

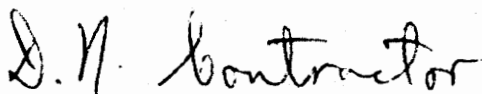
A FINITE ELEMENT ANALYSIS OF DISSOLVED OXYGEN DRAWDOWN AND SULFATE
PRODUCTION IN STRIP MINE SPOIL DAMS, DUE TO PYRITIC CHEMICAL REACTION

by

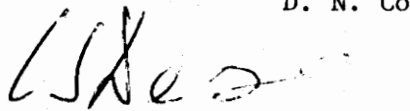
Joseph Henry Amend, III

Dissertation submitted to the Graduate Faculty of the
Virginia Polytechnic Institute and State University
in partial fulfillment of the requirements for the degree of
DOCTOR OF PHILOSOPHY
in
Civil Engineering

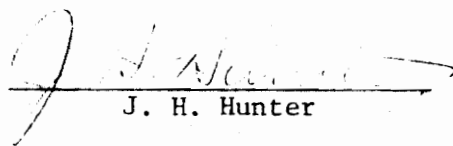
APPROVED:



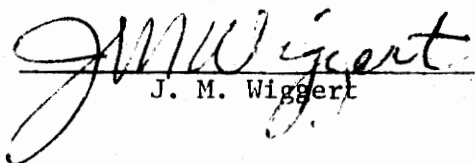
D. N. Contractor, Chairman



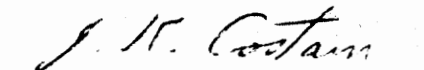
C. S. Desai



J. H. Hunter



J. M. Wiggert



J. K. Costain

May, 1975

Blacksburg, Virginia

LD
5655
V856
1975
A47
c. 2

ACKNOWLEDGEMENTS

The author wishes to express his deepest and heartfelt thanks to everybody, both unnamed and named, who made this thesis possible.

Special thanks are due the following people.

Dinshaw N. Contractor - The author's major advisor without whose constructive criticism and guidance this thesis would not have been possible.

Richard D. Walker - Chairman, Department of Civil Engineering without whose generous financial aid by means of a Graduate Teaching Assistantship this thesis would not have been possible.

Chandrakant S. Desai - Whose guidance in the numerical solution of this thesis and instruction in Finite Element techniques greatly helped the author.

John H. Hunter - Whose criticisms and suggestions during the author's years in Graduate School have been invaluable.

Robert J. Melosh - Who introduced the author to the finite element method, but more importantly, stimulated him intellectually.

Cindy S. Amend - The author's wife and typist of this thesis who shared his defeats and triumphs, never losing faith in him.

TABLE OF CONTENTS

Acknowledgements ii

Table of Contents iii

List of Figures iv

List of Tables viii

Chapter I - Introduction 1

 II - Literature Review 2

 General Background 2

 The Diffusion-Convection Equation 3

 Chemical Reaction 4

 Dispersion Coefficients 7

 III - Problem Derivation 11

 IV - Results 26

 V - Discussion of Results 53

 IV - Closing Remarks and Recommendations for Further
 Study 57

Bibliography 58

Appendix - A. Definition of Terms 61

 B. Description of the Computer Program used in the
 Analysis 63

 C. Computer Program 74

Vita 113

Abstract

LIST OF FIGURES

Figure 1	Typical earth dam cross section	14
Figure 2	Initial continuum discretization.	15
Figure 3	Natural coordinate system and linear isoparametric quadrilateral element	18
Figure 4	Final mesh and node numbering scheme.	27
Figure 5	Nodal dissolved oxygen concentrations in mg/l for isotropic soil permeability (5×10^{-5} cm/sec) and specified oxygen reaction coefficient (1×10^{-4} sec ⁻¹). . .	28
Figure 6	Nodal dissolved oxygen concentrations in mg/l for isotropic soil permeability (5×10^{-5} cm/sec) and specified oxygen reaction coefficient (1×10^{-5} sec ⁻¹). . .	29
Figure 7	Nodal dissolved oxygen concentrations in mg/l for isotropic soil permeability (5×10^{-5} cm/sec) and specified oxygen reaction coefficient (1×10^{-6} sec ⁻¹). . .	30
Figure 8	Nodal dissolved oxygen concentrations in mg/l for isotropic soil permeability (5×10^{-5} cm/sec) and specified oxygen reaction coefficient (1×10^{-7} sec ⁻¹). . .	31
Figure 9	Nodal dissolved oxygen concentrations in mg/l for isotropic soil permeability (5×10^{-5} cm/sec) and specified oxygen reaction coefficient (1×10^{-8} sec ⁻¹). . .	32
Figure 10	Nodal dissolved sulfate concentrations in mg/l for isotropic soil permeability (5×10^{-5} cm/sec) and specified oxygen reaction coefficient (1×10^{-4} sec ⁻¹). . .	33
Figure 11	Nodal dissolved sulfate concentrations in mg/l for isotropic soil permeability (5×10^{-5} cm/sec) and specified oxygen reaction coefficient (1×10^{-5} sec ⁻¹). . .	34

Figure 12	Nodal dissolved sulfate concentrations in mg/l for isotropic soil permeability (5×10^{-5} cm/sec) and specified oxygen reaction coefficient (1×10^{-6} sec ⁻¹).	35
Figure 13	Nodal dissolved sulfate concentrations in mg/l for isotropic soil permeability (5×10^{-5} cm/sec) and specified oxygen reaction coefficient (1×10^{-7} sec ⁻¹).	36
Figure 14	Nodal dissolved sulfate concentrations in mg/l for isotropic soil permeability (5×10^{-5} cm/sec) and specified oxygen reaction coefficient (1×10^{-8} sec ⁻¹).	37
Figure 15	Nodal dissolved oxygen concentrations in mg/l for anisotropic soil permeability ($K_x = 5 \times 10^{-5}$ cm/sec and $K_y = 5 \times 10^{-6}$ cm/sec) and specified oxygen reaction coefficient (1×10^{-4} sec ⁻¹).	38
Figure 16	Nodal dissolved oxygen concentrations in mg/l for anisotropic soil permeability ($K_x = 5 \times 10^{-5}$ cm/sec and $K_y = 5 \times 10^{-6}$ cm/sec) and specified oxygen reaction coefficient (1×10^{-5} sec ⁻¹).	39
Figure 17	Nodal dissolved oxygen concentrations in mg/l for anisotropic soil permeability ($K_x = 5 \times 10^{-5}$ cm/sec and $K_y = 5 \times 10^{-6}$ cm/sec) and specified oxygen reaction coefficient (1×10^{-6} sec ⁻¹).	40
Figure 18	Nodal dissolved oxygen concentrations in mg/l for anisotropic soil permeability ($K_x = 5 \times 10^{-5}$ cm/sec and $K_y = 5 \times 10^{-6}$ cm/sec) and specified oxygen reaction coefficient (1×10^{-7} sec ⁻¹).	41
Figure 19	Nodal dissolved oxygen concentrations in mg/l for anisotropic soil permeability ($K_x = 5 \times 10^{-5}$ cm/sec and $K_y = 5 \times 10^{-6}$ cm/sec) and specified oxygen reaction coefficient (1×10^{-8} sec ⁻¹).	42

