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NUMERICAL MODELLING OF LIQUID WASTE INJECTION INTO POROUS MEDIA SATURATED WITH DENSITY-STRATIFIED FLUID: A PROGRESS REPORT

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by

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for
DYNAMICS OF WASTE INJECTION INTO A TWO-PHASE
FLUID SYSTEM, PHASE I

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ABSTRACT

Waste effluent injected into an aquifer saturated with denser ambient brackish or salt water experiences a buoyant lift. As a result, the effluent migrates both outward from the well and upward in response to the combined effects of injection head and buoyant force. After the injection process has begun, several phenomena can affect the density, shape, and distribution in space and time of the resulting buoyant plume. The most important of these include convection and mechanical dispersion and molecular diffusion.

Previous sandbox and Hele-Shaw laboratory modelling work have provided a basic qualitative understanding of buoyant plume movement in a porous medium. However, these laboratory models cannot correctly simulate dispersion phenomena which may have significant effects on buoyant plume movement and distribution. Consequently, it is necessary to mathematically model the problem using coupled sets of partial differential equations which take into account the effects of dispersion and diffusion, as well as convection. For this problem, there are four unknowns (density, concentration, velocity, and pressure), requiring four equations. The four governing equations are: a motion equation (Darcy's law), a continuity equation, a dispersion equation, and an equation of state. In addition, boundary and initial conditions must be stipulated. In this study, two sets of boundary conditions are used: the first consists of conditions identical to those in the sandbox model studies, and the second models the geology of a specific prototype area. The resulting governing equations and boundary and initial conditions are numerically solved by both the finite difference and the finite element methods. Finally, the numerical models are calibrated with the results of the sandbox model studies mentioned previously.

This report describes in detail formulation of the governing equations and the initial and boundary conditions, and preliminary finite difference modelling work completed to date.

CONTENTS

FIGURES

INTRODUCTION

Background

In Hawai'i, liquid wastes are often disposed of by subsurface injection into the brackish or saline groundwater body which underlies the Ghyben-Herzberg fresh groundwater lens. This method of waste disposal has become fairly commonplace in the past five years with upwards of 170 injection wells now in operation. Injection of waste into the Hawaiian Ghyben-Herzberg lens system presents unique problems because the waste effluents normally are injected into the density-stratified water underlying the freshwater lens. These effluents commonly have a density close to that of fresh water so that the effluent experiences a buoyant uplift superimposed upon any ambient groundwater flow effects. This situation produces a problem with highly complicated boundary conditions which has yet to be theoretically or numerically solved.

The Hele-Shaw (Williams 1977) and sand-packed hydraulic model studies (Wheatcraft, Peterson, and Heutmaker 1976; Heutmaker, Peterson, and Wheatcraft 1977) conducted at the University of Hawaii Water Resources Research Center have provided a basic qualitative understanding of buoyant plume movement in a porous medium. However, the Hele-Shaw and sand-packed hydraulic models are not able to correctly simulate dispersion phenomena which may have significant effects on plume movement and distribution in a prototype situation (this is explained fully in the section entitled "Description of the Injection Process"). As a result, it is necessary to model mathematically the problem using coupled sets of partial differential equations with specified boundary and initial conditions.

Objectives

The purpose of this study is to achieve an understanding of the process of liquid waste injection in Hawai'i through use of mathematical modelling. Many important questions remain to be answered regarding injection into density-stratified aquifers. Some of the important questions to be examined in this study include:

1. What is the extent and distribution of plume migration in three-dimensional space and time?
2. How significant are the effects of mechanical dispersion and molec-

ular diffusion on the effluent plume?

3. What are the relative effects of convection by buoyant force versus convection by injection pressure gradients and to what extent do each of these terms contribute to the total flow regime?

Several specific problems are of particular interest for the Hawaiian situation. Each case has its own unique boundary and initial conditions. The details of these specific cases are outlined in the section entitled "Boundary and Initial Conditions."

In order to answer the questions described above, the physical situation is stated in terms of the appropriate set of governing equations and boundary and initial conditions. The resulting equations are then solved numerically by the finite element method.

Finally, the numerical model calibrated against existing data. Ideally, the calibration procedure would involve using extensive field data collected over a period of years; however for Hawai'i, no such data exists. The numerical model will therefore be calibrated with the results of the sand-packed hydraulic model studies previously mentioned.

MATHEMATICAL FORMULATION

Description of the Injection Process

Waste effluent injected into an aquifer saturated with denser ambient brackish or salt water experiences a buoyant lift. The effluent then migrates outward from the well and upward in response to the combined effects of injection head and buoyant force; this is referred to as a buoyant plume. The initial strength of the buoyant effect is dependent upon the initial density difference between the injected effluent and the ambient groundwater. After the injection process has begun, several phenomena can affect the density, shape, and distribution in space and time of the buoyant plume. These phenomena include convection, mechanical dispersion, molecular diffusion, Rayleigh-Taylor instabilities, entrainment, aquifer elasticity, fluid-aquifer interactions (both geochemical and biological), and change of density as a function of pressure.

