

Modeling the Dispersal of a Marked Fluid in Narragansett Bay

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Introduction

This report summarizes some of the work carried out at the University of Rhode Island in its Sea Grant program for estuarine modeling, and updates parts of the engineering effort in this discipline. Specifically, a numerical model of the convective-diffusive equation of mass conservation is developed for the most general applications, and is coupled with a previously developed tidal-hydrodynamic model of Narragansett Bay (Fig. 1). The computer scheme is then applied to a practical problem, the simulation of the temporal and spatial dispersal of a marked fluid introduced into the Bay at a specific site. Thus an indication of the fate of a foreign substance, which might represent sewage or heated water, can be gained at low cost, and such information can be used in the public and private decision-making process.

The model of water flow is basically the numerical scheme developed by Leendertse (1967), which was adapted to Narragansett Bay by using the appropriate local geometry, bathymetry, river flow data and tidal information as reported by Hess and White (1974). The constituent equation for conservation of mass is similar to that proposed by Leendertse (1970).

To date, the model derived herein has been put to general uses. Mass dispersal from several sections around Narragansett Bay was used as a physical parameter in a simulation by Kramer (in preparation) of the daily spatial distribution of phytoplankton and zooplankton. The concentration of winter flounder larvae in Niantic Bay, Connecticut, and its environs was modeled by Hess et al. (1975). And Alfano (1973) looked at what happened to heated water from the proposed site of a nuclear electric power plant on Narragansett Bay.

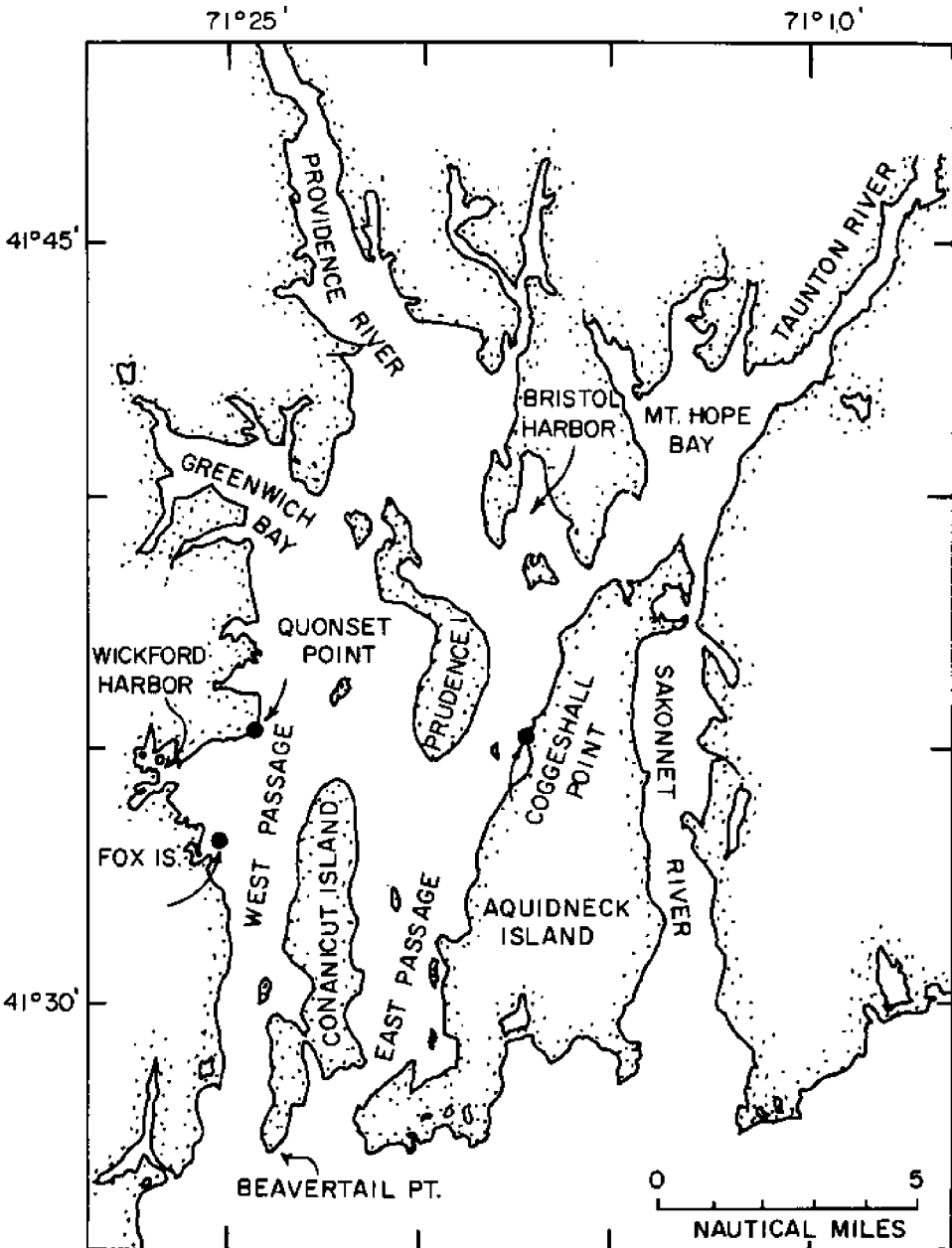


Figure 1. Narragansett Bay.

The Convective - Diffusive Equation

Hydrodynamic inputs are used to simulate the temporal and spatial fate of a species of solute in the water. The conservation of mass equation for any species, or constituent, c (mass per unit-volume), is

$$\frac{\partial c}{\partial t} + \frac{\partial}{\partial x} (uc - D_x \frac{\partial c}{\partial x}) + \frac{\partial}{\partial y} (vc - D_y \frac{\partial c}{\partial y}) + \frac{\partial}{\partial z} (wc - D_z \frac{\partial c}{\partial z}) = q \quad (1)$$

Discussion of turbulent transfer mechanisms is passed over here, and the assumption of simple Fickian diffusion is made. Furthermore, cross-products are neglected and the diffusion coefficient, D , is assumed to be a vector quantity. Internal mass-change processes, such as decay or radiation, are represented by q . Molecular viscosity has been ignored.

The present model assumes that a hydrodynamic model will provide current velocity input. Since the tidal model discussed above is to be used, equation 1 must be integrated from the bottom of the water column ($z = -h$) to the water surface ($z = \eta$). Letting

$$H \equiv \eta + h$$

the result is:

$$\frac{\partial}{\partial t} HC + \frac{\partial}{\partial x} H(AUC - D_x \frac{\partial C}{\partial x}) + \frac{\partial}{\partial y} H(AVC - D_y \frac{\partial C}{\partial y}) = qH \quad (2)$$

where U , V , and C are the vertically-averaged values of the two current vectors and the mass concentration, respectively (see Appendix A). These are evaluated at each grid square (Fig. 2).

The convection factor, A , arises from the non-uniformity of U and C over the vertical. Note that if either U or C is independent of depth, A is unity. A number of examples have occurred from biological applications. The larvae of certain fish species tend to be found in the lower half of the water column, where the currents are less than at the surface, for

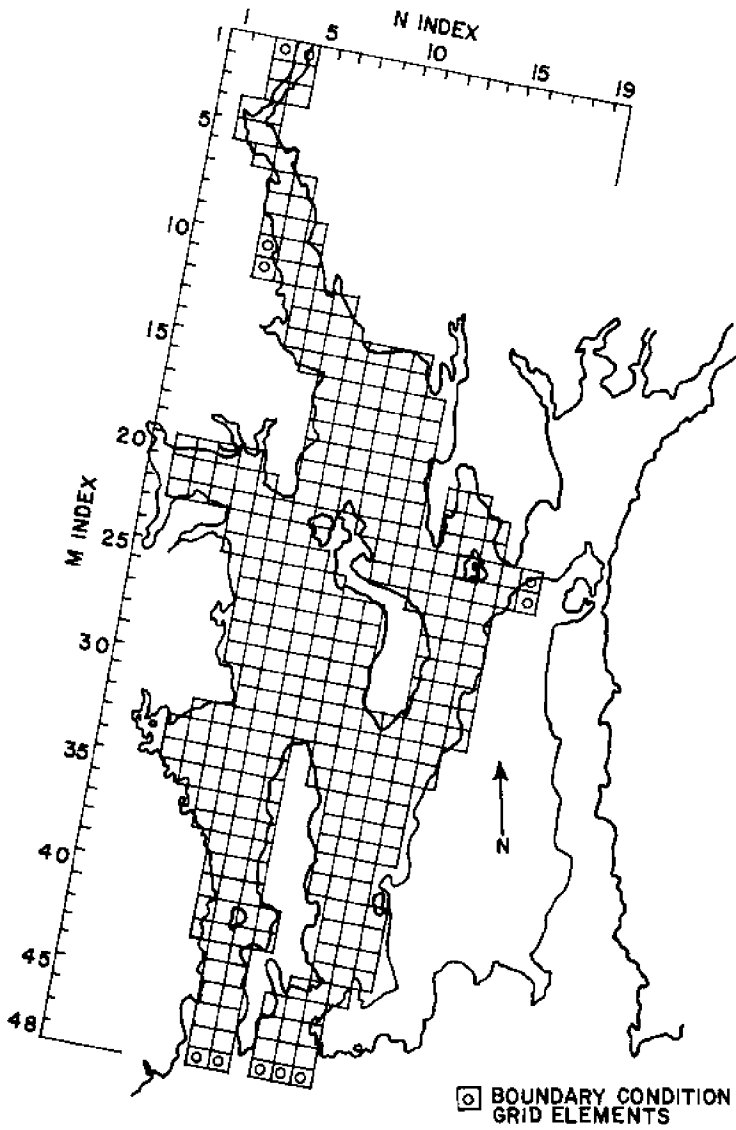


Figure 2. The grid network for Narragansett Bay.

example. In such a case A will be less than unity, but most likely by only a few percent. The opposite is true for the larvae of lobster, which are found primarily within the top meter of the water column. Thus a simulation of lobster larvae dispersal would require a value of A greater than unity. Note that biological concentrations are taken to be the number per unit-volume when all individuals are assumed to be of equal weight.

The numerical values of the diffusion coefficients are found by using the formula proposed by Taylor (1954) and transformed by Harleman (1966) to give

$$D_x = 20 g^{1/2} UH/C_c$$

$$D_y = 20 g^{1/2} VH/C_c$$

where g is gravitational acceleration and C_c the friction constant of Chezy. The diffusion coefficient is recalculated at all grids at each time step.