Figure 20	Nodal dissolved sulfate concentrations in mg/l for anisotropic soil permeability ($K_x = 5 \times 10^{-5}$ cm/sec and $K_y = 5 \times 10^{-6}$ cm/sec) and specified oxygen reaction coefficient (1×10^{-4} sec ⁻¹)	43
Figure 21	Nodal dissolved sulfate concentrations in mg/l for anisotropic soil permeability ($K_x = 5 \times 10^{-5}$ cm/sec and $K_y = 5 \times 10^{-6}$ cm/sec) and specified oxygen reaction coefficient (1×10^{-5} sec ⁻¹)	44
Figure 22	Nodal dissolved sulfate concentrations in mg/l for anisotropic soil permeability ($K_x = 5 \times 10^{-5}$ cm/sec and $K_y = 5 \times 10^{-6}$ cm/sec) and specified oxygen reaction coefficient (1×10^{-6} sec ⁻¹)	45
Figure 23	Nodal dissolved sulfate concentrations in mg/l for anisotropic soil permeability ($K_x = 5 \times 10^{-5}$ cm/sec and $K_y = 5 \times 10^{-6}$ cm/sec) and specified oxygen reaction coefficient (1×10^{-7} sec ⁻¹)	46
Figure 24	Nodal dissolved sulfate concentrations in mg/l for anisotropic soil permeability ($K_x = 5 \times 10^{-5}$ cm/sec and $K_y = 5 \times 10^{-6}$ cm/sec) and specified oxygen reaction coefficient (1×10^{-8} sec ⁻¹)	47
Figure 25	Plot of downstream (node 30) dissolved oxygen deficit production versus isotropic soil permeability for various values of dissolved oxygen reaction coefficient (K)	49
Figure 26	Plot of downstream (node 30) sulfate production versus isotropic soil permeability for various values of the dissolved oxygen reaction coefficient (K)	50

Figure 27	Plot of downstream (node 30) dissolved oxygen concentration versus mixing factor for an isotropic soil permeability = 5×10^{-5} (cm/sec) and a dissolved oxygen reaction coefficient = 1×10^{-4} (sec ⁻¹).	51
Figure 28	Plot of downstream (node 30) sulfate concentration versus mixing factor for an isotropic soil permeability = 5×10^{-5} (cm/sec) and dissolved oxygen reaction coefficient = 1×10^{-4} (sec ⁻¹)	52
Figure 29	Continuum discretization with ICHECK values noted . . .	70

LIST OF TABLES

Table 1	Oxygen Reaction Coefficient as a Function of pH for an Initial Ferrous Ion Concentration of 1000 ppm	8
Table 2	Description of General Input Data	64
Table 3	Description of Nodal Input Data for I th Node	66
Table 4	Description of Elemental Data for J th Element.	68
Table 5	Definition of Boundary Conditions	69

CHAPTER ONE
INTRODUCTION

In recent years much attention has been focused on water quality. Much of this attention has been the result of stringent State and Federal water quality standards. Consequently, it has become increasingly important to be able to predict the effect that a physical process or structure has upon the aquatic environment.

For many years strip mines have been a source of water pollution, but only recently have the mechanisms that cause this pollution come under study. It is the purpose of this study to analyze one aspect of strip mine pollution.

This study investigates the production of sulfates and the removal of dissolved oxygen when water seeps through a dam constructed of strip mine spoil material. Solutions are presented for a wide range of soil permeabilities, chemical reaction coefficients, and dispersion coefficients.

The method of solution is a three part finite element analysis. Part one deals with the steady state seepage problem by solving the Laplacian of the piezometric head. Using this output, parts two and three solve the diffusion-convection equation for the dissolved oxygen and sulfate concentrations. Dissolved oxygen drawdown and sulfate production are the result of chemical reactions taking place within the flow field of the dam.

CHAPTER TWO
LITERATURE REVIEW

General Background

In reviewing the work of previous investigators, there is a conspicuous lack of previous work in the field under study. Recent works by Marino [13]^{*} and Tagaments and Sturnberg [22] are of only peripheral importance. The different initial assumptions and the lack of a chemical reaction greatly limit their applicability to this study. For the same reasons, work by earlier investigators [10, 17] is also deficient.

With respect to this particular analysis, the only relevant studies are those by Guymon [7] and Guymon, Scott, and Hermann [8]. Despite the fact that they investigate a nonreactive medium, the differential equation used in this analysis and their analyses are the same.

The principal source of information for the actual numerical solution is Desai and Abel [5]. The linear isoparametric quadrilateral elements, natural coordinate system, and numerical integration techniques are outlined in detail in their book and this author has made extensive use of these techniques.

^{*}Numbers in brackets refer to references given in the Bibliography

The Diffusion-Convection Equation

The general form of the diffusion-convection equation written in tensor notation [7] is

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x_i} \left[D_{ij} \left(\frac{\partial C}{\partial x_j} \right) - u_i C \right] + Q - KC \quad 2.1$$

In Equation 2.1, C is the state variable, t is time, x_i is the coordinate direction ($i=x,y,z$), u_i is the convection parameter in the i direction, D_{ik} is the positive dispersion tensor, Q is a generalized source term, and K is a generalized sink factor.

Equation 2.1 is a linear nonsymmetric partial differential equation of the parabolic type, with the nonsymmetry arising from the convective terms. Previously these convection terms were the principle difficulty in obtaining satisfactory numerical solutions for the diffusion-convection equation. However, in the past 15 years this problem has been overcome and no longer presents a difficulty [7].

The impetus behind the effort to obtain usable solutions for parabolic partial differential equations is the increasing importance of the class of problems that this type of equation describes [15]: heat conduction in solids, slowing of neutrons in matter, diffusion of vorticity, conduction of long magnetic waves, and seepage of contaminants through porous media.

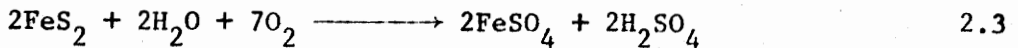
For this analysis Equation 2.1 is written in the x and y cartesian directions and can be stated as follows [7]

$$\frac{\partial C}{\partial t} + \frac{\partial V_x C}{\partial x} + \frac{\partial V_y C}{\partial y} - D_x \frac{\partial^2 C}{\partial x^2} - D_y \frac{\partial^2 C}{\partial y^2} - Q + KC = 0 \quad 2.2$$

In Equation 2.2, V_x and V_y are the bulk fluid velocities in the x and y cartesian directions and D_x and D_y are the dispersion coefficients in the x and y cartesian directions, respectively. Due to the uncertainty in determining the material properties K , D_x , D_y , K_x , and K_y , where K_x and K_y are the soil permeabilities in the x and y directions, the author feels that the increased expense and effort of a three dimensional solution is not justified at this time (1975).

Chemical Reaction

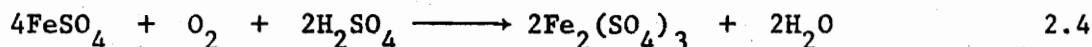
Considerable attention has been given to the reactions that occur in strip mine spoil dams [2, 3, 12, 18, 19, 20]. The principle reaction appears to be [2, 18]



Pyrite (FeS_2) is usually found over, in, and below coal seams and it is common to assume that an excess of this material exists within the impoundment structure [11]. It has been shown [12] that the free oxygen in Equation 2.3 is dissolved oxygen in the water flowing through the reactants and not atmospheric oxygen.

The products of this chemical reaction, iron sulfides and sulfuric acid, readily find their way into streams below the spoil dam. These reaction products can be further oxidized as they are being

transported through or carried away from the dam according to the following reactions [2]



The final result of the above chemical reactions is the precipitation of insoluble iron oxides and oxysulfates onto the stream beds below the dam. These precipitates are known locally as "yellow boy" [11]. Also, the sulfuric acid will remain in solution, further deteriorating the existing water quality.

Several authors [19,20] have postulated that the rate of pyrite dissolution is dependent on three factors: pH, temperature, and dissolved oxygen. Of these three factors, dissolved oxygen appears to be most significant [11].

Kim [12] has stated that the oxidation of the ferrous ion is a slow process, and it is not improbable that for a shallow pond with a large surface area the dissolved oxygen concentration can remain saturated through normal diffusion. However, in a semiconfined area such as an earth dam with nonstatic water conditions, an oxygen deficit can be observed, and in some cases the deficit can be considerable.

Singer and Stumm [19] have observed a linear relationship between dissolved oxygen drawdown and sulfate production using pyritic materials from several Pennsylvania coal seams. In addition, Stauffer

and Levell [20] report first order reaction coefficients for a ferrous ion concentration of 1000 ppm. Table 1 gives reaction coefficients as a function of pH.

Clark [3] observed the following relationship between dissolved oxygen concentration and sulfate production.

$$\frac{d(\text{SO}_4)}{dt} = 0.023(\text{DO})^{0.667} \quad 2.7$$

The units of the left hand side of Equation 2.7 are milligrams of sulfate per gram of pyrite per hour. The DO is the dissolved oxygen concentration expressed in mg/l. The constant 0.0231, therefore, has to have units to balance the equation.