Wheatcraft, Peterson, and Heutmaker (1976) showed that in a sand-packed hydraulic model, the most important mechanism of mass transport is mass displacement by convection. Mechanical dispersion and molecular diffusion did not significantly influence the plume concentration distributions. However, in a Hawaiian prototype aquifer, a representative elementary volume generally is much larger than that of sand in a laboratory model due to the nonhomogeneous nature of the aquifer. The coefficient of hydrodynamic dispersion is, therefore, much larger for the prototype and this difference cannot be scaled for purposes of similitude modelling (Bear 1977). Therefore, a mathematical model of the problem must take into account the effects of hydrodynamic dispersion and molecular diffusion so that an accurate picture can be formulated regarding the relative importance of the dispersion, diffusion, and convection terms in the equations.

For this problem, there are four unknowns, density (ρ), concentration (C), velocity ($\underset{\sim}{q}$), and pressure (P), requiring four equations. The four equations are:

Motion equation (Darcy's law),

$$\underset{\sim}{q} = \frac{\underset{\approx}{k}}{\mu}(\nabla P + \rho \underset{\sim}{g} \nabla z) \; ; \tag{1}$$

Continuity equation,

$$\nabla \cdot (\rho \underset{\sim}{q}) + \rho_0 Q^*(x^*) = -\frac{\partial (n\rho)}{\partial t} \; ; \tag{2}$$

Dispersion equation,

$$\underset{\sim}{q} \cdot \nabla C + \frac{\partial C}{\partial t} = \nabla \cdot (\underset{\approx}{D_h} \nabla C) \; ; \tag{3}$$

Equation of state,

$$\rho = \rho_0 [1 + \beta_c (C - C_0) + \beta_p (P - P_0)] \; . \tag{4}$$

In equation (2), $\rho_0 Q^*(x^*)$ represents a source or sink located at the point x^* in the flow domain with a pumping or injection rate Q^* (with positive or negative sign for respective pumping or injection). The term $\rho_0 Q^*(x^*)$ is defined as:

$$\rho_0 Q^*(x^*) = [n \frac{\partial}{\partial t} \oiiint \rho d\forall + \rho_0 \oiint \underset{\sim}{q} dA] \partial (x - x_i, \; y - y_i) \tag{5}$$

where $\partial \equiv$ Dirac delta function and (x_i, y_i) are the coordinates of the pumping or injection well.

Equations (1) through (5) are a generalized form of the total differential statement of the problem. Now it is necessary to discuss the exact physical conditions, geometry, approximations, and assumptions for the

$k_x \geq k_z \geq 0.01\ k_x$.

6. Changes in density and viscosity caused by varying salt concentration do not significantly affect the hydraulic conductivity. The hydraulic conductivity is, therefore, a second-rank tensor that is constant with respect to space and time, but directional in nature such that:

$$\underset{\approx}{k} = \begin{bmatrix} k_x & 0 & 0 \\ 0 & k_y & 0 \\ 0 & 0 & k_z \end{bmatrix} = \begin{bmatrix} k_x & 0 & 0 \\ 0 & k_x & 0 \\ 0 & 0 & k_z \end{bmatrix} \tag{7}$$

where the coordinate axes are taken to be the principal directions. This assumption introduces a slight error because the lava flow beds dip at an angle of about 7° to 9° from the horizontal. This causes the principal directions to be tilted at the same angle, 7° to 9° from the coordinate axes. This error is relatively small compared to the precision to which values for the hydraulic conductivity are known and will, therefore, be ignored.

7. Although the tensor nature of the hydraulic conductivity is well understood for the general anisotropic porous medium, this is not the case for the coefficient of hydrodynamic dispersion ($D_{hij} = \underset{\approx}{D}$). D_{hij} is known to be a second rank tensor even in isotropic media with principal directions everywhere orthogonal to the average velocity. However, the exact form of the function of D_{hij} for anisotropic porous media is not well known and there has been very little work done in this area (Bear 1977). Therefore, for the purposes of this study, it is necessary to assume that the porous media is isotropic with respect to hydrodynamic dispersion, even though it is being treated as anisotropic with respect to permeability. For isotropic media,

$$D_{hij} = D_{ij} + D^*_{dij} \tag{8.1}$$

where

$$D_{ij} = a_t\ \overline{V}\ \partial_{ij} + (a_i - a_t)\frac{\overline{V}_i \overline{V}_j}{\overline{V}}\ , \tag{8.2}$$

and

$$D^*_{dij} = D_d\ T^*_{ij} \tag{8.3}$$

The tortuosity (T^*_{ij}) is related to the porous medium's intrinsic permeability and is a second-rank tensor. However, it reduces to a scalar (unlike the dispersion coefficient) in an isotropic medium. Since the tortuosity is being used here in an isotropic treatment of dispersion, it may be considered

Hawaiian system and to rewrite accordingly equations (1) through (5).