The Finite - Difference Equations

The vertically-integrated equation is now put into finite-difference formulation for numerical solution. Equation 2 is split into two parts to allow the use of an alternating direction method, in this case analogous to that of Peaceman and Rachford (1955). The only restriction placed on the numerical scheme chosen is that for the case of $C = 1$, it reduces to the continuity equation in the hydrodynamic computations. Using the notation

$$C = C(t)$$

$$C' = C(t + \frac{1}{2}\Delta t)$$

$$C'' = C(t + \Delta t)$$

mass conservation is

(first half time step)

$$\begin{aligned}
& \frac{2}{\Delta t} (H' C')_{n,m} - \frac{2}{\Delta t} (HC)_{n,m} + \frac{A}{\Delta L} (H U' C')_{n,m+\frac{1}{2}} - \frac{A}{\Delta L} (H U' C')_{n,m-\frac{1}{2}} \\
& - \frac{1}{\Delta L^2} (H'D_x')_{n,m+\frac{1}{2}} (C'_{n,m+1} - C'_{n,m}) + \frac{1}{\Delta L^2} (H'D_x')_{n,m-\frac{1}{2}} (C'_{n,m} - C'_{n,m-1}) \\
& + \frac{A}{\Delta L} (HVC)_{n+\frac{1}{2},m} - \frac{A}{\Delta L} (HVC)_{n-\frac{1}{2},m} - \frac{1}{\Delta L^2} (HD_y)_{n+\frac{1}{2},m} (C_{n+1,m} - C_{n,m}) \\
& + \frac{1}{\Delta L^2} (HD_y)_{n-\frac{1}{2},m} (C_{n,m} - C_{n-1,m}) = \frac{1}{2}(q + q')(H + H')_{n,m} \quad (3)
\end{aligned}$$

(second half time step)

$$\begin{aligned}
& \frac{2}{\Delta t} (H'' C'')_{n,m} - \frac{2}{\Delta t} (H' C') + \frac{A}{\Delta L} (H' U' C')_{n,m+\frac{1}{2}} - \frac{A}{\Delta L} (H' U' C')_{n,m-\frac{1}{2}} \\
& - \frac{1}{\Delta L^2} (H'D_x')_{n,m+\frac{1}{2}} (C'_{n,m+1} - C'_{n,m}) + \frac{1}{\Delta L^2} (H'D_x')_{n,m-\frac{1}{2}} (C'_{n,m} - C'_{n,m-1}) \\
& + \frac{A}{\Delta L} (H' V'' C'')_{n,m+\frac{1}{2}} - \frac{A}{\Delta L} (H' V'' C'')_{n-\frac{1}{2},m} - \frac{1}{\Delta L^2} (H'' D_y'')_{n+\frac{1}{2},m} (C''_{n+1,m} - C''_{n,m}) \\
& + \frac{1}{\Delta L^2} (H'' D_y'')_{n-\frac{1}{2},m} (C''_{n,m} - C''_{n-1,m}) = \frac{1}{2}(q' + q'')(H' + H'')_{n,m} \quad (4)
\end{aligned}$$

The above scheme is not the only one admissible. For example, in the first half time step, D_x rather than D_x' could be used without violating continuity.

The equation for the first half time step (3) displays the unknown, C' , in conjunction with derivatives in only the x -direction. In equation 4, C'' occurs only with y -direction derivatives. Thus, the two equations alternate direction, and the implicit equations resulting can be solved by Gaussian elimination. Consider equation 3, which can be recast as

$$P_m C'_{n,m-1} + Q_m C'_{n,m} + R_m C'_{n,m+1} + S_m = 0 \quad (5)$$

where the coefficients P_m , Q_m , and R_m contain known velocities and diffusion coefficients, and the term S_m is a function of the known concentrations C , at the previous time step. The solution of equation 5 is described in Appendix B.

Most of the simulations run with this scheme incorporate the numerical peculiarity known as "upstream differencing" in the convective terms. For a constant depth and a uniform, positive velocity, central differencing produces

$$HU \frac{\partial C}{\partial x} = \frac{HU}{\Delta L} \left[\frac{C_{m+1} + C_m}{2} - \frac{C_m + C_{m-1}}{2} \right] = \frac{HU}{2\Delta L} \left[C_{m+1} - C_{m-1} \right] \quad (6)$$

However, at grids adjacent to sources, the upstream concentration computed with central differencing will be negative; moreover, an unrealistic oscillating solution will propagate upstream. To eliminate these effects, the concentration immediately upstream, rather than the average over two grids, is used in equation 6.

Hence,

$$HU \frac{\partial C}{\partial x} = \frac{HU}{\Delta L} \left[C_m - C_{m-1} \right] \quad \text{for } U > 0$$

$$\text{and } HU \frac{\partial C}{\partial x} = \frac{HU}{\Delta L} \left[C_{m+1} - C_m \right] \quad \text{for } U < 0$$

In general,

$$\frac{\partial C}{\partial x} = \frac{1}{\Delta L} \left[\alpha C_m + (1-\alpha) C_{m+1} - \beta C_m - (1-\beta) C_{m-1} \right]$$

so that central differencing means $\alpha = \beta = 0$. For the case of positive U , upstream differencing results when $\alpha = 1$, $\beta = 0$. Other cases use a weighted

upstream differencing scheme with $\alpha = 3/4$, $\beta = 1/4$ for this example.

Upstream differencing suppresses negative values of concentration, but adds greatly to the effective diffusion. It may be shown that the diffusion coefficient, D^* , can be expressed as

$$D^* = D + \frac{1}{2} |U| \Delta L$$

Even with this large effective coefficient, diffusion is much less important as a transport mechanism than convection, which is usually at least one order of magnitude larger. Upstream differencing is used for the present investigation.

Boundary Conditions

The mathematical problem is properly posed when the initial and boundary conditions are set. For the present study the Bay is assumed to have no marked fluid at the start of the run. The least complex boundary condition is to require zero concentration there for all time. While this is suitable for certain geometrics and constituents, it fails for the present application, and a better approximation must be proposed.

Since the marked fluid originates within the modeled region, it will approach the boundary with a negative gradient (Fig. 3a). The boundary condition proposed for this case (at ebb in Narragansett Bay at Rhode Island Sound, and at flood at Mount Hope Bay) is found by assuming that the curve $C(x,t)$ is locally linear and approaches the boundary at $M = m_a + 1$ by pure translation. Then the boundary condition is then computed from the interior field as

$$C^*_{m_a+1} = \frac{U\Delta t}{2\Delta L} C_{m_a} + \left(1 - \frac{U\Delta t}{2\Delta L}\right) C_{m_a+1}$$

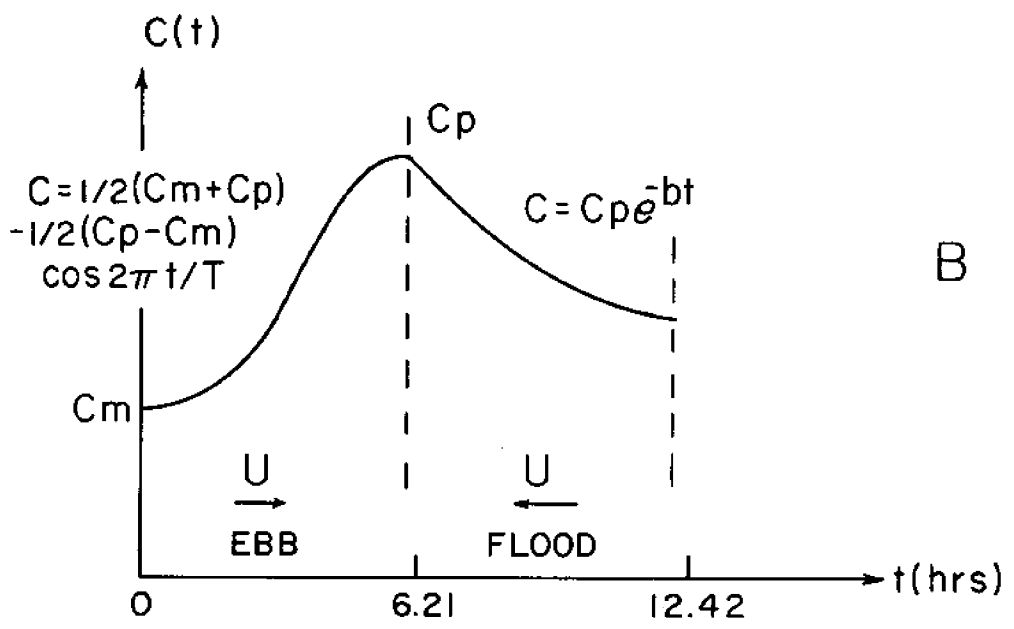
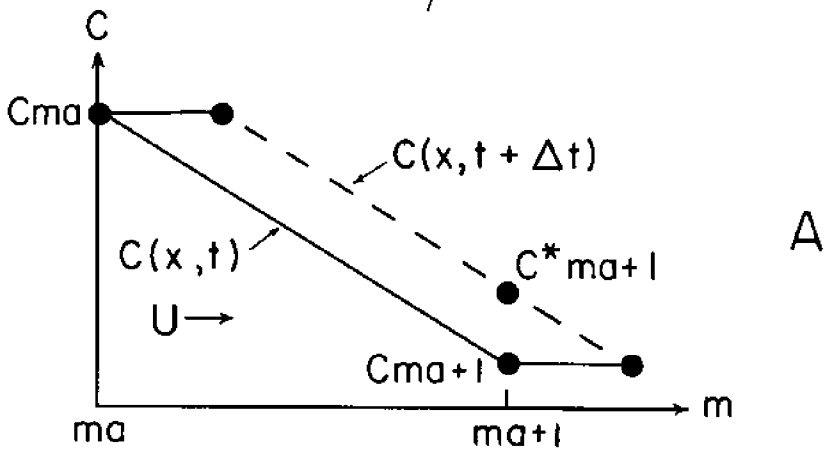


Figure 3. Boundary conditions showing (a) the linear assumption at outflow, and (b) the variation over a full cycle and the decreasing exponential assumption at inflow.

This method of specifying the boundary has worked well without affecting the stability of the computation scheme.

The boundary conditions at inflow are more difficult to compute. Because of the tidal characteristics of Narragansett Bay, the velocity at the mouth is closely approximated by a sine curve. During ebb, or outflow, the concentration at the boundary due to an interior source can be approximated by Fig. 3b

$$\frac{1}{2}(C_m + C_p) - \frac{1}{2}(C_p - C_m) \cos \frac{2\pi t}{T}$$

At flood the concentration is assumed to be a decreasing exponential as depleted Rhode Island Sound water enters the Bay, so that

$$C_F(t) = C_p e^{-bt}$$

Multiplying by a sinusoidal velocity (flow rate), integrating the appropriate expressions over flood and ebb, and specifying that R is the fraction of mass returning on flood, one finds

$$\frac{1 + e^{-bt}}{0.25 + b^2} = \frac{4R(C_m + C_p)}{BC_p}$$

where B is the ratio of the strength of the ebb current to the flood current. When B and R are given and C_m and C_p are found, b can be calculated. Thus, the boundary condition on inflow can be specified analytically. The actual returning mass fraction has not been measured for Narragansett Bay, although it has been found for the Niantic River, a similar embayment, by Hess, Sissenwine and Saila (1975) to be approximately 70 percent. At Rhode Island Sound, R is taken as 50 percent, and at Mount Hope Bay 71 percent.

