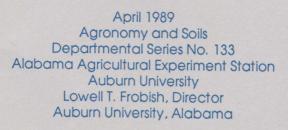
Solution of the One-Dimensional Advection and Two-Dimensional Dispersion Equation







SOLUTION OF THE ONE-DIMENSIONAL ADVECTION AND TWO-DIMENSIONAL DISPERSION EQUATION

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Information contained herein is available to all without regard to race, color, sex, or national origin.

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ABSTRACT

For many transport problems involving 1-D flow, a significant amount of solute might move in the direction transverse to the flow. The analytical description and the experimental determination of transverse solute movement are more complicated than for longitudinal solute movement, and quite often simplifying assumptions are made to predict transverse transport.

This publication reports how the advection-dispersion equation was solved analytically to study transient solute transport in a two-dimensional semi-infinite isotropic porous medium (half-plane) with a step change in concentration along the inlet during 1-D flow. The solution was obtained with Laplace and Fourier transforms and verified with various numerical and analytical solutions. This solution can be used to determine longitudinal and transverse dispersion coefficients in a relatively fast and straightforward manner. It can also be used to evaluate the validity of simplifying assumptions (steady-state, no longitudinal dispersion) for other solutions.

The importance of transverse dispersion for solute transport was investigated numerically for three cases with a finite element code. The first case involved 1-D flow parallel to the interface of two layers with differing pore water velocity. The early arrival of the solute in the low permeability layer and the increase in solute

spreading for both layers, as a result of transverse dispersion, were demonstrated. Two other examples concerned transport of a pollutant from a point source located at the soil surface. The magnitude of the transverse dispersion coefficient influenced the region to which the pollution extended, as well as the intensity of the pollution. Finally, transverse dispersion was shown to affect the movement of a pollutant to a drainage pipe.

INTRODUCTION

Transport of soluble chemicals in porous media, an important topic for many researchers working in engineering, agriculture, and hydrology, is generally assumed to occur by advection and dispersion. Because of the large variability in the field, use of the mass balance equation, on which the advection-dispersion equation or ADE is based, is being questioned to describe transport in natural soils. Although this subject is still under active investigation, application of the ADE is likely to continue for research purposes and as such will be used in this study. From the two terms contributing to the total solute flux, the advective flux is generally known or can easily be obtained by solving the flow problem. The autonomous dispersive flux occurs because of differences in concentrations. Much work has been published on dispersion phenomena, in particular to investigate the dispersion tensor (1). The dispersion in the direction of flow (longitudinal dispersion), is noticeably different from the dispersion perpendicular to the direction of flow (transverse dispersion). The mechanisms causing transverse dispersion are molecular diffusion and "wandering" from the flow path (17).

Solute movement in the transverse direction has to be taken into account for transport modeling whenever a gradient in concentration occurs in that direction (e.g., in the case of a non-uniform solute source or velocity distribution). Assuming that the medium is

isotropic, the 2-D transport equation needs to be used to describe solute transport and both longitudinal and transverse dispersion coefficients need to be known. The solution is generally achieved with numerical methods. However, analytical solutions are available for a number of situations. These solutions possess a greater flexibility and do not suffer from some of the errors associated with numerical solutions. Ogata (12) solved the transport equation analytically for radial dispersion from a circular source while ignoring longitudinal dispersion. Harleman and Rumer (8) presented an analytical solution for the 2-D ADE for steady conditions assuming that longitudinal dispersion could be neglected. Analytical solutions for steady transport, which accounted for longitudinal dispersion, were provided by Grane and Gardner (6) and Verruijt (22). Bruch and Street (3) obtained a series solution for 2-D transport in a finite system. Yule and Gardner (23) used an analytical solution to describe transport from a line source, ignoring longitudinal dispersion. Van Duijn and van der Zee (20) obtained approximate solutions to describe transport parallel to an interface separating two different porous media while neglecting longitudinal dispersion. Furthermore, Bear (1) discussed methods to obtain analytical solutions for some specific problems.

All of the above solutions have some disadvantages, notably the neglect of longitudinal dispersion. Therefore, the objective of this study was to provide an analytical solution for the two-dimensional transport problem which accounts for both longitudinal and transverse dispersion. This solution can be used to determine the two dispersion coefficients simultaneously.

Quantitative information about the dispersion coefficients is generally obtained by displacement experiments (15). The magnitude of the dispersion depends not only on the flow parameters, but also on particle size distribution, particle shape, heterogeneity of the porous medium, the presence of a stagnant phase, and differences in density and viscosity of the displacing and the displaced liquids (14). Compared to the work published on the longitudinal coefficient, $D_{\scriptscriptstyle I}$, relatively few results have been reported on the transverse dispersion coefficient, $\mathbf{D}_{\mathbf{T}}.$ Values for $\mathbf{D}_{\mathbf{T}}$ are more difficult to obtain than values for $D_{_{\hspace{-.1em}I}}$, because the concentration distribution needs to be measured in a direction perpendicular to the flow. In some molecular diffusion. However, Grane and Gardner (6) concluded that "the mechanism of transverse dispersion at high flow rate is dominated by the structure or grain size of the porous medium and influenced only by molecular diffusion." Measurements of slightly, if at all, transverse dispersion coefficients were reported by Simpson (17) and Harleman and Rumer (8). A number of studies have been performed to determine the dependency of $\mathbf{D}_{\!_{\mathbf{T}}}$ on the pore water velocity, and the Reynolds and Peclet numbers (9, 10). Yule and Gardner (23) measured both $D_{_{\rm T}}$ and $D_{_{\rm T}}$ for unsaturated media. Han et al. (7) used media with

Although analytical solutions are useful for simple laboratory investigations (to determine transport parameters), they are of limited value for field and more complex laboratory problems, for which

numerical methods need to be employed to predict solute transport. In addition to the development of an analytical solution, a finite element code was therefore employed to study some more complex transport problems. These problems were selected to meet the primary objective of studying the role of transverse dispersion in transport phenomena.

THEORY

The assumption is made that the transport of a solute is adequately described with the ADE. The advection term is one-dimensional and the dispersion term is two-dimensional. Transport in a homogeneous and isotropic medium during steady flow conditions is given by:

$$\frac{\partial C}{\partial t} = D_L \frac{\partial^2 C}{\partial x^2} - v \frac{\partial C}{\partial x} + D_T \frac{\partial^2 C}{\partial y^2}$$
 (1)

where C is the solute concentration $[ML^{-3}]$, t is time [T], D_L and D_T are the coefficients of longitudinal and transverse dispersion $[L^2T^{-1}]$, respectively, v is the pore water velocity $[LT^{-1}]$, and x and y are positions at the coordinate axes parallel and perpendicular to the direction of flow [L]. The solution domain is a half plane with x ≥ 0 and the other boundaries at infinity. The problem is solved for a prescribed concentration at x=0 (a Dirichlet condition). The initial and boundary conditions are (see also the section on the effect of transverse dispersion on transport):

$$\frac{\partial C}{\partial x}\bigg|_{x\to\infty} = 0 \qquad -\infty < y < +\infty \quad t \ge 0 \qquad (2-a)$$

$$C(0,y,t) = g(y) = \begin{cases} C_{L} & y<0 \\ & t \ge 0 \\ C_{R} & y>0 \end{cases}$$

$$C(x,y,0) = f(x,y) \qquad 0 < x < \infty \quad -\infty < y < \infty \qquad (2-c)$$

$$\frac{\partial \mathbf{C}}{\partial \mathbf{y}}\Big|_{\mathbf{y}\to +\infty} = 0$$
 $0 < \mathbf{x} < \infty$ $t > 0$ (2-d)

Quite often, these are also the experimental conditions for the determination of D_{T} (8). Figure 1 illustrates the problem to be solved.

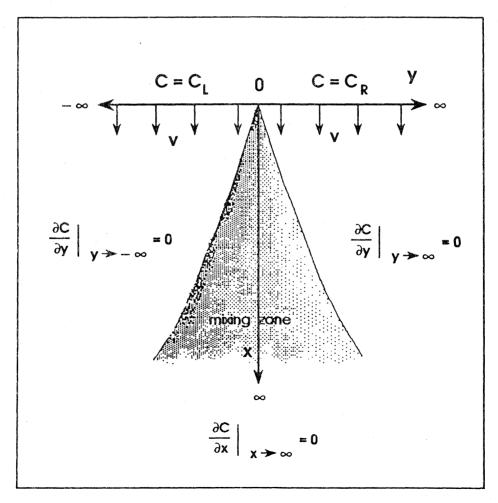


FIG. 1. Schematic of 1-D advection and 2-D dispersion in a half plane for an isotropic medium.

Solutions for this problem were earlier presented for steadystate conditions by Grane and Gardner (6), Harleman and Rumer (8) and Verruijt (22). Grane and Gardner applied a transformation to parabolic coordinates to obtain a diffusion equation. A disadvantage of this transformation complicates procedure is the the that conditions, which is a well known disadvantage of the solution of the 1-D ADE if a moving coordinate system is used. Among others, Harleman and Rumer (8) presented an analytical solution for a semi-infinite system where longitudinal dispersion was ignored $(D_{L_{2},2}^{\frac{\partial^2 C}{\partial L_{2}}} < D_{T_{2},2}^{\frac{\partial^2 C}{\partial L_{2}}})$. However, the transient state solution is usually of interest for contaminant transport. It is therefore desirable to obtain a solution, which facilitates the simultaneous determination of $\mathbf{D}_{\!_{\! 1}}$ and $\mathbf{D}_{\!_{\! T}}.$

Bruch and Street (3) obtained a solution consisting of infinite series for a finite system by using separation of variables. Because the solution procedure is somewhat complicated, and since we deal in effect with a half plane, a different solution technique was used.

The solution of Eq.(1), subject to Eq.(2), can be achieved with a double integral transform, viz. a Laplace transform with respect to t and a Fourier transform with respect to y. This combines solution techniques for the 1-D ADE (21) and the 2-D ADE for steady state conditions (8, 22). It is worthwhile noting that the diffusion equation for a half plane can be solved in a similar way, except that a Laplace transform is taken with respect to x (5).

