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Predicting the quality of waste-disposal seepage for desalination treatment*

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SYNOPSIS

Methods for the prediction of seepage quality from waste-disposal facilities are evaluated for input to the design of desalination treatment facilities. This is done by reference to a waste dump seeping into a near-surface aquifer, the contaminated seepage being collected by scavenger wells. As the quality of contaminated water intercepted by the wells will vary with both space and time, it is necessary for predictive methods to accommodate such variations.

One-dimensional and two-dimensional predictive solute transport models are described and applied to the seepage and scavenger-well example mentioned above. The advantages and disadvantages, in terms of overall applicability, data requirements, and possible accuracy, are described and discussed. While one-dimensional models have the advantages of speed, simplicity, and cost, the frequent requirement of prediction in both space and time necessitates more complex, two-dimensional simulation.

SAMEVATTING

Metodes om die syferwaterkwaliteit van uitskotfasiliteite to voorspel word ge-evalueer met die doel om die resultate te gebruik as 'n inset in die ontwerp van ontsoutingsaanlegte. Die metodes word toegepas op die voorbeeld van 'n uitskothoop waarvan die afloopwater deursyfer na 'n naby-oppervlakte akwifeer. Die besoedelde water word onttrek deur ontrekkingsboorgate. Aangesien die kwaliteit van die water wat so onttrek word varieer met tyd en posisie is dit nodig vir die metodes om hierdie variasies te voorspel.

Een- en tweedimensionele modelle wat die beweging van opgeloste stowwe voorspel word bespreek en toegepas op die bostaande syfering- en ontrekkingsvoorbeeld. Eendimensionele modelle het die voordele van spoed, eenvoudigheid en koste, maar die noodsaaklikheid om posisionele- en tydsvariasies te voorspel verg die gebruik van die meer komplekse tweedimensionele model.

INTRODUCTION

It is expected that, by the turn of the century, South Africa's water usage for domestic, agricultural, municipal, and mining needs will increase by over 200 per cent. Without careful management and more efficient utilization, demand will exceed the supply. Drought conditions have amplified concern about the increased uncontrolled use of water and water pollution resulting from agricultural, industrial, and mining activities. This concern has led to a proliferation of legislation pertaining to the use of water and the disposal of effluents. In future, the common practice of effluent disposal by evaporation will be phased out, and the installation of facilities for desalination treatment will be required.

A major area of concern is the treatment of seepage from gold-tailings dams, ash-disposal areas, dumps of coal-washery discards, and spoil piles from open-cast coal mining. The prediction of seepage quality from these disposal areas for desalination treatment is a complex but very necessary first step in the design of any proposed treatment facility.

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The object of this paper is to present methods for the prediction of seepage quality from waste-disposal facilities. The predictions given here are based on seepage from a waste dump discharging into a near-surface groundwater aquifer and the interception of the resultant contaminated groundwater by a system of scavenger wells. The collected water is considered to be sufficiently contaminated that discharge as effluent is unacceptable, and hence desalination is required. The system to be considered is illustrated schematically in Fig. 1.

It is anticipated that the quality of the effluent from the scavenging wells will vary both with time and well discharge rate. In addition, the quality of seepage arriving at the well will be a function of the initial seepage modified by the effects of advection, dispersion, and attenuation during the transport of the solute from the dump to the well.

The paper addresses the fundamentals of the processes affecting the solute concentrations in the seepage and, given such processes, discusses predictive methods for the estimation of water quality by the use of solute-transport models.

