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MODELING EPISODES IN POLLUTANT DISPERSION
IN LAKE MICHIGAN

by

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ABSTRACT

Numerical simulations of several important episodes in the horizontal dispersion of a conservative substance in thermally-stratified (summer) Lake Michigan were performed. Lake-wide dispersion of chloride during the summer of 1970 was modeled for 125 days using U.S. Weather Service and USEPA data. The results obtained indicated that more useful information might be obtained more easily by simulating local short-term episodes of pollutant movement from single sources. Accordingly, best and worst case 33-day simulations of the dispersion of identical slugs of pollutant from Calumet Harbor were performed. The results for these extreme cases suggested that the disposition of pollutant from any given source is highly dependent upon short-term wind conditions and that such best and worst case modeling might easily provide some of the detailed insights required for water management purposes.

The dispersion model's applicability to unstratified (winter) Lakes Michigan and Ontario is demonstrated for some simple cases.

The numerical model used is readily adaptable to a wide range of episodes of interest. Actual time-varying lake circulations are efficiently approximated by sequences of quasi-steady-state circulations produced by a separate flow model, and time-varying pollutant sources are easily introduced at any point in the lake. A strictly mass-conservative finite-difference formulation ensures numerical stability, even for (potentially) inconsistent circulation data.

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KEYWORDS - computer model/ water circulation/ water pollution/ dispersion/
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A NOTE ON AUTHORSHIP

As principal investigator bearing primary responsibility for this research grant, Dr. Katz is listed as the first author. The work herein, however, has content essentially equivalent to the M.S. thesis (Department of Information Engineering, University of Illinois at Chicago Circle) of Mr. Schwab. Published works drawn from this thesis/research report list Mr. Schwab as the first author and Dr. Katz as the second author.

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INTRODUCTION

To the millions living along its shores, Lake Michigan is a natural resource of tremendous importance, both as a source of clean drinking water and as a place for recreational fishing, boating, and swimming. Widespread use of the lake and its tributaries by industries and municipalities makes enlightened water-quality management essential to the preservation of water quality. The likelihood of making sensible decisions affecting this water quality is enhanced by detailed understanding of the effects of these decisions. Dynamic modeling of aquatic ecosystems is a potentially powerful technique for obtaining the needed insight.

Predictive models, properly constructed, could warn of short-term effects such as algae blooms and dangerous accumulations of bacteria along beaches and also of long-term increases in levels of nutrients and toxic chemicals. Furthermore, such models could estimate the effects of present and future effluent discharges upon these phenomena.

The processes of advective and diffusive dispersion must necessarily be included in any detailed models of localized biological activity in large bodies of water; models for the dispersion of conservative substances under the influence of currents and concentration gradients can be, therefore, looked upon as essential first steps toward overall ecosystem models for the Great Lakes. Existing aquatic biological models which assume horizontal homogeneity in order to concentrate upon vertical changes (e.g., Winter and Pechuzal 1974) or upon kinetics (e.g., Bierman, et al 1973, and Cordeiro, et al 1973) require the addition of horizontal dispersion mechanisms if they are to be more usefully applied to large water bodies. Biological models

including dispersion mechanisms have been applied successfully to estuaries (e.g., Canale, et al 1973, Chen and Orlob 1972, and Schofield and Krutchkoff 1972); and separate conservative-pollutant transport models have been developed for Lake Ontario (Simons 1972) and Lake Erie (Lam and Simons 1974); and for Saginaw Bay (Richardson 1974). Furthermore, the inclusion of biological mechanisms may not be necessary for the preliminary treatment of some important cases involving short-term (time scale of days) movement of non-conservative materials, especially in the near-shore regions of most concern to water resources management. Some results to be shown here, for example, indicate that harmful contaminants (nutrients, fecal coliform, etc.) emanating from the Indiana Harbor Canal as described by Snow and Adamczyk (1974) can, under common wind conditions, begin to accumulate in significant amounts at Chicago beaches and water intakes within a few hours of their discharge.

A finite-difference model for the movement of a generalized conservative pollutant in Lake Michigan will be presented here. This model uses the existing Kizlauskas-Katz (1973, 1974) circulation model to generate step approximations to realistic wind-driven current histories and can simulate many episodes of interest under both thermally-stratified (summer) and homogeneous (winter) conditions for periods of up to several months. The strictly mass-conservative formulation employed ensures computational stability for long simulation periods even when the circulation data used are somewhat inconsistent in terms of water mass conservation, as would be the case for scattered experimental observations.

A four-month (125-day) simulation of chloride dispersion from 28 time-varying sources corresponding to USEPA discharge data and U.S. Weather Service wind data for the summer of 1970 is presented. The usefulness of the

model in the study of extreme cases is then illustrated by 33-day simulations of the movement of identical slugs of pollutant from Calumet Harbor under "best" and "worst" wind conditions culled from actual U.S. Weather Service wind histories. Dispersion of pollutant from a continuous Calumet Harbor source under a constant wind for 60 days is then presented for the unstratified lake, merely to demonstrate the model's applicability to the unstratified case. Emphasis in the Lake Michigan studies was intentionally placed upon the southern tip, especially the Chicago and Lake County shoreline area.

Finally, some results of an application of the circulation and dispersion models to unstratified Lake Ontario for the purpose of comparison with some results of Simons (1972) are shown.

NUMERICAL METHOD

The development of a finite-difference integration procedure for the differential equation governing the two-dimensional dispersion (diffusion and advection) of a conservative pollutant in a vertically-stratified lake with an assumed steady-state flow pattern will now be shown. Here, the flow patterns used will be those obtained from the Kizlauskas-Katz circulation model. (Typical "steady-state" velocity patterns generated by this model are shown in figures 1 through 4, which correspond to epilimnion and hypolimnion flows for SSW and NNE winds at 3.8 m/sec, respectively.) The circulation model used has been shown (Kizlauskas and Katz 1973) to represent some of the observed characteristics of Lake Michigan in summer, such as thermocline tilting and the existence of strong coastal jets in the epilimnion corresponding to the longitudinal components of prevailing winds (Csanady 1967, 1971). The dispersion model developed, however, would work equally well with other forms of circulation data, including those obtained experimentally. Vertical stratification is modeled via two homogeneous layers (depth H and H') separated by an impermeable thermocline (see Figure 5), a commonly used (e.g., Lee and Liggett 1970 and Csanady 1968) idealization of the thermal layering which exists in lakes such as Lake Michigan and Lake Ontario during the summer (Huang 1971, Lee and Liggett 1970). The model also includes the common simplification (e.g., Simons 1972, 1973) of considering vertically-averaged concentrations (C and C') and vertically integrated velocities (\bar{V} and \bar{V}') with separate integrations in each layer.

The assumed impermeability of the thermocline allows the equations for C and C' to be completely independent, provided that H , H' , \bar{V} , and \bar{V}' are

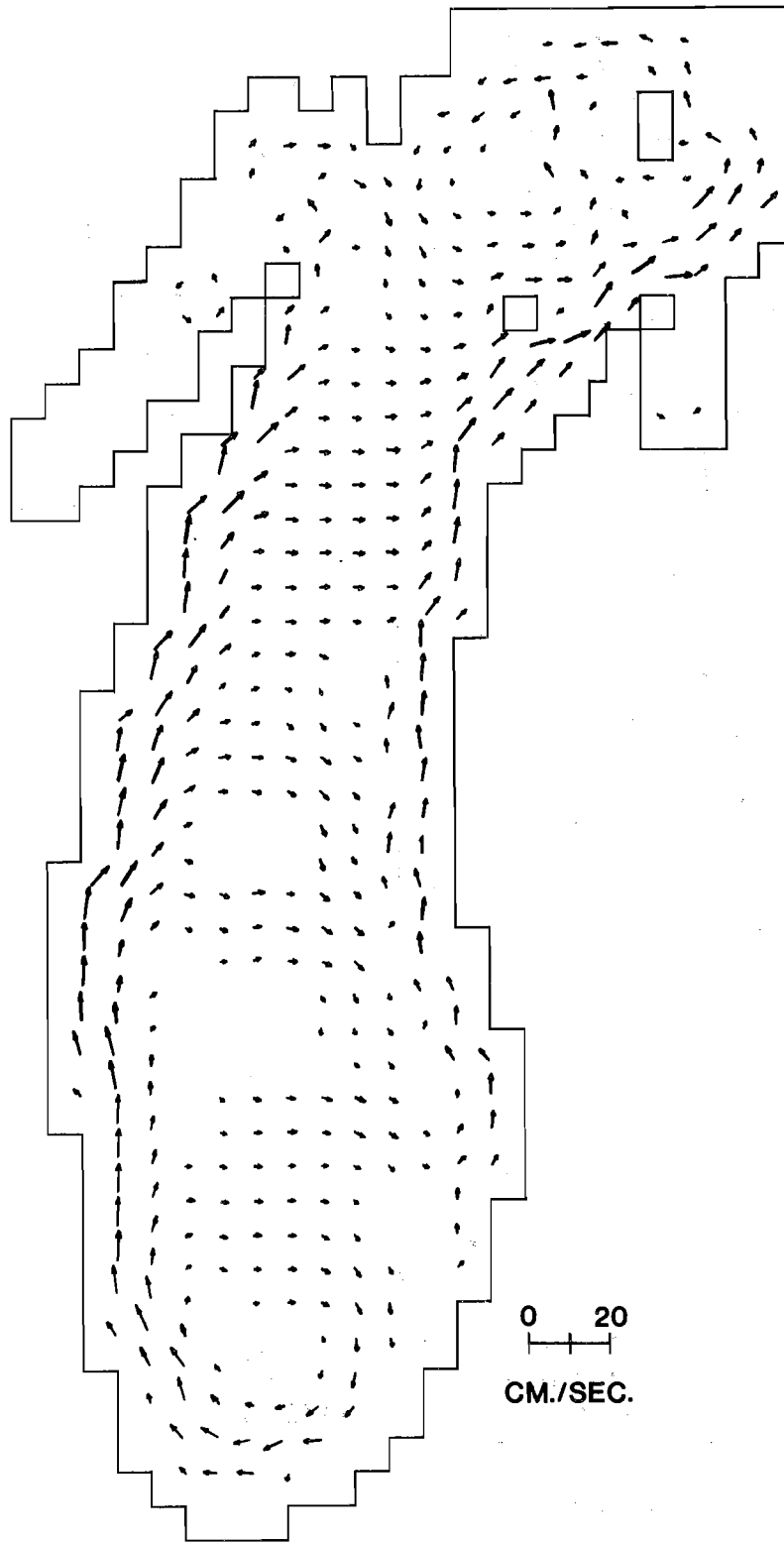


Figure 1. Average Lake Michigan top-layer velocities for a SSW wind @ 3.8 m/sec.

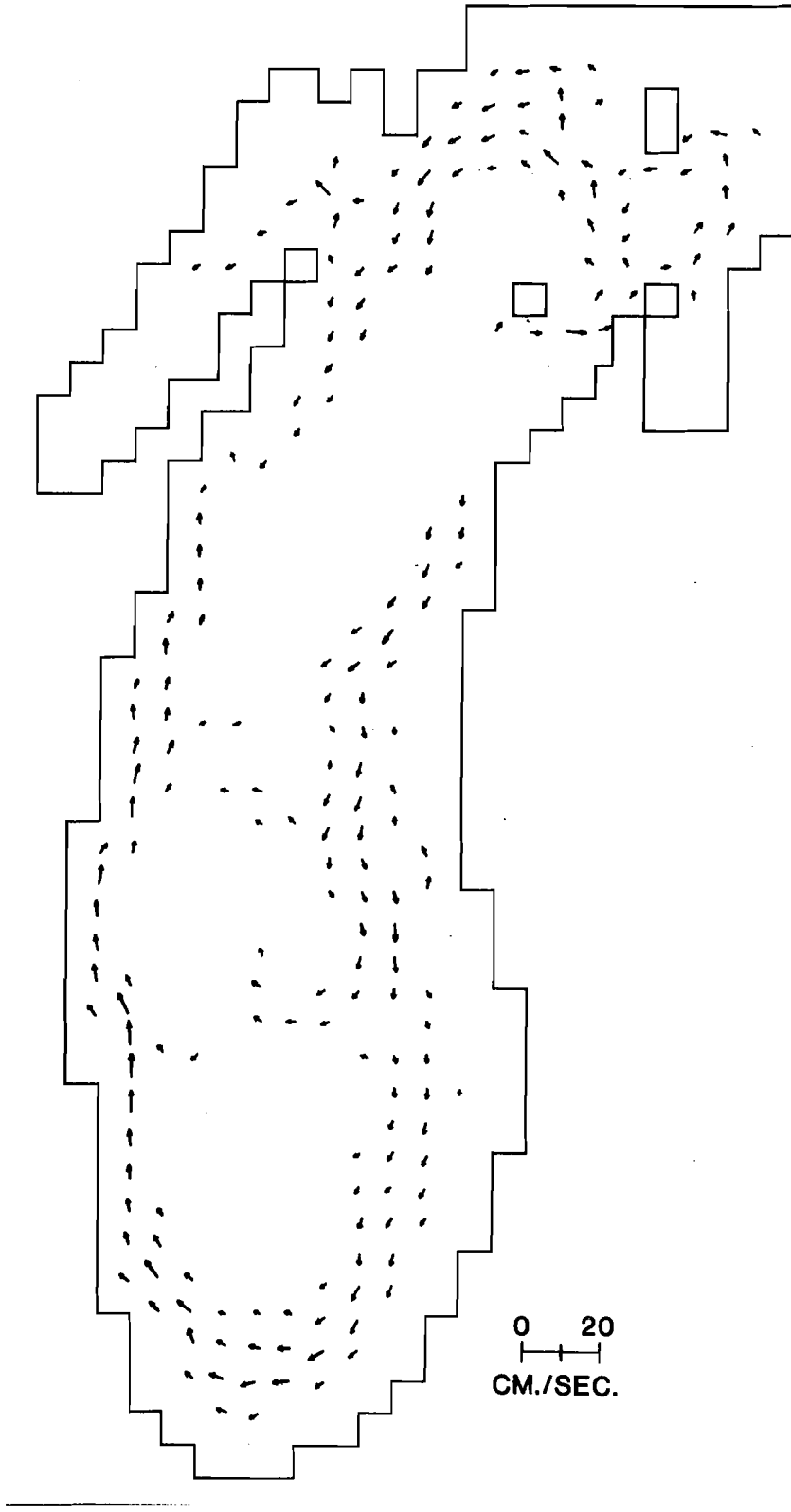


Figure 2. Average Lake Michigan bottom-layer velocities for a SSW wind @ 3.8 m/sec.

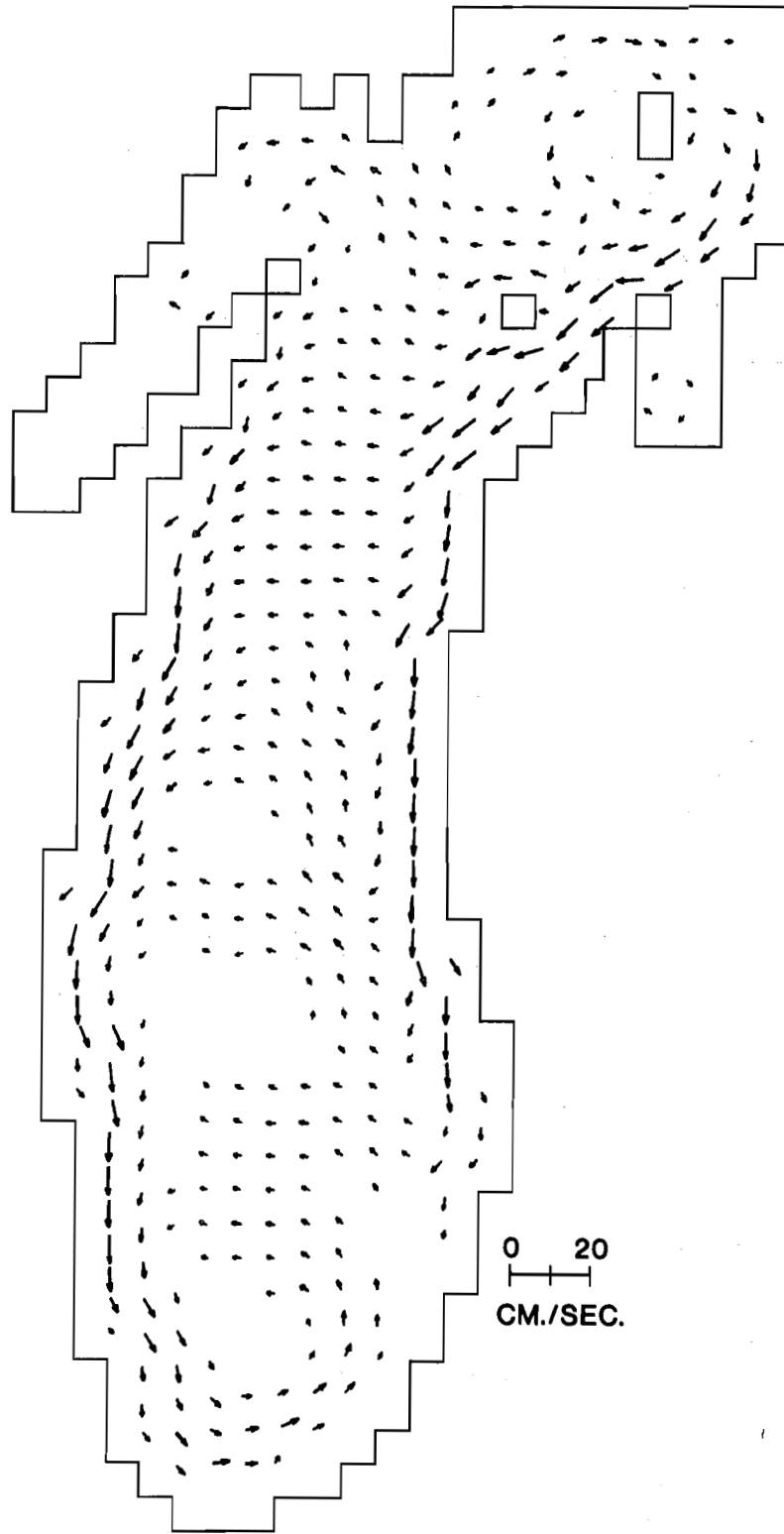


Figure 3. Average Lake Michigan top-layer velocities for a NNE wind @ 3.8 m/sec.

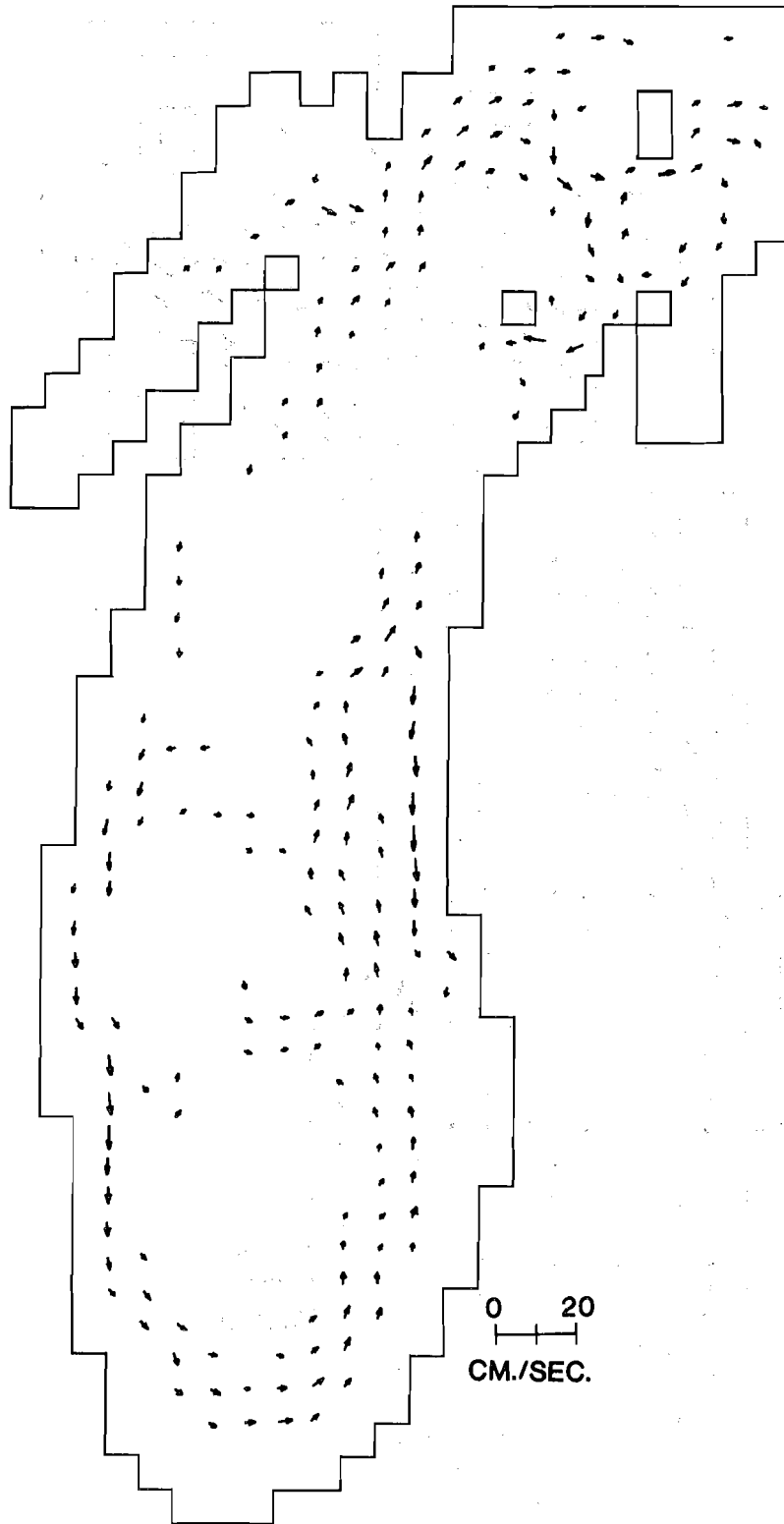


Figure 4. Average Lake Michigan bottom-layer velocities for a NNE wind @ 3.8 m/sec.

