COMPARISON OF ONE-, TWO-, AND THREE-DIMENSIONAL MODELS FOR MASS TRANSPORT OF RADIONUCLIDES

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SECTION 1. SUMMARY

This technical memorandum compares one-, two-, and three-dimensional models for studying regional mass transport of radionuclides in groundwater associated with deep repository disposal of high-level radioactive wastes. In addition, this report outlines the general conditions for which a one- or two-dimensional model could be used as an alternate to a three-dimensional model analysis.

The investigation includes a review of analytical and numerical models in addition to consideration of such conditions as rock and fluid heterogeneity, anisotropy, boundary and initial conditions, and various geometric shapes of repository sources and sinks. Based upon current hydrologic practice, each review is taken separately and discussed to the extent that the researcher can match his problem conditions with the minimum number of model dimensions necessary for an accurate solution.

The primary findings of the report are as follows:

1. Dispersion and diffusion are three-dimensional phenomena. Therefore, any model chosen that assumes dispersion and diffusion to be negligible in any direction may result in misleading conclusions.
2. Radioactive decay is a function of time only, and therefore is independent of the number of space coordinates chosen for model simulation.
3. Vertical cross-sectional models that assume uniform flow conditions perpendicular to the section cannot properly represent the three-dimensional flow towards wells or nuclide repositories. Neither

can they properly represent dispersion in the direction normal to the plane of the cross-section unless very special conditions exist.

4. One-dimensional models are very limited in application to field radionuclide transport. The one-dimensional model, however, has application to laboratory experiments such as sand columns and possibly in combination with other formulations such as one-dimensional flow with three-dimensional dispersion.

5. A "flow" problem may be symmetrical in head distribution but asymmetrical when further consideration is given to mass transport. Three-dimensional dispersion in a one-dimensional uniform flow field is an obvious example of this concept where symmetry in flow and mass transport differ. Use of symmetry conditions for reducing dimensions depends upon both flow and transport consideration.

6. The equivalent replacement of a three-dimensional repository shape in a one- or two-dimensional model study, if desired, should be a line sink. Distortion of head distribution, mass transport velocities, and time-related changes in flow result if a point replacement is used for the actual three-dimensional repository shape.

7. In the event that a point, line, or area equivalent to the true three-dimensional repository is used, one should be aware that errors in calculated heads or flow rates in the system will occur. The relative magnitudes of these errors should be a subject of further research.

8. Consideration of boundary and initial conditions are very important in choosing the number of dimensions for modeling nuclide transport. A test, by cross-section comparisons perpendicular to the coordinate axis to be eliminated, can show when a lower order dimensioned model may be considered for use.

9. The existence of large volumes of heterogeneous fluids presents a moving boundary problem to be dealt with. Not only does one need to consider all of the dimension symmetry and uniformity criteria of stationary boundaries, but one needs to examine the movement of the boundary in time as the physical process takes place.

10. The existence of numerical models allows a means for solving complex one-, two-, or three-dimensional problems but does not help us in deciding which dimensions to include for mass transport of radionuclides. In fact, the approximating features of the numerical models will increase the number of dimension problem decisions.

11. The vertical to horizontal scale contrasts in nodal placement for fully or pseudo three-dimensional models introduces errors that we believe are not fully understood or appreciated. Further study is needed.

SECTION 2. INTRODUCTION

The study of radionuclide mass transport can be accomplished by making use of modeling techniques involving analytical formulas or numerical techniques. These modeling techniques have been, in the past, developed on the basis of one-, two-, or three-dimensional theories and considerations. Quite frequently, the researcher is faced with choosing not only an appropriate formula or numerical technique for solution of a problem, but also with a choice of the number of dimensions to include in the analysis. Under ideal conditions, the researcher can simplify his work, make efficient use of computer time and core storage, and rid himself of handling unnecessary variables when a two-dimensional model can be used to solve his problem just as well as a three-dimensional model. Under further ideal conditions, perhaps the use of a one-dimensional model may provide an accurate solution to a problem.

The purpose of this report is to shed light on the problem of choosing among the one-, two-, or three-dimensional models when studying mass transport of radionuclides. The scope of work in the project task included a general evaluation of the extent a lower order model can adequately simulate the regional flow of radionuclides and a comparison between one-, two-, and three-dimensional flow and quality problems. It should be realized that what is adequate for one use may be insufficient for another. The dimensionality of the model depends on such items as the type of answers sought, the accuracy desired, and the widely varying particulars of the problem to be solved. We have thus developed the necessary concepts in this report which will lead to the specific criteria necessary for choosing the number of dimensions of a model for radionuclide transport.

Consideration was given in this report to such conditions as heterogeneity, anisotropy, and boundary geometry and various sources and sinks as they relate to predictive accuracy. A literature search was conducted and a reference list assembled to the extent that it supports the evaluation and comparison. This task also included studies of one-, two-, and three-dimensional analytical solutions for homogeneous and isotropic cases to show, in the absence of any numerical model approximations, where there is a real need for three-dimensional models. Although there are conceivable regional flow cases where a three-dimensional model may be necessary, an evaluation of modeling techniques (finite-difference versus finite element) was also included to study model approximating procedures still remaining that may cause additional problems in the needs and evaluations process. A selected number of idealized computer simulations was carried out for those areas of particular interest as illustrations of lower dimensional models as equivalents of three-dimensional formulations.

The remainder of the report is in order of discussions concerning analytical models, example solutions, and numerical models. Comparisons among one-, two-, and three-dimensional formulations are made within each of these sections and a list of major conclusions and recommendations given.

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SECTION 3. ANALYTICAL MODELS

The basis for the discussion that follows stems from consideration of groundwater flow in three-dimensions as expressed by analytical formulas. Since many of the classical groundwater equations in one and two dimensional form include assumptions about the third dimension variables, we will discuss the associated validity and possible errors therefore introduced. In the limit, we are thus assuming that the three-dimensional analytical formulas are the true representations of the actual situation and discuss the possibilities of reducing the problem to simpler forms if possible.

Analytical formulas are models themselves. On occasion, the literature on groundwater modeling gives the impression that it is the formula that we are modeling and not the actual physics of the real world. This point is made because it is possible to consider the formula the ultimate answer and forget where the formulas come from in the first place. The formulas themselves contain assumptions. We begin the discussion below by examining what is going on with full three-dimensional formulas themselves as they relate to governing assumptions. For some situations, it is therefore possible that the three-dimensional formulations given in the literature themselves are inadequate for modeling radionuclide transport.

The following analytical modeling part includes a discussion of the three-dimensional formulations and when lower order dimensional analysis may be used. Special attention is then given to source and sink singularity problems, effects of boundary conditions, the separation of local versus regional effects, and the problems associated with heterogeneity and anisotropy. This total part of the report is then concluded by a discussion of the usefulness of analytical formulas in the modeling of radionuclide transport in one, two, and three dimensions. The conclusions section includes a discussion of the difference between one, two, and three dimensional analyses that is independent of modeling technique and therefore applicable to the numerical modeling that follows in the next part of this report.

THREE-DIMENSION EQUATIONS

FLOW EQUATION AND BASIC ASSUMPTIONS

The classical partial differential equation governing the three-dimensional unsteady-state flow of groundwater in a homogeneous and isotropic aquifer was given by Jacob (1950) as:

$$\frac{\partial^2 h}{\partial x^2} + \frac{\partial^2 h}{\partial y^2} + \frac{\partial^2 h}{\partial z^2} = \frac{S_s}{K}\frac{\partial h}{\partial t} \quad * \qquad (1)$$

Equation (1) is of the same form as the fundamental equation of applied physics known as the "diffusion equation." Equations of the same form as Equation (1) appear in the theories of unsteady-state flow of heat and electricity from which solutions to many groundwater flow problems may be obtained by analogy.

Equation (1) can be used, along with appropriate boundary conditions, to solve for head distributions in time and space. The head distribution can then be differentiated with respect to distance, to produce a velocity distribution. The following discussion is centered around the basic assumptions of the above equation, a presentation of example solutions to three-dimensional flow problems, and a review of the possible mechanisms to reduce the three-dimensional problem solution down to either one or two-dimensional representation.

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*Please refer to the "List of Symbols" for definition of terms.

The derivation of Equation (1) was not without additional assumptions as follows.

First, the elemental volume, used in the derivation of the equation, remains constant in dimensions in the lateral directions but is allowed to deform in the vertical direction. Furthermore, it was assumed that the volume of solid materials within the elemental volume remains constant. What is wrong is that a three-dimensional flow field and a one-dimensional stress field are intermixed. The more general approach would combine three-dimensional flow with three dimensional stress. Gambolati (1974) analyzes the range of validity of Equation (1) due this basic assumption. The results of that work indicate that this assumption is not likely to cause problems in deep burial of radionuclides where compaction of groundwater reservoirs is negligible. Gambolati indicates that the three-dimensional stress effects are negligible when the ratio of depth to thickness of aquifer is equal to or greater than 2. The problems would occur in shallow and thick aquifers that compact substantially when pressures of the flowing fluids are reduced.

Secondly, the density gradients in space that exist in reality are assumed to be negligible in Equation (1). These density gradients can be expressed mathematically by the grouping given by Jacob (1950):

$$\rho \beta g \left[\left(\frac{\partial h}{\partial x}\right)^2 + \left(\frac{\partial h}{\partial y}\right)^2 + \left(\frac{\partial h}{\partial z}\right)^2 - \frac{\partial h}{\partial z} \right]$$

and is the pertinent missing component of the left hand side of Equation (1). The reasoning for neglecting this term was that it is quite small in comparison to the first term of Equation (1). Supposedly it is particularly small for low-angle flow with $\partial h/\partial z$ being much less than one.

Thirdly, the specific storage coefficient, S_s, is constant in time and represents a coefficient related to an instantaneous release of water from storage. Fourthly, the flow is confined and therefore no draining of aquifer materials occurs. Fifthly, flow is assumed to be laminar only and therefore turbulent flow is assumed nonexistent. Sixthly, flow is assumed to be statistically irrotational. And finally, no temperature, chemical, radioactive, or bacterial processes are present that would change the fluid viscosity or density either in space or time.

MASS TRANSPORT EQUATION
AND BASIC ASSUMPTIONS

Based upon the derivations of Ogata (1970) and Bear (1972), the three-dimensional equation governing mass transport in saturated, homogeneous and isotropic porous media with adsorption, chemical sorption, and radioactive decay can be given as:

$$\frac{1}{R_d}\left[\frac{\partial}{\partial x}\left(D_x\frac{\partial C}{\partial x}\right) + \frac{\partial}{\partial y}\left(D_y\frac{\partial C}{\partial y}\right) + \frac{\partial}{\partial z}\left(D_z\frac{\partial C}{\partial z}\right)\right]$$

$$-\frac{1}{R_d}\left[\frac{\partial}{\partial x}(v_x D) + \frac{\partial}{\partial y}(v_y C) + \frac{\partial}{\partial z}(v_z C)\right] - \lambda C = \frac{\partial C}{\partial t} \qquad (2)$$

Equation (2), along with appropriate boundary conditions, can be used to obtain concentration distributions in both time and space.

Since velocities of flow are involved in Equation (2), all of the basic assumptions used in the derivation of Equation (1) apply here also. In addition, further assumptions placed on the advective-dispersion Equation (2) are outlined as follows. The coefficient of hydrodynamic dispersion assumes that $D_i = d_i v_i + D^*$ and that the exponent on the velocity term is one. Next, there is assumed that there is no density or viscosity difference between the transported solute and the resident groundwaters.

The system is assumed to be isothermal and that there is no change in porosity with pressure change. The retardation factor and its associated distribution coefficient represents fast and reversible reactions in the presence of linear isotherms. Onsager relationships coupling various forces that can produce other transport are neglected.

No special significance is yet given to these particular assumptions other than to show that a large group of assumptions do exist for three-dimensional formulations. The point to be made is that *the decision on whether to use a one-, two-, or three-*dimensional model is only a part of the decision making process in choosing a model. There are other considerations common to all dimensions which must be kept in mind.

Let us now proceed to consider further assumptions that might be made to reduce a three-dimensional problem down to a two-dimensional one.

TWO-DIMENSION EQUATIONS

PLAN VIEW FLOW EQUATION

For the special case of an uniformly thick and horizontal aquifer of thickness, b, Equation (1) may be reduced to a two-dimensional form by setting $\partial^2h/\partial z^2$ to zero and rewriting the equation of flow as:

$$\frac{\partial^2 h}{\partial x^2} + \frac{\partial^2 h}{\partial y^2} = \frac{S_s b}{Kb}\frac{\partial h}{\partial t} = \frac{S}{T}\frac{\partial h}{\partial t} \qquad (3)$$

The setting of $\partial^2h/\partial z^2$ to zero requires that all of the flow be horizontal in the x and y direction. Equation (3) is thus a plan view model of groundwater flow.

PLAN VIEW MASS TRANSPORT EQUATION

The corresponding mass transport equation for the above plan view flow model comes from Equation (2) with v_z equal to zero and is written as

$$\frac{1}{R_d}\left[D_x\frac{\partial^2 C}{\partial x^2}+D_y\frac{\partial^2 C}{\partial y^2}\right]-\frac{1}{R_d}\left[\frac{\partial}{\partial x}(v_xC)+\frac{\partial}{\partial y}(v_yC)\right]$$
$$-\lambda C=\frac{\partial C}{\partial t} \qquad (4)$$

Equation (4) implies additional simplification other than setting v_z equals zero in Equation (2). Dispersion is a three-dimensional phenomena. Setting v_z equal to zero does not stop dispersion in a two-dimensional flow field from going in the third dimension. So, what we have done for Equation (4) is to add the additional condition that the concentration profile in the z direction is vertically averaged or thoroughly mixed.

CROSS-SECTIONAL VIEW FLOW EQUATION

For the special case of a uniform cross section of an aquifer of unit thickness, Equation (1) may be reduced to a two-dimensional form by setting $\partial^2h/\partial y^2$ to zero and rewriting the equation of flow as

$$\frac{\partial^2 h}{\partial x^2}+\frac{\partial^2 h}{\partial z^2}=\frac{S_s}{K}\frac{\partial h}{\partial t} \qquad (5)$$

Equation (5) is the cross-sectional view model when the flow in the y direction is zero. This type of flow model is popular with radionuclide transport studies. Most often, the right-hand side of Equation (5) is further set to zero to represent the steady-state condition. One can visualize the errors that could be involved in this flow situation by considering how one would simulate a pumping well parallel to the z axis and hope to properly represent the radial flow. In short wells, or any sink that has flow in the y direction, cannot be modeled with this equation.

One acceptable sink for this cross-sectional model would be a horizontal drain of infinite extent laid along the y axis perpendicular to the x-z plane.

CROSS-SECTIONAL VIEW MASS TRANSPORT EQUATION

The corresponding mass transport equation for the above cross-sectional view flow model is derived from Equation (2) by setting v_y equal to zero.

$$\frac{1}{R_d}\left[D_x \frac{\partial^2 C}{\partial x^2} + D_z \frac{\partial^2 C}{\partial z^2}\right] - \frac{1}{R_d}\left[\frac{\partial}{\partial x}(v_x C) + \frac{\partial}{\partial z}(v_z C)\right] - \lambda C = \frac{\partial C}{\partial t} \qquad (5)$$

Here again, the dispersion in the y direction is ignored or at least considered averaged within the unit thickness of the cross-section. Serious errors in mass transport modeling result in this situation occurring since dispersion in the third (y) dimension is restricted. Concentration distribution predicted from point sources with this type of model are over estimated since a diluting mechanism in one of the remaining dimensions is ignored.

One should note that the radioactive decay term λC in Equations (2) and (5) does not depend upon the space coordinates retained and therefore is properly represented in this two-dimensional simplification of the three-dimensional formulation. Thus radioactive decay representation does not lose significance within a reduction of a three-dimensional formulation down to a two or one dimension formulation.

ONE-DIMENSION EQUATIONS

LINEAR FLOW EQUATIONS

In the event that flow is restricted to one direction, the terms $\partial^2h/\partial y^2$ and $\partial^2h/\partial z^2$ of Equation (1) are set to zero to give:

$$\frac{\partial^2 h}{\partial x^2} = \frac{S_s}{K}\frac{\partial h}{\partial t} \tag{6}$$

Equation (6) is for a unit thickness one-dimensional flow situation in the x direction. If one desires that flow be one-dimensional in the y or z directions the coordinate of Equation(6)is adjusted accordingly to either

$$\frac{\partial^2 h}{\partial y^2} = \frac{S_s}{K}\frac{\partial h}{\partial t} \tag{7}$$

or

$$\frac{\partial^2 h}{\partial z^2} = \frac{S_s}{K}\frac{\partial h}{\partial t} \tag{8}$$

These equations are most useful for looking at such problems as the response of aquifers due to fully penetrating rivers, ditches, and filter beds.

On occasion, researchers may desire a model in one-dimensional flow which represents a horizontal and uniform thickness, b, aquifer. In this case either Equation (6) or (7) is used for example as

$$\frac{\partial^2 h}{\partial x^2} = \frac{S_s b}{Kb}\frac{\partial h}{\partial t} = \frac{S}{T}\frac{\partial h}{\partial t} \tag{9}$$

The main restriction on Equations (6) through (9) is that flow is absolutely restricted to one-dimension.

LINEAL MASS TRANSPORT EQUATIONS

Equation (2) can be reduced to one-dimensional form by setting the v_y and v_z terms to zero to yield:

$$\frac{1}{R_d} D_x \frac{\partial^2 C}{\partial x^2} - \frac{1}{R_d}\left[\frac{\partial}{\partial x}(v_x C)\right] - \lambda C = \frac{\partial C}{\partial t} \qquad (10)$$

This equation fits with the one-dimensional flow formula given as Equation (6). Most often, laboratory experiments in sand or rock columns are analyzed by the combination of Equation (6) and (10). Here again, the coordinates y and z may be substituted in Equation (10) to give equations for one-dimensional flow along the other axes.

