MODEL STUDIES OF DISPERSION OF POLLUTANTS IN LAKE VÄNERN

by Ingrid Bork

SMHI Rapporter

HYDROLOGI OCH OCEANOGRAFI
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ABSTRACT

Methods to compute dispersion of pollutants in a known velocity field is described. A Monte-Carlo or random walk technique is used in an example. The velocity field used is two-dimensional, constant in time, but the method can easily be used in a three-dimensional, time dependent velocity field.

A verification study (e.g. dye outlet in a real water body) is needed to prove the applicabilty of the method.

SAMMANFATTNING

Metoder för beräkning av spridning av föroreningar i ett känt hastighetsfält beskrives. En Monte-Carlo eller slumpteknik används i ett exempel. Det använda hastighetsfältet är tvådimensionellt, konstant i tiden, men metoden kan lätt användas i ett tredimensionellt, tidsvariabelt hastighetsfält.

En verifieringsstudie (t ex spårämnesutsläpp i en sjö) behövs för att styrka metodens tillämpbarhet.

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1. INTRODUCTION

Lake Vänern, the largest lake in Sweden, with a volume of 150 km^3, has received increasing attention as a fresh water reservoir, recreation area and fishing-ground as well as waste-water recipient and navigable passage. It is polluted in the north by the pulp mill industry and in the south by small rivers from the densely populated farming district. The yearly amount of fresh water supplied is about 17 km^3 of which 5.2 km^3 is discharged from the nonpolluted Klarälven in the northeastern part of Lake Vänern (see fig 1).

The lake is divided into two basins which are connected by a shallow sound. The maximum depth is about 100 m and situated in the eastern basin. The western basin has a depth of about 70 m.

The inflow of wastes is mainly into the northeastern part of the lake. This has created a significant difference in water quality between the two basins. Until the beginning of the 1960´s, the effluents were becoming increasingly polluted but later because of the closing of factories and cleaner industrial processes this trend was stopped and pollution has been decreasing ever since.

An intense research program was started by SMHI in 1971 to study the circulation and temperature structure of the lake. Extensive field measurements were carried out and model studies of the lake were undertaken.

The computed pictures of the lake´s circulation under different weather conditions (Simons et al 1977) can form a base for studies of the transport and dilution of waste water from sources ashore.

2. DISPERSION MODELS

In an earlier report (Simons et al 1977) is described the application of a numerical model to Lake Vänern. The velocity fields computed in that model can be used to calculate river or waste water transport in the north basin of Lake Vänern. The model gives the horizontal velocity in 4 layers and the vertical velocity at the 3 levels separating the layers. The levels were situated at 10, 20 and 35 m below the surface. The computed velocities are time dependent, driven by wind. These velocities have been used together with a dispersion model to forecast waste water spreading in the lake.

The most common way to model dispersion is by converting the partial differential equations describing it to finite difference form. There are, however, practical limitations associated with the available core on the computer because the numerical simulation of pollution problems involves smaller scales then those controlling the velocity field. To simulate the circulation in Lake Vänern, for example, the whole lake has to be covered by a three-dimensional grid, where a horizontal grid size of 5 km may be sufficient. In such a grid the polluted area covers only a few grid points, which yields a very poor representation of the advective part of the equation (Grotjan, O´Brian 1976). Moreover for spatial constant velocity u and eddy diffusion coefficient A, Gorenflo (1968) showed that -

$$C_x^{t+\Delta t} - C_x^t = -\frac{\Delta t u}{2\Delta x}\left(C_{x+\Delta x}^t - C_{x-\Delta x}^t \right) + \frac{\Delta t A}{\Delta x^2}\left(C_{x+\Delta x}^t - 2C_x^t + C_{x-\Delta x}^t \right)$$

is consistent with the partial differential equation

$$\frac{\partial C}{\partial t} = - u\frac{\partial C}{\partial x} + A\,\frac{\partial^2 C}{\partial x^2}$$

only if $|u\Delta x| < A$

That is, $\Delta x = 5$ km and $u = 0.05$ m/sec would require $A >$ 250 m^2/sec whereas realistic values of A are less then 100 m^2/sec. Alternatively the concentration of pollutant, may be computed by a Monte-Carlo technique avoiding a dependence on grid size. Furthermore, such a probabilistic procedure may be considered as a more realistic simulation of turbulent dispersion than the deterministic description by a partial differential equation involving eddy diffusion coefficients.

