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Project Summary

Plume 3D: Three-Dimensional Plumes in Uniform Ground Water Flow

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A closed-form analytical solution for three-dimensional plumes was incorporated in an interactive computer program. The assumption of an infinite aquifer depth and uniform source mass rate and source location was overcome by using the principal of superposition in space and time. The source code was written in a subset of FORTRAN 77 and can be compiled with FORTRAN IV, FORTRAN 66 as well as FORTRAN 77. As a result, the code is nearly independent of hardware and operating system.

This Project Summary was developed by EPA's Robert S. Kerr Environmental Research Laboratory, Ada, OK, to announce key findings of the research project that is fully documented in a separate report of the same title (see Project Report ordering information at back).

Introduction

The full document describes a mathematical model and the associated computer program that can be used to estimate concentration and distributions in a leachate plume which emanates from one or more point sources. The model includes both linear adsorption and first-order reactions.

The use of the computer program is fairly simple but represents only one tool which can aid in the analysis and understanding of ground-water contamination problems. The user must select the appropriate tools for the problem at hand, based on a sound understanding of the principles of ground-water hydrology, the physical problem, and the assumptions and limitations of the mathematical model.

Model Formulation

The differential equation describing the conservation of mass of a component in a saturated, homogeneous aquifer with uniform, steady flow in the x-direction can be written as

$$R_d \frac{\partial C}{\partial t} + V^* \frac{\partial C}{\partial x} = D_x^* \frac{\partial^2 C}{\partial y^2} + D_z^* \frac{\partial^2 C}{\partial z^2} - R_d \lambda C \quad (1)$$

where

C =	component mass per unit of fluid phase	M/L^3
D_x^* =	dispersion coefficient in x-direction	L^2/t
D_y^* =	dispersion coefficient in y-direction	L^2/t
D_z^* =	dispersion coefficient in z-direction	L^2/t
R_d =	retardation coefficient	
V^* =	average interstitial velocity in x-direction	L/t
x,y,z =	rectangular coordinates	L
λ =	first-order decay constant	$1/t$

The retardation coefficient accounts for partitioning of the component between the fluid and solid phases using a linear adsorption isotherm and is defined as

$$R_d = 1 + \frac{\rho_B}{\theta} K_d \quad (2)$$

where

ρ_B =	bulk density of the aquifer	M/L^3
θ =	effective porosity	
K_d =	distribution constant for a linear adsorption isotherm	$\frac{M/M}{M/L^3}$

A closed-form analytical solution to Equation 1 for an infinite aquifer with a continuous point source of strength M_0 at the origin can be written as (Hunt, 1978; Turner, 1972)

$$C_c = \frac{M_0 \exp\left(\frac{1}{2}\frac{V^*x}{D_x^*}\right)}{8\pi\theta R \sqrt{D_y D_z}}$$

$$\left\{\exp\left(\frac{1}{2}\frac{RU}{D_x}\right) \operatorname{erfc}\left(\frac{1}{2}\frac{R_d R + Ut}{\sqrt{R_d D_x^* t}}\right)\right.$$

$$\left. + \exp\left(-\frac{1}{2}\frac{RU}{D_x^*}\right) \operatorname{erfc}\left(\frac{1}{2}\frac{R_d R - Ut}{\sqrt{R_d D_x^* t}}\right)\right\} \quad (2)$$

where

$$R = \left[x^2 + \frac{D_x^*}{D_y^*} y^2 + \frac{D_x^*}{D_z^*} z^2\right]^{1/2} \quad (3)$$

and

$$U = V^*\left(1 + \frac{4 D_x^* R_d \lambda}{V^{*2}}\right)^{1/2} \quad (4)$$

The steady-state solution for a continuous point source is (Hunt, 1978)

$$C_{c,\infty} = \frac{C_0 Q}{4\pi\theta R \sqrt{D_y^* D_z^*}} \exp\left(\frac{1}{2}\frac{V^*x}{D_x^*} - \frac{UR}{D_x^*}\right) \quad (5)$$

Equations 2 and 5 can be used to calculate the concentrations in a leachate plume under the following assumptions and limitations:

1. The ground-water flow regime is completely saturated.
2. All aquifer properties are constant and uniform throughut the aquifer.
3. The ground-water flow is horizontal, continuous, and uniform throughout the aquifer.
4. The aquifer is infinite in extent.
5. The leachate source is a point located at the origin of the coordinate system.
6. The mass flow rate of the source is constant.
7. At zero time the concentration of leachate in the aquifer is zero.