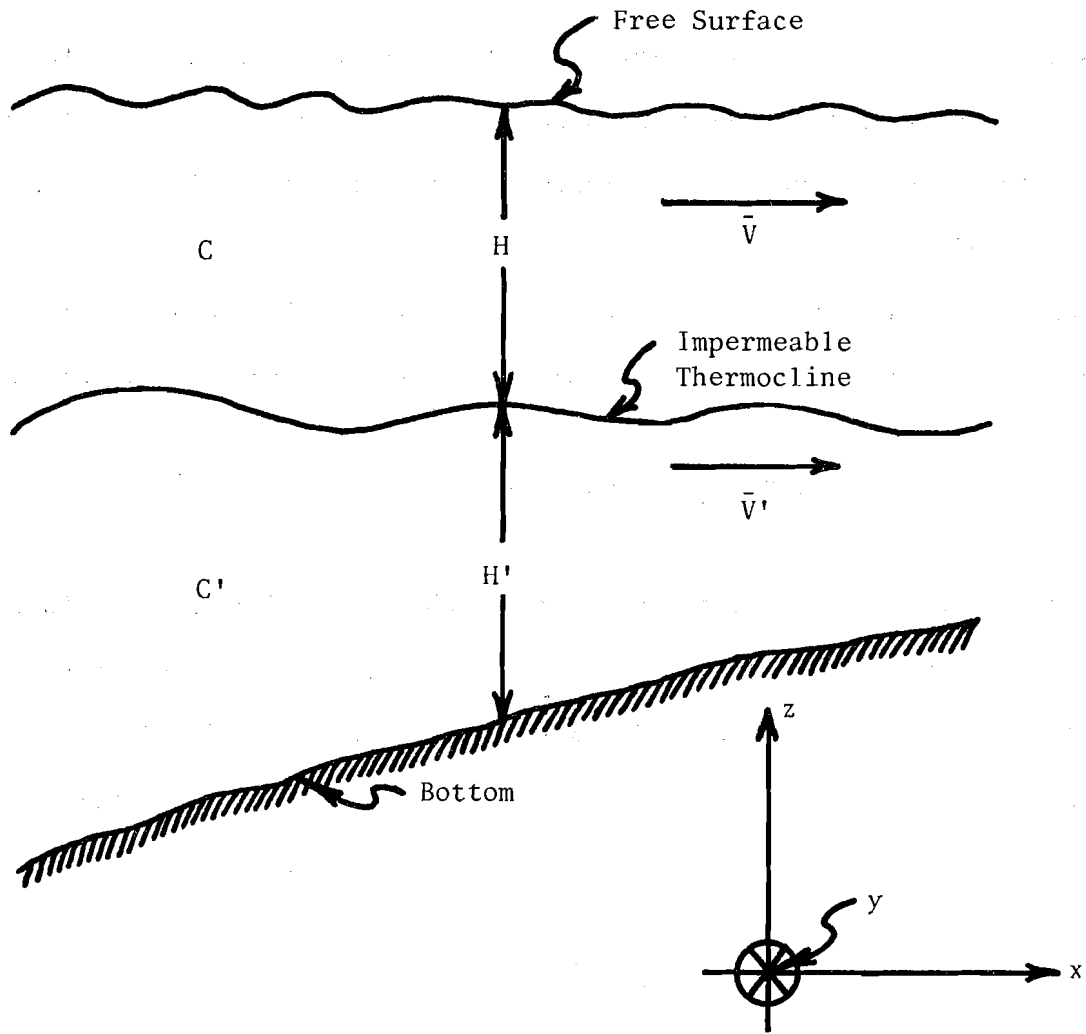


Figure 5. Cross-sectional view of a two-layer lake.

assumed to be known constant or time-varying quantities. Thus, it is possible to consider only one layer at a time with no loss of generality. A rectangular co-ordinate system (Figure 6) divides the map of the entire lake into squares with side Δs , defining cells with depths H_1 at their centers. The C_1 's are pollutant concentrations defined at the cell centers. For purposes of considering five-point differencing schemes, cell 0 is a typical cell, surrounded by cells 1-4.

The two-dimensional second-order partial differential equation governing the dispersion of a conservative pollutant in this case is (Simons 1972)

$$H \frac{\partial C}{\partial t} = - \nabla \cdot [\bar{V}C - HA\nabla(C)] + S(x,y) \quad (1)$$

where the quantities H , C , and \bar{V} are defined above (cf. Figure 5), A is a suitable value of horizontal diffusivity (assumed constant), and $S(x,y)$ is a source term for pollutant introduced to the lake at any point (x,y) .

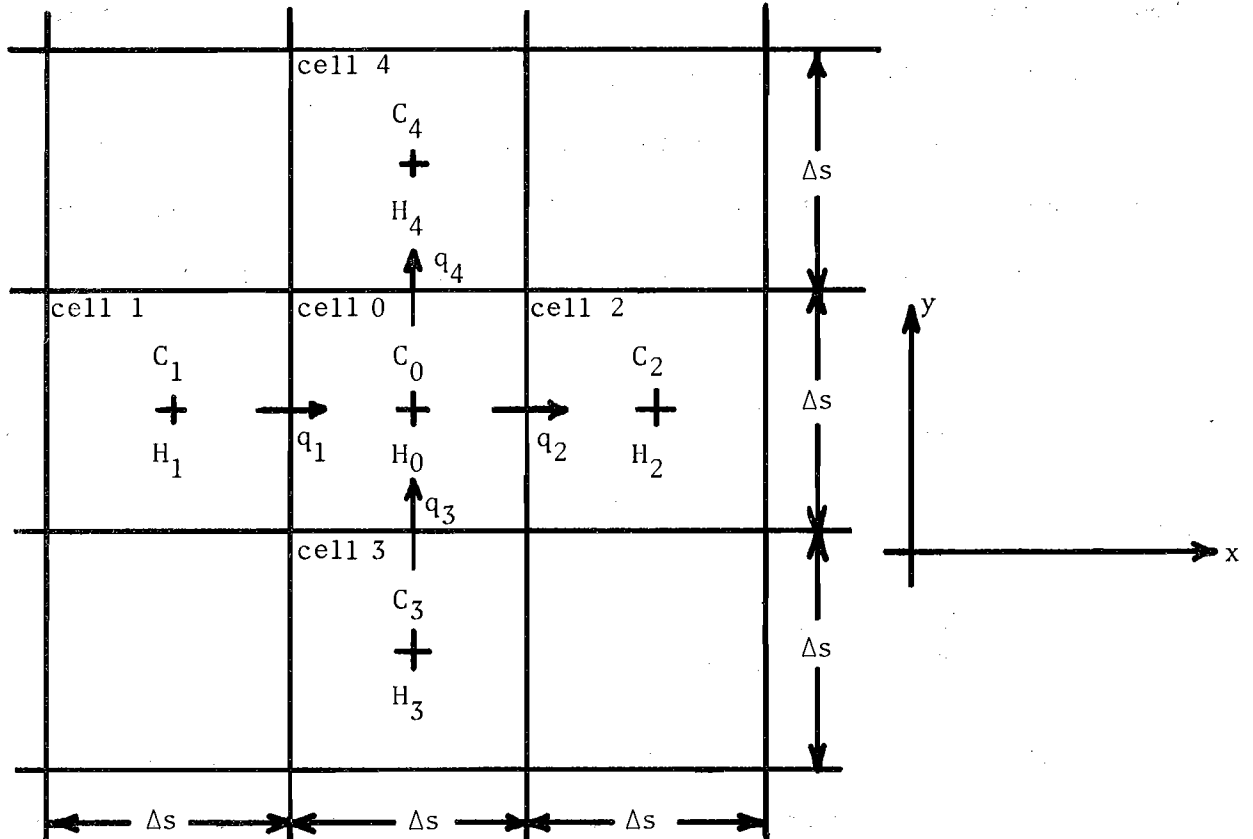
Besides $S(x,y)$, (1) contains one term $f_1 = - \nabla \cdot (\bar{V}C)$ for advection and one term $f_2 = \nabla \cdot [HA\nabla(C)]$ for diffusion. These are expanded below.

$$f_1 = - C \left(\frac{\partial q_x}{\partial x} + \frac{\partial q_y}{\partial y} \right) - q_x \frac{\partial C}{\partial x} - q_y \frac{\partial C}{\partial y} \quad (2)$$

$$f_2 = A \left[H \left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} \right) + \frac{\partial C}{\partial x} \frac{\partial H}{\partial y} + \frac{\partial C}{\partial y} \frac{\partial H}{\partial x} \right] \quad (3)$$

In (2), q_x and q_y are defined by $\bar{V} = q_x \hat{i} + q_y \hat{j}$. Any finite-difference form of equation (1) should satisfy strict mass conservation and minimize error in (single-time-step) approximation of that equation. Strict mass conservation means that the finite-difference scheme should never create or destroy any pollutant within the lake; the advantages of such a scheme in

(a) Top View



(b) Cross-Sectional View through Cell 0

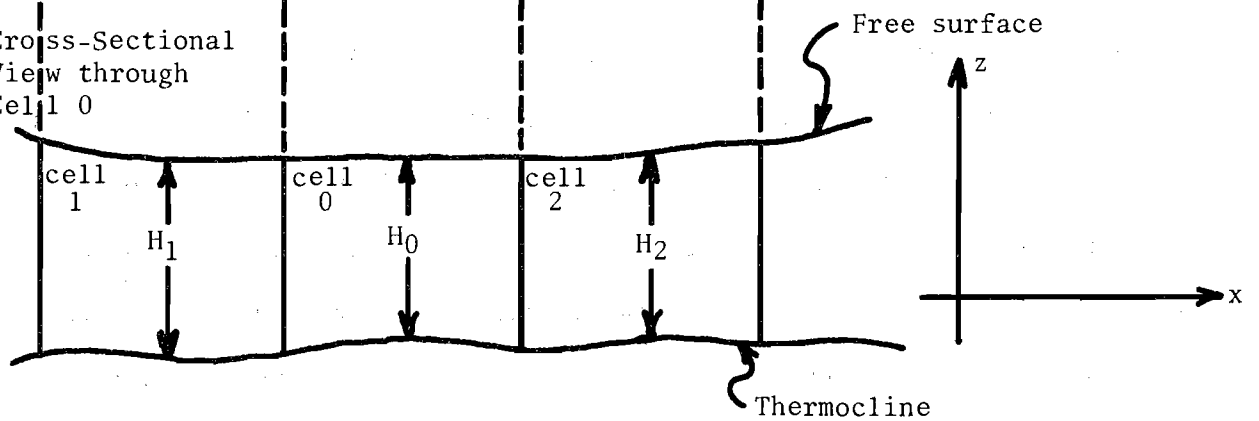


Figure 6. A typical cell and its four surrounding cells in one layer.

preventing changes in pollutant mass (other than those due to pollutant input) are well known (Simons 1973). Mass conservation may only be obtained through a scheme in which any mass transferred from a given cell must be added exactly to the surrounding cells, and vice versa.

It is not at all obvious which finite-differencing scheme will best model equation (1). Analysis (Appendix A) shows, for example, that standard five-point central-difference expressions (Carnahan, et al 1969) such as

$$\frac{\partial C}{\partial x} \approx \frac{C_2 - C_1}{2\Delta s} \quad (4)$$

and

$$\frac{\partial^2 C}{\partial x^2} \approx \frac{C_2 - 2C_0 + C_1}{(\Delta s)^2} \quad (5)$$

lead to both loss of mass conservation and large spatial approximation errors. For the diffusion term f_2 , especially, substitution of expressions such as (4) for the first-order derivatives leads to an error in approximating spatial derivatives which is first-order in Δs .

Consideration of a simple mass balance on cell 0, in which the total mass entering cell 0 during time Δt is approximated in terms of the advective and diffusive fluxes at each side of cell 0, with the values of C and H at a cell boundary set equal to the average of their values in the two cells adjoining that boundary, leads to the following approximation:

$$\begin{aligned}
C_0(t+\Delta t) \cong C_0(t) & \left\{ 1 - \frac{\Delta t}{2H_0(\Delta s)^2} \left[(\Delta s \sum_1^4 (-1)^i q_i) \right. \right. \\
& \left. \left. + A(4H_0 + \sum_1^4 H_i) \right] \right\} \\
& + \sum_1^4 C_i(t) \left\{ \frac{\Delta t [A(H_i + H_0) - (-1)^i q_i (\Delta s)]}{2H_0(\Delta s)^2} \right\} \\
& + (\Delta t)S_0(x,y)
\end{aligned} \tag{6}$$

In (6), $S_0(x,y)$ is the source term for cell 0. Equation (6) (i) may also be derived (Appendix B) by direct finite-differencing of equation (1); (ii) can be shown (Appendix A) to approximate (1) with a second-order error in Δs ; (iii) may be written in the form below:

$$\begin{aligned}
C_0(t+\Delta t) \cong C_0(t) & + (\Delta t)S_0(x,y) \\
& + \sum_1^4 \frac{\Delta t}{2H_0(\Delta s)^2} \{ A[C_i(t) - C_0(t)](H_i + H_0) \\
& - (-1)^i q_i \Delta s [C_i(t) + C_0(t)] \}
\end{aligned} \tag{7}$$

Defining the terms inside the summation as $F_i(t)$, one obtains

$$C_0(t+\Delta t) \cong C_0(t) + (\Delta t)S_0(x,y) + \sum_1^4 F_i(t). \tag{8}$$

Each $F_i(t)$ represents the total (diffusive and advective) inflow of pollutant from cell i to cell 0 in the interval $(t, t+\Delta t)$, and depends upon only the two concentrations adjoining the boundary it represents. (e.g., $F_1(t)$

depends only on $C_1(t)$ and $C_0(t)$.) Furthermore, the dependence of F_i on C_i and C_0 is symmetrical, as may be seen from equation (7) for updating the concentration in cell 0 and the corresponding equation for updating (say) adjoining cell 2 (cf. Figure 6). The pollutant flow from (or to) cell 0 to (or from) cell 2 in the first equation is identical to that in the second equation. Since this situation obtains for all pairs of adjoining cells and thus for all flows, equation (7) (and thus (6)) is strictly conservative of mass in the entire lake. Finally, observe that boundary conditions are easily treated, since the term in (8) corresponding to dispersion across a particular boundary may simply be set to zero if the adjoining cell is dry.

One might consider using a nine-point differencing scheme to obtain a higher-order error in Δs than that obtained from the five-point scheme in equation (8). The author has been unable, however, to formulate a nine-point scheme which will satisfy (more complicated) symmetry conditions analogous to those satisfied by (7) and thus be guaranteed to conserve mass. Furthermore, nine-point schemes would make treatment of the boundary conditions much more difficult.

Saturation Mechanism

Consider again the typical cell 0 and its four neighbors in the finite-difference scheme, as shown in Figure 6. The advective terms of (6) above assume a concentration variation which is piecewise linear in space, as shown in Figure 7, so that the concentration at any cell boundary (except for land-water boundaries) is taken as the average of the concentrations at the centers of the cells forming the boundary. The use of such average concentration values can be shown (Appendix C) to approximate the original

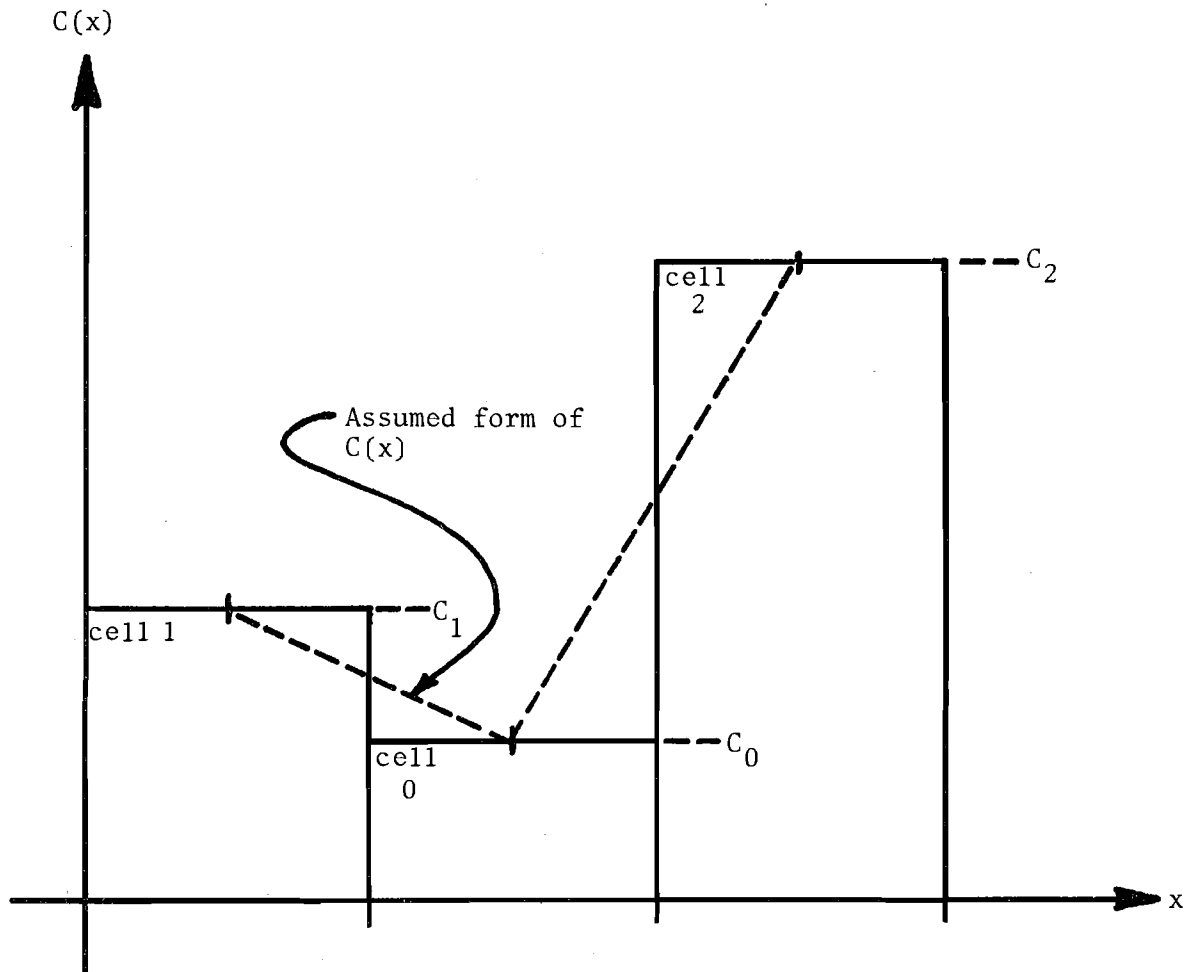


Figure 7. Concentration along a cross-section through cell 0.

differential equation (1) more accurately than does a step approximation proposed elsewhere (Bella and Dobbins 1968) as part of an upstream-differencing scheme. The use of average concentration values, however, leads to certain computational difficulties.

Consider the case depicted in Figure 8, which shows a cross-section of cells 1, 0, and 2, where cell 2 has a fairly large pollutant concentration and cells 0 and 1 have negligible concentration levels. Further, let all flows into cell 0 be zero except for q_2 which is positive. Because the averaging procedure indicates a concentration $C_2/2$ at the boundary (2, 0), and because q_2 is positive as shown, the model indicates that pollutant flows out of cell 0 into cell 2 at the boundary (2, 0), even though $C_0 \cong 0$ (at time t). This flow causes C_0 to become negative at $t+\Delta t$, which is physically unreasonable.