First, the Laplace transform is taken. For completeness the Laplace transforms of C and $\frac{\partial C}{\partial t}$ are given:

$$\mathscr{L}\Big[C(x,y,t)\Big] = \int_0^\infty C(x,y,t) \exp(-pt) dt = \overline{C}(x,y,p)$$
 (3-a)

$$\mathcal{L}\left[\frac{\partial C}{\partial t}\right] = p\overline{C} - C(x, y, 0) \tag{3-b}$$

The Laplace transforms of Eq.(1) and (2) are:

$$p\overline{C} - f = D_{L} \frac{\partial^{2} \overline{C}}{\partial x^{2}} - v \frac{\partial \overline{C}}{\partial x} + D_{T} \frac{\partial^{2} \overline{C}}{\partial y^{2}}$$

$$(4)$$

$$\left. \frac{\partial \overline{C}}{\partial x} \right|_{x \to \infty} = 0 \tag{5-a}$$

$$\overline{C}(0,y,p) = \frac{9}{p} \tag{5-b}$$

Proceed by taking the Fourier transform for the infinite y-domain (18):

$$\mathcal{F}\left[\overline{C}(x,y,p)\right] = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \overline{C}(x,y,p) \exp(i\alpha y) dy = \overline{C}(x,\alpha,p)$$
 (6-a)

$$\mathcal{F}\left[\begin{array}{c} \frac{\partial^2 \overline{C}}{\partial y^2} \end{array}\right] = -\alpha^2 \stackrel{\sim}{\overline{C}} \tag{6-b}$$

The Fourier transforms of Eq. (4) and (5) are

$$D_{L} \frac{d^{2} \overline{\overline{C}}}{dx^{2}} - v \frac{d\overline{\overline{C}}}{dx} - (\alpha^{2} D_{T} + p) \overline{\overline{C}} + \tilde{f} = 0$$
 (7)

$$\frac{\frac{d\overline{C}}{dx}|_{x\to\infty} = 0 \tag{8-a}$$

$$\frac{\tilde{C}}{\tilde{C}}(0,\alpha,p) = \frac{\tilde{g}}{p}$$
 (8-b)

where $\tilde{\mathfrak{f}}$ and $\tilde{\mathfrak{g}}$ are the Fourier transforms of \mathfrak{f} and $\mathfrak{g}.$

A solution of Eq.(7), an ordinary differential equation, subject to Eq.(8) is:

$$\widetilde{\overline{C}}(x,\alpha,p) = A \exp(\lambda_1 x) + B \exp(\lambda_2 x) + \frac{\widetilde{f}}{D_T \alpha^2 + p}$$
(9)

where A and B are constants determined by the boundary conditions and where the roots λ are given by:

$$\lambda_{1,2} = \frac{v}{2D_{L}} + \sqrt{\left(\frac{v}{2D_{L}}\right)^{2} + \frac{D_{T}}{D_{L}}} \alpha^{2} + \frac{p}{D_{L}}$$
(10)

It follows from Eq.(8-a) that A=0. Using the boundary condition at the inlet, Eq.(8-b), we obtain:

$$B = \frac{\tilde{g}}{p} - \frac{\tilde{f}}{D_T \alpha^2 + p}$$
 (11)

Substitution of Eq.(11) into Eq.(9) yields:

$$\tilde{\overline{C}}(x,\alpha,p) = \left(\frac{\tilde{g}}{p} - \frac{\tilde{f}}{D_{T}\alpha^{2} + p}\right) \exp(\lambda_{2}x) + \frac{\tilde{f}}{D_{T}\alpha^{2} + p}$$
(12)

For a solution in the x,y,t-domain, inverse transformations need to be carried out. Although numerical inversion techniques are available, the use of analytical methods is preferred. First, the inverse Laplace transformation is carried out, for which purpose the right-hand side of Eq.(12) is split up into three terms, the first one being:

$$\widetilde{C}_{1}(x,\alpha,t) = \mathscr{Z}^{-1} \left[\widetilde{C}_{1}(x,\alpha,p) \right] = \mathscr{Z}^{-1} \left[\widetilde{\frac{9}{p}} \exp(\lambda_{2}x) \right] \\
= \widetilde{g} \exp\left[\frac{vx}{2D_{L}} \right] \mathscr{Z}^{-1} \left[\frac{1}{p} \exp\left[-\frac{x}{\sqrt{D_{L}}} \sqrt{\frac{v^{2}}{4D_{L}} + D_{T}\alpha^{2} + p} \right] \right]$$
(13)

The inverse Laplace operator is evaluated with the help of the convolution theorem. For the functions h(t) and k(t), with Laplace

transforms $\overline{h}(p)$ and $\overline{k}(p)$, the following convolution integrals can be defined:

$$\mathcal{L}^{-1}\left[\overline{h}(p)\overline{k}(p)\right] = h^*k = \int_0^t h(t-\xi)k(\xi) d\xi = \int_0^t h(\xi)k(t-\xi) d\xi$$
 (14)

where ξ is a dummy variable. Two functions can be distinguished in the expression of Eq.(13), which need to be inverted:

$$\overline{h}(p) = \frac{1}{p} \tag{15-a}$$

$$\overline{k}(p) = \exp\left[-\frac{x}{\sqrt{D_{I}}}\sqrt{\frac{v^{2}}{4D_{L}} + D_{T}\alpha^{2} + p}\right]$$
(15-b)

The inverse expressions, h(t) and k(t), are determined with the help of the shift theorem and a table of Laplace transforms (11):

$$h(t) = 1 ag{16-a}$$

$$k(t) = \frac{x}{t\sqrt{4\pi D_L t}} \exp\left[-\left(\frac{v^2}{4D_L} + D_T \alpha^2\right)t - \frac{x^2}{4D_L t}\right]$$
 (16-b)

Substitution in Eq. (14), results in

$$\widetilde{C}_{1}(x,\alpha,t) = \widetilde{g} \exp\left[\frac{vx}{2D_{L}}\right]$$

$$\times \int_{0}^{t} \frac{x}{\xi \sqrt{4\pi D_{L}\xi}} \exp\left[-\left(\frac{v^{2}\xi^{2} + 4D_{L}D_{T}\alpha^{2}\xi^{2} + x^{2}}{4D_{L}\xi}\right)\right] d\xi$$
(17)

The second term, $\overline{C}_2(x,\alpha,p)$, is inverted in a similar manner, except that no convolution integral is needed.

$$\widetilde{C}_{2}(x,\alpha,t) = \mathscr{U}^{-1} \left[\widetilde{\overline{C}}_{2}(x,\alpha,p) \right] = \mathscr{U}^{-1} \left[-\frac{\widetilde{\mathfrak{f}}}{D_{T}\alpha^{2}+p} \exp(\lambda_{2}x) \right] =$$

$$-\widetilde{\mathfrak{f}} \exp\left[\frac{vx}{2D_{L}}\right] \exp\left[-\left[\frac{v^{2}}{4D_{L}} + D_{T}\alpha^{2}\right] t \right] \mathscr{U}^{-1} \left[\frac{1}{p-(v^{2}/4D_{L})}\right] =$$

$$-\frac{\widetilde{\mathfrak{f}}}{2} \exp(-D_{T}\alpha^{2}t) \left\{ \operatorname{erfc} \left[\frac{x-vt}{\sqrt{4D_{L}t}}\right] + \exp\left[\frac{vx}{D_{L}}\right] \operatorname{erfc} \left[\frac{x+vt}{\sqrt{4D_{L}t}}\right] \right\}$$
(18)

where erfc is the complementary error function. The third term of Eq.(12) can be directly obtained from a table of Laplace transforms:

$$\widetilde{C}_{3}(x,\alpha,t) = \mathcal{L}^{-1}\left[\widetilde{C}_{3}(x,\alpha,p)\right] = \mathcal{L}^{-1}\left[\frac{\widetilde{f}}{D_{T}\alpha^{2}+p}\right] = \widetilde{f} \exp(-D_{T}\alpha^{2}t)$$
 (19)

The resulting expression for $\widetilde{C}(x,\alpha,t)$, the Fourier transform of the analytical solution being sought, is:

$$\widetilde{C}(x,\alpha,t) = \widetilde{C}_1 + \widetilde{C}_2 + \widetilde{C}_3$$
 (20)

The last step of the solution procedure is the application of the inverse Fourier transform to each of the terms in Eq.(20). The inverse transformation of $\widetilde{C}(x,\alpha,t)$ is formally given by:

$$C(x,y,t) = \mathcal{F}^{-1}\left[\widetilde{C}(x,\alpha,t)\right] = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \widetilde{C} \exp(-i\alpha y) d\alpha$$
 (21)

The inverse of the first term of Eq.(20) is determined as follows.

$$C_{1}(x,y,t) = \mathcal{F}^{-1} \left[\widetilde{C}_{1}(x,\alpha,t) \right] =$$
 (22)

$$\int_{0}^{t} \frac{1}{\sqrt{2\pi}} \left\{ \int_{-\infty}^{\infty} \frac{\overset{\circ}{g}x}{\xi \sqrt{4\pi D_{L}\xi}} \exp\left[\frac{vx}{2D_{L}}\right] \exp\left[-\left[\frac{v^{2}\xi^{2}+4D_{L}D_{T}\alpha^{2}\xi^{2}+x^{2}}{4D_{L}\xi}\right]\right] \exp(-i\alpha y) \ d\alpha \right\} d\xi$$

Again, the convolution h^*k was used to determine the inverse of a product of two functions \tilde{h} and \tilde{k} , which are now in the Fourier domain:

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \widetilde{h}(\alpha) \widetilde{k}(\alpha) \exp(-i\alpha y) d\alpha = h^*k = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} h(y)k(y-v) dv$$
 (23)

After inspection of the last expression for $C_1(x,y,t)$ in Eq.(22), the following two functions seem convenient for the convolution integral:

$$\tilde{h}(\alpha) = \tilde{g}$$
 (24-a)

$$\widetilde{k}(\alpha) = \frac{x}{\xi \sqrt{4\pi D_L \xi}} \exp\left[-\left(\frac{x - v\xi}{\sqrt{4D_L \xi}}\right)^2\right] \exp(-D_T \alpha^2 \xi)$$
(24-b)