The use of Equations (6) and (10) is very limited in application to radionuclide transport in the field. Most often, a sand column experiment is the study area where these one-dimensional forms are applicable.

GENERAL COMMENTS AND COMPARATIVE ANALYSIS--BASIC EQUATIONS

On the basis of the above analytical equation discussion one may make general comments and draw some conclusions concerning when to use one-, two-, or three-dimensional models for radionuclide transport analysis.

1. There are a set of basic assumptions which apply to all equations of flow and transport that should also be considered in choosing a model besides the consideration of one-, two- or three-dimensional flow.
2. Dispersion and diffusion are three-dimensional phenomena. Therefore, any model chosen that assumes dispersion and diffusion to be negligible in any direction may result in misleading conclusions.
3. Radioactive decay is a function of time only, and therefore is independent of the number of space coordinates chosen for model simulation.

4. Vertical cross-sectional models that assume uniform flow conditions perpendicular to the section cannot properly represent the three-dimensional flow towards wells or nuclide repositories. Neither can they properly represent dispersion in the direction normal to the plane of the cross-section.
5. One-dimensional models are very limited in application to field radionuclide transport. The one-dimensional model, however, has application to laboratory experiments such as sand columns or possibly in combination with other formulations such as one-dimensional flow with three-dimensional dispersion.

EXAMPLE EQUATION SOLUTIONS

The discussion of basic equations above has been partially instructive in delineating the usefulness of one-, two-, and three-dimensional equations and provides somewhat of a guide in choosing a model to solve a problem. However, boundary and initial conditions have not been addressed as yet. This report section begins to look at the further restrictions of boundaries attached to the basic equations that again have a bearing on choice of model dimensions.

This section of the report covers comparative analyses of selected known solutions to boundary and initial condition problems in one, two, and three dimensions. The comparative analyses further show when and when not a three-dimension problem can be reduced down to a lower order two or even one-dimensional solution.

A special section is included in this section that addresses the question of regional versus local flow due to the geometry of a typical repository. A sneak preview of the results of this part of the report indicates that, when time is included in the flow model, a point sink cannot adequately represent a finite-dimensioned repository even in a regional analysis.

Of special importance in this section is the inclusion of time in the comparisons. A large part of the previous work in radionuclide transport has been centered around steady-state analyses where the flow model is in a steady-flow mode and the transport model is transient. We will consider transient conditions in both flow and transport and provide guidelines for model simulations in this actual four-dimensional scenario.

We will retain the conditions of homogeneous and isotropic porous media in this section. Comments on heterogeneity and anisotropy will be covered later.

SPHERICAL FLOW TO A POINT SINK
IN AN INFINITE PERMEABLE MEDIA

The simplest case of three-dimensional flow in an isotropic-homogeneous aquifer is that of flow to a point sink situated in an unbounded permeable space. Although this situation is not by itself directly applicable to radionuclide transport, it does offer a chance to see a typical three-dimensional flow problem and study how the aquifer response equation might be reduced to simpler forms.

The solution for the above point sink problem can be obtained by applying the appropriate boundary conditions to Equation (1) and solving for the head distribution. Carslaw and Jaeger, 1959, give the nonsteady-state equation of heat flow for this situation and, in terms of the analogous groundwater parameters of this report the solution is:

$$h = (Q/(4\pi Kr)) \text{ erfc } (r/\sqrt{4Kt/S_s}) \tag{11}$$

where:

$r^2 = (x - x')^2 + (y - y')^2 + (z - z')^2$

x', y', z' = location of point sink in rectangular coordinate system

Immediately one recognizes that it is sometimes possible to reduce a three-dimensional problem solution to a one-dimension equation by applying a rectangular to spherical coordinate system transform. For this to be possible the problem solution must be symmetrical about the point source. More will be said about coordinate system transforms as we proceed in the report.

At this juncture let us look at the steady-state solution where $t \to \infty$ and proceed to discuss a convective transport problem. Carslaw and Jaeger also give the steady solution as:

$$h = Q/(4\pi Kr) \tag{12}$$

One may differentiate Equation (12) to obtain the gradient dh/dr to inspect flow velocities as a function of distance r from the point sink. The resulting velocity-related gradient equation is:

$$\frac{\partial h}{\partial r} = - \frac{Q}{4\pi K r^2} \tag{13}$$

The velocity distribution (through use of the equation $v = -K\, \partial h/\partial r$) is seen then to also be a one-dimensional formula in r^2. Therefore, the symmetrical three-dimensional mass transport problem can, in this case, be transformed to a one-dimensional form.

The conclusion to be drawn from this example is that one should look for symmetry and take advantage of it when possible in reducing three-dimensional problems down to lower order solutions. The coordinate system transform is thus a powerful method of simplifying analysis.

SPHERICAL DISPERSION AND DIFFUSION IN AN INFINITE POROUS MEDIA WITHIN A UNIFORM ONE-DIMENSIONAL FLOW

Freeze and Cherry (1979) present a solution of Equation (2), without retardation and decay, for the case of a contaminant movement of an instantaneous slug in a one-dimensional flow field. The contaminant is assumed to originate as an instantaneous slug at a point source at x = 0, y = 0, and z = 0. The mass of contaminant is then carried away from the initial source location by transport in a steady uniform flow field moving in the x direction in a homogeneous and isotropic medium. As the contaminant mass, M, is transported through the system, the concentration distribution at time t was given by

$$C(x,y,z,t) = \frac{M}{8\,(\pi t)^{3/2}\,\sqrt{D_x D_y D_z}}\ \exp\left[-\frac{X^2}{4D_x t} - \frac{Y^2}{4D_y t} - \frac{Z^2}{4D_z t}\right] \quad (14)$$

where X, Y, and Z are distances in the x, y, and z directions from the center of gravity of the contaminant mass. The position of the center of gravity of the contaminant mass at time t will be along the flow path in the x direction at coordinates (x_t, y_t, z_t) where $y_t = z_t = 0$ and $x_t = vt$ where v is the average linear velocity. Therefore in Equation (14) $X = x - vt$, $Y = y$ and $Z = z$.

Without using numbers, one can see that a moving coordinate transform has been employed to simplify the concentration distribution in Equation (14). If one assumes $D_x = D_y = D_z$ Equation (14) can be further simplified to

$$C(r,t) = \frac{M}{8\,(\pi D_x t)^{3/2}}\ \exp\left(-\frac{r}{4D_x t}\right) \quad (15)$$

where C(r,t) is now the concentration distribution radially varying around the mean x-direction flow point of $x_t = vt$. This is an example of using both a coordinate system transform and a moving coordinate system in combination with each other to reduce a three-dimensional problem to a one-dimensional formulation.

One should realize that if the dispersion coefficients are greater than 0 in Equation (14) the concentration distribution is three-dimensional in form. Making an assumption that the dispersion coefficient in one or more directions is zero is risky and can only be done under very special conditions. We are thus re-emphasizing that reducing a three-dimensional dispersion and diffusion problem down to a two- or one-dimensional problem is going to be suspect.

This is even true of long-term simulations where molecular diffusion dominate over dispersion and velocities are very small.

COMPARISON OF POINT AND LINE SINKS IN AN INFINITE NONLEAKY AQUIFER

A large class of three-dimensional flow problems have been solved for the case of partially penetrating wells. In this case the flow is converging three-dimensional near the pumped well and radially two-dimensional at some distance. One extreme case of this situation is where the well just penetrates the top of the aquifer. A solution to the zero penetrating case can be compared to the fully penetrating case to show how, when, and where this three-dimensional flow situation can be considered a two-dimensional flow situation.

Theis (1935), starting with Equation (3), derived the solution for non-steady flow to a fully penetrating well in an infinite nonleaky artesian and horizontal aquifer as:

$$s = \frac{Q}{4\pi T}\int_u^\infty \frac{e^{-u}du}{u} = \frac{Q}{4\pi T}W(u) \qquad (16)$$

where:

$$u = r^2S/(4Tt) \qquad (17)$$

The integral of Equation (16) is known as the "exponential integral" for which tables of values are widely available. The drawdown, s, is uniform in the z direction and flow to the well is thus radial. Equation (16) therefore is a one-dimensional formula in r^2 describing flow in a two-dimensional flow system.

Based upon the work of Jaiswal, et al., (1977) the nonsteady drawdown distribution along the top of the aquifer and around a well of zero penetration and vanishing radius in a nonleaky artesian aquifer of infinite areal extent is given by:

$$s = Q/2\pi Kr\{C(\sqrt{u}, r/b)\} \qquad (18)$$

where:

$$C(\sqrt{u},\ r/b) = \text{erfc}\ \sqrt{u} + \sum_{n=1}^{\infty} 2\ \text{erfc}\ \{\sqrt{1+(2nb/r)^2}\sqrt{u}\}/\sqrt{1+(2nb/r^2)} \qquad (19)$$

The function $C(\sqrt{u}, r/b)$ was not published in tabular form by Jaiswal, et al., (1977) but was given in graphical form as reproduced in Figure 1.

A comparison of Equations (16) and (18) is shown in Figure 2 to illustrate the difference in aquifer response for a given set of aquifer parameters. As seen in Figure 2 the drawdown of head along the top of the aquifer for the nonpenetrating case is much greater than that for the fully-penetrating case. As the distance from the sinks increases, the drawdown curves approach each other asymptotically. With distance the nonpenetrating response curve approaches the fully-penetrating case from beneath. If a figure were presented for drawdowns along the bottom of the aquifer, the reverse conditions of less drawdown for the nonpenetrating would be indicated as compared to the fully-penetrating case. Along the bottom of the aquifer the response curve for the nonpenetrating case would, with distance, approach the fully penetrating case from above.

The distance to the point at which heads for the nonpenetrating and fully penetrating cases are essentially the same has been calculated to be about 2 aquifer thicknesses distant from the sink.

Muskat, 1949 discusses the partial penetrating case for the steady-state condition. Figure 3 shows a cross-sectional comparison of the three-dimensional versus the two-dimensional radially symmetrical problem.

In the final analysis, there are three-dimensional flow cases where a two-dimensional representation may suffice for describing

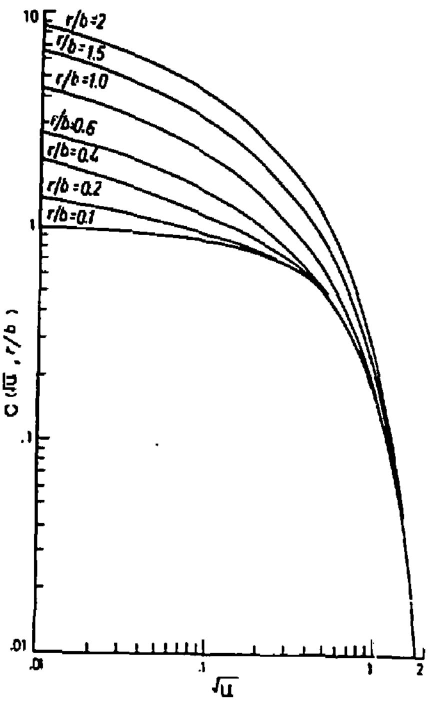


Figure 1. Values of C($\sqrt{u}$, r/b) With $\sqrt{u}$ For Different Values of r/b

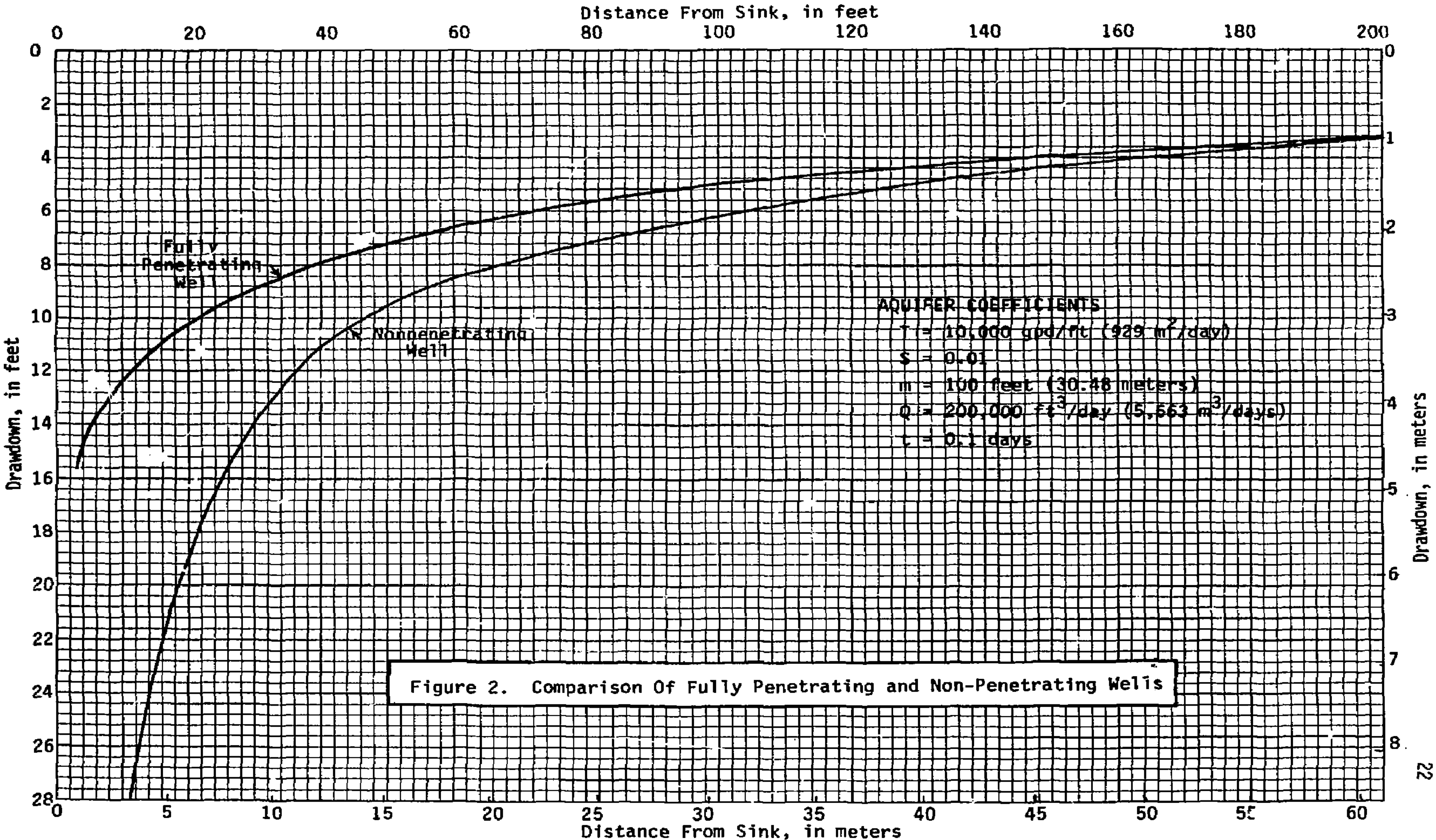
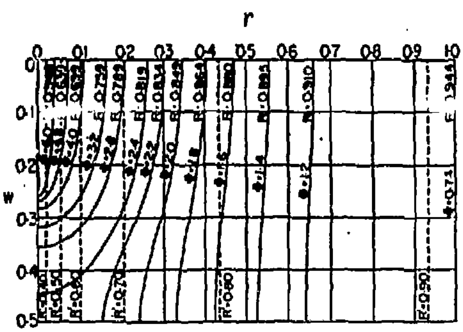


Figure 2. Comparison Of Fully Penetrating and Non-Penetrating Wells



After Muskat (1949)

Figure 3. Calculated Steady-State Potential Distribution About A Well Of Radius = 1/500 Of The Formation Thickness, and 50 Per Cent Penetration. R = Fraction Of Total Potential Drop. External = Boundary Radius = 4 x Formation Thickness. Unit Of Distance = 2 x Formation Thickness. Dashed Curves And R' Correspond To A Strictly Radial-Flow (Complete Well Penetration) System.

the head distribution. However, one must be cautious in assuming that since the flow regime may be reducible in dimensions so is the associated mass transport problem. An examination of Figure 3 shows the variable flow path lengths associated with the partially penetrating case and that the distributions of contaminants therefore are slightly different as compared to a fully penetrating case. This may or may not be of significance--depending upon whether a local or regional problem is under study.

COMPARISON OF ONE-, TWO-, AND THREE-DIMENSIONAL DISPERSION IN A ONE-DIMENSIONAL FLOW FIELD

Bear (1972) gives the one- and two-dimensional equations for dispersion (without adsorption and radioactive decay) of a slug of contaminant introduced into a one-dimensional flow field. Equation (14) illustrates the three-dimensional equivalent. Homogeneous and isotropic conditions are assumed. Inspection of these three equations shows that the peak concentration occurs at the center of gravity of the moving contaminant cloud as given by:

$$\text{one-dimensional dispersion: } C_{max} = \frac{M}{\sqrt{4\pi D_x t}} \qquad (20)$$

$$\text{two-dimensional dispersion: } C_{max} = \frac{M}{4\pi t\sqrt{D_x D_y}} \qquad (21)$$

$$\text{three-dimensional dispersion: } C_{max} = \frac{M}{8(\pi t)^{3/2}\sqrt{D_x D_y D_z}} \qquad (22)$$

For comparative purposes we let $D_x = D_y = D_z = 1$, $t = 1$, and $M = 1$ and calculate C_{max} to be:

one dimension $C_{max} = 1/\sqrt{4\pi} = 0.2821$
two dimension $C_{max} = 1/4\pi = 0.07958$
three dimension $C_{max} = 1/8(\pi)^{3/2} = 0.02245$

The obvious conclusion is that the concentration is a function of the number of dimensions included, all other considerations being the same. Dispersion is a three-dimensional phenomena. Constructing any dimension model and neglecting any one of the dispersion coefficients gives the wrong answer. The trend is that lower order models give higher concentrations.

