Chapter 2

An Efficient Analysis of Pollutant Migration through Soil

R. K. Rowe and J. R. Booker

2.1 INTRODUCTION

The potential for contamination of groundwater is now a major consideration in the design and construction of waste disposal sites in many countries. Often the movement of contaminant from the disposal pit is controlled either by siting the landfill in a natural clayey soil or by constructing a compacted clay liner between the disposal pit and the surrounding soil. The selection of the type and thickness of the liner requires consideration of the expected concentrations at observation points beneath the liner, at the boundaries of the disposal site and possibly, at specific monitoring points outside the site. These contaminant migration analyses can be performed using time-marching finite element techniques [1], however, to obtain accurate results at both small and large times, this requires a relatively refined finite element mesh (to accommodate high concentration gradients at low times) and considerable computational effort.

Many soil deposits are horizontally layered and it is not really necessary to use the finite element method. In these cases, an alternative finite layer procedure proposed by Rowe and Booker [2-6] can be adopted for directly calculating the concentration of contaminants of specified locations and times. This approach, which will be described in this chapter, takes account of the fact that the concentration of contaminant within the disposal pit may decrease as mass is transported into the soil while also allowing for the possible presence of a more permeable underlying stratum (aquifer) beneath the clay liner. The technique to be adopted involves taking the Laplace and, where appropriate, Fourier transforms of the governing equations, finding an analytic solution in transform space and then numerically inverting the transforms to obtain the concentrations of contaminant at selected positions and times.

The solution will be developed initially for the case of 1D (vertical) advective-dispersive transport in layered soil but allowing for horizontal

transport in an underlying aquifer. The procedure will then be generalized to two and three dimensions.

The application of these techniques will be discussed and will be illustrated by a number of examples.

2.2 GOVERNING EQUATIONS

The transport of substances through a saturated clay can often be approximated by a Fickian-type law [7] having the form:

$$f_x = nv_x c - nD_{xx} \frac{\partial c}{\partial x}$$
 (2.1a)

$$f_y = nv_y c - nD_{yy} \frac{\partial c}{\partial y}$$
 (2.1b)

$$f_z = nv_z c - nD_{zz} \frac{\partial c}{\partial z}$$
 (2.1c)

where

c is the concentration of the contaminant of interest at some point (x, y, z) at some time t

n is the porosity of the soil

 f_x, f_y, f_z are the fluxes in the x, y, z Cartesian direction

 v_x , v_y , v_z are the components of the seepage velocity in the x, y and z directions, and

 D_{xx} , D_{yy} , D_{zz} are the coefficients of hydrodynamics dispersion (incorporating the effects of molecular diffusion and mechanical dispersion) in the x, y and z directions.

Consideration of mass balance gives:

$$\frac{\partial f_x}{\partial x} + \frac{\partial f_y}{\partial y} + \frac{\partial f_z}{\partial z} + n \frac{\partial c}{\partial t} + g = 0$$
 (2.2a)

where the quantity g takes account of the possibility of some of the contaminant being absorbed onto the clay skeleton. For equilibrium controlled ion exchange where the concentration of the exchange ion is relatively low, the absorption of this species may be approximated by a linear relationship of the form

$$g = \rho K \frac{\partial c}{\partial t} \tag{2.2b}$$

where

 ρ is the dry density of the solid and K is the distribution coefficient.

The distribution coefficient K may often be estimated from the results of a laboratory column test [8] or may be determined independently [9, 10]. It should of course be determined over a representative range of concentrations which reflect the likely field variation.

For a homogeneous layer in which the pore fluid velocity is uniform, equations (2.1) and (2.2) can be combined to give:

$$(n + \rho K) \frac{\partial c}{\partial t} = nD_{xx} \frac{\partial^2 c}{\partial x^2} + nD_{yy} \frac{\partial^2 c}{\partial y^2} + nD_{zz} \frac{\partial^2 c}{\partial z^2} - nv_x \frac{\partial c}{\partial x} - nv_y \frac{\partial c}{\partial y} - nv_z \frac{\partial c}{\partial z}.$$
 (2.3a)

Equation (2.3a) governs 3D contaminant migration subject to the initial condition that

$$c = c_I \quad \text{at} \quad t = 0 \tag{2.3b}$$

where c_I is the initial (background) concentration.

PROBLEM CONFIGURATION AND BOUNDARY CONDITIONS

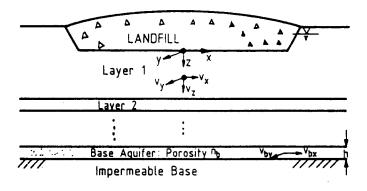
A typical situation is shown schematically in Fig. 2.1. Supposing that at a depth $z = z_n$, the clayey deposit is underlain by a more permeable stratum (base aquifer) of thickness h and porosity n_b . If there is vertical advective transport into the aquifer then, strictly speaking, continuity requires that the base velocity in the aquifer should vary with horizontal position. However, if, as is often the case, the vertical velocity is small compared to the horizontal velocity in the aquifer then, as a first approximation, the base velocity may be assumed to be uniform and horizontal. If it is also assumed that the concentration in the aquifer is uniform across its thickness, then consideration of conservation of mass within a small element of the aquifer between (x, x + dx), (y, y + dy)gives:

s:

$$n_b h \, dx dy \, c(x, y, z_n, t) = dx \, dy \int_0^t f_z(x, y, z_n, \tau) \, d\tau$$

$$-h \, dy \int_0^t \left[f_x(x + dx, y, z_n, \tau) - f_x(x, y, z_n, \tau) \right] \, d\tau$$

$$-h \, dx \int_0^t \left[f_y(x, y + dy, z_n, \tau) - f_y(x, y, z_n, \tau) \right] \, d\tau \qquad (2.4)$$



(a) Schematic of Landfill

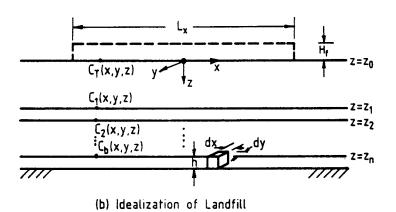


Figure 2.1 Problem under consideration.

which follows from the observation that the mass of contaminant in the element at time t is equal to the total mass transported into the element from the overlying clay less the net mass transported out of the element in the x and y Cartesian directions. Assuming again that mass transport is governed by Fick's Law, dividing throughout by the pore volume n_bh dx dy, and taking the limit as dx and dy tend to zero then gives:

$$c(x, y, z_n t) = \int_0^t \left[\frac{f_z(x, y, z_n, \tau)}{n_b h} - \frac{v_{bx}}{n_b} \frac{\partial c(x, y, z_n, \tau)}{\partial x} - \frac{v_{by}}{n_b} \frac{\partial c(x, y, z_n, \tau)}{\partial y} \right] d\tau$$

$$+ D_{Hx} \frac{\partial^2 c(x, y, z_n, \tau)}{\partial x^2} + D_{Hy} \frac{\partial^2 c(x, y, z_n, \tau)}{\partial y^2} d\tau \qquad (2.5a)$$

where

 n_b is the base aquifer porosity

h is the thickness of the base aquifer

 v_{bx} , v_{by} are the components of the superficial velocity in the x and y directions in the base aquifer (The superficial velocity is the seepage velocity, multiplied by the porosity.)

 D_{Hx} , D_{Hy} are the coefficients of hydrodynamic dispersion in the x and y directions in the base aquifer.

Adopting the following notation

 $c_b = c(x, y, z_n, \tau)$ is the concentration in the aquifer at (x, y, z_n) at time τ :

 $f_{bz} = f_z(x, y, z_n, \tau)$ is the flux into the aquifer at (x, y, z_n) at time τ ;

 $f_{bx} = f_x(x, y, z_n, \tau)$ is the flux in the x direction in the base aquifer at time τ ; and

 $f_{by} = f_y(x, y, z_n, \tau)$ is the flux in the y direction in the base aquifer at time τ .

Equation (2.5a) can be rewritten as

$$c_b = \int_0^t \left(\frac{f_{bz}}{n_b h} - \frac{v_{bx}}{n_b} \frac{\partial c_b}{\partial x} - \frac{v_{by}}{n_b} \frac{\partial c_b}{\partial y} + D_{Hx} \frac{\partial^2 c_b}{\partial x^2} + D_{Hy} \frac{\partial^2 c_b}{\partial y^2} \right) d\tau \qquad (2.5b)$$

Thus the presence of a base aquifer can be modelled as a boundary condition by invoking equation (2.5). Of course when analysing a layered deposit for 2D or 3D conditions an aquifer could also be modelled as an additional layer in the deposit rather than as a boundary condition to the clayey deposit.