FUNDAMENTALS OF SOLUTE TRANSPORT

Usually, the dominant process of solute transport is that of advection. This is where solutes are carried by the bulk motion of flowing groundwater, itself a function of hydraulic head differentials and material permeabilities. During advective motion, there are two major processes that cause a decrease in the concentrations of solutes in seepage. These are hydrodynamic dispersion and

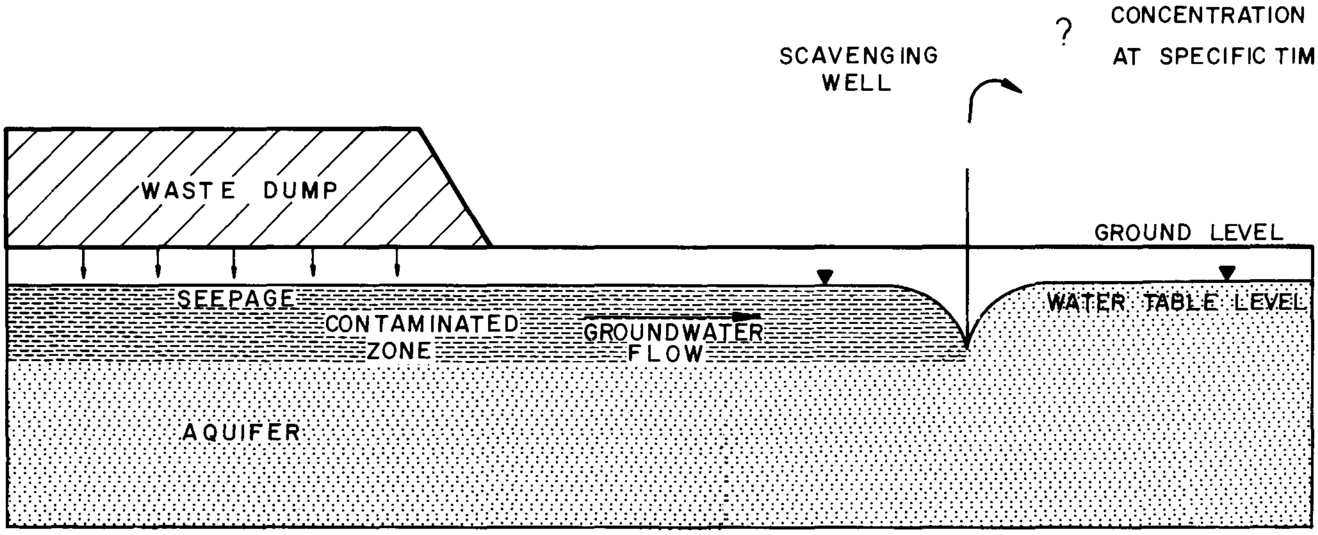

Fig. 1—Illustrative system for the prediction of seepage quality at a scavenging well

hydrogeochemical attenuation.

Hydrodynamic Dispersion

Hydrodynamic dispersion can be sub-divided into two processes:

- molecular diffusion (otherwise known as ionic diffusion), due to the thermo-kinetic energy of the solute species themselves; and
- mechanical dispersion, due essentially to the physical nature of groundwater flow.

Molecular Diffusion

Molecular diffusion is the process in which ionic or molecular constituents move by kinetic activity in the direction of their concentration gradient. Diffusion can occur in the absence of any bulk hydraulic movement of water and ceases only when concentration gradients become non-existent.

The mass of diffusing substance passing through a given cross-section per unit time is proportional to the concentration gradient and is known as Fick's First Law. It can be expressed as

$$F = -D\frac{dC}{dx},$$

where

F = mass flux, or mass of solute per unit area per unit time
D = diffusion coefficient
C = solute concentration
dC/dx = concentration gradient (a negative quantity in the direction of diffusion).

As diffusion coefficients for electrolytes in aqueous solutions are well known, the estimation of this quantity poses little problem.

In geological materials, these coefficients are significantly smaller than for aqueous solutions only, owing to the effects of the solid phase on flow distances. Termed the tortuosity, this will reduce the coefficient of molecular diffusion by approximately 50 per cent.

If D_1 is defined as the coefficient of hydrodynamic dispersion, then,

$$D_1 = ax_1 \bar{v} + D^*,$$

where

ax_1 = dynamic dispersivity of a given porous medium
$\bar{v}$ = average linear groundwater velocity
D^* = coefficient of molecular diffusion.