DEVELOPMENT OF 3-D ANALYTICAL MODEL AND TEST OF DIMENSION ASSUMPTIONS OF REPOSITORY

A distinction between regional and local effects had been made in studying the various aspects of radionuclide transport from waste repositories. Various definitions have been heard of what a local or regional problem is. One prevalent definition that has been stated is that a regional problem exists when the source of the radionuclides can be considered a point. With this definition, a local problem therefore exists when you can't consider the source a point. We were concerned that this definition needed clarification and that the true three-dimensional aspects be looked into. With the regional/local and point source/repository configuration questions in mind, we proceeded to develop two analytical formula models that would shed light on differences involved.

The development of the three dimensional models are first outlined, the results of the simulations given and discussed, and then conclusions are drawn.

Development of Theory for Comparison of Three-Dimensional Flow Analysis to and from Repositories of Various Shapes

Analytical equations developed from point-source potential theory can be applied to a groundwater aquifer to obtain solutions for the potential fields around various sink configurations (lines, areas, cylinders, volumes, etc.). This combined with the use of the method of images (since potential theory is a linear system) will enable the modeling not only of a source or sink in an infinite aquifer but also the boundary conditions inherent to a particular aquifer.

The starting point for the development of the analytical solutions is the potential field of an instantaneously discharged point sink from Carslaw and Jaeger (1959), namely

$$S_p = \frac{Vol/S_s}{8(\pi \underline{k} t)^{3/2}} \, e^{-r_p^2/4\underline{k}t} \tag{23}$$

where:

S_p = potential at point defined by r_p

Vol/S_s = instantaneous volume depletion

The term r_p can be applied to a one-, two-, or three-dimensional potential field and can be defined for each as

$r_p = x_p - x'$ (1-D potential field)

$r_p = \sqrt{(x_p - x')^2 + (y_p - y')^2}$ (2-D potential field)

$r_p = \sqrt{(x_p - x')^2 + (y_p - y')^2 + (z_p - z')^2}$ (3-D potential field)

where:

x_p, y_p, z_p = are the coordinates of the point of interest

x', y', z' = are the coordinates of the point sink

Integration of Equation (23) with respect to time yields a solution for a continuously discharging point sink

$$S_p = \frac{1}{8(\pi \underline{k})^{3/2}} \int_0^t q \, e^{-r_p^2/4\underline{k}(t-t')} \frac{dt'}{(t-t')^{3/2}}$$

Assuming q (continuous flow rate = $Vol/S_s t$) to be constant

$$S_p = \frac{q}{4(\pi \underline{k})^{3/2}} \int_{1/\sqrt{t}}^{\infty} e^{-r_p^2 \tau^2/4\underline{k}} \, d\tau$$

where:

$\tau = (t-t')^{-\frac{1}{2}}$

This integral and the constants can be rearranged to obtain the complementary error function (erfc),

$$S_p = \frac{q}{4\pi \underline{k} r_p} \, \text{erfc}\,(r_p/\sqrt{4\underline{k}t}) \tag{24}$$

or $$S_p = \frac{DIS}{4\pi \underline{k} r_p \cdot S_s} \, \text{erfc}\,(r_p/\sqrt{4\underline{k}t}) = \frac{DIS}{4\pi K r_p} \, \text{erfc}\,(r_p/\sqrt{4Kt/S_s})$$

This is the equation of the potential field from a continuously discharging point sink of strength DIS.

Equation (24) forms the basis for generation of the potential due any configuration of source or sink producing at a constant rate. The following discussion explains how a potential distribution around a line, area, and slab are generated.

Equation (24) is now integrated to obtain the potential field of a continuously discharging line sink of length L along the x-axis. Figure 4 shows the relationships of dimensions. The line potential equation is thus:

$$S_p = \frac{1}{4\pi KL} \int_0^L \frac{DIS}{r_p} \ erfc(r_p/(\sqrt{4Kt/S_s}))dx'$$

where r_p is as defined previously. This can be rearranged to obtain

$$S_p = \frac{DIS}{4\pi KL} \int_0^L erfc(r_p/(\sqrt{4Kt/S_s}))/r_p \ dx' \qquad (25)$$

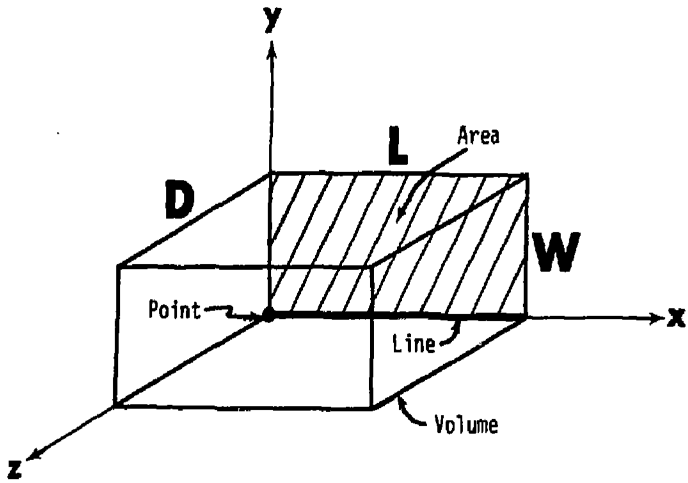
Integration can now be performed in the y-dimension to obtain a rectangular areal sink with dimensions L by W

$$S_p = \frac{DIS}{4\pi KLW} \int_0^W \int_0^L erfc(r_p/(\sqrt{4Kt/S_s}))/r_p dx' \ dy' \qquad (26)$$

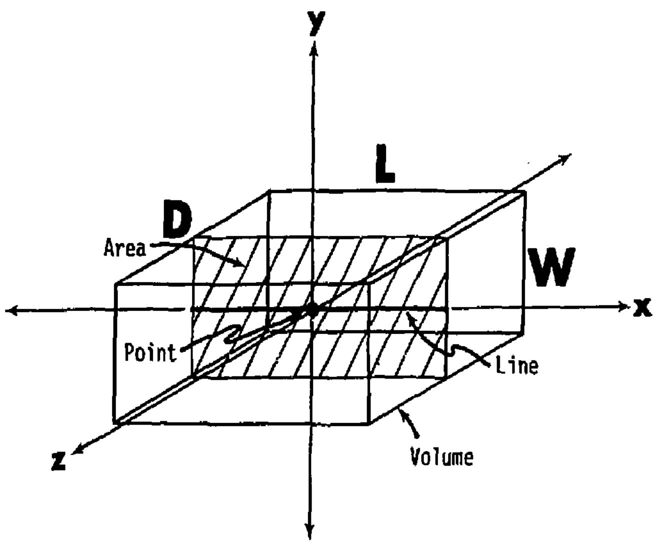
Likewise integration in the z-dimension enables one to obtain a solution for the potential field due to a continuously discharging volume sink of dimensions L by W by D

$$S_p = \frac{DIS}{4\pi KLWD} \int_0^D \int_0^W \int_0^L erfc(r_p/(\sqrt{4Kt/S_s}))/r_p dx' \ dy' \ dz' \qquad (27)$$

In summary, from the equation for a continuously discharging point sink of strength DIS (Equation (24)), we were able to obtain analytical equations for sinks of the same strength for 1-D, 2-D, and 3-D sinks in 1-D, 2-D, or 3-D potential fields (Equations (25)-(27)). These equations can be applied to infinite aquifers to obtain the potential fields.



(A)



(B)

Figure 4. Dimension Labels And Definition For Asymmetric (A) And Symmetric (B) Repository Models

Boundary conditions can now be modeled by the use of the method of images since potential theory is represented by linear partial differential equations. The only boundary conditions modeled were infinite planes in the x-z planes as illustrated by Figure 5. The distance of the plane barrier boundaries are A and B respectively for the lower and upper plane barriers. Also illustrated is the sink configurations and their appropriate dimensions. The general equation that follows for the modeling of these barriers is for a three-dimensional sink and potential field as:

$$S_p = \frac{DIS}{4\pi KLWD} \int_0^D \int_0^W \int_0^L \{ erfc(r_p/(\sqrt{4Kt/S_s}))/r_p + \sum_{i=I}^{\infty} \Big[erfc(r_{pAi}/(\sqrt{4Kt/S_s}))/r_{pAi} + erfc(r_{pBi}/(\sqrt{4Kt/S_s}))/r_{pBi} \Big] \} \, dx' \, dy' \, dz' \qquad (28)$$

where

$$r_{pAi} = \sqrt{(x_p - x')^2 + (y_p - D_{Ai})^2 + (z_p - z')^2}$$

$$\begin{aligned} D_{A1} &= -2A - y' \\ D_{A2} &= D_{A1} - 2\,(B - y') \\ D_{A3} &= D_{A2} - 2\,(A + y') \\ D_{A4} &= D_{A3} - 2\,(B - y') \qquad \text{recursive equation for Boundary A} \\ D_{A5} &= D_{A4} - 2\,(A + y') \\ &\vdots \end{aligned}$$

$$r_{pBi} = \sqrt{(x_p - x')^2 + (y_p - D_{Bi})^2 + (z_p - z')^2}$$

$$\begin{aligned} D_{B1} &= 2B - y' \\ D_{B2} &= D_{B1} + 2\,(A + y') \\ D_{B3} &= D_{B2} + 2\,(B - y') \\ D_{B4} &= D_{B3} + 2\,(A + y') \qquad \text{recursive equation for Boundary B} \\ D_{B5} &= D_{B4} + 2\,(B - y') \\ &\vdots \end{aligned}$$

The solution for Equations (25)-(28) were obtained by numerical integration since the erfc itself is not analytically integrable.

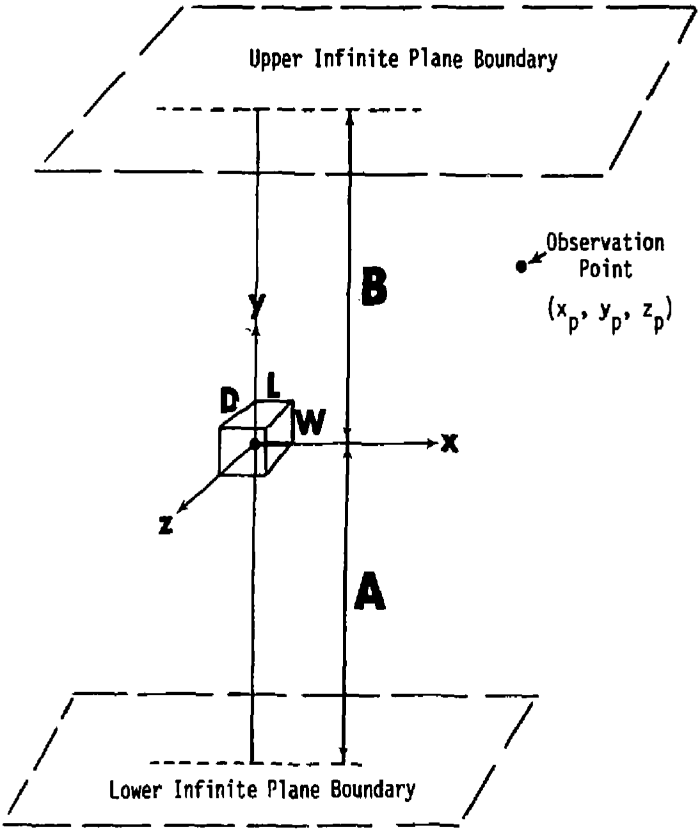


Figure 5. Position and Shape Dimensions Of Repositories Between Impermeable Upper And Lower Boundaries

The infinite series in Equation (28) is truncated to 100 image terms as the larger order image sinks were assumed to have negligible influence on the resulting potention comparisons at (x_p, y_p, z_p).

The complementary error function of Equation (28) was computed via a function subroutine which uses a rational function approximation. Numerical integration was performed by using the three-eighths rule

$$\int_{x_0}^{x_3} f(x)dx \simeq \frac{3h}{8}(f_0 + 3f_1 + 3f_2 + f_3)$$

where

$f(x)$ = the integrand

x_0, x_3 = integral limits

h = the equally spaced interval from $x_0 - x_1 - x_2 - x_3$

f_0, f_1, f_2, f_3 = function values at x_0, x_1, x_2, x_3

Since the potential at (x_p, y_p, z_p) was a linear function of DIS, DIS was assumed to be unity and then any other potential for a different DIS (sink strength) could be computed remembering that DIS must be steady or constant with time ($\partial DIS/\partial t = 0$).

Description of Computer Codes. Two computer codes were written to study the flow to repositories of various shapes. The first program (see Appendix A) was written on the basis of the repository shapes and positioning as defined in Figure 4A and Figure 5. The second program (see Appendix B) was written on the basis of the origin of the coordinate system being at the centroid of the repository shapes as defined in Figure 4B. Two programs were written in this manner so that both asymmetric and symmetric results could be conveniently studied.

The program codes were written in the FORTRAN IV language for a Control Data Corporation Cyber 175 system operating on the NOS batch time-sharing subsystem. Documentation of the program is included so that one may obtain an understanding of the operation of the code or actually use it if desired.

Results of Computer Model Simulations. Two sets of computer runs were made with the asymmetrical and symmetrical models to test for response of the various shaped repositories. Table 1 gives the results for the asymmetrical model and Table 2 gives the values for the symmetrical one. The differences in aquifer response for the various repository shapes is sometimes very subtle. Although graphical comparisons will be given, on occasion statements will be made strictly on the basis of tabular comparisons.

The first conclusion that can be drawn on a basis of a scan of the point, line, area, and volume columns of both Tables 1 and 2 is that the point sink response is the worst equivalent of a respository that has three dimensions. This is true no matter the time, distance from, or position of repository between the top and bottom of the system flow boundaries. Although there are differences that are exaggerated when the observation point is close to the sink center, it appears that the better equivalent of a three-dimensional sink (actual repository shape) is either a line or area. Therefore, if a researcher insists upon a two-dimensional model study, replace the three-dimensional repository with an equivalent line or area but not a point.

The second conclusion that can be drawn directly from the Tables is that the point, line, area, and volume shape responses approach each other with greater distances from the center of the sink. We use the word "approach" rather than the words "becomes equal" since theoretically differences always exist. It appears, for the homogeneous and isotropic conditions used, that the same rule of partially penetrating wells of twice the aquifer thickness distance away from the various sinks is sufficient such that potentials approach each other there and beyond. Figures 6, 7, and 8 help in visualizing this shape-distance-potential relationship. Figure 6 shows distance-head decline graphs for the

Table 1. Computer Model Results for Various Repository Shapes (Asymmetric Model)

Sequence number	Coordinate distance in meters x_p	y_p	z_p	Hydraulic conductivity in cm/sec	Time in days	Upper and lower boundary position in meters B	A	Repository shape* and change in head per unit flow rate, in meters/(l/sec) Point	Line	Area	Volume
1	10,000	100	0	4.72×10^{-7}	365,000	1,000	1,000	.00834	.009480	.009482	.009472
2	10,000	100	0	4.72×10^{-7}	365,000	500	500	.01040	.012270	.012280	.012270
3	1,000	100	0	4.72×10^{-5}	300	200	100	.23860	.33260	.32720	.32191
4	10,000	100	0	4.72×10^{-6}	365,000	500	500	.84400	.86860	.86880	.86870
5	5,000	100	0	4.72×10^{-7}	365,000	1,000	1,000	1.0061	1.11880	1.11900	1.11840
6	1,000	100	0	4.72×10^{-5}	365,000	200	100	3.6186	3.78490	3.73580	3.72500
7	1,000	100	0	4.72×10^{-5}	365,000	200	100	3.9213	4.08760	4.0386	4.0278
8	3,000	100	0	4.72×10^{-7}	365,000	1,000	1,000	4.7453	5.19790	5.19910	5.19770
9	2,000	100	0	4.72×10^{-7}	365,000	1,000	1,000	9.6532	10.56940	10.57280	10.58070
10	1,000	100	0	4.72×10^{-7}	3,650,000	10,000	10,000	15.4480	17.9460	17.9585	18.2323
11	1,000	100	0	4.72×10^{-7}	365,000	1,000	1,000	20.9852	23.8367	23.85410	24.09170
12	1,000	100	0	4.72×10^{-6}	365,000	200	100	28.0023	29.6833	29.1868	29.0789
13	1,000	100	0	4.72×10^{-6}	3,650,000	200	100	36.1859	37.8490	37.3579	37.2461
14	1,000	100	0	4.72×10^{-7}	365,000	200	100	146.9160	162.8239	159.6473	158.6269
15	1,000	100	0	4.72×10^{-7}	3,650,000	200	100	280.2410	296.8327	291.8678	290.7893
16	300	100	0	4.72×10^{-7}	3,650,000	200	100	421.4970	482.7085	477.4180	--
17	0	-1000	0	4.72×10^{-7}	3,650,000	10,000	10,000	15.5313	15.3633	15.2814	15.1177
18	0	0	1000	4.72×10^{-7}	3,650,000	10,000	10,000	15.5313	15.3602	15.3599	17.8121
19	1,000	0	0	4.72×10^{-7}	3,650,000	10,000	10,000	15.5313	18.0767	18.0767	17.8128
20	500	100	0	4.72×10^{-7}	365,000	1,000	1,000	38.5638	50.5847	50.7638	47.7035
21	0	-500	0	4.72×10^{-7}	365,000	1,000	1,000	41.0097	39.6778	39.3422	38.1677
22	0	-800	0	4.72×10^{-7}	365,000	1,000	1,000	30.7759	30.3377	30.1456	29.7309
23	0	-200	0	4.72×10^{-7}	365,000	1,000	1,000	90.5320	76.8171	75.5081	66.6374
24	0	-100	0	4.72×10^{-7}	365,000	1,000	1,000	174.7815	117.1566	114.1117	88.4901