The numerical scheme described herein has been widely used by the authors and others to model mass transport in several coastal waterways. Stability is virtually assured when driven by a hydrodynamic model with

the same time step. Accuracy is a function of time step and grid mesh size and the quality of current vector input. Analytical distributions of concentrations can be modeled to desired accuracy for known values of turbulent diffusion. Verification studies of the concentration model are not presently available. Preliminary model predictions by Kramer (in preparation) indicate that gross features of diffusion and mixing are accurately reproduced.

Multiple Time Steps

The numerical computation scheme derived (Equations 3, 4) uses velocities calculated in the hydrodynamic model and has the same time step, Δt . However, the equation of mass conservation for a constituent can be solved with high accuracy with a longer time step, using the intermediate velocity components in a reformulated numerical equation, as shown in Sissenwine, Hess and Salla (1975).

The present equations, 3 and 4, are based on the continuity equations in the hydrodynamic computations, and each conserves mass. Adding these two equations and setting $D_x = D_y = 0$, and $C = C' = C'' = 0$ yield a third equation which also conserves mass

$$\frac{H'' - H}{\Delta t} + \frac{\partial}{\partial x} (H + H')U' + \frac{\partial}{\partial y} (HV + H'V'') = 0 \quad (7)$$

but has an effective time step of $2\Delta t$. Equation 7 can be used as a basis for a new constituent equation, or the process can be continued to produce even longer time steps. Using an effective time step of $6\Delta t$, and calculating the coefficients once (employing one tidal cycle of currents recursively), a real time reduction by a factor of 10 has been attained.

Case Studies

The concentration model was put to use by simulating discharges into Narragansett Bay at two locations, Quonset Point (grid N=7, M=31) and Coggeshall Point (N=17, M=29), near the location of United States Navy property at Melville. At the first location mass was injected at a constant rate for the entire length of the simulation, while at the second, injection was constant for three tidal cycles and zero thereafter.

Mass was introduced at the Quonset Point location at a nearly constant rate, so the concentration in that grid before convection or diffusion increased by 268.8 units per hour. For example, if the units of concentration were parts per billion (ppb), then adding mass to the grid at the rate of 43 pounds per hour at that point would increase the concentration at the rate of 268.8 ppb per hour.

The spreading of the isopleths around the Quonset Point source is shown in Figs. 4, 5 and 6. After 3 hours and high water slack is approached, the threshold contour has moved north approximately 2 nautical miles although the area of maximum concentration is located very close to the source. Successive drawings show the progress of the spread. The southerly position of the isopleth of value 50 has moved at the average rate of 1.5 nautical miles per day. The extension of the concentrate is primarily in the direction of the predominant currents, or north-south, with lateral spread occurring at a slower rate. Spread into the East Passage takes at least three tidal cycles.

The concentration at Fox Island (N=6, M=36), shown in Fig. 7, rises rapidly after ten hours when the concentrate first spreads to the island. If mass is injected continuously into the Bay and there is some constant percentage removal rate (in this case 50 percent), there is some time at which the concentration, averaged over a tidal cycle, will become constant. The model was run for 20 cycles (about 40 minutes of IBM 360/55 time), but after ten

days this equilibrium had not been reached (Fig. 8). However, an approximate curve can be fitted through the tidal means, which is

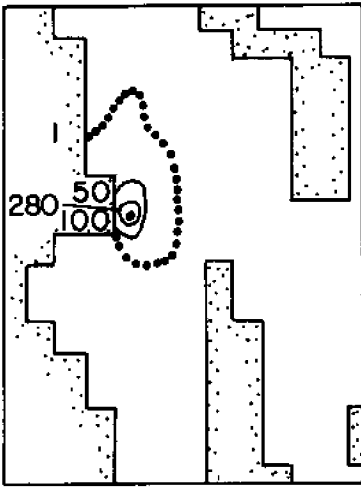
$$C = 660 [1 - 1/\exp(0.1 \text{ DAY} - 0.025)].$$

Employing this relationship it can be seen that it requires about 23 days for the concentration at Fox Island to reach 90 percent of equilibrium, averaged over a tidal period.

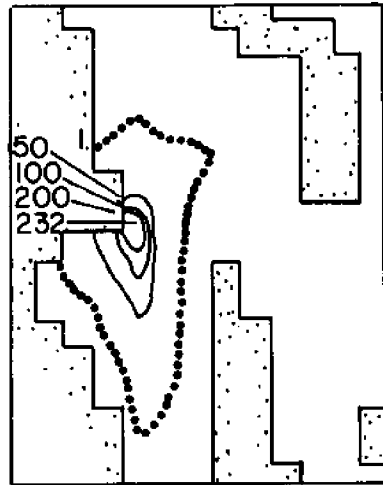
Mass was injected into the Coggeshall Point location at a nearly constant rate for three tidal cycles, then the injections were ceased. As with the previous location, the concentration without convection or diffusion was increased by 268.8 parts per hour. In this case the equivalent mass rate would be 46 pounds per hour in that grid square if the concentration were measured in ppb.

The isopleths are plotted in Figs. 9 through 12. By the end of the first full tidal cycle there is significant concentration (more than 25 ppb) in most of the upper East Passage. The region of highest concentration remains small and near the point of injection. After four tidal cycles the 25-ppb isopleth has moved down toward Newport Harbor, and westward into the West Passage. The extent of the area is primarily north-south, as was the case in the Quonset Point source.

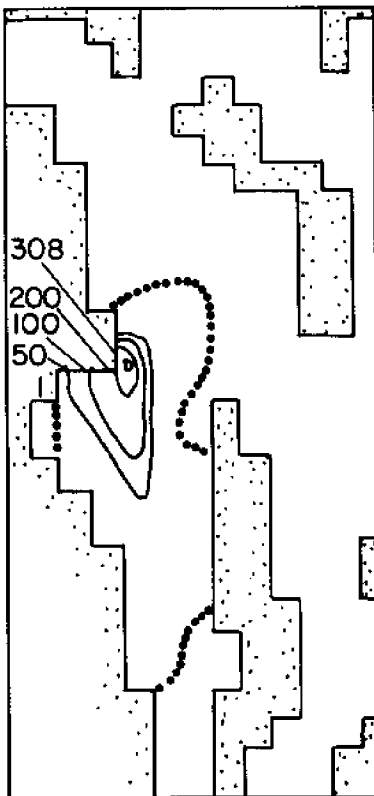
After the end of the injection period, flushing quickly reduces the peaks of concentration. At the source point (N=17, M=29) three days is sufficient to reduce the mass to 10 percent of its maximum value (Fig. 13). The loss, which appears to be exponential, is approximately 28 percent of the mass from the injection point every two days.



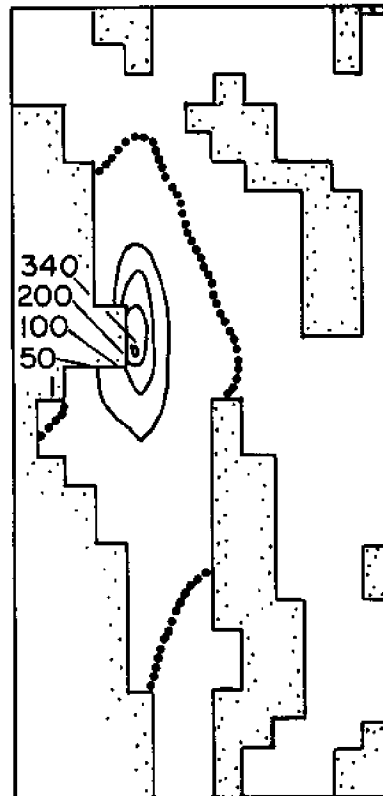
3 HOURS



6 HOURS



9 HOURS



12 HOURS

Figure 4. Concentrations in the West Passage for 12 hours during a continuous injection of mass just off Quonset Point.

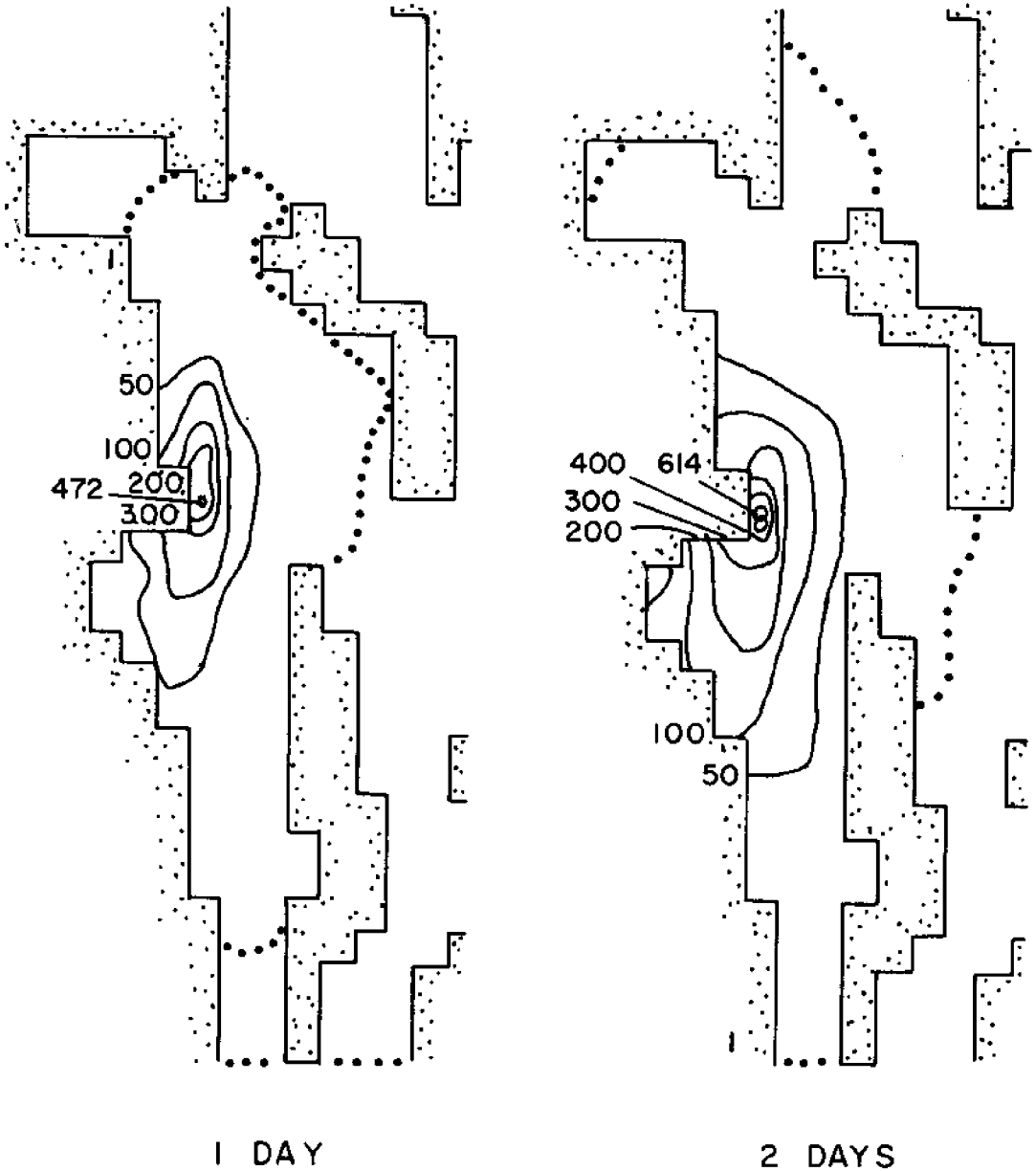


Figure 5. Concentrations in the West Passage at one and two days during a continuous injection at Quonset Point.