A MONTE - CARLO METHOD

The term Monte-Carlo or random walk method implies a computational procedure to simulate statistical processes by a game. The rules of the game are adjusted to the special process under consideration. Sokolnikoff et al 1966, for example, illustrate how to construct a statistical process to make partial differential equations solvable by a Monte Carlo method. Especially suitable are random walk techniques to model turbulent dispersion as it is a random process by nature and therefore, the rules of the game are made by direcly reproducing the features of the physical process.

In his discussion of random walk study Bugliarello (1964), for example, presented a simulation of diffusion from an instantaneous point source in the centerline of a laminar parabolic two-dimensional velocity field. Thompson (1971) computed the three-dimensional development of a smoke plume under the influence of a turbulent wind field, known from measurements. Alternatively, the mean velocity field can be derived from a separate model study, as done by Maier-Reimer (1973, 1975) who modeled horizontal waste dispersion in the North Sea.

In all these approaches, the dispersion of a passive admixture is simulated by letting a series of particles move with the time averaged ambient velocity. Turbulent transport is modeled by an additional random displacement of each particle at each time step. Thus, the motion of each particle is described by the following equations (Thompson 1971, Maier-Reimer 1973/1975).

$$\frac{dx}{dt} = \bar{u} + \mu_u P_u$$

$$\frac{dy}{dt} = \bar{v} + \mu_v P_0$$

$$\frac{dz}{dt} = \bar{w} + \mu_w P_w + f\ (\rho\ \text{particle})$$

In this basicly heuristic formulation the Ps are known scales of turbulent velocity components and the μs are random numbers between -1 and +1 chosen independently from a prescribed distribution function. The last term in the third equation represents buoyancy of the suspended matter. The advection velocity ($\bar{u}$, $\bar{v}$, $\bar{w}$) is taken at the position of the specific particle under consideration and at the corresponding time. A particle reaching a rigid wall or the surface is reflected to simulate zero transport through that kind of boundary. If it is rather complicated to incorporate geometrical reflection in the simulation process, due to irregular topography for example, it is sufficient to define a small velocity prependicular to the wall to prevent particles to move through the wall.

By tracking a number N of particles, each representing a certain quantity Q of admixture, its mean concentration after a time

t in a volume V (x, y, z) = Δx Δy Δz around (x, y, z) is

$$C\,(x,\,y,\,z) = \frac{Q}{V\,(x,y,z)} \sum_{i=1}^{N} \delta^{\Delta x \Delta y \Delta z}$$

$$\text{with } \delta^{\Delta x \Delta y \Delta z}_{(i)} = \begin{cases} 1 \text{ if} & x - \frac{\Delta x}{2} \leq x(i) \leq x + \frac{\Delta x}{2} \text{ and} \\ & y - \frac{\Delta y}{2} \leq y(i) \leq y + \frac{\Delta y}{2} \text{ and} \\ & z - \frac{\Delta z}{2} \leq z(i) \leq z + \frac{\Delta z}{2} \\ 0 \text{ otherwise} & \end{cases}$$

That is, the concentration C is statistically interpretated as the probability for a particle to be in the volume V(x,y, z) at time t.

The choice of $\overset{=\text{bouyancy}}{f}$ (ρ particle) and P is entirely due to convenience. Thompson (1971), for example, simulates buoyancy in a two-dimensional model by $f = \Gamma(x)\,(I(x)-z)$ where I(x) is the equilibrium height and Γ(x) a buoyancy parameter. As Γ is not dependent on z, i.e. changes in buoyancy due to varying ambient density are neglected. the particle tends to <u>rise</u> to equilibrium height I(x). To simulate <u>sedimentation</u> of matter in water,

$$f = \frac{\rho_{\text{particle}} - \rho_{\text{ambient}}}{\rho_{\text{ambient}}}\, g\Delta t$$

may be more realistic. In a lot of problems this kind of buoyancy effect may, however, be completely ignored. Ambient density stratification, on the other hand, will modify P_v by assuming a decrease in turbulent mixing due to very stable stratification or increased mixing under unstable conditions, respectively.