Without actually determining \tilde{g} , which is the Fourier transform of a step function, it is clear that h(y) must equal g(y). To determine the inverse of $\tilde{k}(\alpha)$, note that:

$$\mathcal{F}^{-1}\left[\exp(-D_{\mathrm{T}}\alpha^{2}\xi)\right] = \frac{1}{\sqrt{2\xi D_{\mathrm{T}}}}\exp\left[-\frac{y^{2}}{4\xi D_{\mathrm{T}}}\right]$$
(25)

The resulting h(y) and k(y) are:

$$h(y) = g(y) = \begin{cases} C_L & y < 0 \\ C_R & y > 0 \end{cases}$$
 (26-a)

$$k(y) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \tilde{k}(\alpha) \exp(-i\alpha y) d\alpha =$$

$$= \frac{x}{\xi \sqrt{4\pi D_L \xi}} \exp\left[\left(\frac{x - v\xi}{\sqrt{4D_L \xi}}\right)^2\right] \frac{1}{\sqrt{2\xi D_T}} \exp\left[-\frac{y^2}{4\xi D_T}\right]$$
(26-b)

From Eq. (23) it follows that:

$$h^*k = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \frac{xh(v)}{\xi \sqrt{4\pi D_L \xi}} \exp\left[-\left(\frac{x-v\xi}{\sqrt{4D_L \xi}}\right)^2\right] \frac{1}{\sqrt{2\xi D_T}} \exp\left[-\frac{(y-v)^2}{4\xi D_T}\right] dv \qquad (27)$$

This expression is evaluated by using the substitution $\rho=(\upsilon-y)/2\sqrt{\xi D_T}$, Eq.(26-a) and the properties of the error function (4):

$$h^*k = \frac{x}{\xi \sqrt{4\pi D_L \xi}} \exp\left[-\left(\frac{x - v\xi}{\sqrt{4D_L \xi}}\right)^2\right] \left\{\frac{C_L}{2} \operatorname{erfc}\left[\frac{y}{\sqrt{4\xi D_T}}\right] + \frac{C_R}{2} \operatorname{erfc}\left[-\frac{y}{\sqrt{4\xi D_T}}\right]\right\}$$
(28)

This result can be substituted in Eq.(22) to obtain the following expression for $C_1(x,y,t)$:

$$C_{1}(x,y,t) = \int_{0}^{t} h^{*}k \ d\xi =$$

$$\int_{0}^{t} \frac{x}{\xi \sqrt{4\pi D_{L}\xi}} \exp\left[-\left(\frac{x-v\xi}{\sqrt{4D_{L}\xi}}\right)^{2}\right] \left\{\frac{C_{L}}{2} \operatorname{erfc}\left[\frac{y}{\sqrt{4\xi D_{T}}}\right] + \frac{C_{R}}{2} \operatorname{erfc}\left[-\frac{y}{\sqrt{4\xi D_{T}}}\right]\right\} d\xi$$
(29)

The second term, $C_2(x,y,t)$, is given as follows:

$$C_{2}(x,y,t) = -\frac{1}{2} \left\{ erfc \left[\frac{x-vt}{2\sqrt{D_{L}t}} \right] + exp \left[\frac{vx}{D_{L}} \right] erfc \left[\frac{x+vt}{2\sqrt{D_{L}t}} \right] \right\} \mathcal{F}^{-1} \left[\tilde{f} exp(-D_{T}\alpha^{2}t) \right]$$
(30)

The Fourier inverse term in Eq.(30) is obtained with the convolution theorem, with:

$$\tilde{h}(\alpha) = \tilde{f}$$
 (31-a)

$$\tilde{\mathbf{k}}(\alpha) = \exp(-D_{\mathrm{T}}\alpha^2 \mathbf{t})$$
 (31-b)

For convenience, it is assumed that the initial concentration is constant, viz. $C_{\underline{i}}$. Making use of Eq.(25) results in the following inverse functions:

$$h(y) = f(x, y) = C_{i}$$
 (32-a)

$$k(y) = \frac{1}{\sqrt{2D_T t}} \exp\left(-\frac{y^2}{4D_T t}\right)$$
 (32-b)

The inverse transformation can now be carried out by using the properties of erfc and applying the same substitution variable ρ :

$$\mathcal{F}^{-1}\left[\tilde{f} \exp(-D_{T}\alpha^{2}t)\right] = h*k = \frac{C_{i}}{\sqrt{4\pi D_{T}t}} \int_{-\infty}^{\infty} \exp\left(-\frac{(y-\upsilon)^{2}}{4D_{T}t}\right) d\upsilon = C_{i}$$
 (33)

Hence:

$$C_{2}(x,y,t) = -\frac{C_{i}}{2} \left\{ erfc \left[\frac{x-vt}{\sqrt{4D_{L}t}} \right] + exp \left[\frac{vx}{D_{L}} \right] erfc \left[\frac{x+vt}{\sqrt{4D_{L}t}} \right] \right\}$$
(34)

The last term, $C_3(x,y,t)$, was already evaluated in Eq.(33):

$$C_3(x,y,t) = \mathcal{F}^{-1} \left[\tilde{f} \exp(-D_T \alpha^2 t) \right] = C_i$$
 (35)

The resulting expression for C(x,y,t) is:

$$C(x,y,t) = \int_{0}^{t} \frac{x}{\xi \sqrt{4\pi D_{L}\xi}} \left\{ \frac{C_{L}}{2} \operatorname{erfc} \left[\frac{y}{2\sqrt{D_{T}\xi}} \right] + \frac{C_{R}}{2} \operatorname{erfc} \left[-\frac{y}{2\sqrt{D_{T}\xi}} \right] \right\} \times \exp \left[-\left[\frac{x-v\xi}{2\sqrt{D_{L}\xi}} \right]^{2} \right] d\xi - \frac{C_{i}}{2} \left\{ \operatorname{erfc} \left[\frac{x-vt}{2\sqrt{D_{L}t}} \right] + \exp \left[\frac{vx}{D_{L}} \right] \operatorname{erfc} \left[\frac{x+vt}{2\sqrt{D_{L}t}} \right] \right\} + C_{i}$$

$$(36)$$

The integral in Eq.(36) needs to be evaluated numerically, which is conveniently done with the Gauss-Chebyshev quadrature. The computer program to calculate C(x,y,t), including the function EXF(A,B) to obtain exp(A)erfc(B), is given in the Appendix. Notice that the solution was kept quite general by not specifying f and g. In many other instances, a simpler expression arises if C_L or C_R and C_i are equal to 0. Transport of solutes which are linearly retarded, because of reactions with the solid phase of the medium, can be described by dividing the parameters D_I , D_T , and V with the retardation coefficient.

VALIDATION OF ANALYTICAL SOLUTION

The solution presented in Eq.(36), including the numerical integration of the first term, was validated via comparison with various numerical and analytical solutions for specific values of C_L , C_R , and C_i . First, the steady state solution of Eq.(1) is used under the assumption that longitudinal dispersion can be ignored. This solution was obtained via the Fourier transform of y (18):

$$C(x,y) = \frac{C_L}{2} \operatorname{erfc} \left[\frac{y}{\sqrt{4D_T x/v}} \right] + \frac{C_R}{2} \operatorname{erfc} \left[-\frac{y}{\sqrt{4D_T x/v}} \right]$$
(37)

The program to evaluate Eq.(37) is also listed in the Appendix.

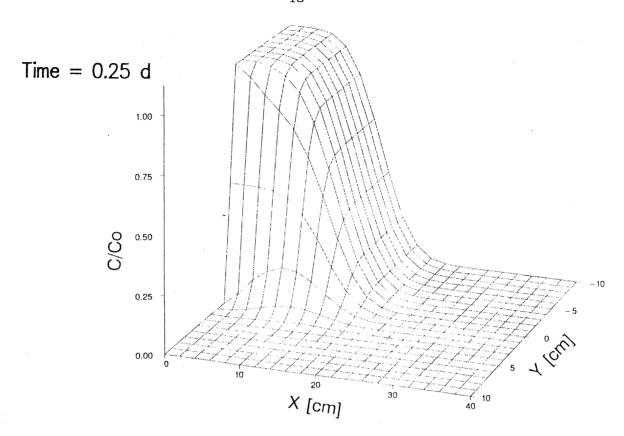
During the validation a porous medium with the following arbitrary transport parameters was assumed: $D_L=25~{\rm cm}^2/{\rm d}$, $D_T=5~{\rm cm}^2/{\rm d}$, v=50 cm/d, see table 1. All concentrations were conveniently expressed as dimensionless quantities C/C_o , with C_o being equal to unity. The dimensionless inlet and initial concentrations were: $C_L=1$, $C_R=0$, $C_i=0$. Figure 2 shows the solutions for various times according to Eq.(36). The solution for larger times was virtually identical to the steady-state solution given by Eq.(37). The "invasion" of the solute into the medium and the flattening of the step front can clearly be observed.

The solution of equations describing transport problems usually requires experimental determination of the transport parameters. Experimental conditions as sketched in figure 1 allow the simultaneous determination of D_L and D_T . Breakthrough curves, C=C(L,y,t), can be

Table 1. List of Physical and Mathematical Parameters for Calculations

Fig	. Ur	nits	Layer	r v	θ	α_{L}	DL	α_{T}	$^{\mathrm{D}}_{\mathrm{T}}$	Δx	Δу	Δt
	L	Т		LT ⁻¹		L	L^2T^-	1 L	L ² T ⁻¹	L	L	T
2	cm	d	_	50	-	-	25		5	_	-	
4	m	d	_	0.4	0.4	20	8	4	1.6	60	30	100
6 7 8	cm	d	I	10 100	0.4	2 0.5		0.5 0.1		1	.5 or .25	0.01
10 11 12	cm	hr	I II	2.5 2.5	0.4	2 2	5 5	0.1 .1/.5	0.25 .25/1.25	10	2.5	2.5
14 15 16	cm	d		s ig	0.4	10	-	1.0/5.	0 -	1	1	0.05

^{*} See figure 14 for additional information.



