beta_t]^T$  is Brownian motion process with:

$$E\{dw_t \ dw_t^T\} = I \ dt \quad (4)$$

At a closed boundary a particle is reflected so there will be no transfer of mass through such a boundary.

To show that the model (2)-(4) is indeed consistent with the advection-diffusion equation we note that the stochastic process  $(X_t, Y_t)$  is Markov and that the probability function  $p(x, y, t)$ ,  $t \geq t_0$ , is determined by the Fokker-Planck equation (Jazwinski, 1970):

$$\begin{aligned} \frac{\partial p}{\partial t} = & -\frac{\partial}{\partial x} \left[ \left[ U + \left( \frac{\partial H}{\partial x} D \right) / H + \frac{\partial D}{\partial x} \right] p \right] - \frac{\partial}{\partial y} \left[ \left[ V + \left( \frac{\partial H}{\partial y} D \right) / H + \frac{\partial D}{\partial y} \right] p \right] \\ & + \frac{1}{2} \frac{\partial^2}{\partial x^2} (2Dp) + \frac{1}{2} \frac{\partial^2}{\partial y^2} (2Dp) \end{aligned} \quad (5)$$

with the initial condition:

$$p(x, y, t_0) = \delta(x - x_0) \delta(y - y_0). \quad (6)$$

The particle concentration  $C(x, y, t)$  is related to this probability function through:

$$C(x, y, t) = p(x, y, t) / H(x, y, t) \quad (7)$$

By substituting equation (7) into the Fokker-Planck equation (5), the advection-diffusion equation can be derived:

$$\frac{\partial(HC)}{\partial t} = -\frac{\partial(HUC)}{\partial x} - \frac{\partial(HVC)}{\partial y} + \frac{\partial}{\partial x}(DH \frac{\partial C}{\partial x}) + \frac{\partial}{\partial y}(DH \frac{\partial C}{\partial y}). \quad (8)$$

The initial condition for the concentration can be obtained similarly by substituting the equation (6) into equation (7). At a closed boundary the condition  $\partial C / \partial x = 0$  is used to model the fact that there is no transfer of pollutants through such a boundary.

We have now shown that the model (2)-(4) is consistent with the well-known advection-diffusion equation (8). As a consequence we can either solve the equation (8) numerically or simulate the stochastic equation (2)-(3) for many different particles.

The random walk model (2)-(3) can easily be modified to take into account mechanisms such as decay, sedimentation or evaporation. The statistical error introduced by the use of a finite number of particles can be approximated using a Poisson distribution with parameter  $n$  for the probability that  $k$  particles are located within a certain small area, where  $n$  is the number of particles that are actually found in this area after the simulation.

### 3 Random flight model

As noted in the introduction, the random walk model (2)-(4), and thus the advection-diffusion equation (8), does only describe the dispersion of particles in turbulent fluid flow accurately if they have been in the flow much longer than a certain Lagrangian time scale  $T_L$ . This time scale is a measure of how long the particle takes to lose memory of its initial turbulent velocity (Fisher et al., 1979). This shortcoming of the random walk model is caused by the fact that the driving noise in the stochastic differential equation (2)-(3) is modelled as a Brownian motion process and, as a consequence, has independent increments. For time scales  $\ll T_L$  it is however more realistic to assume that these increments are correlated in time: particles with a certain velocity at time  $t$  are likely to travel with approximately the same velocity at time  $t+\Delta t$ ,  $\Delta t \ll T_L$ . Therefore we have improved the random walk model (2)-(3) by introducing a random flight model that describes the position as well as the velocity of the particle at time  $t$ . We developed the model such that it is, for long simulation periods, again consistent with the advection-diffusion equation (8). In the following we first formulate this particle model and then we show that this model has indeed the correct asymptotic behaviour. Consider that the particle position and particle velocity are described by:

$$dX_t = [U + \sigma U_t + (\frac{\partial H}{\partial x} D)/H + \frac{\partial D}{\partial x}] dt, \quad (9)$$

$$dU_t = -(1/T_L)U_t dt + \gamma d\alpha_t, \quad (10)$$

$$dY_t = [V + \sigma V_t + (\frac{\partial H}{\partial y} D)/H + \frac{\partial D}{\partial y}] dt, \text{ and} \quad (11)$$