Although, the modeling principle can be looked upon as an entirely heuristic approach, there is some theoretical justification for it.

Consider a simple one-dimensional case (compare Maier-Reimer 1973), where a large number N of particles, which do not interact, undergo a sequence of random displacements (μPΔt), each of which is independent from all the preceding displacements. Then the probability to find a particle at position x at time t = KΔt is

$$F\,(x,t) = NF\,\Big(\sum_{k=1}^{K} \mu P \Delta t\Big)$$

and according to the law of large numbers, F is a Gaussian distribution.

$$F\ (x,t) = \frac{N}{\sqrt{2\Pi\sigma_x^2}} \quad \exp\ \left(- \frac{x^2}{2\sigma_x^2} \right)$$

with the variance $\sigma_x^2 = \sigma_x^2\ (t) = \frac{1}{N-1} \sum_{i=1}^{N} (x_i - \bar{x})^2$

$$\bar{x} = \frac{1}{N} \sum_{i=1}^{N} x_i$$

According to Gauss´law of error propagation, σ_x^2 increases linearly with time: $\sigma_x^2\ (t) = 2\ At$.

This is the solution to the Fickian diffusion equation.

$F_t = A\ F_{xx}$ with $\sigma_x^2 = 2\ At$ and

the initial condition $F(x,0) = 0$ for $x \neq 0$,

boundary condition $F(x,t) = 0$ for $x \to \pm\ \infty$

and $\int_{-\infty}^{+\infty} F(x,t)\ dx = N$.

This result is a consequence of the relation between the one-dimensional diffusion coefficient A and the probability $\ell\ (\Delta)$ for a particle to move the distance between Δ and $\Delta + d\Delta$ during the small time interval Δt (Einstein 1905):

$$A = \frac{1}{\Delta t} \int_{-\infty}^{+\infty} \frac{\Delta^2}{2}\ \ell(\Delta)\ d\Delta \ / \int_{-\infty}^{+\infty} \ell(\Delta)\ d\Delta$$

with $\int_{-\infty}^{+\infty} \ell(\Delta)\ d\Delta = 1$, $\ell(\Delta) = \ell(-\Delta)$ and $\ell(\Delta) \neq 0$ only for

small $|\Delta|$.

As $\ell(\Delta)$ is different from zero only for small values of Δ the distribution can be cut off at $\pm\ p\Delta t$, i.e.

$$A = \frac{1}{2\Delta t} \int_{-p\Delta t}^{+p\Delta t} \Delta^2\ \ \ell(\Delta)\ d\Delta$$

As the effective diffusion coefficient is only a function of the variance of $\ell(\Delta)$ not of the special form of ℓ, a simple rectangular distribution is sufficient for modelling a constant diffusion coefficient (Maier-Reimer 1975). With

$$\ell(\Delta) = \frac{1}{2P\Delta t} \quad \text{if} \quad \Delta \in \left[-P\Delta t, P\Delta t\right]$$

$$0 \text{ otherwise}$$

The turbulence scale P is thus related to the diffusion coefficient by $P = \sqrt{\frac{6A}{\Delta t}}$

In reality, however, the value of A is merely a sensitive guess and it may be even easier to prescribe the maximum distance a particle is allowed to move during Δt due to turbulent transport. The modeller is free to choose different values for P_u, P_v and P_w to count for anisotropy. The P_s may also vary in time and space as a function of $\bar{u},\bar{v},\bar{w}$, and stability, whenever information about such dependency is available.

RESULTS

For demonstration purpose, pollution from two outlets A and B (see fig 1) is modelled, assuming that the admixture is well mixed over a depth H. At source A, Q kg sec^{-1} are released into the water and at source B, 3 × Q kg sec^{-1}. Each source is simulated seperately by releasing one particle every ten minutes. I.e. a particle starting at point A represents 600 × Q kg and a particle stating at C represents 1800 × Q kg. The particles are then transported by a steady horizontal velocity field (see fig 1), its trajectory being modified due to isotropic turbulence.