Mechanical Dispersion

Mechanical dispersion, a three-dimensional process that is most significant in the principal direction of groundwater flow, causes spreading of a seepage front, and hence dilution. It results from the following:

- differential velocity of groundwater in intergranular/interfracture spaces due to the drag effect of the rough edges of the solid particles;
- differential flow through rates due to the differences in the sizes of the actual pores in the porous medium, i.e. volume differences in interstitial pore space;
- differences in the flow length of different particles due to the tortuous nature of the flow in a porous medium, some particles taking a far longer path length, and hence time, to travel the same linear distance down hydraulic gradient.

The net result of the processes is dispersion. Dispersion in the longitudinal direction down hydraulic gradient towards the scavenging well is significantly larger than transverse dispersion, either vertically or laterally. Such dispersion causes a decrease in the concentrations of solutes in seepage as a result of dilution.

Hydrogeochemical Attenuation

The term *attenuation* is used for a number of processes, which are mainly chemical but can be physiochemical and biochemical, that can change the concentration of solutes by reaction with either the solid aquifer material or the existing interstitial water in the porous medium. The reactions between the solid phase and the solute, essentially transfer processes, are likely to be of prime importance in a saturated medium, unless there is a great difference between the interstitial groundwater and a solute plume passing through the aquifer. Hydrogeochemical attenuation processes can be subdivided into a large range of reactions, but these can be essentially grouped as follows:

- acid–base (neutralization) reactions
- dissolution–precipitation reactions (which can be pH dependent)
- co-precipitation reactions
- absorption–desorption reactions
- oxidation–reduction (redox) reactions
- ion-exchange or ion-fixation reactions
- chemical complexation
- radioactive decay (applicable only to radiogenic species).

Attenuation is a fundamental concept of solute removal. Therefore, in any determination of the actual, residual downstream concentration at a scavenging well of any solute discharged from a waste-disposal facility, it is important to assess the total attenuation of the aquifer materials through which solutes will be transported.

PREDICTIVE METHODS FOR SEEPAGE QUALITY

The fundamental processes that would affect seepage quality from the base of a waste-disposal facility to a scavenging well have been discussed briefly, and it is appropriate to return to the application of predictive models to the illustrative system given in Fig. 1. This diagram and variations of the diagram will be used to show three different types of predictive solute transport models. A particular example of each of these models is described, and each model is applied to an illustrative system, with an account of its data input requirements, model constraints, and output.

Model 1: One-dimensional Analytical Model ADVTAT

Fig. 2 illustrates the case of one-dimensional flow from a waste dump to a well. Seepage from the dump is being carried to the well at a finite rate, and during the process the concentration of dissolved species in the seepage is being modified. The concentration of any particular constituent arriving in the scavenging well will vary with time. At some stage, the concentration may reach a stable, steady-state condition. The one-dimensional model, ADVTAT, allows this varying concentration with time at the scavenging well to be predicted.

Basis of the Model

The ADVTAT model is based on the equation of Ogata and Banks[1] for one-dimensional advective/dispersive flow in a porous medium. The equation is

$$\frac{C}{C_o} = \tfrac{1}{2}\left[erfc\left(\frac{L - \bar{v}t}{2\,D_L T}\right) + \exp\left(\frac{\bar{v}_L}{D_L}\right) erfc\left(\frac{L + \bar{v}t}{2\,D_L T}\right)\right],$$

where

C = present concentration of solute
C_o = original concentration of solute
L = longitudinal distance along the flow path
$\bar{v}$ = average linear groundwater velocity
t = simulation time
D_L = coefficient of longitudinal dispersion
$erfc$ = complementary error function.

In most practical cases, the simulation time, t, or the flow path, L, are large, and hence the value of the third term in the equation becomes very small.

The Ogata–Banks equation has been modified by Diering and Smith[2] to include the effects of hydrogeochemical attenuation by the addition of a retardation factor (R). This relates the relative velocity of the attenuated or retarded species to the average linear groundwater velocity, i.e.

$$R = \frac{V}{V_c},$$

where

V = average linear groundwater velocity
V_c = velocity of retarded species.

