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paper to appear in the proceedings
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ABSTRACT

To predict the dispersion of pollutants in shallow water in case of a calamity one can adopt an Eulerian point of view and solve the well-known two-dimensional advection-diffusion equation numerically or one can use a stochastic Lagrangian particle model. The Lagrangian approach is mass conserving, while concentrations can never become negative. However, for long simulation periods many particles are required to obtain acceptable results. To combine the best of the two approaches we developed in this paper a particle model that is exactly consistent with the general advection-diffusion equation and use this stochastic model only to describe the spreading of the pollutant during the period short after the calamity. From a certain time, when the particles are spread over a large area we determine the concentration and solve the advection-diffusion equation numerically by means of an ADI/FEM-scheme.

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 pollutants are required in taking adequate arrangements. 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 exactly mass conserving or may introduce negative concentrations in case of steep gradients. Since in practice the initial concentration is usually a delta-like function, we may expect serious problems (Van Stijn, Praagman and Van Eijkeren 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 is exactly 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 (Heemink 1989). This stochastic approach is mass conserving, while concentrations can never become negative. Furthermore, relevant subgrid details of the particle distribution can be obtained. Another important advantage of stochastic modelling of dispersion in turbulent fluid flow lies in its simplicity. It is well-known that the advection–diffusion equation does only describe dispersion accurately if the diffusing particles have been in the flow longer than a Langrangian 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 (Heemink 1989). Within the Eulerian framework this tends to be more complicated and in general results in an additional set of partial-differential equations that has to be solved numerically together with the advection–diffusion equation (closure problem). A disadvantage of random walk models is that for long simulation periods the particles are spread over a large area and many particles are required to obtain acceptable results.

To combine the best of the two approaches we develop a particle model to describe the dispersion process during the period short after the deployment of the pollutant. From a certain time, when the particles are spread over a larger area we determine the concentration and solve the advection–diffusion equation numerically using an unconditionally stable ADI/FEM scheme. In section 2 we describe our random walk model and show that it is exactly consistent with the two–dimensional advection–diffusion equation. Here both the depth of the water as the dispersion coefficient is allowed to vary in space. In section 3 the ADI/FEM scheme is introduced. Finally in section 4 realistic applications of the approach to predict the dispersion of pollutants in the Eastern Scheldt estuary and in the North Sea are discussed.

2. RANDOM WALK MODEL

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. H, U and V are assumed to satisfy the continuity equation:

$$\frac{\partial H}{\partial t} + \mathrm{div}\ (\underline{U}H) = 0 \qquad (1)$$

The deterministic background flow field $\underline{U} = [U \quad V]^T$ and the water depth H are usually determined by running a numerical hydrodynamic model.

To model dispersion in a shallow water area, we describe the position $\underline{X}_t = (X_t, Y_t)$ of a particle injected into the water at time $t=t_0$ at (X_{t_0}, Y_{t_0}) by means of the following Itô stochastic differential equation (Arnold 1974):

$$d\underline{X}_t = \left[\underline{U} + (D \text{ grad } H)/H + \text{grad } D\right] dt + \sqrt{2D}\, d\underline{\omega}_t \tag{2}$$

Here D(x,y) is the dispersion coefficient and $\underline{\omega}_t$ is a Brownian motion process with:

$$E\{d\underline{\omega}_t \, d\underline{\omega}_t^T\} = I \, dt \tag{3}$$

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

Since the stochastic process $\underline{X}_t$ is Markov, the probability p(x,y,t) to find a particle at time $t \geq t_0$ at position (x,y) is determined by the Fokker-Planck equation (Jazwinski 1970):

$$\frac{\partial p}{\partial t} = - \text{div} \left(\left[\underline{U} + (D \text{ grad } H)/H + \text{grad } D\right] p \right) + \text{div grad } (Dp) \tag{4}$$

whereas the initial condition is given by:

$$p(x,y,t_0) = \delta(x-x_0)\delta(y-y_0) \tag{5}$$

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

$$c = p/H \tag{6}$$

By substituting equation (6) into the Fokker-Planck equation (4), the advection-diffusion equation can be derived:

$$\frac{\partial Hc}{\partial t} = - \text{div } (\underline{U}Hc) + \text{div } (D \text{ grad } c) \tag{7}$$

The initial condition for the concentration can be obtained similarly by substituting the equation (5) into equation (6). At a closed boundary the condition $\partial c/\partial n=0$ is used.