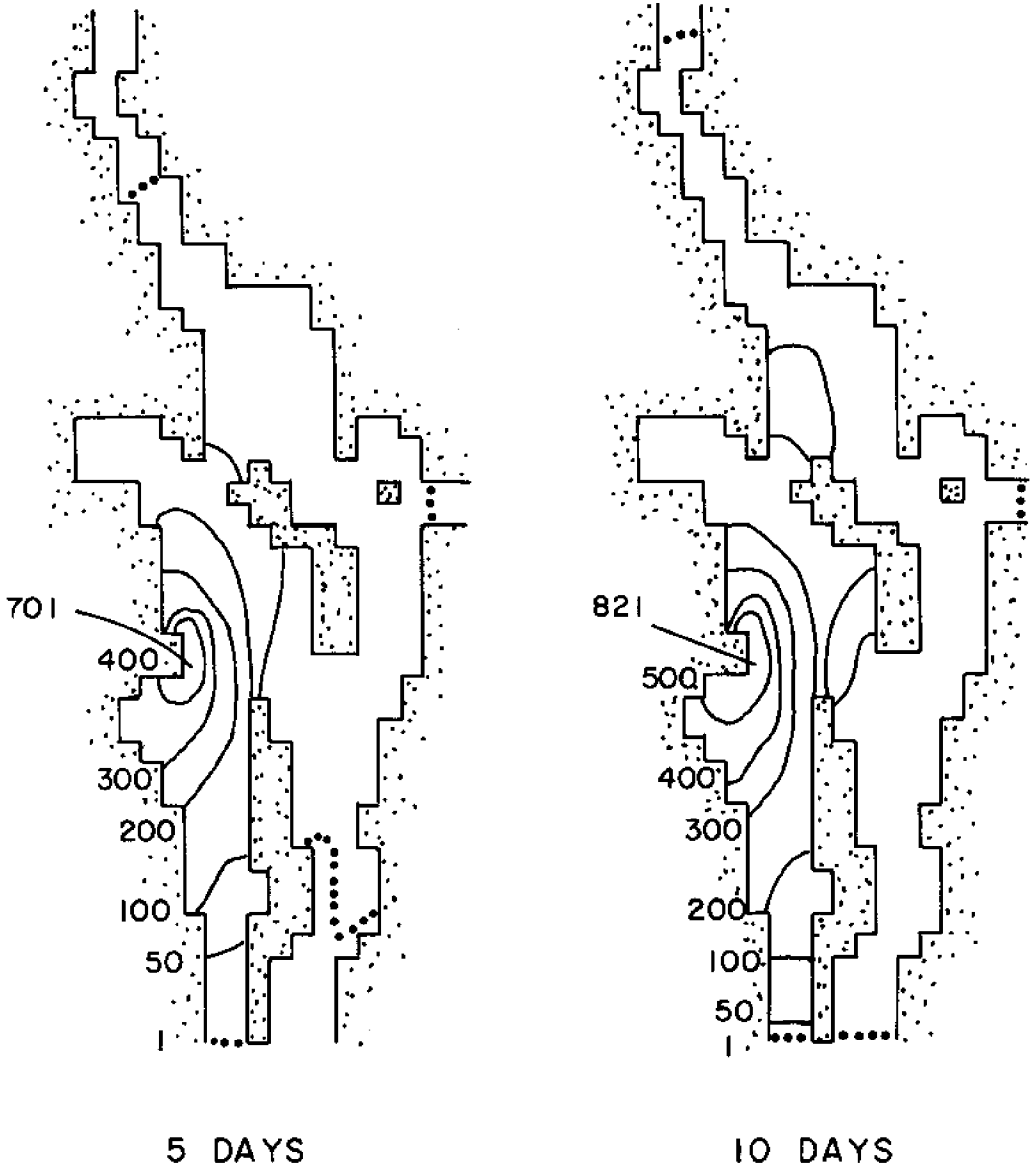


Figure 6. Concentrations in the West Passage after five and ten days during a continuous injection at Quonset Point.

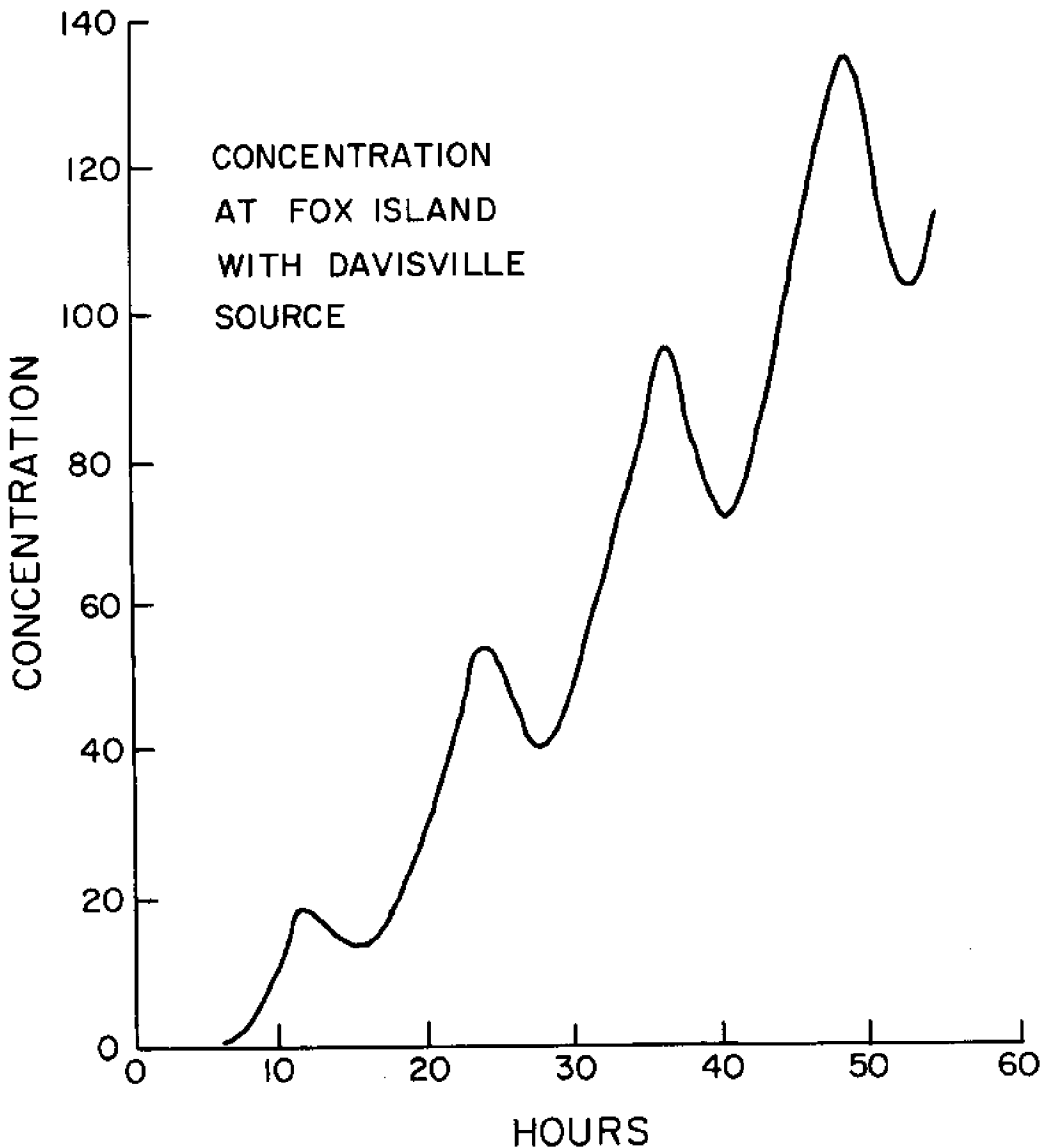


Figure 7. Concentration at Fox Island during the Quonset Point injection for the first 60 hours. Six hours is required before significant concentrations occur at the island which is two miles south of the injection point, but the increase is rapid thereafter.