Imposed Conditions, Approximations, and Assumptions

Some conditions must be imposed that complicate the mathematical statement of the problem, i.e., retain generality, in order to achieve more realistic and accurate answers in light of the real physical situation. These conditions are addressed first, then simplifying assumptions and approximations will be presented.

1. Formation of buoyant plumes in an ambient groundwater flow regimes is transient and three-dimensional in nature. One of the most important questions to be addressed in this study is: how wide (horizontally) is the plume at some point of interest downgradient, e.g., the coastline, in an ambinet flow field; and, how long after injection does it take for a specified concentration of the plume to reach the coastline from the point of injection? The horizontal and vertical distributions of effluent plume concentrations, therefore, require the use of a transient, three-dimensional set of equations.

2. In the formulation of the groundwater quality problem, $\rho = \rho(C, P)$ and the right-hand side of equation (2) becomes:

$$\frac{\partial(n\rho)}{\partial t} = \rho\frac{\partial n}{\partial t} + n\frac{\partial\rho}{\partial p}\frac{\partial p}{\partial t} + n\frac{\partial\rho}{\partial C}\frac{\partial C}{\partial t} \tag{6}$$

3. The porous medium will be assumed to be nondeformable, thus eliminating the term $\rho(\partial n/\partial t)$ from the right-hand side of the continuity equation (eq. 6).

4. Fluid density variations are only a function of concentration. This approximation is valid because density variations due to concentration are much larger than either density variations due to pressure or variations with respect to space.

5. In Hawai'i, the aquifers are known to be anisotropic in the x-z plane, with $k_x > k_z$. Estimates of the ratio $k_x > k_z$ generally range from 10 to 100. Although no quantitative work has been done to determine this ratio, anisotropy must be taken into account when dealing with the x-z (vertical) plane since it has the potential of affecting both dispersive and bulk mass transport. Any anisotropy that exists in the horizontal plane is probably small compared to that in the vertical plane and can generally be ignored. Therefore $k_x = k_y$ will be assumed and solutions will be obtained for 0.1

a scalar.

8. Injection will take place from a line source rather than from a point source. A line source is numerically simulated by a series of closely spaced point sources.

Governing Equations

With the above considerations, the governing equations (1-4) reduce to the following:

Darcy's law,

$$q_x = -\frac{k_x}{\mu}\frac{\partial P}{\partial x} , \tag{9.1}$$

$$q_y = -\frac{k_x}{\mu}\frac{\partial P}{\partial y} , \tag{9.2}$$

$$q_z = -\frac{k_z}{\mu}\left(\frac{\partial P}{\partial z} + \rho g\right) , \tag{9.3}$$

Continuity equation,

$$\frac{\partial q_x}{\partial x} + \frac{\partial q_y}{\partial y} + \frac{\partial q_z}{\partial z} + Q^*(x^*) = -\frac{n\rho_0\beta_c}{\rho}\frac{\partial C}{\partial t} , \tag{10}$$

Dispersion equation:

$$\underset{\sim}{q} \cdot \nabla C + \frac{\partial C}{\partial t} = \nabla \cdot (\underset{\approx}{D}_h \nabla C) ,$$

or,

$$\begin{aligned} q_x\frac{\partial C}{\partial x} + q_y\frac{\partial C}{\partial y} + q_z\frac{\partial C}{\partial z} &= \frac{\partial}{\partial x}\left(D_{xx}\frac{\partial C}{\partial x} + D_{xy}\frac{\partial C}{\partial y} + D_{xz}\frac{\partial C}{\partial z}\right) \\ &+ \frac{\partial}{\partial y}\left(D_{yx}\frac{\partial C}{\partial x} + D_{yy}\frac{\partial C}{\partial y} + D_{yz}\frac{\partial C}{\partial z}\right) \\ &+ \frac{\partial}{\partial z}\left(D_{zx}\frac{\partial C}{\partial x} + D_{zy}\frac{\partial C}{\partial y} + D_{zz}\frac{\partial C}{\partial z}\right) . \end{aligned} \tag{11}$$

Equation of state,

$$\rho = \rho_0[1 + \beta_c(C - C_0)] .$$

These are the equations which must be solved by the numerical scheme. However, in order to complete the mathematical statement of the problem, it is necessary to stipulate the boundary and initial conditions.

Boundary and Initial Conditions

Two separate sets of boundary conditions will be examined. Case I will consist of injection into the caprock of very simple geometry, so that the boundary and initial conditions are identical to those in the sand-packed hydraulic model studies. Case 2 will be similar to case 1, except with irregular geometry that closely models the geology of a specific area. Use of the finite element method will easily allow for widely varying geometries without re-formulation of the numerical algorithms and more cases will be studied if time permits. Boundary conditions are, in effect, reduced to input data for the finite element program.

