Computer Simulation of Waste Transport in Groundwater Aquifers

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IN GROUNDWATER AQUIFERS

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ABSTRACT

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A computer simulation of the convective-dispersive process of the movement of pollutants in groundwater systems was developed and tested for several conditions. An implicit numerical technique was used to solve the flow equation and the method of characteristics used to solve the convective-dispersion equation.

The model was tested by applying it to longitudinal dispersion problem and the longitudinal and lateral dispersion problem. The tensorial nature of the dispersion coefficient was demonstrated by solving a problem in the rotated coordinate system. The model was successfully used to solve the salt-water interface problem.

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INTRODUCTION

Description of Problem

The rapid growth of the world's population is placing an ever increasing demand upon fresh water supplies. This has resulted in groundwater becoming an important water supply in many regions. Efficient management of groundwater aquifers will require an understanding of the water quality problems created by sea water intrusion, recharge of surface water into aquifers, underground waste disposal, and interaction between groundwater aquifers and adjacent surface streams.

Since pollutants, wastes, and recharge waters are normally miscible with the native groundwater an understanding of the mechanics of miscible fluid displacement is necessary for the analysis of groundwater quality problems. The desired end result of such an analysis is the prediction of the concentration of wastes as they move through an aquifer, and their ultimate effect on the waters of adjoining lands or streams. The concentrations are dependent upon the magnitude and distribution of flow velocities within the porous medium, upon the geometry of the porous structure, and upon the nature of the waste material (i.e., time of decay for radionuclides). The mixing of the wastes in groundwater is greater

than can be accounted for by molecular diffusion and has been dubbed dispersion by Scheidegger (1954).

A complete description of this work may be found in "Dispersion in Ground Water Flow Systems" by D. L. Reddell, Ph.D. Dissertation, Colorado State University, December 1969.

Purposes and Objectives

Many basic studies have been conducted to explain the physical relationships of the dispersion process [Bear (1961), Scheidegger (1961), Bearn and Bachmat (1967), Hoopes and Harleman (1965) . These studies have resulted in analytical and approximate solutions for simple flow problems with simple boundary conditions. However, no analytical solutions have been obtained which will adequately describe groundwater quality problems on an aquifer wide basis.

Because of the rapid advances in digital computer technology, an opportunity exists for simulating complex flow problems on the digital computer. The objective of this study is to develop a computer simulation for the mass transport of a waste product miscible with the native groundwater. The theory is developed for three-dimensional, nonhomogeneous, unsteady flow fields, with density and viscosity variations between the waste and groundwater. However, the simulation is tested for only two-dimensional flow problems and onisotropic mediums are not investigated.

PROCEDURE

The techniques of investigation are entirely computer oriented. No attempt is made to obtain experimental results. The basic differential equations are derived in their most general form. This reduces the number of assumptions which are ordinarily used. Thus, the variation of such parameters as porosity, permeability, fluid pressure, fluid density, fluid viscosity, and dispersion coefficients are all considered.

The basic differential equations were then written in finite difference form and numerical techniques developed for solving the set of equations on the computer. The reliability of the computer simulation was checked by comparison with known analytical solutions of some simple problems.

RESULTS

Differential Equations

When working with waste transport, it is necessary to require the conservation of mass for each component present. In this study, only two components were considered, a waste material and the native groundwater. Therefore, two equations of mass conservation are required to describe the system. One of these equations will be for the combined masses of both components (i.e., waste + groundwater) and the other equation will be for the waste material only.

A fundamental flow equation for the mixture of miscible fluids is derived by combining the conservation of mass equation for the mixture, Darcy's law, and an equation of state describing the pressure volume-temperature-concentration relationship. The result is an equation involving two dependent variables, pressure and concentration. Using shorthand tensor notation, this equation may be expressed as:

$$\frac{\partial}{\partial x_i}\left[\frac{\rho \Delta A_i}{\mu} K_{x_i}\left(\frac{\partial p}{\partial x_i}+\rho g\frac{\partial h}{\partial x_i}\right)\right]\Delta x_i = \rho\phi\Delta V\left(\beta+c_f\right)\frac{\partial p}{\partial t}+\delta\phi\Delta V\frac{\partial c}{\partial t}+\rho Q\cdots(1)$$