The resultant negative concentration in cell 0 could simply be set to zero, since it is usually small in magnitude compared with C_2 . The resulting addition of total pollutant, over the entire lake, could become quite significant after many iterations and in the long run would therefore destroy the otherwise strictly mass-conservative nature of the algorithm.

One might consider simply banning any advective flows of pollutant from an empty cell. This step, however, would not properly prevent negative concentrations in the case of a cell which contained a very small original concentration, or a cell which experienced a very small inflow during the time step. Such cells might easily be flushed by a large flow across boundary (2, 0). Alternatively, it might be determined beforehand whether a given flow would flush cell 0. In practice, with q_1, q_2, q_3 and/or $q_4 \neq 0$, such a determination would require checking of all the pollutant transfers into

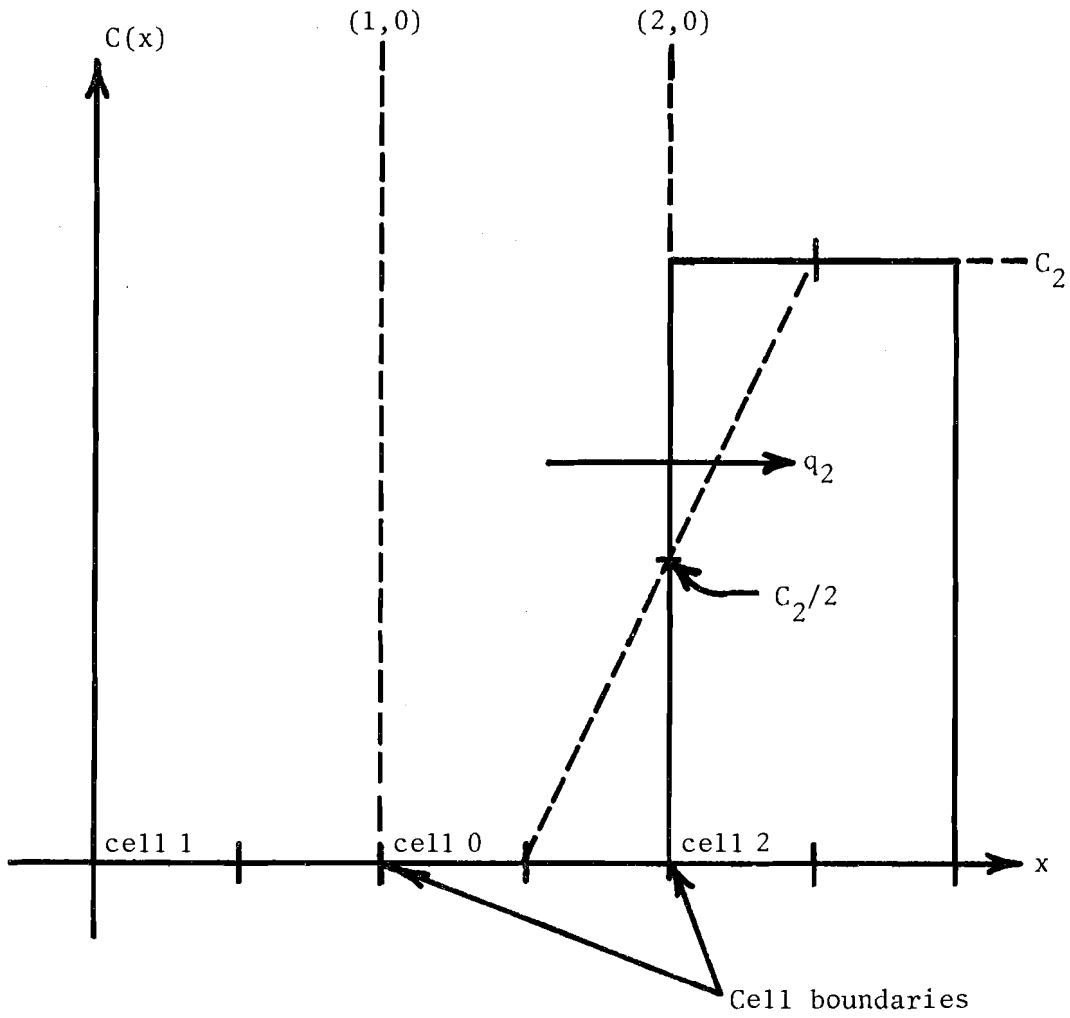


Figure 8. A case in which negative concentrations occur.

and out of cell 0 prior to every concentration updating in that cell.

Thus, to avoid the previously mentioned loss of mass conservation or a priori checking, the following saturation mechanism for pollutant flows was used to prevent the occurrence of negative concentrations.

During the time interval $(t, t+\Delta t)$, for each application of equation (8) to any cell 0, $-F_i$ is the total outflow from cell 0 at the boundary $(i, 0)$.

$C_0(t+\Delta t)$ is first evaluated using equation (8); if $C_0 \geq 0$, the value of $C_0(t+\Delta t)$ is allowed to stand, and no additional computation is necessary in cell 0 until the entire lake has been updated. If the above value of $C_0(t+\Delta t) < 0$, this negative concentration $C_0(t+\Delta t)$ is added to the concentrations in cells 1, 2, 3, and/or 4 at time $t+\Delta t$, in the proportion in which these cells contributed to the outflow from cell 0, and $C_0(t+\Delta t)$ is set to zero. In other words, if pollutant flow from cell 0 saturates with $C_0(t+\Delta t) < 0$, $C_i(t+\Delta t)$ ($i = 1, 2, 3, 4$) is decreased by an amount

$$K_i = \frac{F_i'}{F_1' + F_2' + F_3' + F_4'} \left| C_0(t+\Delta t) \right| \frac{H_0}{H_i} \quad (9)$$

where $F_i' = F_i$ if $F_i < 0$, and $F_i' = 0$, otherwise. Obviously,

$\sum K_i H_i = H_0 C_0(t+\Delta t) =$ ("negative pollutant mass" in cell 0) / $(\Delta s)^2$, so that the above correction procedure is, in fact, mass conservative.

The corrections K_i are added to the $C_i(t+\Delta t)$'s after all cells in the entire lake have been updated, to make the saturation mechanism solely dependent upon conditions at time t and thus to avoid any bias in the treatment of cells which might not have been reached in the "marching" procedure.

If the concentration in one of the cells adjoining cell 0 is very small in comparison with any one of the others, it is possible that one or more

successive corrections might cause such a cell to have a negative concentration at the end of the correction procedure. Such over-correction is prevented in the following way:

If C_i ($i = 1, 2, 3, 4$) is very small in comparison with C_j ($j = 1, 2, 3, 4, j \neq i$), with $F_i < 0$ and $F_j < 0$, cell i could be over-corrected and C_i could become negative. Also, if cell i is subject to over-correction, then $|F_i| \ll |F_1' + F_2' + F_3' + F_4'|$, because the flow F_i would clearly not be enough to flush cell i if a return of some small fraction of $C_0(t+\Delta t)$ is enough to flush cell i . Therefore, over-corrections are avoided by not including cell i ($i = 1, 2, 3, 4$) in the corrections of cell 0 if $|F_i| < 0.01|F_1' + F_2' + F_3' + F_4'|$, and absorbing cell i 's share of the correction in the other cells surrounding cell 0 , to maintain mass conservation.

This modification may be applied whether or not an over-correction would, in fact, occur. If including cell i in the corrections to cell 0 would cause over-correction in cell i , because C_i is too small, this modification prevents the over-correction. If C_i is sufficiently large as to prevent over-correction, and the modification is applied anyway (due to $|F_i| < 0.01|F_1' + F_2' + F_3' + F_4'|$), the correction procedure is only modified by (at most) 1% of the total correction to C_0 . This particular modification to prevent over-correction was chosen over others largely because of its uncomplicated (single-decision) criterion.

Spatial and Temporal Step Sizes Used for Lake Michigan

For Lake Michigan, a grid spacing of $\Delta s = 10.8\text{km}$ was used, giving a system of 24 squares by 46 squares, with a time step of $\Delta t = 1$ hour. For this system, in tests run for over 3000 hours, the total pollutant mass

appearing in the lake never differed from the amount introduced by more than a few tenths of one per cent, the slight error being apparently introduced by machine round-offs.

Treatment of Sources

A time-varying pollutant source may be introduced in any cell in the lake. The fraction of pollutant introduced into each layer from a given river or stream source is, in practice, taken as the fraction of the total depth at the source corresponding to that layer; that fraction is, of course, a function of thermocline position. This scheme of apportioning pollutant input between the two layers assumes essentially complete mixing at a point source in a two-layer region. This assumption is a reasonable first approximation in the absence of either experimental data or a detailed plume model for actual mixing at the mouths of the various rivers and streams. The available discharge data were deemed of insufficient quality to justify the use of one of the available river plume models (e.g., Paul and Lick 1974; Strazisar and Prah1 1973).

Horizontal Eddy Diffusivity Values

Empirical estimates of the horizontal diffusivity A in (1) range from $10^4 \text{ cm}^2/\text{sec}$ to $10^5 \text{ cm}^2/\text{sec}$ (Murthy 1970 and Okubo 1971, quoted by Simons 1972). In extensive tests of the model, diffusion was a relatively small effect in comparison with wind-driven advection, even for the larger diffusivity considered, i.e., the value of A had little effect upon the more significant pollutant concentration contours generated as the Lake Ontario results to follow show. For the Lake Michigan results to follow, $10^5 \text{ cm}^2/\text{sec}$ diffusivity was used throughout.

Homogeneous Lake Model

Both the circulation and pollutant dispersion models used are readily adaptable to single-layer (winter) lakes, as will also be shown.

Use of Steady-State Circulations

To approximate actual time-varying circulations with sequences of "steady-state" circulations in the first two applications shown and thus simplify the computational procedure, each simulation period was divided into sub-periods of from three to nine days in length. Within each sub-period the observed wind had essentially the same direction and speed. Steady-state circulations had already been computed and stored for each of sixteen "standard" 3.8 m/sec (8.5 mph) winds (N, NNE, NE, ENE, E, etc.) and an approximate wind history was formed by selecting the closest approximation to the mean observed wind for each subperiod from among the sixteen standard winds. This use of step approximation to actual circulations seems reasonable, especially in light of some recent current-meter observations (Snow and Adamczyk 1974).

APPLICATIONS

125-Day Chloride Dispersion Simulation

Chloride dispersion corresponding to the 125-day period from May 28, 1970 through September 29, 1970 was simulated using U.S. Weather Service daily wind data for Chicago during that period as the basis for an approximate wind history for the entire lake. The use of Chicago data corresponds to the intentional emphasis upon modeling the southern end of the lake. Nineteen sub-periods were used in approximating observed winds; these sub-periods, their average observed winds, and the standard winds used to approximate them, are listed in Table 1.

The model's pollutant inputs were based upon all available USEPA chloride and stream flow measurements for streams and rivers discharging into Lake Michigan for the given period. There are 27 such sources listed in the available data, with measurements usually reported no more often than once a month. Often only a few data points were taken over a number of years for a given source. Considerable interpolation was, therefore, necessary; in general, the input level from each source during each of the sub-periods listed in Table 1 was taken as the mean of the two data points encompassing all or most of the sub-period. In cases where the data were especially insufficient, long-term average discharge values were used; such cases generally involved smaller sources. The most significant sources, mostly on the eastern shore of the lake, generally had the best data available. In addition to the river and stream flows mentioned, a single very significant industrial discharge directly into the lake at Manistee, Michigan, was included; the average discharge value for this source, as obtained from the USEPA, was used.

Table 1. 125-day wind history (5/28/70 - 9/29/70).

| Subperiod # | Dates (1970) | Average Wind Direction (Degrees from North) | Average Wind Speed (m/sec) | Nearest Standard 3.8m/sec Wind |
|-------------|--------------|---|----------------------------|--------------------------------|
| 1 | 5/28-6/1 | 162 | 4.6 | SSE |
| 2 | 6/2 -6/6 | 32 | 5.0 | NNE |
| 3 | 6/7 -6/13 | 183 | 4.8 | S |
| 4 | 6/14-6/21 | 173 | 4.5 | S |
| 5 | 6/22-6/28 | 177 | 4.6 | S |
| 6 | 6/29-7/3 | 246 | 4.8 | WSW |
| 7 | 7/4 -7/11 | 305 | 4.4 | NW |
| 8 | 7/12-7/19 | 231 | 4.5 | SW |
| 9 | 7/20-7/23 | 60 | 4.1 | ENE |
| 10 | 7/24-7/30 | 197 | 3.8 | SSW |
| 11 | 7/31-8/2 | 257 | 3.4 | WSW |
| 12 | 8/3 -8/11 | 91 | 3.9 | E |
| 13 | 8/12-8/18 | 204 | 3.7 | SSW |
| 14 | 8/19-8/23 | 242 | 3.4 | WSW |
| 15 | 8/24-8/30 | 210 | 4.2 | SSW |
| 16 | 8/31-9/6 | 171 | 4.2 | S |
| 17 | 9/7 -9/13 | 190 | 4.7 | S |
| 18 | 9/14-9/20 | 177 | 3.6 | S |
| 19 | 9/21-9/29 | 229 | 4.3 | SW |

All 28 chloride sources and their mean discharge levels over their respective periods of record are listed in Table 2.

Because insufficient data were available for a realistic initial chloride distribution, the lake was assumed to be free of chloride at the start of the simulation period (zero initial conditions). This use of zero initial conditions obviously causes the model to underestimate long-term chloride levels and to overestimate short-term dispersion somewhat due to unrealistic concentration gradients near sources.

Figures 9 through 16 show computed chloride distributions for the period considered. In all of these figures, the numbers outside the lake boundary indicate the locations of the chloride sources as listed in Table 2. Figures 9, 10, 11, and 12 show top-layer distributions at 32, 64, 95, and 125 days, respectively, after the start of simulation; Figures 13, 14, 15, and 16 show bottom-layer distributions at the same four elapsed times.

Because of the simplifying assumptions (particularly the assumption of zero initial conditions) and approximations made in adapting the available data, the model cannot presume to give a precise picture, in time and space, of chloride concentrations in Lake Michigan during the summer of 1970. Some general conclusions may be drawn, however, regarding the general behavior of chloride (and other conservative pollutants released near shore) under realistic wind conditions. The model exhibits the "coastal entrapment" (Csanady 1973) observed in the actual lake; that is, most of the pollutant discharged clearly tends to stay near its sources, and dispersion is dominated by strong coastal flows resulting in relatively low concentration levels far offshore. Under steady wind conditions, few large pollutant accumulations are observed, but during periods of highly variable winds the changing

Table 2. Lake Michigan chloride sources.

| Source # | Source | Average Chloride Discharge (g/sec) |
|----------|--|------------------------------------|
| 1 | Ford River | 42.7 |
| 2 | Portage Creek | 3.4 |
| 3 | Whitefish River | 26.7 |
| 4 | Manistique River | 140.3 |
| 5 | Pine River | 67.9 |
| 6 | Elk River | 31.4 |
| 7 | Boardman River | 31.9 |
| 8 | Betsie River | 42.9 |
| 9 | Manistee River | 4130.8 |
| 10 | Pere Marquette River | 880.7 |
| 11 | Pentwater River | 62.4 |
| 12 | White River | 766.5 |
| 13 | Muskegon River | 1398.6 |
| 14 | Black Creek | 85.4 |
| 15 | Grand River | 3600.6 |
| 16 | Kalamazoo River | 1437.5 |
| 17 | Black River | 282.7 |
| 18 | St. Joseph River | 1768.8 |
| 19 | Galien River | 55.7 |
| 20 | Root River | 250.7 |
| 21 | Kewaunee River | 24.2 |
| 22 | Peshtigo River | 26.6 |
| 23 | Menominee River | 140.5 |
| 24 | Oconto River | 115.7 |
| 25 | Sheboygan River | 125.2 |
| 26 | Fox River | 1516.8 |
| 27 | Milwaukee River | 442.5 |
| 28 | Paper Co. Discharge at Manistee, Mich. | 2000.0 |

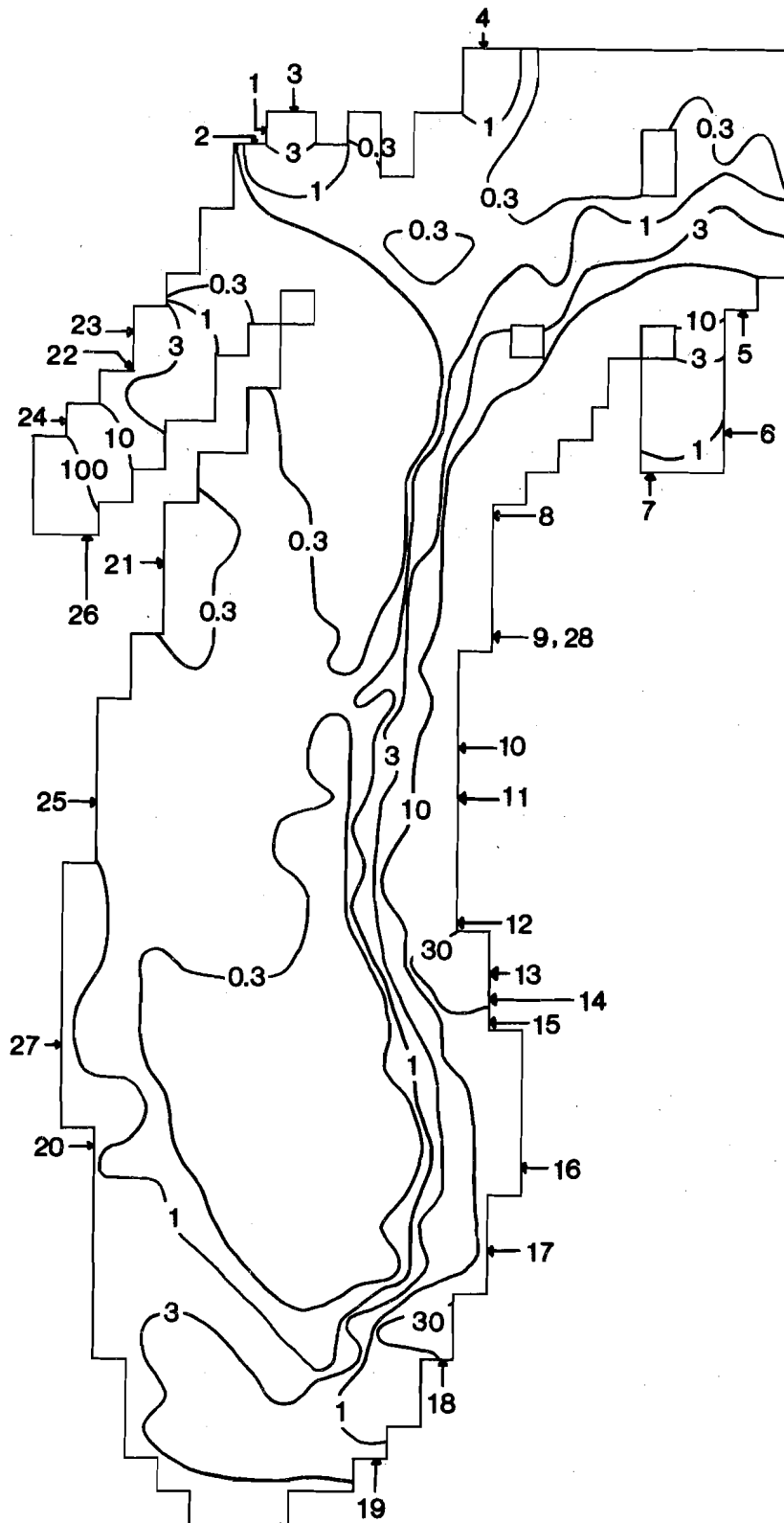


Figure 9. 125-day chloride dispersion simulation: Lake Michigan top-layer chloride concentration contours for June 28, 1970 (32 days elapsed time) in units of 10^{-8} g/cm^3 .