CASE 1. The initial conditions for case 1 are (see Fig. 1):[1]

$$C = C(z,0) \tag{13.1}$$

$$P = P(z,0) \doteq \int_{z_0}^{z} \rho g \, dz + P_0 \tag{13.2}$$

Equation 13.1 is not a function which can be analytically determined, but rather it is a set of ordered pairs of numbers (C,z) that defines the transition zone curve for a particular field (or laboratory model) situation. Hence 13.2 can be determined from 13.1 because ρ is strictly a function of C.

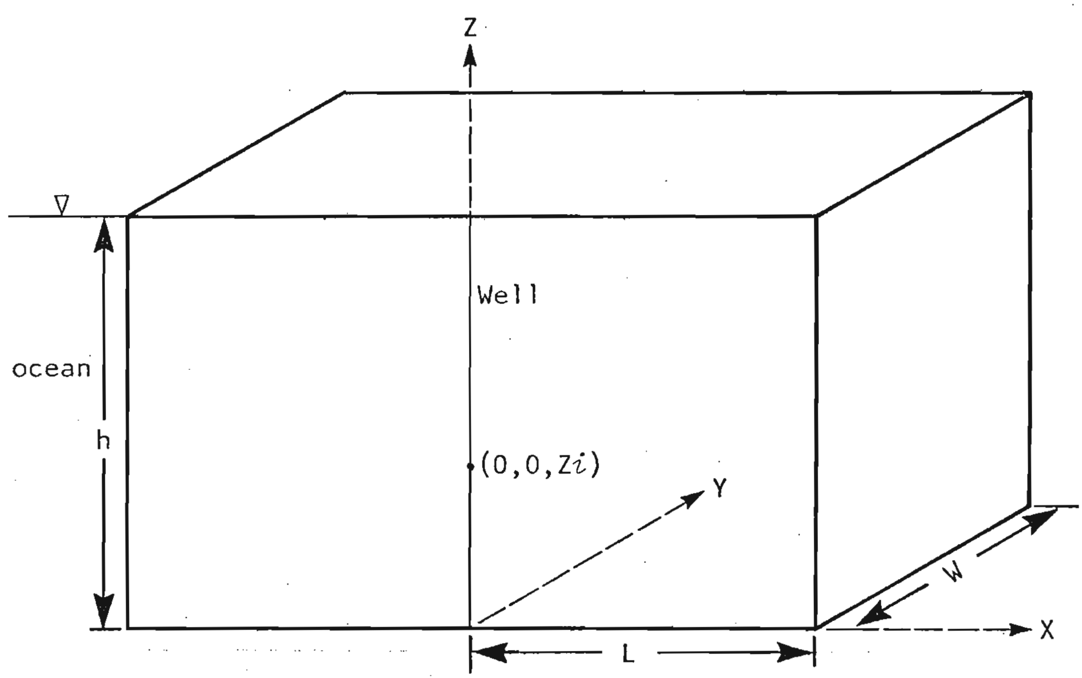

FIGURE 1. BOUNDARY CONDITIONS FOR CASE 1, INJECTION INTO CAPROCK WITH SIMPLE GEOMETRY

[1]The notation used in the following section is: $f = f(x,y,z,t)$. A missing parameter indicates that f is not a function of that parameter. A parameter (x,y,z or t) replaced with a constant indicates that the replaced parameter is held constant at the particular value while other parameters vary over their normal range.

The boundary conditions for case 1 are as follows (see Fig. 1):

$$\frac{\partial C}{\partial z}(x,y,0) = \frac{\partial C}{\partial z}(x,y,h) = 0 \quad , \tag{14.1,2}$$

$$\frac{\partial C}{\partial y}(x,0,z) = \frac{\partial C}{\partial y}(x,w,z) = 0 \tag{14.3,4}$$

$$C(-L,y,z) = C_s \tag{14.5}$$

$$C(L,y,z) = C(z) \tag{14.6}$$

$$\frac{\partial P}{\partial y}(x,0,z) = 0 \tag{14.7}$$

$$\frac{\partial P}{\partial z} = (x,w,z) = 0 \tag{14.8}$$

$$\frac{\partial P}{\partial z}(x,y,0) = -\rho(x,y,0)g \tag{14.9}$$

$$\frac{\partial P}{\partial z}(x,y,h) = -\rho(x,y,h)g \tag{14.10}$$

$$P(-L,y,z) = -g\int_{z_0}^{z}\rho(-L,y,z)dz + P_{0,-L} \tag{14.11}$$

$$P(L,y,z) = -g\int_{z_0}^{z} (L,y,z)dz + P_{0,L} \tag{14.12}$$

CASE 2. In Hawai'i, injection usually takes place in the coastal caprock aquifers such as the injection well facility at the Waimanalo Sewage Treatment Plant on O'ahu. Figure 2 is a cross section of a hypothetical coastal caprock aquifer. The functions ζ_1, ζ_2, and ζ_3 can be designed to specify boundary surfaces for a particular geometry based on known geologic information for an injection well facility. The initial conditions for case 2 are:

$$C = C(x,y,z,0) \quad , \tag{15.1}$$

$$P = P(x,y,z,0) \quad . \tag{15.2}$$

The boundary conditions are:

$$\frac{\partial C}{\partial \zeta}(\zeta_1) = \frac{\partial}{\partial \zeta}(\zeta_2) = 0 \quad , \tag{16.1,.2}$$

$$\frac{\partial C}{\partial y}(x,0,z) = \frac{\partial C}{\partial y}(x,\infty,z) = 0 \tag{16.3,.4}$$

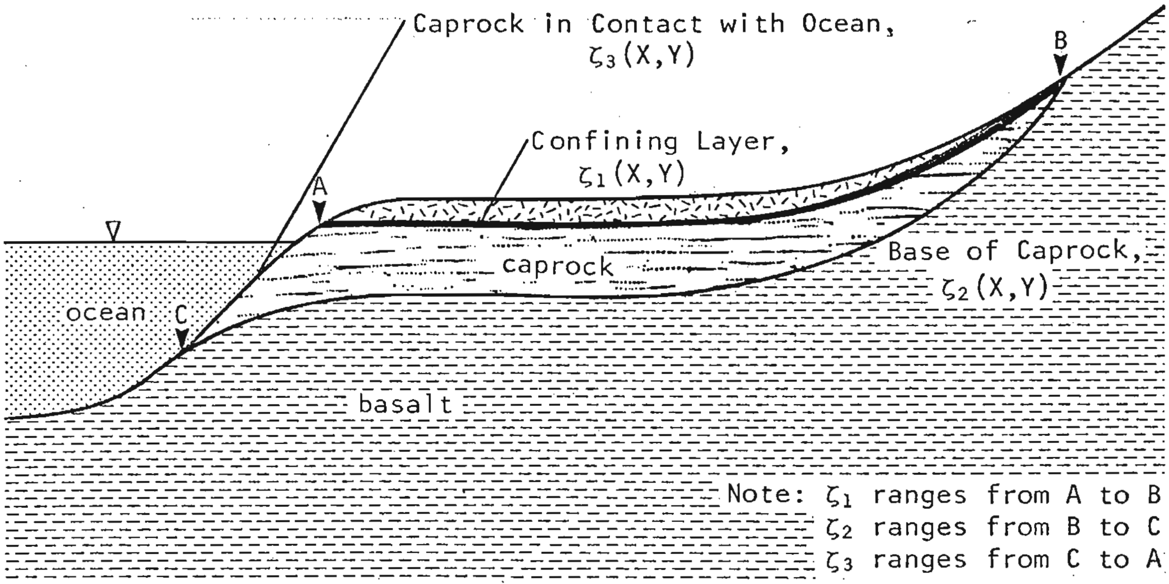

FIGURE 2. BOUNDARY CONDITIONS FOR CASE 2, CAPROCK WITH IRREGULAR GEOMETRY

$$C(\zeta_3) = C_s \tag{16.5}$$

$$\frac{\partial P}{\partial n}(\zeta_1) = 0 \tag{16.6}$$

$$\frac{\partial P}{\partial n}(\zeta_2) = 0 \tag{16.7}$$

$$P(\zeta_3) = -g\int_{z_0}^{z} \rho(z)dz + P_{0,\zeta_3} \tag{16.8}$$

PROGRESS REPORT AND FUTURE WORK

The equations and boundary conditions for case 1 have been formulated into a numerical algorithm with the finite difference method (FDM). It was decided to solve case 1 with the FDM before a finite element solution was achieved. Thus, the answers from the finite difference program would provide a check for the finite element program. The solution procedure used in the finite difference program was the alternating direction implicit (ADI) method (Fig. 3 is a flow chart for the ADI method). Some difficult problems were encountered during the coding of the combined motion-continuity equation. As can be seen from the flow chart, the program outputs concentrations, pressures, and velocities as a function of time and space. At the present time, only concentration and pressure distributions without the effects of ambient