We have shown that the model (2)-(3) is consistent with the well-known advection-diffusion equation (7). As a consequence we can either solve the equation (7) numerically or simulate the stochastic equation (2) for many different particles.

The random walk model 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.

The stochastic differential equation (2) cannot in general be solved analytically and has to be integrated numerically. Defining a fixed mesh $\{t_i=t_0+i\Delta t,\ i = 1, 2, \dots\}$, the simplest Euler scheme for the random walk model consistent with the Îto definition of a stochastic integral is:

$$\underline{\bar{X}}_{t_{k+1}} = \underline{\bar{X}}_{t_k} + \left[\underline{U} + (D \text{ grad } H)/H + \text{grad } D\right]\Delta t + \sqrt{2D}\,\Delta\underline{\omega}_k \qquad (8)$$

Here $\underline{\bar{X}}_t$ is the numerical approximation of $\underline{X}_t$, while $\underline{\bar{X}}_{t_0}=\underline{X}_{t_0}$. Furthermore, $\Delta\underline{\omega}_k$ is Gaussian with zero mean and variance $I\Delta t$. Each time step $\Delta\underline{\omega}_k$ is determined using a random generator. It can be shown that for the Euler scheme (8) we have (Talay and Pardoux 1985):

$$E\{\|\underline{\bar{X}}_{t_k}-\underline{X}_{t_k}\|^2\}=O(\Delta t) \qquad (9)$$

Rümelin (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 in general the best integration scheme that can be obtained is $O(\Delta t^2)$ in the sense of equation (9). To obtain this order of accuracy one can take the Milshtein scheme. However, in the multi-dimensional case Rümelin showed that in general (D both a function of x and y) it is impossible 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. Therefore we employ a second order midpoint rule to approximate this drift.

The back ground flow is usually computed by means of a numerical model. Therefore U, V and H are only available at 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. A straightforward bilinear or higher order interpolation procedure will not conserve mass. As a consequence these interpolation procedures create sources and sinks that respectively repulse and attracts particles. In instationary conditions and if the stochastic part of the random walk model is sufficiently strong, both the numerical error in the interpolation and the error introduced by the integration scheme have a random character. As a consequence, 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 the random term is small, we expect numerical artefacts. Particles may, e.g., be "caught" by a numerically introduced sink. To eliminate these problems in stationary conditions we propose an interpolation procedure that is based on fitting a streamfunction.

3. ADI/FEM METHOD

As noted before, in practice accidents are modelled by a delta-like source function. Most Eulerian methods for solving the advection-diffusion equation (7) are not suited for resolving such steep gradients. Even after the evolution of a point source for some time calculated with a strict Lagrangian method, the gradients in the concentration profile are still large with respect to the grid used. In Van Stijn, Praagman and Van Eijkeren (1987) it was shown that if the profile is confined to a few grid meshes, only a small number of methods satisfy practical demands like accuracy, effectiveness and non-negativeness. This last property is especially important in case of chemical or biological interactions.

Usually schemes are tested on problems with an exact description of the velocity field. However, if equations of motion are introduced for both velocities and waterlevel it is important to take care that its discretization and that of the advection-diffusion equations are compatible. In the Netherlands the WAQUA package is widely used for the simulation of shallow water flow. These non-linear equations are solved with an efficient composite ADI-technique (Stelling 1983) which is almost marginally and unconditionally stable. To comply with this technique an ADI time splitting is chosen for the advection-diffusion part as well. In Van Stijn and Praagman (1988) it is shown that for this predominantly hyperbolic equation it is necessary to use a Finite Element approach for the spatial approximation. This is indicated as follows. For the sake of simplicity only the advective part of (7) will be treated. Denote the operators Λ_x and Λ_y by:

$$\Lambda_x = \tfrac{1}{2}\,\Delta t\,\frac{\partial U\bullet}{\partial x} \quad , \quad \Lambda_y = \tfrac{1}{2}\,\Delta t\,\frac{\partial V\bullet}{\partial y} \ . \tag{10}$$

Then for constant $\underline{U}$ and H and for D=0 the ADI time-splitting of equation (7) can be written in the two stages:

$$(1 + \Lambda_x)\,\tilde{c} = (1 - \Lambda_y)\,c^n, \qquad (1 + \Lambda_y)\,c^{n+1} = (1 - \Lambda_x)\,\tilde{c}, \tag{11}$$

where $\tilde{c}$ is an intermediate function and $c^n(x,y) = c(x,y,t_n)$.