Table 1. Concluded

Sequence number	Coordinate distance in meters			Hydraulic conductivity in cm/sec	Time in days	Upper and lower boundary position in meters		Repository shape* and change in head per unit flow rate, in meters/(l/sec)			
	x_p	y_p	z_p			B	A	Point	Line	Area	Volume
25	300	0	0	$4.72x10^{-7}$	365,000	1,000	1,000	62.0047	126.9282	126.7049	91.1571
26	300	100	0	$4.72x10^{-7}$	365,000	1,000	1,000	59.1642	96.1902	97.9269	79.4568
27	0	-1000	0	$4.72x10^{-7}$	365,000	1,000	1,000	29.2830	28.9325	28.7523	28.4167
28	0	-10	0	$4.72x10^{-7}$	365,000	1,000	1,000	1693.80	265.607	240.568	118.2191
29	0	-25	0	$4.72x10^{-7}$	365,000	1,000	1,000	681.091	207.254	195.710	112.7033
30	1,000	100	0	$4.72x10^{-5}$	36.5	200	100	.0005694	.00253612	.0025162	.0022373
31	-1,000	100	0	$4.72x10^{-7}$	365,000	1,000	1,000	20.9769	18.8123	18.8222	18.6719
32	125	0	1000	$4.72x10^{-7}$	365,000	1,000	1,000	20.8791	20.9809	20.9810	23.8502
33	125	5	1000	$4.72x10^{-7}$	365,000	1,000	1,000	20.8790	20.9808	20.9815	23.8509
34	125	5	1125	$4.72x10^{-7}$	365,000	1,000	1,000	18.6737	18.7487	18.7493	21.0656
35	0	0	1000	$4.72x10^{-7}$	365,000	1,000	1,000	21.0321	20.8311	20.8311	23.6304

*L = 250 m, W = 10m, and D = 250 m, when applicable $S_s = 3.281x10^{-5}m^{-1}$

Table 2. Computer Model Results for Various Repository Shapes (Symmetrical Model)

Sequence number	Coordinate distances in meters x_p	y_p	z_p	Repository shape* and change in head per unit flow rate in meters/(l/sec) Point	Line	Area	Volume
36	0	900	0	29.6417	29.5469	29.5473	29.4534
37	0	700	0	32.7893	32.6406	32.6412	32.4945
38	0	500	0	41.0015	40.6434	40.6446	40.2966
39	0	200	0	90.5249	85.8059	85.8190	81.7593
40	0	100	0	174.7745	147.4298	147.4917	128.9628
41	0	50	0	343.5274	228.2399	228.4749	173.8912
42	5000	0	0	1.0034	1.0051	1.0051	1.0047
43	3000	0	0	4.7493	4.7552	4.7553	4.7523
44	2000	0	0	9.6541	9.6677	9.6677	9.6588
45	1000	0	0	21.0321	21.1182	21.1182	21.0657
46	550	0	0	36.0009	36.5391	36.5388	36.2429
47	0	0	5000	1.0034	1.0030	1.0030	1.0047
48	0	0	3000	4.7493	4.7463	4.7464	4.7523
49	0	0	2000	9.6541	9.6452	9.6452	9.6588
50	0	0	1000	21.0321	20.9809	20.9810	21.0657
51	0	0	550	36.0009	35.7329	35.7326	36.2429
52	0	0	250	73.2637	70.71819	70.71423	75.90547
53	0	0	150	118.3480	108.2366	108.2205	129.72777
54	150	0	0	118.3480	168.47071	168.2202	129.72777
55	150	150	150	70.8651	70.61156	70.61224	70.64081

*L = 250 m, W = 10 m, and D = 250 m, when applicable $S_s = 3.281 \times 10^{-5} m^{-1}$

A = 1000 m, B = 1000 m, K = 4.72×10^{-7} cm/sec, t = 365,000 days

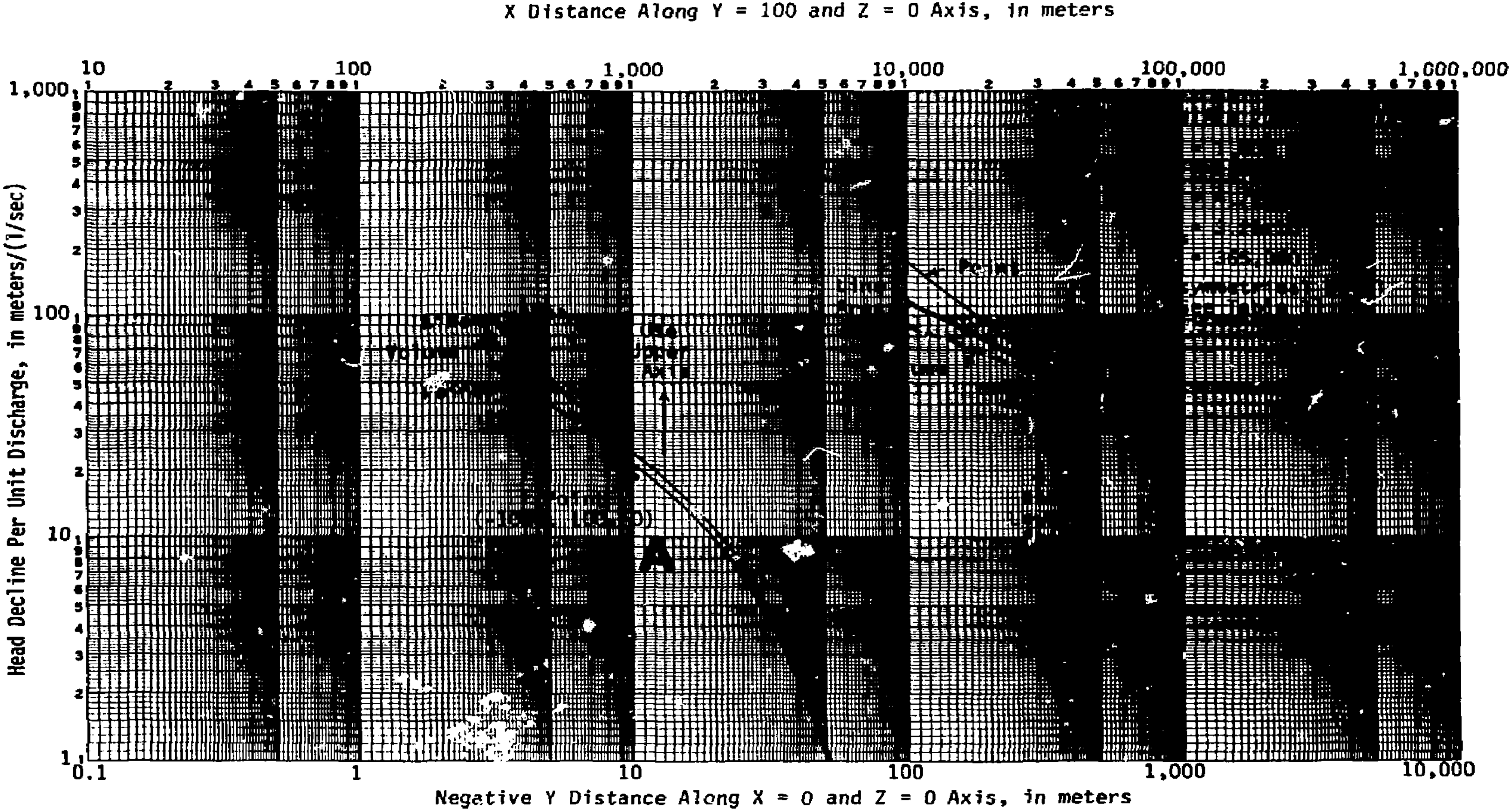


Figure 6. Distance-Head Decline Relationships Viewed Along Asymmetrical Axes, in meters

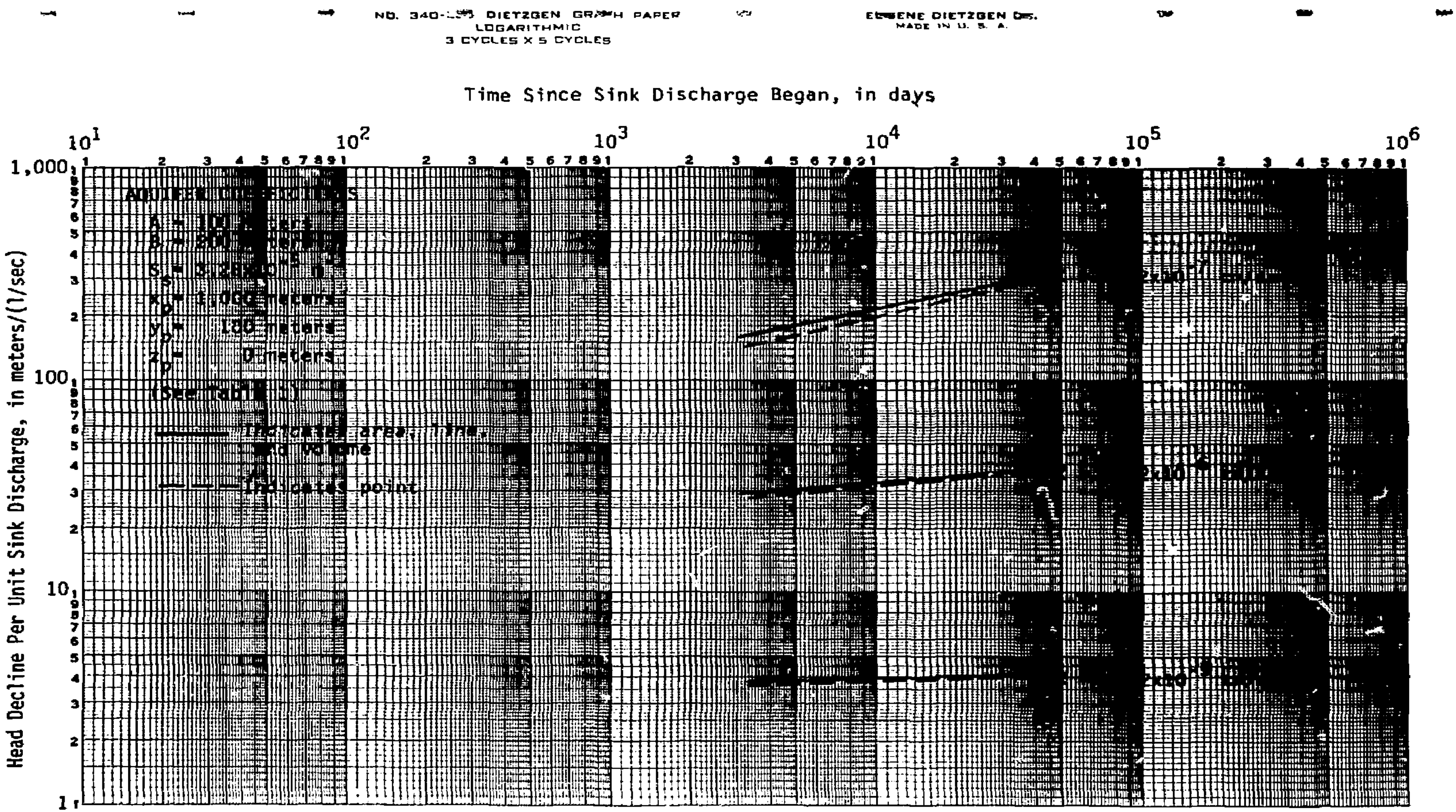


Figure 7. Time-Head Decline Relationships Near Repository As A Function Of Hydraulic Conductivity

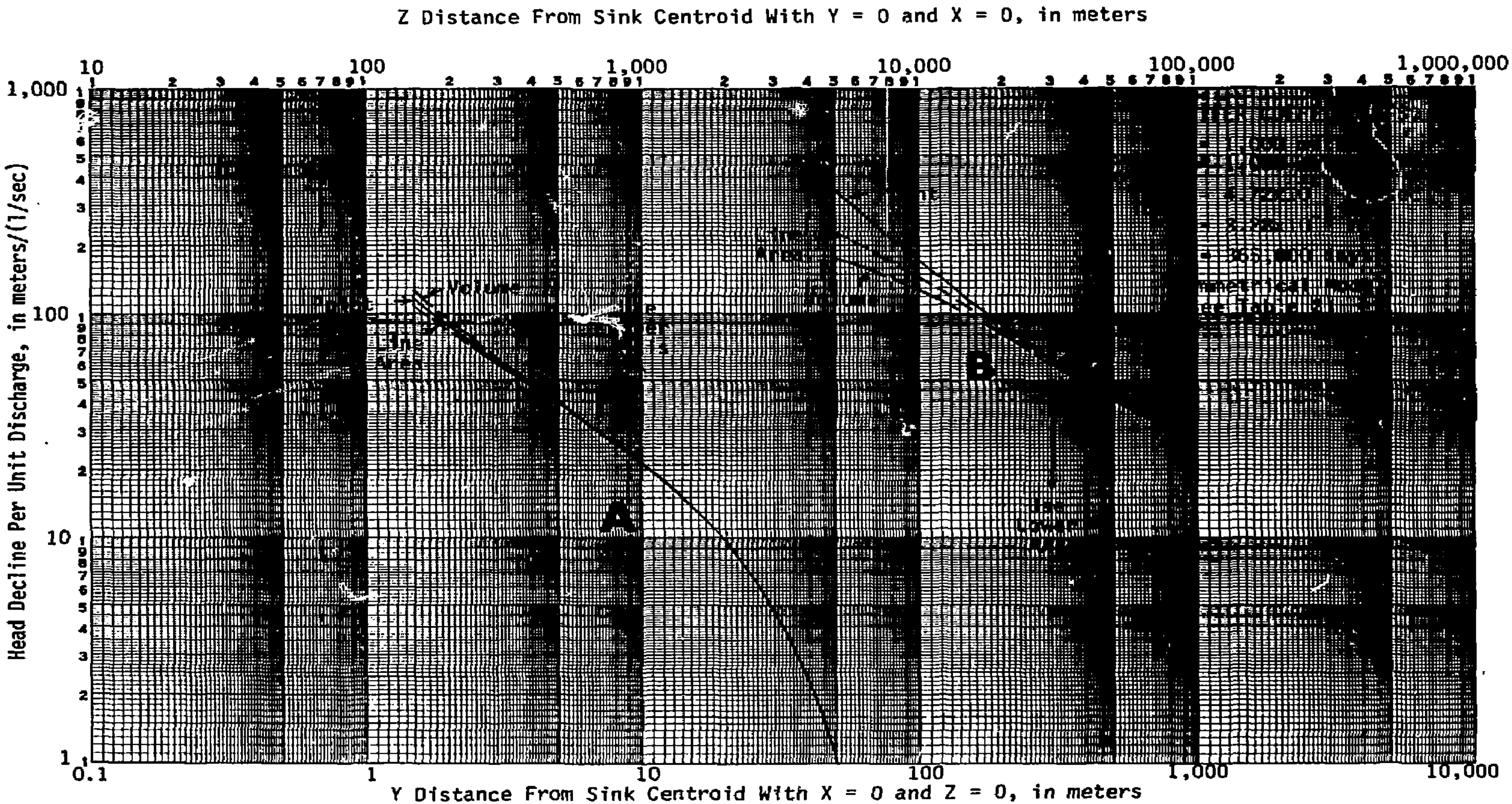


Figure 8. Distance-Head Decline Relationships Viewed From Centroids Of Repository

asymmetrical model runs. In the case shown the flow system thickness is 2000 meters and the curves approach each other in the range of 4000 meters.

Although the response curves approach one another with distance, Figure 6 illustrates clearly that the curves "are" different. First of all, the magnitudes of head declines are different and secondly the slopes of the various curves are different. Notice in the group A curves of Figure 6 that the point response is, in magnitude, smaller than the other shapes. Since the curves of group A are approaching one another with distance, one can realize that the slope of the point response curve is less than the other response curves (at least along the x axis with $y = 100$ and $z = 0$). The slope comparison relates to the mass transport velocities in that flow to the point sink, along the axis displayed, is less than those towards the line, area, and volume sinks. Although the velocities toward the point sink are less than the other shapes along the axis displayed, there are other axes along which the point sink related velocities are greater than the other shapes (see group B on Figure 6). The main conclusion to be drawn from this discussion is that the velocity distribution around the various shaped sinks is asymmetrical. Although by conservation of mass principals, the total flow towards the sinks of various shapes is equal, the flow velocity distribution is distorted in three-dimensional space.

Figure 7 illustrates the time-response and permeability related response associated with the repository shapes as viewed at a point about 3 aquifer thicknesses from the sink centroids. The main conclusions to be drawn from this comparison is that the point sinks, in all cases of varying permeability, always have less head declines than the other shapes and that the comparative difference in heads decreases with time. During early times, Figure 7 shows significant differences in heads between the point and other repository shapes. Excess water taken from storage elsewhere in the immediate vicinity of the point sink accounts for this difference. Not only is there a space distortion (see previous paragraphs) but there is also a time-wise variation involved.

Figure 8 illustrates a selected group of distance-response curves for the symmetrical model. Figure 8 shows the distance-head decline relationships from the views of along the major coordinate axes. From these views, the comparative distortions of head declines for the various repository shapes is less than the asymmetrical case (compare Figures 6 and 8). Notice also in Figure 8 that the distance out to which all shapes have essentially the same head decline is considerably less than twice the aquifer thickness.

The explanation for the relative magnitudes of head declines with distance, as illustrated in Figures 6 and 8 may be generalized by considering where the centroid of the sink shape is located relative to the observation point. The head declines will generally be greatest the closer one is to this centroid. However, as the observation point gets close to the sink, it becomes a matter of the relative magnitudes of the dimension L, W, and D and the closeness of the observation point to the edges of the repository boundaries.

An important concept should be made concerning whether a flow-rate versus a head condition should be specified on the equivalent point, line, or area replacement of the actual three-dimensional repository. The model simulations of this section used a constant and equal flow-rate boundary condition on the repository shapes. An examination of the head decline distributions close to the sink boundaries show the large differences that are experienced (see Tables and Figures). As one goes away from the various shaped sinks, the head distributions approach one another. Now, it should not be difficult to imagine the relative magnitudes of sink flow rates that would result if one would specify a constant and equal head on each of the sink shapes. It is beyond the scope of this project to describe the proper way to adjust the size of each of the equivalent shaped sinks such that both the head and flow rate properly simulates the three-dimensional repository. It may be mentioned, however, that this type of study could be made (see Prickett and Lonnquist, 1972, page 61 for a similar analysis). The results of this shape equivalent study indicates the importance of looking into this question in some future research.