In many practical situations, the mass of solute in the landfill (or lagoon) will be limited and the mass will reduce with time as pollutant is transported from the landfill. The simplest such case is where the landfill is filled relatively quickly having a concentration c_0 and height of fluid H_f at completion. The height of fluid H_f represents the volume of leachate (which depends on the porosity of the landfill and the location of the watertable) divided by the average plan area of the landfill. The initial concentration c_0 and height of leachate H_f can be estimated for a given landfill. Assuming that the concentration in the landfill is spatially homogeneous but may vary with time as mass is transported into the clay, conservation of mass requires that:

$$AH_f c_{LF}(t) = AH_f c_0 - \int_0^t \left(\int \int_A f_T \, \mathrm{d}A \right) \, \mathrm{d}\tau. \tag{2.6a}$$

where

A is the plan area of the landfill;

 H_f is the equivalent height of leachate (fluid);

 $c_{LF}(t)$ is the concentration of the contaminant within the landfill at time t;

 c_0 is the initial concentration of contaminant within the landfill (i.e. at t = 0); and

 $f_T = f_z(x, y, z_0, \tau)$ is the flux entering the soil from the landfill at the point (x, y, z_0) at time τ and may be calculated from (2.1).

Equation (2.6a) simply says that the mass of contaminant within the landfill at time t is equal to the original mass of contaminant within the landfill (at t=0) less the mass of contaminant transported into the soil over the area of the landfill between time $\tau=0$ and $\tau=t$. Dividing (2.6a) throughout by AH_f then gives an expression for the concentration c_{LF} within the landfill at time t

$$c_{LF}(t) = c_0 - \frac{1}{AH_f} \int_0^t \left(\iint f_T \, \mathrm{d}A \right) \, \mathrm{d}\tau \tag{2.6b}$$

Clearly, the limit as the volume of fluid in the landfill tends to infinity $(H_f \to \infty)$ corresponds to a constant surface concentration.

2.4 1D SOLUTION

The simplest case which can be considered is that of one-dimensional contaminant transport in the clayey deposit, parallel to the z direction as shown in Fig. 2.1. It is assumed that this deposit is divided into a number of layers by node planes $z = z_0, z_1, \ldots, z_n$ and that each layer, $(z_{k-1} \le z < z_k)$ may be considered homogeneous. Thus the vertical flux per unit area per unit time at a point in layer k is given by (2.1) viz.:

$$f_z = nv_z c - nD_{zz} \frac{\partial c}{\partial z}.$$
 (2.1c)

For 1D mass transport in the clayey deposit, the equation governing pollutant migration (2.3) reduces to

$$(n + \rho K) \frac{\partial c}{\partial t} = nD_{zz} \frac{\partial^2 c}{\partial z^2} - nv_z \frac{\partial c}{\partial z}.$$
 (2.7a)

Subject to the initial condition

$$c = c_1(z_{k-1} \le z \le z_k)$$
 at $t = 0$ (2.7b)

where the quantities n, v_z , D_{zz} , ρ , K and c_I assume constant values appropriate for the layer k under consideration.

Equations (2.1c) and (2.7) can be simplified by introducing the Laplace Transform

$$(\bar{c}, \bar{f_z}) = \int_0^\infty (c, f_z) e^{-st} dt \qquad (2.8)$$

yielding

$$\bar{f}_z = nv_z\bar{c} - nD_{zz} \frac{\partial \bar{c}}{\partial z}$$
 (2.9)

$$(n + \rho K)(s\tilde{c} - c_I) = nD_{zz} \frac{\partial^2 \tilde{c}}{\partial z^2} - nv_z \frac{\partial \tilde{c}}{\partial z}. \qquad (2.10)$$

Equation (2.10) has a solution of the form

$$\tilde{c} = E + A e^{\alpha z} + B e^{\beta z} \tag{2.11a}$$

where $m = \alpha$, β are the roots of the equation

$$nD_{zz}m^2 - nv_z m - (n + \rho K)s = 0$$
 (2.11b)

$$_{\beta}^{\alpha} = \frac{v_z}{2D_{zz}} \pm \left(\frac{v_z^2}{4D_{zz}^2} + \frac{s(n + \rho K)}{nD_{zz}}\right)^{\frac{1}{2}}$$
 (2.11c)

and

$$E = c_I/s = -\frac{(n + \rho K)c_I}{nD_{zz}\alpha\beta}.$$
 (2.11d)

Evaluating equations (2.11) in terms of the concentrations at the nodal planes z_i , z_k (where j = k - 1) yields the interpolation formulae

$$\bar{c} = (\bar{c}_j - E) \left\{ \frac{e^{\alpha(z - z_k)} - e^{\beta(z - z_k)}}{e^{\alpha(z_j - z_k)} - e^{\beta(z_j - z_k)}} \right\}
+ (\bar{c}_k - E) \left\{ \frac{e^{\alpha(z - z_j)} - e^{\beta(z - z_j)}}{e^{\alpha(z_k - z_j)} - e^{\beta(z_k - z_j)}} \right\} + E$$
(2.12)

and thus

$$\frac{\tilde{f}_{z}}{nD_{zz}} = (\tilde{c}_{j} - E) \left(\frac{\beta e^{\alpha(z-z_{k})} - \alpha e^{\beta(z-z_{k})}}{e^{\alpha(z_{j}-z_{k})} - e^{\beta(z_{j}-z_{k})}} \right) + (\tilde{c}_{k} - E) \left(\frac{\beta e^{\alpha(z-z_{j})} - \alpha e^{\beta(z-z_{j})}}{e^{\alpha(z_{k}-z_{j})} - e^{\beta(z_{k}-z_{j})}} \right) + (\alpha + \beta)E.$$
(2.13)

20 Numerical Methods in TRANSIENT AND COUPLED PROBLEMS

If we denote the depth of the sublayer by $\lambda = z_k - z_j$ this then gives the layer matrix relating nodal concentrations and nodal fluxes

$$\begin{bmatrix} \bar{f}_{zj} \\ -\bar{f}_{zk} \end{bmatrix} = nD_{zz} \begin{bmatrix} \frac{\beta e^{-\alpha\lambda} - \alpha e^{-\beta\lambda}}{e^{-\alpha\lambda} - e^{-\beta\lambda}} & \frac{(\beta - \alpha)}{e^{\alpha\lambda} - e^{\beta\lambda}} \\ \frac{-(\beta - \alpha)}{e^{-\alpha\lambda} - e^{-\beta\lambda}} & \frac{-(\beta e^{\alpha\lambda} - \alpha e^{\beta\lambda})}{e^{\alpha\lambda} - e^{\beta\lambda}} \end{bmatrix} \begin{bmatrix} \bar{c}_j - E \\ \bar{c}_k - E \end{bmatrix} + (\alpha + \beta)EnD_{zz} \begin{bmatrix} 1 \\ -1 \end{bmatrix}$$
(2.14a)

which may be written

$$\begin{bmatrix} \tilde{f}_{zj} \\ -\tilde{f}_{zk} \end{bmatrix} = \begin{bmatrix} Q_k & R_k \\ S_{zk} & T_k \end{bmatrix} \begin{bmatrix} \tilde{c}_j - E \\ \tilde{c}_k - E \end{bmatrix} + (\alpha + \beta) E n D_{zz} \begin{bmatrix} 1 \\ -1 \end{bmatrix}.$$
 (2.14b)

Rearranging then gives:

$$\begin{bmatrix} \bar{f}_{zj} \\ -\bar{f}_{zk} \end{bmatrix} = \begin{bmatrix} Q_k & R_k \\ S_k & T_k \end{bmatrix} \begin{bmatrix} \bar{c}_j \\ \bar{c}_k \end{bmatrix} - \begin{bmatrix} U_k \\ V_k \end{bmatrix}$$
 (2.14c)

where

$$U_k = [Q_k + R_k - (\alpha + \beta)nD_{zz}]E$$

$$V_k = [S_k + T_k + (\alpha + \beta)nD_{zz}]E$$

and where α, β, E are defined by (2.11c) and (2.11d).