From this point the spatial discretization can be performed by applying the Galerkin Finite Element Method, using a Cartesian combination of linear basis functions φ for c, viz.

$$c^n(x,y) = \sum_{i,j} c^n_{i,j}\,\varphi_i(x)\varphi_j(y). \tag{12}$$

This yields the following approximation for the first stage of (11)

$$\begin{aligned}\frac{\Delta x}{6}\left[\tilde{c}_{i-1,j} + 4\tilde{c}_{i,j} + \tilde{c}_{i+1,j}\right] + U\,\frac{\Delta t}{4}\left[\tilde{c}_{i+1,j} - \tilde{c}_{i-1,j}\right] &= \\ \frac{\Delta y}{6}\left[c^n_{i,j+1} + 4c^n_{i,j} + c^n_{i,j-1}\right] - V\,\frac{\Delta t}{4}\left[c^n_{i,j+1} - c^n_{i,j-1}\right]&\end{aligned} \tag{13}$$

It can be proved that this Galerkin procedure attains the highest degree of accuracy if the stencil is limited to five grid points. Equation (13) shows that the coefficients of the time derivative have been distributed in space in accord with the ADI structure, which means that the three-diagonal structure of the ADI matrix is not distroyed. Moreover, the usual mass matrix from the Finite Element Method (FEM) is recovered. In many applications, especially in structural dynamics this mass matrix is lumped (i.e. diagonalized) without loss of accuracy. However, in case of the present hyperbolic equation, lumping can degradate the accuracy of the FEM approach substantially. In fact this causes the usual ADI method to be produced, which brings about high wavenumber oscillations. The phase properties of the ADI/FEM method, as given in (13), are such that only relative few $2\Delta x$ spurious oscillations emerge. This makes the method not positive. A mass conserving Forester filter, that selectively smoothes out the $2\Delta x$ waves is able to make the method almost non-negative. Due to the symmetry in the two stages of (13) the ADI/FEM method is unconditionally stable for the Cauchy initial value problem.

4. APPLICATIONS

In this section we describe realistic applications of our approach in the Eastern Scheldt estuary and in the North Sea. The tidal back ground flows are determined using WAQUA models of the Eastern Scheldt and the Continental Shelf respectively. Since the tidal movement is not stationary, it is possible to use bilinear interpolation for the particle models to obtain the water velocity and depth at arbitrary position. The results of the application in the Eastern Scheldt estuary can be found in the figures 1–5. Here

1000 particles are released at Zijpe at t_0 = 18:00, September 1, 1975. The particle distribution is shown each 6 hours. After 24 hours the distribution of the particles is sufficiently smooth and the dispersion process can be simulated using the ADI/FEM method. A similar application in the North Sea can be found in the figures 6–9. The Continental Shelf model used to determine the tidal movement is shown in figure 6. Here 1000 particles are released near the coast of Belgium at t_0 = 00:00, March 14, 1976. After nine days the concentration is determined and the ADI/FEM method is used to continue the simulation.