While the overall correlation of Clark's data is nonlinear, a strong linearity exists for the dissolved oxygen values ranging from 1 to 16 mg/l. The maximum amount of oxygen that can be dissolved in water under atmospheric pressure occurs at 0° C. This value is 14.62 mg/l [21]. This value is well within the range of linearity of Clark's data and it appears that the nonlinearity occurs at oxygen concentrations exceeding those that can occur in nature.

From Equation 2.7 it can be seen that the dissolved oxygen concentration must be known before the sulfate reaction coefficients and concentrations can be determined. The average elemental dissolved oxygen concentration is calculated, and this value is used in calculating the elemental sulfate reaction coefficients. After the

elemental sulfate reaction coefficients are known, the nodal sulfate concentrations can be calculated.

Due to the uncertainty in determining a specific criterion for specifying generalized reaction coefficients, their determination is left to the program user. As a first approximation, values from the middle range in Table 1 can be used. It is advisable, however, to determine experimentally the numerical values for a specific case under study.

To be dimensionally compatible with Equation 2.2, the reaction coefficient must have units of time⁻¹. To be dimensionally compatible with this analysis, the units of the reaction coefficient must be sec⁻¹.

Dispersion Coefficients

There are few instances encountered in engineering where less is known about a phenomena than the present state of knowledge of field dispersion coefficient values. Previous studies [9, 10, 14, 17] have dealt almost exclusively with laboratory soil column tests and do not even vaguely represent the dispersion processes that occur in a discontinuous and nonhomogeneous flow medium such as a strip mine spoil dam.

For this reason, Guymon [7] has postulated a linear relationship between bulk fluid velocity and dispersion coefficient.

$$D_i = d_i V_i$$

TABLE 1
OXYGEN REACTION COEFFICIENT AS A FUNCTION OF pH FOR AN INITIAL
FERROUS ION CONCENTRATION OF 1000 PPM (After Stauffer and Levell [20])

<u>pH</u>	<u>Oxygen reaction coefficient (min⁻¹)</u>
4.50	1.50×10^{-5}
4.70	2.63×10^{-3}
4.75	3.48×10^{-3}
4.80	5.17×10^{-3}
5.10	8.09×10^{-3}
5.18	1.19×10^{-2}
5.35	3.03×10^{-2}

In the preceding equation D_i is the dispersion coefficient, expressed in cm^2/sec , in the i^{th} cartesian coordinate direction, d_i is the mixing factor in the i^{th} direction, and V_i is the elemental bulk fluid velocity in the i^{th} direction.

Intuitively, it can be reasoned that the more discontinuous a flow field is, the higher the mixing factor and dispersion coefficient. Considering laminar flow in a closed conduit, it is evident that very little mixing will occur, and therefore, the dispersion coefficient and mixing factor would be small. However, for turbulent flow a much greater amount of mixing will occur due to eddies set up in the conduit. The same result can be obtained if obstructions are placed in the laminar flow medium. While laminar flow is maintained, much more mixing occurs due to the distortion of the flow paths of the fluid particles. These irregularities are greatly magnified when considering a laminar flow regime such as an earth dam where the material can be anisotropic and highly discontinuous. It is, therefore, logical to assume that the more tortuous the fluid path through a dam is, the higher the values of the dispersion coefficient and mixing factor.

It is evident from examination of Equation 2.8 that even though the spoil material may be homogeneous and isotropic, the x and y direction dispersion coefficients will not be equal, for the x and y fluid velocities are constantly changing and are a function of the point in the flow field which is under study.

Guymon [6] suggests that the only method to accurately determine the dispersion coefficient is to obtain dispersion data and adjust the

mixing factor values until a good correlation is obtained between the calculated and observed data. As an initial guess Guymon [9a] suggests a value of 5 miles (8.50×10^5 cm) for the mixing factor.

At this time (1975) the only acceptable method for the determination of field values of the dispersion coefficient is the empirical correlation of field and calculated data by use of the mixing factor. In this study, unless specifically noted otherwise, the value of the mixing factor in both the x and y directions will be 8.50×10^5 cm (5 miles).

CHAPTER THREE

PROBLEM DERIVATION

The overall problem is approached in three steps. The first step calculates the bulk fluid velocities in the earth dam flow field. This is accomplished by solution of the following equation [4,5]

$$K_x \frac{\partial^2 \phi}{\partial x^2} + K_y \frac{\partial^2 \phi}{\partial y^2} = 0 \quad 3.1$$

for the nodal piezometric head (ϕ) and using this value to calculate the average x and y velocities in each element. The assumptions made in the seepage problem are steady state, saturated laminar flow, and constant soil permeabilities in the x and y directions in each element. The permeabilities, however, may vary in a stepwise manner from element to element. These assumptions will also apply to all other parts of the analysis. If the permeabilities in the x and y directions are equal, Equation 3.1 will reduce to the well-known Laplace Equation for flow through porous media.

The variational statement of Equation 3.1 is written as follows [5]

$$A = \iint \frac{1}{2} \left[K_x \left(\frac{\partial \phi}{\partial x} \right)^2 + K_y \left(\frac{\partial \phi}{\partial y} \right)^2 \right] dx dy \quad 3.2$$

The variational method used for the solution of the seepage problem is presented in detail in Desai and Abel [5] and is one of many solutions available [16, 23, 24]. Desai and Abel's method was selected because of the inherent advantages in merging the velocity, dissolved oxygen concentration (DOC), and sulfate production parts of the analysis.

Two types of boundary conditions occur in the flow problem. The first one is

$$\phi = \bar{\phi} \quad 3.3$$

where $\bar{\phi}$ is a prescribed boundary potential. This is known as the Dirichlet or head boundary condition [4]. This condition is imposed when the state variable is defined to have a specific value at a given node. This condition occurs on the upstream face, seepage surface, and downstream face of the dam.

The second condition is

$$\frac{\partial \phi}{\partial n} = 0 \quad 3.4$$

when n indicates the outward normal of the flow boundary. Equation 3.4 states that there is no change in fluid potential normal to the boundary. This condition occurs along the base of the dam and is called the Neumann or flow boundary condition [4].

Along the free surface both the Dirichlet and Neumann conditions must be satisfied. This is accomplished by allowing no fluid flow normal to the free surface and comparing the total head and elevation head. If the difference between the total and elevation head is not within a given tolerance, the free surface nodes are repositioned, allowing no normal flow until the difference is less than a specified tolerance.

A second step is the determination of the DOC. This is accomplished in six steps that are common to all finite element analyses [5].

Discretization of the Continuum Figure 1 illustrates the continuum to be subdivided. It is a typical earth dam cross-section in which the major features of the dam are labeled.

Figure 2 shows the initial discretization of the dam. It has been subdivided into roughly square elements that to some extent approximate the shape and configuration of a flow net. Only a rough estimate of the free surface needs to be made for its position is calculated in the program. The method of node numbering is also illustrated in Figure 2. This method of node numbering was selected as being the most efficient for working with the free surface adjustment.