Noting that both the flux f_z and concentrations c must be continuous, the layer matrices defined by equation (2.14) may be assembled for each layer in the deposit to give

$$\begin{bmatrix} Q_{1} & R_{1} \\ S_{1} & T_{1} + Q_{2} & R_{2} \\ S_{2} & T_{2} + Q_{3} & R_{3} \\ \vdots & \vdots & \vdots \\ S_{n-1} & T_{n-1} + Q_{n} & R_{n} \\ S_{n} & T_{n} \end{bmatrix} \begin{bmatrix} \tilde{c}_{T} \\ \tilde{c}_{1} \\ \tilde{c}_{2} \\ \vdots \\ \tilde{c}_{n-1} \\ \tilde{c}_{b} \end{bmatrix} = \begin{bmatrix} \tilde{f}_{T} + U_{1} \\ V_{1} + U_{2} \\ \vdots \\ V_{n-1} + U_{n} \\ -\tilde{f}_{b} + V_{n} \end{bmatrix}$$

$$(2.15)$$

where

 \tilde{c}_T , \tilde{f}_T are the values of concentration and flux at the top of the deposit; and

 $\bar{c}_b = \bar{c}_n$, $\bar{f}_b = \bar{f}_n$ are the values of concentration and flux at the base of the deposit.

We now wish to solve this equation subject to the appropriate boundary conditions.

Equation (2.15) describes vertical contaminant migration in a clayer deposit for 1D conditions. If this deposit is underlain by a far more permeable stratum with ground-water flow in the horizontal direction at a superficial velocity v_b , then solute will be transported away from the landfill at a rate dependent on the velocity, porosity and geometric dimensions of this layer. The concentration in this base aquifer will only tend to zero when the base velocity is sufficiently large to remove the discharged leachate. However, in many cases the velocity will be relatively small and there will be a change in concentration with time in this stratum. To provide a means of estimating this concentration in a one dimensional analysis, it will be assumed that the concentration $c_b(t)$ in the base aquifer does not vary with vertical or horizontal position and that solute transport in this layer is only by horizontal advection. Thus for a landfill of length L (where the length is the dimension of the landfill parallel to the base velocity v_b), the general equation (2.5) governing the concentration in the base reduces to

$$c_b = \int_0^t \left(\frac{f_{bz}}{n_b h} - \frac{v_b}{n_b} \frac{c_b}{L} \right) d\tau \tag{2.16}$$

where c_b represents an average concentration in the aquifer beneath the landfill.

It is implicitly assumed here that the permeable stratum is confined by a lower impermeable boundary and so the volume of water in this permeable stratum, beneath the landfill, depends on its thickness, h. Thus, the assumption that c_b is independent of position is likely to be most appropriate when h is no more than a few metres. This approximation is considered to be adequate for many practical situations; the more general two-dimensional case where the concentration varies with lateral position beneath the landfill will be considered in the next section.

Taking the Laplace transform of (2.16) gives

$$\bar{c}_b = \frac{\bar{f}_b}{sn_b h} - \frac{\hat{v}_b \bar{c}_b}{sn_b L} \tag{2.17}$$

This can be rewritten in the form

$$\bar{f_b} = \Omega \bar{c}_b \tag{2.18a}$$

where

$$\Omega = h[n_b s + v_b/L]. \tag{2.18b}$$

Substituting (2.18a) into the last equation of (2.15) then gives

$$S_n \bar{c}_{n-1} + (T_n + \Omega) \bar{c}_b = V_n \tag{2.19}$$

which now replaces the last equation of (2.15).

22 Numerical Methods in TRANSIENT AND COUPLED PROBLEMS

Now considering the boundary condition at the top nodal plane $z = z_0$, the top concentrate c_T is equal to that in the landfill i.e.:

$$c_T = c_{LF} \qquad t > 0 \tag{2.20}$$

and for the 1D case, the equation for the concentrations in the landfill (2.6b) reduces to

$$c_{LF}(t) = c_0 - \frac{1}{H_f} \int_0^t f_T d\tau.$$
 (2.21a)

Taking the Laplace transform, this becomes

$$\bar{c}_{LF} = \frac{\bar{c}_0}{s} - \frac{\bar{f}_T}{sH_f}.$$
 (2.22)

Combining (2.20) and (2.22) and the first equation of (2.15) then gives:

$$\bar{c}_{LF} = \frac{\bar{c}_0}{s} - \frac{\bar{f}_T}{sH_f} \tag{2.22}$$

Combining (2.20) and (2.22) and the first equation of (2.15) then gives:

$$(Q_1 + sH_f)c_{LF} + R_1c_1 = c_0H_f + U_1. (2.23)$$

Replacing the first and last equation of (2.15) by (2.23) and (2.19) then gives the complete set of equations.

$$\begin{bmatrix} Q_1 + sH_f & R_1 \\ S_1 & T_1 + Q_2 & R_2 & 0 \\ 0 & S_2 & T_2 + Q_3 & R_3 \\ & & & & S_{n-1} & T_n + Q_n & R_n \\ & & & & & & & & \\ 0 & S_n & T_n + \Omega \end{bmatrix} \begin{bmatrix} \tilde{c}_{LF} \\ \tilde{c}_1 \\ \tilde{c}_2 \\ \tilde{c}_{n-1} \\ \tilde{c}_b \end{bmatrix} = \begin{bmatrix} c_0H_f + U_1 \\ V_1 + U_2 \\ V_2 + U_3 \\ V_{n-1} + U_n \\ V_n \end{bmatrix}$$

where c denotes the concentration in layer plane $z = z_j$; Q_k , R_k , S_k , T_k , U_k and V_k are defined by equation (2.14); and Ω is defined by (2.18b). Equation (2.24) can now be solved giving \bar{c}_j at each node plane. The Laplace transform can then be inverted using a very efficient scheme proposed by Talbot [12]. Using this approach an accuracy of order 10^{-6} and 10^{-10} can typically be achieved using 11 and 18 sample points respectively. For many practical problems an accuracy of 10^{-6} is more than adequate. The theory described above has been coded in program POLLUTE [11] and can be run on both mini and micro computers.

2.5 2D SOLUTION

The procedure described in the previous section can be readily generalized for contaminant transport in both the x and z directions. Again, it is assumed that the deposit is divided into a number of layers with node planes $z = z_0, z_1, \ldots z_n$

and that each layer $k(z_{k-1}, \le z \le z_k)$ may be considered as homogeneous. Thus from equation (2.1) the fluxes f_x , f_z transported in the x and y directions within layers k are given by

$$f_x = nv_x c - nD_{xx} \frac{\partial c}{\partial x}$$
 (2.1a)

$$f_z = nv_z c - nD_{zz} \frac{\partial c}{\partial z}.$$
 (2.1c)

For 2D transport in the soil, the equation governing contaminant migration (2.3) reduces to

$$(n + \rho K) \frac{\partial c}{\partial t} = nD_{xx} \frac{\partial^2 c}{\partial x^2} + nD_{zz} \frac{\partial^2 c}{\partial z^2} - nv_x \frac{\partial c}{\partial x} - nv_z \frac{\partial c}{\partial z}$$
(2.25a)

and

$$c = c_I(z_{k-1} \leqslant z \leqslant z_k, -\infty \leqslant x \leqslant \infty) \quad \text{at } t = 0$$
 (2.25b)

where the quantities n, v_x , v_z , D_{xx} , D_{zz} , ρ , K and c_I are constants appropriate to the layer k under consideration.