CONCENTRATION AT FOX ISLAND

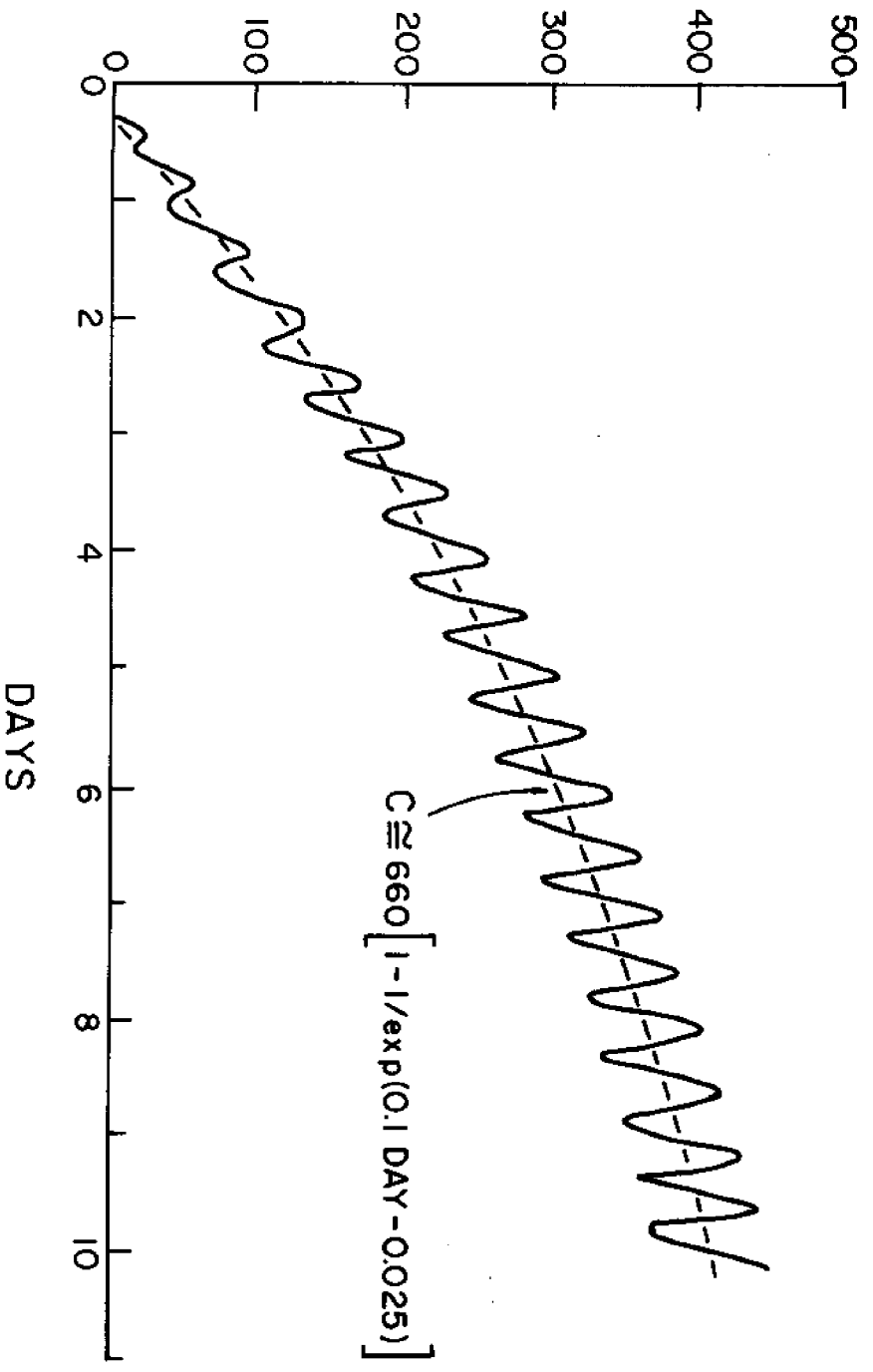


Figure 8. Fox Island concentration for the first ten days. Flattening of curve of averaged concentrations indicates that equilibrium is being approached.

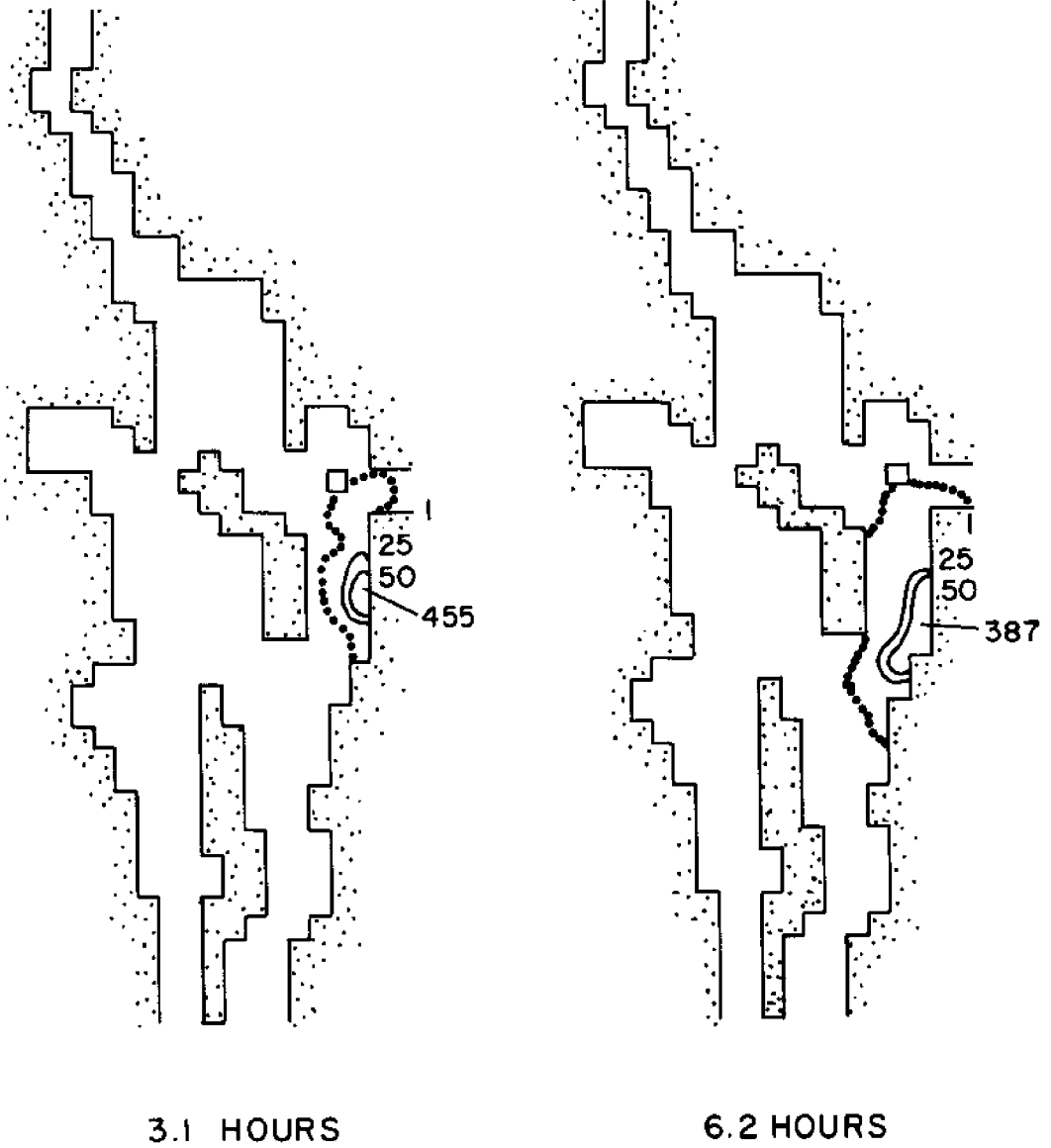


Figure 9. Concentration at 3.1 and 6.2 hours in Narragansett Bay due to injection at Coggeshall Point.

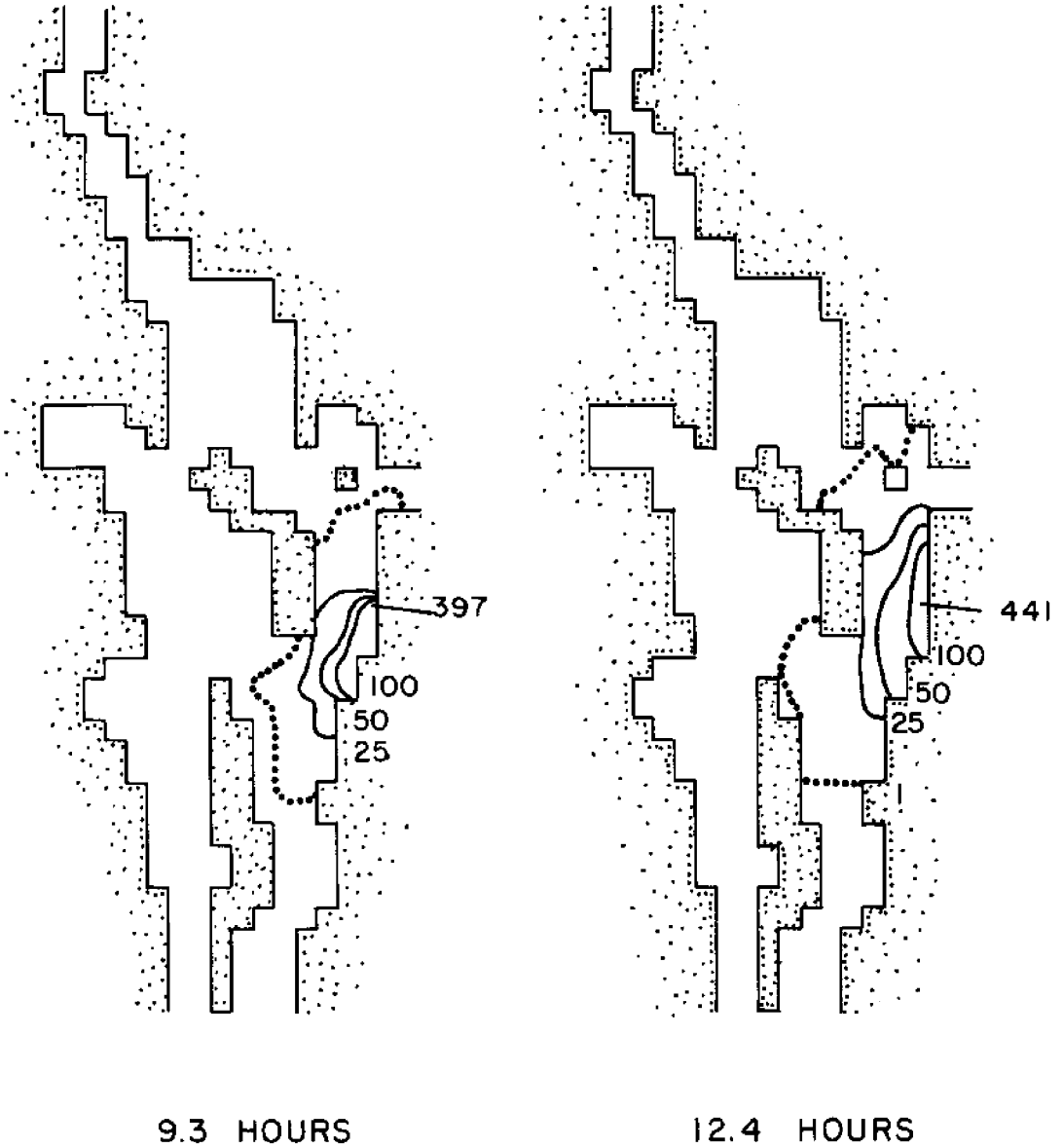


Figure 10. Concentration in Narragansett Bay after 9.3 and 12.4 hours of injection at Coggeshall Point.