It should be noted that the number of elements and their positions in the continuum are arbitrary and the choice is left to the program user. The mesh configuration that is used in this analysis was chosen to facilitate the free surface determination and to keep the computer

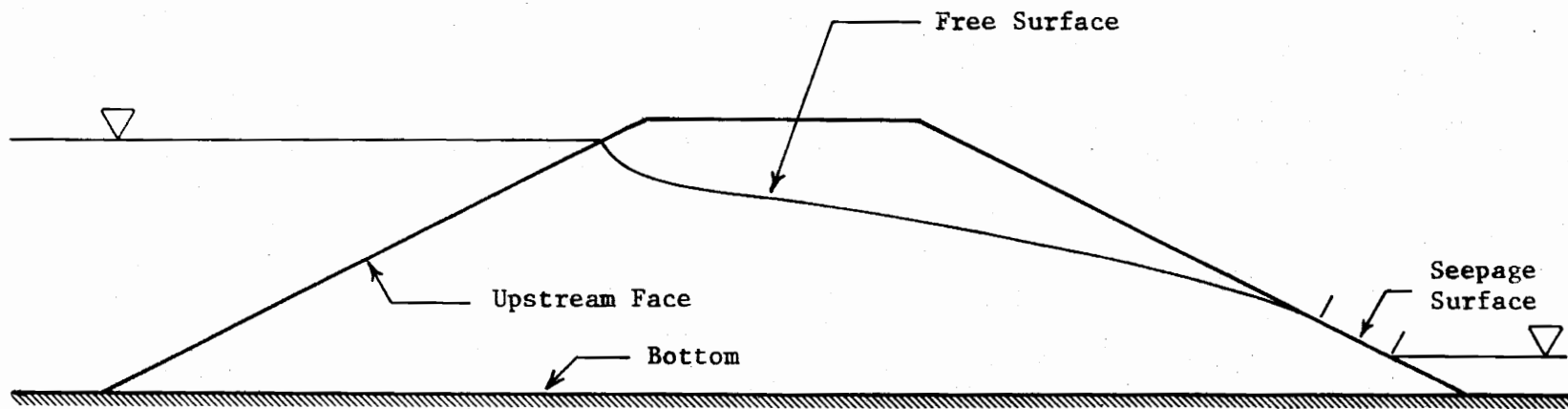


Figure 1 Typical earth dam cross section

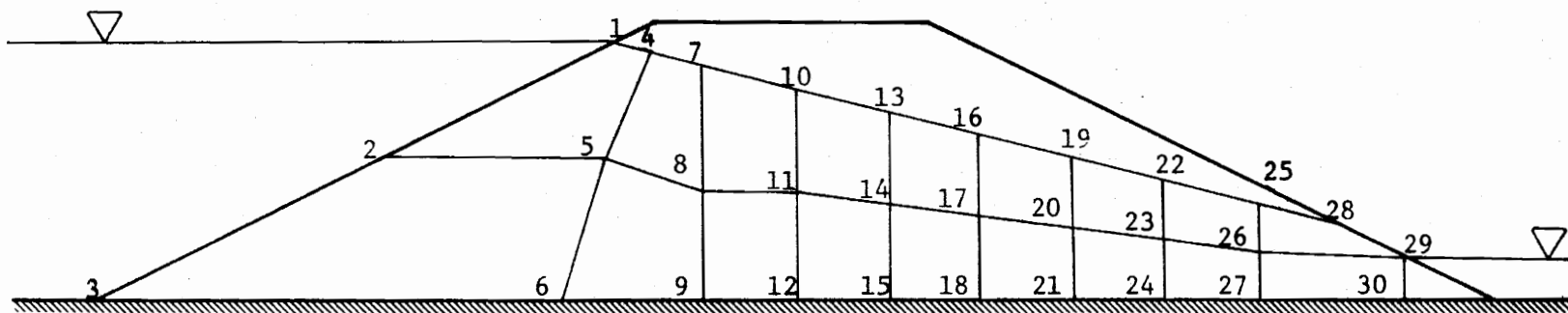


Figure 2 Initial continuum discretization

storage requirements to a minimum. In addition, in view of the difficulty in accurately determining the material properties, K_x , K_y , D_x , D_y , and K , the extra expense of a finer mesh is not justified at this time.

Because of the physical properties of the flow medium, the soil in the elements is rigid. The continuum will not deform in the circumstances under study. However, the initial node positions will move during the iterations to determine the correct position of the free surface.

Selection of the Field Variable Model The field variable model selected for this analysis is the dissolved oxygen concentration, hereafter referred to as DOC. This term is defined as the amount of dissolved oxygen present in the water.

A natural coordinate system is used, which in conjunction with the linear isoparametric quadrilateral elements, simplifies the problem formulation and equation derivation. In addition, these selections tend to normalize the numerical values of the resulting matrix equations.

Using the linear isoparametric elements, the field variable is assumed to vary linearly across an element according to the following equation

$$C = c_i N_i + c_j N_j + c_k N_k + c_l N_l \quad 3.5$$

In Equation 3.5, c_i is the DOC of element node i and N_i is the shape function at the same node and is defined to be

$$N_i = \frac{1}{4}(1 + ss_i)(1 + tt_i) \quad 3.6$$

s and t are the local coordinates and s_i and t_i are the natural coordinates of the i^{th} node of an element. Figure 3 shows a general isoparametric quadrilateral with the appropriate node numbers with natural coordinate values of the nodes. The corresponding nodal cartesian coordinates are also defined.

Equation 3.5 can be written

$$C = \{z^T\} \{c_n\} \quad 3.7$$

In Equation 3.7, $\{z^T\}$ and $\{c_n\}$ are defined as follows:

$$\{z^T\} = \{N_i \ N_j \ N_k \ N_l\} \quad 3.8$$

$$\{c_n\}^T = \{c_i \ c_j \ c_k \ c_l\} \quad 3.9$$

The subscripts used in Equations 3.8 and 3.9 refer to the node definitions in Figure 3.

While natural coordinates have computational advantages over cartesian coordinates, the following equations must be used in converting from one coordinate system to another [5]:

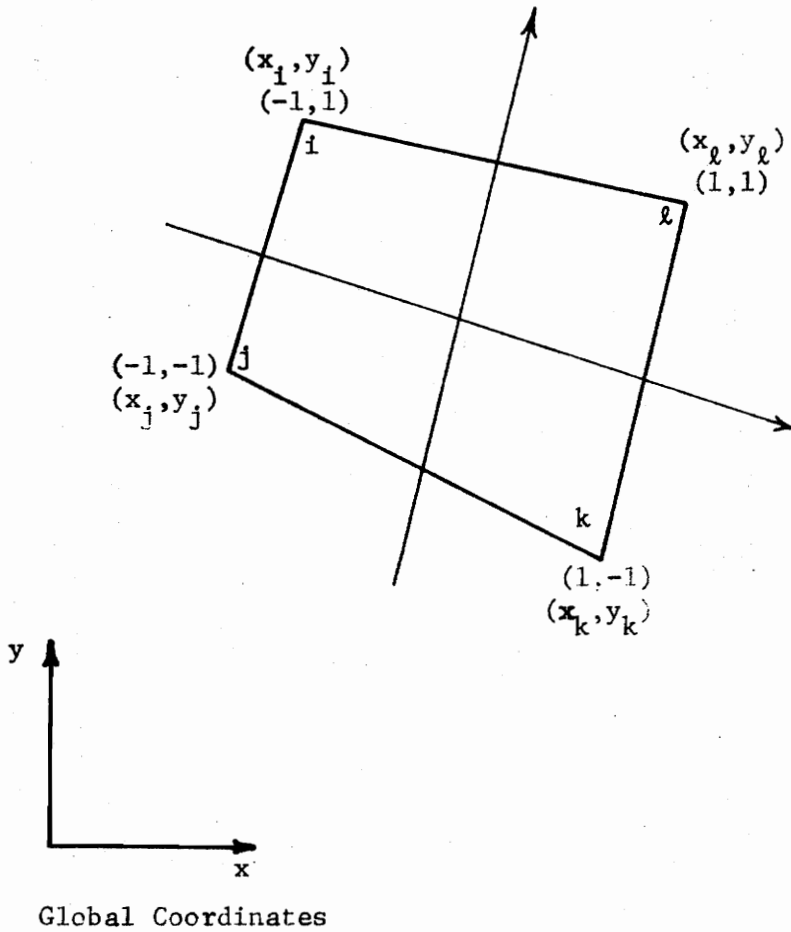


Figure 3 Natural coordinate system and linear isoparametric quadrilateral element (after Desai and Abel [5])

$$\begin{Bmatrix} \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} \end{Bmatrix} = [J^{-1}] \begin{Bmatrix} \frac{\partial}{\partial s} \\ \frac{\partial}{\partial t} \end{Bmatrix} \quad 3.10$$

and

$$dx dy = \det |J| ds dt \quad 3.11$$

J in the preceding equations is the Jacobian matrix and is defined [5]

$$[J] = \begin{Bmatrix} \frac{\partial}{\partial s} \{z^T\} \\ \frac{\partial}{\partial t} \{z^T\} \end{Bmatrix} \begin{Bmatrix} \{x_n\} \\ \{y_n\} \end{Bmatrix} \quad 3.12$$

In the previous equation x_n and y_n are the cartesian coordinates of the elemental nodes.