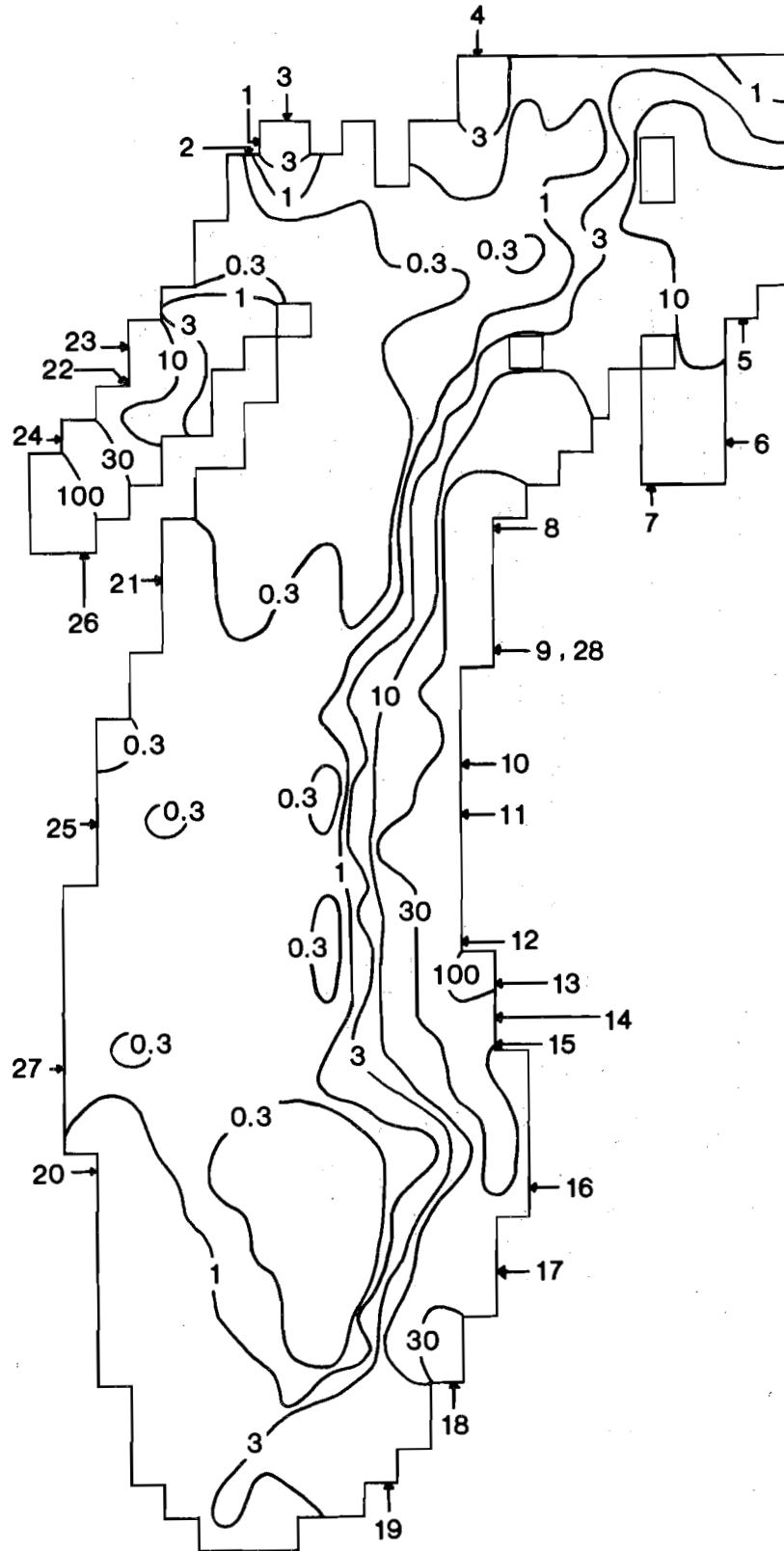


Figure 10. Same as Figure 9, but for July 30, 1970 (64 days elapsed time).

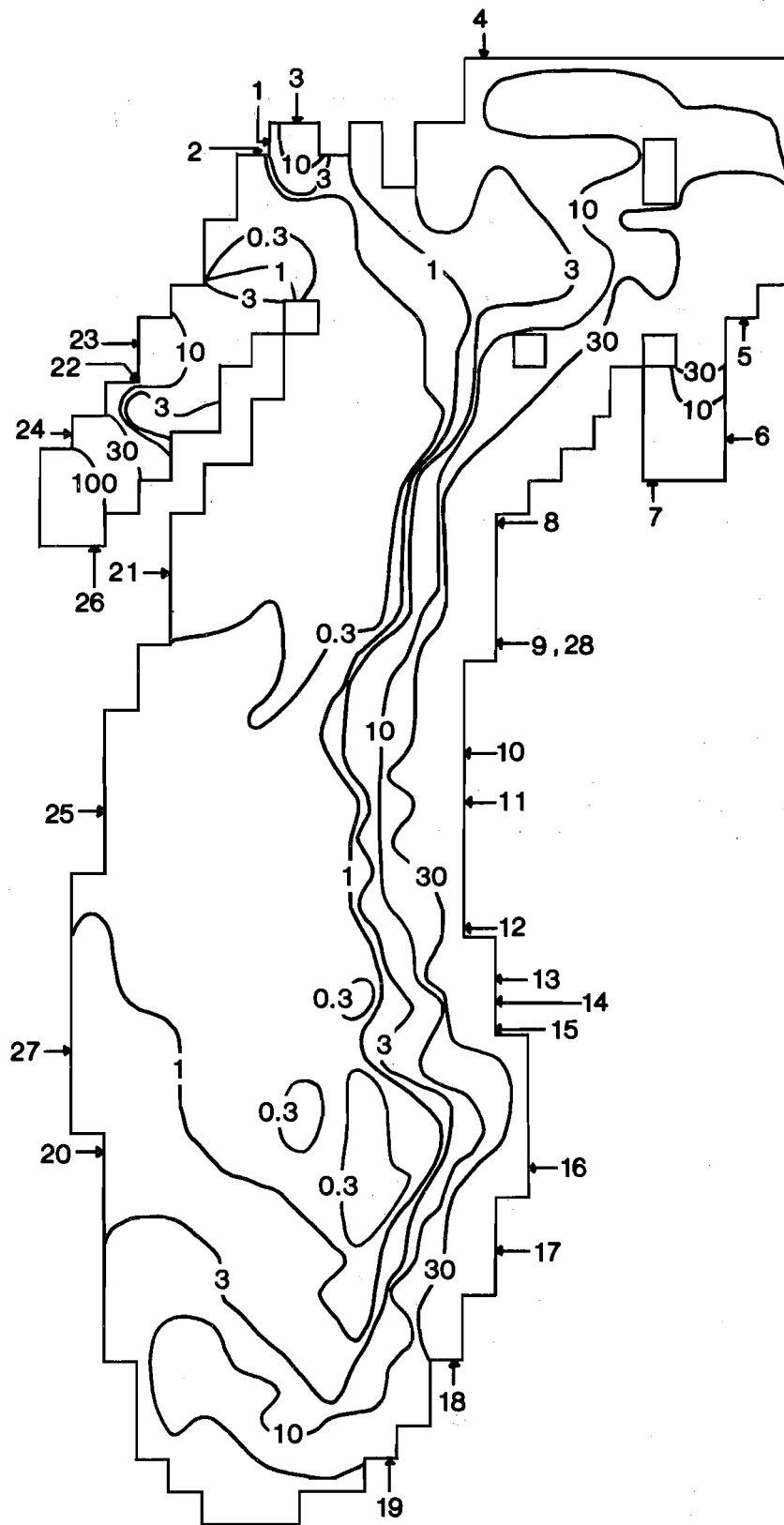


Figure 11. Same as Figure 9, but for August 30, 1970 (95 days elapsed time).

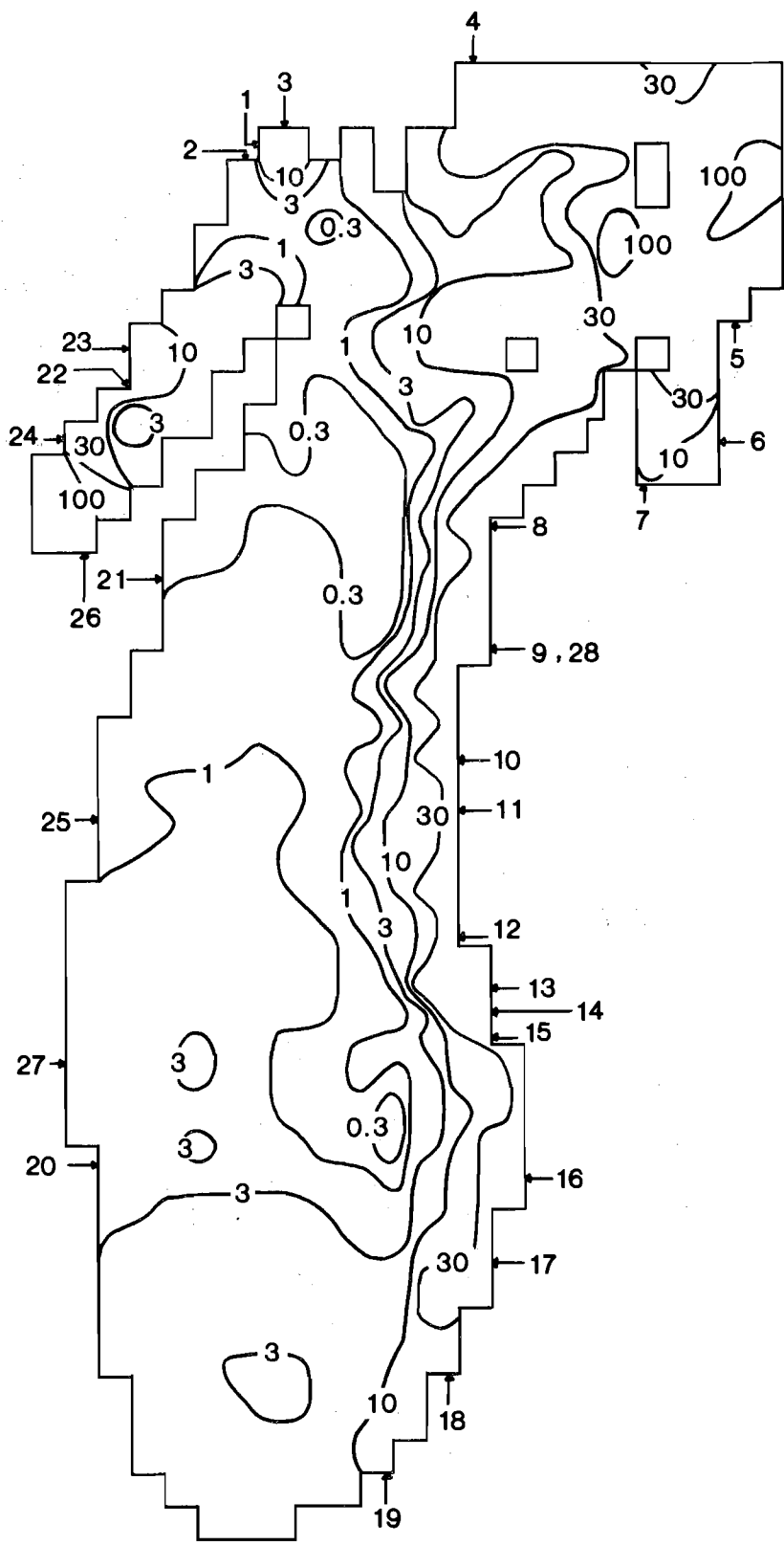


Figure 12. Same as Figure 9, but for September 30, 1970 (125 days elapsed time).

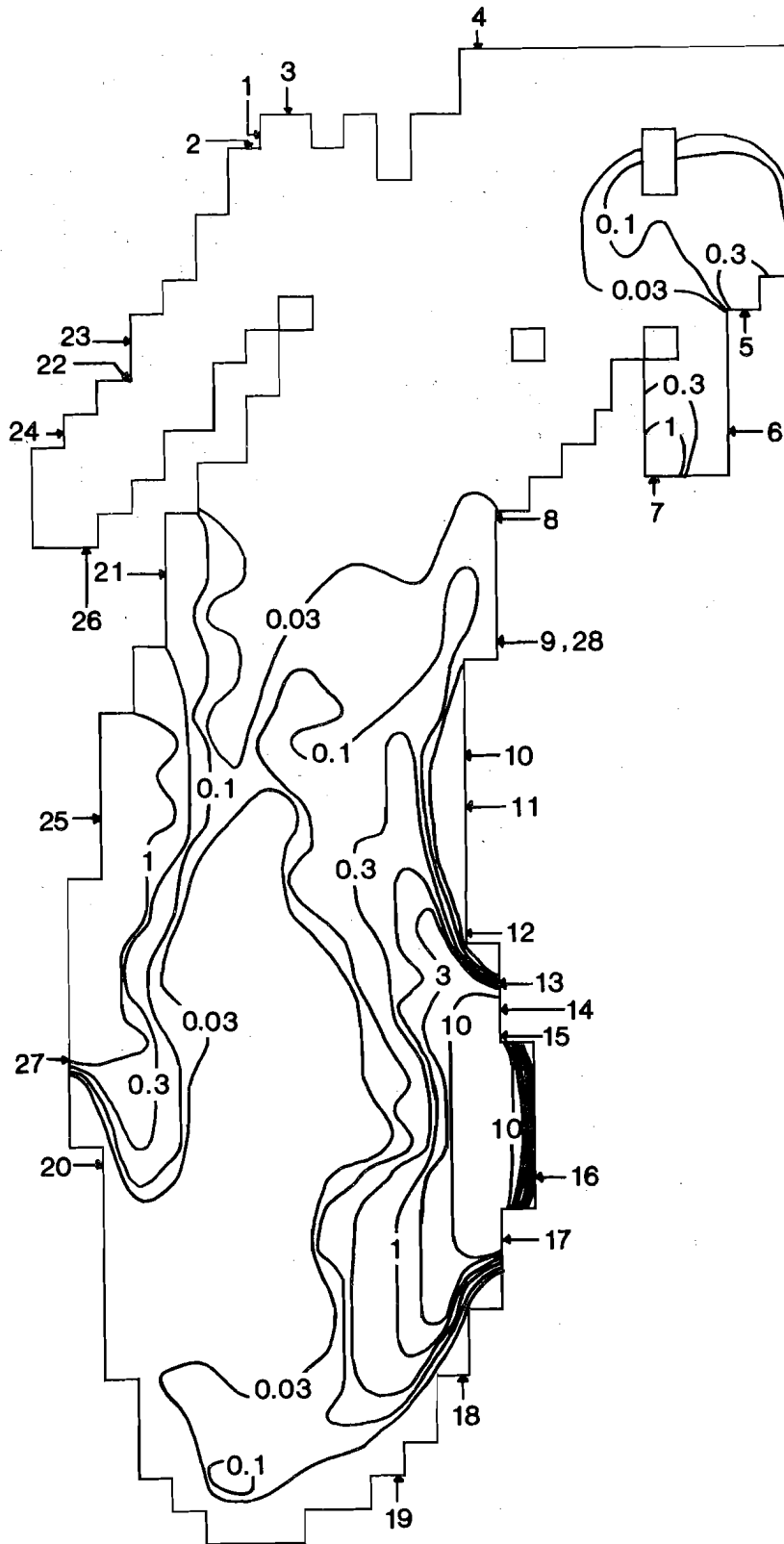


Figure 13. 125-day chloride dispersion simulation: Lake Michigan bottom-layer chloride concentration contours for June 28, 1970 (32 days elapsed time) in units of 10^{-8} g/cm^3 .

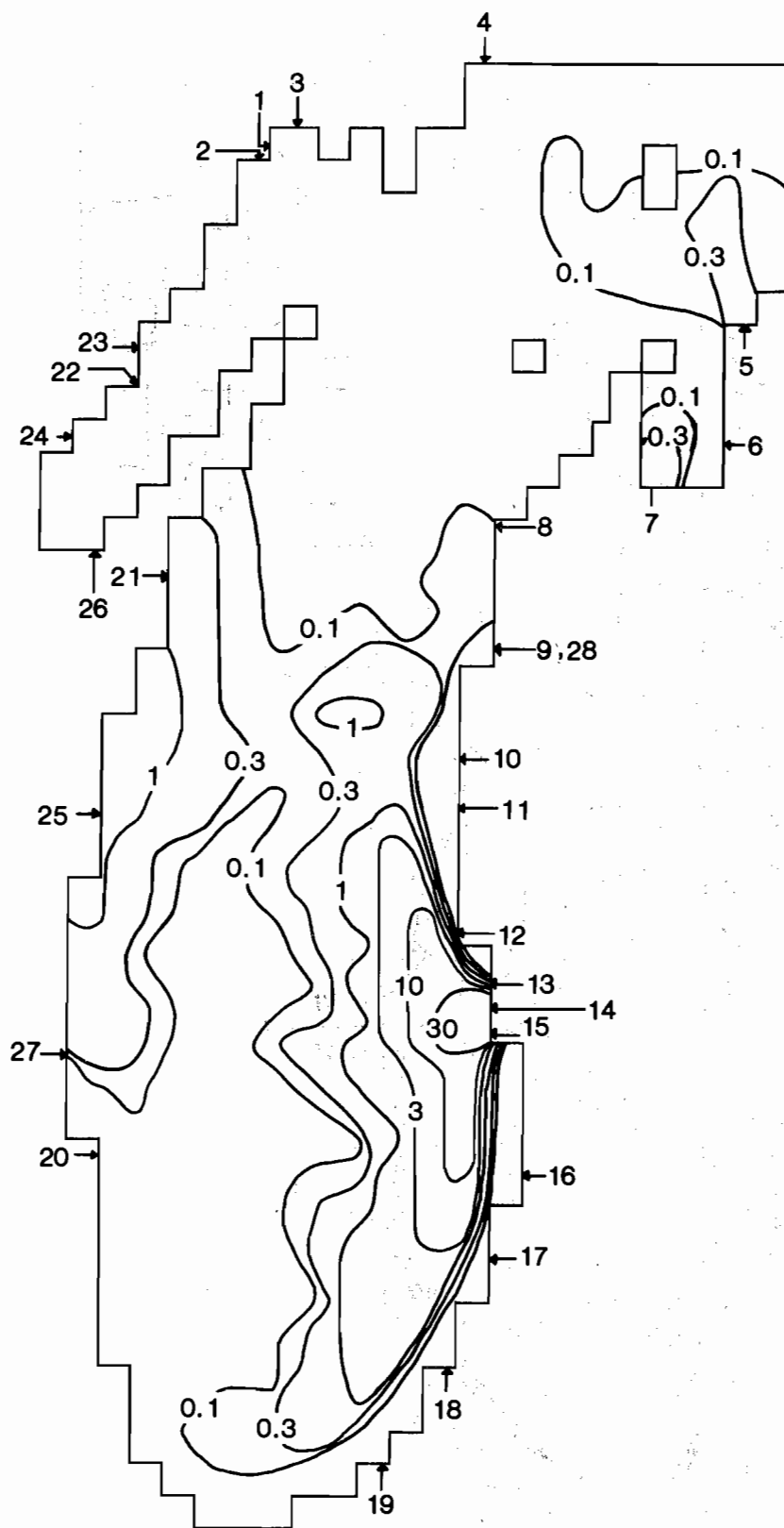


Figure 14. Same as Figure 13, but for July 30, 1970 (64 days elapsed time).

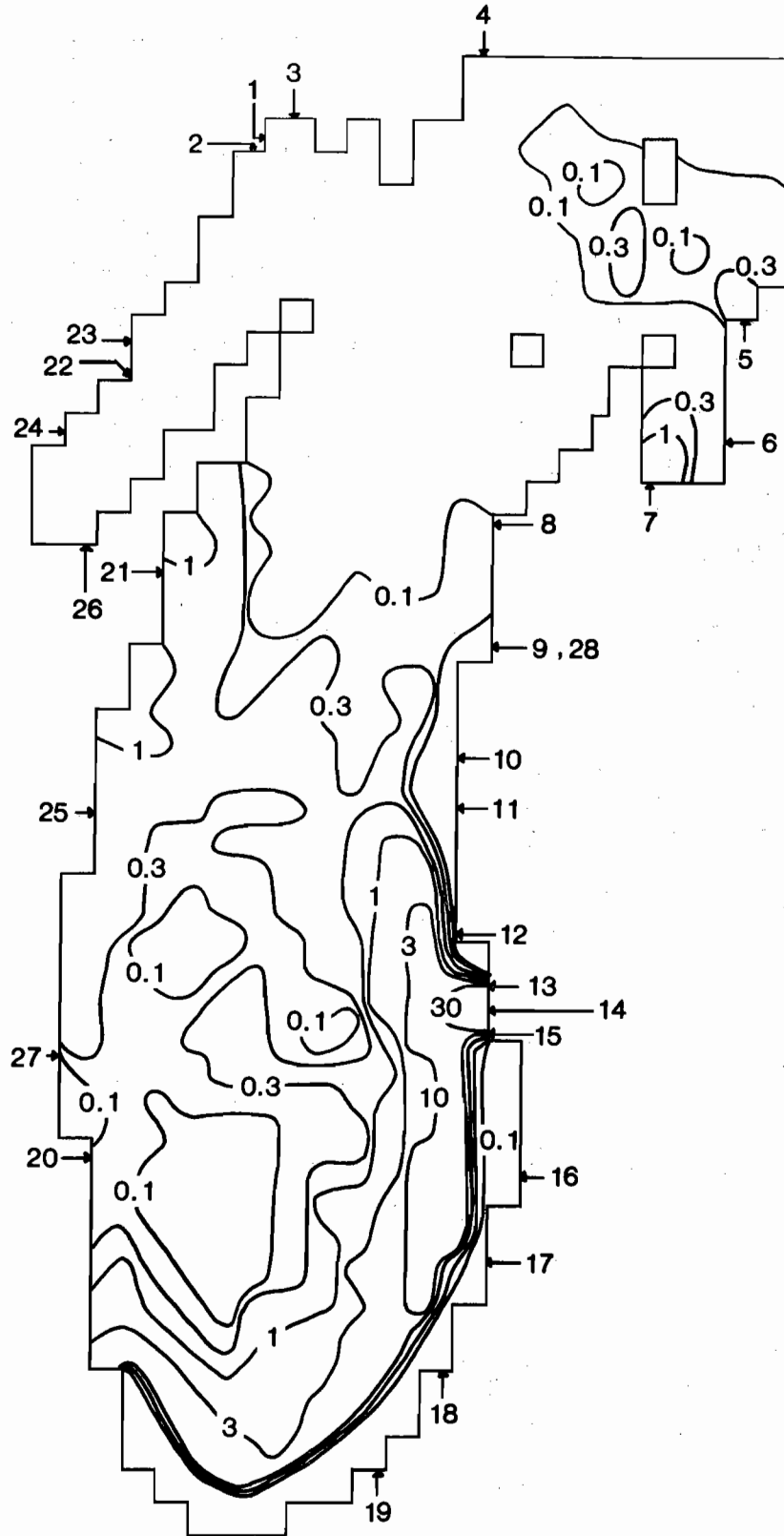


Figure 15. Same as Figure 13, but for August 30, 1970 (95 days elapsed time).