GENERAL COMMENTS AND COMPARATIVE ANALYSIS -- SOLVED EQUATIONS

On the basis of the above example solved equation discussion one may make further general comments and draw some conclusions concerning when to use one-, two-, or three-dimensional models for radionuclide transport analysis.

1. The use of the coordinate system transform is again illustrated to be a powerful technique for reducing a three-dimensional "flow" problem down to either two- or one-dimensional forms. The problem must, for these cases, be strictly symmetrical in the directions of one or more of the axes.

2. A "flow" problem may be symmetrical in head distribution but asymmetrical when further consideration is given to mass transport. Three-dimensional dispersion in a one-dimensional uniform flow field is an obvious example of this concept where symmetry in flow and mass transport differ.

3. The use of a moving coordinate system, on occasion, simplifies the equations of mass transport. An example of this would be in having the coordinate system origin move with the mean flow and having the dispersion equation in terms of distances from this mean-flow center. Application of this concept is restricted to straight line steady flow, however.

4. There are problems which result in part of the flow field being three-dimensional while other parts are essentially two-dimensional. The effects of partial penetration of a well or repository in an aquifer is an example of this case wherein flow beyond about two aquifer thicknesses can possibly be considered a good approximation of two-dimensional flow.

5. As with the conclusions drawn from the basic equation section of this report, a reaffirmation of the concept of error arises again in ignoring one of the directions of dispersion. A comparison of concentration distributions of three-dimensional dispersion in a one-dimensional flow field reconfirms this conclusion. Ignoring any direction of dispersion yields a higher concentration distribution than the actual true three-dimensional phenomena.

6. The equivalent replacement of a three-dimensional repository shape in a one- or two-dimensional model study should be a line sink. Distortion of head distribution, mass transport velocities, and time-related changes in flow result if a point replacement is used for the actual three-dimensional repository shape.

SECTION 4. GEOHYDROLOGIC CONSIDERATIONS

The entire discussion above concerns the hydrology of groundwater formations that are homogeneous and isotropic. Thus, the comparative analyses of three-versus two- and one-dimensional flow in the above work shows where a three-dimensional representation is needed for the homogeneous and isotropic cases only. In reality, homogeneous and isotropic conditions are rare, if not nonexistent. The comparative analyses above show even under certain ideal and simplified conditions, that there is on occasion a need for full three-dimensional representation of mass transport of radionuclides.

The above analyses also assume that the flowing fluid is homogeneous. We can come closer to idealizing the fluid conditions to homogeneous situations than we can geologic formation homogeneity. However, consideration of heterogeneous fluids must be addressed as it relates to dimensions used in modeling radionuclide transport. The existence of density gradients, multiphase flow, and temperature related viscosity variations demand attention.

External boundary conditions and configurations are also extremely important in the choice of one-, two-, or three-dimensional models for radionuclide transport since these boundaries produce a direct control over the flow directions.

The following discussions thus address these further complications to the modeling of radionuclide transport processes and outlines the dimensionality problems that accompany such complications.

HETEROGENEITY OF GEOLOGIC FORMATIONS

Freeze and Cherry, 1979, give an adequate definition of formation heterogeneity for our purposes as follows. If the hydraulic conductivity is independent of position within a geologic formation, the formation is homogeneous. Freeze and Cherry continue by defining three broad classes of geologic environments that represent heterogeneous environments as 1) layered heterogeneity, 2) trending heterogeneity, and 3) discontinuous heterogeneity. Expansion in discussion of these three types of heterogeneity follows.

Layered heterogeneity is common in geologic formations and most frequently is related to essentially horizontal sedimentary and unconsolidated deposits and the process by which the layers were formed. In this case, each horizontal layer might be considered homogeneous, but heterogeneous in the vertical direction as one passes from one layer to the next, each layer having a different hydraulic conductivity as shown in Figure 9 A.

Trending heterogeneity, as illustrated in the horizontal plan view of Figure 9 B is a typical result of sedimentation processes that create deltas, coastal plains, and alluvial fans. Freeze and Cherry, 1979, indicate that trending heterogeneity in large consolidated sedimentary formations can attain gradients of 2-3 orders of magnitude in a few miles. Formations whose conductivity is a function of joint and fracture concentration are further examples of this type of trending heterogeneity.

Discontinuous heterogeneity occurs in the presence of faults or other large-scale stratigraphic features as illustrated by Figure 9 C as an example. These discontinuities may occur in the vertical section as well as the horizontal plan view.

The existence of heterogeneous hydraulic conductivity adds a further complication to the modeling of radionuclide mass transport. Heterogeneity is one of the principal reasons why researchers turn to numerical techniques for solutions rather than to struggle with highly complex mathematical or analytical formulations.

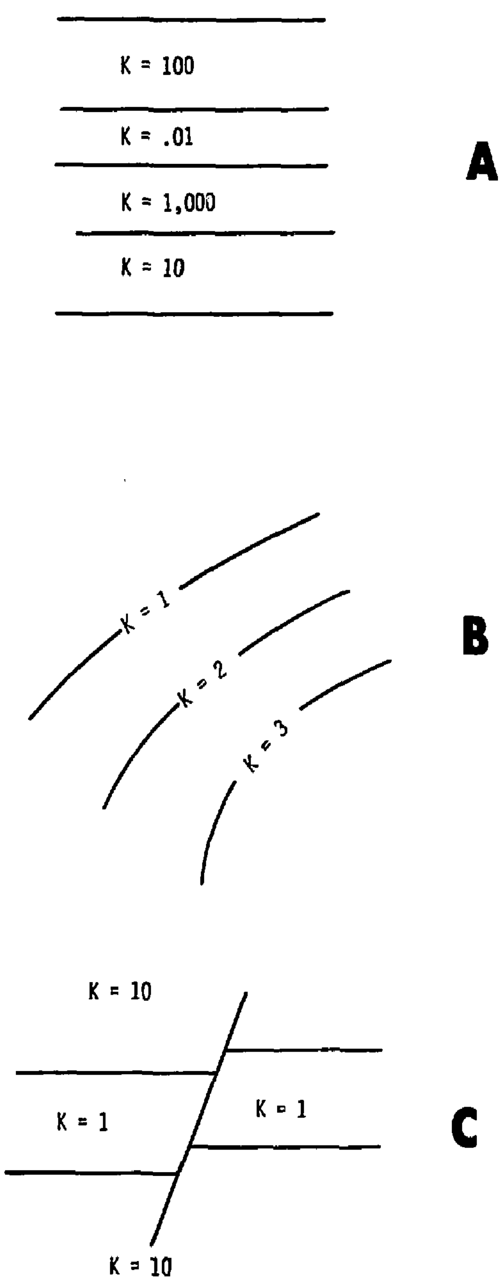


Figure 9. Vertical Cross Section Showing Layered Heterogeneity (A), Horizontal View Showing Trending Heterogeneity (B), And Fault-Type of Heterogeneity (C).

The number of analytical solutions to flow problems in heterogeneous geologic formations is small as compared to the homogeneous counterpart. Most of the analytical formulas available in the literature (see Walton, 1970, for examples up to that date) apply to the layered heterogeneity type. Leaky artesian conditions (layered aquifer, confining layer, and source bed properties), storage from confining layers (aquifer and contrasting confining bed properties), and the multilayered aquifer/confining layer sequence are examples of the available layered heterogeneity analytical solutions. However, two of the basic assumptions that appear in most of these theories and solutions is that radial symmetry in the plan view exists and vertical flow only occurs in the cross section of confining layers. In other words, a three-dimensional analytical representation of radionuclide transport in a heterogeneous environment is very restrictive.

One may draw the conclusion at this point in the report that the existence of heterogeneity is a condition which forces the researcher to consider three-dimensional models more than he would when dealing with homogeneous environments. The general rule for neglecting one or more of the dimensions in a flow model still, however, is generally the same as before. If all of the flow is parallel to the layer or discontinuity or perpendicular to the trend heterogeneities, then one may consider dropping one of the dimensions from a full three-dimensional analysis. However, the existence of dispersion and diffusion phenomena in a heterogeneous formation still presents problems that may not be ignored.

Symmetry and moving coordinate systems can also be utilized in studying flow in heterogeneous environments. On occasion, a curvilinear coordinate system laid out along the axes of the heterogeneity configuration may eliminate the necessity of even another dimension in the analysis of sinuously varying heterogeneities.

ANISOTROPY

According to Freeze and Cherry, 1979, if the hydraulic conductivity is independent of the direction of measurement at a point in a geologic formation, the formation is isotropic at that point. If the hydraulic conductivity varies with the direction of measurement at a point in a geologic formation, the formation is anisotropic at that point.

In an anisotropic formation there are three principal directions of anisotropy which are always perpendicular to one another. The hydraulic conductivities in these directions are maximum. If the magnitudes of the three principal direction hydraulic conductivities are equal, the formation is isotropic, whereas an anisotropic formation will have differing magnitudes.

The primary cause of anisotropy on the small scale is the orientation of clay minerals in sedimentary rocks and unconsolidated sediments. On a large scale there is a relationship between layered heterogeneity and anisotropy. In the layered case, each layer may be homogeneous in two directions but anisotropic considering flow in the remaining direction.

The usual mechanism for dealing with anisotropic hydraulic conductivity is to align the coordinate system axes along the principal directions of anisotropy. Derivation of analytical formulas is made simpler by this mechanism. In actuality, considering the cross products possible there are six components of hydraulic conductivity in addition to the three principal components. The authors of this report know of no analytical solution for flow or mass transport that includes all nine components applied to a real field problem. What you do see in the literature are solutions for anisotropic conditions that consider only principal anisotropy directions aligned coincident with the coordinate axes and the assumption of cross-product permeabilities equaling zero.

In homogeneous but anisotropic groundwater formations analysis is complicated by the fact that streamlines and equipotential are not orthogonal. It may be mentioned that a "transformed section" may be constructed for some anisotropic flow problems that allows application of orthogonality of streamlines and equipotential lines (see Freeze and Cherry, 1979) for solutions. This technique involves expanding one of the scales of the region of flow, applying isotropic equations, and then inverting the results. This technique does not reduce a three-dimensional problem down to a two- or one-dimensional form and therefore, is not totally applicable to the problem at hand.

The main conclusion to be drawn herein is that the presence of anisotropic conditions puts additional restrictions on the use of two- or one-dimensional models in place of full three-dimensional ones. Here again, as above, one must examine flow directions of the problem and judge whether any component of flow can be neglected along one or more of the principal directions of anisotropy. If the resulting judgment in flow is anything but zero, errors will occur in lower order dimension models.

Anisotropic conditions not only apply to hydraulic conductivity but also to dispersivity and its effect on mass transport. The directional properties of the coefficient of dispersion is also (like conductivity) a nine component problem although the nature of the dispersion process is the cause rather than the permeability variations. No mathematical solutions are known for the situation involving both dispersion and hydraulic conductivity anisotropy. As has been said repeatedly dispersion is a three-dimensional phenomena and adding to the problem, the complication of anisotropic conductivity can make the choice of one-, two-, or three-dimensional models lean toward the higher order simulations.

DELIMITING BOUNDARY CONDITIONS

The equations discussed above were derived mainly on the basis of infinite extent groundwater formations and geologic strata. Some of the equations assumed parallel upper and lower no flow boundaries. The presence of delimiting boundaries, whether they for example be no flow, constant flux, or constant head vastly controls the direction of flow in the problem under study.

We have seen above that the geometry of sources and sinks have a profound effect on whether a problem can be reduced from a three-dimensional representation down to either a two- or one-dimensional formulation. The keys to choosing minimum dimensions for flow modeling were based on the flow directions produced by the source or sink and the degree to which one could take advantage of symmetry. The same sort of keys apply to boundary conditions as they also affect flow directions.

External or delimiting boundaries come in a variety of forms and shapes with prescribed conditions. There are three basic types of prescribed boundary conditions; first the prescribed potential, second the prescribed flux, and third the free surface boundary. The prescribed potential boundary exists in groundwater situations when the porous formation is in contact with a fluid continuum--a boundary along which there is no change in potential such as a tunnel, the sea, large lake, or perennial river. The prescribed flux boundary exists in groundwater situations where the flow normal to the boundary is fixed in space and time. The condition of vanishing flux or zero flow is a special case of the prescribed flux boundary and is called an impervious boundary. In two-dimensional flow, an impervious boundary is also a streamline. The free surface boundary is used to denote that surface on which the pressure is atmospheric.

Although the prescribed conditions along the above types of boundaries are important in the solution of problems it is more important, in our task, to consider the geometric shape of the boundaries as it relates to dimensions needed for modeling radionuclide transport.

The shape of the boundaries delimiting the region being modeled can be made up of an infinite variety of shapes. For a simple example in a typical vertical cross-sectional model in two-dimensions, the missing third dimension is usually prescribed to be of unit thickness. This amounts to specifying two limiting and parallel impervious boundaries spaced either side of the unit thickness. At the other extreme the two-dimensional plan view groundwater model may be confronted by edge boundaries such as fully penetrating meandering rivers, coastal shore lines, or lakes. In this type of plan view model one may assume that the top and bottom conditions are no flow boundaries so that the flow in the vertical third dimension can be ignored.

Strictly speaking, if the boundary shapes have variability in any one of the three dimensions, then one must use a model that includes the capability to map that variability. A first test to check on this would be to slice numerous cross-sections of the groundwater system normal to the axis desired to be eliminated in the analysis. If all cross sections produce identical boundary shapes, then you can then further consider eliminating that dimension--the further exceptions would be made on the basis of heterogeneity, anisotropic conditions, source of sink configuration, and dispersion effects.

Just as the viewing distance from the source and sink has something to do with whether one can adequately model a three-dimensional with a lower dimension model, so does the viewing distance from the boundaries. If one is sufficiently removed, spatially, from a boundary of complex shape, the solution to a three-dimensional problem may be reduced to consideration of a lower number of dimensions. Despite the information available about viewing distance from such items as partially penetrating wells where a three-dimensional problem becomes a two-dimensional one (beyond two aquifer thicknesses), no generalization can be offered for equivalent acceptable distances from shaped boundaries.

According to Freeze and Witherspoon (1967), in a complex topographic and geologic system, small differences in the location of points of recharge can make the difference between recharge water entering a minor local system or a major regional system. The implications of this are thus disturbing when considering eliminating even one-dimension from a radionuclide waste repository modeling study.

INITIAL CONDITIONS

When the problem under study is time dependent (unsteady flow), certain conditions, called initial conditions, must be specified everywhere in the region being considered at the particular instant of time at which the physical process begins. Example initial conditions would be hydraulic head or pressures existing at every point in the domain under study. Usually, the head or pressure distribution used as initial conditions represents a steady-state condition.

In the event that one would like to eliminate one or more dimensions from the analysis on the basis of initial condition symmetry or uniformity, the same cross-sectional test can be used as was described in the delimiting boundary condition section above.

HETEROGENEOUS FLUIDS

The above discussions have been made on the basis of an assumed homogeneous fluid. There is the distinct possibility that the regional and local flows related to radionuclide transport will involve more than one type of fluid. Existence of steam, gas, oil, and water of varying density are all to be expected somewhere in the hydrogeologic system.

The coexistence of more than one type of fluid in a porous medium such as gas and water does not of itself invalidate the concept of homogeneous fluid flow. First of all one of the fluids may be immobile while the other is mobile. In addition, if the water and gas mixture is flowing at pressures that maintain the gas in solution, its only effect will be to reduce the viscosity of the water as it flows from place to place.

According to Muskat, 1949, as long as other phases are immobile, the flow of the water phase may be considered as equivalent to that of a homogeneous fluid, except that the numerical value of the hydraulic conductivity must be adjusted to take account of the effect of the other phases. What Muskat was getting at was a description of a moving boundary problem. In particular a permeability must be associated with each fluid phase as if the individual phases were flowing separately in parallel channels. And their interaction is expressed by the fact that the numerical values of the permeability for the separate phases are determined by the volumetric distribution of the fluid saturation of the rock among all the phases. The permeability is no longer a constant but is a separate function for each phase of the local phase distribution within the porous medium. Thus, superposed on its granular structure, which is dynamically characterized by its homogeneous-fluid permeability, a porous medium carrying a heterogeneous fluid may be considered as possessing a local structure defined by the saturation distribution of the several fluid phases, which in turn determine the local permeabilities for the individual phases.

The sensitivity of the heterogeneous fluid possibilities as it relates to regional (as opposed to local) transport of radionuclides is controversial. Certainly the volume of the overall system being studied, in relation to the volume of rocks actually containing other phases of fluids, must dictate to a large extent the overall accuracy loss if one were to ignore these complications.

Although not totally a problem of different phases, the density gradients due various solute concentrations or temperature variations (due both the earths' natural thermal gradient and heat produced at the repository site) cause additional viscosity and buoyant forces that lead to heterogeneous fluid flow concepts.

Much like any other boundary condition, the symmetry or uniformity of the areas of heterogeneous fluids must be accounted for if it is desired to reduce the three-dimensional scenario down to two or one-dimensional form.

GENERAL COMMENTS ON GEOHYDROLOGIC CONSIDERATIONS

On the basis of the above discussions, one may make general comments and draw conclusions concerning when to use one-, two-, or three-dimensional models for radionuclide transport analyses.

1. The existence of heterogeneous and anisotropic conditions may cause flow in unexpected directions and thus complicate an analysis. The use of two- or one-dimensional flow models in this instance must be predicated upon the third dimension flow being zero.

2. Consideration of boundary and initial conditions are very important in choosing the number of dimensions for modeling nuclide transport. A test, by cross-section comparisons perpendicular to the coordinate axis to be eliminated, can show when a lower order dimensioned model may be considered for use.