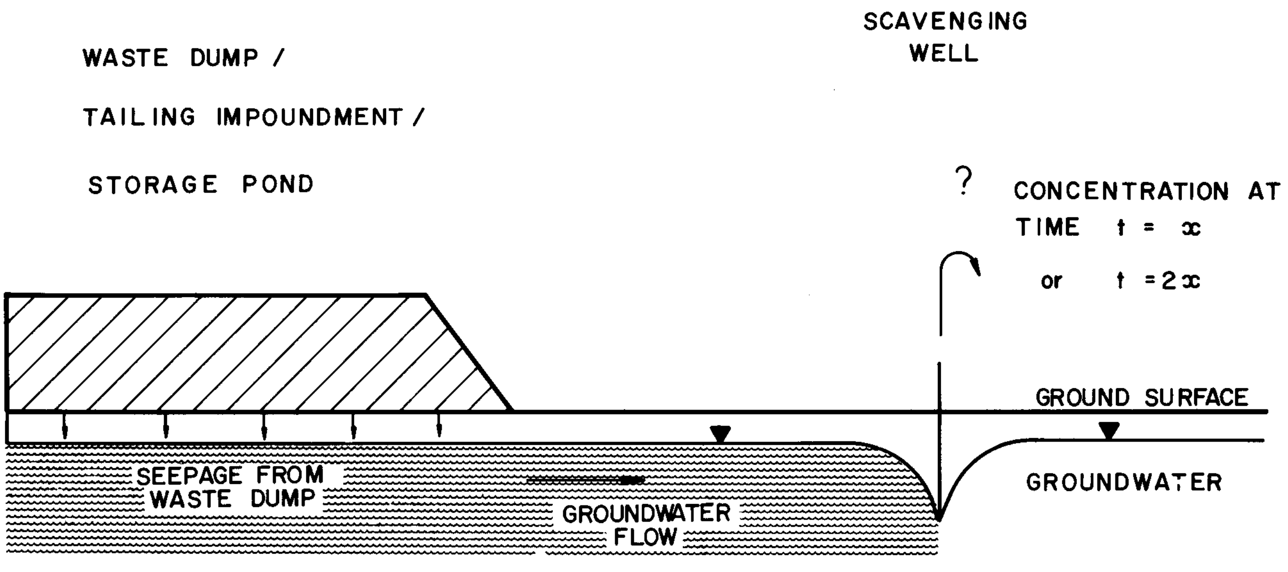

Fig. 2—Model 1: A one-dimensional solute-transport model—ADVTAT

The relative velocity, V/V_c, is related to the estimated hydrogeochemical partition coefficient, K_d, by the following equation:

$$\frac{V}{V_c} = 1 + \frac{P_b}{n} \cdot K_d,$$

where

P_b = bulk density of solid phase
n = porosity of solid phase
K_d = partition coefficient.

The following are typical input parameters, together with their possible derivations:

- bulk density and porosity—a geotechnical testing programme;
- partition coefficients—attenuation testing programme;
- flow path—physical measurement to a downstream control point, i.e. the scavenging well;
- velocity—hydraulic gradient (maximum value) and permeability from field or laboratory measurements;
- dispersivity—based on literature values and previous experience of model calibrations by the use of historic data;
- simulation time—as required.

Model Output

The model output comprises a listing of the actual concentration relative to the initial concentration for a solute in the seepage at a specific line at the scavenging well. This can be plotted automatically on a graph of concentration versus flow distance for any specific time interval, as shown in Fig. 3. The expected concentrations for any particular parameter can be predicted and these data used as input to the design of desalination plants and their operating parameters.

A one-dimensional, analytical model such as ADVTAT has the advantage of being simple and relatively straightforward to use. It is limited, however, in that it can deal only with saturated flow in one dimension in a homogeneous medium. It is often necessary to be able to ascertain concentrations in more than one dimension, i.e. spatially, and hence two- or three-dimensional models are required.