$$dV_t = -(1/T_L)V_t dt + \gamma d\beta_t. \quad (12)$$

Here  $U_t$  and  $V_t$  are the stochastic velocity of the particle in respectively the  $x$ - and  $y$ -directions induced by the turbulent fluid flow. Furthermore,  $\sigma$  is a space varying parameter,  $\gamma$  and  $T_L$  are constants and, as we will see,  $D = \frac{1}{2}(T_L \sigma \gamma)^2$  again turns out to be the well known dispersion coefficient. The spreading of the particles does not depend on  $\gamma$  and  $\sigma$  but only on the product  $\gamma\sigma$ . In practice usually  $D(x,y)$  and  $T_L$  are specified,  $\gamma$  is chosen to be 1 while  $\sigma(x,y)$  is determined using the relation between all these variables. The reason why we introduced the additional parameter  $\sigma$  is explained at the end of this section. The particle is injected at time  $t=t_0$ , at position  $(X_{t_0}, Y_{t_0})$  and with initial velocity  $(U_{t_0}, V_{t_0})$ .

By introducing the additional equations (10) and (12) for the turbulent velocities  $U_t$  and  $V_t$ , we in fact assume that the turbulence is isotropic and that the coloured noise processes  $U_t$  and  $V_t$  are both stationary with zero mean and with an exponential Lagrangian autocovariance:

$$E\{U_{t+\tau}U_t\} = E\{V_{t+\tau}V_t\} = \frac{1}{2}T_L\gamma^2 e^{-|\tau|/T_L} \quad (13)$$

The approach described above can easily be extended by introducing equations for the acceleration and third and higher order derivatives of the position. In this way the Lagrangian autocovariance of the velocity processes can be modelled more accurately and it becomes possible to take into account the characteristics of the turbulent fluid flow.

Over time periods much longer than  $T_L$ , i.e.  $t-t_0 \gg T_L$ , the model is again consistent

with the advection-diffusion equation (8), since for  $(t-t_0)/T_L \rightarrow \infty$  or  $T_L \rightarrow 0$  while D is constant, equations (9)-(12) reduce to the stochastic differential equations:

$$dX_t = \left[ U + \left( \frac{\partial H}{\partial x} D \right) / H + \frac{1}{2} \frac{\partial D}{\partial x} \right] dt + \sqrt{2D} d\alpha_t \quad (14)$$

$$dY_t = \left[ V + \left( \frac{\partial H}{\partial y} D \right) / H + \frac{1}{2} \frac{\partial D}{\partial y} \right] dt + \sqrt{2D} d\beta_t \quad (15)$$

The equations (14) and (15) have to be interpreted, in fact by definition, in the Stratonovich sense (Arnold, 1974). The corresponding Itô equations are given by the random walk model (2)-(3) and, as a consequence, the asymptotic model (14)-(15) is consistent with the advection-diffusion equation (8).

The random flight process is again Markovian and the probability function  $p(x,y,u,v,t)$  is determined by the Fokker-Planck equation:

$$\begin{aligned} \frac{\partial p}{\partial t} = & -\frac{\partial}{\partial x} \left[ [U + \sigma u + (\frac{\partial H}{\partial x} D) / H + \frac{\partial D}{\partial x}] p \right] - \frac{\partial}{\partial y} \left[ [V + \sigma v + (\frac{\partial H}{\partial y} D) / H + \frac{\partial D}{\partial y}] p \right] \\ & + \frac{\partial}{\partial u} \left( \frac{pu}{T_L} \right) + \frac{\partial}{\partial v} \left( \frac{pv}{T_L} \right) + \frac{1}{2} \frac{\partial^2}{\partial u^2} (yp) + \frac{1}{2} \frac{\partial^2}{\partial v^2} (yp) \end{aligned} \quad (16)$$

with initial condition:

$$p(x,y,u,v,t_0) = \delta(x-x_0)\delta(y-y_0) \frac{1}{\pi T_L \gamma^2} e^{-\frac{u^2+v^2}{T_L \gamma^2}}. \quad (17)$$

Here we have chosen the initial velocity distribution to be consistent with equation (13).