Equation (2.1a), (2.1c), (2.25a) and (2.25b) can be simplified by the introduction of a Laplace transform:

$$(\bar{c}, \bar{f}_x, \bar{f}_z) = \int_0^\infty (c, f_x, f_z) e^{-st} dt$$
 (2.26)

and a Fourier transform

$$(C, F_x, F_z) = \frac{1}{2\pi} \int_{-\infty}^{\infty} (c, f_x, f_z) e^{-i\xi x} dx$$
 (2.27)

yielding

$$\bar{F}_x = nv_x \bar{C} - nD_{xx} i\xi \bar{C} \tag{2.28a}$$

$$\bar{F}_z = nv_z\bar{C} - nD_{zz} \frac{\partial \bar{C}}{\partial z}$$
 (2.28b)

and

$$(n+\rho K)(s\bar{C}-C_I) = -\xi^2 nD_{xx}\bar{C} + nD_{zz}\frac{\partial^2 \bar{C}}{\partial z^2} - i\xi nv_x\bar{C} - nv_z\frac{\partial \bar{C}}{\partial z}. \quad (2.29)$$

This equation has the solution

$$\bar{C} = E + A e^{\alpha z} + B e^{\beta z}$$
 (2.30a)

where $m = \alpha, \beta$ are the roots of the equation:

$$nD_{zz}m^2 - nv_z m - [i\xi nv_x + \xi^2 nD_{xx} + (n + \rho K)s] = 0$$
 (2.30b)

and

$$E = \frac{(n + \rho K)C_I}{\xi^2 n D_{xx} + i\xi n v_x + (n + \rho K)s} = -\frac{(n + \rho K)C_I}{n D_{zz} \alpha \beta}.$$
 (2.30c)

Evaluating equation (2.30) in terms of concentration of the nodal planes z_i , $z_k (j = k - 1)$ yields the interpolation formulae:

$$\bar{C} = (\bar{C}_j - E) \left\{ \frac{e^{\alpha(z-z_k)} - e^{\beta(z-z_k)}}{e^{\alpha(z_j-z_k)} - e^{\beta(z_j-z_k)}} \right\} + (\bar{C}_k - E) \left\{ \frac{e^{\alpha(z-z_j)} - e^{\beta(z-z_j)}}{e^{\alpha(z_k-z_j)} - e^{\beta(z_k-z_j)}} \right\} + E$$
(2.31)

and thus

$$\frac{\bar{F}_z}{nD_{zz}} = (\bar{C}_j - E) \left\{ \frac{\beta e^{\alpha(z-z_k)} - \alpha e^{\beta(z-z_k)}}{e^{\alpha(z_j-z_k)} - e^{\beta(z_j-z_k)}} \right\} + (\bar{C}_k - E) \left\{ \frac{\beta e^{\alpha(z-z_j)} - \alpha e^{\beta(z-z_j)}}{e^{\alpha(z_k-z_j)} - e^{\beta(z_k-z_j)}} \right\} + (\alpha + \beta)E.$$
(2.32)

Notice that (2.31) and (2.32) have precisely the same form as (2.12) and (2.13) since only the definition of α , β and E differ. Consequently, the layer matrix also takes the same form as (14a) and can be written as

$$\begin{bmatrix} \bar{F}_{zj} \\ -\bar{F}_{zk} \end{bmatrix} = \begin{bmatrix} Q_k & R_k \\ S_k & T_k \end{bmatrix} \begin{bmatrix} \bar{C}_j \\ \bar{C}_k \end{bmatrix} - \begin{bmatrix} U_k \\ V_k \end{bmatrix}$$
 (2.33)

where Q_k , R_k , S_k , T_k , U_k and V_k are as defined in (14) but where in this case α , β , E are defined by (2.30b) and (2.30c).

Noting again that the flux \tilde{F}_z and concentrations \tilde{C} must be continuous the layer matrices defined by (2.33) may be assembled for each layer k in the deposit to give

$$\begin{bmatrix} Q_{1} & R_{1} & & & & & \\ S_{1} & T_{1} + Q_{2} & R_{2} & & & & \\ & S_{2} & T_{2} + Q_{3} & R_{3} & & & \\ & & S_{n-1} & T_{n-1} + Q_{n} & R_{n} \\ & & S_{n} & & T_{n} \end{bmatrix} \begin{bmatrix} \bar{C}_{T} \\ \bar{C}_{1} \\ \bar{C}_{2} \\ \bar{C}_{n-1} \\ \bar{C}_{b} \end{bmatrix} = \begin{bmatrix} \bar{F}_{T} + U_{1} \\ V_{1} + U_{2} \\ V_{n-1} + U_{n} \\ -\bar{F}_{b} + V_{n} \end{bmatrix}$$
(2.34)

where \bar{F}_T and \bar{F}_b are the transformed fluxes at the top $(z=z_0)$ and bottom $(z=z_n)$ nodal plane respectively and \bar{C}_T and \bar{C}_b are the corresponding transforms of the concentrations at these points. It should be noted that this matrix will not usually be symmetric but it is tridiagonal and hence solution of these equations is computationally trivial.

Equation (2.34) must be solved subject to the appropriate boundary conditions. Considering the lower boundary first, suppose that the clay layer is

underlain by a more permeable stratum of thickness h and porosity n_b . Assuming that the concentration is uniform across the thickness h but may vary with position x, the general equation governing the concentration in the base aquifer (2.5) reduces to

$$c_b = \int_0^t \left(\frac{f_{bz}}{n_b h} - \frac{v_{bx}}{n_b} \frac{\partial c_b}{\partial x} + D_{Hx} \frac{\partial^2 c_b}{\partial x^2} \right) d\tau$$
 (2.35)

If (2.35) is transformed using (2.26) and (2.27) it is found that:

$$\vec{F_h} = \Omega \vec{C_h} \tag{2.36a}$$

where

$$\Omega = h [n_b s + i \xi v_b + n_b D_{Hx} \xi^2]. \tag{2.36b}$$

Thus substituting (2.36a) into the last equation of (2.34) gives

$$S_n \bar{C}_{n-1} + (T_n + \Omega) \bar{C}_b = V_n.$$
 (2.37)

Replacing the last equation of (2.34) by (2.37) allows the horizontal advective—dispersive transport in the aquifer to be modelled as a boundary condition. Clearly, the same result could also be achieved by modelling the aquifer as a layer of the deposit. If this aquifer layer is underlain by a no-flux boundary, this can then be simulated by setting $-F_b = 0$ in the last equation of (2.34) which now becomes.

$$S_n \bar{C}_{n-1} + T_n \bar{C}_b = V_n \tag{2.38}$$

The boundary condition at the upper boundary can be developed for the case where there is a finite mass of contaminant within the landfill of length L (see Fig. 2.1). Assuming that the concentration of contaminant within this landfill is spatially homogeneous but may vary with time as mass is transported into the underlying soil, the two dimensional version of (2.6) can be written

$$c_{LF}(t) = c_0 - \frac{1}{LH_f} \int_0^t \int_{-L/2}^{L/2} f_T \, \mathrm{d}x \, \mathrm{d}t$$
 (2.39)

and so the concentration on the nodal plane $z = z_0$ is given by

$$c_T = c(x, z = z_0, t) = c_{LF}(t) -L/2 \le x \le L/2 c_T = c(x, z = z_0, t) = 0 |x| > L/2. (2.40)$$

Taking the Laplace and Fourier transforms of (2.40) then gives

$$\bar{C}_T = \frac{1}{2\pi} \int_{-L/2}^{L/2} \bar{C}_{LF} e^{-i\xi x} dx = \frac{L}{2\pi} \bar{C}_{LF} \frac{\sin(\xi L/2)}{(\xi L/2)}$$
 (2.41)

where \tilde{C}_{LF} is as yet unknown.

To determine \bar{C}_{LF} let us firstly define $\bar{\chi}$ such that

$$\bar{\chi} = \bar{F_T} \tag{2.42}$$

for the reference case where \bar{F}_T is determined by solving (2.34) (with the appropriate base boundary condition), subject to the condition that $\bar{C}_{LF} = 1$ and hence, from (2.41),

$$\bar{C}_T = \frac{L}{2\pi} \frac{\sin(\xi L/2)}{(\xi L/2)}.$$
 (2.43)

It follows that in general

$$\bar{F}_T = \bar{\chi} \bar{C}_{LF}. \tag{2.44}$$

Taking the Laplace transform of (2.39) gives

$$\bar{c}_{LF} = \frac{c_0}{s} - \frac{1}{sLH_f} \int_{-L/2}^{L/2} \bar{f}_T \, \mathrm{d}x \tag{2.45}$$