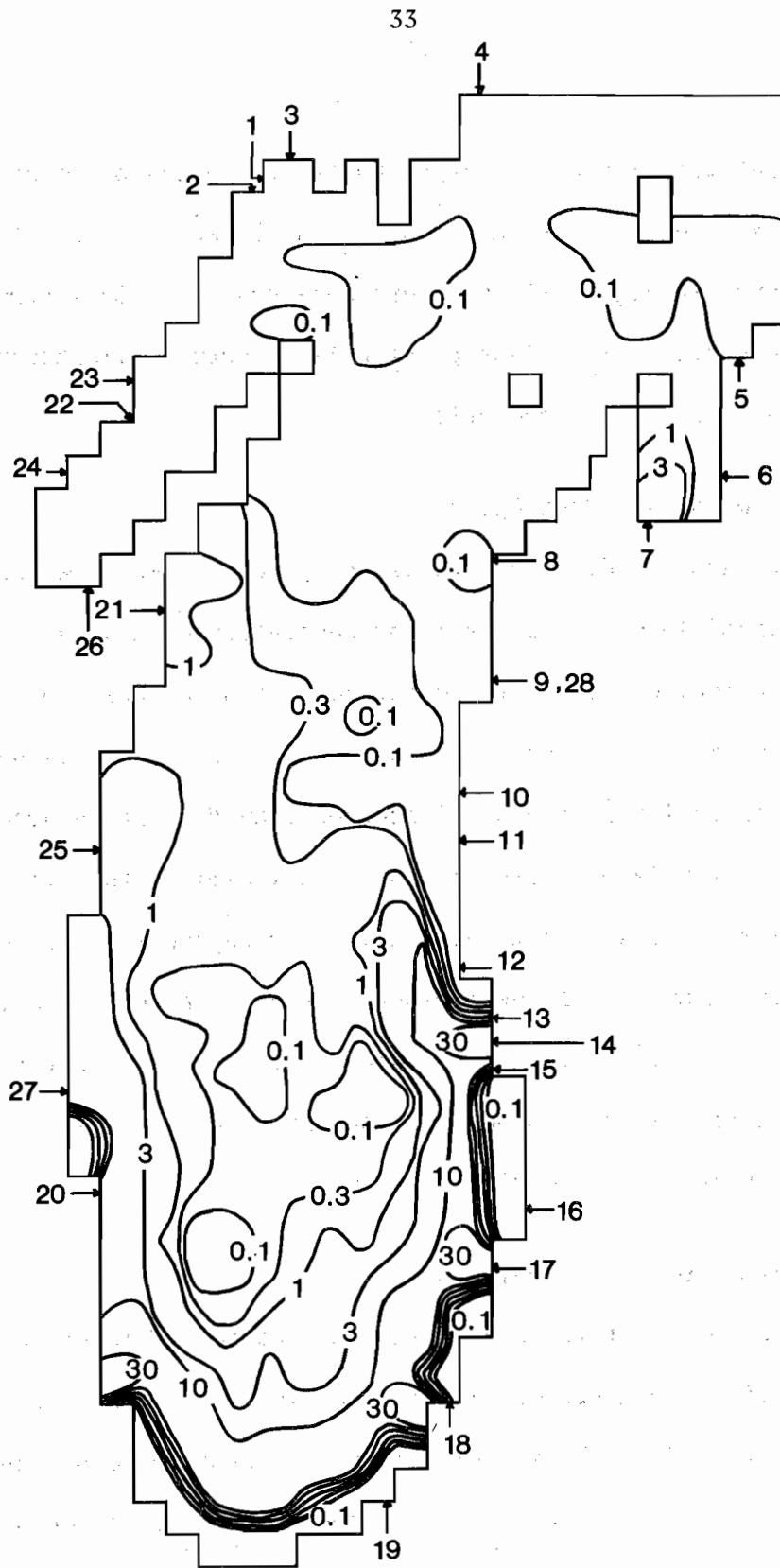


Figure 16. Same as Figure 13, but for September 30, 1970 (125 days elapsed time).

circulation patterns may cause large short-term build-ups in areas far removed from major sources. Such build-ups may be seen in almost the center of the top layer in Figure 12, and were observed often in intermediate results not shown here. This last point will be better illustrated by the best and worst cases described below.

Definition of Worst and Best Cases

A "worst case" is defined here as an episode in which a "slug" of pollutant discharged into the lake remains concentrated in an area (particularly a nearshore region) close to its source for a considerable period of time (say several weeks). A "best case", similarly, is defined as an episode in which a slug of pollutant rapidly disperses away from its source and nearby areas. Because top-layer flows are not at all similar to bottom-layer flows, best and/or worst cases do not necessarily correspond for the two layers. Only top-layer examples will be presented here. Wind conditions for the probable occurrence of best and worst cases were determined through experimentation with the dispersion model; such wind conditions are, however fairly common in the Chicago area during the summer.

Worst Case 33-Day Episode Simulation

A worst case is apt to occur during any period of large, abrupt changes in wind direction; such periods often occur in Chicago, in the summer, as prevailing south and southwest Gulf winds are interrupted by the passage of successive cold fronts. The example presented here corresponds to one such period, July 30, 1971 through August 31, 1971 (33 days). For this period, an approximate history of standard winds was fitted to the observed average winds for seven sub-periods, as described above; the sub-periods and their

average and standard winds are listed in Table 3. For purposes of illustration, a slug of pollutant (10^4 g/sec for 24 hours on July 30) was assumed to be discharged into Calumet Harbor from a single source, with zero initial concentration elsewhere.

Figures 17 through 19 show computed pollutant distributions at 7, 25, and 32 days, respectively, after the pollutant slug's introduction.

Best Case 33-Day Episode Simulation

A best case is apt to occur during any period in which the wind maintains an almost constant direction. The Chicago area frequently has month-long periods of prevailing south and southwest winds, with accompanying high temperatures. Results are given here for such a period, lasting 33 days from August 24, 1970 through September 29, 1970. The sub-periods used, their average winds, and their nearest standard winds are listed in Table 4. A slug of pollutant identical to that used for the worst case above was introduced on August 24. Figures 20 through 22 show calculated concentration patterns at 6, 20, and 32 days, respectively, after the introduction of this slug.

Comparison of Worst and Best Cases

In the worst case (Figures 17-19), the pollutant slug remains concentrated near its point of release for the entire 33-day period due to the absence of a prolonged, steady current. In the best case (Figures 20-22), the slug quickly disperses over much of the top layer due to a nearly constant coastal current. The concentration at Calumet Harbor after 32 days is approximately 10^{-8} g/cm³ in the worst case, but is only about 3×10^{-10} g/cm³ in the best case. Notice also that in the best case the "center" of

Table 3. Worst case wind history (7/30/71 - 8/31/71).

| Subperiod # | Dates (1971) | Average Wind Direction (Degrees from North) | Average Wind Speed (m/sec) | Nearest Standard 3.8m/sec Wind |
|-------------|--------------|---|----------------------------|--------------------------------|
| 1 | 7/30-8/2 | 233 | 4.2 | SW |
| 2 | 8/3 -8/6 | 50 | 4.4 | NE |
| 3 | 8/7 -8/13 | 220 | 4.3 | SW |
| 4 | 8/14-8/17 | 50 | 3.9 | NE |
| 5 | 8/18-8/24 | 190 | 4.4 | S |
| 6 | 8/25-8/28 | 320 | 4.4 | NW |
| 7 | 8/29-8/31 | 100 | 3.3 | E |

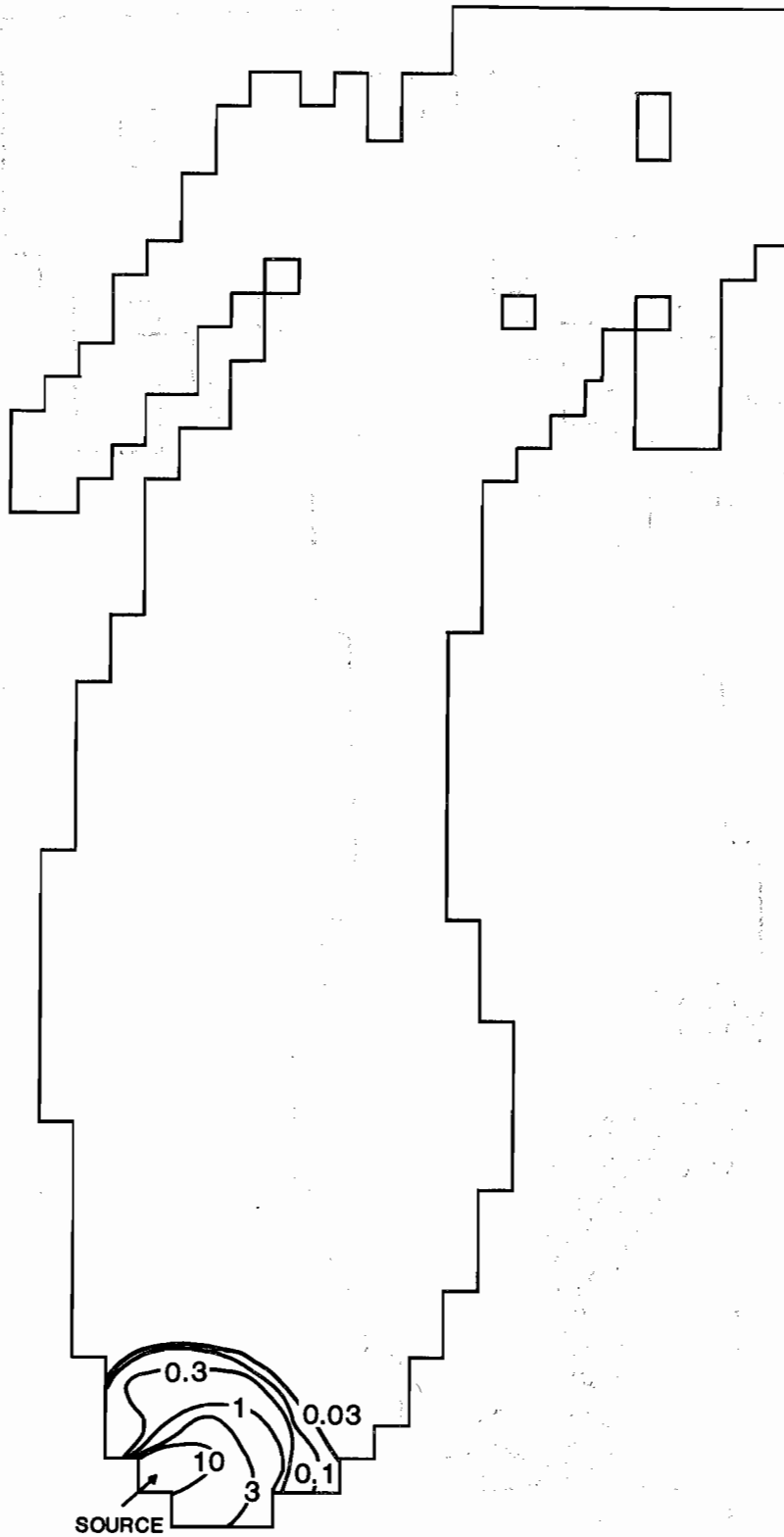


Figure 17. Worst case 33-day episode simulation: pollutant distribution 7 days after the introduction of a pollutant slug at Calumet Harbor (units of 10^{-8} g/cm³).

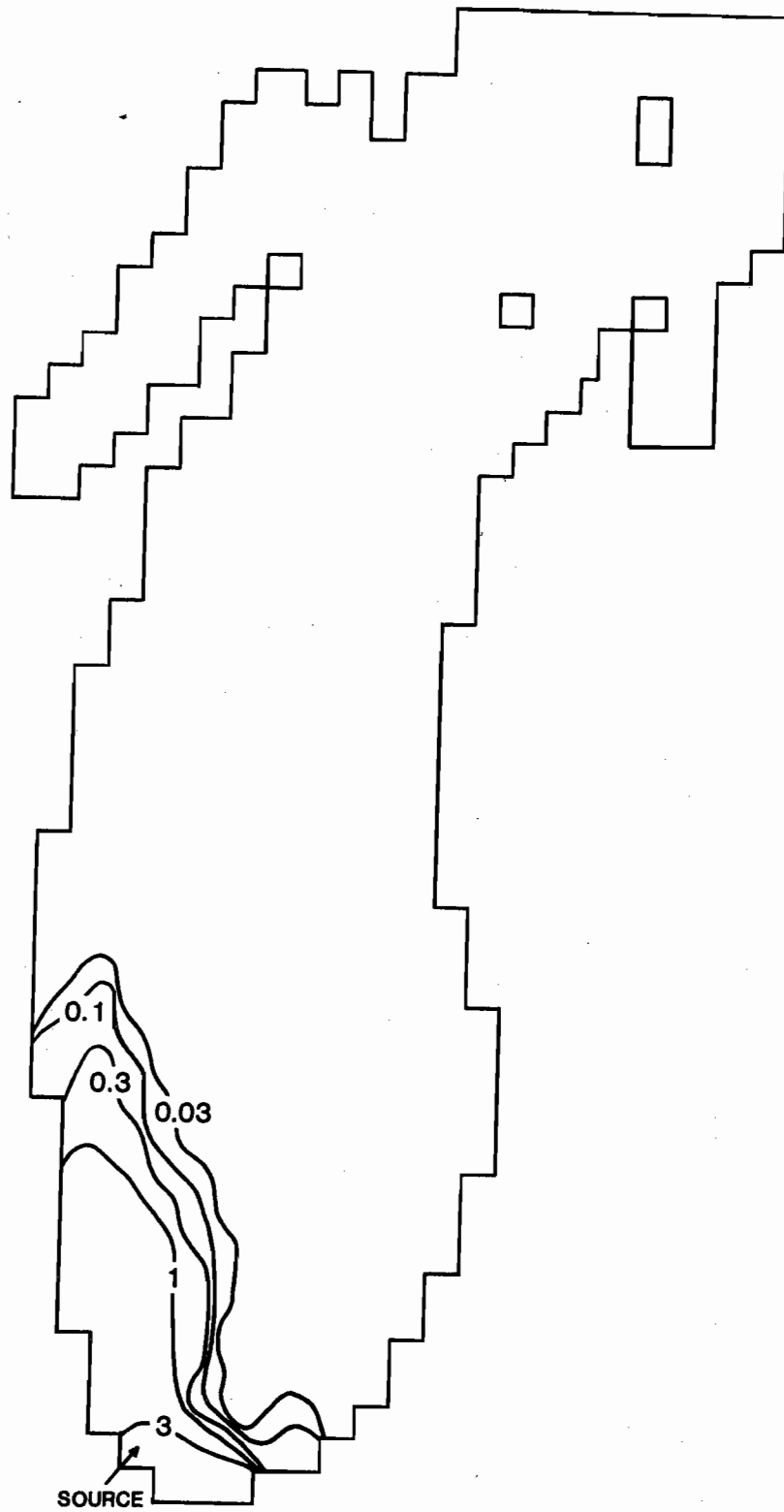


Figure 18. Same as Figure 17, but 25 days after the slug's introduction.

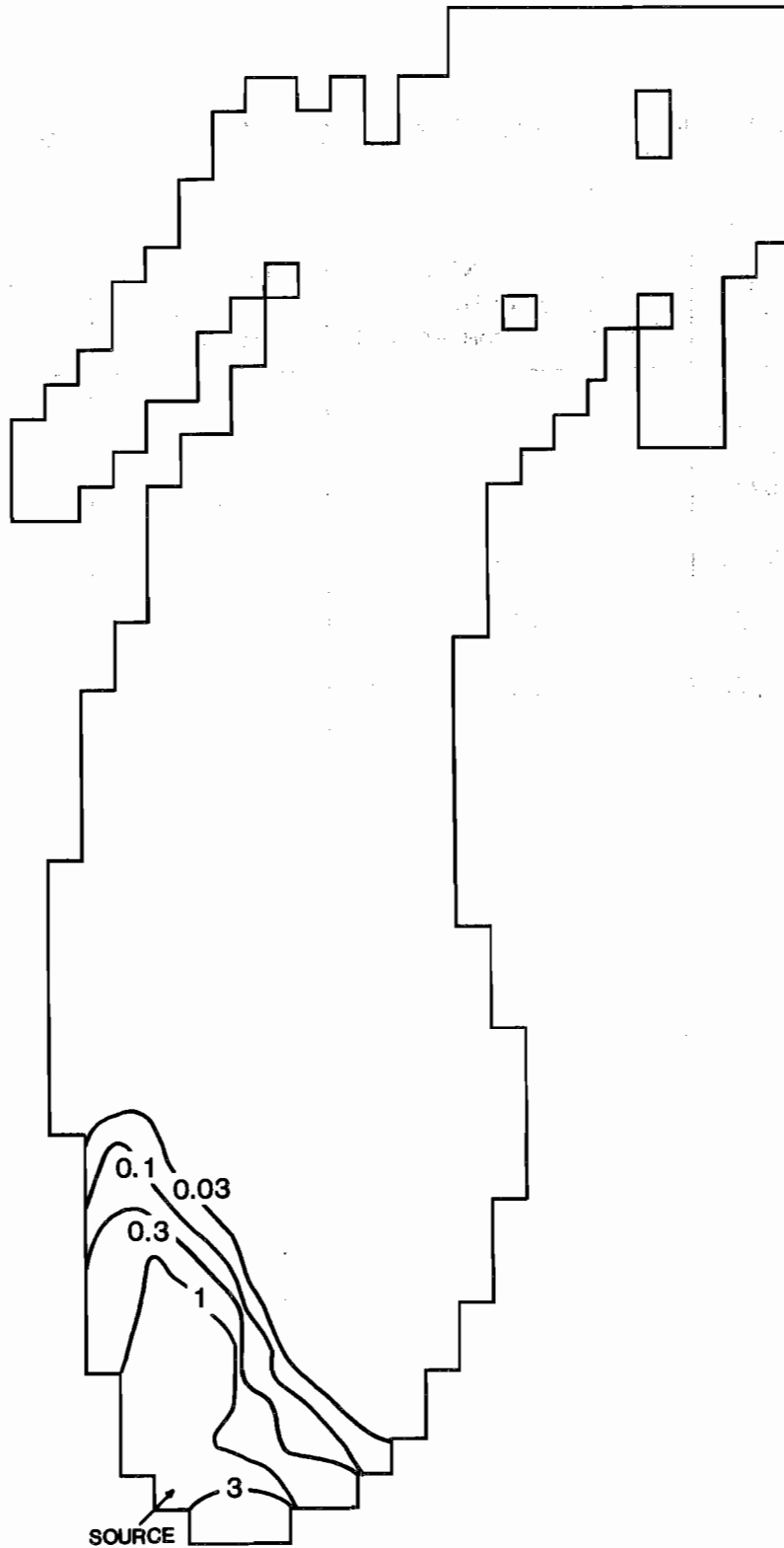


Figure 19. Same as Figure 17, but 32 days after the slug's introduction.