The particle concentration  $C(x,y,t)$  is given by:

$$C(x,y,t) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} p(x,y,u,v,t) du dv / H(x,y,t). \quad (18)$$

By introducing the moments:

$$\langle u \rangle(x,y,t) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} u p(x,y,u,v,t) du dv / H(x,y,t) \quad (19)$$

$$\langle v \rangle(x,y,t) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} v p(x,y,u,v,t) du dv / H(x,y,t) \quad (20)$$

$$\langle u^2 \rangle(x,y,t) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} u^2 p(x,y,u,v,t) du dv / H(x,y,t) \quad (21)$$

$$\langle v^2 \rangle(x,y,t) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} v^2 p(x,y,u,v,t) du dv / H(x,y,t) \quad (22)$$

we are able to derive from the Fokker-Planck equation (16) the following parabolic set of equations:

$$\frac{\partial(HC)}{\partial t} = -\frac{\partial(HUC)}{\partial x} - \frac{\partial(HVC)}{\partial y} - \frac{\partial}{\partial x}(H\sigma) - \frac{\partial}{\partial y}(H\sigma<v>) \quad (23)$$

$$\frac{\partial(H<u>)}{\partial t} = -\frac{\partial}{\partial x}(H\sigma<u^2>) - H<u>/T_L \quad (24)$$

$$\frac{\partial(H<v>)}{\partial t} = -\frac{\partial}{\partial y}(H\sigma<v^2>) - H<v>/T_L \quad (25)$$

$$\frac{\partial(H<u^2>)}{\partial t} = -2H<u^2>/T_L + H\gamma^2 C \quad (26)$$

$$\frac{\partial(H<v^2>)}{\partial t} = -2H<v^2>/T_L + H\gamma^2 C \quad (27)$$

The particle concentration can be determined by solving the closed set of partial-differential equations (23)-(27).

We have shown above that the random flight model (9)-(12) is consistent with the set of equations (23)-(27). This illustrates one of the advantages of stochastic modelling of dispersion. While the random flight model (9)-(12) can be implemented very simply, it is not an easy task to solve the corresponding set of partial-differential equations numerically.

Taking the limit  $T_L \rightarrow 0$ , while  $D = \frac{1}{2}(T_L\sigma\gamma)^2$  is constant, the set of equations (23)-(27) reduce to the advection-diffusion equation (8) and again we have shown that for  $t-t_0 \gg T_L$  the random flight model is consistent with this equation.

The non-linear equation (8) as well as the set of non-linear equations (23)-(27) cannot in general be solved analytically. However in the absence of the background flow it is possible to determine analytical solutions for the linearised case. Studying these approximate solutions is important to develop insight into the behaviour of the model shortly after the deployment of the particles. It is a well-known fact that for the linear random walk model the variance of the position of a particle at time  $t$ , released at time  $t_0$ , is  $2D(t-t_0)$  (Taylor, 1921). It is easy to show that using the linear random flight model, the variance of a particle released with a Gaussian initial velocity with zero mean and variance  $\frac{1}{2}T_L\gamma^2$  is, shortly after the deployment  $D(t-t_0)^2$ . For long simulation periods the behaviour of the random flight model is similar to that of the random walk model.

Finally we note that, if necessary,  $T_L$  and  $\gamma$  are allowed to vary in space. However, in this case it is not possible to derive a closed set of partial-differential equations for the moments of the probability function  $p(x,y,u,v,t)$ . The resulting set of equations is infinite and we are faced with a closure problem. This is in fact the reason why we have introduced the parameter  $\sigma(x,y)$  into the model (9)-(12) and, in addition, have chosen  $\gamma$  to be constant such that  $D=0.5(T_L\sigma\gamma)^2$ . In this case it becomes possible to derive a closed set of partial-differential equations for the moments of  $p(x,y,u,v,t)$  and to avoid the closure problem (or to solve it implicitly).

#### 4 Numerical approximation

The stochastic differential equations (2)-(3) or (9)-(12) cannot in general be solved analytically and have to be integrated numerically (Kloeden and Platen, 1989). In this section we only consider the random walk model since the numerical approximation of the random flight model does not give rise to new conceptual problems. Defining a fixed mesh  $\{t_i=t_0+i\Delta t, i=1,2,\dots\}$ , the simplest Euler scheme for the random walk model con-

sistent with the Itô definition of a stochastic integral is:

$$\bar{X}_{t_{k+1}} = \bar{X}_{t_k} + \left[ U + \left( \frac{\partial H}{\partial x} D \right) / H + \frac{\partial D}{\partial x} \right] \Delta t + \sqrt{2D} \Delta \alpha_k , \quad (28)$$

$$\bar{Y}_{t_{k+1}} = \bar{Y}_{t_k} + \left[ V + \left( \frac{\partial H}{\partial y} D \right) / H + \frac{\partial D}{\partial y} \right] \Delta t + \sqrt{2D} \Delta \beta_k . \quad (29)$$

