



# The combination of a random walk method and a hydrodynamic model for the simulation of dispersion of dissolved matter in water

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## ABSTRACT

A three-dimensional particle model with random walk has been applied to simulate the dispersion of dissolved matter in water. The particle model uses flow information obtained with a hydrodynamic model. This flow information is only available at discrete grid points. The grid is curvilinear in the horizontal plane and uses the sigma-coordinate in the vertical. The advective part of the particle model reproduces closed streamlines in recirculation zones. A reflection principle at closed boundaries is given, which does not introduce an artificial diffusion.

## INTRODUCTION

Three-dimensional (3D) hydrodynamic simulations are often executed to analyze water quality problems. The advection-diffusion equation is widely accepted that it gives a sufficient mathematical-physical description of the transport process. It takes into account the local flow velocities and the dispersion coefficients obtained with a hydrodynamic model. Two approaches are known for the solution of the advection-diffusion equation. The Eulerian approach uses conservation equations for fixed control volumes, and finite difference approximations of the advection-diffusion equation are derived. In the second, the so-called Lagrangian approach, (random) trajectories of suspended particles immersed in the fluid are calculated. The equivalence of both approaches follows from the probability density function of a random, Lagrangian, trajectory [3].

If standard Eulerian algorithms are used in the simulation of dispersion of contaminant, the solution sometimes suffers from problems associated with



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the used grid and the discretization of gradients. Negative concentration might occur, especially if steep concentration gradients are present. Here a particle method, also referred to as a random walk method, may form an alternative. It overcomes the aforementioned deficiencies and the algorithm resembles the simple, intuitive meaning of the underlying physical process.

For the 3D simulation of flows, finite difference methods are usually used, introducing boundary fitted horizontal coordinates and/or the so-called sigma-coordinate along the vertical. Then the flow information is only available at discrete grid points. The main question to be considered here is: how to formulate a random walk method in terms of particle displacements, while taking into account the flow information available at discrete grid points?

## THE HYDRODYNAMIC MODEL

Advection and dispersion of contaminant are determined by the local flow velocities and the diffusion coefficients. Therefore, the hydrodynamic model that solves the free surface water flow problem and generates these quantities, will be considered first. To obtain a schematization, suited for complex irregular geometries, curvilinear orthogonal coordinates are used for the horizontal direction. For the vertical direction the so-called sigma-coordinate, [8], is used, yielding a constant depth-independent vertical resolution. Figure 1 illustrates the used notation:

$(x_1, x_2, x_3)$  the coordinate system in the physical space,  
 $(\xi^1, \xi^2, \xi^3) = (\xi, \eta, \sigma)$  the coordinate system in the computational space,  
 $\zeta$  the water level elevation above the plane of reference  $x_3 = 0$ ,  
 $d$  the depth below the plane of reference  $x_3 = 0$ ,  
 $H = \zeta + d$  the water depth,

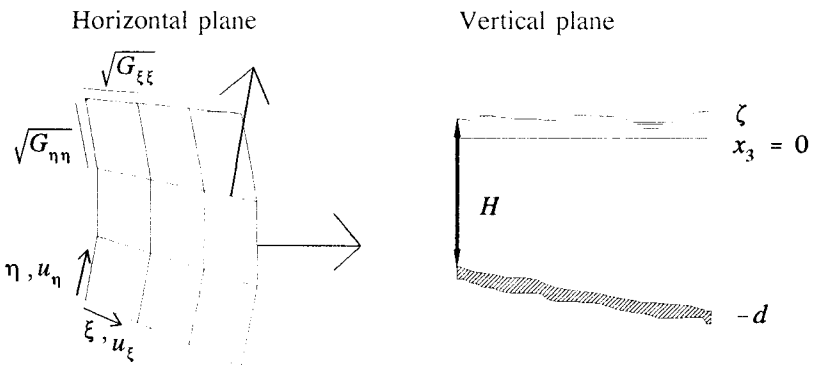


Fig.1: Physical domain

$\sqrt{G_{\xi\xi}}$  the increment of arc length along the coordinate line  $\eta = \text{constant}$ ,  
 $\sqrt{G_{\eta\eta}}$  the increment of arc length along the coordinate line  $\xi = \text{constant}$ ,  
 $u_\xi$  the horizontal velocity component in  $\xi$ -direction,  
 $u_\eta$  the horizontal velocity component in  $\eta$ -direction,  
 $\omega$  the vertical velocity component relative to a  $\sigma$ -plane,  
 $\sigma = (x_3 - \zeta) / H$  The sigma transformation.