Table 4. Best case wind history (8/24/70 - 9/29/70).

| Subperiod # | Dates (1970) | Average Wind Direction (Degrees from North) | Average Wind Speed (m/sec) | Nearest Standard 3.8/sec Wind |
|-------------|--------------|---|----------------------------|-------------------------------|
| 1 | 8/24-8/30 | 210 | 4.2 | SSW |
| 2 | 8/31-9/6 | 171 | 4.2 | S |
| 3 | 9/7 -9/13 | 190 | 4.7 | S |
| 4 | 9/14-9/20 | 177 | 3.6 | S |
| 5 | 9/21-9/29 | 229 | 4.3 | SW |

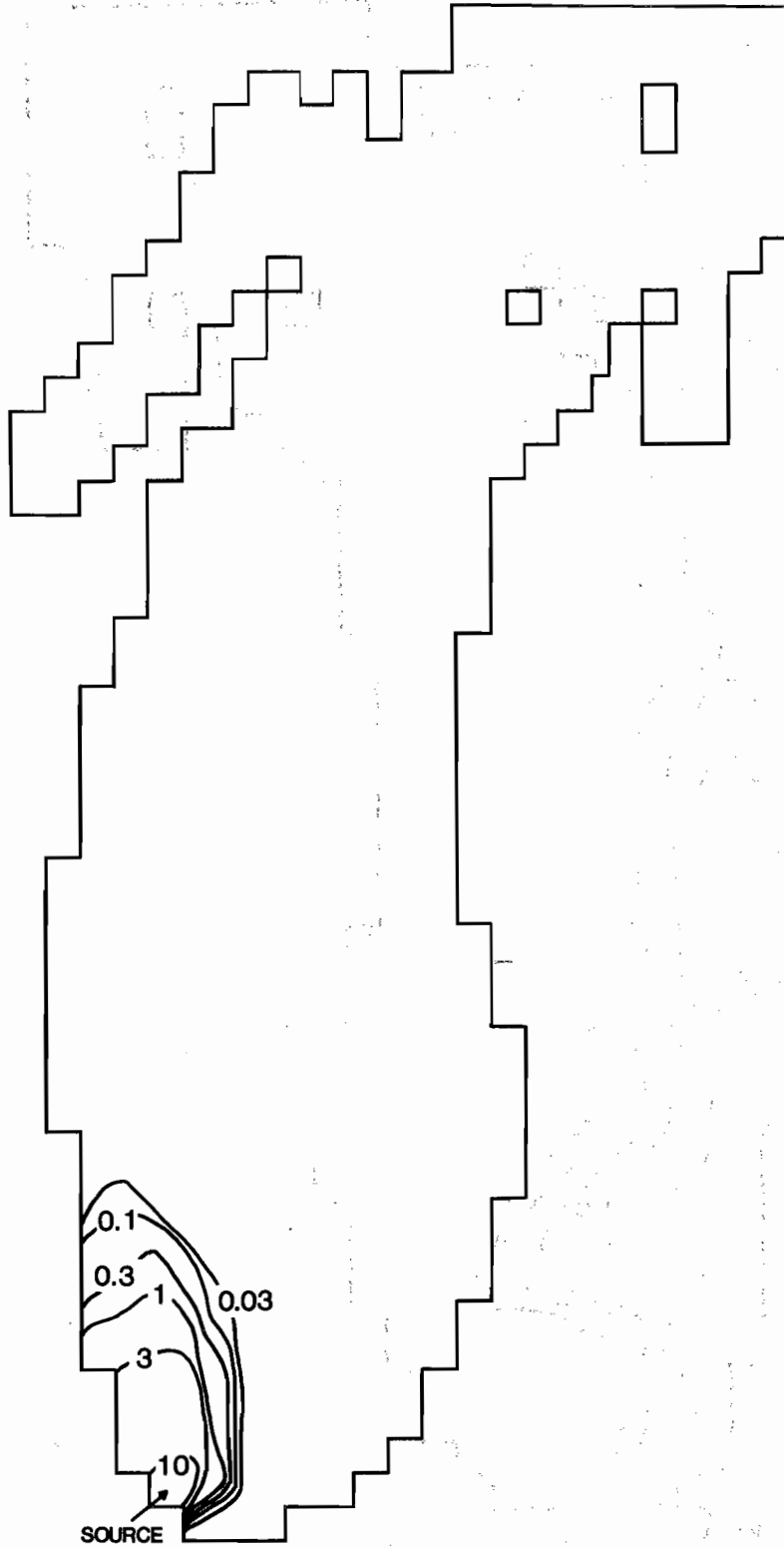


Figure 20. Best case 33-day episode simulation: pollutant distribution 6 days after the introduction of a pollutant slug at Calumet Harbor (units of 10^{-8} g/cm³).

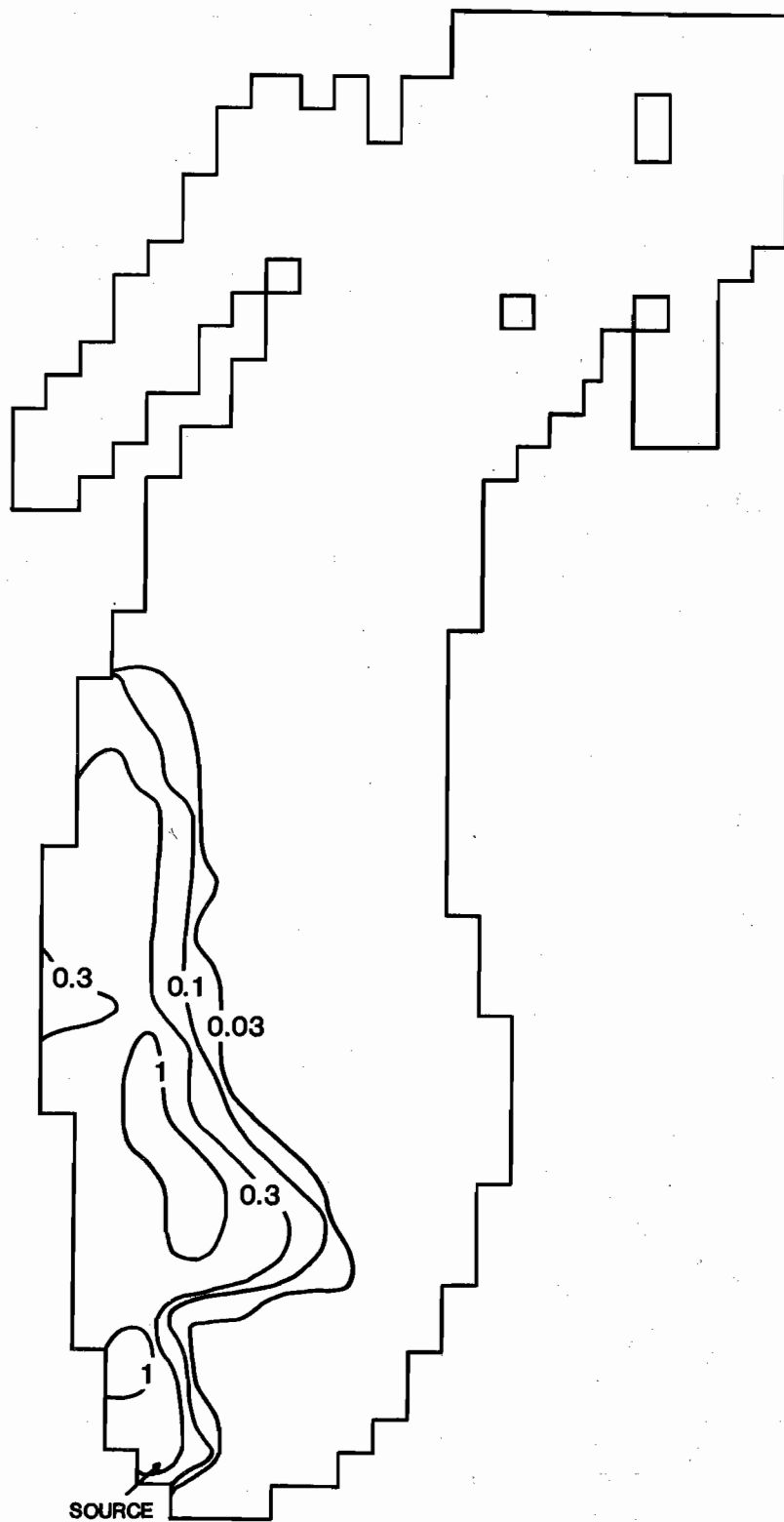


Figure 21. Same as Figure 20, but 20 days after the slug's introduction.

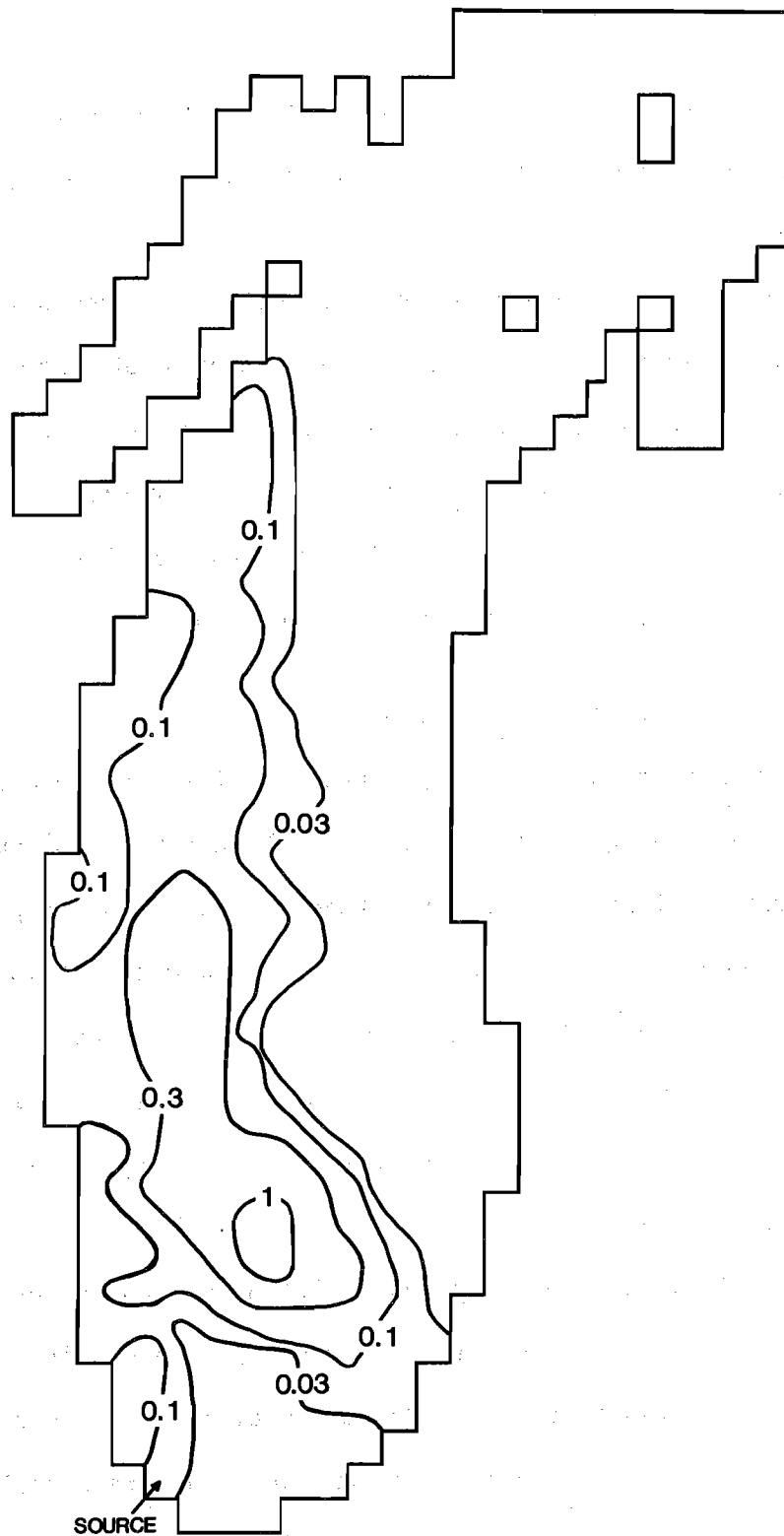


Figure 22. Same as Figure 20, but 32 days after the slug's introduction.

the slug (the region of greatest concentration) moves out to the center of the lake while in the worst case it remains along the shore, near the southern tip.

In general, then, the disposition of pollutant from any coastal source seems to be highly dependent upon the particular wind history for the period considered. It seems altogether possible to find an actual wind history which could produce a worst case situation (with possibly significant pollutant buildup) in almost any region along the Lake Michigan shoreline, due to the predominant effects of wind-driven advection.

Single-Layer Lake Michigan Simulation

As a demonstration of the applicability of the circulation and dispersion models to a homogeneous (winter) Lake Michigan, some sample results were generated. Figure 23 shows a "steady-state" velocity pattern corresponding to homogeneous flow for a 3.8 m/sec SSW wind. This pattern is quite similar, in general, to those of Figures 1 and 2 which are for stratified flow under the same wind; the ranges of average velocity calculated are roughly the same, and the characteristic coastal jets are present in both sets of results.

Figures 24 and 25 show computed pollutant concentration contours at 30 and 60 days, respectively, after the beginning of a continuous discharge of 5000 g/sec into Calumet Harbor, under the prevailing circulation shown in Figure 23. Such extended periods of constant wind are unrealistic, but can provide useful insight into the speed and direction of pollutant movement under particular conditions (as in a search for probable best and worst case situations).

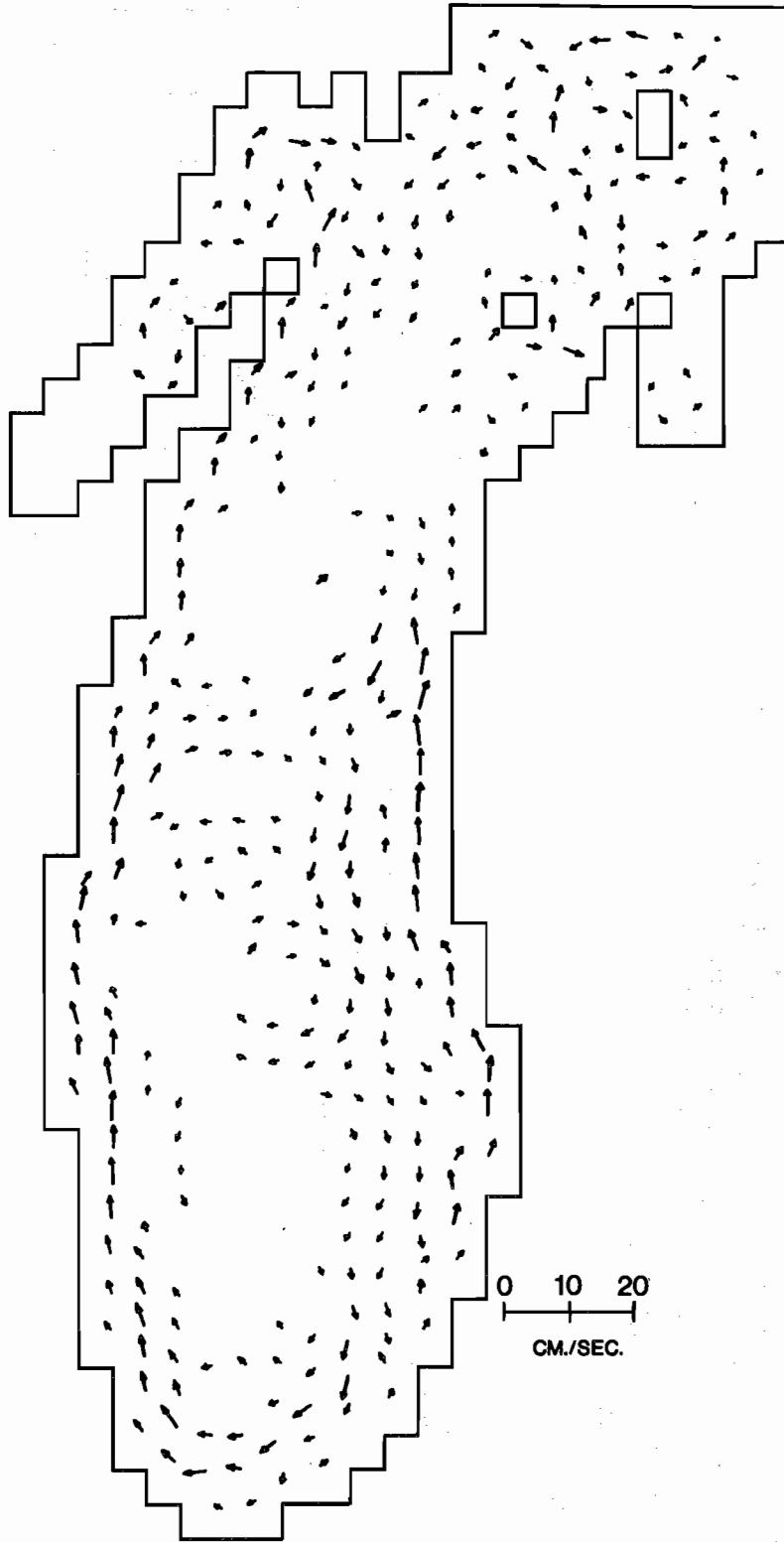


Figure 23. Single-layer Lake Michigan simulation: average velocities for a SSW wind @ 3.8 m/sec.

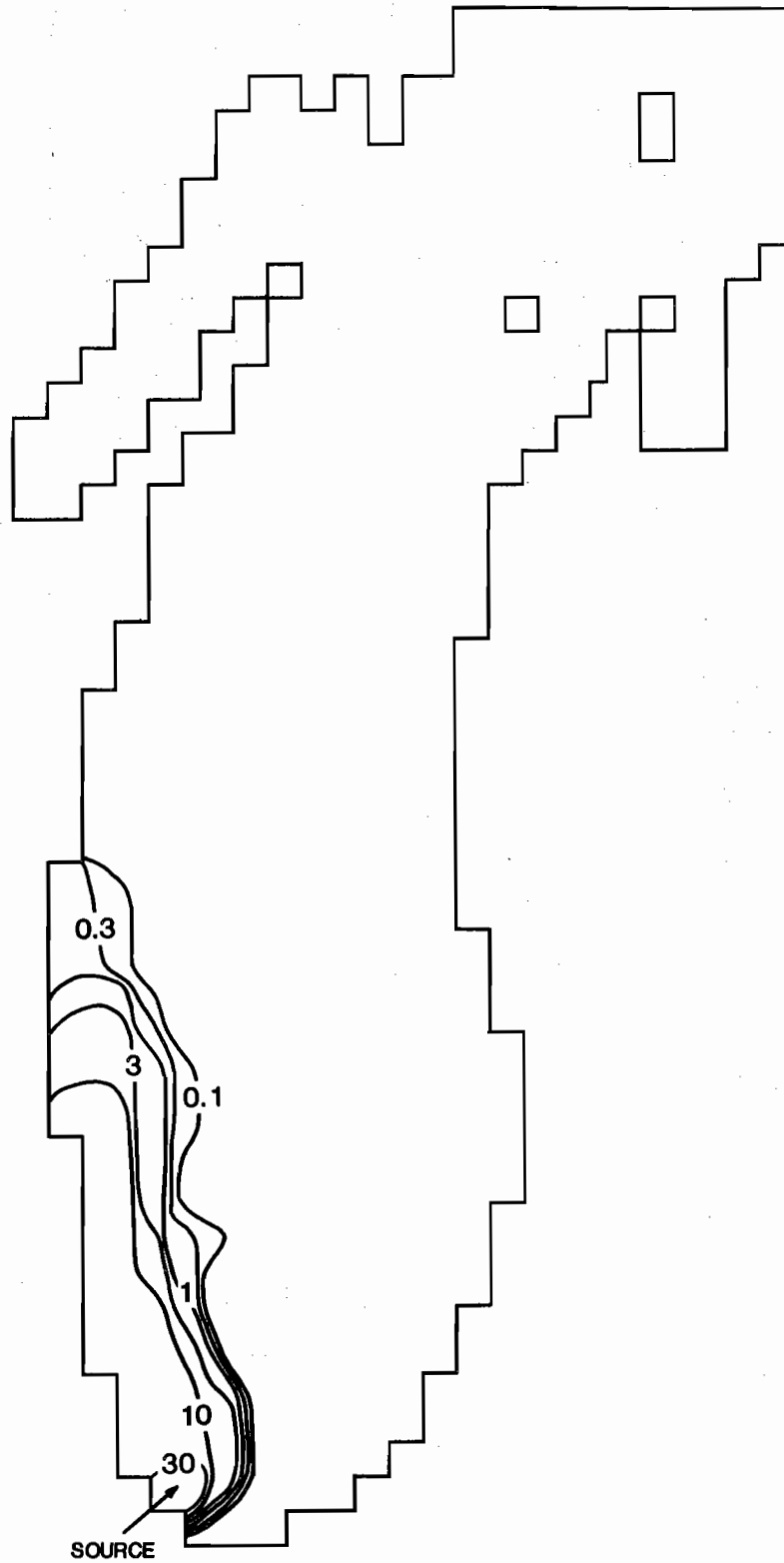


Figure 24. Single-layer Lake Michigan simulation: pollutant concentration contours for the circulation of Figure 23, thirty days after the start of a continuous discharge into Calumet Harbor.