Derivation of the Finite Element Equations Assuming no internal oxygen sources and steady state conditions, the elemental diffusion-convection equation (Equation 2.2) can be written

$$V_x \frac{\partial C}{\partial x} + V_y \frac{\partial C}{\partial y} - D_x \frac{\partial^2 C}{\partial x^2} - D_y \frac{\partial^2 C}{\partial y^2} + KC = 0 \quad 3.13$$

The variational statement corresponding to Equation 3.13 is [8]

$$\chi = \iint \exp(\beta) \left[\frac{D_x}{2} \left(\frac{\partial C}{\partial x} \right)^2 + \frac{D_y}{2} \left(\frac{\partial C}{\partial y} \right)^2 + \frac{KC^2}{2} \right] dx dy \quad 3.14$$

where

$$\beta = - \frac{X V_x}{D_x} - \frac{Y V_y}{D_y} \quad 3.15$$

x and y are the cartesian coordinates of the point at which β is being evaluated.

The elemental material property matrix can be formulated in a natural coordinate system and is written as follows:

$$[k] \{c\} = \{r\} \quad 3.16$$

In the preceding equation $[k]$ is the elemental material property matrix and is defined [5] as

$$[k] = \iint \exp(\beta') \left[[B^T] [D] [B] + \{N^T\} \{N\} \right] \det|J| \, dsdt \quad 3.17$$

$\{c\}$ is the vector of unknown nodal oxygen concentrations, and $\{r\}$ is a column vector formed by applying the appropriate boundary conditions. This procedure will be discussed later. The $[B]$ matrix of Equation 3.17 is defined as follows:

$$[B] = [b_i \ b_j \ b_k \ b_l] \quad 3.18$$

The b terms of Equation 3.18 are defined as follows:

$$\{b_n\} = [J^{-1}] \begin{Bmatrix} \frac{\partial N_n}{\partial s} \\ \frac{\partial N_n}{\partial t} \end{Bmatrix} \quad 3.19$$

The $[D]$ matrix in Equation 3.17 is the matrix of principle dispersion coefficients

$$[D] = \begin{bmatrix} D_x & 0 \\ 0 & D_y \end{bmatrix} \quad 3.20$$

and $\{N\}$ in Equation 3.17 is a vector of nodal shape functions

$$\{N\} = \{N_i \ N_j \ N_k \ N_l\} \quad 3.21$$

where the values of the shape functions are defined by Equation 3.6.

In the transformation of Equation 3.14 to Equation 3.17, it is necessary to transform the exponent β because it is a function of the x and y cartesian directions. The transformed exponent β' becomes

$$\beta' = -\frac{X' V_x}{D_x} - \frac{Y' V_y}{D_y} \quad 3.22$$

X' and Y' are defined as follows [5]:

$$\begin{Bmatrix} X' \\ Y' \end{Bmatrix} = \begin{bmatrix} \{z^T\} & \{0\} \\ \{0\} & \{z^T\} \end{bmatrix} \begin{Bmatrix} \{x_n\} \\ \{y_n\} \end{Bmatrix} \quad 3.23$$

To make the integration of Equation 3.16 manageable, it is assumed that the material properties D_x , D_y , K_x , K_y , and K are constant across any given element. These parameters, however, may vary in a stepwise manner from element to element. In addition, the bulk fluid

velocities, V_x and V_y , are assumed to be a constant across an element.

The generation of the elemental material property matrix is accomplished by a numerical integration technique of the following form [5]:

$$\int_{-1}^1 \int_{-1}^1 (\text{Integrand}) \det|J| \, dsdt = \sum_{i=1}^4 W_i (\text{Integrand}) \bigg|_{s_i, t_i} \det|J| \bigg|_{s_i, t_i} \quad 3.24$$

In the preceding equation, W_i is a weighting factor. For four point integration, $W_i = 1.0$, s_i and t_i are ± 0.577350289189626 [1]. A four point numerical integration is performed and the resulting four answers summed to form the element material property matrix.

Assembly of Algebraic Equations Before the element equations are assembled into the global matrix, the boundary conditions are imposed. While the boundary conditions could be imposed at the system level, they are imposed at the element level to reduce the number of calculations and the amount of computer storage required.

There are two types of boundary conditions encountered in this part of the analysis. The first condition is that certain nodes are defined to have specific DOC values. This occurs along the upstream face of the dam and along the free surface. Along these surfaces the oxygen concentration is defined to be the saturation oxygen concentration. This condition is similar to the boundary condition

described by Equation 3.3, the only difference being that the DOC values are used instead of the fluid potentials.

The following form is used to specify the state variable to have a specific value. Consider the elemental material property matrix

$$\begin{bmatrix} k_{ii} & k_{ij} & k_{ik} & k_{il} \\ k_{ji} & k_{jj} & k_{jk} & k_{jl} \\ k_{ki} & k_{kj} & k_{kk} & k_{kl} \\ k_{li} & k_{lj} & k_{lk} & k_{ll} \end{bmatrix} \begin{bmatrix} c_i \\ c_j \\ c_k \\ c_l \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} \quad 3.25$$

To define $c_i = R_a$ and $c_j = R_b$ the preceding equation becomes

$$\begin{bmatrix} 1.0 & 0 & 0 & 0 \\ 0 & 1.0 & 0 & 0 \\ 0 & 0 & k_{kk} & k_{kl} \\ 0 & 0 & k_{lk} & k_{ll} \end{bmatrix} \begin{bmatrix} c_i \\ c_j \\ c_k \\ c_l \end{bmatrix} = \begin{bmatrix} R_a \\ R_b \\ -k_{ki}R_a - k_{kj}R_b \\ -k_{li}R_a - k_{lj}R_b \end{bmatrix} \quad 3.26$$

It should be noted that any combination of nodes may be defined to have specific values and not just i and j, depending on the type of boundary condition to be imposed. The terms on the right-hand side of Equation 3.2 comprise the $\{r\}$ vector defined in Equation 3.16.

The second type of boundary condition is the specification that the oxygen concentration gradient normal to an impervious boundary is zero. This condition exists along the impervious base of the dam.

This condition is analogous to the boundary condition described by Equation 3.4, the only difference being that the DOC instead of the fluid potential ϕ is used. An additional advantage of the variational method is that this boundary condition is implicitly included in the problem formulation.

After the boundary conditions have been imposed, the constrained elemental material property matrices are summed to obtain the constrained global material property matrix. This matrix is symmetric, banded, and of rank NN, where NN is the number of nodes in the continuum discretization.

Solution of the Nodal Field Variable Vector A linear simultaneous equation solver is used for the solution of the oxygen concentration vector. By subtracting the DOC from the saturation oxygen concentration, the dissolved oxygen deficit is found.

Computation of the Elemental Resultants from the Nodal Field Variable Amplitudes This step of the finite element analysis is not needed since the object of the analysis was the field variable vector.

Step three of this analysis is the determination of the sulfate production. Referring to Equation 2.7, it can be seen that the sulfate reaction coefficient cannot be calculated until the dissolved oxygen concentrations are known. By taking the average of the nodal dissolved oxygen concentrations, the average elemental sulfate reaction coefficient can be calculated using Equation 2.7.

With the sulfate reaction coefficients known, the finite element analysis outlined for step two is repeated and the nodal sulfate

concentrations are calculated. The only difference between the DOC and sulfate solutions is that no sulfate recharge exists, that is the sulfate production will accumulate as water flows through the dam towards the downstream face.

CHAPTER FOUR

RESULTS

In order to determine the extreme values of the dissolved oxygen and sulfate concentrations, several example problems were solved. The initial discretization of the continuum is the same as in Figure 2. A saturated dissolved oxygen concentration of 12.47 mg/l is used in all cases. While all the data presented represent numerically stable solutions, the range of variation of the material properties encountered in practice will be much less.

Figure 4 represents the earth dam cross section and final mesh discretization that is used in this study. This mesh also illustrates the node numbering scheme that is used.