The fluxes related to dispersion are calculated with a horizontal eddy-viscosity/diffusivity,  $D_H$ , and a vertical eddy viscosity/diffusivity,  $D_V$ . They represent the transport due to turbulence.  $D_H$  and  $D_V$  are obtained with a so-called  $k$ - $\epsilon$  turbulence model and will vary in time and space.

The hydrodynamic model solves the flow field at discrete grid points. The  $u_\xi$ ,  $u_\eta$ ,  $\omega$ ,  $D_H$  and  $D_V$  that are obtained in this way, will be used to simulate the dispersion of dissolved matter.

### 3D RANDOM WALK MODEL

In Cartesian coordinates, the three-dimensional dispersion of contaminant in water is described by the mass balance equation, i.e., the advection-diffusion equation [4]:

$$\frac{\partial C}{\partial t} + \sum_{i=1}^3 \frac{\partial}{\partial x_i} (u_i C) = \frac{\partial}{\partial x_1} \left( D_H \frac{\partial C}{\partial x_1} \right) + \frac{\partial}{\partial x_2} \left( D_H \frac{\partial C}{\partial x_2} \right) + \frac{\partial}{\partial x_3} \left( D_V \frac{\partial C}{\partial x_3} \right) \quad (1)$$

$C$  is the concentration of transported substance and  $u_i$  the local flow velocity in  $x_i$ -direction. The three-dimensional particle model, consistent with (1) is formulated in terms of successive particle displacements  $d\mathbf{X} = (dX_1, dX_2, dX_3)^T$  by the following Itô stochastic differential equations [6]:

$$\begin{aligned} dX_1 &= (dX_1)_{\text{drift}} + (dX_1)_{\text{ran}} = \left( u_1 + \frac{\partial D_H}{\partial x_1} \right) dt + \sqrt{2D_H} dW_1(t) \\ dX_2 &= (dX_2)_{\text{drift}} + (dX_2)_{\text{ran}} = \left( u_2 + \frac{\partial D_H}{\partial x_2} \right) dt + \sqrt{2D_H} dW_2(t) \\ dX_3 &= (dX_3)_{\text{drift}} + (dX_3)_{\text{ran}} = \left( u_3 + \frac{\partial D_V}{\partial x_3} \right) dt + \sqrt{2D_V} dW_3(t) \end{aligned} \quad (2)$$

The well-known Wiener-Levy process  $W(\cdot)$ , provides the characterization of equation (2). The increments,  $d\mathbf{W}(t)$ , are independent stochastic variables.  $d\mathbf{W}(t)$  is Gaussian distributed with mean zero and variance  $dt$ . The equation that governs the time evolution of the (conditional) probability density function of the particle positions, given an initial condition satisfies the Fokker-Planck equation. This equation matches equation (1), which shows the equivalence of the random walk model with the transport equation (1), see for instance



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[2,5,7,9]. Equation (2) is not yet suitable for simulations, since the hydrodynamic model yields the velocities  $u_\xi$ ,  $u_\eta$ ,  $\omega$  in curvilinear coordinates, instead of the velocities  $u_i$ ,  $i=1,2,3$  at discrete grid points. Therefore equation (2) must be transformed to the  $(\xi, \eta, \sigma)$ -space, which leads to particle displacements in the transformed space, denoted with  $(\sqrt{G_{\xi\xi}}d\xi, \sqrt{G_{\eta\eta}}d\eta, Hd\sigma)$ :