Here  $\bar{X}_{t_k}$  and  $\bar{Y}_{t_k}$  are the numerical approximations of  $X_t$  and  $Y_t$  respectively, while  $\bar{X}_{t_0} = X_{t_0}$  and  $\bar{Y}_{t_0} = Y_{t_0}$ . Furthermore,  $\Delta \alpha_k$  and  $\Delta \beta_k$  are Gaussian with zero mean and variance  $\Delta t$ . Each time step  $\Delta \alpha_k$  and  $\Delta \beta_k$  are determined using a random generator. It can be shown that for the Euler scheme (28)-(29) we have (Pardoux and Talay, 1985):

$$E\{(\bar{X}_{t_k} - X_{t_k})^2\} = O(\Delta t) , \quad (30)$$

$$E\{(\bar{Y}_{t_k} - Y_{t_k})^2\} = O(\Delta t) . \quad (31)$$

Rumelin (1982) showed that it is very hard to obtain higher order schemes for non-linear stochastic differential equations. In the one-dimensional case he showed that efficient integration schemes of  $O(\Delta t^2)$  can be obtained. To obtain this order of accuracy one can take the Milstein scheme. However, in the multi-dimensional case Rumelin showed that, in general ( $D$  both a function of  $x$  and  $y$ ), it is very hard to construct a scheme that has a higher order of convergence than the Euler scheme. Therefore, we use this scheme to approximate the stochastic part of the random walk model.

Since in most practical problems the spatial variation of  $D$  is small, the Euler scheme, is, with respect to the stochastic part of the differential equation, sufficiently accurate and allows a large time step. It is however the deterministic drift that usually causes numerical problems. In case the background flow strongly varies in space and time we have to use a small time step or a more accurate numerical scheme.

As noted before, the back ground flow is usually computed by means of a hydrodynamic numerical model. Therefore  $U$ ,  $V$  and  $H$  are only available at the grid points. However, if we want to solve the random walk model, these quantities have to be known at every position and we are faced with an interpolation problem. Despite the fact that the finite difference scheme used to solve the hydrodynamic equations may be mass conserving, a straightforward bilinear or higher order interpolation procedure will not conserve mass. As a consequence the interpolation procedures create sources and sinks that respectively repulse and attract particles. In instationary conditions the numerical errors created by the interpolation are different at each time step and appear to have a random character. As a consequence, in such cases these errors are masked by the random term in the model and serious problems are not likely to occur. However in stationary conditions and if, in addition, the random term is very small, we expect numerical artefacts. Particles may, e.g., be "caught" by a numerically introduced sink. To eliminate these numerical problems in stationary conditions we propose an interpolation procedure that is based on fitting a quadratic streamfunction  $\Psi$ . Furthermore, to avoid numerical problems involving the integration of the back ground flow, we integrate this deterministic part of the particle model analytically.

## 5 Numerical experiments

In this section we describe some simple experiments to show that the particle models (2)-(3) and (9)-(12) have the correct asymptotic behaviour. Moreover, we illustrate the numerical problems described in section 4. We consider a simple square reservoir with a length of 25 km. We start the simulations at time  $t_0$  using the random flight model with