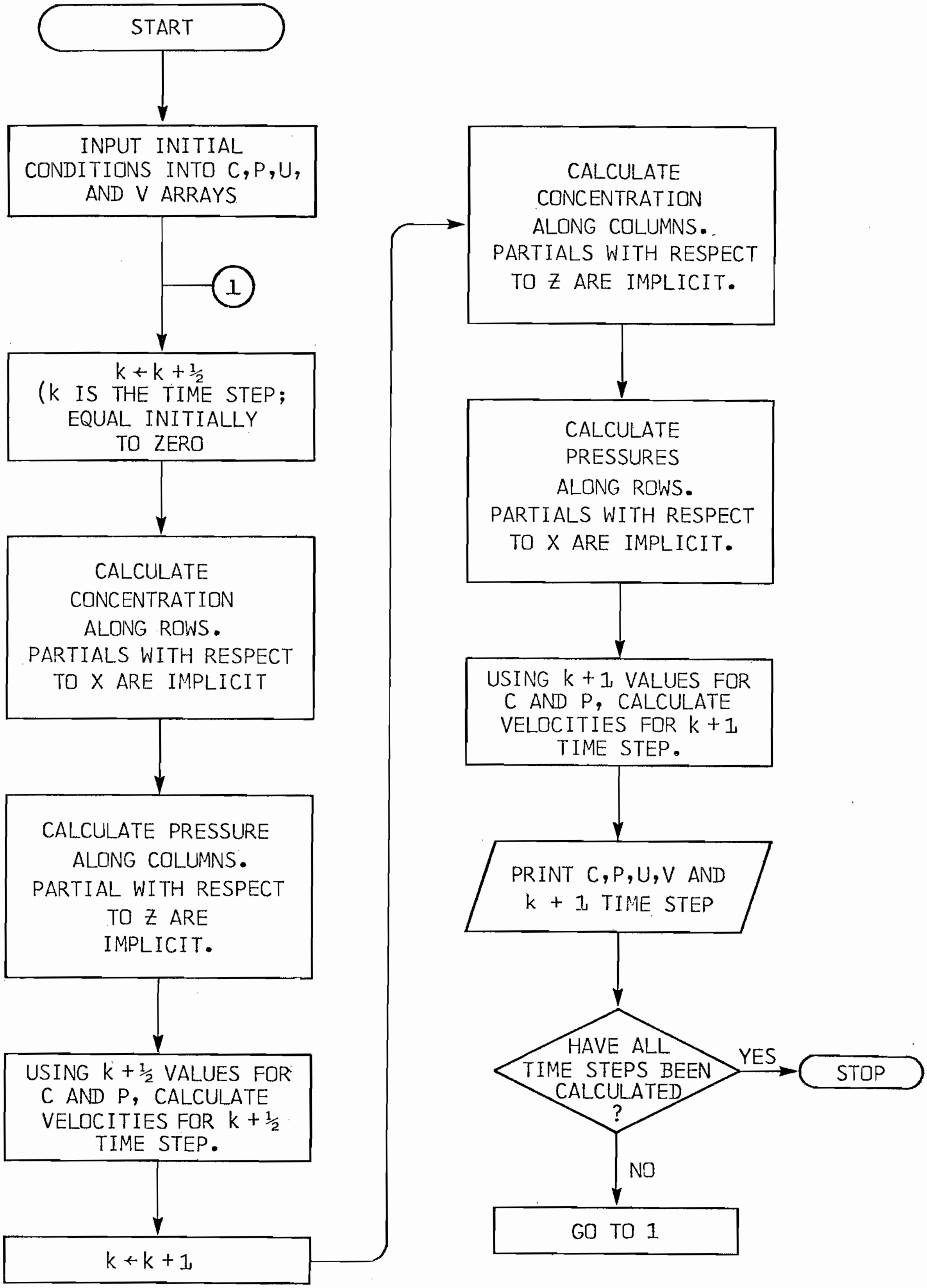

FIGURE 3. FLOW CHART FOR ALTERNATING DIRECTION IMPLICIT (A.D.I.) ALGORITHM

flow are available, and Figures 4 and 5 illustrate the general nature of the concentration outpus. Figure 4 illustrates the effects of molecular diffusion on the transition zone as a function of time in the interior of the model (75 cm from the ocean). Figure 5 illustrates the effects of molecular diffusion from the ocean on the freshwater lens as a function of distance inland from the ocean. Concentrations at the initial conditions