$$\begin{aligned}
 d\xi &= \frac{1}{\sqrt{G_{\xi\xi}}}u_\xi dt + \frac{1}{G_{\xi\xi}}\frac{\partial D_H}{\partial \xi}dt - \frac{1}{HG_{\xi\xi}}\frac{\partial x_3}{\partial \xi}\frac{\partial D_H}{\partial \sigma}dt + (d\xi)_{\text{ran}} \\
 d\eta &= \frac{1}{\sqrt{G_{\eta\eta}}}u_\eta dt + \frac{1}{G_{\eta\eta}}\frac{\partial D_H}{\partial \eta}dt - \frac{1}{HG_{\eta\eta}}\frac{\partial x_3}{\partial \eta}\frac{\partial D_H}{\partial \sigma}dt + (d\eta)_{\text{ran}} \quad (3) \\
 d\sigma &= \frac{1}{H}\omega dt + \frac{1}{H^2}\frac{\partial D_V}{\partial \sigma}dt - (d\sigma)_{\text{nonorthogonal}} + (d\sigma)_{\text{ran}}
 \end{aligned}$$

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advection
space-varying  
diffusivity
nonorthogonality
stochastic  
forcing

As in (2), the particle is subjected to a displacement due to the local flow velocity and the space-varying diffusivity. Additional terms, given in (3), are due to the nonorthogonal sigma-transformation. Finally equation (3) introduces:

$$\begin{aligned}
 (d\sigma)_{\text{nonorthogonal}} &= \frac{1}{H\sqrt{G_{\xi\xi}}}\frac{\partial x_3}{\partial \xi}\left(\frac{1}{\sqrt{G_{\xi\xi}}}\frac{\partial D_H}{\partial \xi} - \frac{1}{H\sqrt{G_{\xi\xi}}}\frac{\partial x_3}{\partial \xi}\frac{\partial D_H}{\partial \sigma}\right)dt \\
 &+ \frac{1}{H\sqrt{G_{\eta\eta}}}\frac{\partial x_3}{\partial \eta}\left(\frac{1}{\sqrt{G_{\eta\eta}}}\frac{\partial D_H}{\partial \eta} - \frac{1}{H\sqrt{G_{\eta\eta}}}\frac{\partial x_3}{\partial \eta}\frac{\partial D_H}{\partial \sigma}\right)dt \quad (4)
 \end{aligned}$$

$$(d\xi^i)_{\text{ran}} = \left(\frac{\partial \xi^i}{\partial x_1} \quad \frac{\partial \xi^i}{\partial x_2} \quad \frac{\partial \xi^i}{\partial x_3}\right)^T \cdot \left((d\mathbf{X})_{\text{ran}} - \left(\frac{\partial \mathbf{X}}{\partial t}\right)dt\right) \quad (5)$$

## NUMERICAL ASPECTS

The numerical aspects of the 3D random walk algorithm are now summarized:

- A finite number of particles is released in the flow area. Their initial position and mass are determined by the initial concentration distribution. In discharge applications, particles are released at the discharge location. If the initial concentration is distributed over more than one grid cell, particles are released uniformly within these cells. The number of injected particles is determined by the concentration in the corresponding cell.

- After the release of particles, their trajectories are computed. For that purpose, equation (3) must be discretized. The position of the particle,  $(\mathbf{E}_1^n, \mathbf{E}_2^n, \mathbf{E}_3^n)^T$ , at time  $t_n = n\Delta t$  is computed by evaluation of

$\Xi_i^n = \Xi_i^{n-1} + \Delta \Xi_i^{n-1}$ ,  $i=1,2,3$ . The increment  $\Delta \Xi_i^{n-1}$  is determined by equation (3). The local flow velocities and the eddy-diffusivities are evaluated explicitly in time, i.e., at time  $t_{n-1}$  at the previous particle location, as required by the Itô interpretation of equation (2).