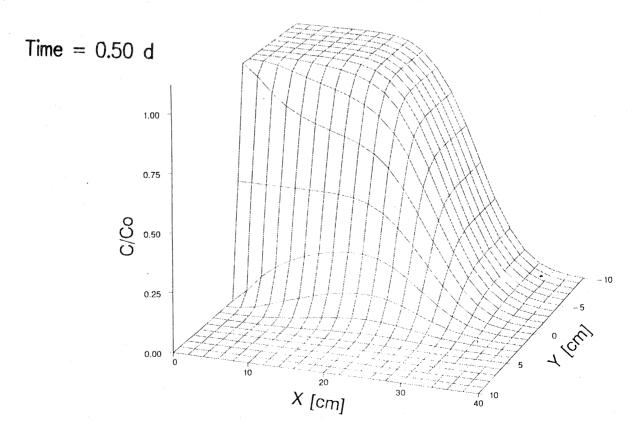
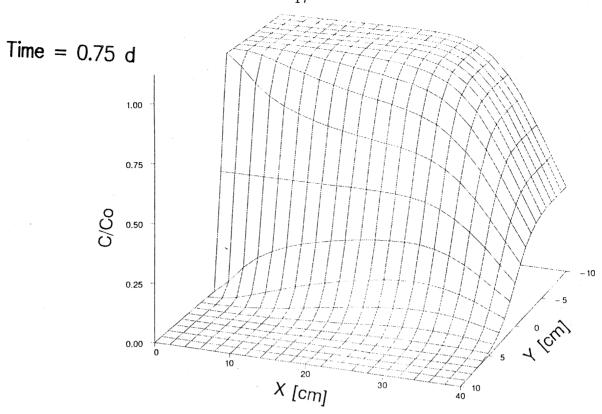


FIG.2. Solution of the 1-D advection and 2-D dipersion equation for various times.



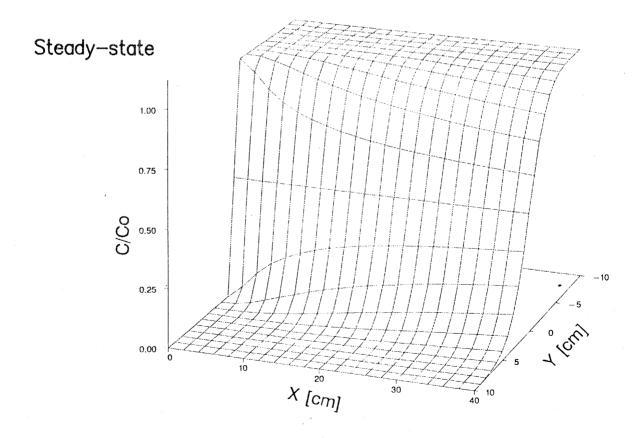


FIG.2. Solution of the 1-D advection and 2-D dipersion equation for various times.

measured at an arbritray position x=L for a sufficient number of y-values. The steady state profile, $C=C(L,y,\infty)$, can be used to determine D_T according to Eq.(37). Values for D_L can be determined subsequently with Eq.(36) via an iteration procedure.

Next, the half-plane solution (Eq.(36)) was compared with the solution by Bruch and Street (3). The mathematical problem studied by these authors obeys the following boundary and initial conditions:

$$C(0,y,t) = \begin{cases} C_0 & 0 \le y \le \varepsilon & t > 0 \\ 0 & \varepsilon \le y \le n & t > 0 \end{cases}$$
 (38-a)

$$\frac{\partial C}{\partial y}\bigg|_{y=0} = 0 \qquad x > 0 \qquad t > 0 \tag{38-b}$$

$$\frac{\partial C}{\partial y}\bigg|_{\substack{y=n\\0}} = 0 \qquad x > 0 \qquad t > 0 \qquad (38-c)$$

$$|C(\omega, y, t)| = \text{bounded}$$
 $0 \le y \le n_0 \quad t > 0$ (38-d)

$$C(x, y, 0) = 0$$
 $x > 0 0 \le y \le n_0$ (38-e)

The solution presented by Bruch and Street (3) is:

$$\frac{\varepsilon C_{o}}{2n_{o}} \left\{ \operatorname{erfc} \left[\frac{x - vt}{\sqrt{4D_{L}t}} \right] + \exp \left(\frac{vx}{D_{L}} \right) \operatorname{erfc} \left[\frac{x + vt}{\sqrt{4D_{L}t}} \right] \right\} + \sum_{n=1}^{\infty} \left\{ \frac{C_{o}}{n\pi} \sin(\frac{n\pi\varepsilon}{n_{o}}) \cos(\frac{n\pi y}{n_{o}}) \right\}$$

$$\times \left[\exp \left[\frac{x}{2} \left(\frac{v}{D_{L}} - \sqrt{\left(\frac{v}{D_{L}}\right) + \left(\frac{2n\pi}{n_{o}}\right)^{2} \frac{D_{T}}{D_{L}}} \right) \right] \operatorname{erfc} \left[\frac{x - D_{L}t}{\sqrt{\left(\frac{v}{D_{L}}\right)^{2} + \left(\frac{2n\pi}{n_{o}}\right)^{2} \frac{D_{T}}{D_{L}}}}{\sqrt{4D_{L}t}} \right]$$

$$+ \exp \left[\frac{x}{2} \left(\frac{v}{D_{L}} + \sqrt{\left(\frac{v}{D_{L}}\right)^{2} + \left(\frac{2n\pi}{n_{o}}\right)^{2} \frac{D_{T}}{D_{L}}} \right) \right] \operatorname{erfc} \left[\frac{x + D_{L}t}{\sqrt{\left(\frac{v}{D_{L}}\right)^{2} + \left(\frac{2n\pi}{n_{o}}\right)^{2} \frac{D_{T}}{D_{L}}}}}{\sqrt{4D_{L}t}} \right] \right] \right\}$$

This solution was evaluated numerically with a computer program containing the EXF(A,B)-function. The geometry according to figure 1 was obtained by shifting the y-coordinate by a distance ε to the left. figure 3 contains the results obtained with this solution as well as the results obtained with the half-plane solution. The results are almost identical.

For many situations, numerical methods need to be employed in order to solve the 2-D ADE. To demonstrate the effects of transverse dispersion on contaminant transport, some simple problems, which were solved with a finite element code, will be presented in the next section. But first the input parameters of the code will be discussed and a comparison will be made between numerical and analytical results.

The code solves 2-D flow and transport problems in isotropic media and was validated for a variety of transport problems. Somewhat arbitrary values were used for the calculations, which represent situations encountered in the laboratory or field. The relevant data for the calculations of all examples are listed in the table 1. It should be noted that dimensions of parameters are quite often omitted, since any set of consistent units can be used.

The apparent dispersion tensor, $\mathbf{D}_{\mathbf{a}}$, accounts for mechanical dispersion and molecular diffusion and can be defined according to Bear (1):

$$\mathbf{p}_{\mathbf{a}} = \begin{pmatrix} \mathbf{p}_{\mathbf{x}\mathbf{x}} & \mathbf{p}_{\mathbf{x}\mathbf{y}} \\ \mathbf{p}_{\mathbf{y}\mathbf{x}} & \mathbf{p}_{\mathbf{y}\mathbf{y}} \end{pmatrix} \tag{40}$$

with

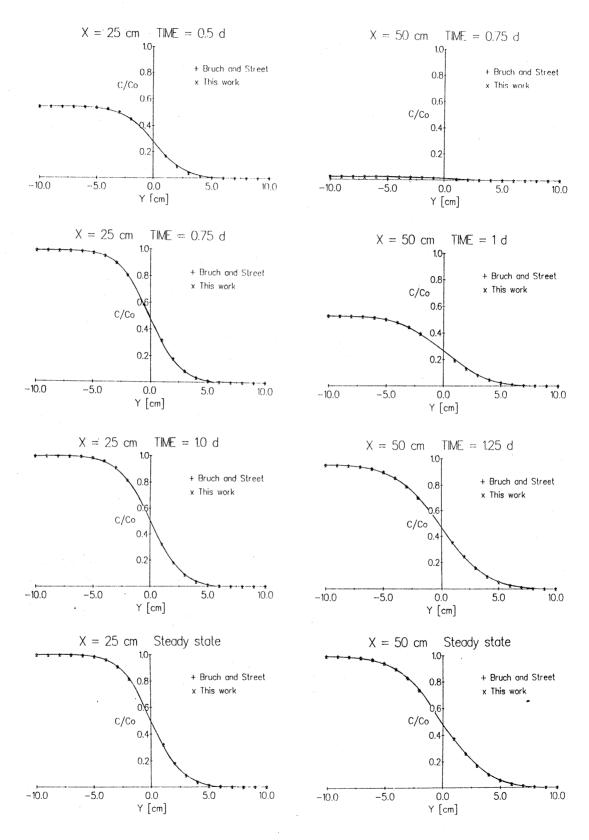


FIG.3. Comparison of the half-plane solution with the semi-infinite strip solution by Bruch and Street (3).

$$D_{xx} = \alpha_{T} |q| + (\alpha_{L} - \alpha_{T}) q_{x}^{2} / |q| + D_{xx}^{*}$$

$$D_{xy} = (\alpha_{L} - \alpha_{T}) q_{x} q_{y} / |q| = D_{yx}$$

$$D_{yy} = \alpha_{T} |q| + (\alpha_{L} - \alpha_{T}) q_{y}^{2} / |q| + D_{yy}^{*}$$
(41)

where q denotes the average Darcy velocity with components q_x and q_y and vector norm |q| $[LT^{-1}]$, α_L and α_T are the transverse and longitudinal dispersivity [L], respectively, and D_{xx}^* and D_{yy}^* are components of the apparent coefficient of molecular diffusion $[L^2T^{-1}]$. For a volumetric water content θ , the velocity and dispersion terms in Eq.(1) are rewritten as $v=q_x/\theta$, $D_L=D_{xx}/\theta$, $D_T=D_{yy}/\theta$ and it is assumed that $D_{yx}=D_{xy}=0$. The grid system and the time step are chosen based on the dimensionless Peclet and Courant number. The restraints were: $\frac{\Delta x}{\alpha_L} < 5$, $\Delta y \le \Delta x$, and $\frac{v\Delta t}{\Delta x} < 1$.