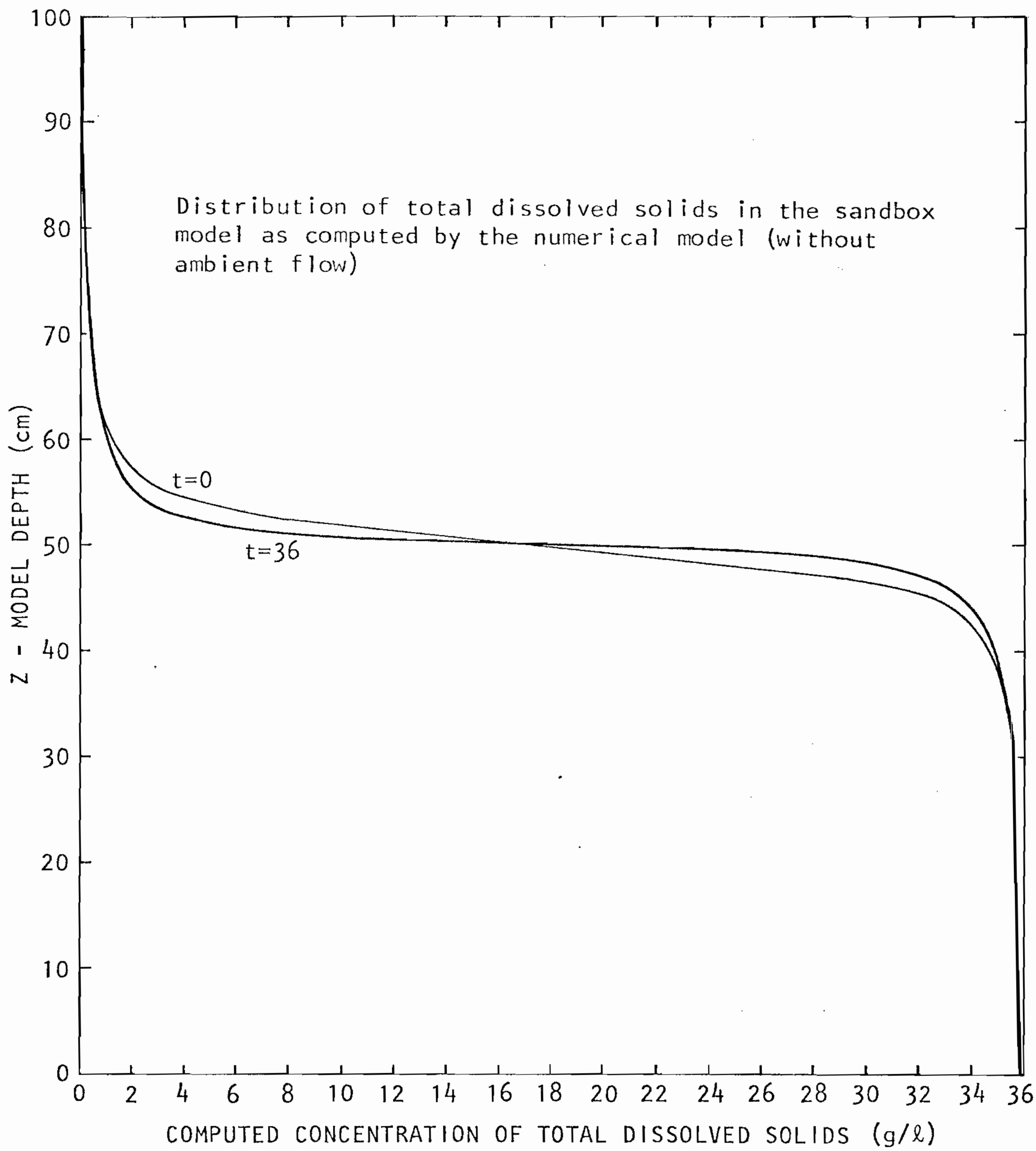

FIGURE 4. EFFECT OF DIFFUSION ON THE TRANSITION ZONE

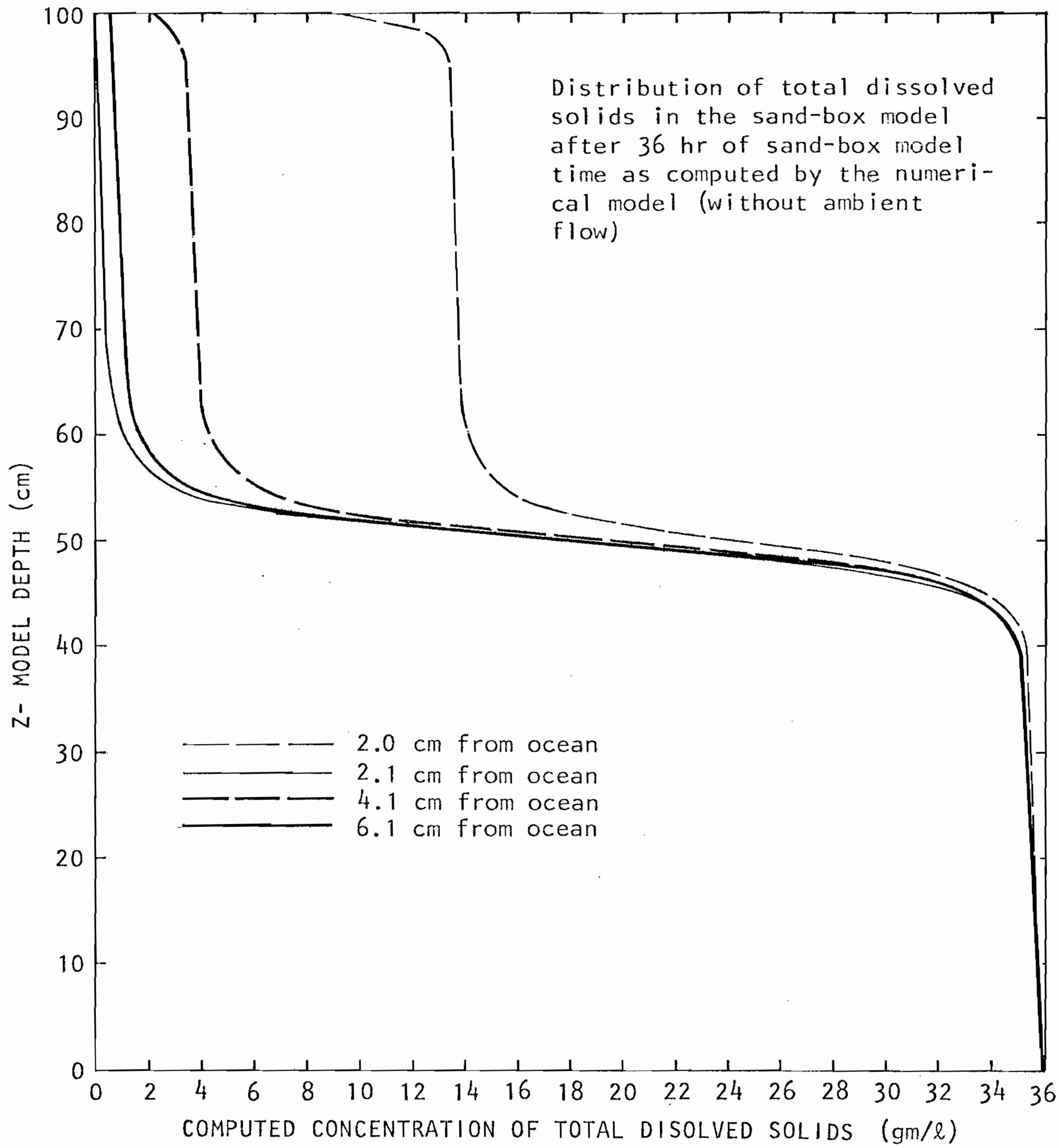

FIGURE 5. EFFECT OF DIFFUSION FROM THE SEA ON THE FRESH WATER LENS

were computed artificially to represent an average concentration distribution that was measured as an initial condition in the sand-box model. Singularities in the coefficient matrix were encountered due to certain curious relationships between the boundary conditions and the ADI method itself. These problems have nearly been solved and complete results for case 1 will shortly be available. In addition, work has also begun on the solution of case 1 by the finite element method (FEM). George Pinder, of Princeton

University, has supplied a FEM code which provides automatic mesh generation and efficient matrix solving routines for coupled sets of transient nonlinear three-dimensional partial differential equations. Using the method of weighted residuals, systems of matrix equations will be generated from the governing equations and boundary conditions. Subroutines that generate these matrix equations will then be coded and used as input to the program provided by Pinder. Using this program will save time during the developmental stage since matrix solving routines and generation of system topology (the character of the finite element mesh) are common to all FEM problems.