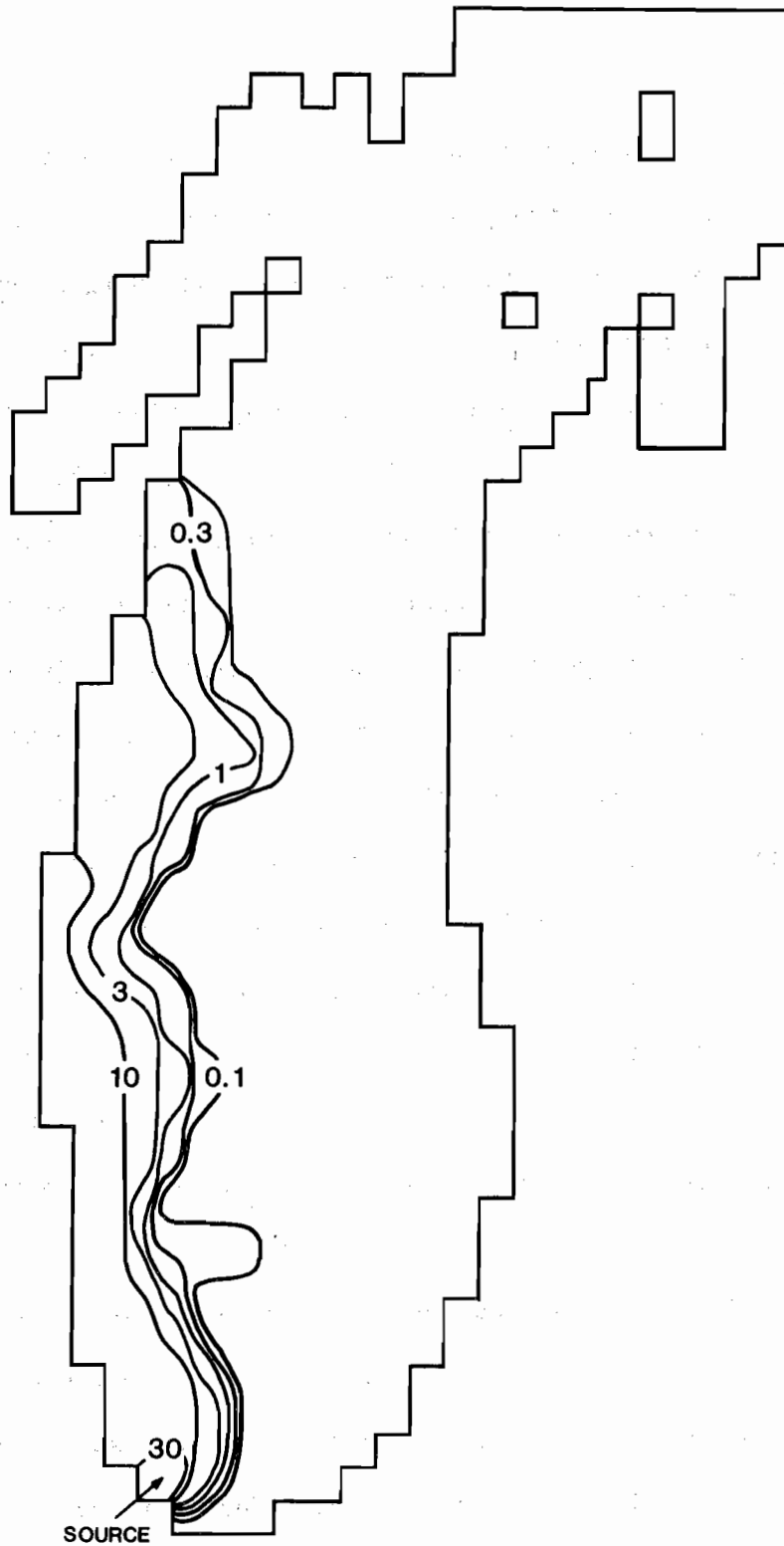


Figure 25. Same as Figure 24, but 60 days after the start of the pollutant discharge.

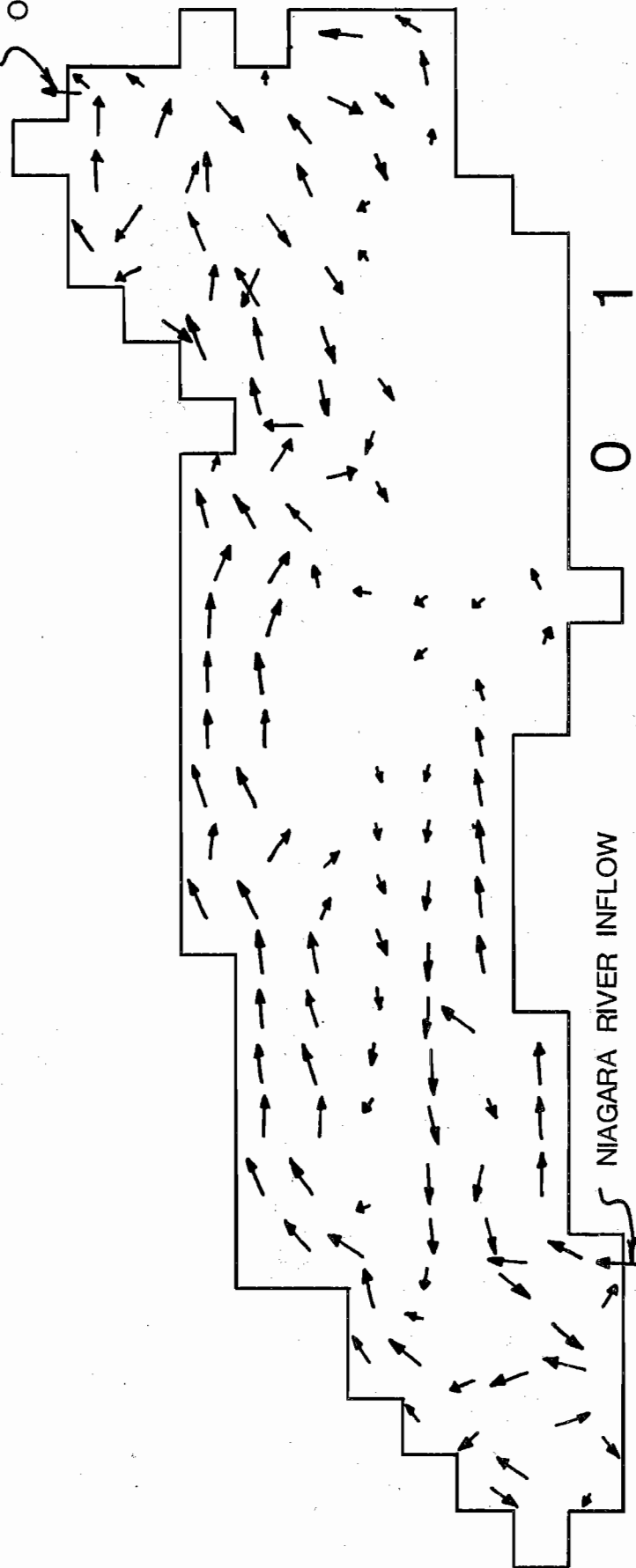
Lake Ontario Simulation

The circulation and dispersion models were adapted for use on a homogeneous Lake Ontario. Two steady-state circulations were computed, one driven only by the Niagara and St. Lawrence River discharges (no wind), and one driven by a constant NW wind with a wind stress magnitude of $0.16 \text{ cm}^2/\text{sec}^2$ and the two river discharges. A long-term average value of $5.9 \times 10^8 \text{ cm}^3/\text{sec}$ (Simons 1972) was used for each river discharge. Figures 26 and 27 show the velocity patterns for the "no-wind" and wind-driven cases, respectively.

For a demonstration of the dispersion model, the cell at the mouth of the Niagara River was assigned a fixed concentration of 10 (arbitrary units) and pollutant contours were generated (starting from zero initial conditions elsewhere), for two extreme values of diffusivity, for 180 days of dispersion under each of the two circulations. Figures 28 and 29 show results for the case of no wind with diffusivities of 10^4 and $10^5 \text{ cm}^2/\text{sec}$, respectively. Figures 30 and 31 show results for the wind-driven case, for the same two diffusivities. As can be seen from these figures, diffusivity values within the range considered had little effect upon the disposition of the bulk of the pollutant introduced. Diffusion seems to have great importance only in regions well removed from strong coastal flows.

The Lake Ontario results shown here have been compared with some similar unverified numerical results of Simons (1972). The same general behavior of circulation and pollutant movement was found in these results, although considerable quantitative discrepancies existed. These discrepancies might have arisen from the use of a coarser grid (10.8 km vs. 5 km) and the use of a long-term average wind stress for the wind-driven case here.

ST. LAWRENCE RIVER
OUTFLOW



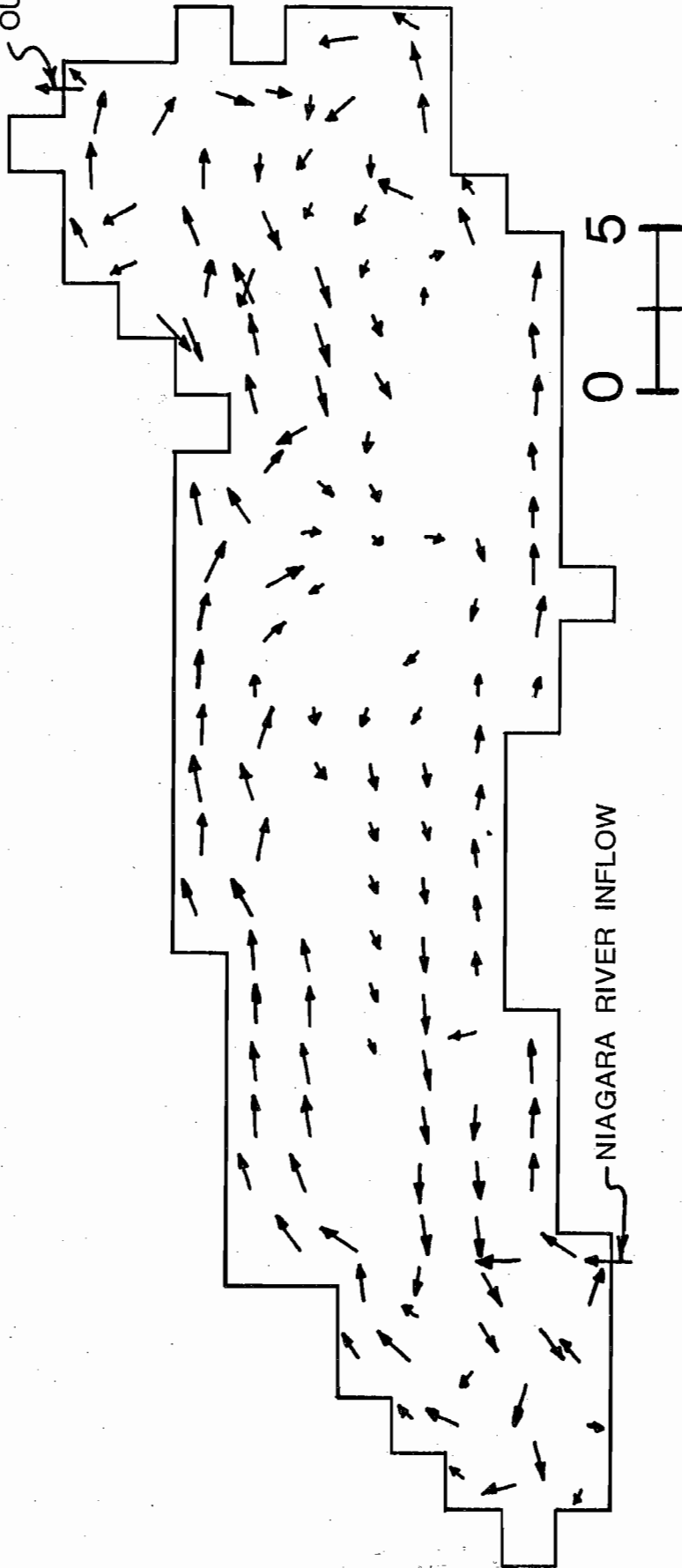
0 1

CM./SEC.

Figure 26. Lake Ontario simulations: computed velocities for the "no-wind" case.

ST. LAWRENCE RIVER
OUTFLOW

50



CM./SEC.

Figure 27. Lake Ontario simulations: computed velocities for a NW wind with a wind stress magnitude of $0.16 \text{ cm}^2/\text{sec}^2$.

ST. LAWRENCE RIVER
OUTFLOW

51

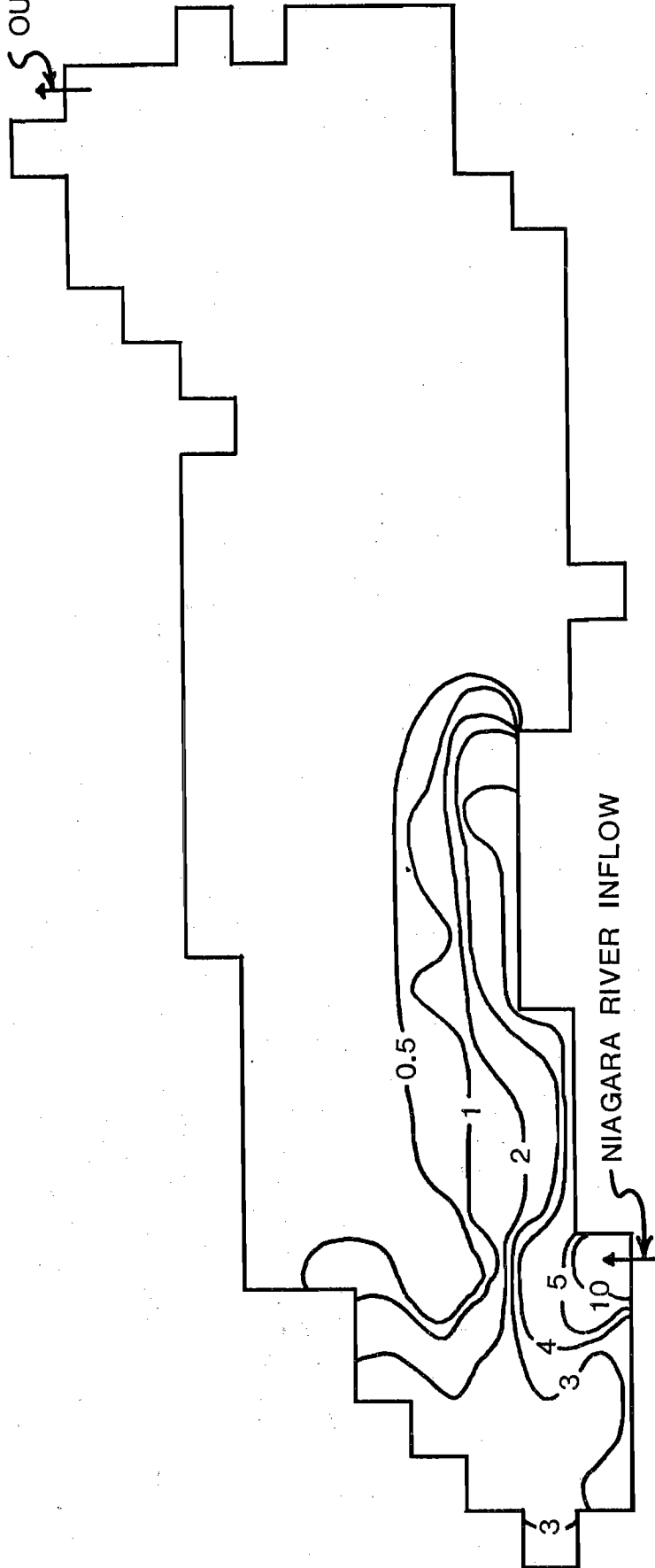


Figure 28. Lake Ontario simulations: pollutant concentration contours (180 days elapsed time) for the "no-wind" case with diffusivity equal to $10^4 \text{ cm}^2/\text{sec}$.

ST. LAWRENCE RIVER
OUTFLOW

52

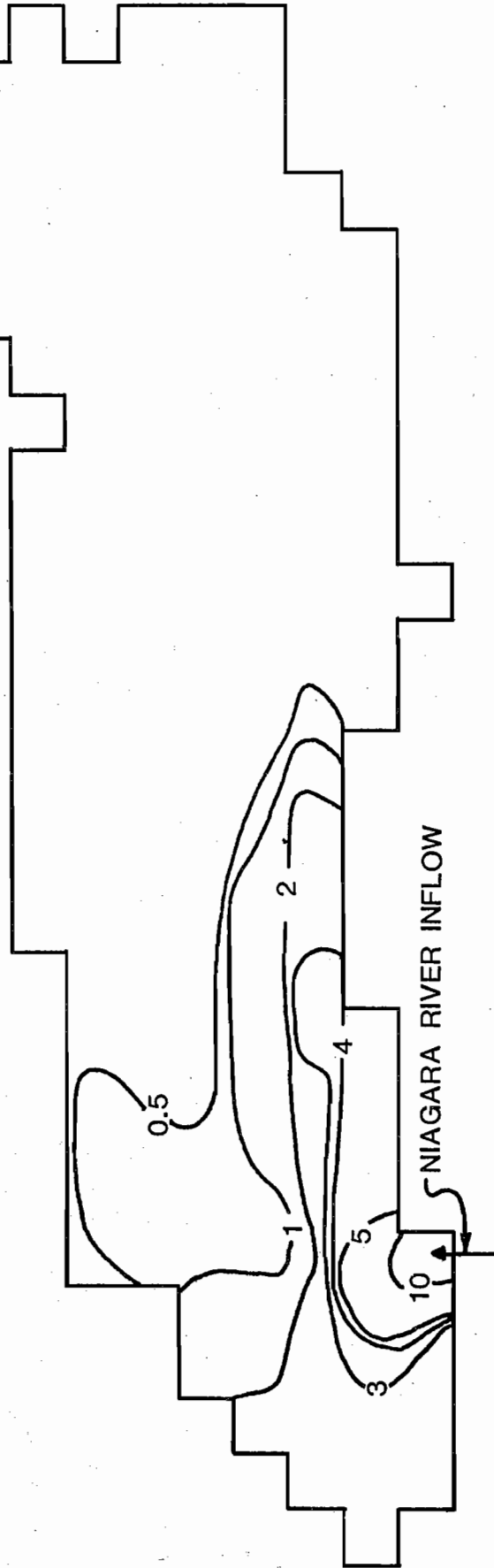


Figure 29. Same as Figure 28, but with diffusivity equal to $10^5 \text{ cm}^2/\text{sec}$.

ST. LAWRENCE RIVER

OUTFLOW

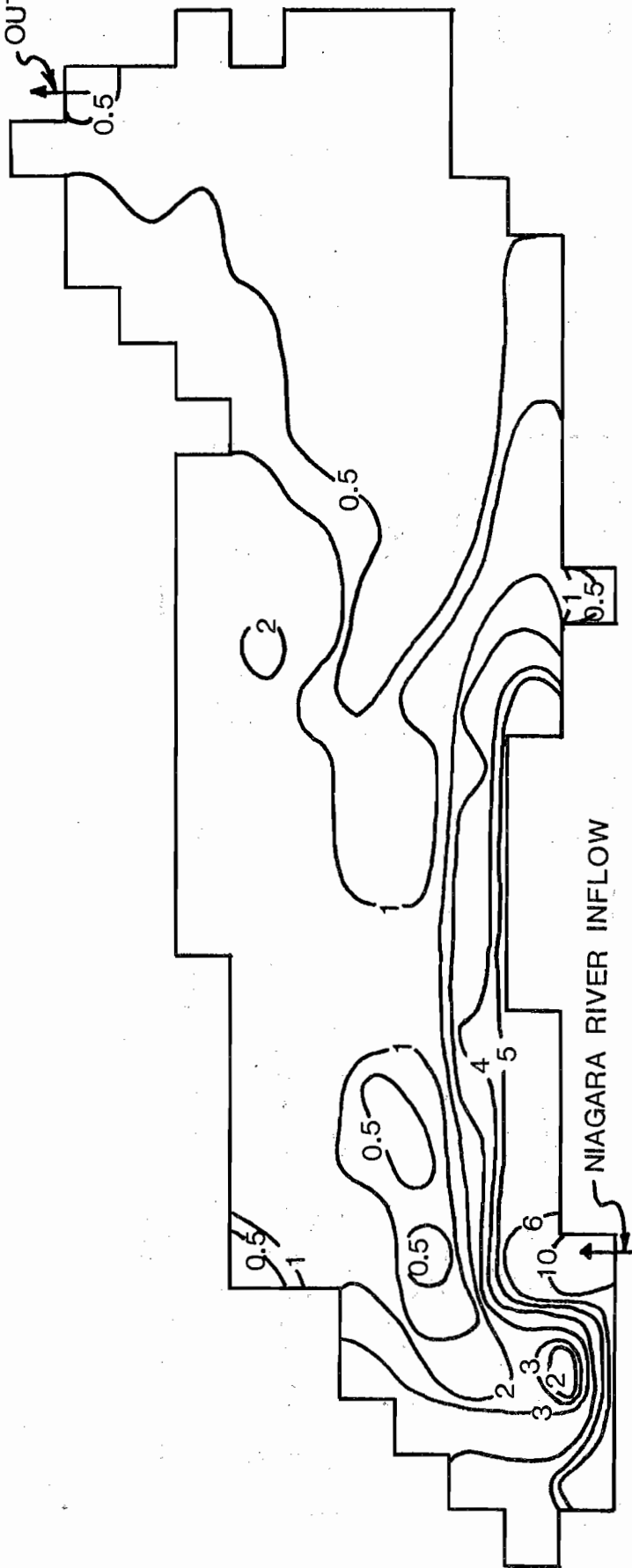


Figure 30. Lake Ontario simulations: pollutant concentration contours (180 days elapsed time) for the wind-driven case with diffusivity equal to $10^4 \text{ cm}^2/\text{sec}$.