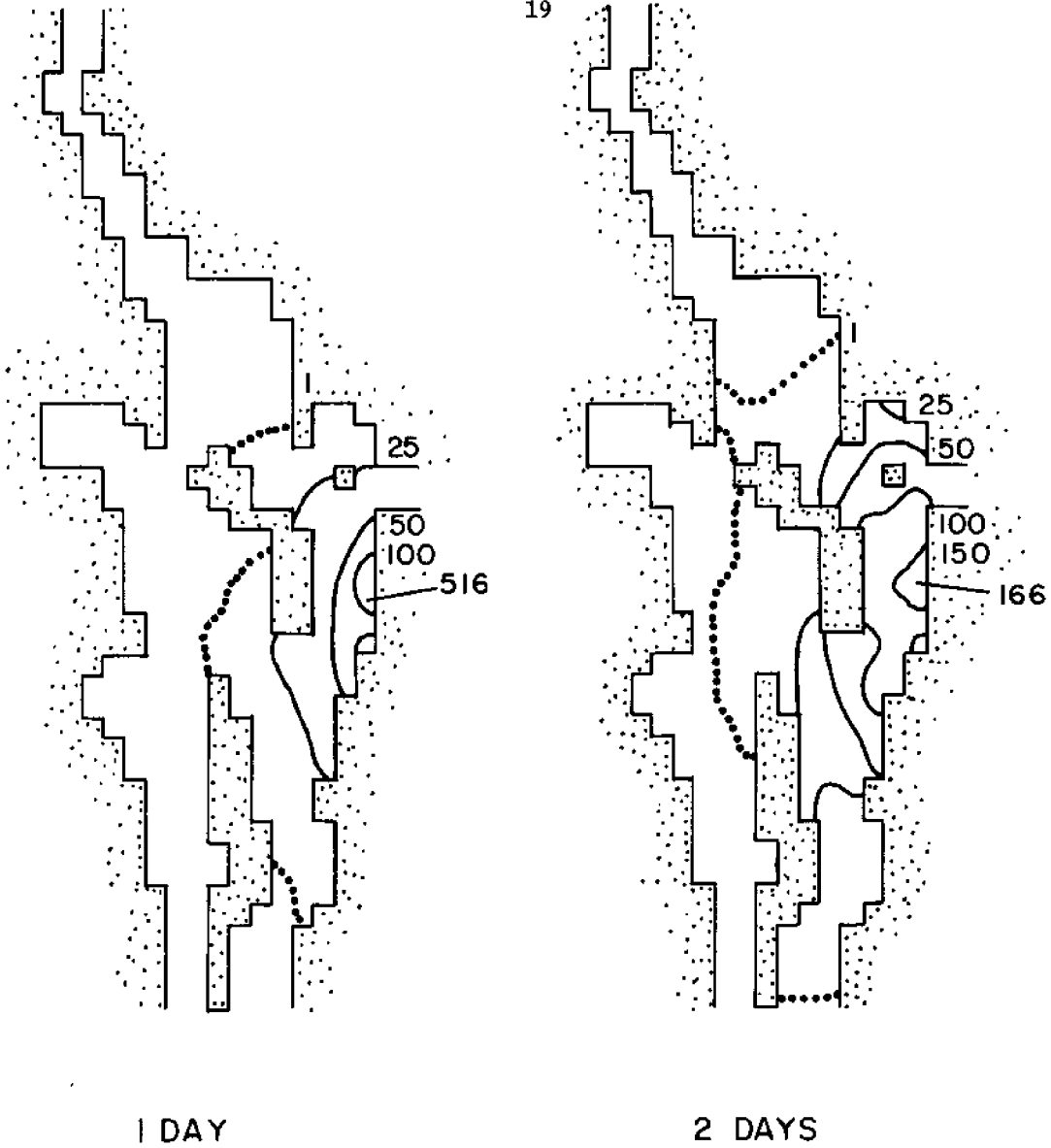


Figure 11. Concentration in Narragansett Bay after one and two full days. Injection ceases midway through the second day.

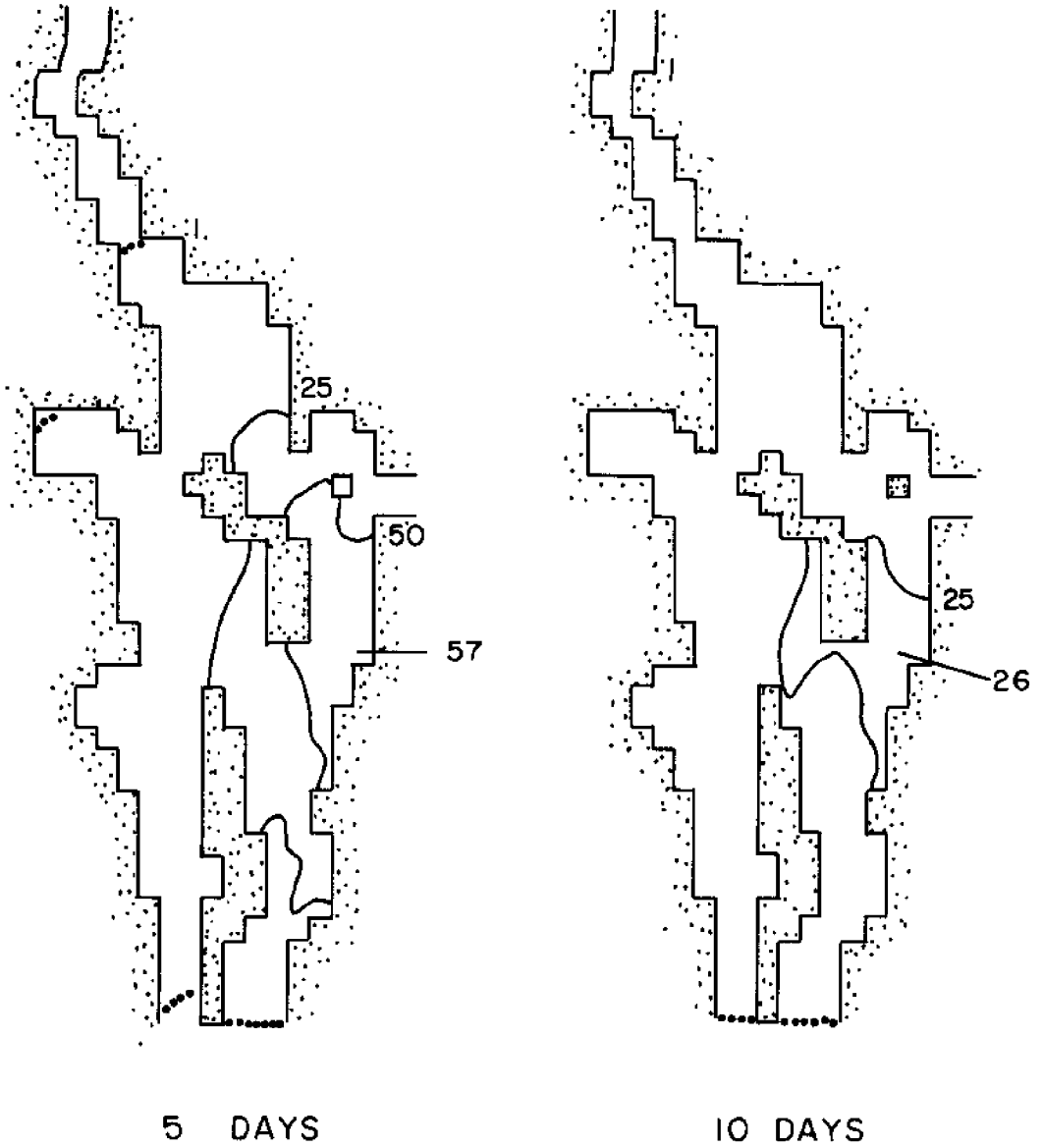


Figure 12. Concentrations in Narragansett Bay after five and ten full days. Rapid decrease of peak concentrations shows that flushing is efficient.

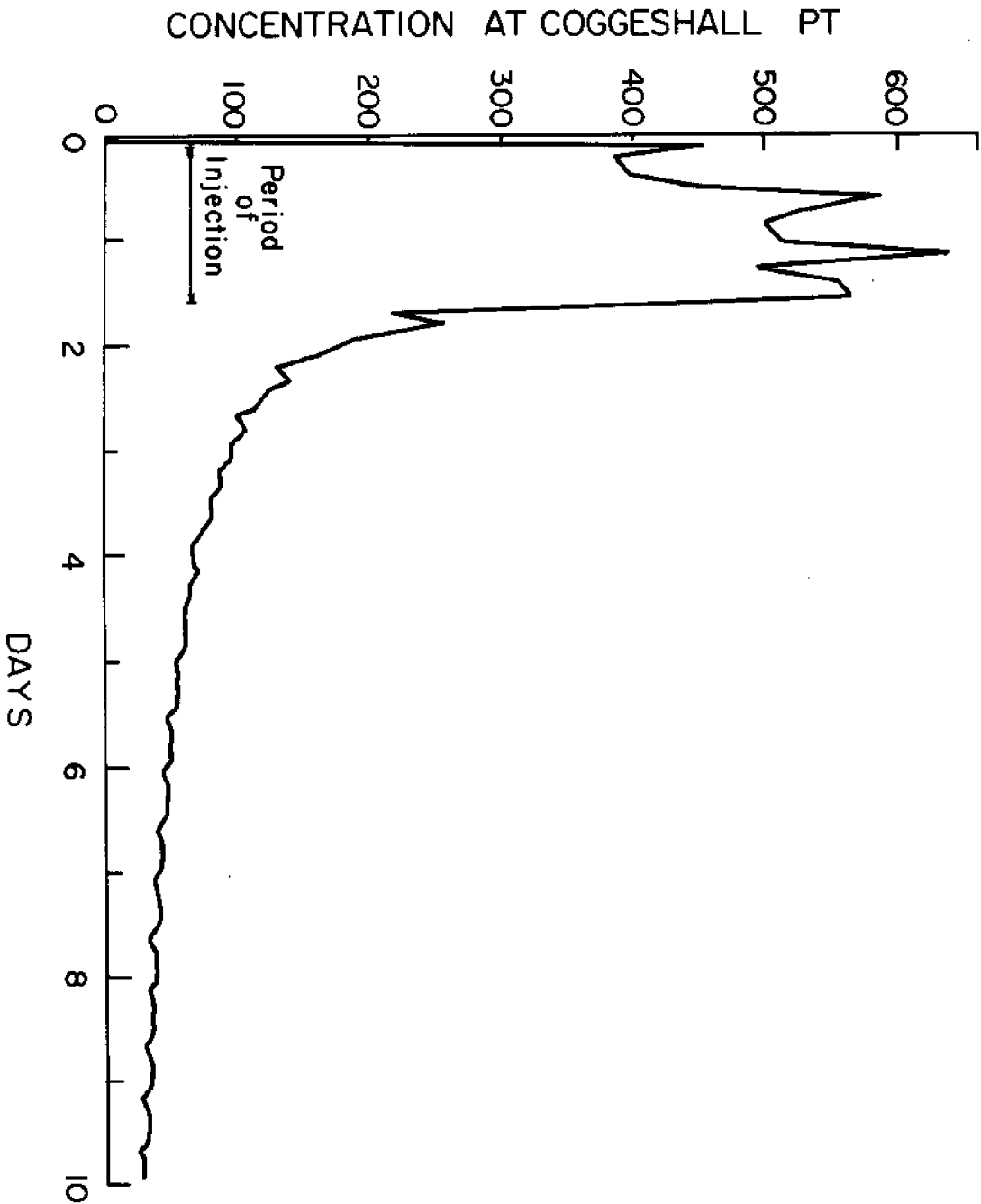


Figure 13. Concentration at Coggeshall Point, the place of injection, for ten days. Decay is rapid when injection ceases -- about 15 percent of the remaining mass at that point is lost every day.