Two-dimensional Models

Two-dimensional models and their application to the prediction of solute concentration are given as Models 2 and 3 below. Three-dimensional models of solute transport are not appraised in this paper. In general, the data requirements for three-dimensional models are so severe that few practical situations can meet such requirements, and hence their general practical applicability is questionable.

Model 2: A Two-dimensional Finite-difference Model, AQUISOL

Fig. 4 is a representation in plan of seepage from a waste dump to a line of scavenging wells. It is apparent that the concentration of species arriving at each well may be different. Hence, there is a variation in concentration spatially, as well as in time. A two-dimensional predictive model is therefore required that is capable of reproducing time-dependent variations in concentration. One such model is AQUISOL.

The AQUISOL model is based largely on the aquifer-simulation model of Prickett and Lonnquist[3], and the model of Prickett *et al.*[4], which is based on discrete-particle, random-walk solute transport.

AQUISOL is a finite-difference model, using a modified interactive alternating direction implicit method to solve the set of finite-difference equations. This is a form of the backward-difference formulation and, as such, is stable for all types of problems with, for instance, rapid changes in abstraction patterns, short- or long-period analysis, uneven time steps, and boundary effects (Rushton and Redshaw[5]).

The model can simulate one- or two-dimensional, non-steady groundwater flow in heterogeneous, anisotropic aquifers under unconfined, semi-confined, and confined conditions. Solute transport is simulated by the generation of a mass of discrete particles, each representing a specific mass of solute, which are transported by advection in the model. Dispersion is simulation by a random-walk procedure.