ST. LAWRENCE RIVER
OUTFLOW

54

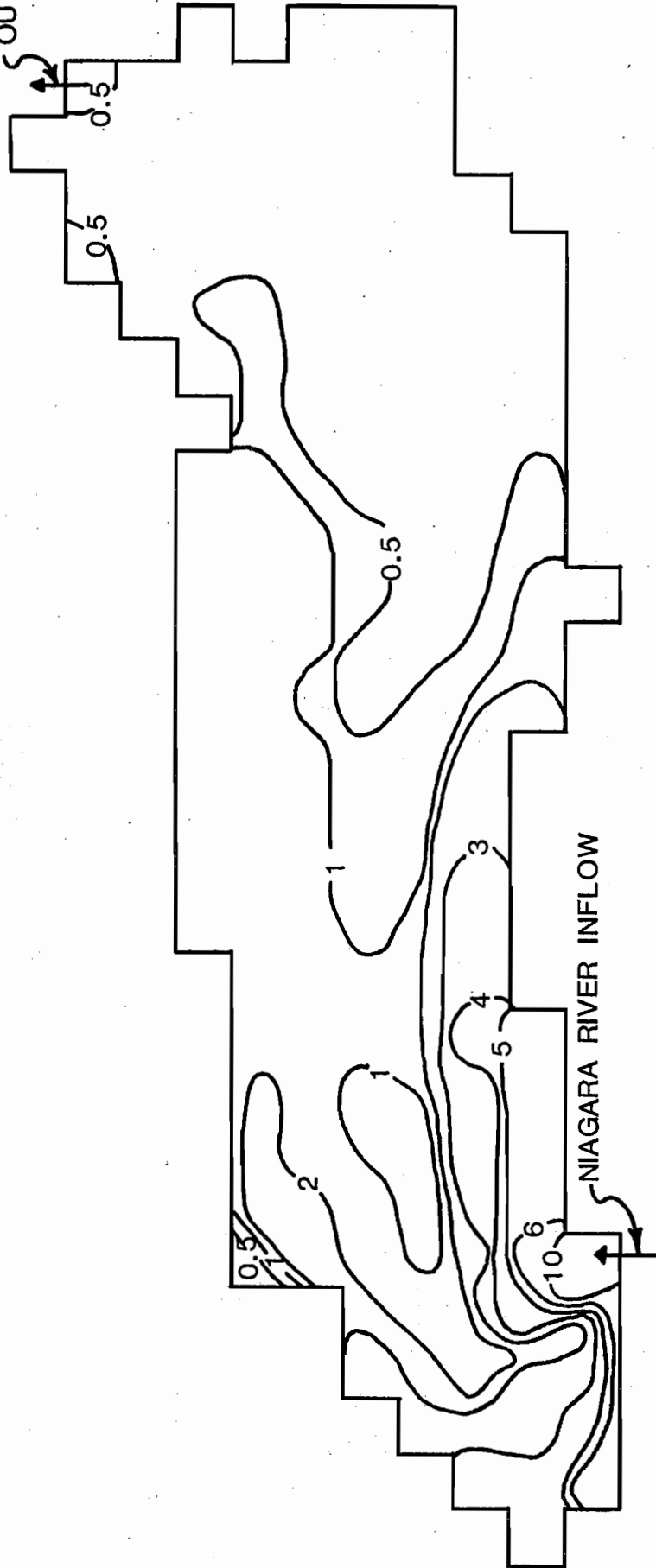


Figure 31. Same as Figure 30, but with diffusivity equal to $10^5 \text{ cm}^2/\text{sec}$.

CONCLUSIONS

Several important conclusions may be drawn from the results presented here regarding the use of numerical models in simulations directed toward water quality management. The 125-day pollutant dispersion results shown indicate the difficulties involved in any such long-term simulation of pollutant buildup from multiple discharges; the effects of individual sources are almost impossible to discern, and highly detailed wind, loading, and initial conditions data, as well as careful local matching of wind stresses and diffusivities, are necessary if any really useful quantitative results are to be obtained. While detailed wind data are available for a number of points along the Lake Michigan shore, and fairly realistic wind-stress fields could probably be derived, initial pollutant concentration data are not presently available. Obtaining whole-lake pollutant distributions would require a large, intensive research effort. The need for initial values might be overcome by starting a model from zero initial conditions and allowing it to run until a quasi-steady state, supposedly representing actual lake conditions, was achieved. Such a simulation, however, would still require far better discharge data for all important sources than are now available, and would still need to be verified quantitatively before the results could be taken seriously. Given presently available data, the modeling of short-term episodes based upon local data seems to be a far more promising avenue toward providing the insights required for the making of water-management decisions.

The Lake Michigan best and worst case results shown here, for example, tend to indicate that a large pollutant slug (resulting, for example, from a storm discharge from a combined sewer system or from a river and canal trib-

utary system) introduced into a strong coastal jet will be quickly diluted and "spread out" along the shore, fading into the background pollutant level for a given region. Such an indication implies that such slugs probably are of little importance at any great distance from their sources and that knowledge of local background values may, therefore, be sufficient for verification and use of local worst case models. It might be far easier to verify a model for local episodes than to verify a whole-lake model.

The best and worst case results also clearly indicate that long-term average values of water-quality parameters are of little use in predicting possible extreme cases, because the disposition of pollutant from any given source is so highly dependent upon particular wind conditions.

Therefore, it seems clear that effluent discharge standards for Lake Michigan should be based either upon a search for worst cases or upon a predictive real-time simulation. The latter might be used to indicate the need for a reduction in the amounts discharged, based on Weather Service wind predictions.

SUGGESTIONS FOR FUTURE WORK

The most pressing need is for a verification of the existing models for use in local short-term predictive simulation of worst cases. Attempts at such verification, using water-intake data, will commence shortly. The use of turbidity measurements extracted from earth satellite observations of Lake Michigan is also being considered as a means of model calibration. The inclusion of three-dimensional dispersion (including pollutant movement through the thermocline in summer) would also provide valuable insight; we are currently developing a three-dimensional model. A high-resolution near-shore model must then be developed if whole-lake or large regional dispersion models are to be adapted successfully to the study of localized biological activity. Simulation of local dispersion in the area of Calumet Harbor, for example, might provide extremely useful knowledge of that region and its interactions with the rest of the lake, and is being considered as a possible future project.

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APPENDIX A

1. A Standard Central-Difference Approach to the Dispersion Equation (1). Equation (1) above may be rewritten (neglecting the source term), by simple substitution of equations (2) and (3), as

$$H \frac{\partial C}{\partial t} = -C \left(\frac{\partial q_x}{\partial x} + \frac{\partial q_y}{\partial y} \right) - q_x \frac{\partial C}{\partial x} - q_y \frac{\partial C}{\partial y} + A \left[H \left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} \right) + \frac{\partial C}{\partial x} \frac{\partial H}{\partial x} + \frac{\partial C}{\partial y} \frac{\partial H}{\partial y} \right] \quad (10)$$

Let all of the individual derivatives in (10) be replaced by standard central-difference approximations such as (4) and (5) above. Taylor-series expansion of the right-hand sides of (4) and (5) show that these expressions are exact to within error terms containing no powers of the space increment Δs which are less than 2. Thus, (4) and (5) are second-order approximations. The approximation for (10) which results when such second-order approximations are substituted is (for the center of cell 0, as shown in Figure 6)

$$H_0 \frac{\partial C}{\partial t} \approx \frac{q_1(C_1 - C_2 - 2C_0) + q_2(C_1 - C_2 + 2C_0) + q_3(C_3 - C_4 - 2C_0) + q_4(C_3 - C_4 + 2C_0)}{4\Delta s} + \frac{A}{4(\Delta s)^2} [C_1(H_1 - H_2 + 4H_0) + C_2(H_2 - H_1 + 4H_0) + C_3(H_3 - H_4 + 4H_0) + C_4(H_4 - H_3 + 4H_0)] \quad (11)$$

In the derivation of (11), the values of q_x and q_y at the center of cell 0 were taken as the averages of the values of q_x and q_y at the boundaries of cell 0.

$$q_{x_0} \approx \frac{q_2 + q_1}{2} \quad (12)$$

$$q_{y_0} \approx \frac{q_4 + q_3}{2}; \quad (13)$$

From the first term of equation (11) it is apparent that, for example, advective pollutant flow across the boundary (2,0) of cell 0 is represented by a term of the form

$$g_2 = \frac{q_2(C_1 - C_2 + 2C_0)}{4\Delta s} \quad (14)$$

in equation (11). If an equation similar to (11) were written for cell 2, the advective flow across (2,0) would be represented by a term involving C_0 , C_2 , and the concentration in the cell to the right of cell 2 instead of C_0 , C_1 , and C_2 . Therefore, the advective pollutant flow across (2,0) would have a different calculated value depending upon which cell was used as the center for the finite-difference approximation. Equation (11), then, is obviously not strictly conservative of pollutant mass. It may be shown similarly that approximations using more than five points are also not mass conservative, because they employ cells other than those adjoining a given boundary to estimate the dispersion across that boundary and are, thus, not symmetrical with respect to that boundary.

Taylor-series expansion of the right-hand side of (11) (about the center of cell 0) shows that the equation is exact to within an error whose most significant term is

$$\epsilon_1 = \frac{A}{12} (\Delta s) \left[\frac{\partial^3 H}{\partial x^3} (C_1 - C_2) + \frac{\partial^3 C}{\partial x^3} (H_1 - H_2) + \frac{\partial^3 C}{\partial y^3} (H_3 - H_4) + \frac{\partial^3 H}{\partial y^3} (C_3 - C_4) \right] \quad (15)$$

Equation (11) is only a first-order approximation of equation (10). The first-order error terms of ϵ_1 arise from the product terms

$$\frac{\partial C}{\partial x} \frac{\partial H}{\partial x} \quad \text{and} \quad \frac{\partial C}{\partial y} \frac{\partial H}{\partial y}$$

in (10). Products of second-order approximations such as (4) are only first-order approximations.

2. A. Mass-Balance Approach to the Dispersion Equation (1).

Consider the boundary (2,0) between cells 0 and 2, as shown in Figure 6. If the concentration at this boundary is assumed to be

$$C_{2,0} \approx \frac{C_0 + C_2}{2}, \quad (16)$$

the average of C_0 and C_2 , the advective mass transfer from cell 0 to cell 2 during the time interval $(t, t+\Delta t)$ is approximately

$$G_1 = q_2(\Delta s)C_{2,0}(\Delta t) = \frac{q_2(\Delta s)(C_0 + C_2)(\Delta t)}{2}. \quad (17)$$

If the thickness of the lake's top layer at the boundary (2,0) is assumed to be

$$H_{2,0} = \frac{H_2 + H_0}{2}, \quad (18)$$

the average of H_2 and H_0 , then the diffusive pollutant mass transfer from cell 0 to cell 2 is approximately

$$G_2 = \frac{A(\Delta t)(C_0 - C_2)H_{2,0}(\Delta s)}{\Delta s}, \quad (19)$$

during the interval $(t, t+\Delta t)$. The total pollutant mass flow across the

boundary (2,0) in (t, t+Δt) is approximately

$$G_3 = G_1 + G_2 = \frac{\Delta t}{2} [q_2(\Delta s)(C_0 + C_2) + A(C_0 - C_2)(H_2 + H_0)]. \quad (20)$$

Expressions similar to G_3 may be derived for the other three horizontal boundaries of cell 0. The total mass in cell 0 at t+Δt is, then,

$$\begin{aligned} M_0(t+\Delta t) \cong M_0(t) - \frac{\Delta t}{2} \left\{ [\Delta s \sum_1^4 (-1)^i q_i] + A(4H_0 + \sum_1^4 H_i) \right\} \\ + \sum_1^4 C_i(t) \left\{ \frac{\Delta t}{2} [A(H_i + H_0) - (-1)^i q_i(\Delta s)] \right\} \end{aligned} \quad (21)$$

where all the C_i 's and H_i 's are for time t, and sources are neglected. To obtain an equation in terms of concentration, both sides of equation (21) are divided by $H_0(\Delta s)^2$, the approximate volume of cell 0, to obtain

$$\begin{aligned} C_0(t+\Delta t) = \frac{M_0(t+\Delta t)}{H_0(\Delta s)^2} \cong C_0(t) \left\{ 1 - \frac{\Delta t}{2H_0(\Delta s)^2} [\Delta s \sum_1^4 (-1)^i q_i + A(4H_0 + \sum_1^4 H_i)] \right\} \\ + \sum_1^4 C_i(t) \left\{ \frac{\Delta t [A(H_i + H_0) - (-1)^i q_i(\Delta s)]}{2H_0(\Delta s)^2} \right\} \end{aligned} \quad (22)$$

If the source term $[S_0(x,y)](\Delta t)$ is now added to equation (22), equation (22) becomes equation (6), above, the finite-difference equation used in this paper.

Taylor-series expansion of the right-hand side of equation (6) about the center of cell 0 shows that (6) approximates the differential equation (1) with an error having

$$\begin{aligned}
\epsilon_2 = A(\Delta s)^2 & \left\{ \frac{1}{6} \left[\frac{\partial C}{\partial x} \frac{\partial^3 H}{\partial x^3} + \frac{\partial H}{\partial x} \frac{\partial^3 C}{\partial x^3} + \frac{\partial C}{\partial y} \frac{\partial^3 H}{\partial y^3} + \frac{\partial H}{\partial y} \frac{\partial^3 C}{\partial y^3} \right] \right. \\
& + \frac{1}{4} \left[\frac{\partial^2 C}{\partial x^2} \frac{\partial^2 H}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} \frac{\partial^2 H}{\partial y^2} \right] + \frac{1}{12} H_0 \left(\frac{\partial^4 C}{\partial x^4} + \frac{\partial^4 C}{\partial y^4} \right) \left. \right\} \\
& - \frac{1}{2} (\Delta s)^2 \left\{ \frac{1}{3} \left[q_{x_0} \frac{\partial^3 C}{\partial x^3} + q_{y_0} \frac{\partial^3 C}{\partial y^3} \right] + \frac{1}{2} \left[\frac{\partial q_x}{\partial x} \frac{\partial^2 C}{\partial x^2} + \frac{\partial q_y}{\partial y} \frac{\partial^2 C}{\partial y^2} \right] \right. \\
& \left. + \frac{1}{4} \left[\frac{\partial C}{\partial x} \frac{\partial^2 q_x}{\partial x^2} + \frac{\partial C}{\partial y} \frac{\partial^2 q_y}{\partial y^2} \right] + \frac{1}{12} C_0 \left[\frac{\partial^3 q_x}{\partial x^3} + \frac{\partial^3 q_y}{\partial y^3} \right] \right\}
\end{aligned} \tag{23}$$

as its most significant term. Hence (6) is a second-order approximation of (1), and thus represents (1) more accurately, for sufficiently small Δs , than does (11).

APPENDIX B

A Direct Finite-Difference Derivation of Equation (6).

The partial differential equation (1) may be rewritten as

$$H \frac{\partial C}{\partial t} = - \frac{\partial(q_x C)}{\partial x} - \frac{\partial(q_y C)}{\partial y} + A \left[\frac{\partial}{\partial x} \left(H \frac{\partial C}{\partial x} \right) + \frac{\partial}{\partial y} \left(H \frac{\partial C}{\partial y} \right) \right] + S(x,y) \quad (24)$$

The derivatives in (24) may be approximated as follows for the center of cell 0:

$$\frac{\partial(q_x C)}{\partial x} \cong \frac{(q_x C)_{2,0} - (q_x C)_{1,0}}{\Delta s} \quad (25)$$

$$\frac{\partial(q_y C)}{\partial y} \cong \frac{(q_y C)_{4,0} - (q_y C)_{3,0}}{\Delta s} \quad (26)$$

$$\frac{\partial}{\partial x} \left(H \frac{\partial C}{\partial x} \right) \cong \frac{\left(H \frac{\partial C}{\partial x} \right)_{2,0} - \left(H \frac{\partial C}{\partial x} \right)_{1,0}}{\Delta s} \quad (27)$$

$$\frac{\partial}{\partial y} \left(H \frac{\partial C}{\partial y} \right) \cong \frac{\left(H \frac{\partial C}{\partial y} \right)_{4,0} - \left(H \frac{\partial C}{\partial y} \right)_{3,0}}{\Delta s} \quad (28)$$

In equations (25)-(28), the subscript i,o indicates that a quantity is evaluated at the boundary (i,o) of cell 0, as shown in Figure 6. However,

$$(q_x C)_{i,o} \cong q_i \frac{C_i + C_o}{2} \quad (i = 1, 2) \quad (29)$$

and

$$(q_y C)_{i,o} \cong q_i \frac{C_i + C_o}{2} \quad (i = 3, 4), \quad (30)$$

where the value of C at the boundary $(i,0)$ is taken to be the average of C_i and C_0 . Similarly,

$$\left(H \frac{\partial C}{\partial x} \right)_{i,0} \cong \pm \frac{H_i + H_0}{2} \frac{C_i - C_0}{\Delta s} \quad (i = 1, 2) , \quad (31)$$

and

$$\left(H \frac{\partial C}{\partial y} \right)_{i,0} \cong \pm \frac{H_i + H_0}{2} \frac{C_i - C_0}{\Delta s} \quad (i = 3, 4) , \quad (32)$$

where the + signs are used for even values of i , and the minus signs for odd values of i .

By substituting equations (31) and (32) into expressions (25)-(28), and then substituting the resulting expressions into (24), one obtains equation (6), the equation derived from a mass balance in Appendix A.

APPENDIX C

Comparison of Equation (6) with an Equation Using a Step Variation
in Concentration.

If it is assumed that the concentration in cell i is everywhere the same as at its center (a step approximation to $C(x,y)$), the method of Bella and Dobbins (1968) may be extended simply to the two-dimensional case of Figure 6 to obtain an advection term which is strictly conservative of pollutant mass and does not create spurious negative concentrations which must be corrected.

Let $S_0(x,y) = 0$, and let the diffusivity $A = 0$; then, advection is the only process involved in pollutant dispersion. Furthermore, assume that q_1 , q_2 , q_3 , and q_4 are all positive as shown in Figure 6. (The formulation here requires different expressions if q_1 , q_2 , q_3 , and/or q_4 are negative.) The differential equation (1) may be approximated, for advection only, by

$$H_0 \frac{\partial C}{\partial t} \cong \frac{1}{\Delta s} [C_1 q_1 + C_3 q_3 - C_0 (q_2 + q_4)]. \quad (33)$$

Equations of the form shown in (33) are symmetrical with respect to the boundaries; such equations conserve pollutant mass. Also, since in equation (33) no pollutant is advected from a cell with concentration zero at its center, no spurious negative concentrations will occur in computation.

Taylor-series expansion of the right-hand side of (33) about the center of cell 0, however, shows that the error in (33) has

$$\epsilon_3 = \frac{1}{2} (\Delta s) \left[\frac{\partial C}{\partial x} \frac{\partial q_x}{\partial x} + \frac{\partial C}{\partial y} \frac{\partial q_y}{\partial y} + \frac{\partial^2 C}{\partial x^2} q_{x_0} + \frac{\partial^2 C}{\partial y^2} q_{y_0} \right] \quad (34)$$

as its most significant term. Equations such as (33), then, are only first-order approximations to (1) and are therefore less accurate approximations than the advection terms of (6) for sufficiently small Δs .