Using the mesh presented in Figure 4, the seepage surface is the part of the downstream dam face between nodes 28 and 29. Node 29 is also the intersection of the downstream face of the dam and the downstream water level.

Figures 5 - 14 give the nodal concentrations for dissolved oxygen and sulfate ions for the isotropic permeability 5×10^{-5} cm/sec and various values of the oxygen reaction coefficient.

Figures 15 - 24 give the nodal concentrations for dissolved oxygen and sulfate ions for the anisotropic flow field in which the x direction permeability is 5×10^{-5} cm/sec and the y direction permeability is 5×10^{-6} cm/sec and various values of the oxygen reaction coefficient.

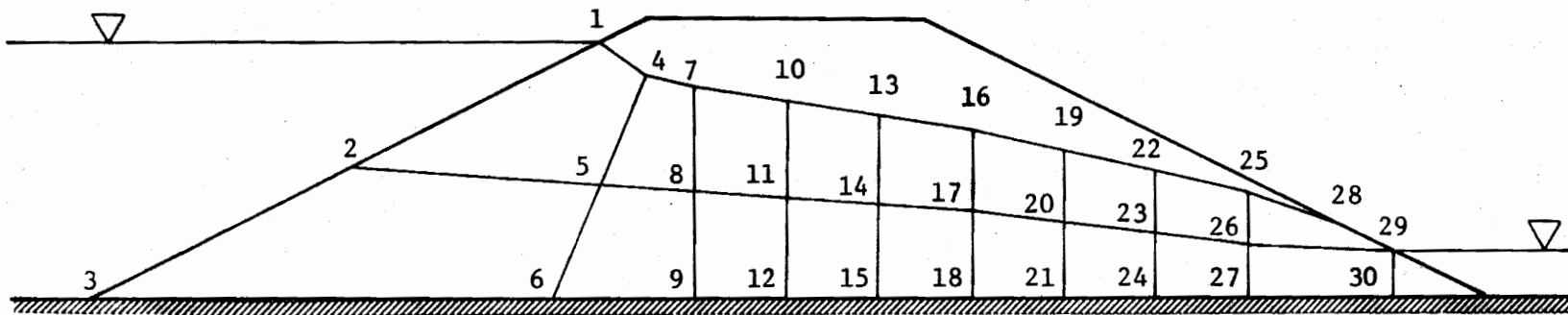


Figure 4 Final mesh and node numbering scheme

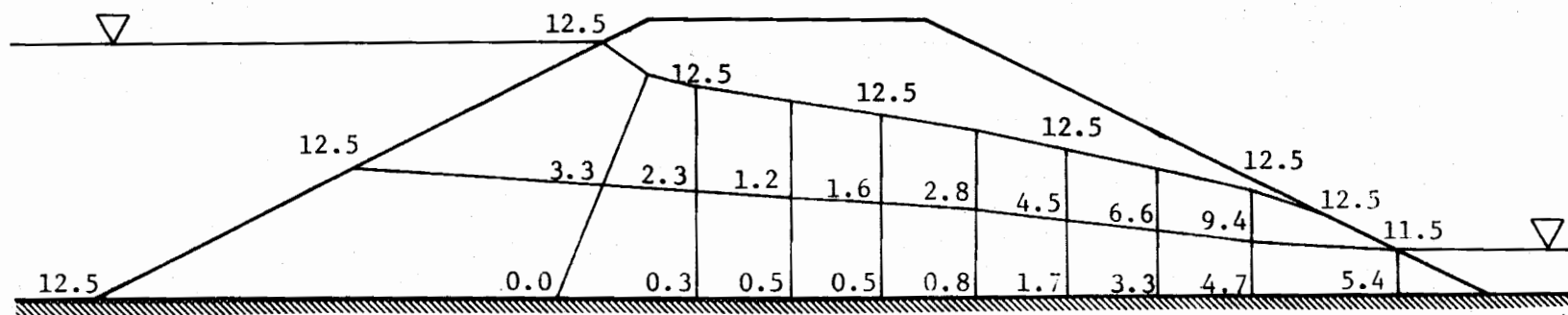


Figure 5 Nodal dissolved oxygen concentrations in mg/l for isotropic soil permeability (5×10^{-5} cm/sec) and specified oxygen reaction coefficient (1×10^{-4} sec⁻¹)

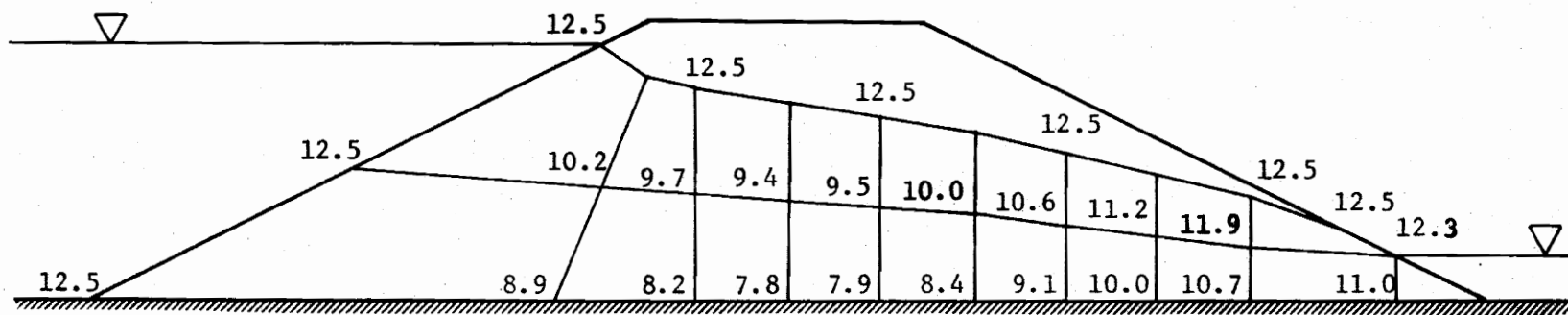


Figure 6 Nodal dissolved oxygen concentrations in mg/l for isotropic soil permeability (5×10^{-5} cm/sec) and specified oxygen reaction coefficient (1×10^{-5} sec $^{-1}$)

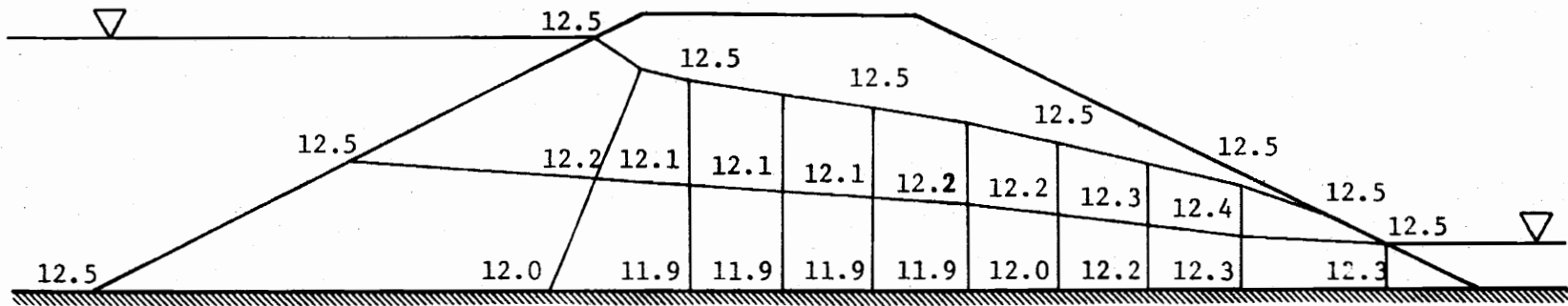


Figure 7 Nodal dissolved oxygen concentrations in mg/l for isotropic soil permeability (5×10^{-5} cm/sec) and specified oxygen reaction coefficient (1×10^{-6} sec⁻¹)