The results of the code were compared with the analytical solution using $v_x=0.4$ m/d, $\alpha_L=20$ m, $\alpha_T=4$ m, which is assumed to represent a "field situation." A rectangular grid, with $\Delta x=60$ m and $\Delta y=30$ m, was used for the calculations with a timestep of 100 d. The boundary and initial conditions, for the numerical solution, were as follows:

$$C(x,y,0) = 0.25 C_0 0 < x < 600, -150 < y < 150$$
 (42-a)

$$C(0,y,t) = \begin{cases} C_{o} & y < 0, t > 0 \\ 0.5 C_{o} & y > 0, t > 0 \end{cases}$$
(42-b)

The resulting concentration profiles in the transverse direction, for various t and x, are given in figure 4. The comparison between the analytical and numerical solution is fair, with the best agreement found at larger times.

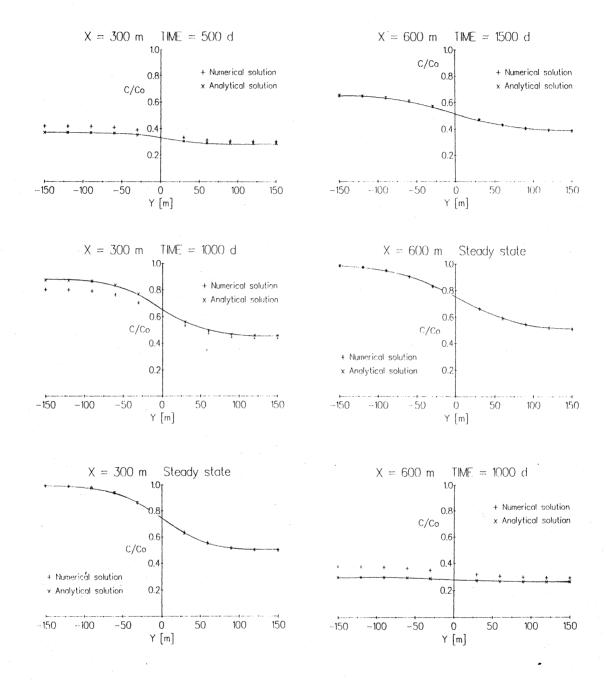


FIG. 4. Comparison of the analytical (half-plane) and the numerical (finite element) solution.

Based on the results in this section, the analytical solution given by Eq.(36) was concluded to be sufficiently validated.

THE EFFECT OF TRANSVERSE DISPERSION ON SOLUTE TRANSPORT

A sensitivity analysis was conducted to investigate the effect of transverse dispersion for three transport problems. Concentration distributions were determined with a finite element code.

The first example concerned a two-layer medium, each layer with its own characteristics, and flow occurring in the same direction as the interface. The physical and mathematical characteristics, including the grid system, are shown in figure 5. The influence of transverse dispersion during flow along such an interface has been studied by a number of authors for different inlet conditions (16, 19, 20, 22). The problem is of interest to study the early occurrence of a solute in a

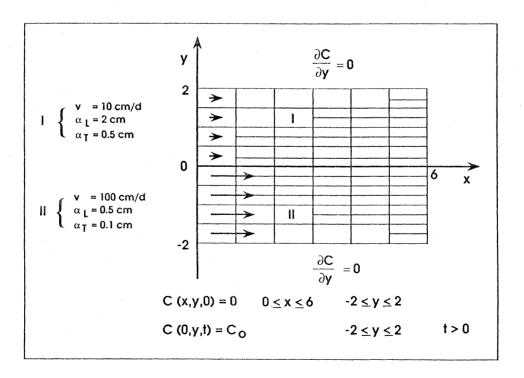


FIG.5. Physical and mathematical characteristics of transport in a two-layer medium with advection along the interface.

low permeability layer as a result of transverse dispersion or to study mixing of salt and fresh water. Furthermore, a layered medium is a simplification of a heterogeneous medium, and can therefore be used to investigate transport in heterogeneous media. In particular, the combined effect of longitudinal and transverse dispersion on the overall spreading needs to be considered in such a case.

Figure 6 shows the concentration profiles in the transverse direction at x=2 and 6 for various times. To get an impression of the effect of transverse dispersion, results in the absence of transverse dispersion (1-D transport) are included as well. It should be noted that transverse dispersion causes movement of the solute from the high to the low permeability layer. This is particularly important at the early stage, virtually all the solute in the low permeability layer is then present due to (transverse) dispersive rather than advective transport.

For the half-plane solution it was assumed that a first- or concentration-type boundary condition could be used at the inlet. However, Parker and van Genuchten (1984) showed for 1-D transport that the use of a third- or flux-type boundary condition is more appropriate. Although the solution for the steady-state problem is not influenced by the inlet condition, the solution for the transient problem will be. Therefore a comparison was made between results obtained with the finite element code for the two conditions. Figure 7 shows concentration profiles at x=6 which were obtained by using a flux and a concentration boundary condition. As is the case for 1-D

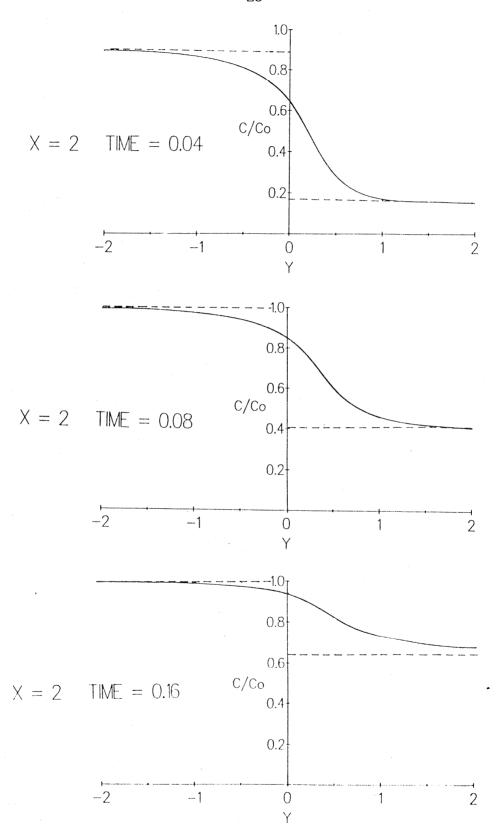


FIG. 6A. Concentration profiles in the transverse direction at various times, with transverse dispersion (solid line, 2-D transport) and without transverse dispersion (dashed line, 1-D transport), at x=2.

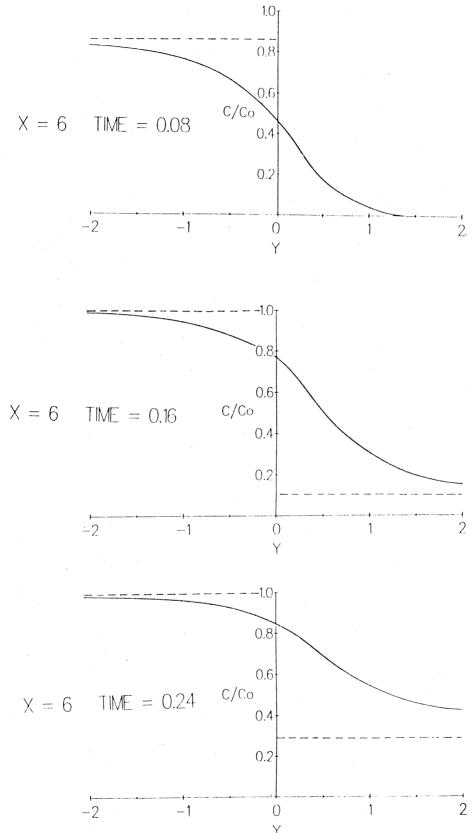


FIG.6B. Concentration profiles in the transverse direction at various times, with transverse dispersion (solid line, 2-D transport) and without transverse dispersion (dashed line, 1-D transport), at x=6.



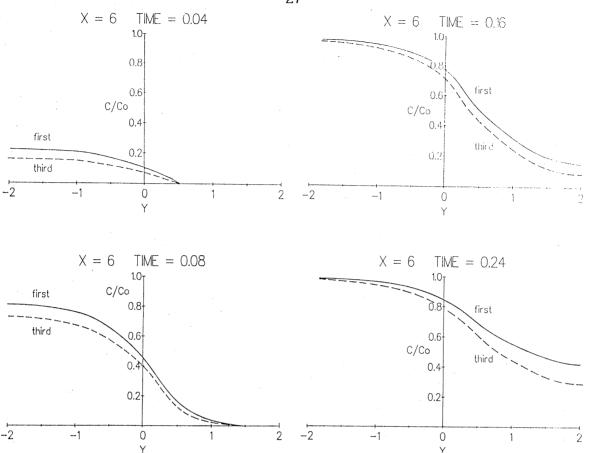


FIG. 7. Concentration profiles in the transverse direction at x=6 for various times, using a first- and third-type boundary condition.

transport, the profile obtained with the flux boundary lies below the profile obtained with the concentration boundary condition. At the initial stage, a mass balance error is involved in the use of the first-type boundary condition at the inlet. This error is considered to be minor, except for systems with a small length in the longitudinal direction during the inital stage of solute displacement.

Transverse dispersion also has an impact on the longitudinal concentration profile because it tends to annihilate concentration gradients orthogonal to the direction of flow. Figure 8 shows concentration profiles in the direction of flow as determined by the 1-

and 2-D transport equation. The results imply that application of the 1-D ADE to determine longitudinal dispersion coefficients in a (heterogeneous) medium with, for whatever reason, concentration gradients in the transverse direction, leads to erroneous values for D_L . Also included is the front, which would occur if D_T =0 (1-D transport). Longitudinal dispersion causes the front to spread symmetrically around the step front in the direction of flow. Lateral dispersion causes the front to deviate from symmetry in this direction. Because of differences in D_T and V for both layers, no symmetry will occur in the lateral direction.

The next example concerns 2-D transport from a bounded surface area in a two-layer medium with an interface perpendicular to the direction of flow. The bottom part of the medium, layer II, consists of particles of a different size and shape resulting in a higher value for α_T than for layer I. A schematic of the problem is given in Figure 9, which also includes the mathematical conditions and the physical parameters. The problem is symmetrical about y=0. To evaluate how transverse dispersion causes a contaminant to deviate from the advective flow path, the path being determined by the location of the point source and the flow field, solute transport was simulated for two different values of α_T for the bottom layer. To illustrate the transverse dispersion, the longitudinal dispersion was assumed to be identical for both layers.