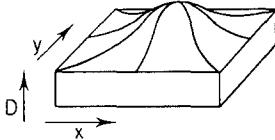


Figure 1

**Figure 1.** Space-varying dispersion coefficient

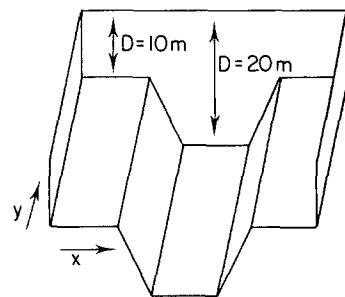


Figure 2

**Figure 2.** Space-varying depth of the water

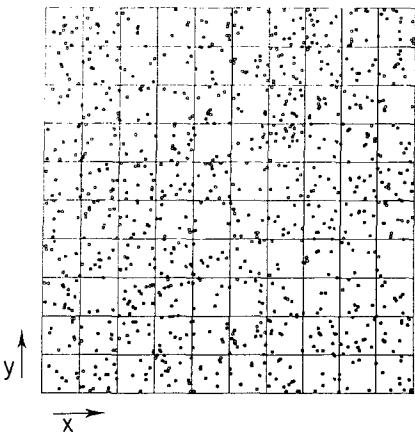


Figure 3

**Figure 3.** Asymptotic particle distribution using the random walk model

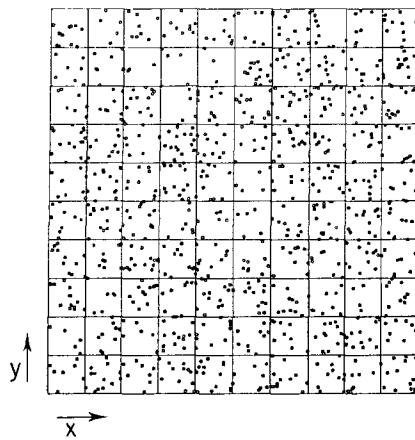


Figure 4

**Figure 4.** Asymptotic particle distribution using the random flight model

1000 particles at the middle of the reservoir and with zero initial velocity.

### 5.1 Experiment 1

We neglected the background flow and took the depth  $H=10m$ . The dispersion coefficient was chosen to vary in space (see Figure 1). For the random flight model we, in addition, chose  $T_L=5$  hours. In this case it is easy to show that the particle distribution will have to become uniform for sufficiently large simulation times. In the Figures 3 and 4 the particle distribution is drawn after 800 time steps of 30 min. for respectively the random walk model and the random flight model, showing the correct asymptotic behaviour. Such behaviour can easily be verified more objectively by using the fact that if the particle distribution is uniform, the number of particles in one small square of Figure 3 or 4 should be Poisson distributed with parameter  $10 = (\text{total number of particles}) \times (\text{volume of the reservoir}) / (\text{volume of the small square part of the reservoir})$ . By counting the number of particles in all the small squares and by comparing the results with a

**Table 1.** The probability to find  $k$  number of particles in a small square of the Figures 3 and 4 using a Poisson distribution compared with the actual number of small squares where  $k$  particles are found in these figures

number of particles $k$ in one small square	probability to find $k$ particles in a small square using a Poisson distribution with parameter 10	relative number of small squares where $k$ particles are found in Figure 3	relative number of small squares where $k$ particles are found in Figure 4
3	0.01	-	0.02
4	0.02	0.04	0.02
5	0.04	0.03	0.06
6	0.06	0.09	0.02
7	0.09	0.06	0.08
8	0.11	0.12	0.11
9	0.13	0.13	0.16
10	0.13	0.13	0.14
11	0.11	0.09	0.07
12	0.09	0.07	0.08
13	0.07	0.09	0.09
14	0.05	0.04	0.06
15	0.03	0.05	0.04
16	0.02	0.04	0.02
17	0.01	0.01	-
18	0.01	0.01	0.02

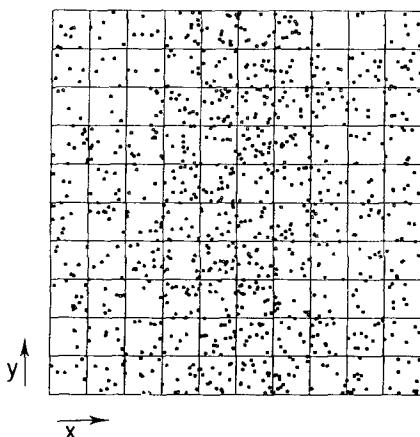


Figure 5

**Figure 5.** Asymptotic particle distribution in case of a space-varying depth

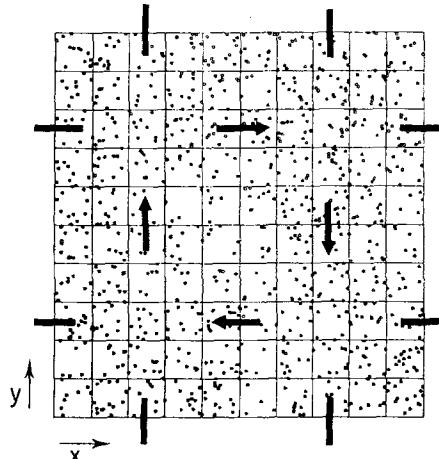


Figure 6

**Figure 6.** Asymptotic particle distribution using a stream function interpolation and an analytic integration of the background flow

Poisson distribution it has been verified that the asymptotic particle distribution is indeed uniform (see Table 1).