Now from the Fourier inversion theorem

$$\bar{f}_T = \int_{-\infty}^{\infty} \bar{F}_T e^{i\xi x} d\xi \qquad (2.46)$$

and hence

$$\int_{-L/2}^{L/2} \bar{f}_T \, \mathrm{d}x = \int_{-\infty}^{\infty} \int_{-L/2}^{L/2} \bar{F}_T \, \mathrm{e}^{i\xi x} \, \mathrm{d}x \, \mathrm{d}\xi$$

$$= \int_{-\infty}^{\infty} \frac{L \sin(\xi L/2)}{(\xi L/2)} \, \bar{F}_T \, \mathrm{d}\xi$$
(2.47)

substituting (2.44) and (2.47) into (2.45) then gives

$$\bar{c}_{LF} = \frac{c_0}{s} - \frac{1}{sLH_f} \int_{-\infty}^{\infty} \frac{L \sin(\xi L/2)}{(\xi L/2)} \, \bar{C}_{LF} \bar{\chi} \, d\xi$$
(2.48)

which upon solving for \tilde{c}_{LF} gives

$$\tilde{c}_{LF} = \frac{LH_f c_0}{sLH_c + \Lambda} \tag{2.49a}$$

where

$$\Lambda = \int_{-\infty}^{\infty} \frac{2 \sin (\xi L/2)}{\xi} \, \bar{\chi} \, dz. \qquad (2.49b)$$

The reference concentrations \tilde{c}_{rj} at the nodal planes are obtained for the reference condition where $\tilde{c}_{LF} = 1$ by invoking

$$\bar{c}_{rj} = \int_{-\infty}^{\infty} \bar{C}_j \, \mathrm{e}^{i\xi x} \, \mathrm{d}\xi \qquad (1 \leqslant j \leqslant n)$$
 (2.50)

and by performing the integration using numerical quadrature. The transform coefficients \tilde{C}_j in (2.50) are obtained by solving (2.34) subject to the appropriate base boundary condition (2.37) and (2.38) and the top boundary condi-

tion (2.43). At the same time the quantity Λ can be determined from (2.42) and (2.49b). The concentration \tilde{c}_{LF} can then be determined from (2.49a) and hence the concentrations of the nodal planes are given by

$$\bar{c}_j = \bar{c}_{LF} \cdot \bar{c}_{rj}. \tag{2.51}$$

It then only remains to invert the Laplace transform.

The theory described above for 2D conditions has been coded in program MIGRATE [13]. The major computational effort involved is associated with the numerical inversion of the Fourier and Laplace transforms for the locations and times of interest. The Fourier transform can be efficiently inverted using 20 point Gauss quadrature. The width and number of integration subintervals which are needed to achieve a reasonable accuracy (say 0.1%) depends somewhat on the geometry and properties of the problem under consideration. These parameters can be determined from a few trial calculations for a representative point and time of interest. (Similarly, it should be noted that numerical experiments are also required to determine an appropriate finite element mesh and time integration procedure if alternative finite element or finite difference codes are used.) The Laplace transform can again be inverted using Talbot's algorithm.

3D SOLUTIONS

The governing equations for the 3D case are given by (2.1) and (2.3). The development of the solution for this case follows along the same lines as that for the 2D case described in the previous section except that here the Fourier transform take the form

$$(C, F_x, F_y, F_z) = \frac{1}{4\pi^2} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} (c, f_x, f_y, f_z) e^{-i\xi x - i\eta y} dx dy. \quad (2.52)$$

Thus taking the Laplace and Fourier Transform of (2.3) gives

$$(n + \rho K)(s\bar{C} - C_I) = -\xi^2 n D_{xx}\bar{C} - \eta^2 n D_{yy}\bar{C} + n D_{zz} \frac{\partial^2 \bar{C}}{\partial z^2}$$
$$-i\xi n v_x \bar{C} - i\eta n v_y \bar{C} - n v_z \frac{\partial \bar{C}}{\partial z}$$
(2.53)

for any layer k $(z_{k-1} \le z \le z_k)$.

This also has a solution of the form

$$\bar{C} = E + A e^{\alpha z} + \beta e^{\beta z}$$
 (2.54a)

where $m = \alpha, \beta$ are the roots of the equation

$$nD_{zz}m^2 - nv_z m - [i\xi nv_x + i\eta nv_y + \xi^2 nD_{xx} + \eta^2 nD_{yy} + (n + \rho K)s] = 0$$
 (2.54b)

and

$$E = \frac{-(n + \rho K)c_I}{nD_{zz}\alpha\beta}.$$
 (2.54c)

The layer matrices take precisely the same form as that given by (2.14) and (2.33) but where α , β , E are defined by (2.54b) and (2.54c) above. The layer matrices may then be assembled for each layer in the deposit to give (2.34) which again must be solved subject to the appropriate boundary conditions in a similar manner to that described for the 2D case.

Considering horizontal flow in a base aquifer of thickness h and porosity n_b , the equation governing the variation in concentration (within the aquifer) with lateral position and time is given by (2.5b).

Thus taking the Fourier and Laplace transforms of (2.5b) it is found that

$$\bar{F_b} = \Omega \bar{C_b} \tag{2.55a}$$

where

$$\Omega = h [n_b s + i \xi v_{bx} + i \eta v_{by} + n_b D_{Hx} \xi^2 + n_b D_{Hy} \eta^2]$$
 (2.55b)

which can then be substituted into the last equation of (2.34) to give

$$S_n \bar{C}_{n-1} + (T_n + \Omega) \bar{C}_b = V_n$$
 (2.56)

as was the case for 2D conditions.

At the upper boundary the constant mass boundary condition in 3D is given by (2.6) which for the case of a rectangular landfill of length L and width W can be written

$$c_{LF}(t) = c_0 - \frac{1}{WLH_f} \int_0^t \int_{-W/2}^{W/2} \int_{-L/2}^{L/2} f_T \, dx \, dy \, d\tau \qquad (2.57)$$

and so the concentration on the nodal plane $z = z_0$ is given by

Taking the Laplace and Fourier transforms of (2.58) then gives

$$\bar{C}_T = \frac{1}{4\pi^2} \int_{-L/2}^{L/2} \int_{-W/2}^{W/2} \bar{c}_{LF} e^{-i\xi x - i\eta y} dx dy$$

$$= \bar{c}_{LF} \frac{LW}{4\pi^2} \frac{\sin(\xi L/2)}{(\xi L/2)} \frac{\sin(\eta W/2)}{(\eta W/2)}$$
 (2.59)

where \tilde{c}_{LF} is as yet unknown.

The quantity $\bar{\chi} = \bar{F_T}$ can then be determined by solving (2.34) with the appropriate base boundary conditions and α , β , E, Ω defined by (2.54b),

(2.54c) and (2.55b) for the case where

$$\tilde{c}_T = \frac{LW}{4\pi^2} \frac{\sin(\xi L/2)}{(\xi L/2)} \frac{\sin(\eta W/2)}{\eta W/2}.$$
 (2.60)

Taking the Laplace transform of (2.57) and invoking the Fourier inversion theorem the procedure described for the 2D case may be followed to give

$$\bar{c}_{LF} = \frac{WLH_f c_0}{sLWH_f + \Lambda} \tag{2.61a}$$

where

$$\Lambda = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{4 \sin(\xi L/2) \sin(\eta W/2)}{\xi \eta} \bar{\chi} d\xi d\eta \qquad (2.61b)$$

The reference concentrations \hat{c}_{rj} at the nodal plane can now be obtained from the Fourier inversion theorem, viz

$$\bar{c}_{rj} = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \bar{C}_j e^{i\xi x + i\eta y} d\xi d\eta \qquad 1 \leqslant j \leqslant n$$
 (2.62)

by numerical quadrature. The transform coefficients \bar{C}_j in (2.62) are obtained by solving (2.34) subject to the appropriate boundary conditions (2.37) or (2.38) and the top boundary condition (2.60) by adopting the values of α , β , E, Ω defined by (54b), (54c) and (55b). At the same time the quantity Λ can also be determined from (2.61b). The concentrations \tilde{c}_{LF} can then be calculated from (2.61a) and hence the concentrations at the nodal plane are given by (2.51). The Laplace transform can then be numerically inverted using Talbot's algorithm.

RESULTS

The theory described in this chapter is amenable to the analysis of contaminant migration for a wide range of geometries and combinations of conditions. Rowe et al. [8] have shown how this approach can be used to determine the coefficient of hydrodynamic dispersion (which includes the effects of molecular diffusion) and the sorption potential (ρK) from the back analysis of results from a single laboratory column test. The application of the theory for the analysis of field problems has been demonstrated by Rowe et al. [8] and Quigley and Rowe [13].