where

$\Delta x_i \ (i=1,2,3)$ = dimensions of volume element,

$\Delta A_i \ (i=1,2,3)$ = cross-sectional area of element perpendiular to

ΔV = volume of element = $\Delta X, \Delta X, \Delta X$

$x_i \ (i=1,2,3)$ = cartesion coordinate system

t = time

ρ = fluid density at reservoir conditions

K_{Xi} = absolute permeability in X_i direction,

μ = viscosity of fluid mixture of reservoir conditions,

P = pressure of fluid mixture at reservoir conditions,

g = acceleration of gravity,

h = elevation of volume element,

ϕ = reservoir porosity,

β = fluid compressibility,

C_f = formation compressibility factor,

α = proportionality factor relating concentration and density,

C = concentration of waste material in native groundwater,

ρ_p = mass density of any produced fluid, and

Q = production terms with units of L^3/T and is positive when a sink and negative when a source.

To obtain Eq. 1 in its present form the following assumptions have been made: (1) Darcy's law is applicable, (2) single phase flow (3) isothermal flow, (4) a linear relationship between porosity and pressure, (5) size of volume element does not vary with time, and (6) a linear relationship between density, pressure, and concentration.

Another equation may be obtained by combining the conservation of mass equation for the waste material, Frick's law, and an equation of state. This equation is given by:

$$\frac{\partial c}{\partial t} = \frac{\rho}{\phi \Delta A_i (\rho - \alpha c)} \frac{\partial}{\partial x_i}\left[(D_{ij} + D_d T_{ij})\phi \Delta A_i \frac{\partial c}{\partial x_j}\right] - V_i \frac{\partial c}{\partial x_i} \left(\frac{\rho c_p - c \rho_p}{\rho - \alpha c}\right) \frac{Q}{\phi \Delta V} \quad \cdots (2)$$

where D_{ij}' = dispersion coefficient which is a second rank tensor,

D_d = molecular diffusion coefficient,

T_{ij} = a porous media "tortuosity" factor which is also a second rank tensor,

V_i = seepage velocity of fluid mixture in i^{th} direction,

C_p = concentration of waste in produced fluid, and

all other terms are as described previously.

Assumptions necessary to obtain Eq. 2 are: (1) diffusion is described by Frick's law, (2) the convective mixing called dispersion may be described by a Frickian process, (3) single phase flow, and (4) compressibility effect on concentration are neglected. The double summation convention of tensors is implied in the use of Eq. 2. Also, it might be noted from a practical point that $D_{ij} + D_d T_{ij}$ is a parameter determinted in the field just like permeability or porosity. For this reason it is sometimes referred to as the hydro-dynamic dispersion coefficient and given the single designation D_{ij}'.

Because of the interrelationship among several of the parameters, the following additional equations are also used:

$$V_i = -\frac{k x_i}{\mu \phi}\left[\frac{d p}{d x_i} + \rho g \frac{d h}{d x_i}\right] \quad \ldots \ldots \ldots \ldots \ldots \ldots (3)$$

$$\phi = \phi_{org}\left[1 + C_f (p - p_{org})\right] \quad \ldots \ldots \ldots \ldots \ldots (4)$$

$$\rho = \rho_{org} + \beta \rho_{org}(p - p_{org}) + \alpha(c - c_{org}] \quad \ldots \ldots \ldots \ldots (5)$$

$$\mu = \mu_{org} + \lambda(c - c_{org}) \quad \ldots \ldots \ldots \ldots \ldots (6)$$

where org = subscript referring to original value,

λ = proportionality factor relating concentration and viscosity, and

all other terms are as previously described.

Computer Simulation

The task of finding a suitable numerical approximation to the convective-dispersion process has been a particularly difficult task. Eq. 1 is a typical second-order equation of parobolic type and has been successfully treated by numerical methods. Neglecting the convective terms of Eq. 2, it would also be a second order equation of parobolic type. However, if the dispersion terms in Eq. 2 are neglected, then the convective transport portion is a first-order equation of hyperbolic type, and has been treated numerically with some success in one dimension. However, extension of two or more dimensions has proven difficult. Usually one of two things happens: (1) the numerical solution develops oscillations or (2) it becomes smeared by artificial dispersion resulting from the numerical process. When transport and dispersion are considered simultaneously, this numerical dispersion may dominate the low physical dispersinity which characterizes miscible displacement.

A technique introduced by Gardner et.al. (1964) is used as the basic numerical scheme for solving Eq. 2. They did not consider the tensorial nature of the dispersion coefficient which adds some difficulty to the problem.

The region of interest is broken up into the usual grid network. In addition to this, a set of moving points is also introduced. Each moving point has associated with it a concentration, which

varies with time. To begin the simulation, an implicit finite

difference form of Eq. 1 is written for each grid in the region.