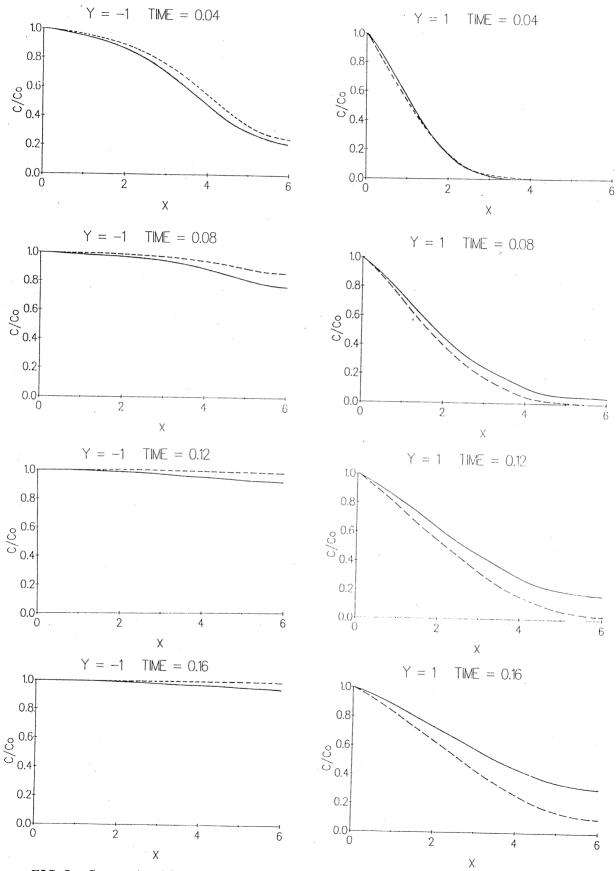


FIG. 8. Concentration profiles in the longitudinal direction in layers I and II at |y|=1 for various times, with transverse dispersion (solid line) and without transverse dispersion (dashed line).

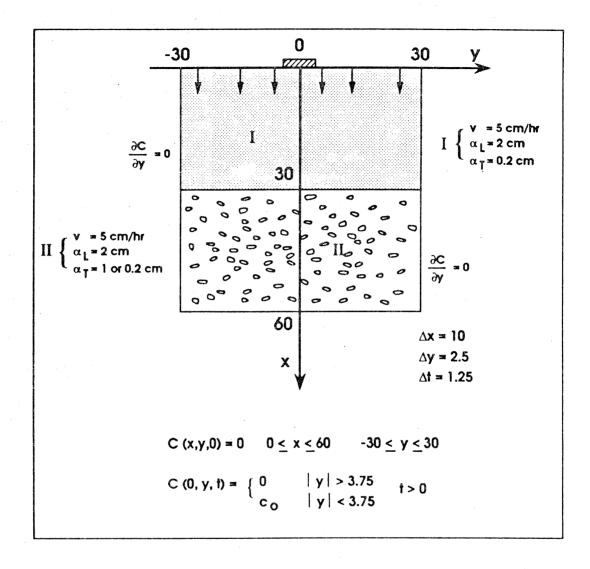


FIG.9. Physical and mathematical characteristics of transport in a two-layer medium with flow perpendicular to the interface.

Lines of equal dimensionless concentration C/C for various times are shown in figure 10A for equal α_T -values for both layers and in figure 10B for an α_T -value that is 5 times greater for the bottom than the top half of the profile. The shape of the plume in figure 10B differs from the one in figure 10A once the front reaches the bottom

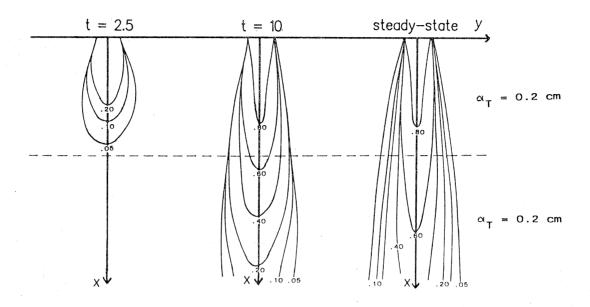


FIG. 10A. Lines of equal concentration, C/C $_{\rm O}$, at various times with ($\alpha_{\rm T}$) $_{\rm I}$ =($\alpha_{\rm T}$) $_{\rm II}$.

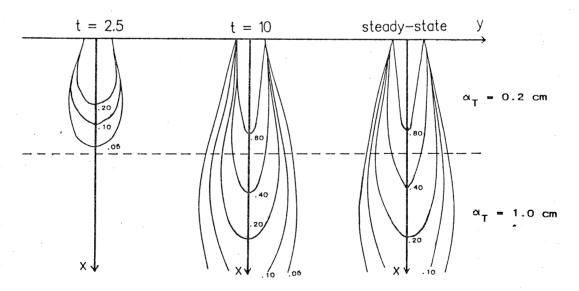


FIG. 10B. Lines of equal concentration, C/C $_{\rm o}$, at various times with ($\alpha_{\rm T}$) $_{\rm I}^{\neq}(\alpha_{\rm T})_{\rm II}$.

layer. The plume is restricted to a small area, with relatively high concentrations, in figure 10A, whereas figure 10B shows that, because of the increase in α_r , the plume spreads out over a larger area in layer II with relatively low concentrations. Even the concentrations in the top layer are influenced by the degree of spreading in the bottom layer. This is also shown in figure 11, which shows the longitudinal profile for various values of y and t. Breakthrough curves at various positions are presented in figure 12. An increase in transverse dispersion (x>30) lowers the maximum concentration of the solute (e.g., x=60 and y=0), but increases the area where the solute will occur (e.g., x=60 and y=10). The interpretation of these results depends on the type of contaminant. If low levels of solute are acceptable, increased transverse dispersion is favorable contrast in substances which already pose a threat at low concentrations and need to be removed.

The last example, illustrated in Fig. 13, deals with 2-D transport from the surface in an isotropic medium. At depth d, drainage pipes with spacing l are present to collect the contaminant to prevent it from reaching an underlying aquifer. A likely approach to do so is to optimize 1/d and the flow regime. However, this is beyond the scope of this analysis, which merely concerns the effect of transverse dispersion.

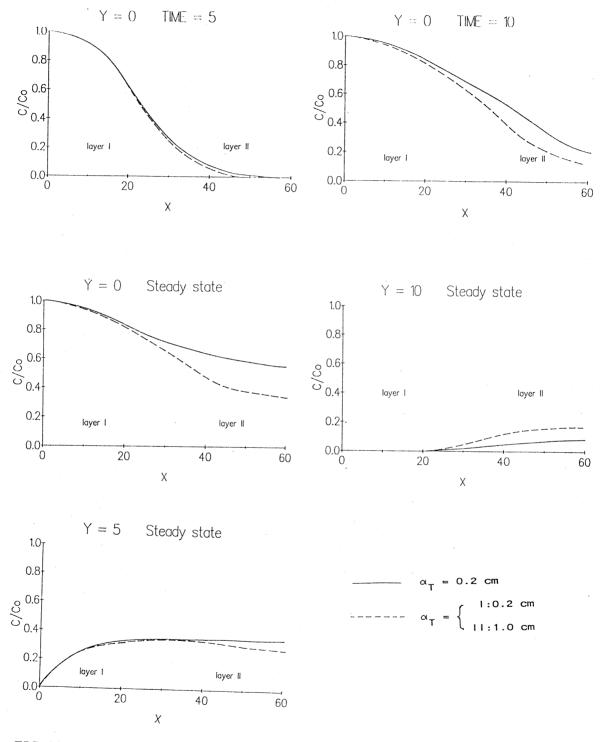


FIG.11. Concentration profiles in the longitudinal direction for various values of y and t.

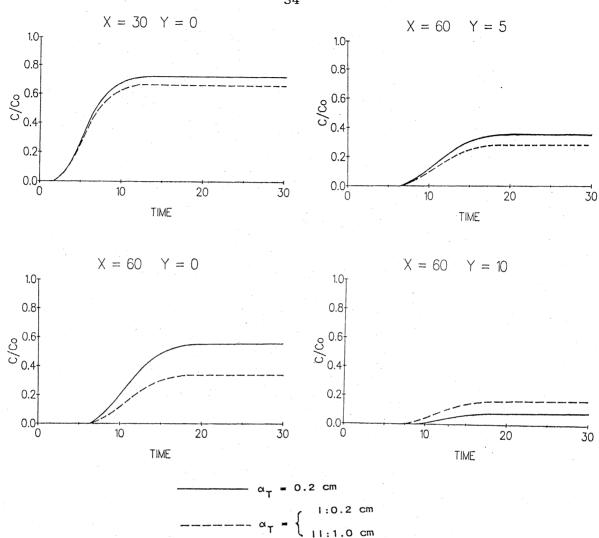
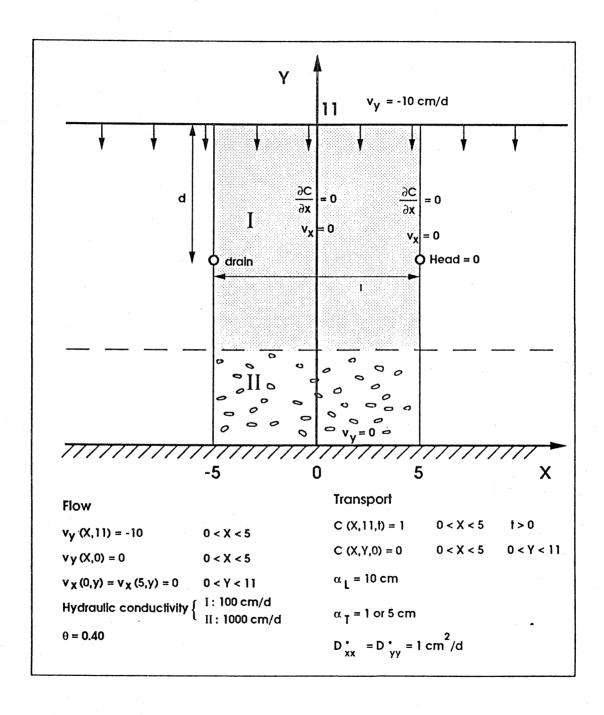


FIG. 12. Breakthrough curves at various positions during transport in a two-layer medium with the interface perpendicular to the direction of flow.