### 5.2 Experiment 2

We now introduce a space varying depth (see Figure 2). In this case the number of particles observed in a certain area will have to become, for sufficient large simulation times, linearly dependent with the depth of the water. In Figure 5 the particle distribution is

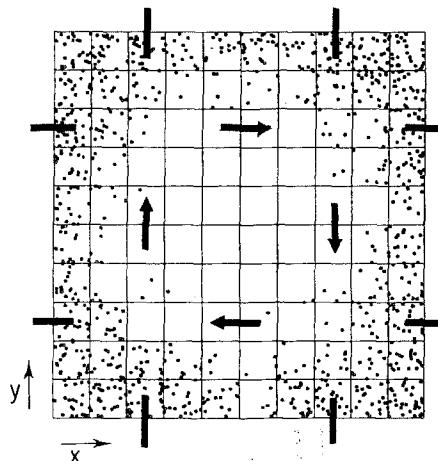


Figure 7a

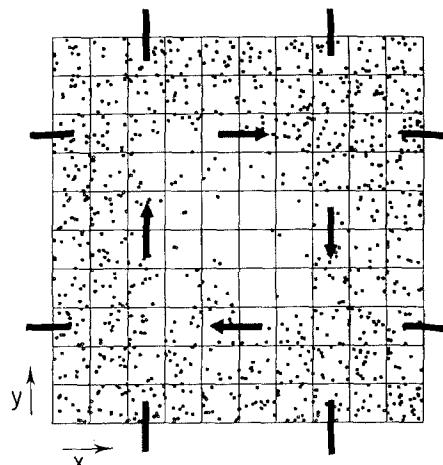


Figure 7b

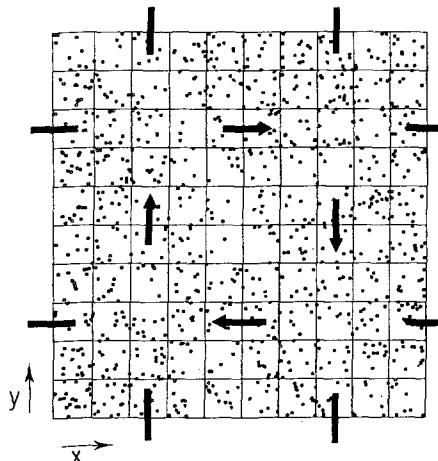


Figure 7c

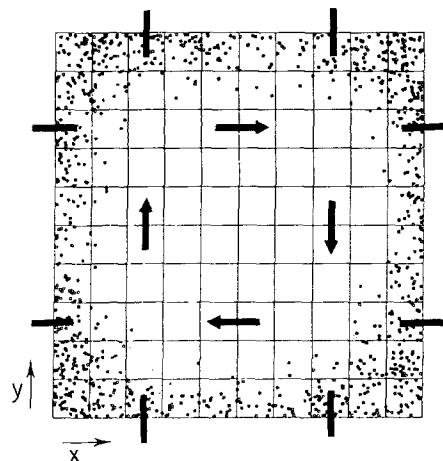


Figure 8

**Figure 7.** Asymptotic particle distribution using a stream function interpolation and an Euler scheme to integrate the background flow: (a)  $\Delta t=30$  min.; (b)  $\Delta t=5$  min.; (c)  $\Delta t=1$  min

**Figure 8.** Asymptotic particle distribution using bilinear interpolation and an Euler scheme with  $\Delta t=1$  min. to integrate the back ground flow

drawn after 800 time step of 30 min., again showing the correct behaviour. In the area where the depth  $H=10$  m (the sides) the averaged number of particles in a small square of Figure 5 should be  $7.14 = (\text{total number of particles}) \times (\text{volume of the reservoir}) / (\text{volume of the small squary part of the reservoir})$ , while in the area where  $H=20$  m (the central part) this number should be 14.28. From Figure 5 we find respectively 7.35 and 14.10 for these numbers.