The theory can also be readily used to perform sensitivity studies to indicate the effects of uncertainty regarding design parameters on the expected concentration of contaminant at proposed monitoring points beneath or adjacent to waste disposal sites. One problem of particular interest is that where the waste disposal site is separated from an underlying aquifer by a thin layer of relatively impermeable soil. This situation may arise naturally as a result of glaciation. For example, in Southern Ontario, Canada, it is not uncommon to encounter

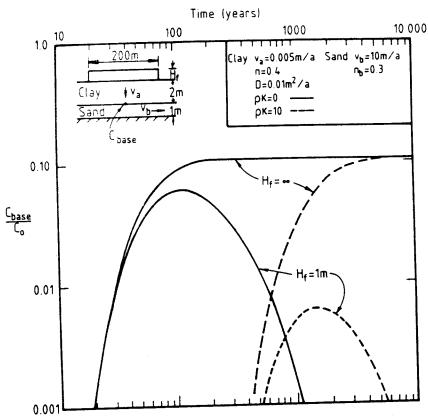


Figure 2.2 Variation in base concentration with time showing the effect of height of leachate (H_f) and sorption (ρK) : 1D Analysis.

Intuitively, one would expect that the advective (superficial) velocity v_a in the clay would have a significant effect on the concentrations of contaminant within the aquifer. That this is so is illustrated by the results given in Figure 2.3. Recognizing the role of advection in the transportation of contaminant, it is clearly desirable to design landfills to minimize any downward seepage and in some cases it may be desirable to design a system which gives rise to upward flow from the aquifer into the landfill. However, it should be emphasized that contamination of the aquifer can occur due to downward diffusion even when there is opposing upward seepage into the landfill (e.g. see the results for $v_a = -0.005$ m/a in Figure 2.3).

Provided that the mass of contaminant is finite, there will be a maximum (peak) concentration within the aquifer (c_{bmax}) which will occur at some time t_{max} . The magnitude and time of occurrence of this maximum will be the primary quantity of interest in the design and evaluation of landfills separated from aquifers by either a natural or man-made clay liner. Among other things, these quantities c_{bmax} and t_{max} will depend on the height of leachate (H_f) and the advective velocity within the clay (v_a) as illustrated in Figure 2.4. A com-

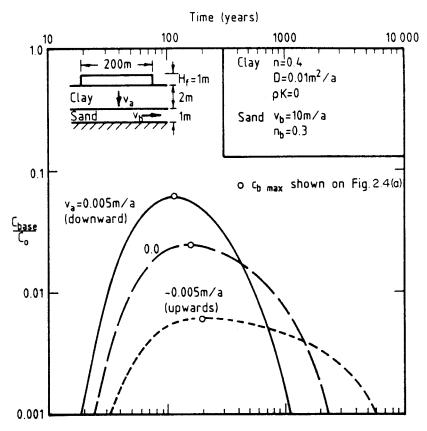


Figure 2.3 Variation in base concentration with time showing the effect of advective velocity v_a : 1D analysis.

parison of Figure 2.4(a) ($\rho K = 0$) and Figure 2.4(b) ($\rho K = 10$) clearly shows that the effect of the height of leachate is substantially greater for a reactive species ($\rho K = 0$), this appears to be true irrespective of the advective velocity, v_a .

The modified 1D approach (Section 2.4) used in the preceding example is the simplest of the proposed models which could be used. To make the problem tractable within this 1D framework, it was necessary to assume that the concentration within the aquifer directly beneath the landfill was spatially homogeneous at all times and that mass transport out of the aquifer directly beneath the landfill was only due to the horizontal advective velocity. This is equivalent to assuming that the coefficient of hydrodynamic dispersion in the aquifer is infinite directly beneath the landfill and zero at all points outside the boundary of the landfill. This is clearly an oversimplication of the actual situation and this raises the question 'what is the effect of the aquifer model upon predicted concentrations?'

If the 2D or 3D formulations are adopted (Sections 2.5 and 2.6), the conditions in the aquifer can be modelled in the following ways.

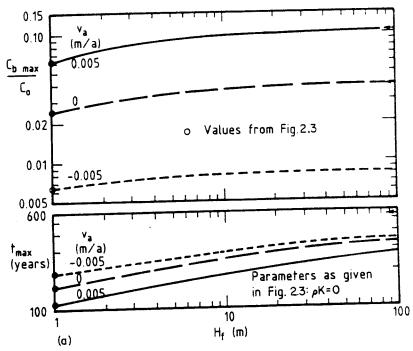


Figure 2.4 (a) Effect of leachate height H_f upon maximum base concentration: and time to reach maximum base concentration: 1D analysis: $\rho K = 0$.

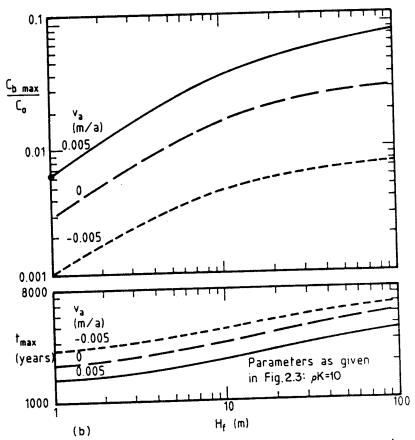


Figure 2.4(b) Effect of leachate height upon maximum base concentration and time to reach maximum base concentration: 1D analysis, $\rho K = 10$.

34 Numerical Methods in TRANSIENT AND COUPLED PROBLEMS

- (1) As a boundary condition (see Section 2.3). This approach allows for spatial variations in concentration within the horizontal plane of the aquifer as well as advective dispersive transport within the aquifer itself. Thus this advective dispersive transport will depend on the horizontal velocity within the aquifer v_{bx} , v_{by} and the coefficient of hydrodynamic dispersion in the acquifer (D_{Hx}, D_{Hy}) . However, this approach does assume that the concentration in the acquifer is uniform in the vertical direction (i.e. $D_v = \infty$) and that the acquifer is underlain by an inpenetrable boundary (i.e. zero flux across this boundary).
- (2) As a physical layer having prescribed velocity components v_{bx} , v_{by} and coefficients of hydrodynamic dispersion D_v , D_{Hx} , D_{Hy} . This approach allows for spatial variations in concentration both vertically and horizontally within the aquifer. Treating the aquifer as a physical layer (i.e. in a manner similar to the clay but with different parameters) permits us to examine two cases:
 - (i) where the aquifer is underlain by an impenetrable boundary (as we assumed in (1) above); or
 - (ii) where the aquifer is underlain by an additional layer (or layers) of clay (and/or sand).

Considering firstly, case (i) where the aquifer is assumed to be underlain by an impenetrable boundary, 2D analyses were performed for the problem shown in Figure 2.5 using the parameters given in Table 2.1. Figure 2.5 shows

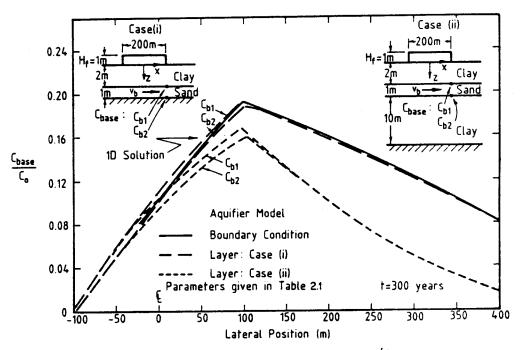


Figure 2.5 Concentration plume in aquifier at 300 years.

Table 2.1 Parameters used to obtain Figures 2.5 and 2.6

Layer	Quantity	Symbol (units)	Value
Clay	Vertical advective velocity Porosity Sorption potential Coefficient of hydrodynamic	υ _α (m/a) n ρΚ	0.0 0.4 0.0
	dispersion (horizontal and vertical)	$D(m^2/a)$	0.01
Sand	Horizontal advective velocity Porosity Sorption potential Coefficient of hydrodynamic	$egin{aligned} v_b({ m m/a}) & n_b & ho K \end{aligned}$	1.0 0.3 0.0
	Dispersion: Horizontal Vertical (layered case) Vertical (boundary condition)	$D_H(\mathrm{m}^2/\mathrm{a})$ $D_v(\mathrm{m}^2/\mathrm{a})$ $D_v(\mathrm{m}^2/\mathrm{a})$	1.0 0.2 ∞

the concentration plumes obtained at t = 300 years using methods (1) and (2) above. Method 1 implicitly assumes that the concentration c_{base} is vertically uniform within the aquifer. Method 2 makes no a priori assumption regarding the spatial variation of concentration and the calculated values at the top (c_{b1}) and bottom (c_{b2}) of the aquifer are both shown in Figure 2.5. For the parameters considered, there is relatively little vertical variation in concentration within the aquifer and the results obtained by treating the aquifer as a physical layer (Method 2) closely bound the results from the computationally simpler approach where the aquifer is treated as a boundary condition (Method 1).