At each time step the position of every particle is determined. Its advection velocity components are found by linear interpolation of the four surrounding velocities. The random velocity components are chosen - independent from one another - out of the same interval (+ 32 cm sec^{-1}, -32 cm sec^{-1}), corresponding to an isotropic diffusion coefficient of 10^5 cm^2 sec^{-1}. Fig 2 and 3 show the particle distribution after 3, 6 and 9 days for source A and B, respectively. For the tenth day both distributions are plotted in the same picture (fig 4) and the corresponding isolines are drawn, taking into account the different strength of source A and B. The combined effect of both sources yields a concentration of

$A_H = 10\ m^2/s$

$\Rightarrow \Delta t = 600\ s.$

$$C\ (x,y) = \frac{Q\ \Delta\ t}{\Delta x\ \Delta y\ H} \left[\sum_{\substack{i=1\\A}}^{N} \delta_{(i_A)} + 3\sum_{\substack{i=1\\B}}^{N} \delta_{(i_B)} \right]$$

where H is the depth of the layer in which the pollutant is mixed. In fig 5 Q is chosen so that

$$\frac{Q \times 600\ sec}{1.000m \times 1.000m \times H} = 1\ kg/m^3.$$

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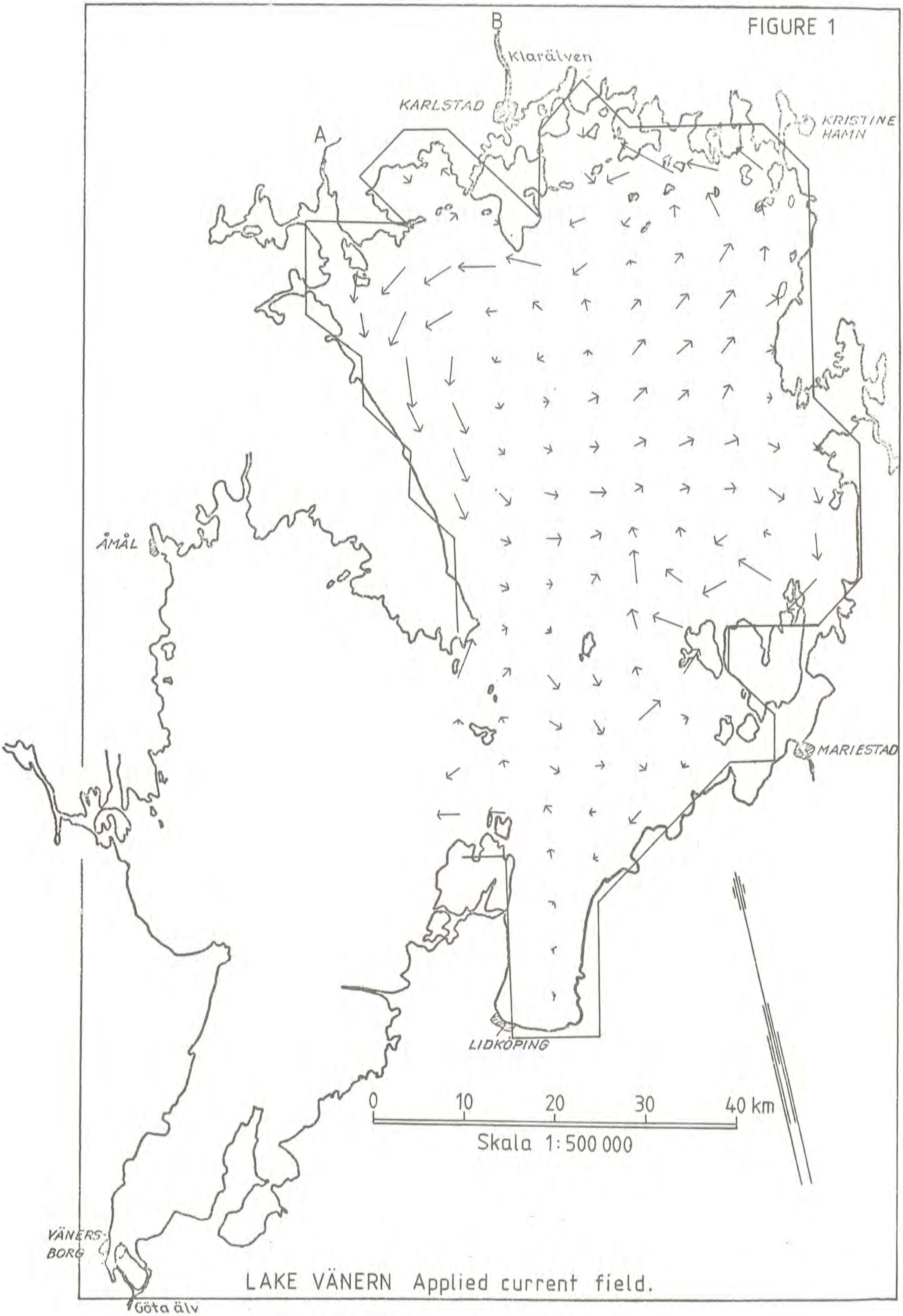
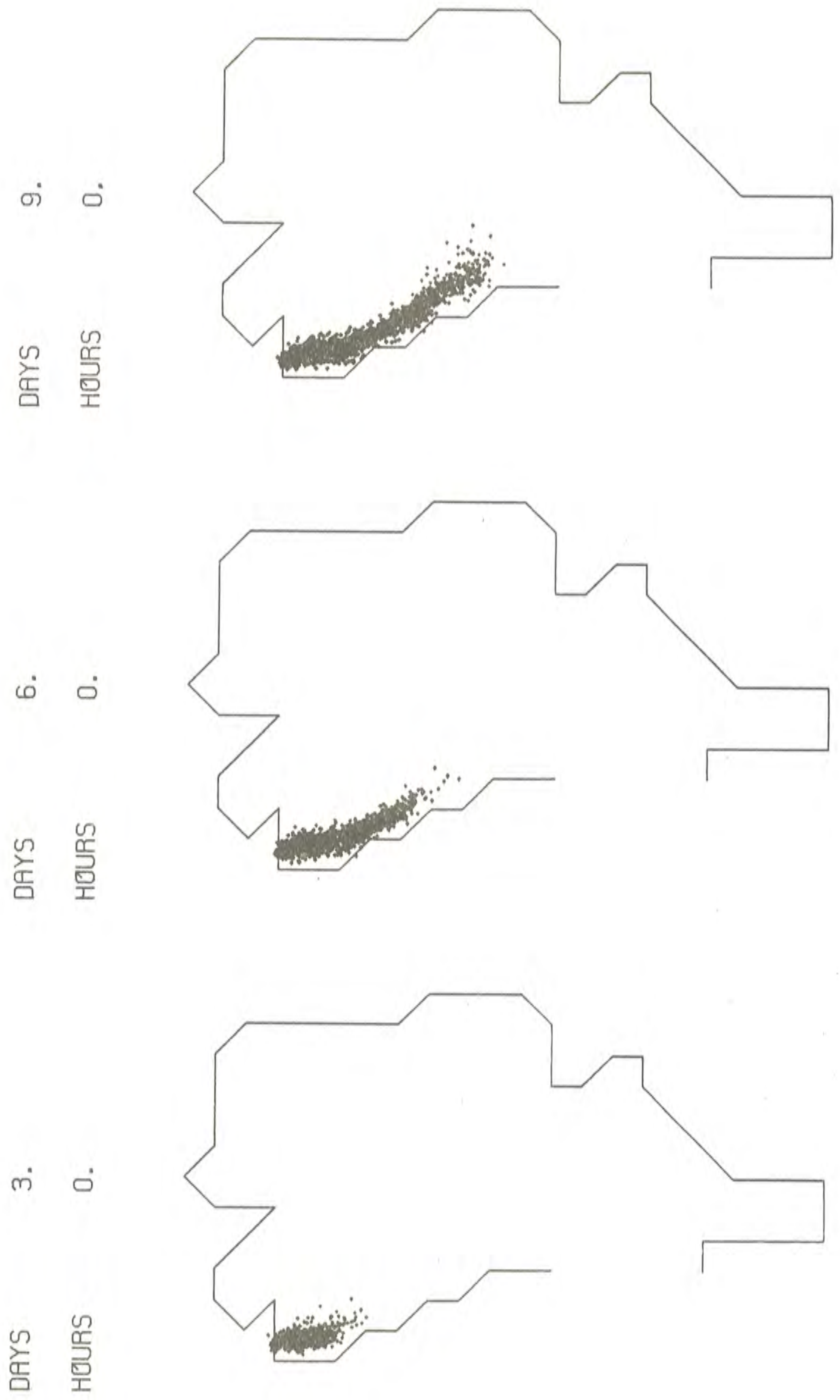
FIGURE 1