 $FIG.\,13.$ Characteristics of the flow and transport problem from the soil surface to a drain.

First, the (steady) flow regime was determined with the code followed by the solution of the transport problem. Because of the symmetry, a solution for the region 0<x<5 was sufficient. The grid system is shown in figure 14, along with equipotential lines and the velocity field, which were obtained by using arbitrary values for the hydraulic conductivity and assuming an impervious bottom. The ADE was solved for this velocity field, using two values for α_T , namely 1 and 5 cm. Because of the low velocity at certain positions, molecular diffusion contributes significantly to the overall dispersion.

Lines of equal concentration at various times are given in figure 15. The concentration profile is clearly influenced by the advection term, as indicated by the pattern around the drain; relatively high concentrations exist above the pipe. The solute will move in a direction orthogonal to the radial flow field as a result of transverse dispersion. An increase in α_T causes the higher solute concentration to reach the aquifer (x<5) sooner. Furthermore, a better recovery (removal via the drain) of the contaminant is achieved in case of a low value of α_T . This is also illustrated in figure 16, which contains breakthrough curves for y=7 (just above the drainage pipe) and y=3 (at the boundary with the aquifer). Close to the drainage pipe (x=4 and y=7) the concentration is higher for α_T =1 cm than for α_T =5 cm indicating that more solute can be removed from the system at lower values for α_T . At the other three locations, the higher transverse dispersion leads to higher solute concentrations.

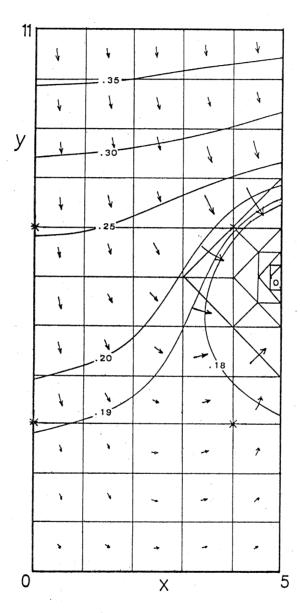


FIG.14. Grid system, velocity field and equipotential lines for the problem sketched in figure 13.

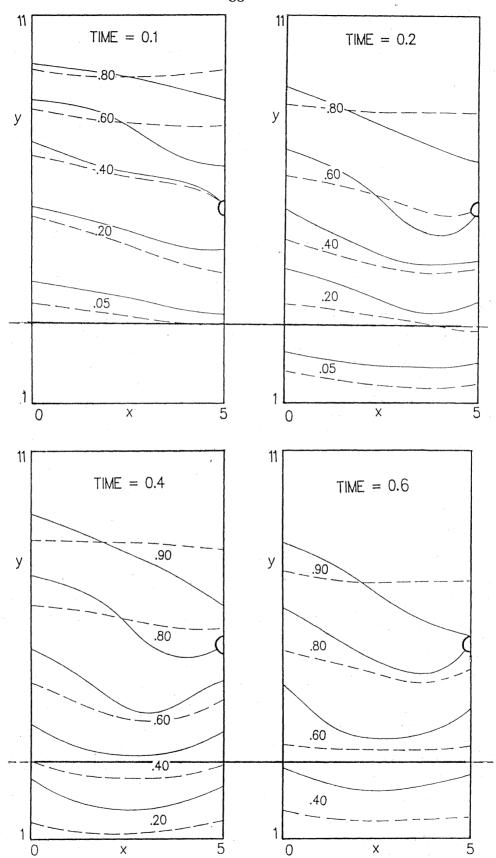


FIG.15. Lines of equal concentration C/C $\,$ at various times with $\alpha_{\mbox{\scriptsize T}}$ equal to 1 cm (solid line) or 5 cm (dashed line).

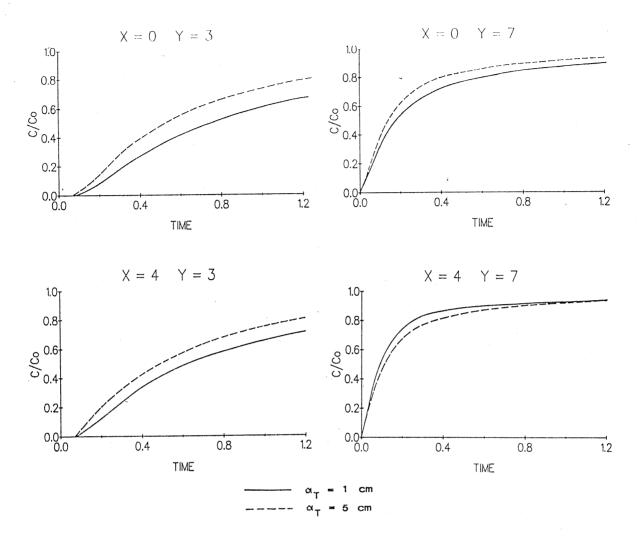


FIG. 16. Breakthrough curves at various positions for transport to a drain.

Finally, the "smoothness" of the concentration profiles in figure 15 (especially for α_T =5 cm), despite the changes in the flow vector, is pointed out. This is attributed to (transverse) dispersion, which has a tendency to annihilate concentration gradients.

SUMMARY AND CONCLUSIONS

An analytical solution was obtained for the 2-D ADE for a semi-infinite medium (half-plane) with 1-D flow using a double integral transform. Although the solution contains an integral expression, this using Gauss-Chebyshev could conveniently be evaluated half-plane solution was validated with various quadrature. The analytical and numerical solutions. Excellent agreement was found with other analytical solutions, whereas the numerical solution showed reasonable agreement with the half-plane solution. The solution can be used to determine values for $\boldsymbol{D}_{\!\!\!\boldsymbol{I}}$ during transient conditons and for $\boldsymbol{D}_{\!\!\!\boldsymbol{T}}$ during steady-state.

A finite element code was used in a sensitivity analysis to investigate the effect of transverse dispersion on transport. The first case involved transport in a medium consisting of two layers with different velocities and flow in the same direction as the interface. The computations pointed out that a substantial amount of solute moved from the high to the low permeability layer. This explained the "early" appearance of solute in the low permeability region and is one of the reasons for an increase in dispersion in heterogeneous media.

Two cases of point source pollution were considered: first, the development of a solute plume during downward flow was shown to depend on transverse dispersion, and second, the transport in a non-uniform flow field to a drainage pipe was studied. Attempts to collect the pollutant depend, among other things, on the value of the transverse dispersivity.

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APPENDIX. Listing of Computer Programs

ANLOTR: Solution of the 1-D advection and 2-D dispersion equation according to Eq.(36) (transient).