The assumptions of an infinite aquifer depth and a uniform source mass rate can be overcome by using the principles of superposition in space and time, respectively (Walton, 1962). Both of these provisions have been incorporated in the computer program developed in this project. Superposition is also used to include multiple sources.

Computer Program

The closed-form analytical solutions for the two-dimensional plumes as presented above have been incorporated in an interactive computer program. The source code has been written in a subset of FORTRAN 77 and can be compiled with FORTRAN IV, FORTRAN 66, as well as FORTRAN 77 compilers. As a result, the code is almost entirely independent of hardware and operating systems. Those changes that may be required to implement the code on a given system, such as assigning logical devices, are clearly identified.

The program has been developed for interactive use and requires input data under two modes of operation—"Basic Input Data" and "Edit." The basic input data listed in Table 1 are required to initiate a new problem. The user is prompted for the required data through a series of input commands.

Table 1. *Input Data Required for the Analytical Three-Dimensional Plume Model*

Title - Units for length, time, and concentration
Saturated thickness (for aquifer of finite depth)
Effective porosity
Ground water interstitial velocity
Retardation coefficient
Longitudinal dispersion coefficient
Transverse dispersion coefficient
Vertical dispersion coefficient
First-order decay constant
Type of solution (transient or steady-state)
Number of sources
Location and rate schedules for each source
Coordinates of observation points
Observation times (for transient solution)

Once the basic input data have been entered, the problem as currently defined is listed and the program enters the "edit" mode. The two character edit commands listed in Table 2 can be used to redefine the problem, run the calculations, and terminate the program.

The program has been written to require a minimum of machine resources and will run on both 8 and 16 bit microcomputers under CP/M, MS-DOS, and PC-DOS as well as larger minicomputers and mainframe machines.

Summary

The models and computer codes developed in this project are intended to serve as additional tools in the analysis of ground-water contamination problems. The user must select the best tool for the problem at hand based on a sound understanding of the principles of ground-water hydrology, the physical problem, and the limitations of the mathematical model(s). Unfortunately, these computer programs cannot substitute for an understanding of the processes and mechanisms of solute transport in ground-water systems or sound judgement based on training and experience.

Table 2. *Edit Commands*

Command	*Variable changed/Execution*
ST	*Saturated Thickness*
PO	*Porosity*
VX	*New Seepage Velocity*
RD	*Retardation Coefficient*
DE	*Decay Constant*
DX	*X-Dispersion Coefficient*
DY	*Y-Dispersion Coefficient*
DZ	*Z-Dispersion Coefficient*
RT	*Source Rate Schedule*
OB	*Observation Points*
XC	*X-Coordinates*
ZC	*Z-Coordinates*
YC	*Y-Coordinates*
TC	*Observation Times*
AS	*Aquifer Sectioning*
CS	*Change Solution/Sources*
MU	*Menu of Edit Commands*
LI	*List input data*
RN	*Run*
NP	*New Problem*
DN	*Done*

References

Hunt, B., 1978, "Dispersive Sources in Uniform Ground-Water Flow," *Journal of The Hydraulics Division, ASCE, Vol. 104, No. HY1*, pp. 75-85.

Turner, G. A., 1972, *Heat and Concentration Waves*, Academic Press, New York, New York, 233 pp.

Walton, W. C., 1962, "Selected Analytical Methods for Well and Aquifer Evaluation," Bulletin 49, Illinois State Water Survey, Urbana, Illinois, 81 pp.

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The complete report, entitled "PLUME 3D: Three-Dimensional Plumes in Uniform Ground Water Flow," (Order No. PB 85-214 443/AS; Cost: $11.50, subject to change) will be available only from:

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