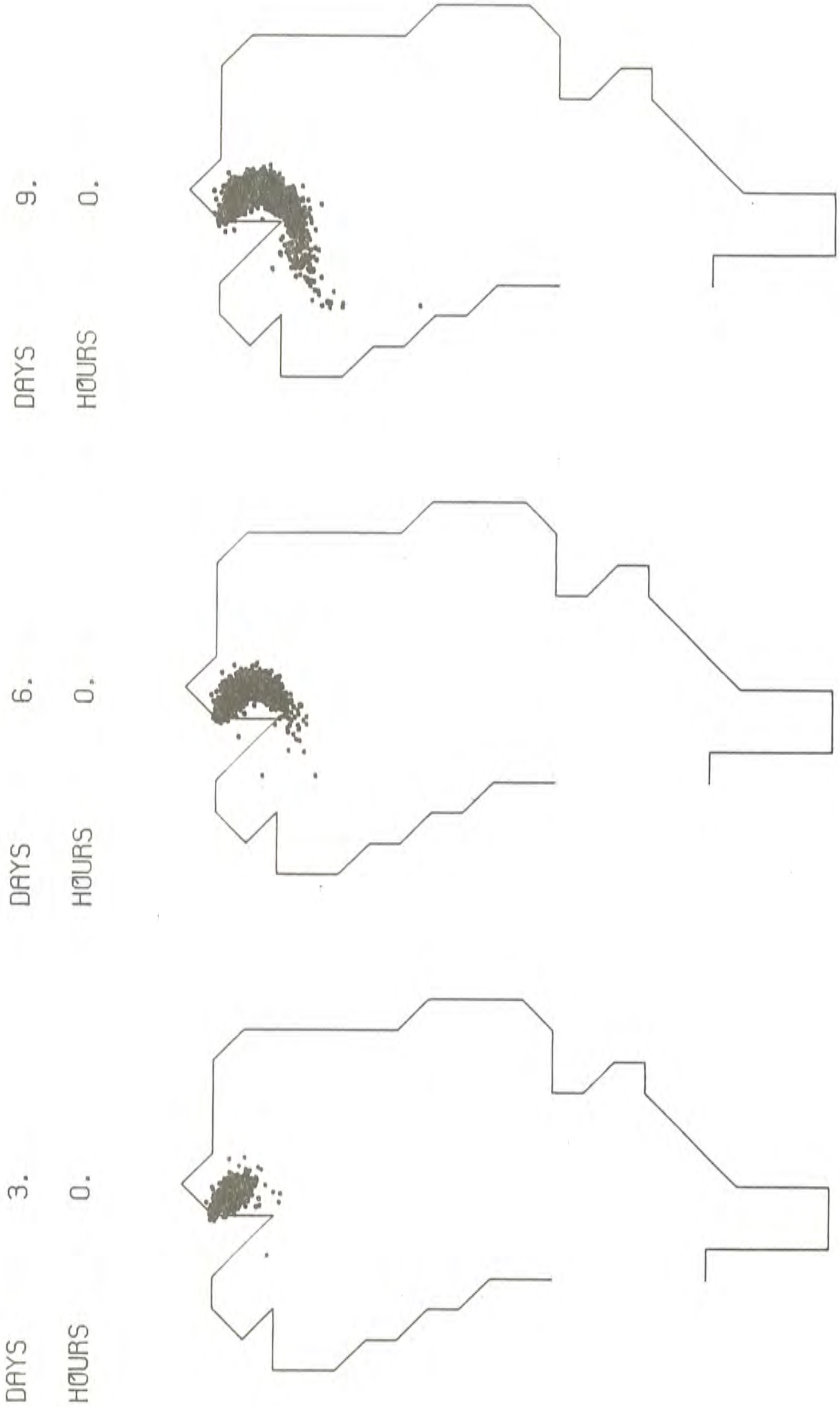
LAKE VÄNERN Applied current field.