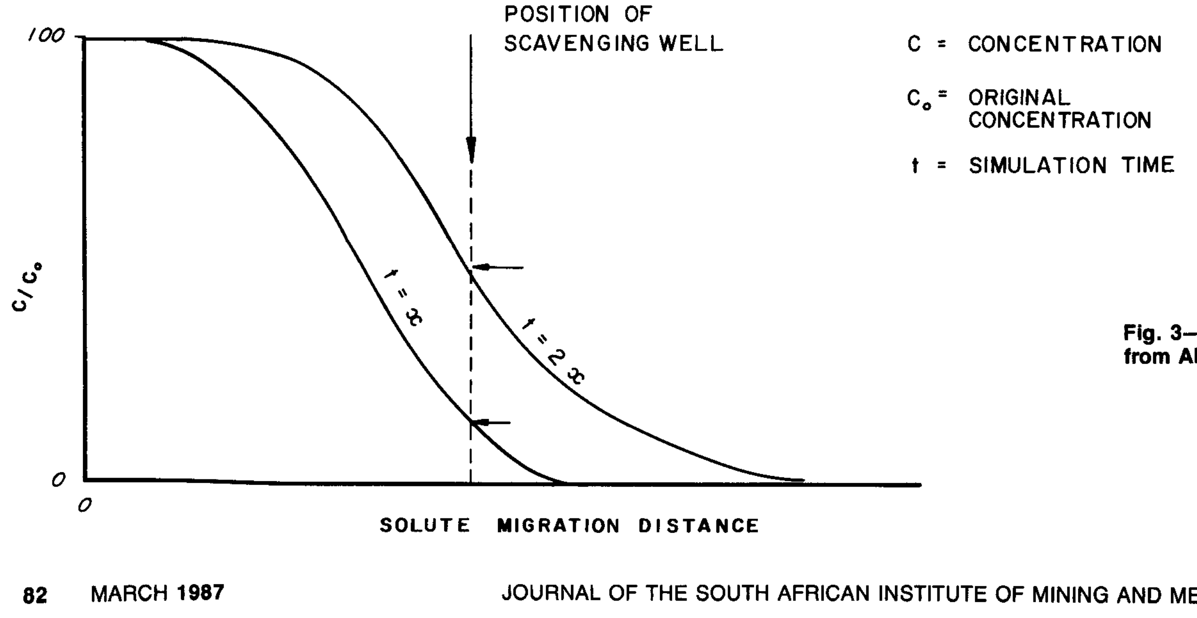

Fig. 3—The output from ADVTAT

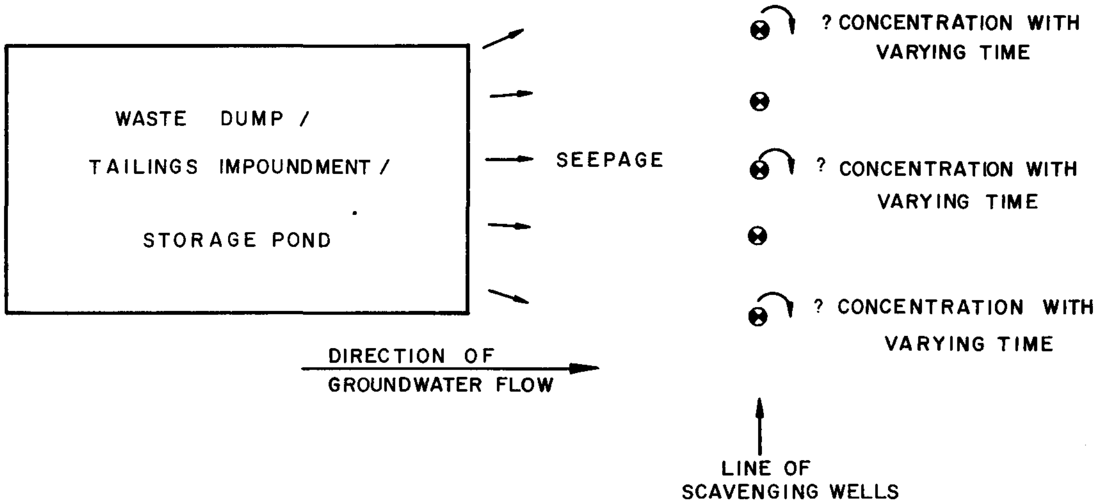

Fig. 4—Model 2: A two-dimensional (plan) solute-transport model—AQUISOL

The following features can be incorporated into the model:

- variable rate abstraction
- recharge
- induced recharge from a lake or stream
- evapotranspiration directly from a near-surface water table
- conversion from water table to confined or semi-confined conditions
- variable aquifer thicknesses
- variable hydraulic conductivity and storativity
- anisotropic hydraulic conductivity and transmissivity
- confined, semi-confined, and water-table conditions
- constant rate leakage through the base of an aquifer
- automatic data contouring for head distribution and concentration.

The program includes a predictor, which significantly accelerates convergence at each time step, thus economizing on the number of iterations required and reducing running costs.

The output for Model 2 would consist of piezometric head values at all nodes of the finite element grid, as well as concentration values at those nodes. The nodes corresponding to the positions of scavenger wells will give predicted effluent concentrations at those wells for the simulated time intervals. If required, these data can be contoured by the use of a subroutine, CPLOT.

Model 3: A Two-dimensional Finite-element Model, QSOL

In the third example of concentration prediction, the illustrative system is modelled in section rather than in plan. The difference between this model and Model 1 is that the vertical variation of seepage concentration in the aquifer is required, since there is vertical differentiation of species. Such a variation may affect the concentration of the seepage arriving at the scavenger well, particularly if the abstraction rate from these wells varies. Model 3, QSOL, is illustrated in Fig. 5, which indicates the requirement for a two-dimensional model capable of predicting transient concentration levels in a non-homogeneous concentration system.

QSOL is a general-purpose program, in that steady state or transient saturated flow, which is confined or unconfined, can be modelled. Non-homogeneous and anisotropic material can be modelled in plan or in section. Extraction or scavenger wells, as well as rainfall recharge or evaporation, can be modelled. QSOL is a Galerkin finite-element program that uses two-dimensional linear, isoparametric, quadrilateral elements. QSOL is written primarily for efficient execution on a 16-bit minicomputer, rather than on a main-frame computer. Numerous ancillary programs supplement QSOL with respect to mesh generation, plotting, and graphic output of results.