Appendix A

Given the equation

$$\frac{\partial c}{\partial t} + \frac{\partial}{\partial x} uc + \frac{\partial}{\partial y} vc + \frac{\partial}{\partial z} wc - \frac{\partial}{\partial x} D_x \frac{\partial c}{\partial x} - \frac{\partial}{\partial y} D_y \frac{\partial c}{\partial y} - \frac{\partial}{\partial z} D_z \frac{\partial c}{\partial z} = q \quad (1)$$

the Leibniz rule for differentiating within an integral is most useful:

$$\frac{d}{dt} \int_a^b \frac{\partial F}{\partial x}(x, z) dz = \frac{\partial}{\partial x} \int_a^b F(x, z) dz - F(x, b) \frac{\partial b}{\partial x} + F(x, a) \frac{\partial a}{\partial x} \quad (2)$$

Here the integration is from the bottom ($z = -h$) to the surface ($z = \eta$).

Note also that (see Egleston and Dean, 1966, p. 20)

$$\frac{\partial \eta}{\partial t} = w - u \frac{\partial \eta}{\partial x} - v \frac{\partial \eta}{\partial y} \quad (3)$$

The vector component $F_{\hat{n}}$ in the surface normal direction, \hat{n} , is

$$F_{\hat{n}} = F_z \cos\theta - F_x \sin\theta$$

$$\text{but } \sin\theta \approx \frac{\partial \eta}{\partial x}$$

$$\text{and } \cos\theta \approx 1$$

$$\text{so } F_{\hat{n}} \approx F_z - \frac{\partial \eta}{\partial x} F_x \quad (4)$$

At the bottom

$$F_{\hat{n}} = -F_z - \frac{\partial h}{\partial x} F_x \quad (5)$$

The vertically-averaged quantities may be defined as

$$\frac{1}{H} \int_{-h}^{\eta} u dz = U \quad (6a)$$

$$\frac{1}{H} \int_{-h}^{\eta} v dz = V \quad (6b)$$

$$\frac{1}{H} \int_{-h}^{\eta} c dz = C \quad (6c)$$

where $H = h + \eta$. Therefore the velocities and concentration can be defined in terms of their means

$$u = [1 + e(z)]$$

$$v = [1 + f(z)]$$

$$c = [1 + g(z)]$$

Thus

$$\int_{-h}^{\eta} u c dz = UC \int_{-h}^{\eta} (1+e+g+eg) dz = UC \left[H + \int_{-h}^{\eta} eg dz \right] \equiv AHUC \quad (7)$$

Integrating each term in equation 1, and further noting that

$$\partial h / \partial t = u(z = -h) = v(z = -h) = w(-h) = 0$$

$$\int_{-h}^{\eta} \frac{\partial c}{\partial t} dz = \frac{\partial}{\partial t} \int_{-h}^{\eta} c dz - c(\eta) \frac{\partial \eta}{\partial t} = \frac{\partial AHUC}{\partial t} - c(\eta) \frac{\partial \eta}{\partial t} \quad (8a)$$

$$\int_{-h}^{\eta} \frac{\partial}{\partial x} (uc) dz = \frac{\partial}{\partial x} AHUC - (uc) \Big|_{\eta} \frac{\partial \eta}{\partial x} \quad (8b)$$

$$\int_{-h}^{\eta} \frac{\partial}{\partial y} (vc) dz = \frac{\partial}{\partial y} AHVC - (vc) \Big|_{\eta} \frac{\partial \eta}{\partial y} \quad (8c)$$

$$\int_{-h}^{\eta} \frac{\partial}{\partial z} w c dz = (wc) \Big|_{\eta} \quad (8d)$$

Assuming that D_x and D_y are independent of depth,

$$\int_{-h}^{\eta} \frac{\partial}{\partial x} D_x \frac{\partial c}{\partial x} dz = \frac{\partial}{\partial x} HD_x C - \left(D_x \frac{\partial c}{\partial x} \right) \Big|_{\eta} \frac{\partial \eta}{\partial x} - \left(D_x \frac{\partial c}{\partial x} \right) \Big|_{-h} \frac{\partial \eta}{\partial x} \quad (8e)$$

$$\int_{-h}^{\eta} \frac{\partial}{\partial y} D_y \frac{\partial c}{\partial y} dz = \frac{\partial}{\partial y} HD_y C - \left(D_y \frac{\partial c}{\partial y} \right) \Big|_{\eta} \frac{\partial \eta}{\partial y} - \left(D_y \frac{\partial c}{\partial y} \right) \Big|_{-h} \frac{\partial \eta}{\partial y} \quad (8f)$$

$$\int_{-h}^{\eta} \frac{\partial}{\partial z} D_z \frac{\partial c}{\partial z} dz = D_z \frac{\partial c}{\partial z} \Big|_{\eta} - D_z \frac{\partial c}{\partial z} \Big|_{-h} \quad (8g)$$

$$\int_{-h}^{\eta} q dz = Hq \quad (8h)$$

The four surface terms in (8a, b, c, d) can be grouped so

$$-c(\eta) \frac{\partial \eta}{\partial x} - c(\eta)u(\eta) \frac{\partial \eta}{\partial x} - c(\eta)v(\eta) \frac{\partial \eta}{\partial y} + c(\eta)w(\eta) = 0$$

by virtue of the surface condition (3). Also, the surface and bottom terms in 8e, f, g are simply the turbulent flux normal to the top and bottom surfaces (c.f. equations 4 and 5), which equals zero. Thus

$$\frac{\partial}{\partial t} HC + \frac{\partial}{\partial x} H(AUC - D_x \frac{\partial C}{\partial x}) + \frac{\partial}{\partial y} H(AVC - D_y \frac{\partial C}{\partial y}) = qH$$

is the vertically-integrated form of the mass equation.

Appendix B

The general recursive relation at grid m is

$$P_m C_{m-1} + Q_m C_m + R_m C_{m+1} = S_m \quad (1)$$

Consider the first computational grid in the row at the lower (value of the index m) end as $m = m_a = 2$. If the boundary is open (water-bound), then C_1 is specified. If closed, $P_2 = 0$ and C_1 may have any value. Then equation 1 can be recast as C_2 in terms of C_3 ,

$$C_2 = \frac{S_2 - P_2}{Q_2} C_1 - \frac{R_2 C_3}{Q_2} \equiv F_2 - G_2 C_3 \quad (3)$$

Now at the next grid, $m = 3$, equation 1 is

$$P_3 C_2 + Q_3 C_3 + R_3 C_4 = S_3$$

but with equation 2

$$P_3(F_2 - G_2 C_3) + Q_3 C_3 + R_3 C_4 = S_3$$

or

$$C_3 = \frac{S_3 - P_3 F_2}{Q_3 - P_3 G_2} - \frac{R_3}{Q_3 - P_3 G_2} C_4 = F_3 - G_3 C_4$$

Continuing this trend, the simple relationship arises

$$C_m = F_m - G_m C_{m+1} \quad (3)$$

where

$$F_m \begin{cases} = \frac{S_m - P_m F_{m-1}}{Q_m - P_m G_{m-1}} & m > m_a \\ = C_{m-1} & m = m_a - 1 \end{cases} \quad (4)$$

$$G_m \begin{cases} = \frac{R_m}{Q_m - P_m G_{m-1}} & m > m_a \\ = 0 & m = m_a - 1 \end{cases} \quad (5)$$

Proceeding up the grid row to the last interior square at $m = m_b$,

$$C_{m_b} = F_{m_b} - G_{m_b} C_{m_b+1}$$

Now, if the boundary is open, C_{mb+1} is known, and, if closed

$R_{mb} = G_{mb} = 0$, so C_{mb} is again known. Then, using equation 3, the unknowns

C_m are computed successively down the grid row.

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Computer Program SALT Listing

Note: The following constants are used in the program:

AU = 1.0	C7 = 200.*SQRT(AG)
C1 = AL*AT	C8 = AU/AL
C2 = AT	C10 = 2.*C7/(AL**2)
C3 = AL**2	

```

SUBROUTINE SALT(NST, ISTEP, AL, AG, NHR)
  COMMON /F(30,50), SEP(30,50), U(30,50), UP(30,50), V(30,50), VP(30,50)
  1  U(10,50), U(30,50), TEF(10,50), MRD(100), MRD(100), NPRINT(100),
  2  NORD(10), NORD(10), INUM(30,50), JNUM(500), AL, A2, A3, A4, A5, A6, AT,
  3  RMAX, MMAX, NIND(,MININD, MAXST, MIND, MIND)
  COMMON /C(20,50), CNP(30,50), C1, C2, C3, C7, C8, C10
  DIMENSION A(48), R(48), P(48), C(48), R(48), S(48), KONVPT(30)
  DIMENSION ILTNEF(20), IINVF(20), TEXTU(20), TEXTV(20)
  LOGICAL TEST, RE/CIN
  JB=MHR
  CMAG=1000.
  IF(NST.EQ.10*(NST/10)) JB=15
  IF(NST.EQ.10*(NST/10)) JA=12
  JR=0
  JA=0
  PR=.1001
  MMAX=MMAX-1
  MMAX=MMAX-1
C
C   COMPUTE C/P ALONG ROWS IN SECOND HALF OF TIMESTEP
C
  ND=1
  IF(ISTEP.EQ.1) GO TO 400
  200 IF(NUM.(N,MIND) GO TO 600
  NSRCH=MRD(NUM)/1000000
  R  =MRD(NUM)/10000 -MSRCH*100
  RF  =MRD(NUM)/100 -MSRCH*10000 -M*100
  I  =MRD(NUM) -MSRCH*1000000 -M*10000 -NF*100
  IA=MSRCH/10
  IR=MSRCH-10*IA
  LL=L-1
  LP=L+1
  NFF=NF-1
  NMR=M+1
  NM=M-1

  N=NFF
  GAMMAC=.5*VP(N,M)/(ABS(VP(N,M))+ER)+.5
  TEMP4=.5*(H(N,M)+H(N,MM))+SF(N,M)+SE(N+1,M)
  TEMP8=.5*(H(N,M)+H(N,MM))+SEP(N,M)+SEP(N+1,M)
  TEMP22=C8*TEMP4*VP(N,M)
  TEMP23=C10*ABS(VP(N,M))*TEMP8**2/(C(N,M)+C(N+1,M))
C
  DO 220 N=NF, L
    NM=N-1
    NNN=N+1
    NN=N-1
    ALFAC=.5*U(N,M)/(ABS(U(N,M))+ER)+.5
    BETAC=-.5*U(N,MM)/(ABS(U(N,MM))+ER)+.5
  C   DELTAC=-.5*VP(NM,M)/(ABS(VP(NM,M))+ER)+.5
    DELTAC=1.-GAMMAC