3. The existence of large volumes of heterogeneous fluids presents a moving boundary problem to be dealt with. Not only does one need to consider all of the dimension symmetry and uniformity criteria of stationary boundaries given in 2 above, but one needs to examine the movement of the boundary in time as the physical process is likely to take place.

SECTION 5. NUMERICAL MODELS

The basic concepts of one-, two-, and three-dimensional modeling of radionuclide transport and when a three-dimensional scenario may be reduced in dimensions has been essentially outlined by the discussions given in Parts 1. and 2. above. In actuality, the model used is of secondary concern in the study of radionuclide transport. The choice of one-, two-, or three-dimensional models of any sort should be based first upon the problem boundary and initial condition scenario.

It is of interest to note while numerical techniques allow solution of extremely complex problems, that numerical models all contain sets of approximations that may affect the accuracy of the solution. Some of these approximations concern space dimensions and thus have a bearing on the two- versus three-dimension model comparisons addressed in this report.

The purpose of this section of the report will be to outline the problem areas of model approximating procedures to the extent that the one-, two-, and three-dimensional solutions are fully understood. The discussion is in order o⁻ a brief description of the major techniques used in numerical simulation of mass transport, a library and description of present three-dimensional models used for both flow and mass transport, and then a discussion of the approximating procedures for the various techniques and how they affect the dimension subject accuracy.

BRIEF BACKGROUND ON NUMERICAL TECHNIQUES

Briefly, there are two major types of numerical techniques available for studying radionuclide transport problems: i.e., the finite-difference and finite-element techniques. A cursory background of these two techniques is given below as a beginning point for further discussion concerning these techniques.

In the case of finite-difference models, the continuous derivatives of the appropriate differential equations are replaced by ratios of the changes in variables over a small finite interval defined by a finite-difference grid. The intersections of the grid are called nodes. The scheme here is an approximation of the true aquifer but reduces a continuous boundary-value or initial-value problem to the solution of a set of algebraic equations. Since there is one algebraic equation for each node of the model grid, a large set of simultaneous equations must be solved. Recently, the finite-difference method has been applied to almost every conceivable groundwater flow problem imaginable. The method is essentially fully developed and numerous publications are available which describe and apply the technique to problems in one-, two-, or three-dimensions. Presently, finite-difference models are very popular, are easily understood, and are applied to nearly the full range of groundwater flow problems that exist.

Two main approaches are available for solving the differential equations of groundwater flow using the finite-element method. Finite elements may be used in conjunction with either a variational formulation of or a Galerkin method of generating approximate integral equations.

The variational formulation is where some quantity F, when minimized, yields the solution to the differential equation of interest. The quantity F is defined as an integral functional of the unknown heads over the whole aquifer domain. The process of minimizing the functional of the whole aquifer domain is usually accomplished by the Ritz method in conjunction with subdividing the aquifer into finite elements. The finite elements generally consist of simple shapes such as triangles or quadrilaterals joined by nodes at the boundaries of each element. The functional is then minimized by writing the functional as piecewise linear functions applicable to each element, differentiating the element functionals with respect to the heads, and solving the resulting set of algebraic equations.

Briefly, Galerkin's method assumes there exists an infinite series which exactly represents the solution of the differential equation of interest. The infinite series solution is made up of unknown coefficients, to be determined, and a set of known basis functions. The original Galerkin formulation assumed that each basis function was defined over the entire domain of interest. However, with the computer, the basis functions are defined as piecewise continuous functions over subdivided areas (finite elements) of the total region. The finite elements most often used here are the triangular and the deformed isoparametric quadrilateral. Since digital computers work with finite numbers, the exact solution is not realized and an approximation is thus sought. The difference between the exact and the approximate solution is called a residual R. The Galerkin method continues by attempting to minimize the residual R by considering yet another set of known basis functions. In the Galerkin method the two sets of above basis functions are the same. Using the theory of orthogonal functions, the residual R is forced to a minimum by requiring that R be orthogonal to all possible values of the chosen basis functions. The result of this total process is a set of N approximating integral equations where N is the total number of element nodes of the model. The N equations are solved by numerical integration yielding the unknown coefficients spoken of above completing the series type of solution.

Each of the above techniques have their advantages and disadvantages. There are also several numerical models existing that combine the best parts of each technique. And on occasion, numerical models of the above type are extended in their application by the addition of subsidiary techniques such as random walk, discrete kernel generators, and stochastic model subroutines. In any event, we shall concern ourselves only with the types of approximating procedures that are inherent in the two major techniques and applicable to three versus two dimensional models.

SELECTED THREE-DIMENSIONAL MODEL CODES

It is of some interest to note that considerable progress has been made in the development of three-dimensional numerical models in the last five years. Most of the development came during the years 1975-1976. It seems as though, prior to this time, that researchers were still getting accustomed to one- and two-dimensional models, arguing about the superiority of one numerical scheme over the other, and racing toward two-dimensional development of mass transport models.

Table 3 is a listing of three-dimensional models that were found as a result of a selected search of the groundwater literature and the Holcomb Research Institute (Butler University, Indianapolis, Indiana) International Clearinghouse on Groundwater Models. The models listed in Table 3 range in complexity from quasi 3D saturated-steady-flow models up to saturated/unsaturated transient models with solute transport, radioactive decay, compaction, and ion exchange reactions. The list of models and the solved processes claimed is impressive.

A comparable list of two-dimensional models is not given since they are not only voluminous but are readily available in Bachmat, et. al., 1978. Very little is lost here in the comparison since the three-dimensional models of Table can be reduced to two-dimensional form by setting appropriate parameters to zero.

Forty-eight three-dimensional groundwater models are listed in Table 3 of which twenty-seven are flow models. Of these, 20 handle only the saturated zone, and seven can handle either the saturated or the unsaturated zone. Specializations include two agricultural models, one cost and pumping optimization model, two models connected to surface water systems, one model that handles seepage faces, five models that specify themselves as quasi

Table 3. Summary of Selected 3D Models

Modeler	Hydrologic zones or phases	Processes	Method of solution	Availability	Past applications	Documentation	Date completed	Institution	Special Features
Wilsdon	saturated	steady flow, head prediction	FE	yes	field	listing & description, users manual in progress	Sept. 1976	Australian government	core & mass storage
Blanc	saturated, confined or unconfined	steady or unsteady flow, head prediction	FE or FD, point or block successive over-relaxation	no	some field	?	?	ABLAB, France	flexible mesh size & configuration, multilayered
Prudhomme, Henry & Biesel	saturated, confined or unconfined	steady or nonsteady flow, head prediction	FD, Gauss-Seidel w/line successive over-relaxation	no	many field	Listing & manual	1968	Geohydraulique, France	user oriented, possible surface connection
Cloet O'Orval et al	saturated, confined or unconfined	steady or unsteady flow, head prediction	FD, Gauss-Seidel	no	?	?	1972-1977	BURGEAP, France	multilayered, hierarchy of grids
Trescott & Larson	saturated, confined or unconfined	steady or unsteady flow, head prediction	FD, strongly implicit	yes	many field	complete	1976	USGS	multilayered, storativity of aquitards, user oriented
Kuiper	stream & aquifer	steady flow, stream-aquifer relationship	FE, subdomain variant of weight residual	yes	little field	poor	Dec 1976	Iowa Geological Survey	multilayered, specific to Iowa
Narasimhan	unsaturated & saturated	steady or unsteady flow, deformation, heads predicted	integrated FD	yes	none, general algorithm-academic exercise	complete	Feb 1975	UC Berkeley	Elastic or nonelastic deformation, hysteresis, versatile

Table 3. Continued

Modeler	Hydrologic zones or phases	Processes	Method of solution	Availability	Past applications	Documentation	Date completed	Institution	Special features
Verge & Frind	unsaturated & saturated	steady or unsteady flow, predicts piezometric & capillary head	FE, Galerkin	yes	field: flow in vicinity of radioactive waste facility	complete	October 1975	University of Waterloo, Ontario	several unsaturated strata, specific storativity, arbitrary anisotropy, user oriented
Freeze	saturated & unsaturated coupled to stream	Darcian nonsteady flow and open channel flow	FD, line successive overrelaxation	yes	research, field once on an experimental water shed	complete	1971	IBM, US	no overland flow, storativity, soil moisture retention, versatile, large computer time & storage requirements
Barends	saturated or semi-saturated	steady & unsteady flow, gives heads & flow nets	FE or Gauss-Seidel or Gauss elimination	?	field	complete	December 1975	Netherlands Laboratory or Soil Mechanics	variety of options, interfaces
Lantz et al	gas & water pressure & phase saturation	flow, geothermal flow	FD-LSOR or direct inversion	no	?	complete	1975	INTERCOMP	2 modifications: geothermal model & fractured matrix model, user oriented
Gupta, Tanji, & Luthin	saturated	convection & dispersion	FE, Galerkin	yes	field	user manual and examples	November 1975	UC Davis	stability under extreme conditions, multilayered aquifer
Pinder & Cole	saturated	convection & dispersion	FE, Galerkin	?	?	not available	1974	Princeton University	special equation solver
Segol	saturated & unsaturated	convection, dispersion, decay, & adsorption	FE	yes	none yet	complete	August 1976	University of Waterloo, Ontario	user oriented element size limited by computer

Table 3. Continued

Modeler	Hydrologic zones or phases	Processes	Method of solution	Availability	Past applications	Documentation	Date completed	Institution	Special features
Lantz et al	saturated	convection, dispersion, decay, & adsorption	FD, line successive over-relaxation	no	many field	complete	1975	INTERA, US	user oriented, convergence under extreme conditions
Cazal	saturated	conservative convection & conduction, noncoupled flow, steady state	FD, point successive over-relaxation	no	none, program is in experimentation	none	January 1977	Universite de Bordeaux III, France	multilayered aquifer, instable for extreme parameter contrasts, wells
Kitching	saturated, confined or unconfined	unsteady, analyzes pump tests	FD, successive over-relaxation	no	some field	description only	1976	Institute of Geological Sciences, London	axial symmetry, cylindrical coordinates
O'Neill	saturated	conservative, convection & conduction, coupled with flow	isoparametric FE with Galerkin solution	after publication	none	in preparation	1977	Yale University	porous medium with double porosity-fractures & pores, temperature & flow coupled thru viscosity, special solution scheme, different velocity in pore & fractures
Sorey	saturated	conservative, convection & conduction, coupled flow	Integrated FD	yes	research & field	complete	June 1974	USGS	heterogeneous, isotropic, compressible porous medium, no sources or sinks, conductive solid phase, nonhomogeneous liquid, thermal equilibrium between solid & liquid, numerical dispersion restricts step size, user oriented
Narasimhan	saturated zone of compressible groundwater	flow, coupled elastic and nonelastic deformation	Integrated FD	yes	none	manual & references	1976	UC Berkeley	nonlinear state functions, stress dependent permeability and void ratio, arbitrary sources and sinks, general coordinates
Pinder	saturated	subsurface flow & transport	general FE scheme completed with a block iterative equation solver	yes	?	complete (?)	1976	Princeton University	general purpose code for solving transient, nonlinear, partial differential equations in one or two dependent variables

Table 3. Continued

Modeler	Hydrologic zones or phases	Processes	Method of solution	Availability	Past applications	Documentation	Date completed	Institution	Special features
Narasimhan & Witherspoon	saturated, single compressible fluid	conduction, convection, elastic or nonelastic vertical deformation	integrated FD, accelerated iterative scheme	yes	none	complete	1976	UC Berkeley	Arbitrary heterogenity, isotropy, nonlinear state function, coupled flow, heat & deformation, automatic adjustment of time step
Lantz et al	saturated, heterogeneous confined layer	nonsteady flow, convection, dispersion, radioactive decay, adsorption desorption; forced & natural thermal convection, conduction & dispersion	FD, line successive-relaxation or direction inversion	yes	some by USGS	complete	1975	INTERA & INTERCOMP	source-sink terms, single solute, concentration & temperature dependent density & viscosity, new option of N constituents, first order reactions, pressure effects on enthalpy, user oriented
Joradat Blanc	saturated, water supply system	cost determination, flow	LP	?	?	?	?	Arlab, France	cost includes drilling, pumps & surface network, conjunctive simulation & optimization, static
Prickett & Lonnquist	saturated, confined or unconfined	steady or unsteady flow, leakage thru confining layer	FD, iterative alternating direction implicit	yes	many field	complete	1971	Illinois State Water Survey	quasi-3D, user oriented, multilayered
Kitching	two layers separated by clay, phreatic or saturated	steady or unsteady flow, leakage thru clay	FD, alternating direction explicit	no	some field	complete	1974	Institute of Geological Sciences	isotropic aquifer
Barriere, Gaillard, Jardin, Jouhet & Normand	saturated & unsaturated root zone	steady or unsteady flow to determine irrigation distribution	FD, Gauss elimination for steady flow, alternating direction implicit for unsteady flow	no	some field	complete	1975	SOGREAH, France	designed for agricultural studies, input includes crop information, control card options, user oriented
McCracken & Voss	saturated	transient flow & transport	FE	limited	?	?, limited availability	1976	Princeton University	general purpose code, user must prepare "driver" program to establish form of partial differential equation

Table 3. Continued

Modeler	Hydrologic zones or phases	Processes	Method of solution	Availability	Past applications	Documentation	Date completed	Institute	Special features
Robertson	saturated & unsaturated	steady or unsteady flow, vertical perc. from ponds or perched groundwater, dispersion, radioactive decay, linear adsorption	ponds to perched-analytical to transport eqs; perched flow-2D FD explicit; unsat-1D explicit hop-scotch procedure	property of USGS, unpublished	one	Description published, listing and instructions unpublished	November 1976	USGS	Several reacting solutes, perched water bodies, quasi-3D, custom designed to Idaho sight
Levassor	mono or multilayered connected to surface water	flow, linearity of system, superposition	FE, simplex	yes	little field	operating instructions programmer oriented	1975	Ecole des Mines de Paris	multilayered connected to rivers, optimization of well field, exploitation, quasi-3D
Shibasaki, Kamata, Harado, Miyamoto, Masuhara, Murakami	saturated, 2 aquifers	flow, leakage, squeezing & subsidence	FD, alternating direction implicit	?	?	?	two versions: March 1970 March 1971	Research Group for Water Balance, Japan	quasi-3D, subsidence caused by squeezing from a semi-pervious confining layer
Kamata, Fujisaki & Oka	multi-aquifer system	flow & subsidence	FE, Galerkin	?	under testing	?	October 1976	Research Group for Water Balance, Japan	quasi-3D, forecasts heads and land subsidence in a multiaquifer system
Cooley & Peters	saturated, semi-confined aquifer	steady flow	FE	?	?	?	1972	Army Corps of Engineers	unisymmetric cylindrical coordinates
Neuman, Feddes, Bresler	saturated-unsaturated system with or without plants	unsteady flow, soil evaporation, evapotranspiration due to plant uptake	FE and Gaussian elimination	yes	many field	complete	1974	Agricultural Research Organization, Israel	several plant species, 3D with axial symmetry, maximize rate of evaporation or evapotranspiration subject to Darcy's law, user oriented
Neuman & Witherspoon	saturated groundwater with free surfaces	nonsteady seepage	implicit interative FE with Gaussian elimination	yes, but author's aid is recommended	not widely applied must be used with caution	complete	1970	UC Berkeley	3D with axial symmetry, seepage faces, user oriented

Table 3. Continued

Modeler	Hydrologic zones or phases	Processes	Method of solution	Availability	Past applications	Documentation	Date completed	Institution	Special features
Narasimhan & Neuman	saturated, unsaturated, confined, unconfined	steady or unsteady flow, leaky, nonleaky	mixed explicit-implicit finite elements	?	tested against theoretical & experimental results	under preparation	1976	Lawrence Berkeley Lab & University of Arizona	user oriented, any desired linear or nonlinear relationship between dependent variables & parameters
Chorley & Frind	saturated, multi-aquifer	flow, leakage	iterative FE in aquifers and aquitards	?	?	?	1978	University of Waterloo, Ontario	quasi 3D, multiple aquifers, permeability contrast of at least 2 orders of magnitude between aquifers & aquitards, storage in aquitards
Winter	saturated	steady flow	FD strongly implicit	?	?	?	1978	USGS	flow near lakes
Charbeneau & Street	confined or leaky aquifers	steady or unsteady flow & transport-convection & dispersion	FE, Galerkin	?	?	?	1979	Stanford University	handles point singularities, artificial recharge
Narasimhan & Witherspoon	saturated or unsaturated flow in deformable porous medium	flow, elastic or non-elastic deformation	integrated FD, mixed implicit-explicit	?	10 examples given	at least references on theory algorithm & applications	1979	UC Berkeley	hysteresis, handles soil consolidation, infiltration, drainage & generation of fluid pressures
Gambolati	saturated	time dependent flow, consolidation	FE	?	?	?	1977	IBM Scientific Center, Italy	deviations from Theis
Duguid & Lee	saturated	flow through fractured porous medium	FE, Galerkin	?	?	?	1977	Princeton University	isotropic primary porosity, anisotropic fractures

Table 3. Concluded

Modeler	Hydrologic zones or phases	Processes	Method of solution	Availability	Past applications	Documentation	Date completed	Institutes	Special features
Frind & Verge	saturated, unsaturated	steady or unsteady flow	Galerkin, FE	?	?	?	1978	University of Waterloo, Ontario	flexible, convenient for user, choice of integration schemes & matrix solvers
Rodarte	multiple leaky aquifers	flow	theory only	?	?	?	1976	Universidad Autonoma Metropolitana, Mexico City	equations for large & small values of time
Gambolati	deformable aquifer	flow, horizontal deformation	theory only	?	?	?	1974	IBM Scientific Center, Venice	small deformation in comparison to stress, homogeneous & isotropic media
Bredehoeft & Pinder	multiple leaky aquifers	steady & unsteady flow, leaky thru aquitards	iterative FD scheme	yes	many field	complete	1970	USGS	quasi-3D, storage in confining layers
Neuman & Witherspoon	confined 2-aquifer system	flow	FE	?	?	?	1969	UC Berkeley	infinite, radial aquifer
Jovandel & Witherspoon	multilayered aquifers	transient flow	FE	?	?	?	1969	Pahlavi University, Iran; UC Berkeley	handles up to 13-layer isotropic or anisotropic aquifer

3D or axially symmetric, eight that are multiaquifer and layered with leakage between layers, one that models flow through fractures, one model that is designed to specifically analyze pump tests, and one model which determines flow nets. Of the total, at least eight consider themselves completely documented and available. One of these (see Frind and Verge) has been used for flow in the vicinity of a radioactive waste disposal facility.