Now let us consider case (ii) where the aquifer is underlain by an additional layer of clay (in this case 10 m of clay is assumed to be resting on an impenetrable base). It is found that (see Figure 2.5) the concentration plume is almost the same as that obtained for case (i) near the upstream edge of the landfill but gives rise to considerably smaller concentrations near the downstream edge of the landfill and at points outside the landfill ($x \ge 100$ m). This decrease in concentration represents a natural attenuation as mass is transported into the lower clay layer by diffusion. The results given at the top and bottom of the aquifer indicate that there is a small concentration gradient in the vertical direction within the aquifer.

Analyses similar to those performed to obtain Figure 2.5 were repeated for different times to give the variation in concentration with time. Figure 2.6 summarizes the results for a point beneath the downstream edge of the landfill (x = 100 m) and a point well outside the landfill (x = 400 m). For the sake of

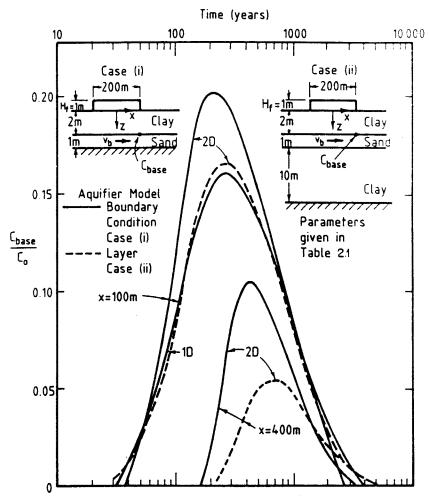


Figure 2.6 Concentration in aquifier beneath edge of landfill (x = 100 m): effect of model.

clarity, only the concentrations calculated at the top of the aquifer (c_{b1}) are shown. A number of observations can be made regarding these results.

Firstly, it is evident that there is a natural attenuation of contaminant plume as it advances along the aquifer (x > 100 m). The attenuation arises due to diffusion of contaminant into the adjacent clay. Thus the maximum concentration reached at x = 400 m is substantially less (by at least a factor of 2) than that obtained at the edge of the landfill x = 100 m.

Secondly, consideration of possible diffusion into a clay layer beneath the aquifer (case ii) gives rise to additional attenuation of contaminant concentration. At the edge of the landfill (x = 100 m), diffusion into the lower clay layer reduces the maximum concentration (compared to case i) by approximately 20%. The effect increases with distance away from the landfill and at x = 400 m diffusion into the lower clay reduces the maximum concentration by

almost a factor of two. Thus the modelling of the aquifer as a boundary condition in a 2D analysis provides a conservative estimate of the contaminant concentrations within the aquifer.

The modified 1D analysis which also treats the aquifer as a boundary condition gives an estimate of the concentration that may be expected in the aquifer directly beneath the landfill. The results obtained for the present problem are shown in Figures 2.5 and 2.6. Comparing these results with those obtained at x = 100 m from the 2D analysis indicates that for this case the modified 1D approach slightly overestimates the time required to attain the maximum concentration and underestimated the magnitude of the maximum concentration. However, in this case and a number of other cases examined [6] the discrepancy, which was typically less than 30%, may be acceptable in preliminary calculations.

It can be shown analytically that the total mass present in the aquifer at any time t, for any base velocity v_b , is equal to the mass into the aquifer calculated from the 1D solution for $v_b = 0$, i.e.

$$m(t) = \int_{-\infty}^{\infty} \int_{0}^{t} f_{z}(x, z_{n}, \tau) d\tau dx = L \int_{0}^{t} f_{1D}(z_{n}, \tau) d\tau$$

in which L is the 'width' of the landfill;

is the flux into the aquifer at time τ determined from the 1D solu $f_{1\mathrm{D}}(z_n,\tau)$ tion for $v_b = 0$;

 $f_z(x, z_n, \tau)$ is the flux into (or out of) the aquifer at time τ and position x from the 2D solution for the actual value of v_b .

It should be noted that the total mass present in the aquifer $(-\infty \le x \le \infty)$ at any time t will be less than the total mass that has passed into the aquifer directly beneath the landfill (-L/2 < x < L/2) up to this time t. The difference between these masses is due to diffusion from the aquifer back into the clay outside the landfill (i.e. |x| > L/2). At large time the mass of contaminant which has diffused into the clay is quite large. It is also interesting to observe that the total mass remaining in the aquifer at any given time is independent of the base velocity v_b (although the total mass which has, at some time, moved into the base does depend on v_b).

OTHER FINDINGS

The problem of a clayey layer underlain by a thin aquifer examined in the previous sections has been considered in more detail by Rowe and Booker [2-6]. In these studies consideration was given to the effects of the height of leachate $H_{\rm f}$, the advective velocity v_a , the horizontal advective velocity (referred to as the 'base velocity', v_b), the coefficient of hydrodynamic dispersion in the vertical and horizontal direction (D_H, D_v) , the sorption potential (ρK) ,

the thickness of the clay layer, the thickness of the aquifer, and the dimensions of the landfill. As a result of these studies, it was observed that:

- (1) If the base velocity is greater than zero, then the concentration of pollutant in the aquifer beneath the liner will reach a maximum value, c_{bmax} , at some time t_{max} , and will decrease for greater times. This maximum value can be used in design to ensure that the contamination of the groundwater never exceeds a specified level.
- (2) Geochemical reactions (sorption) can greatly affect the magnitude of the maximum base concentration as well as the time required to reach this maximum. The sorption potential will depend on the species of contaminant being considered and the chemical properties of the clay. For reactive species, the clay absorbs pollutant when the concentration is increasing. Once the concentration at a point reaches a maximum value, the sorbed contaminant may remain fixed to the clay or, in the worst case, may be released back into the pore fluid as the concentration drops. This beneficial buffering role for some species of pollutant is only apparent if the finite mass of pollutant in the landfill is considered.
- (3) The effect of sorption is greatest for low to moderate volumes of leachate (i.e. leachate height less than 10 m). Sorption may be particularly important in designing for hazardous substances such as NH₄ and heavy metals although careful consideration of the chemical properties of the clay is necessary.
- (4) The maximum base concentration can be decreased by increasing clay liner thickness. However, the design of the liner may be optimized by also considering the effects of leachate height, base velocity and any geochemical reaction.
- (5) The consideration of advection velocity does not alter the trends described above. Downward advective transport increases the maximum base concentration and decreases the time required to reach this concentration.
- (6) Diffusion of contaminant from the aquifer into the surrounding clay will provide natural attenuation of contaminant in the aquifer. The maximum concentration reached at any point outside the boundaries of the landfill will never reach the maximum value at the edge of the landfill. This phenomenon may be used in specifying the buffer zone required around a landfill to ensure the groundwater quality outside the buffer is never degraded below allowable levels due to contamination from the landfill.
- (7) The magnitude of the maximum concentration in the aquifer beneath the landfill decreases:
 - (a) with decreasing mass of contaminant in the landfill; and
 - (b) with increasing base velocity.
 - (8) There is a critical base velocity which will result in the maximum concen-

tration of contaminant at a point in the aquifer away from the landfill. Velocities either larger or smaller than the critical velocity will result in a smaller peak concentration in the aquifer at the point of interest. Thus it is not necessarily conservative to design for only the maximum and minimum expected velocities in the aquifer and a range of values between these limits should be considered.

(9) Except for the case where the dispersion coefficient is very high or the advective velocity is very low, advection is the predominant mechanism for

mass transport within the aquifer.

(10) Increasing thickness of the aquifer (all other things being equal) tends to decrease the concentration at the edge of the landfill. This is primarily a result of increased dilution due to a correspondingly higher flow of water through the aquifer. However, at points well away from the landfill, the calculated maximum concentration may actually increase with increasing thickness of the aquifer (again, all other things being equal) because the relative diffusion into the surrounding clay layers is reduced.

(11) Increasing the dimensions of the landfill increases the maximum concentration at both the edge and at points 'downstream' (with respect to the direction of advective flow within the aquifer) of the landfill. This is a result of an increased mass loading of the aquifer which arises from a larger total

mass of contaminant within the landfill.