### 5.3 Experiment 3

Let us now consider the case of a depth  $H = 10$  m and a dispersion coefficient  $D=10m^2/s$  and let us introduce a constant background flow at the grid points of a space staggered grid. The chosen background flow satisfies the discretised continuity equation. In this

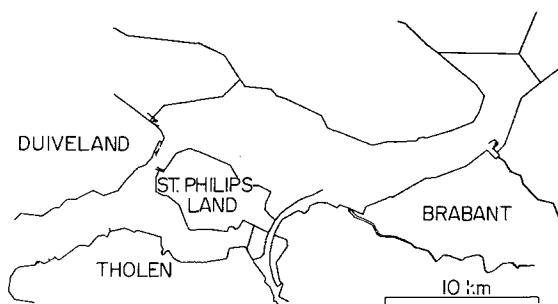


Figure 9. Keeten-Volkerak, a part of the Eastern Scheldt estuary

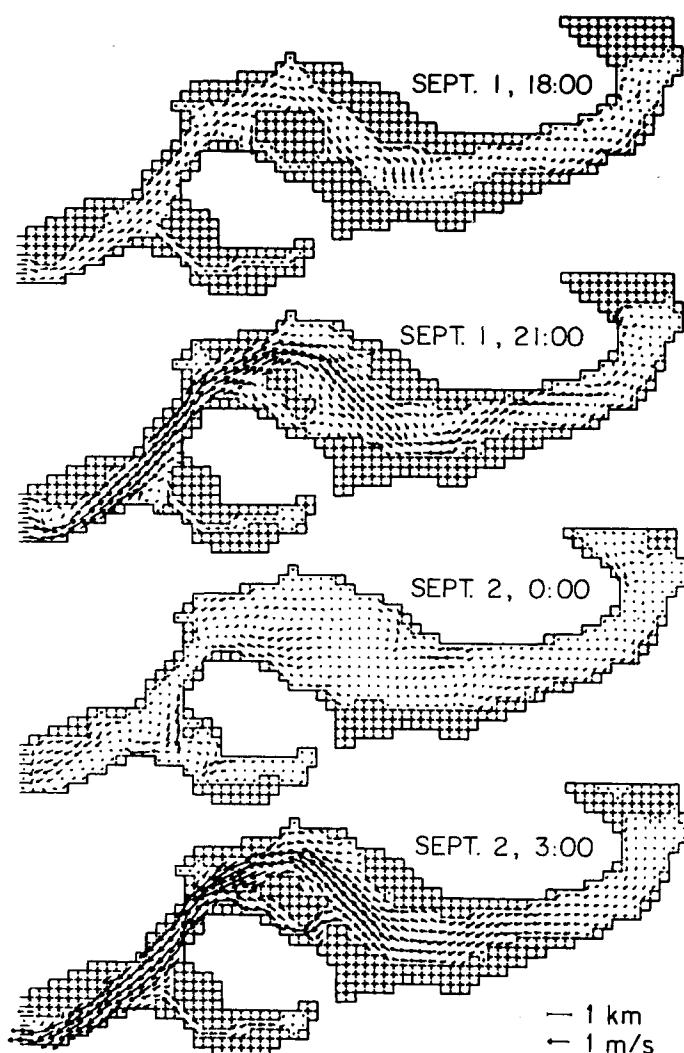
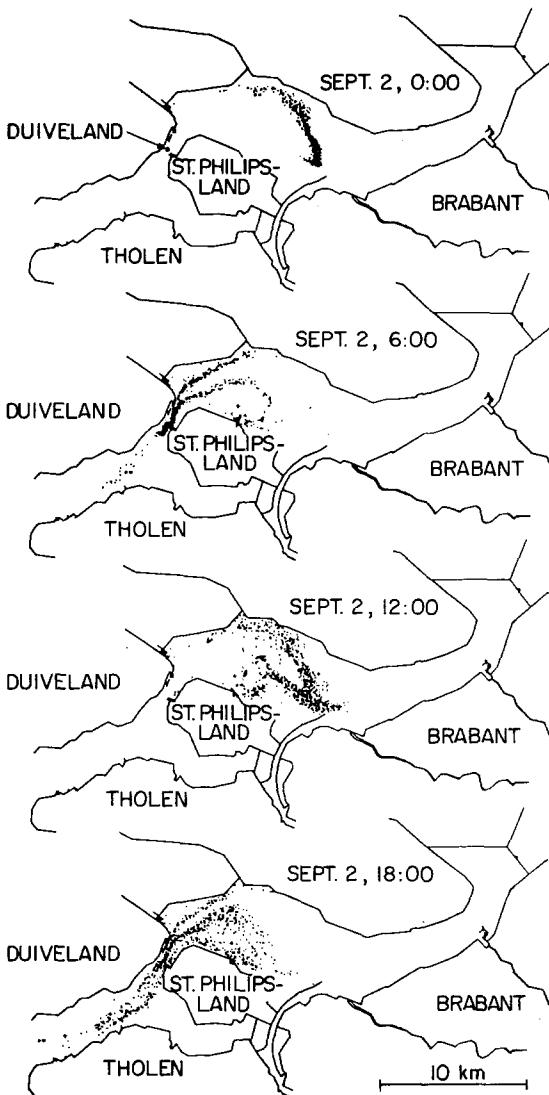