```

```

GAMMAC=.5*VP(N,M)/(ABS(VP(N,M))+ER)+.5
C
TEMP1=(.25*(H(N,M)+H(NN,M)+H(N,MM)+H(NN,MM))+SEP(N,M))/AT
TEMP2=(.25*(H(N,M)+H(NN,M)+H(N,MM)+H(NN,MM))+SE(N,M))/AT
C
TEMP3=.5*(H(NN,M)+H(NN,MM))+SE(N,M)+SE(NN,M)
TEMP3=TEMP4
TEMP4=.5*(H(N,M)+H(N,MM)+SE(N,M)+SE(NNN,M))
TEMP5=.5*(H(N,MM)+H(NN,MM))+SE(N,M)+SE(N,MM))
TEMP6=.5*(H(N,M)+H(NN,M)+SE(N,M)+SE(N,MMM))
TEMP7=TEMP8
TEMP8=.5*(H(N,M)+H(N,MM))+SEP(N,M)+SEP(N+1,M))
C
TEMP20=CR*TEMP3*VP(NN,M)
C
TEMP21=C10*ABS(VP(NN,M))*TEMP3**2/(C(N,M)+C(NN,M))
TEMP20=TEMP22
TEMP21=TEMP23
TEMP22=CR*TEMP4*VP(N,M)
TEMP23=C10*ABS(VP(N,M))*TEMP6**2/(C(N,M)+C(N+1,M))
TEMP24=CR*TEMP5*U(N,MM)
TEMP25=C10*ABS(U(N,MM))*TEMP5**2/(C(N,M)+C(N,MM))
TEMP26=CR*TEMP6*U(N,M)
C
TEMP27=C10*ABS(U(N,M))*TEMP6**2/(C(N,M)+C(N,MMM))
C
P(N)=-((1.-DELTA C)*TEMP20+TEMP21)
Q(N)=TEMP1+GAMMAC*TEMP22+TEMP23-DELTA C*TEMP20+TEMP21
R(N)=(1.-GAMMAC)*TEMP22-TEMP23
S(N)=-CN(N,MM)*((1.-BETAC)*TEMP24+TEMP25)
I+CN(N,M)*(-TEMP2+ALFAC*TEMP26-BETAC*TEMP24+TEMP27+TEMP25)
J+CN(N,MMM)*((1.-ALFAC)*TEMP26-TEMP27)
TEST=.FALSE.
IF(NM.EQ.JA) TEST=.TRUE.
IF(TEST) WRITE(6,1200) N,M,P(N),Q(N),R(N),S(N)
IF(TEST) WRITE(6,1200) N,M,TEMP1,TEMP2
IF(TEST) WRITE(6,1200) N,M,TEMP20,TEMP21,TEMP22,TEMP23
IF(TEST) WRITE(6,1200) N,M,TEMP24,TEMP25,TEMP26,TEMP27
IF(TEST) WRITE(6,1200) N,M,ALFAC,BETAC,GAMMAC,DELTA C
1200 FORMAT( //,3X,'N=',I2,2X,I2,2X,7(F10.4,2X))
220 CONTINUE
B(NFF)=0.
A(NFF)=CNP(NFF,M)
IF(TEST) WRITE(5,1200) N,M,A(NFF),CNP(LP,M)
DP 240 N=NF,L
NN=N-1
F1=Q(N)-P(N)*B(NN)
A(N)=-((S(N)+P(N)*A(NN))/F1)
240 B(N)=R(N)/F1
* = L
DP 245 I=NF,L
NP=N+1
CNP(N,M)=A(N)-B(N)*CNP(NP,M)
IF(TEST) WRITE(6,1200) N,M,CN(N,M),CNP(N,M)
245 * = N-1
NLM=NIM+1
GO TO 208
C
C
C
C

```

```

C      COMPUTE CNP ALONG COLUMNS IN FIRST HALF OF TIMESTEP
C      C
C      C
C      C
400 IF(NUM.EQ.NIND) GO TO 402
   NSRCH=NBD(NUM)/1000000
   N      =NBD(NUM)/10000  -NSRCH*100
   MF     =NBD(NUM)/100-NSRCH*10000-N*100
   L      =NBD(NUM)-NSRCH*1000000-N*10000-MF*100
   IA=NSRCH/10
   IB=NSRCH-10*IA
   NN=N-1
   NNN=N+1
   LL=L-1
   LLL=L+1
   LP=L+1
   MFF =MF-1
   M=MFF
   ALFAC=.5*UP(N,M)/(ABS(UP(N,M))+ER)+.5
   TEMP4=.5*(H(N,M)+H(NN,M)+SE(N,M)+SE(N,M+1))
   TEMP2=.5*(H(N,M)+H(NN,M)+SEP(N,M)+SEPP(N,M+1))
   TEMP22=C8*TEMP4*UP(N,M)
   TEMP23=C10*ABS(UP(N,M))*TEMP2**2/(C(N,M)+C(N,M+1))
C
   DC 420 M=MFF,1
   MMM=M+1
   MNN=M-1
   MNM=N-1
   RETAC=1.-ALFAC
   ALFAC=.5*UP(N,M)/(ABS(UP(N,M))+ER)+.5
   RETAC=-.5*UP(N,MM)/(ABS(UP(N,MM))+ER)+.5
   GAMMAC=.5*V(N,M)/(ABS(V(N,M))+ER)+.5
   DELTAC=-.5*V(NM,M)/(ABS(V(NM,M))+ER)+.5
   TEMP1=(.25*(H(N,M)+H(NN,M)+H(N,MM)+H(NN,MM))+SEP(N,M))/AT
   TEMP2=(.25*(H(N,M)+H(NN,M)+H(N,MM)+H(NN,MM))+SE(N,M))/AT
   TEMP2=TEMP4
C
   TEMP3=.5*(H(N,MM)+H(NN,MM)+SE(N,M)+SE(N,MM))
   TEMP4=.5*(H(N,M)+H(NN,M)+SE(N,M)+SE(N,MM))
   TEMP5=.5*(H(NN,M)+H(NN,MM)+SE(N,M)+SE(NN,M))
   TEMP6=.5*(H(N,M)+H(N,MM)+SE(N,M)+SE(NNN,M))
   TEMP7=TEMP3
   TEMP8=.5*(H(N,M)+H(NN,M)+SE(N,M)+SE(N,M+1))
C
   TEMP20=C8*TEMP3*UP(N,MM)
C
   TEMP21=C10*ABS(UP(N,MM))*TEMP3**2/(C(N,M)+C(N,MM))
   TEMP20=TEMP22
   TEMP21=TEMP23
   TEMP22=C8*TEMP4*UP(N,M)
   TEMP23=C10*ABS(UP(N,M))*TEMP8**2/(C(N,M)+C(N,M+1))
   TEMP24=C8*TEMP5*V(N,M)
   TEMP25=C10*ABS(V(NN,M))*TEMP5**2/(C(N,M)+C(NN,M))
   TEMP26=C8*TEMP6*V(N,M)
   TEMP27=C10*ABS(V(N,M))*TEMP6**2/(C(N,M)+C(NNN,M))
C
C
C
P(M)=-((1.-RETAC)*TEMP20+TEMP21)
Q(M)=TEMP1 +ALFAC*TEMP22 +TEMP23-BETAC*TEMP20 +TEMP21
R(M)=(1.-ALFAC)*TEMP22-TEMP23
S(M)=-C(NN,M)*((1.-DELTAC)*TEMP24+TEMP25)+

```

```

1 CN(N,M)*(-TEMP2+GAMMAC*TEMP26 -DELTAC*TEMP24+TEMP27+TEMP25)
2 +CN(NNN,M)*((1.-GAMMAC)*TEMP26-TEMP27)
TEST=.FALSE.
IF(NUM.EQ.JR) TEST=.TRUE.
IF(TEST) WRITE(6,1200) N,M,P(M),Q(M),R(M),S(M)
IF(TEST) WRITE(6,1200) N,M,TEMP1,TEMP2
IF(TEST) WRITE(6,1200) N,M,TEMP20,TEMP21,TEMP22,TEMP23
IF(TEST) WRITE(6,1200) N,M,TEMP24,TEMP25,TEMP26,TEMP27
IF(TEST) WRITE(6,1200) N,M,ALFAC,BETAC,GAMMAC,DELTAC

```

```

420 CONTINUE
P(MFF)=0.
A(MFF)=CNP(N,MFF)
IF(TEST) WRITE(6,1200) N,M,A(MFF),CNP(N,LP)
DO 440 M=MF,L
MM=M-1
F1=C(M)-P(M)*B(MM)
A(M)=-((S(M)+P(M)*A(MM))/F1)
440 B(M)=R(M)/F1
M=L
DO 445 T=MF,L
MP=M+1
CNP(N,M)=A(M)-B(M)*CNP(N,MP)
IF(TEST) WRITE(6,1200) N,M,CN(N,M),CNP(N,M)
445 M=M-1
NUM=NUM+1
GO TO 400
462 CONTINUE

```

C
C
C
C

PRINT OUT

```

IF(NST.EQ.1) GO TO 509
IF(NST.EQ.MAXST) GO TO 509
IF(NST.NE.1P*(NST/IP)) GO TO 520
509 CONTINUE
TIME=FLUAT(NST)*AT/1800.
WRITE(6,5024) NST,TIME
5024 FORMAT(1H1,'AVERAGED CONCENTRATION FOR SECOND HALF TIMESTEP',15,
1 5X,'TIME = ',F6.2,'HRS. ')
DO 508 N=1,NMAX
508 KONVRT(N)=N
M=0
WRITE(6,6001) M,(KONVRT(N),N=1,NMAX)
DO 510 M=1,NMAX
DO 512 N=1,NMAX
512 KONVRT(N)=(CN(N,M)+CNP(N,M))*5*CMAG+.5
IF(NST.EQ.MAXST) WRITE(7,6002) (KONVRT(N),N=1,NMAX)
6002 FORMAT(20I4)
510 WRITE(6,6001) M,(KONVRT(N),N=1,NMAX)
6001 FORMAT(1X,I2,1X,30I4)
520 CONTINUE
600 CONTINUE

```

C

RETURN
END