SSTR : Solution of the 1-D advection and 1-D dispersion equation according to Eq.(37) (steady-state).

```
ANLOTR
//ANLOTR JOB (AYL59FL,124), 'FEIKE LEIJ', MSGCLASS=P,
// NOTIFY=AYL59FL, MSGLEVEL=(1,1), REGION=1024K, TIME=(1,59)
/*ROUTE PRINT RMT4
/*JOBPARM LINES=10
//STEP1 EXEC WATFIV
//WATFIV.SYSIN DD *
/JOB FEIKE.TIME=(5).PAGES=60
      INTEGER I,J,K,NUMX/11/,NUMY/11/,UP/50/
     REAL ARG1, ARG2, CLEFT/1./, CRIGHT/0.5/, CZERO/1./, CIN/0.25/
     REAL B(21), C(21), CON(21,21), D(21), DL/8./, DT/1.6/
     REAL XPOS(21), YPOS(21), VELO/0.40/
     REAL DELX/60./,DELY/30./,DUM,NOEM(400),TERM1,TERM2
     REAL TIME, FACT(100), HELP(100), NO/0.0/
     REAL ROOT(100), STU(21), LOTERM(100), TRTERM(100)
      REAL DELTIM/500./, TIMMAX/3000./, UPR/50./
C
C VARIABLES
C
     NUMX
               : NUMBER OF NODES IN X-DIRECTION
C
               : NUMBER OF NODES IN Y-DIRECTION
     NUMY
C
               : ELUENT CONCENTRATION FOR X<0
     CLEFT
C
     CRIGHT
               : ELUENT CONCENTRATION FOR X>0
C
               : TOTAL SOLUTE CONCENTRATION
     CZERO
C
     CIN
               : INITIAL CONCENTRATION
C
               : LONGITUDINAL DISPERSION COEFFICIENT
                                                       L2/T
     DL
C
     DT
               : TRANSVERSE DISPERSION COEFFICIENT
                                                       L2/T
C
                                                        L/T
               : PORE WATER VELOCITY
     VELO
C
               : INCREMENT IN X-DIRECTION
                                                         L
     DELX
C
                                                         L
     DELY
               : INCREMENT IN Y-DIRECTION
C
     DELTIM
               : INCREMENT IN TIME
                                                         Т
C
              : MAXIMUM TIME FOR ANALYTICAL SOLUTION
     TIMMAX
C
     PRINT, 1 *
                                ANLOTR
                                                                 大 I
     PRINT, '*
     PRINT, 1 *
                ANALYTICAL SOLUTION OF THE ADVECTION-DISPERSION
                EQUATION FOR 2-D TRANSPORT IN A SEMI-INFINITE
     PRINT, 1*
     PRINT, '* MEDIUM WITH A STEP INPUT FUNCTION AND A 1-ST TYPE
                                                                 * I
     PRINT, 1*
                                                                 大 I
                     BOUNDARY CONDITION AT THE INLET
                                                                 * 1
     PRINT. '*
     C
C INITIALIZE COORDINATE SYSTEM
C
     XPOS(1)=0.0
     DO 10 I=2, NUMX
         XPOS(I)=XPOS(I-1)+DELX
  10
     CONTINUE
Ċ
     YPOS(1) = -0.5*(NUMY - 1)*DELY
     DO 20 K=2, NUMY
```

```
YPOS(K) = YPOS(K-1) + DELY
     CONTINUE
  20
C
C INITIALIZE POSITION DEPENDENT AND TIME INDEPENDENS VARIABLE
C
      DO 40 I=1, NUMX
          C(I)=VELO*XPOS(I)/DL
  40
      CONTINUE
C
      TIME=DELTIM
      WHILE (TIME.LE.TIMMAX) DO
C
C INITIALIZE POSITION AND TIME DEPENDENT VARIABLES
C
      DO 70 I=1, NUMX
         STU(I)=1.253314137*XPOS(I)/(UPR*(SQRT(DL*TIME)))
         B(I)=0.5*(XPOS(I)-VELO*TIME)/(SQRT(DL*TIME))
         D(I)=0.5*(XPOS(I)+VELO*TIME)/(SQRT(DL*TIME))
     CONTINUE
  70
C
C EVALUATE THE INTEGRAL
C
      DO 100 K=1, NUMY
         DO 90 I=2, NUMX
C
             TERM1=0.0
             DO 80 J=1,UP
                DUM = ((2*J-1)*1.570796327)/UPR
                ROOT(J) = COS(DUM)
                 FACT(J) = SORT(1.-ROOT(J))/(ROOT(J)+1.)
                LOTERM(J) = SQRT(2.*TIME*DL*(ROOT(J)+1.))
                TRTERM(J) = SORT(2.*TIME*DT*(ROOT(J)+1.))
                HELP(J)=0.5*TIME*VELO*(ROOT(J)+1.)
                ARG1=-((XPOS(I)-HELP(J))/LOTERM(J))**2
                ARG2=YPOS(K)/TRTERM(J)
                  TERM1=TERM1+0.5*STU(I)*FACT(J)*(CLEFT*EXF(ARG1,ARG2)+
                        CRIGHT*EXF(ARG1,-ARG2))
   80
             CONTINUE
             TERM2=CIN*(1.-0.5*(EXF(NO,B(I))+EXF(C(I),D(I))))
             CON(I,K)=TERM1+TERM2
         CONTINUE
   90
  100 CONTINUE
C SUPER IMPOSE INLET CONDITIONS
      DO 105 \text{ K}=1,\text{NUMY}
          IF (YPOS(K).LT.-0.00001) THEN
              CON(1,K) = CZERO
          ELSE IF (YPOS(K).GT.0.0001) THEN
              CON(1,K)=CIN
          ELSE
```

```
CON(1,K) = (CIN + CZERO)/2.
           ENDIF
 105
      CONTINUE
C
       PRINT, '
       PRINT, 'TIME=', TIME
C
       PRINT, ' '
       PRINT.'
                                                 X-COORDINATES'
       PRINT, ' '
 PRINT 113,' ',(XPOS(I),I=1,11)
113 FORMAT(' ',A8,11F8.3)
       PRINT 113, ' ', (XPOS(I), I=12, NUMX)
C
       PRINT, '
       DO 120 K=1, NUMY
          PRINT 112, YPOS(K), (CON(I,K), I=1,11)
 112
          FORMAT(' ',12F8.3)
          PRINT 114, ' ', (CON(I,K), I=12, NUMX)
          FORMAT(' ', A8, 10F8.3)
 114
 120
      CONTINUE
\mathbf{C}
      TIME=TIME+DELTIM
      ENDWHILE
C
      STOP
      END
C
      REAL FUNCTION EXF(Q,Z)
\mathbf{C}
      REAL LOEF, Q, Z, T, STUP1, STUP2, XX, YY, QQ, BOUND/100./
C
      EXF=0.0
      STUP1=ABS(Q)
      QQ=Q-Z*Z
      STUP2=ABS(QQ)
C
      IF (STUP1.GT.BOUND .AND. Z.LE.O.O) GO TO 40
      IF(Z.NE.O.) GO TO 31
      IF(Q.LE.-BOUND) THEN
           LOEF=0.
      ELSE
           LOEF=EXP(Q)
      ENDIF
      EXF=LOEF
      GO TO 40
  31 IF(STUP2.GT.BOUND .AND. Z.GT.0.0) GO TO 40
      IF(QQ.LT.-BOUND) GO TO 34
      XX = ABS(Z)
      IF (XX .GT. 3.0) GO TO 32
         T=1.0/(1.0+0.3275911*XX)
```

```
YY=T*(.2548296-T*(.2844967-T*(1.421414-
            T*(1.453152-1.061405*T)))
     GO TO 33
        YY=0.56418958/(XX+.5/(XX+.1/(XX+1.5/(XX+2./
 32
           (XX+2.5/(XX+1.)))))
 33 IF(QQ.LE.-BOUND) THEN
         LOEF=0.
     ELSE
         LOEF=EXP(QQ)
     ENDIF
     EXF=YY*LOEF
C
 34 IF (Q.LE.-BOUND) THEN
         LOEF=0.
      ELSE
         LOEF=EXP(Q)
      ENDIF
      IF(Z.LT.O.) EXF=2.*LOEF-EXF
C
     CONTINUE
 40
C
      RETURN
      END
/G0
```

```
//SSTR JOB (AYL59FL,124), 'FEIKE LEIJ', MSGCLASS=P,
// NOTIFY=AYL59FL, MSGLEVEL=(1,1), REGION=1024K, TIME=(1,59)
/*ROUTE PRINT RMT4
/*JOBPARM LINES=10
//STEP1 EXEC WATFIV
//WATFIV.SYSIN DD *
/JOB FEIKE, TIME=(5), PAGES=60
C
      INTEGER I, J, K, NUMX/11/, NUMY/49/, UP
      REAL CIN/0.0/, CON(11,49), CZERO/1.0/, DT/5./
      REAL XPOS(11), YPOS(49), VELO/50./, ARG(11,49)
      REAL DELX/5./, DELY/0.5/, NO/0.0/
C
C VARIABLES
C
             : NUMBER OF NODES IN X-DIRECTION
     NUMX
C
     YMUN
             : NUMBER OF NODES IN Y-DIRECTION
C
             : INITIAL CONCENTRATION
     CIN
C
     CZERO
             : TOTAL CONCENTRATION
C
             : PORE WATER VELOCITY
                                                     L/T
     VELO
C
             : TRANSVERSE DISPERSION COEFFICIENT
                                                     L2/T
     DT
C
             : SPACE STEP IN X-DIRECTION
                                                      L
     DELX
C
                                                      L
     DELY
             : SPACE STEP IN Y-DIRECTION
C
     PRINT, 1*
                                   SSTR
     PRINT, '*
                                                                  <del>*</del> 1
                ANALYTICAL SOLUTION OF THE ADVECTION-DISPERSION
     PRINT, '*
                 EQUATION FOR 2-D TRANSPORT IN A SEMI-INFINITE
     PRINT, '*
     PRINT, '* MEDIUM WITH A STEP INPUT FUNCTION AND A 1-ST TYPE
                  BOUNDARY CONDITION AT THE INLET, LONGITUDINAL
     PRINT, '*
                  DISPERSION IS IGNORED. STEADY-STATE APPROXIMATION *'
     PRINT, '*
     PRINT, '*
     C
C INITIALIZE COORDINATE SYSTEM
C
     XPOS(1)=0.0
      DO 10 I=2, NUMX
         XPOS(I) = XPOS(I-1) + DELX
  10
     CONTINUE
C
      YPOS(1)=-0.5*(NUMY-1)*DELY
      DO 20 K=2.NUMY
          YPOS(K) = YPOS(K-1) + DELY
  20
     CONTINUE
C
      DO 100 K=1, NUMY
        DO 90 I=2, NUMX
         ARG(I,K)=0.5*YPOS(K)/(SQRT((DT*XPOS(I))/VELO))
         CON(I,K)=0.5*CZERO*EXF(NO,ARG(I,K))+0.5*CIN*EXF(NO,-ARG(I,K))
  90
        CONTINUE
```

```
100 CONTINUE
C
C SUPER IMPOSE INLET CONDITIONS
      DO 105 K=1, NUMY
          IF (YPOS(K).LT.-0.00001) THEN
              CON(1,K) = CZERO
          ELSE IF (YPOS(K).GT.0.0001) THEN
              CON(1,K)=CIN
              CON(1,K)=(CIN+CZERO)/2.
          ENDIF
 105
      CONTINUE
C
      PRINT, '
      PRINT, ' X-COORDINATES'
      PRINT,
      PRINT 113, ' ', (XPOS(I), I=1, NUMX)
 113
     FORMAT(' ',A8,11F8.3)
C
      PRINT,
      DO 120 K=1, NUMY
         PRINT 112, YPOS(K), (CON(I,K), I=1, NUMX)
 112
         FORMAT(' ',12F8.3)
 120
      CONTINUE
C
C
      STOP
      END
C
      REAL FUNCTION EXF(Q,Z)
C
      REAL LOEF, Q, Z, T, STUP1, STUP2, XX, YY, QQ, BOUND/100./
C
      EXF=0.0
      STUP1=ABS(Q)
      QQ=Q-Z*Z
      STUP2=ABS(QQ)
С
      IF (STUP1.GT.BOUND .AND. Z.LE.O.O) GO TO 40
      IF(Z.NE.O.) GO TO 31
      IF(Q.LE.-BOUND) THEN
          LOEF=0.
      ELSE
          LOEF=EXP(Q)
      ENDIF
      EXF=LOEF
      GO TO 40
 31 IF(STUP2.GT.BOUND .AND. Z.GT.0.0) GO TO 40
      IF(QQ.LT.-BOUND) GO TO 34
      XX=ABS(Z)
```

```
IF (XX .GT. 3.0) GO TO 32
        T=1.0/(1.0+0.3275911*XX)
         YY=T^*(.2548296-T^*(.2844967-T^*(1.421414-
             T*(1.453152-1.061405*T))))
     GO TO 33
       YY=0.56418958/(XX+.5/(XX+.1/(XX+1.5/(XX+2./
  32
            (XX+2.5/(XX+1.)))))
  33 IF(QQ.LE.-BOUND) THEN
          LOEF=0.
      ELSE
          LOEF=EXP(QQ)
      ENDIF
      EXF=YY*LOEF
C
  34 IF(Q.LE.-BOUND)THEN
          LOEF=0.
      ELSE
          LOEF=EXP(Q)
      IF(Z.LT.O.) EXF=2.*LOEF-EXF
C
      CONTINUE
  40
C
      RETURN
      END
/G0
```