Figure 10. Tidal flow patterns in the Keeten-Volkerak model



**Figure 11.** Simulation of a calamity in the Keeten-Volkerak. The arrow in the first figure indicates the location where the pollutants was released in the water at 18:00, September 1, 1975

case the particle distribution should again become uniform. In the Figures 6-8 we show the results of the random walk model after 400 hours for a number of different interpolation and integration methods. Here the dark lines represent the grid points where the velocity normal to the closed boundary is zero, while the arrays indicate the grid points where the background flow is prescribed. Figure 6 illustrates that using a streamfunction interpolation method and integrating the background flow analytically, the correct behaviour is observed: the particle distribution appears to be uniform. Here we note that in this experiment it is not our intention to verify this again in an objective sense, but we concentrate our attention on the various numerical problems that might occur. Using a numerical integration scheme instead of integrating the background flow analytically, we see from Figure 7 that the time step has to be very small to reduce the outward drift that is introduced by the numerical integration scheme. Choosing a time step of 5 or 30

minutes, the asymptotic particle distribution is far from uniform. With a time step of 1 minute, the numerical errors introduced by the numerical integration scheme are very small and negligible with respect to the random forcing and the particle distribution appears to be uniform again. Finally we see in Figure 8 that using bilinear interpolation instead of a stream function interpolation method, the sources and sinks that are created numerically have a dramatical effect on the asymptotic particle distribution, that should again be uniform.

## 6 Application

In this section we describe a realistic application of the random walk model (2)-(3) in the Keeten-Volkerak, a part of the Eastern Scheldt estuary in the south western part of the Netherlands (Figure 9). The tidal back ground flow is determined using a numerical model with a grid size of 400 m and a time step of 1.25 min. The tidal flow at the grid points of the model during one tidal cycle are shown in Figure 10. Here the dotted lines indicate the area that is above the water-level. This area is not permanently dry but may be flooded in case of high water. Since the tidal movement in the Eastern Scheldt is not stationary, it is possible to use bilinear interpolation to obtain the water velocity and depth at arbitrary position. Furthermore, to approximate the drift of the stochastic differential equation, we employ the mid point rule, a second order iterative scheme, with time step  $\Delta t=1.25$  min. The dispersion coefficient was in this case chosen to be  $D=1m^2/s$ . For a discussion on the choice of the dispersion coefficient the reader is referred to Van Dam (1981). The results of particle dispersion can be found in Figure 11. Here 1000 particles are released at Zijpe at low water at  $t_0=18:00$ , September 1, 1975. The particle distribution is shown each 6 hours until 18:00, September 2, 1975. One of the main reason to use a particle model in this application is to avoid the numerical problems that occur when the advection-diffusion equation is solved numerically in case of high concentration gradients. From the results shown in Figure 11 we see that the spatial concentration variations remain very high during a number of tidal cycles. As a consequence, an Eulerian approach is not able to produce acceptable results in this case (Van Stijn et al., 1988). Furthermore, the spreading of the pollutant is too complex to employ a simple analytical approximation to model the spreading during a period shortly after the release of the pollutant. Therefore, we preferred the particle model.

## 7 Conclusions

In this paper we developed a number of particle models to describe the dispersion of pollutants in shallow water. By deriving the Fokker-Planck equation, it is possible to compare the Lagrangian models with their Eulerian equivalent. The various numerical problems of the implementation have been discussed and illustrated with some simple experiments. Finally a realistic application of one of the particle models is described.

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