Initial values of ρ, μ, C and ϕ are used and a Gauss-elimination

matrix solver is used to obtain new values of the pressure at

time $t+\Delta t$. These values of pressure are then used in Eq. 3 to

obtain values for the seepage velocity. Then each moving point

is moved to a new location, using the local velocity and time

increment. Each grid is investigated for all moving points located

within its boundaries, and is assigned a concentration equal to the

arithmetic average of the moving points inside it. The effect of

dispersion is obtained by neglecting the convective terms of Eq. 2

and writing an explicit finite difference form of the remaining

dispersion terms. The change in concentration due to dispersion

in each grid is then added to each of the moving points located

within that particular grid. This gives the new concentration

at $t+\Delta t$.

The effects of the change in pressure and concentration are

then used to obtain new values of $\phi, \rho,$ and μ from Eqs. 4, 5, and 6.

The process is then repeated by solving Eq. 1 again for the new

pressures at $t+2\Delta t$, moving the points, getting average con-

centrations, and correcting for dispersion. In this manner the

solution is advanced step by step into time.

Careful evaluation of the numerical errors involved in

the above numerical technique has shown accuracies which exceeded

original expectations. With as few as two to four moving points

per grid, excellent results have been obtained. Increasing the

number of moving points beyond four, appears to have little effect

on the results. Although rigorous proof of convergence and stability was not obtained for the combined numerical simulation, trial runs indicate that as the space dimensions and time increment approach zero, the solution tends to approach more closely those given by the available analytic solutions. A stability criterion was developed for the explicit solution of the dispersion effect, and it appears that as long as these stability requirements are met, the overall solution is stable.

It is apparent from these calculations that the treatment of the dispersion coefficient as a second rank tensor improves the solution. The amount of improvement is not available at this time. However, for long periods of time, use of the tensor form of the dispersion coefficient may be very important. Additional work will be done in this area.

SUMMARY AND CONCLUSIONS

A computer simulation sequence is presented which enables rational predictions of contominant concentrations moving through groundwater aquifers. Throughout the analysis, major emphasis has been placed on realistically evaluating actual situations. The groundwater aquifer is assumed heterogeneous with respect to permeability and porosity, treatment of the dispersion coefficient as a second rank tensor is maintained, and the effects of changes in density, viscosity, and concentration are introduced into the system. A brief description of the computer simulation is given.

Such a flexible approach should contribute to the much needed progress toward a detailed analysis of waste transport in groundwater aquifers. It is recommended that work begin immediately on applying these developments to a field situation to determine the merits of this computer simulation in a field condition.

REFERENCES

Bear, Jacob, 1961, "On The Tensor Form of Dispersion in Porous Media", _Journal of Geophysical Research_, Vol. 66, No. 4, April 1961, pp. 1185-1198.

Bear, Jacob and Y. Bachmat, 1967, "A Generalized Theory of Hydrodynamic Dispersion in Porous Media", _Pub. No. 72_, International Association of Scientific Hydrology, Symposium of Haifa, March 1967, pp. 7-16.

Gardner, A. O., D. W. Peaceman, and A. L. Pozzi, Jr., 1964, "Numerical Calculation of Multidimensional Miscible Displacement by the Method of Characteristics", _Journal of the Society of Petroleum Engineers_, March 1964, pp. 26-36.

Hoopes, J. A. and D. R. F. Harlemon, 1965, "Waste Water Recharge and Dispersion in Porous Media", _Technical Report No. 75_, Hydrodynamics Laboratory, M.I.T., June 1965, 166 pp.

Scheidegger, A. E., 1954, "Statistical Hydrodynamics in Porous Media", _Journal of Applied Physics_, Vol. 25, No. 8, August 1954, pp. 994-1001.

Scheidegger, A. E., 1961, "General Theory of Dispersion in Porous Media", _Journal of Geophysical Research_, Vol. 66, No. 10, October 1961, pp. 3273-3278.

PUBLICATIONS:

White, N. F. and D. K. Sunada, Ground Water Quality Study of
    Severence Basin, Weld County, Colorado, Civil Engineering
    Department CER 66NFW-DKS5, Colorado State University,
    April 1966 - 29p.

Reddell, D. L., Dispersion in Ground Water Flow Systems, Ph.D.
    dissertation, Colorado State University, Fort Collins,
    Colorado, Dec. 1969, 225 pp.