Various conditions of solute transport, together with adsorption or radioactive decay of solutes, can be model-

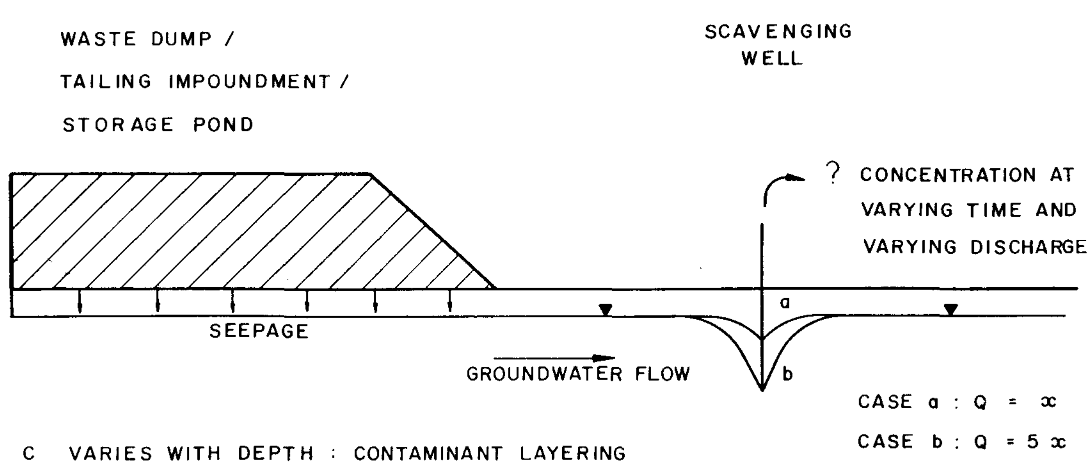

Fig. 5—Model 3: A two-dimensional (sectional) solute-transport model—QSOL

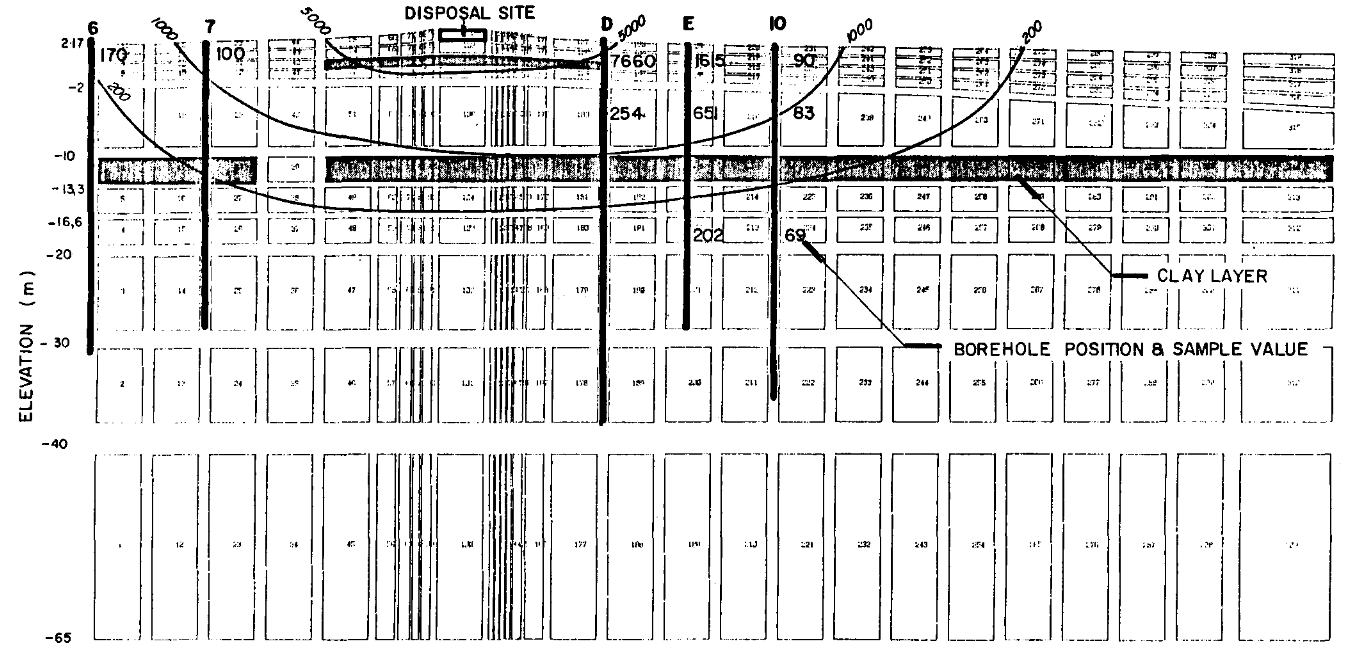

Fig. 6—A typical output from QSOL

led by use of the advective–dispersion equation.

Briefly, QSOL requires the region of interest of the aquifer to be subdivided into quadrilateral finite elements. The flow properties required for the elements include permeabilities, saturated thicknesses, initial heads, and leakage coefficients. Flow boundaries can be modelled as impermeable or as constant-head boundaries (i.e. permeable). At each time-step of the modelling process, output of fluid heads, flow velocities, and solute concentrations is provided at each node.

The equation, incorporating both seepage and solute transport, with areal, two-dimensional transport of a non-conservative solute that may undergo attenuation, is as follows:

$$\frac{\mathrm{d}}{\mathrm{d}x}\left(D_{xx}\frac{\mathrm{d}c}{\mathrm{d}x}\right) + \frac{d}{\mathrm{d}x}\left(D_{xy}\frac{\mathrm{d}c}{\mathrm{d}y}\right) + \frac{\mathrm{d}}{\mathrm{d}y}\left((D_{yy}\frac{\mathrm{d}c}{\mathrm{d}y}\right) +$$

$$\frac{\mathrm{d}}{\mathrm{d}\bar{y}}\left(D_{yx}\frac{\mathrm{d}c}{\mathrm{d}x}\right) - \frac{\mathrm{d}}{\mathrm{d}x}(cq_x) - \frac{\mathrm{d}}{\mathrm{d}y}(cq_y) - \frac{\mathrm{d}}{\mathrm{d}t}(nbc) -$$

$$\frac{\mathrm{d}}{\mathrm{d}t}(P_b bS) + Qc' + \frac{K'}{l'}(h - h_w)\, c'' = 0$$

where

b = saturated aquifer thickness
c = concentration
c' = concentration of discharged effluent
c'' = concentration of fluid discharging through leakage
D = dispersion coefficient
K' = hydraulic conductivity of confining bed
l' = thickness of confining bed
q = mass average flux vector
Q = rate of effluent withdrawal
n = porosity of aquifer material
P_b = bulk density of solid matrix
S = concentration of adsorbed material expressed as mass of solute per unit mass of porous medium.

A typical output for a QSOL section model is shown in Fig. 6. Although this particular example does not incorporate scavenger wells, it does show variations in the vertical and horizontal concentrations of seepage from a waste-disposal facility where the aquifer below the site is non-homogeneous and anisotropic.

SUMMARY

While most effluent streams are more or less predictable in terms of bulk volume and concentration, it is difficult to predict the quality of the seepage from waste-disposal facilities. The net effect of seepage quality is related to such factors as time, discharge rates, and characteristics of the subsite material.

This paper has illustrated how predictive solute transport models can be used to aid in the assessment of seepage quality prior to desalination treatment. The particular system modelled, a scavenger wellfield downstream of a waste dump, demonstrates the application of one-dimensional and two-dimensional solute transport models (plan and sectional) that are capable of predicting the concentrations of transient effluent discharge at the wells with variations in discharge rates.

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