There are thirteen solute transport models, all of which handle convection. Of these, eleven handle only the saturated zone, while two handle both saturated and unsaturated flow. Other processes are handled by fewer models. Five handle conduction, seven handle dispersion, four account for adsorption, one allows desorption, four allow radioactive decay, one allows compaction, one handles thermal processes, one is coupled to surface water, one handles fractures, and two are designed for multiple leaky aquifers. Some of the models handle several of the above processes and one says that it can also handle more than one contaminant. At least five models are considered available and completely documented. The model by Robertson and Grove was designed for studying a nuclear waste disposal site in Idaho.

The remainder of the three-dimensional models include items such as compaction and geothermal processes.

A study of the literature concerning these models shows that the main reasons for using a three-dimensional model are because of real-world variability in three dimensions of the geologic and hydrogeologic fluid environments, the three-dimensional variations in shapes of limiting boundary conditions, and the three-dimensional flow to partially penetrating sources and sinks. These conditions have already been discussed in previous sections of this report and do not differ appreciably from the reasons behind the development of the 3D models included in the references and in Table 3.

The items that haven't been discussed are some of the approximations still remaining in the full three-dimensional numerical techniques that influence further thought about three- versus two-dimensional models. That discussion now follows.

FINITE-DIFFERENCE APPROXIMATIONS

One of the basic assumptions used in a rectangular grid finite-difference approximation of a two-dimensional flow equation like Equation (3) is that flow is restricted to the x and y directions only. What this means is that the finite-difference representation of head differentials are in terms of heads measured only at grid intersections, or nodes, lined up at discrete points along the major axes. In this case, the end result of this approximation process is that flow in the finite-difference model is not a true two-dimensional situation but a restricted x-y flow direction situation. The errors involved in this approximation are kept at a minimum by either making the grid interval small in areas where the actual flow is other than strictly in the x and y directions or by lining up the coordinate axes of the grid along the major flow directions. The first lesson to be learned here is that reducing a three-dimension system down to a two-dimensional formulation and then approximating the remainder with a finite-difference scheme involves further consideration of directions of flow. Ignoring this situation may make a perfectly fit three-to-two-dimensional transformed model totally inaccurate because of the x-y finite difference direction assumption. Secondly, it should be realized that even a full three-dimensional finite-difference representation assumes flows are restricted to the x, y, and z directions only. The same type of alignment errors in the three-dimensional model occur as in the two-dimensional representation.

The size of the finite-difference grid also controls, on occasion, the accuracy of the finite-difference approximation. There are occasions where the size of the finite-difference grid does not affect the accuracy of the problem being solved. The key to whether accuracy is impaired by size of grid is dependent on the head, pressure, or concentration distribution. If the variables are straight line functions along the major axes of the coordinate system, there is no error in the finite-difference approximation. For three- or two-dimensional groundwater problems this no error situation is uncommon. For one-dimensional flow problems it is more common. Flow around wells, repositories, lakes, outcrops, and other discharge or recharge points or areas are common instances where close attention should be given to reducing the size of the grid interval to minimize discretization error problems.

Approximating boundary conditions with finite-difference approximations is more difficult than finite-element techniques. Usually, rectangular step-wise changes are made with finite-difference grids along the equivalent smooth or complex real world boundary. A three-dimensional problem is distorted via this type of approximating procedure and is not reduced in importance when passing to a two-dimensional form.

The usual procedure for modeling a three-dimensional groundwater problem is to include a scale distortion in the vertical dimension as compared to the horizontal. Serious errors are commonly involved with this scale distorting procedure particularly where head gradients vary steeply. For example, typical horizontal scales for a regional flow problem are one node per several hundred feet or meters. Typical vertical scales might be only a few feet or meters per node. As a result, vertical transfer of water between layers is concentrated on the basis of large horizontal area contributions from one overlying aquifer to the next. In the event that a repository is located at one of these large scale nodes (where normally gradients would be steep and directionally influenced) errors in flow-rates to or from the repository will occur. As the vertical to horizontal scale contrast increases, so does the error. Quite frequently the situation is somewhat overcome by reducing a three-dimensional problem down to a two-dimensional cross-section problem. In this case more nodes in the vertical section can be used without exceeding core storage. However, you still lose the third dimension when cross-sectional models are used for analysis.

In the mass transport category of study, the scale distortion problems are extremely important since the finite-difference approximating procedures are much the same as the flow procedures.

The accuracy of the mass transport model is directly related to the accuracy of the flow model used for convective and dispersive components of the mass transport model. An accurate representation of gradients (flow velocities) is thus all important. While head distributions may be quite close to the correct values, it is the gradient distribution that is more important in mass transport studies.

Finite-difference grids come in many shapes and forms. The literature includes approximations available for squares, rectangles, triangles, polygons, cylinders, spheres, and curvilinear nets. In general, the use of higher order grid shapes will yield higher accuracy since flow directions and boundary configurations may be modeled more closely.

The time-related discretizing approximations in finite-difference techniques vary from backward, to forward, to central differences along the time axis. Not only is the size of the time increment related to accuracy but so is the method (central differences as an example).

Remson et al., 1971, and Pinder and Gran, 1977, give ezcellent evaluations of the above approximating procedures and their resulting errors with the exception of the vertical/horizontal scale distortion errors. Further study appears to be needed in the scale distortion area.

FINITE-ELEMENT APPROXIMATIONS

Many of the same approximating errors mentioned above in the finite-difference section also apply to the finite-element approximating process. For instance, the spacing size of the element nodes and the overall number of nodes is proportional to the accuracy of the results. Since the finite-element technique is essentially a polynomial fitting procedure, a general increase in accuracy is however experienced compared to the same number of node finite-difference procedures.

The same type of errors in the vertical versus horizontal scale of node spacing is experienced in the finite-element method as the finite-difference method.

Use of higher-order geometric elements such as isoparametric quadrilaterals allows the finite element technique to model more closely complex boundary, source, and sink geometrics. When the geometry of the real world problem is complex, finite elements are superior to finite-difference techniques.

The finite-difference schemes are used primarily for the time-domain in the finite-element technique and have the same approximating error problems associated with them.

Generally speaking, the use of higher order basis functions gives higher accuracy in the finite-element method. In the authors' opinion, however, these higher order basis functions are of dubious value in the vicinity of singularities. The recent paper by Charbeneau and Street, 1979, addresses special problems around singularities.

One may note by reviewing the literature that finite-element models have a tendency to be designed to be special purpose models. In particular, finite-element nets are usually lined up along the likely flow paths. One must be very cautious about this flow-path alignment tendency in that it does not lull the researcher into believing that all solutions, independent of changes of boundary potentials and sink flow rates are of equal accuracy. Since the modeling of radionuclide mass transport may involve a large number of flow direction unknowns, one must be cautions about predesigning the finite-element grid in preferential directions. It would be better to use more elements of uniform spacing rather than fewer elements aligned in specific directions.

USE OF COMBINED NUMERICAL AND ANALYTICAL MODELS

One idea for reducing the number of dimensions needed for modeling mass transport of radionuclides is by combining a three-dimensional analytical formula with a two-dimensional numerical model. For example, a partially penetrating well may be simulated in a two-dimensional plan view model by making an adjustment to the computed nodal head value for fully penetrating conditions. The adjustment for additional drawdown due the partially penetrating condition would come from a standard analytical formula. This combination method works as long as the boundary and initial conditions of the analytical formula and the specified homogeneity/anisotropic parameters mesh with the numerical model. Prickett and Lonnquist, 1971, show how this analytical and numerical model combination works for simulating wells of various radii.

It may be possible to combine a vertical cross-sectiona two-dimensional flow model with one-, two- or three-dimensional dispersion formula to map the dispersive movement of a contaminant in the dimension excluded from the flow model.

Jacob, 1950, developed an analytical method for adjusting the height of the water table in a plan view model to account for reduction in the saturated thickness of flow due pumping from a phreatic aquifer. One must be cautious with this adjustment since the law of conservation of mass is not obeyed.

It is also possible to combine one numerical technique with another to arrive at a solution of a three-dimensional problem with a two-dimensional model. As mentioned above, a random walk model may be coupled to a two-dimensional flow model to allow dispersive solute movement in the direction excluded from the flow model.

GENERAL COMMENTS AND CONCLUSIONS ON NUMERICAL MODELS

Based upon the discussion above, some main conclusions may be drawn as they relate to one-, two-, or three-dimensional modeling.

1. The existence of numerical models allows a means for solving complex one-, two-, or three-dimensional problems but does not help us in deciding which dimensions to include for mass transport of radionuclides. In fact, the approximating features of the numerical models will increase the number of dimension problem decisions.

2. The vertical to horizontal scale contrasts in nodal placement for fully or pseudo three-dimensional models introduces errors that we believe are not fully understood or appreciated. Further study is needed.

3. It may be possible to combine a numerical technique in two-dimensional representation with a three-dimensional analytical formula to arrive at a solution to a fully three-dimensional problem.

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SECTION 7. LIST OF SYMBOLS

b = aquifer thickness
C = concentration
D_i = dispersion coefficient = $d_i v_i + D^*$ in the i direction
D^* = diffusion coefficient
d_i = dispersivity in the i direction
e = base of the Naperian logarithm = 2.71828
g = gravitational constant
h = head
h_R = head at radius R from point sink
h_w = head at radius r_s from well or sink
K = hydraulic conductivity
$\underline{k}$ = aquifer diffusivity = K/S_s
M = mass of contaminant per unit dimensions
m = aquifer thickness
Q = flow rate
R_d = retardation coefficient
r = radial distance
r_p = radial distance from observation point to point sink
r_w = radius of well or spherical sink
S = storage coefficient
S_s = specific storage = $\gamma\theta\beta(1 + \alpha/\theta\beta)$
s = drawdown
s_p = potential at a point defined at r_p
T = aquifer transmissivity
t = time
Vol/S_s = instantaneous volume discharge (L^4)
v_i = specific discharge in i direction unless otherwise noted
x,y,z = space coordinates
α = reciprocal of the modulus of elasticity of skeleton of aquifer
β = reciprocal of the modulus of elasticity of water
γ = unit weight of water
λ = radioactive decay constant
μ = dynamic viscosity
θ = porosity of aquifer
ρ = density of water

SECTION 8. APPENDICES

APPENDIX A

ASYMMETRICAL REPOSITORY MODEL FORTRAN CODE

```
C....  CDM PROGRAM VARISINK/3D
C....  PROGRAM FOR EXECUTION ON CDC CYBER 175 TIME-SHARING SYSTEM AT U OF I.
C....  INTERACTIVE PROGRAM TO DETERMINE THE DRAWDOWN AT A POINT WITH
C....   COORDINATES (XP,YP,ZP) DUE TO A POINT, LINE, AREAL, AND
C....   3-D SINKS OF EQUAL STRENGTH WITH PARALLEL PLANE IMPERMEABLE BOUNDARIES
C....   IN THE X-Z PLANE AT DISTANCES OF ADIST AND BDIST.
C
C
C....  ANNOTATED DEFINITION OF VARIABLES:
C....    XP=X-COORDINATE OF POINT IN FT
C....    YP=Y-COORDINATE OF POINT IN FT
C....    ZP=Z-COORDINATE OF POINT IN FT
C....    X =VARIABLE OF INTEGRATION ALONG X-AXIS
C....    Y =INTEGRAND ARRAY USED FOR INTEGRATION ALONG THE X-AXIS
C....    XX=VARIABLE OF INTEGRATION ALONG THE Y-AXIS
C....    YY=INTEGRAND ARRAY USED FOR INTEGRATION ALONG THE Y-AXIS
C....    XXX=VARIABLE OF INTEGRATION ALONG THE Z-AXIS
C....    YYY=INTEGRAND ARRAY USED FOR INTEGRATION ALONG THE Z-AXIS
C....    LENGTH=LENGTH OF SINK IN FT ALONG X-AXIS
C....    WIDTH=WIDTH OF SINK IN FT ALONG Y-AXIS
C....    DEPTH=DEPTH OF SINK IN FT ALONG Z-AXIS
C....    K=PERMEABILITY IN GPD/FT**2
C....    T=TIME IN DAYS
C....    SS=STORAGE COEFFICIENT IN FT-1
C....    TAREA=DRAWDOWN DUE TO LINE SINK IN FT
C....    TTARE=DRAWDOWN DUE TO AREAL SINK IN FT
C....    TTT=DRAWDOWN DUE TO 3-D SINK IN FT
C....    BDIST=ABS DISTANCE TO UPPER INFINITE PLAIN BOUNDARY(+Y DIRECTION) IN FT
C....    ADIST=ABS DISTANCE TO LOWER INFINITE PLAIN BOUNDARY(-Y DIRECTION) IN FT
C....    EXXA,EXXB,RFIA,RFIB-USED FOR IMAGE WELL COMPUTATIONS
      PROGRAM MAIN(INPUT,OUTPUT)
      DIMENSION X(4),Y(4),XX(4),YY(4),XXX(4),YYY(4)
      REAL K,LENGTH
      LOGICAL POINT,LINE,D2,D3
      POINT=LINE=D2=D3=.TRUE.
C
C....  INPUT DATA AND PARAMETERS
C
      K=0.01$ SS=1E-05 $ T=365000. $ LENGTH=820. $ WIDTH=33.$XP=0984.
      YP= 0328.$ ZP=0000.$ DEPTH=820. $ BDIST=3280. $ ADIST=3280.
      PRINT*," OBS POINT COORDINATES (",XP,",",YP,",",ZP,")"
      CONST=1.37/SQRT(K*T/SS)
      TTT=0.0
C
```

```
C....  DEFINE THE NUMBER OF DIVISIONS FOR INTEGRATION IN EACH DIMENSION
C....   NOTE:  NDIV MUST BE DIVISABLE BY 3 FOR 3/8 THS RULE INTEGRATION.
C
      NDIV=12
      NUP=NDIV/3
C
C....  Z-DIMENSION INTEGRATION LOOP
C
      DO 80 III=1,NUP
      DO 81 IIJ=1,4
C     IF(IIJ.EQ.1.AND.III.EQ.1) XXX(IIJ)=1E-50
      IF(IIJ.EQ.1.AND.III.EQ.1) XXX(IIJ)=0.0
      IF(IIJ.EQ.1.AND.III.GT.1) XXX(IIJ)=XXX(4)
      IF(IIJ.GT.1) XXX(IIJ)=XXX(IIJ-1)+DEPTH/FLOAT(NDIV)
      TTARE=0.0
C
C....  Y-DIMENSION INTEGRATION LOOP
C
      DO 40 I=1,NUP
      DO 41 IJ=1,4
C     IF(IJ.EQ.1.AND.I.EQ.1) XX(IJ)=1E-50
      IF(IJ.EQ.1.AND.I.EQ.1) XX(IJ)=0.0
      IF(IJ.EQ.1.AND.I.GT.1) XX(IJ)=XX(4)
      IF(IJ.GT.1) XX(IJ)=XX(IJ-1)+WIDTH/FLOAT(NDIV)
C     X(2)=1E-50
      X(4)=0.0
      RP=SORT((XP-0.0)**2+(YP-XX(IJ))**2+(ZP-XXX(IIJ))**2)
      Y(4)=114.6*ERFC(CONST*RP)/RP/K
C....  ADD EFFECTS OF 100 IMAGES DUE TO EACH OF THE TWO BOUNDARIES FOR THE POINT
      EXXA=XX(IJ)
      EXXB=XX(IJ)
      A=ADIST+XX(IJ)
      B=BDIST-XX(IJ)
      DO 7 IKI=1,50
      IF(IKI/2.NE.IKI*2)EXXA=EXXA-2.*A
      IF(IKI/2.EQ.IKI*2) EXXA=EXXA-2.*B
      IF(IKI/2.NE.IKI*2) EXXB=EXXB+2.*B
      IF(IKI/2.EQ.IKI*2) EXXB=EXXB+2.*A
      RPIA=SORT((XP-X(4))**2+(YP-EXXA)**2+(ZP-XXX(IIJ))**2)
      RPIB=SORT((XP-X(4))**2+(YP-EXXB)**2+(ZP-XXX(IIJ))**2)
    7 Y(4)=Y(4)+114.6*ERFC(CONST*RPIA)/RPIA/K
     $+114.6*ERFC(CONST*RPIB)/RPIB/K
C....  OUTPUT FOR POINT SINK IN M/LPS
      IF(POINT)PRINT*," POINT SINK DRAWDOWN(M/LPS)= ",Y(4)
     $*4.830842995
      POINT=.FALSE.
      TAREA=0.0
C
C....  X-DIMENSION INTEGRATION LOOP
C
      DO 45 J=1,NUP
      X(1)=X(4)
      Y(1)=Y(4)
      DO 10 II=2,4
      X(II)=X(II-1)+LENGTH/FLOAT(NDIV)
C....  DETERMINE THE EFFECT OF THE REAL WELL
      RP=SORT((XP-X(II))**2+(YP-XX(IJ))**2+(ZP-XXX(IIJ))**2)
      Y(II)=114.6*ERFC(CONST*RP)/RP/K
```

```
C....  ADD EFFECTS OF 100 IMAGES DUE TO EACH OF THE TWO BOUNDARIES
       EXXA=XX(IJ)
       EXXB=XX(IJ)
       A=ADIST+XX(IJ)
       B=BDIST-XX(IJ)
       DO 5 IKI=1,50
       IF(IKI/2.NE.IKI*2)EXXA=EXXA-2.*A
       IF(IKI/2.EQ.IKI*2) EXXA=EXXA-2.*B
       IF(IKI/2.NE.IKI*2) EXXB=EXXB+2.*B
       IF(IKI/2.EQ.IKI*2) EXXB=EXXB+2.*A
       RPIA=SQRT((XP-X(II))**2+(YP-EXXA)**2+(ZP-XXX(IIJ))**2)
       RPIB=SQRT((XP-X(II))**2+(YP-EXXB)**2+(ZP-XXX(IIJ))**2)
     5 Y(II)=Y(II)+114.6*ERFC(CONST*RPIA)/RPIA/K
      $+114.6*ERFC(CONST*RPIB)/RPIB/K
    10 CONTINUE
       CALL INTEG(X,Y,AREA,LENGTH/FLOAT(NDIV))
       TAREA=TAREA+AREA
    45 CONTINUE
C.... OUTPUT FOR 1-D SINK IN M/LPS
       IF(LINE)PRINT*," L ..E SINK DRAWDOWN(M/LPS)= ",TAREA
      $*4.830842995/LENGTH," LENGTH=",X(4)
       LINE=.FALSE.
    41 YY(IJ)=TAREA
       CALL INTEG(XX,YY,ARE,WIDTH/FLOAT(NDIV))
    40 TTARE=TTARE+ARE
C....  OUTPUT FOR 2-D SINK IN M/LPS
       IF(D2)PRINT*," AREAL SINK DRAWDOWN(M/LPS)=",TTARE
      $*4.830842995/(LENGTH*WIDTH)," LENGTH=",X(4)," WIDTH=",XX(4)
       D2=.FALSE.
    81 YYY(IIJ)=TTARE
       CALL INTEG(XXX,YYY,A,DEPTH/FLOAT(NDIV))
     0 TTT=TTT+A
C.... OUTPUT FOR 3-D SINK IN M/LPS
       PRINT*," 3D SINK DRAWDOWN(M/LPS)=",TTT*4.830842995/(LENGTH*
      +WIDTH*DEPTH)," LENGTH=",X(4)," WIDTH=",XX(4)," DEPTH=",XXX(4)
       STOP
       END
```

```
      SUBROUTINE INTEG(X,Y,AREA,H)
C....  SUBROUTINE TO INTEGRATE A FUNCTION DEFINED AT DISCRETE ARRAY
C....    AT EQUALLY SPACED INTERVALS H.
C....   THREE-EIGHTS RULE INTEGRATION(CUBIC POLYNOMIAL FIT)
C....   POINTS X,Y APPROXIMATED BY A CUBIC EQUATION.  THE APPROXIMATION
C....   OF THE INTEGRAL IS THEN COMPUTED BY THE INTEGRATION
C....   OF THE FITTED CUBIC OVER THE INTERVAL BETWEEN X(1) AND X(4).
      DIMENSION X(4),Y(4),C(4,5),COEFF(4)
      AREA=(Y(1)+3.*Y(2)+3.*Y(3)+Y(4))*3.*H/8.
      RETURN
      END
      FUNCTION ERFC(X)
C....  FUNCTION SUBROUTINE TO APPROXIMATE THE COMPLEMENTARY ERROR FUNCTION.
C     READ*,X
      IF(X.GT.5.0) GO TO 10
      ERFC=1.+.278393*X+.230389*X*X+.000972*X*X*X+.078108*X*X*X*X
      ERFC=ERFC*ERFC*ERFC*ERFC
      ERFC=1./ERFC
C     PRINT*,X,ERFC
      RETURN
   10 PI=ACOS(-1.)
C     PRINT*,PI
      ERFC=1/X-1/(2*X**3)+3/(4*X**5)-15/(8*X**7)+105/(16*X**9)
     +-945/(32*X**11)
      CON=EXP(-AMIN1(X*X,500.))/SQRT(PI)
      ERFC=ERFC*CON
      RETURN
      END
```