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LIST OF SYMBOLS

Symbol	Description
a_l	longitudinal dispersivity (L)
a_t	transverse dispersivity
C	concentration of sea water in total dissolved solids (mass/length^3, m/l^3)
C_0	initial concentration (m/l^3)
D_d	coefficient of molecular dispersion (length^2/time, l^2/t)
$\underset{\sim}{g}$	acceleration of gravity (l/t^2)
$\underset{\approx}{k}$	intrinsic permeability tensor (second rank) (l^2)
k_x	intrinsic permeability in x-direction (l^2)
k_y	intrinsic eprmeability in y-direction (l^2)
k_z	intrinsic permeability in z-direction (l^2)
n	porosity (dimensionless)
P	pressure (force/l^2, f/l^2)
P_0	initial pressure at top of aquifer (f/l^2)
$\underset{\sim}{q}$	specific discharge vector (l/t)
$\overline{V}$	magnitude of specific discharge vector (l/t)
β_c	density coefficient; relates change in density to change in concentration (l^3/m)
β_p	coefficient of compressibility for water (l^3/t)
μ	dynamic viscosity ($m/l\text{-}t$)
ρ_0	density of fresh water (m/l^3)
ρ	density of fluid (m/l^3)
$\not{V}$	control volume
∇	differential operator: $\underset{\sim}{i}(\partial/\partial x) + \underset{\sim}{j}(\partial/\partial y) + \underset{\sim}{k}(\partial/\partial z)$
∇Z	gradient of Z = 1 in z-direction, = 0 otherwise

Symbol	Description
$\sim$	vector symbol
$\approx$	second-rank tensor symbol
$\frac{\partial}{\partial n}$	normal derivitive of a function with respect to a line or surface