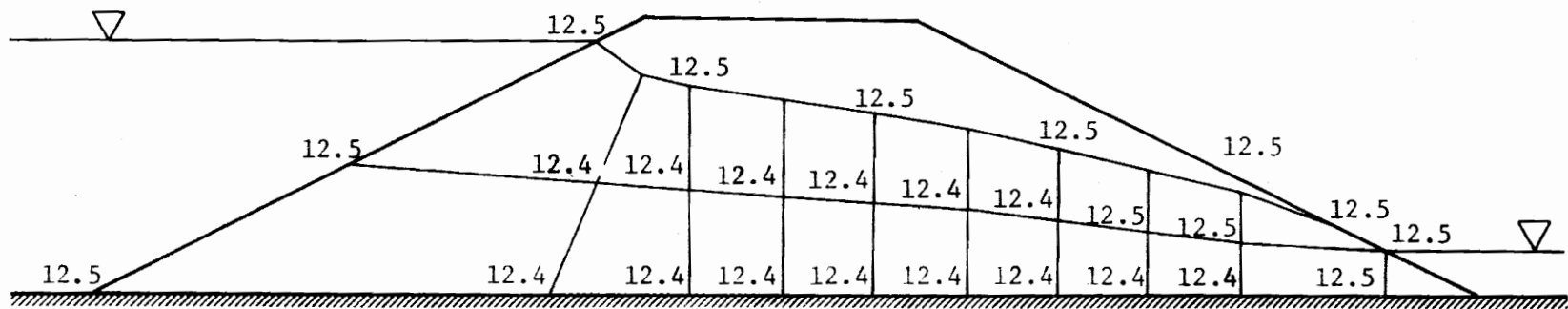


Figure 8 Nodal dissolved oxygen concentrations in mg/l for isotropic soil permeability (5×10^{-5} cm/sec) and specified oxygen reaction coefficient (1×10^{-7} sec $^{-1}$)

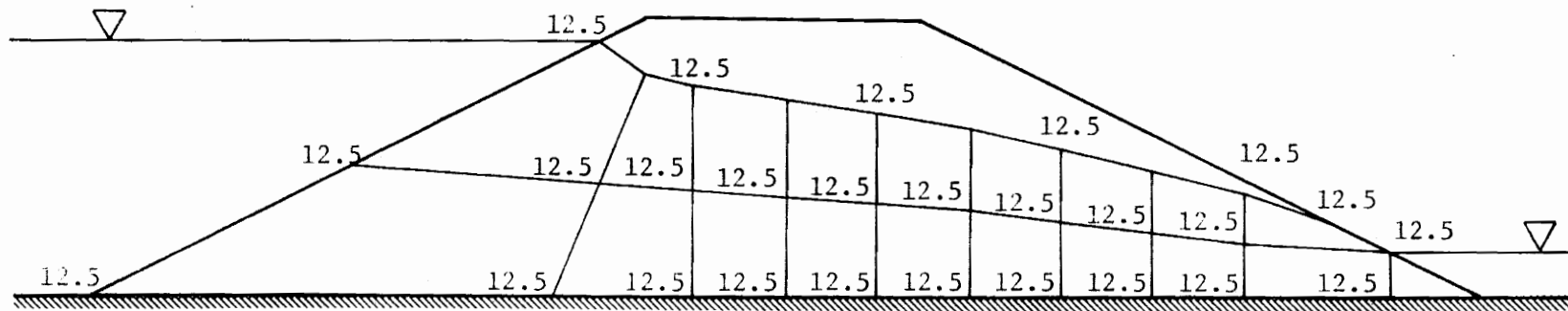


Figure 9 Nodal dissolved oxygen concentrations in mg/l for isotropic soil permeability (5×10^{-5} cm/sec) and specified oxygen reaction coefficient (1×10^{-8} sec⁻¹)

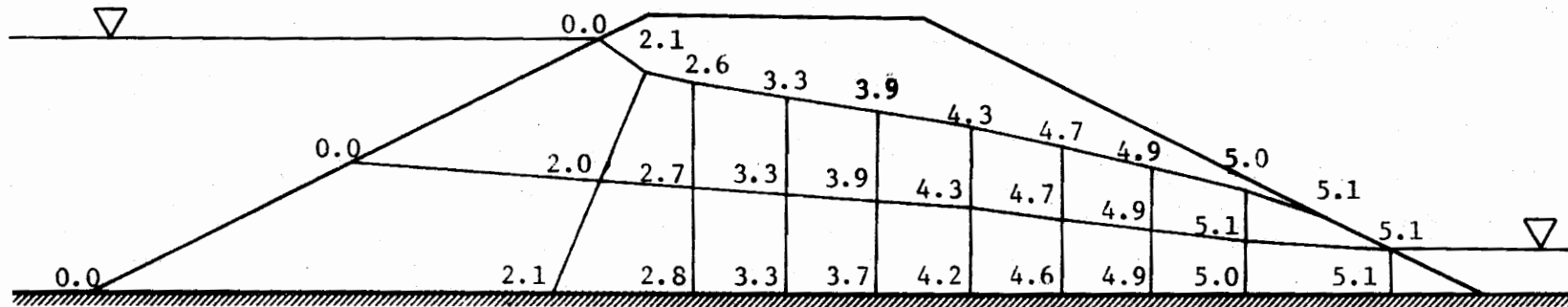


Figure 10 Nodal dissolved sulfate concentrations in mg/l for isotropic soil permeability (5×10^{-5} cm/sec) and specified oxygen reaction coefficient (1×10^{-4} sec $^{-1}$)

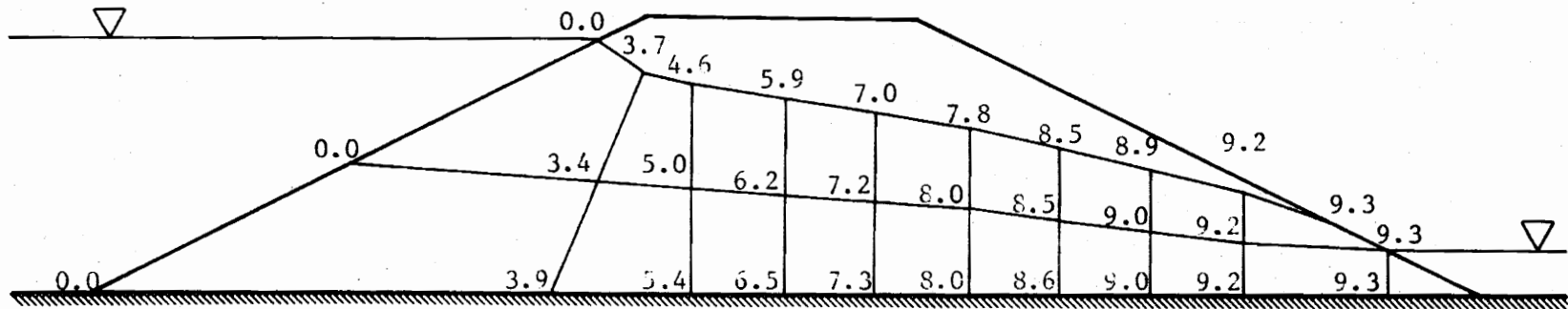


Figure 11 Nodal dissolved sulfate concentrations in mg/l for isotropic soil permeability (5×10^{-5} cm/sec) and specified oxygen reaction coefficient (1×10^{-5} sec $^{-1}$)

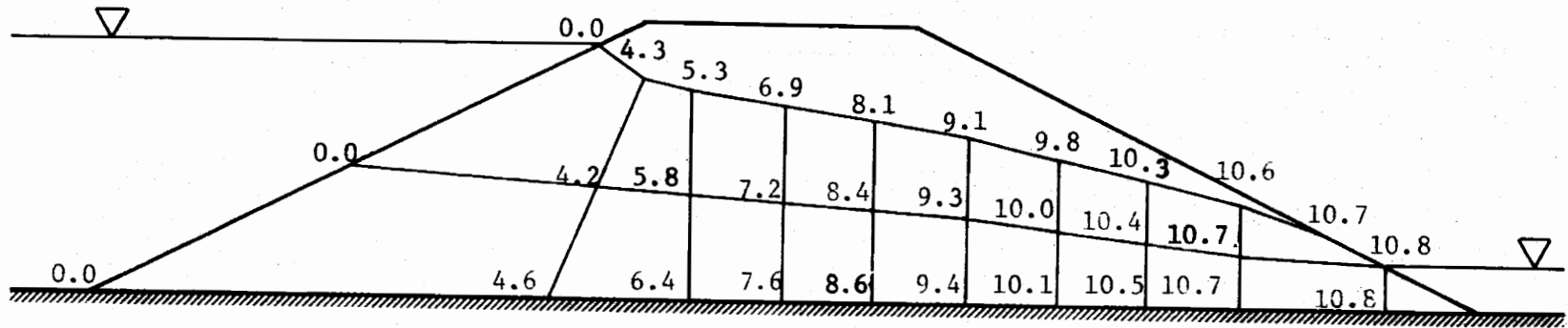


Figure 12 Nodal dissolved sulfate concentrations in mg/l for isotropic soil permeability ($5/10^{-5}$ cm/sec) and specified oxygen reaction coefficient (1×10^{-6} sec $^{-1}$)