● For the integration of the velocity field, in the absence of the stochastic component, an algorithm is used such that numerical streamlines are solved exactly. For that purpose the discrete velocity field is interpolated within each grid cell, such that at each point in the continuous space, the continuity equation is satisfied. The streamline equation becomes,  $i=1,2,3$ :

$$dx_i = u_i^{\text{ext}} dt \quad \text{approximated with} \quad \Delta X_i^n = \int_{t_{n-1}}^{t_{n-1} + \Delta t} u_i^{\text{ext}} d\tau \quad (6)$$

$u_i^{\text{ext}}$  is achieved by linear interpolation of the velocity-field using the grid cell information. Then the streamline equation (6) is solved analytically. Since the divergence of  $\underline{u}^{\text{ext}}$  corresponds with the discretized continuity equation of the hydrodynamic model, a mass conserving hydrodynamic model gives a mass conserving advection step in the particle model as well.

● The diffusion coefficients at the particle's location, are computed by linear interpolation. The spatial derivatives are approximated by finite differences.

● The random variable,  $\Delta W_i$  is determined by  $\sqrt{3 \Delta t} U_i$ , where  $U_i \in (-1, 1)$  is a pseudo random number,  $i=1,2,3$ , as in [9].

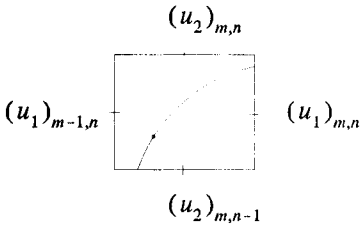
● Output consists of cell-averaged concentrations, which are obtained by counting the number of particles in each grid cell.

● At the model boundaries, boundary conditions have to be imposed. At open boundaries a zero concentration is imposed, which can be realized by absorption of particles [1]. At closed boundaries, a zero normal-flux boundary is usually imposed, which is realized by reflection of particles [1]; a particle that hits a boundary under a certain angle, will be retraced towards its starting point, instead of obeying perpendicular reflection.

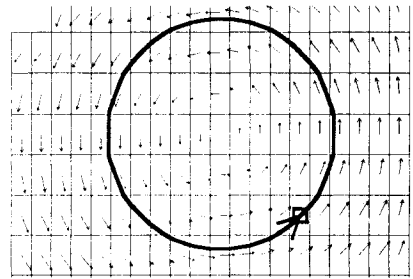
### EXAMPLE 1: CLOSED STREAMLINES IN A VORTEX FLOW

In a vortex flow all streamlines are closed curves. To illustrate the advection step in the particle method, a circular vortex flow is observed. Here a staggered, rectangular grid is defined wherein the velocity components at the centres of each grid side are used to compute the particle trajectory. These velocity components are analytically determined. For a normalized grid cell,  $x_i \in (0, 1)$ ,  $i=1,2$ , the streamline equation (6) becomes for  $i=1$ :

$$\frac{\partial x_1}{\partial t} = ((u_1)_{m,n} - (u_1)_{m-1,n}) x_1 + (u_1)_{m-1,n} \quad (7)$$



**Fig.2:** Normalized grid cell

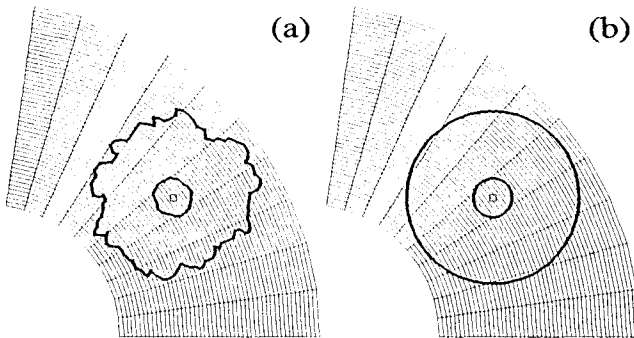


**Fig.3:** Closed orbit in a vortex flow

Then for each grid cell, as depicted in figure 2, equation (7) is solved analytically. In a stationary flow field, the procedure does not depend on  $\Delta t$  and closed orbits are produced, as shown in figure 3.