FIGURE 2



POLLUTION FROM OUTLET A.

FIGURE 3

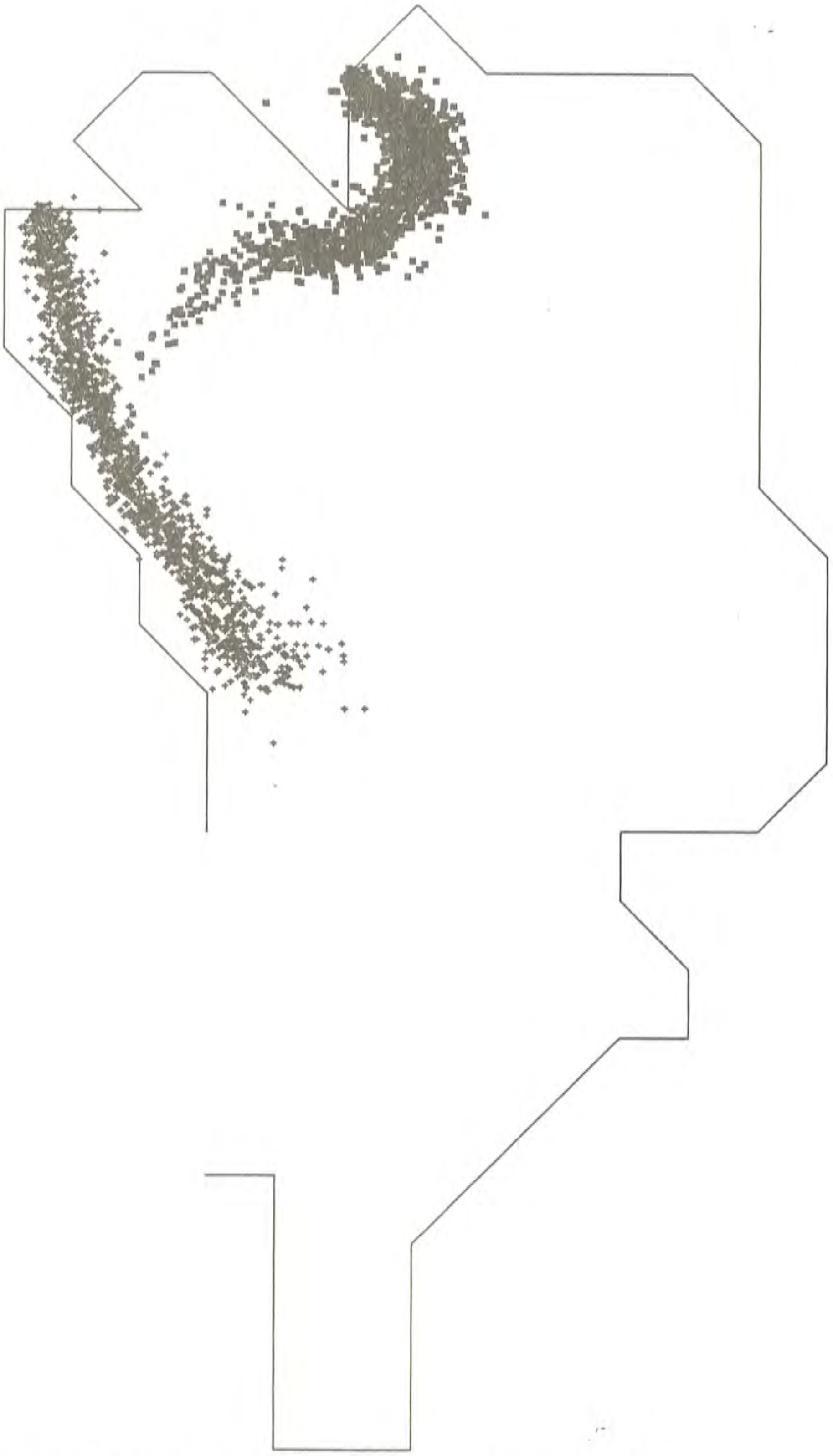


POLLUTION FROM OUTLET B.