APPENDIX B

SYMMETRICAL REPOSITORY MODEL FORTRAN CODE

```
C....   PROGRAM FOR EXECUTION ON CDC CYBER 175 TIME-SHARING SYSTEM AT U OF I.
C....   INTERACTIVE PROGRAM TO DETERMINE THE DRAWDOWN AT A POINT WITH
C....   COORDINATES (XP,YP,ZP) DUE TO A POINT, LINE, AREAL, AND
C....   3-D SINKS OF EQUAL STRENGTH WITH PARALLEL PLANE IMPERMEABLE BOUNDARIES
C....   IN THE X-Z PLANE AT DISTANCES OF ADIST AND BDIST.
C
C
C....  ANNOTATED DEFINITION OF VARIABLES:
C....    XP=X-COORDINATE OF OBSERVATION POINT IN FT
C....    YP=Y-COORDINATE OF OBSERVATION POINT IN FT
C....    ZP=Z-COORDINATE OF OBSERVATION POINT IN FT
C....    X =VARIABLE OF INTEGRATION ALONG X-AXIS
C....    Y =INTEGRAND ARRAY USED FOR INTEGRATION ALONG THE X-AXIS
C....    XX=VARIABLE OF INTEGRATION ALONG THE Y-AXIS
C....    YY=INTEGRAND ARRAY USED FOR INTEGRATION ALONG THE Y-AXIS
C....    XXX=VARIABLE OF INTEGRATION ALONG THE Z-AXIS
C....    YYY=INTEGRAND ARRAY USED FOR INTEGRATION ALONG THE Z-AXIS
C....    LENGTH=LENGTH OF SINK IN FT ALONG X-AXIS
C....    WIDTH=WIDTH OF SINK IN FT ALONG Y-AXIS
C....    DEPTH=DEPTH OF SINK IN FT ALONG Z-AXIS
C....    K=PERMEABILITY IN GPD/FT**2
C....    T=TIME IN DAYS
C....    SS=STORAGE COEFFICIENT IN FT-1
C....    TAREA=DRAWDOWN DUE TO LINE SINK IN FT
C....    TTARE=DRAWDOWN DUE TO AREAL SINK IN FT
C....    TTT=DRAWDOWN DUE TO 3-D SINK IN FT
C....    BDIST=ABS DISTANCE TO UPPER INFINITE PLAIN BOUNDARY(+Y DIRECTION) IN FT
C....    ADIST=ABS DISTANCE TO LOWER INFINITE PLAIN BOUNDARY(-Y DIRECTION) IN FT
C....    EXXA,EXXB,RRIA,RRIB-USED FOR IMAGE WELL COMPUTATIONS
      PROGRAM MAIN(INPUT,OUTPUT)
      DIMENSION X(4),Y(4),XX(4),YY(4),XXX(4),YYY(4)
      REAL K,LENGTH
      LOGICAL LINE,D2,D3,DEBUG
      LINE=D2=D3=.TRUE.
C
C....  INPUT DATA AND PARAMETERS
C
      K=0.01$ SS=1E-05 $ T=365000. $ LENGTH=820. $ WIDTH=33.$XP=00000.
      YP= 0000.$ ZP= 3281.$ DEPTH=820. $ BDIST=3281. $ ADIST=3281.
      DEBUG=.FALSE.
      PRINT*," OBS POINT COORDINATES (",XP,",",YP,",",ZP,")"
      CONST=1.87/SQRT(K*T/SS)
C....  COMPUTE THE POINT DRAWDOWN WITH BOUNDARIES
      RR=SQRT((XP-0.0)**2+(YP-0.0)**2+(ZP-0.0)**2)
      Y(4)=114.6*ERFC(CONST*RR)/RR
```

```
C....  ADD EFFECTS OF 100 IMAGES DUE TO EACH OF THE TWO BOUNDARIES FOR THE POINT
       EXXA=0.0
       EXXB=0.0
       A=ADIST+0.0
       B=BDIST-0.0
       DO 7000 IKI=1,50
       IF(IKI/2.NE.IKI*2)EXXA=EXXA-2.*A
       IF(IKI/2.EQ.IKI*2) EXXA=EXXA-2.*B
       IF(IKI/2.NE.IKI*2) EXXB=EXXB+2.*B
       IF(IKI/2.EQ.IKI*2) EXXB=EXXB+2.*A
       RPIA=SQRT((XP-0.0)**2+(YP-EXXA)**2+(ZP-0.0)**2)
       RPIB=SQRT((XP-0.0)**2+(YP-EXXB)**2+(ZP-0.0)**2)
 7000 Y(4)=Y(4)+114.6*ERFC(CONST*RPIA)/RPIA/K
     $+114.6*ERFC(CONST*RPIB)/RPIB/K
C....  OUTPUT FOR POINT SINK IN M/LPS
       PRINT*," POINT SINK DRAWDOWN(M/LPS)= ",Y(4)
     $*4.830842995
C
C....  DEFINE THE NUMBER OF DIVISIONS FOR INTEGRATION IN EACH DIMENSION
C....   NOTE:  NDIV MUST BE DIVISABLE BY 3 FOR 3/8 THS RULE INTEGRATION.
C
       NDIV=12
       NUP=NDIV/3
C
C....  Z-DIMENSION INTEGRATION LOOP
C
       TTT=0.0
       DO 80 III=1,NUP
       DO 81 IIJ=1,4
       IF(IIJ.EQ.1.AND.III.EQ.1) XXX(IIJ)=0.0
       IF(IIJ.EQ.1.AND.III.GT.1) XXX(IIJ)=XXX(4)
       IF(IIJ.GT.1) XXX(IIJ)=XXX(IIJ-1)+DEPTH/FLOAT(NDIV)
C
C....  Y-DIMENSION INTEGRATION LOOP
C
       TTAPE=0.0
       DO 40 I=1,NUP
       DO 41 IJ=1,4
       IF(IJ.EQ.1.AND.I.EQ.1) XX(IJ)=0.0
       IF(IJ.EQ.1.AND.I.GT.1) XX(IJ)=XX(4)
       IF(IJ.GT.1) XX(IJ)=XX(IJ-1)+WIDTH/FLOAT(NDIV)
       X(4)=0.0
       RP=SQRT((XP+LENGTH/2.0)**2+(YP-(XX(IJ)-WIDTH/2.0))**2
     $+(ZP-(XXX(IIJ)-DEPTH/2.0))**2)
       Y(4)=114.6*ERFC(CONST*RP)/RP/K
```

```
C....  ADD EFFECTS OF 100 IMAGES DUE TO EACH OF THE TWO BOUNDARIES FOR THE POINT
      EXXA=XX(IJ)-WIDTH/2.0
      EXXB=XX(IJ)-WIDTH/2.0
      A=ADIST+XX(IJ)-WIDTH/2.0
      B=BDIST-XX(IJ)+WIDTH/2.0
      DO 7 IKI=1,50
      IF(IKI/2.NE.IKI*2) EXXA= EXXA-2.*A
      IF(IKI/2.EQ.IKI*2) EXXA=EXXA-2.*B
      IF(IKI/2.NE.IKI*2) EXXB=EXXB+2.*B
      IF(IKI/2.EQ.IKI*2) EXXB=EXXB+2.*A
      RRIA=SQRT((XP-(X(4)-LENGTH/2.0))**2+(YP-EXXA)**2
     $+(ZP-(XXX(IIJ)-DEPTH/2.0))**2)
      RRIB=SQRT((XP-(X(4)-LENGTH/2.0))**2+(YP-EXXB)**2
     $+(ZP-(XXX(IIJ)-DEPTH/2.0))**2
    7 Y(4)=Y(4)+114.6*ERFC(CONST*RRIA)/RRIA/K
     $+114.6*ERFC(CONST*RRIB)/RRIB/K
C
C....  X-DIMENSION INTEGRATION LOOP
C
      TAREA=0.0
      DO 45 J=1,NUR
      X(1)=X(4)
      Y(1)=Y(4)
      DO 10 II=2,4
      X(II)=X(II-1)+LENGTH/FLOAT(NDIV)
C....  DETERMINE THE EFFECT OF THE REAL WELL
      RR=SQRT((XP-(X(II)-LENGTH/2.0))**2+(YP-(XX(IJ)-WIDTH/2.0))**2
     $+(ZP-(XXX(IIJ)-DEPTH/2.0))**2)
      Y(II)=114.6*ERFC(CONST*RR)/RR/K
C....  ADD EFFECTS OF 100 IMAGES DUE TO EACH OF THE TWO BOUNDARIES
      EXXA=XX(IJ)-WIDTH/2.0
      EXXB=XX(IJ)-WIDTH/2.0
      A=ADIST+XX(IJ)-WIDTH/2.0
      B=BDIST-XX(IJ)+WIDTH/2.0
      DO 5 IKI=1,50
      IF(IKI/2.NE.IKI*2) EXXA= EXXA-2.*A
      IF(IKI/2.EQ.IKI*2) EXXA=EXXA-2.*B
      IF(IKI/2.NE.IKI*2) EXXB=EXXB+2.*B
      IF(IKI/2.EQ.IKI*2) EXXB=EXXB+2.*A
      RRIA=SQRT((XP-(X(II)-LENGTH/2.0))**2+(YP-EXXA)**2
     $+(ZP-(XXX(IIJ)-DEPTH/2.0))**2)
      RRIB=SQRT((XP-(X(II)-LENGTH/2.0))**2+(YP-EXXB)**2
     $+(ZP-(XXX(IIJ)-DEPTH/2.0))**2)
    5 Y(II)=Y(II)+114.6*ERFC(CONST*RRIA)/RRIA/K
     $+114.6*ERFC(CONST*RRIB)/RRIB/K
   10 CONTINUE
```

```
      CALL INTEG(X,Y,AREA,LENGTH/FLOAT(NDIV))
      TAREA=TAREA+AREA
      IF(DEBUG.AND.LINE)PRINT*," AREA=",AREA," TAREA=",TAREA
      IF(DEBUG.AND.LINE)PRINT*," X-ARRAY ",X
      IF(DEBUG.AND.LINE)PRINT*," Y-ARRAY ",Y
C.... OUTPUT FOR 1-D SINK IN M/LPS
      IF(ABS(XX(IJ)-WIDTH/2.0).LT.1E-05.AND.
     $ABS(XXX(IIJ)-DEPTH/2.0).LT.1E-05.AND.LINE.AND.ABS(X(4)-LENGTH).LT.
     $1E-05)
     $PRINT*," LINE SINK DRAWDOWN(M/LPS)= ",TAREA
     $*4.830842995/LENGTH," LENGTH=",X(4)
      IF(ABS(XX(IJ)-WIDTH/2.0).LT.1E-05.AND.
     $ABS(XXX(IIJ)-DEPTH/2.0).LT.1E-05.AND.LINE.AND.ABS(X(4)-LENGTH).LT.
     $1E-05)
     $LINE=.FALSE.
   45 CONTINUE
   41 YY(IJ)=TAREA
      CALL INTEG(XX,YY,ARE,WIDTH/FLOAT(NDIV))
      TTARE=TTARE+ARE
C....  OUTPUT FOR 2-D SINK IN M LPS
      IF(
     $ABS(XXX(IIJ)-DEPTH/2.0).LT.1E-05.AND.D2.AND.ABS(XX(4)-WIDTH).LT.
     $1E-05)
     $PRINT*," AREAL SINK DRAWDOWN(M/LPS)=",TTARE
     $*4.830842995/(LENGTH*WIDTH)," LENGTH=",X(4)," WIDTH=",XX(4)
   40 IF(
     $ABS(XXX(IIJ)-DEPTH/2.0).LT.1E-05.AND.D2.AND.ABS(XX(4)-WIDTH).LT.
     $1E-05)
     $D2=.FALSE.
   81 YYY(IIJ)=TTARE
      CALL INTEG(XXX,YYY,AA,DEPTH/FLOAT(NDIV))
   80 TTT=TTT+AA
C.... OUTPUT FOR 3-D SINK IN M/LPS
      PRINT*,"  3D SINK DRAWDOWN(M/LPS)=",TTT*4.830842995/(LENGTH*
     +WIDTH*DEPTH)," LENGTH=",X(4)," WIDTH=",XX(4)," DEPTH=",XXX(4)
      STOP
      END
```

```
      SUBROUTINE INTEG(X,Y,AREA,H)
C....  SUBROUTINE TO INTEGRATE A FUNCTION DEFINED AT DISCRETE ARRAY
C....    AT EQUALLY SPACED INTERVALS H.
C....   THREE-EIGHTS RULE INTEGRATION(CUBIC POLYNOMIAL FIT)
C....   POINTS X,Y APPROXIMATED BY A CUBIC EQUATION.  THE APPROXIMATION
C....   OF THE INTEGRAL IS THEN COMPUTED BY THE INTEGRATION
C....   OF THE FITTED CUBIC OVER THE INTERVAL BETWEEN X(1) AND X(4).
      DIMENSION X(4),Y(4),C(4,5),COEFF(4)
      AREA=(Y(1)+3.*Y(2)+3.*Y(3)+Y(4))*3.*H/8.
      RETURN
      END
      FUNCTION ERFC(X)
C....  FUNCTION SUBROUTINE TO APPROXIMATE THE COMPLEMENTARY ERROR FUNCTION.
C     READ*,X
      IF(X.GT.5.0) GO TO 10
      ERFC=1.+.278393*X+.230389*X*X+.000972*X*X*X+.078108*X*X*X*X
      ERFC=ERFC*ERFC*ERFC*ERFC
      ERFC=1./ERFC
C     PRINT*,X,ERFC
      RETURN
   10 PI=ACOS(-1.)
C     PRINT*,PI
      ERFC=1/X-1/(2*X**3)+3/(4*X**5)-15/(8*X**7)+105/(16*X**9)
     +-945/(32*X**11)
      CON=EXP(-AMIN1(X*X,500.))/SQRT(PI)
      ERFC=ERFC*CON
      RETURN
      END
```