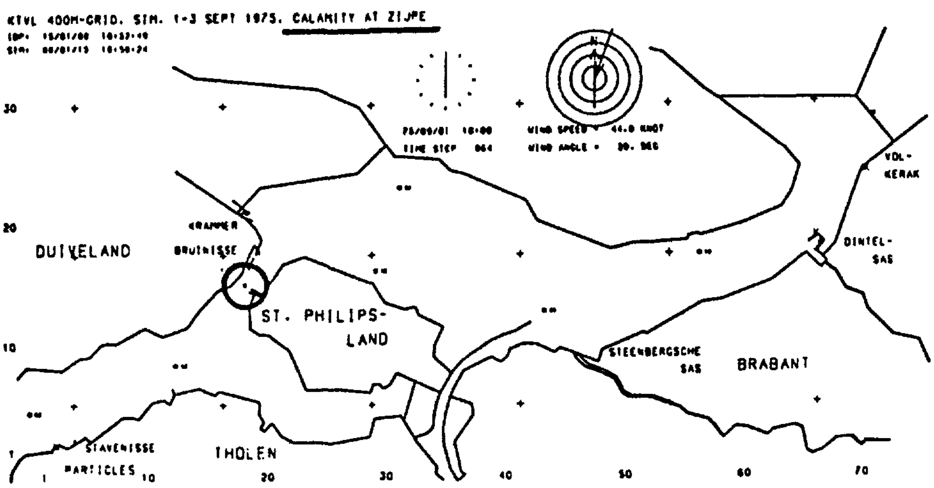

Figure 1: The Eastern Scheldt model

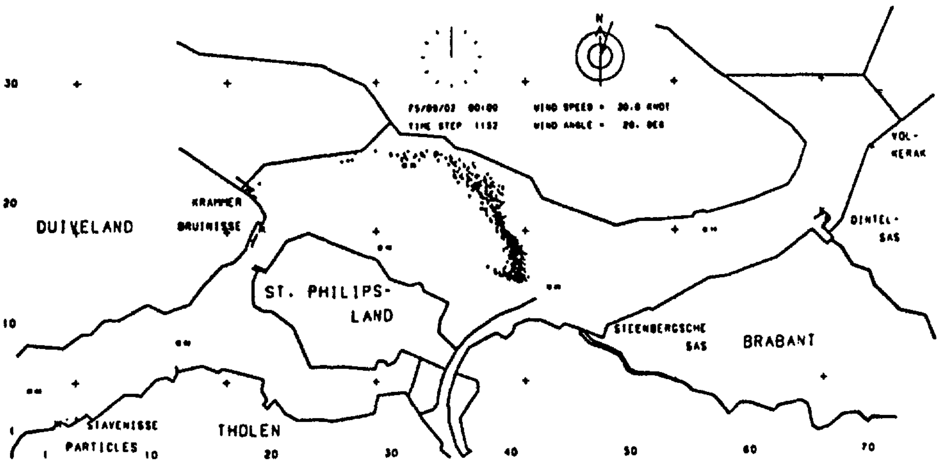

Figure 2: The particle distribution 6 hours after the calamity

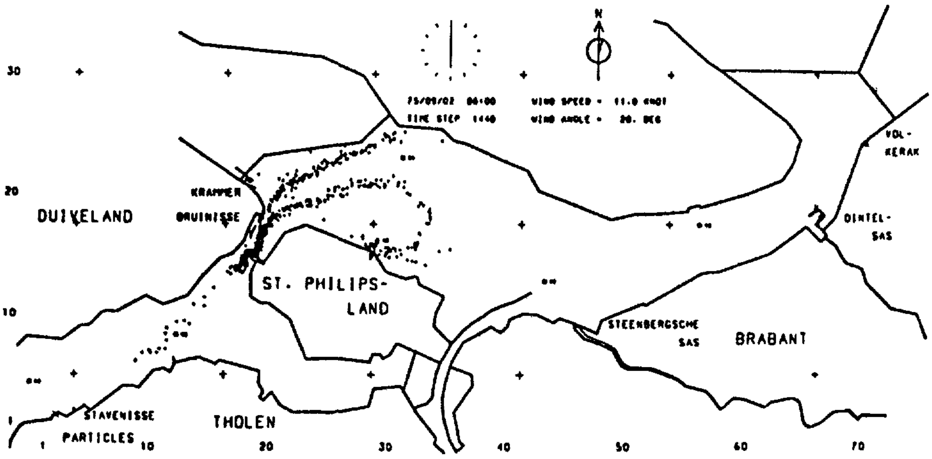