FIGURE 4

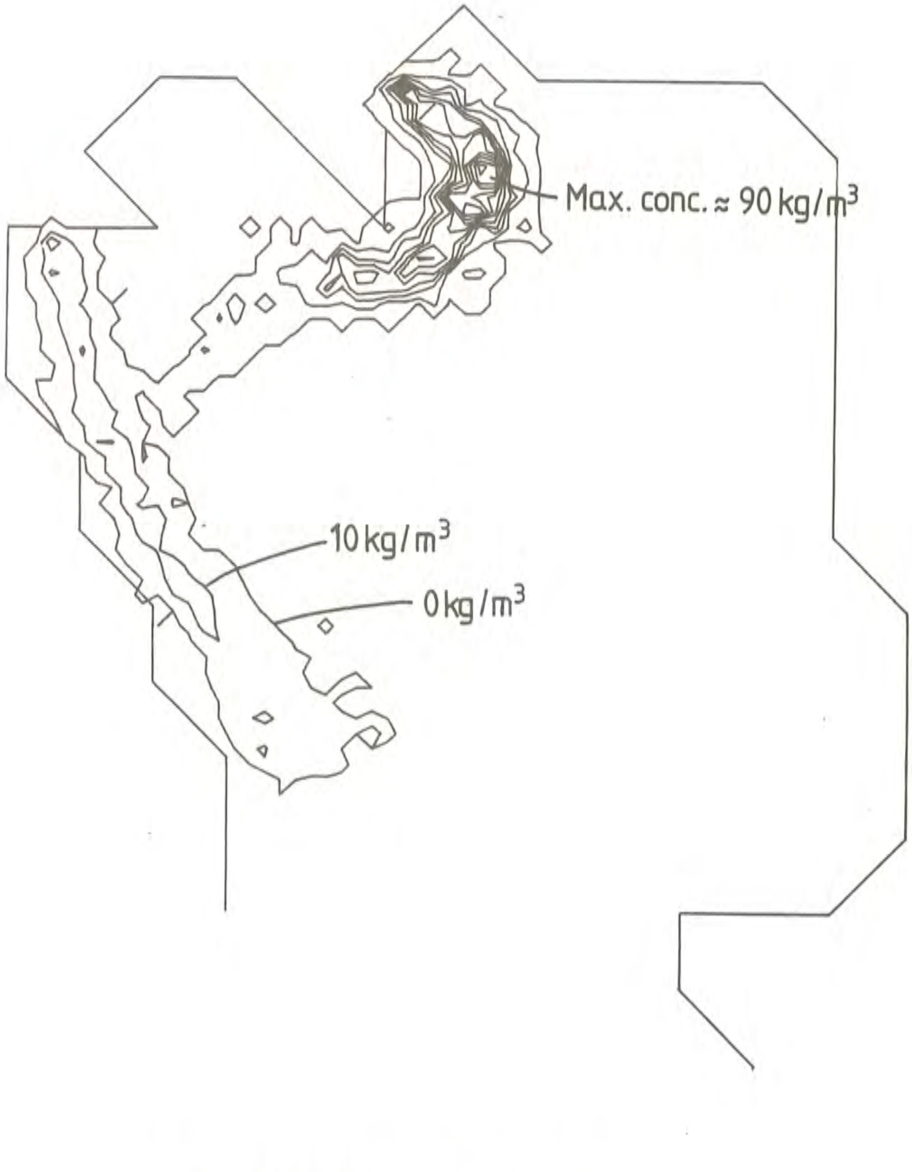
DAYS 10.

HOURS 0.



COMBINED EFFECT OF POLLUTION FROM A AND B.

FIGURE 5



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