**EXAMPLE 2: A DISCHARGE PROBLEM; DISPERSION OF POLLUTANT**

This second example illustrates diffusive transport in a curved grid. Here the discharge of an initial slug of mass is simulated in a two-dimensional horizontal (2DH) domain. If equation (1) is solved with a finite differencing method on a curvilinear grid, the polluted region becomes curved and oval shaped, amplified by the steep concentration gradient at initial state. This is a result of discretization errors that propagate along the coordinate lines of the grid. The solver should produce circular concentration isolines. Here, the particle method is applied to test grid-dependency of the solution. The averaged grid dimensions are 1m x 7.7m. At the discharge location a mass of  $M = 76\text{kg}$  has been released in a zero flow field. The horizontal diffusivity  $D_H = 0.1\text{m}^2/\text{s}$ . 400000 particles are injected, which reduces the stochastic



**Fig.4:** Concentration isolines for  
(a) Particle method (b) Analytical computations

error in the estimation of the concentration to negligible proportions. Figure 4 shows contour lines after a simulation time of  $t = 100\text{s}$  ( $\Delta t = 1\text{s}$ ). The inner contour line is the isoline of concentration  $C = M \exp(-1/2) / (4\pi t D_H)$   $\text{kg/m}^2$  per unit depth. Theoretically this should be a circle  $\{(x_1, x_2) \in \mathbb{R}^2 \mid x_1^2 + x_2^2 = \sigma^2(t)\}$  where  $\sigma(t)$  is the spread in  $x_1$ - and  $x_2$ -direction at time  $t$ . The other orbit represents the isoline of minimum positive cell-averaged concentration value, as observed in the particle simulation. Since such a low concentration value is considered, a larger deviation from a circle has been expected. The time step has been chosen such that the particle crosses one grid line per time step at the most. Locally, the curved coordinate lines are approximated with straight lines parallel to the grid cell edges. A particle travels  $\Delta t$  time in a direction that is a linear combination of these approximated coordinate lines. So, a particle that moves within a grid cell is not aware of the curvature of the grid; a time step reduction will not benefit the result. This kind of grid dependency appears to be small.

#### ADDITIONAL EXAMPLES

After studying advection and diffusion problems separately, other tests were executed to demonstrate the applicability of the described particle method in hydrodynamic applications. The results of these tests are sketched briefly.

● Flow in a square harbour, boarding a river - The corresponding stationary depth-averaged flow pattern has been calculated with the flow solver PHOENICS. These flow results have been used in the particle model, (i) to compute horizontal flow patterns, and (ii) to predict the dispersion of heating water inside the harbour. Closed streamlines are obtained inside the harbour. The particle model showed a good resemblance with a traditional finite difference model.

● Flow over a sill - The recirculation zone behind a sill has been computed with the hydrodynamic model TRISULA using the sigma-transformation. Again, the particle model proved to be meaningful in producing closed streamlines and concentration distributions of a dissolved contaminant.

● Anisotropic diffusion in a reservoir - Qualitative results are obtained by running an anisotropic space-varying diffusion test in a sigma-grid. Particle simulations showed:

- (1) Omission of the nonorthogonality terms, as expressed in equation (3), results in an excessive artificial migration of particles. The influence of nonorthogonality on the particle displacement may not be neglected.
- (2) Due to the stochastic approximation technique, (small amplitude) oscillations can not be avoided, but remain acceptable.
- (3) A drift is observed if the information of the diffusion coefficients is restricted to grid nodes. This nonphysical drift is due to the linear



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approximation technique and the finite differencing procedure, to obtain the spatial derivatives, as they appear in equation (3). Then the accuracy of the particle method is reduced but statistical tests show the correct asymptotic behaviour.

(4) If the flow information is given at the continuous flow region (not restricted to grid nodes), the particle method yields good results..

### CONCLUSIONS

The description and the effectiveness of a particle method, using discrete Eulerian flow information, have been demonstrated. If the Eulerian flow information is given with respect to a curvilinear grid, the particle method shows a grid dependency. This dependency is small in comparison with: (1) the time step error, due to the time integration procedure, (2) the stochastic error, due to the initial number of particles, and (3) the discretization error, arising in equation (3) for the computation of particle displacements. Application of nonorthogonal grids requires correction terms in the computation of particle displacement. In applications where traditional Eulerian methods fail, the particle method proved to be an adequate alternative.

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