Figure 3: The particle distribution 12 hours after the calamity

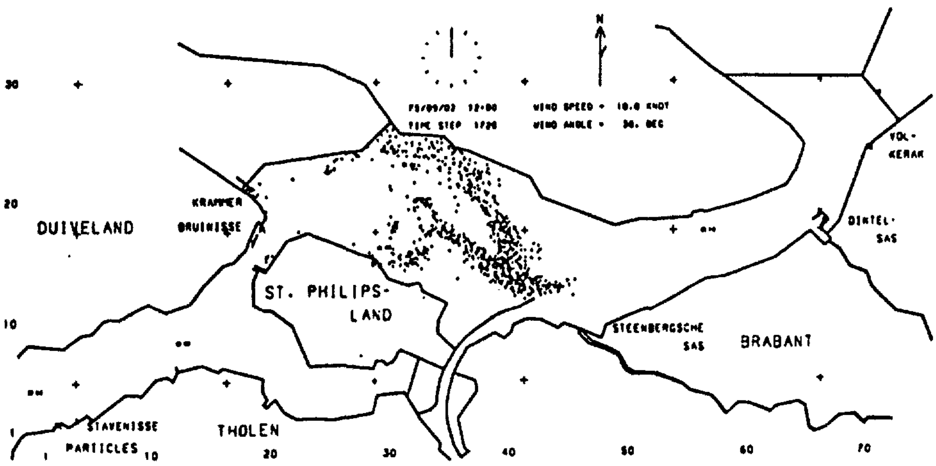

Figure 4: The particle distribution 18 hours after the calamity

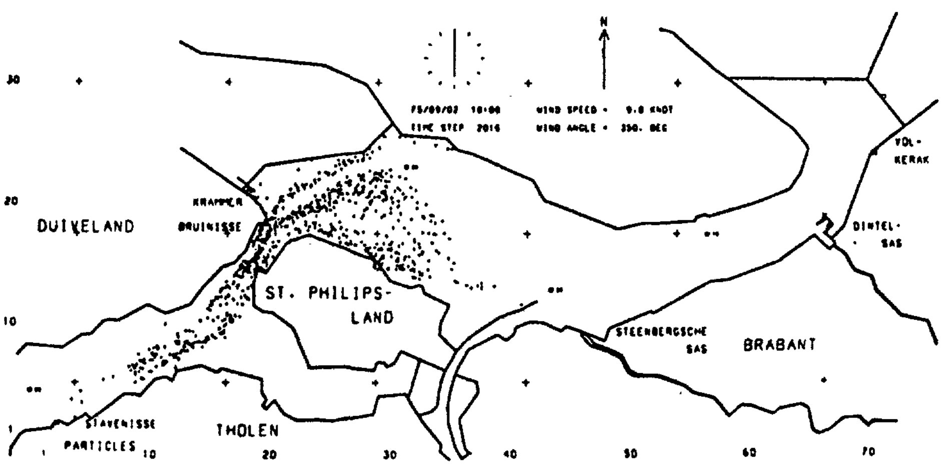

Figure 5: The particle distribution 24 hours after the calamity.