CHOICE OF ANALYSIS

The semianalytic methods of analysis developed in this chapter assume that the soil stratigraphy consists of horizontal layers in which there is no variation in properties in the horizontal plane. Clearly, this will not be the case in all field situations. Nevertheless, in many practical cases the stratigraphy is sufficiently regular that it can be reasonably idealised as having horizontal layering. For problems involving complicated stratigraphy, it will usually be necessary to adopt a more general numerical technique (e.g. the finite element method) but even in these cases the techniques proposed here may be useful in developing preliminary estimates of concentrations as well as for providing benchmark results against which finite element calculations can be checked.

The primary advantage of the semianalytic techniques as compared to alternative numerical approaches, is that it is possible to directly determine the concentration of contaminant at specific points and times without determining the entire concentration field at previous times. In many applications, it is really only necessary to determine the magnitude and time of occurrence of the maximum expected base concentration at a few specific points which will usually be specified as monitoring points in the aquifer (e.g. beneath the landfill and at a few points outside the landfill). Using a 'binary chop' algorithm (which can be readily incorporated into the computer program), the maximum concentration expected to occur at the point can usually be determined to a precision of 0.1% or better by evaluating the concentration at these points for seven times. Clearly, even fewer times would be required if one has a reasonable initial estimate of the time at which the maximum will occur. Since the data preparation time is also quite small, sensitivity studies can be easily performed to determine the effect of uncertainty regarding input parameters (e.g. v_b , v_a , ρK , etc) upon the calculated maximum concentrations at the specified monitoring points.

The question of whether the 1D, 2D or 3D formulation is adopted will, of course, depend on the specific problem. The computational effort involved in performing a 3D analysis may be less than that involved in performing a 3D finite element or finite difference analyses but it is, nevertheless, sufficiently large to predicate against performing 3D sensitively analyses for most practical applications.

Provided reasonable engineering judgement is exercised in selecting appropriate cross sections for analysis, it is considered that a 2D analysis will be adequate for the vast majority of applications. A full 3D analysis may be warranted to check the most critical case identified from the 2D analyses.

The modified 1D approach is ideally suited to the analysis of laboratory column tests and other similar 1D situations. It may also be useful for:

- (1) Obtaining an estimate of the contaminant migration through the clay liner at the sides of the landfill.
- (2) Identifying when significant concentrations are to be expected in the aquifer.
- (3) Providing an initial estimate of the magnitude of the peak concentration (and its time of occurrence) in the aquifer beneath the landfill, thereby minimizing the amount of computation required to get accurate values for these quantities from a subsequent 2D analysis.

REFERENCES

- Anderson, M. P. Using models to simulate the movement of contaminants through groundwater flow systems CRC Critical Reviews in Environmental Control, 9(2) 97-156, 1979.
- 2. Rowe, R. K., and Booker, J. R. A novel technique for the analysis of 1D pollutant migration, Proceedings of the International Conference on Numerical Methods for Transient and Coupled Problems, Venice, 699-702, 1984a.
- 3. Rowe, R. K., and Booker, J. R. The analysis of pollutant migration in a non-homogeneous soil. *Geotechnique*, 32(4), 601-612, 1984b.
- 4. Rowe, R. K., and Booker, J. R. A finite layer technique for calculating 3D pollutant migration in soil. Geotechnique, 36(2), 205-214, 1986.

- 5. Rowe, R. K., and Booker, J. R. 1D pollutant migration in soils of finite depth, Journal of Geotechnical Engineering, ASCE, 111 (GT4), 479-499, 1985a.
- 6. Rowe, R. K., and Booker, J. R. 2D pollutant migration in soils of finite depth, Canadian Geotechnical Journal, 22(4), 429-436, 1985b.
- 7. Gillham, R. W., and Cherry, J. A. Predictability of solute transport in diffusion-controlled hydrogeologic regimes Proc. Symp. on Low Level Waste Disposal: Facility Design, Construction and Operating Practices, Nuclear Regulatory Commission, Washington, D.C. 1982.
- 8. Rowe, R. K., Caers, C. J., Booker, J. R., and Crooks, V. E. Pollutant migration through clayey soils, Proceedings of XI International Conference on Soil Mechanics and Foundation Engineering, 1293-1298, San Francisco, 1985.
- 9. Griffin, R. A., Cartwright, K., Shimp, N. F., Steele, J. D., Ruch, R. R., White, W. A., Hughes, G. M., and Gilkeson, R. H. Attenuation of pollutants in municipal landfill leachate by clay minerals. Environmental Geology Notes, Nos. 78 and 79, Illinois State Geological Survey, Urbana, Ill., 1976.
- 10. Griffin, R. A., Frost, R. R., and Shimp, N. F. Effect of pH on removal of heavy metal from leachate by clay minerals. Residual Management by Land Disposal (W.H. Fuller, ed.), United States Environment Protection Agency, EPA-600/ 9-76-015, Cincinnati, Ohio, 1976, pp. 259-268.
- 11. Rowe, R. K., and Booker, J. R. Program POLLUTE 1D Pollutant migration analysis program, Distributed by SACDA, The Faculty of Engineering Science, The University of Western Ontario, London, Ontario N6A 5B9, 1983.
- 12. Talbot, A. The accurate numerical integration of Laplace transforms, J. Inst. Maths. Applics. 23, 97-120, 1979.
- 13. Rowe, R. K., Booker, J. R., and Caers, C. J. Migrate 2D pollutant migration through a non-homogeneous soil: user manual. Available through SACDA, Faculty of Engineering Science, University of Western Ontario, 1985.
- 14. Quigley, R. M., and Rowe, R. K. Leachate migration through clay below a domestic waste landfill, Sarnia, Ontario, Canada, Chemical Interpretation and Modelling Philosophies, Proceedings of International Symposium on Industrial and Hazardous Waste, Alexandria, 1985.

NOTATION

$A \\ c = c(x, y, z, t)$	plan area of the landfill concentration of contaminant at any point (x, y, z) within the clay layer at
$c_T = c(x, y, z_0, t)$	time t concentration of contaminant at the top of the clay layer $(z = z_0)$
$C_b = C_{\text{base}}$	$=c(x, y, z_n, t)$ concentration of contaminant within the base aquifer at position (x, y)
Cbmax	concentration of contaminant ever reached at position (x, y) in the base aquifer
c_I	initial (background) concentration concentration of contaminant within the landfill
CLF Co	initial concentration of contaminant within the landfill
<i>c</i> ₀ <i>c</i> ̄	Laplace transform of c
С	Fourier transform of c
D_{xx}, D_{yy}, D_{zz}	coefficient of hydrodynamic dispersion (including diffusion and mechanical dispersion) in the x , y and z Cartesian directions
D	isotropic coefficient of hydrodynamic dispersion

42 Numerical Methods in TRANSIENT AND COUPLED PROBLEMS

D_{Hx}, D_{Hy}	horizontal coefficient of hydrodynamic dispersion in x , y directions in the base aquifer
$f_x = f_x(x, y, z, t)$	the flux in the x direction
$f_{v} = f_{v}(x, y, z, t)$	the flux in the y direction
	the flux in the z direction
	the vertical flux entering the top of the clay layer at position (x, y)
$f_b = f_z(x, y, z_n, t)$	the vertical flux entering the base aquifer at position (x, y)
$\bar{f}_x, \bar{f}_y, \bar{f}_z, \bar{f}_T, \bar{f}_b$	Laplace transforms of f_x , f_y , f_z , f_T , f_b
F_x, F_y, F_z, F_T, F_b	Fourier transforms of f_x , f_y , f_z , f_T , f_b
H_f	equivalent height of leachate (volume of leachate per unit plan area)
h	thickness of aquifer
K	distribution coefficient
L	width of the landfill parallel to the velocity v_b
n	porosity of the clay layer
n_b	porosity of the base aquifer
t, τ	time
v_x, v_y, v_z	horizontal $(x \text{ and } y)$ and vertical (z) components of the seepage velocity
v_a	apparent (Darcy, superficial) vertical = nv_z
v_b	apparent (Darcy, superficial) horizontal velocity in the base aquifer
v_{bx}, v_{by}	components of the apparent velocity in the base aquifer
x, y	horizontal distance from the centre of the landfill
Z	vertical distance below the base of the landfill
ρ	dry density of the soil soilds
λ	thickness of a layer