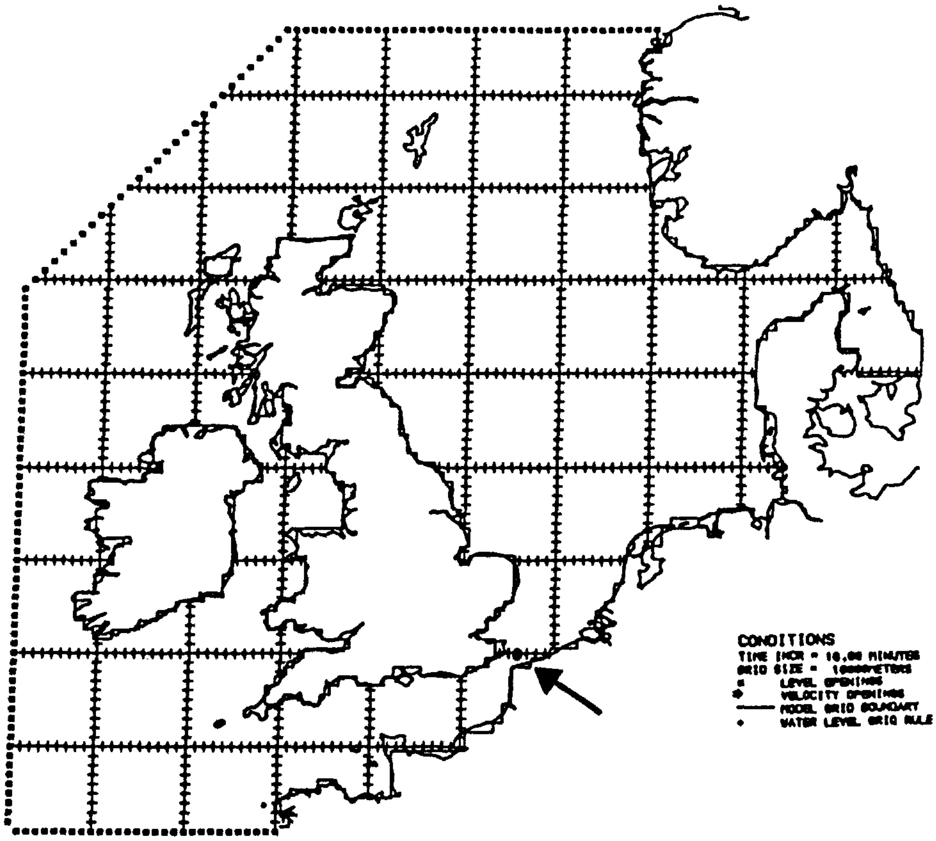

Figure 6: The Continental Shelf model

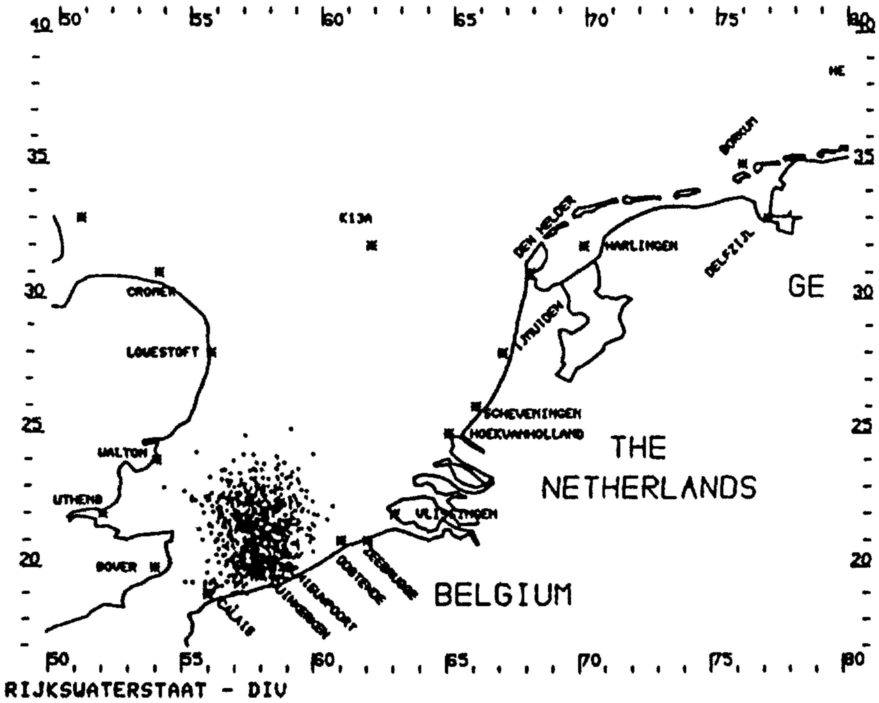

Figure 7: The particle distribution 9 days after the calamity

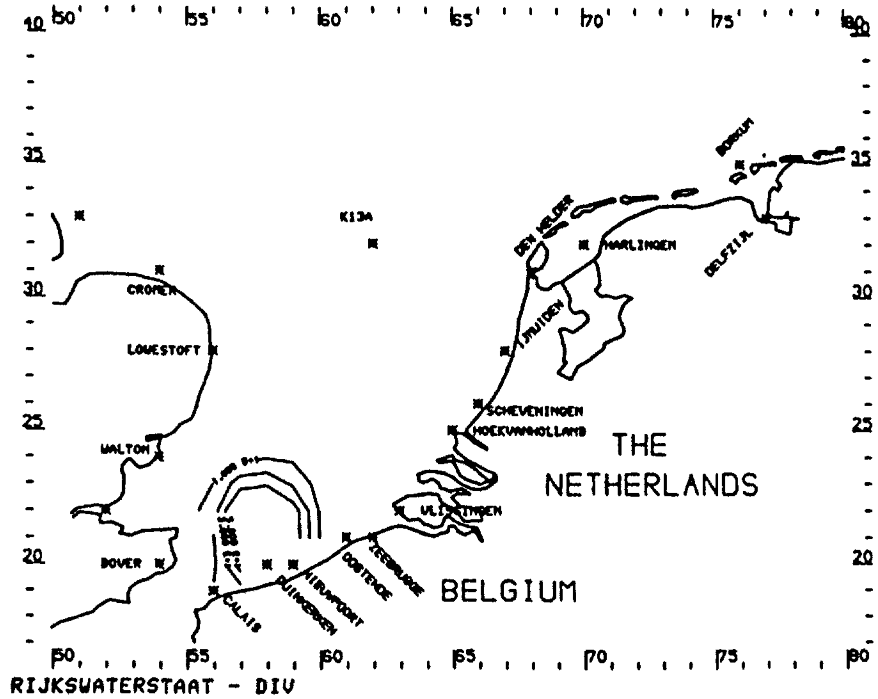

Figure 8: The concentration of the pollutant determined from the particle distribution shown in figure 7

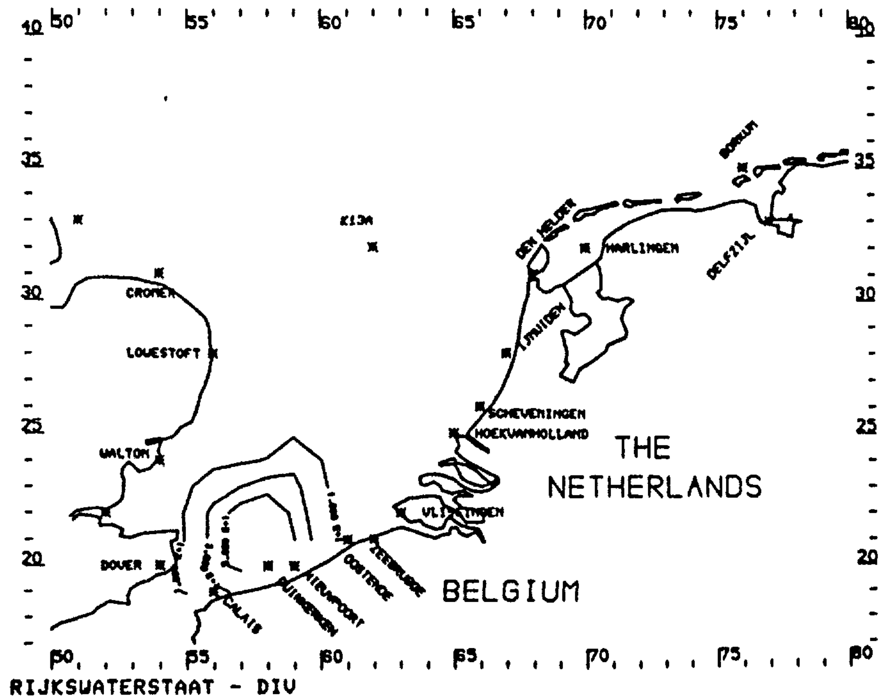

Figure 9: The concentration of the pollutant 15 days after the calamity

5. CONCLUSIONS

The advection-diffusion is difficult to treat numerically, especially in case of calamities when steep gradients need to be resolved. Therefore in this paper we develop a particle model to describe the dispersion process of the pollutant during the period short after a calamity. By interpreting the advection-diffusion equation as a Fokker-Planck equation, it is possible to derive an Itô stochastic differential equation for the position of one particle of the pollutant. This particle model is exactly consistent with the advection-diffusion equation. From a certain time the concentration of the pollutant is determined and the advection diffusion is solved numerically using an ADI/FEM method. Realistic applications of the approach show that in this way numerical difficulties can be avoided.

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