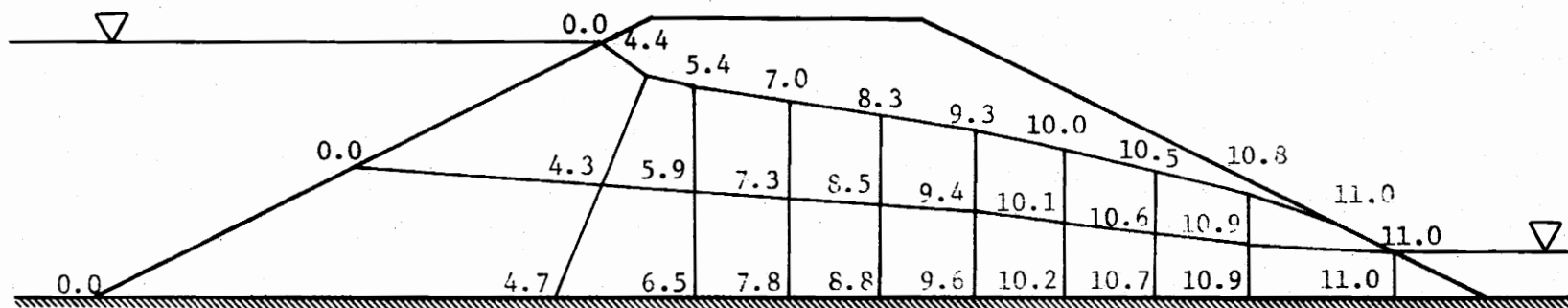


Figure 13 Nodal dissolved sulfate concentrations in ng/l for isotropic soil permeability (5×10^{-5} cm/sec) and specified oxygen reaction coefficient (1×10^{-7} sec $^{-1}$)

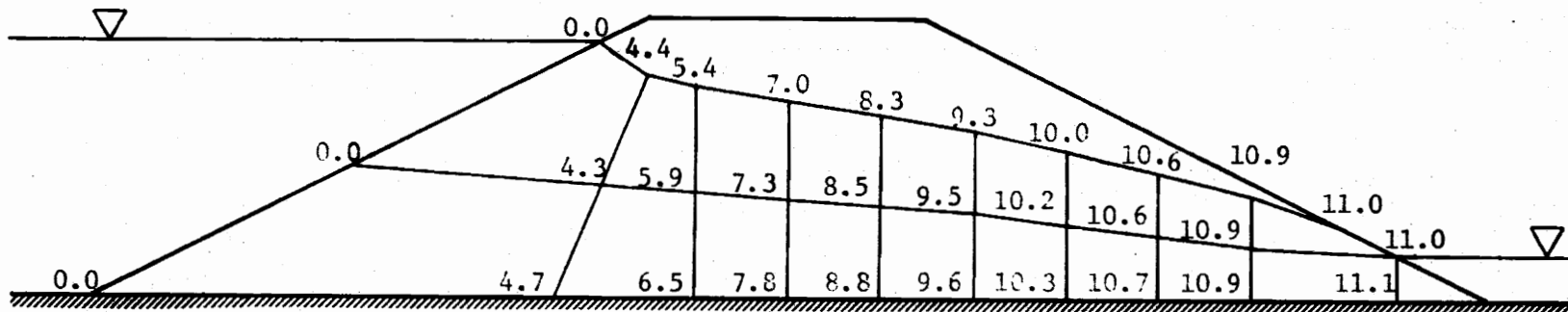


Figure 14 Nodal dissolved sulfate concentrations in mg/l for isotropic soil permeability (5×10^{-5} cm/sec) and specified oxygen reaction coefficient (1×10^{-8} sec $^{-1}$)

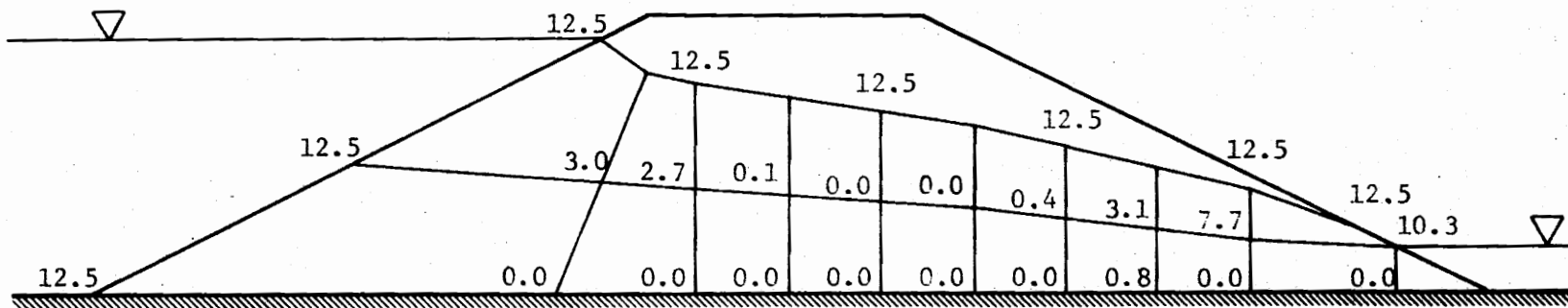


Figure 15 Nodal dissolved oxygen concentrations in mg/l for anisotropic soil permeability ($K_x = 5 \times 10^{-5}$ cm/sec and $K_y = 5 \times 10^{-6}$ cm/sec) and specified oxygen reaction coefficient (1×10^{-4} sec $^{-1}$)

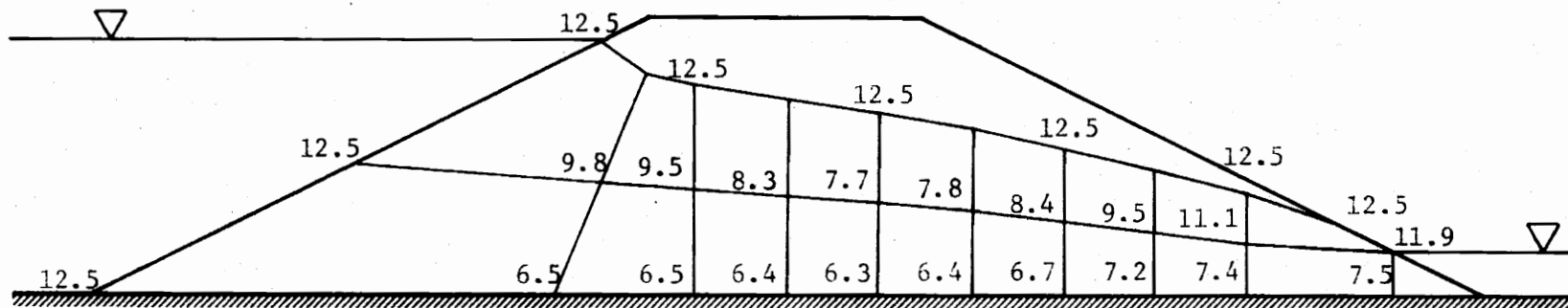


Figure 16 Nodal dissolved oxygen concentrations in mg/l for anisotropic soil permeability ($K_x = 5 \times 10^{-5}$ cm/sec and $K_y = 5 \times 10^{-6}$ cm/sec) and specified oxygen reaction coefficient (1×10^{-5} sec $^{-1}$)

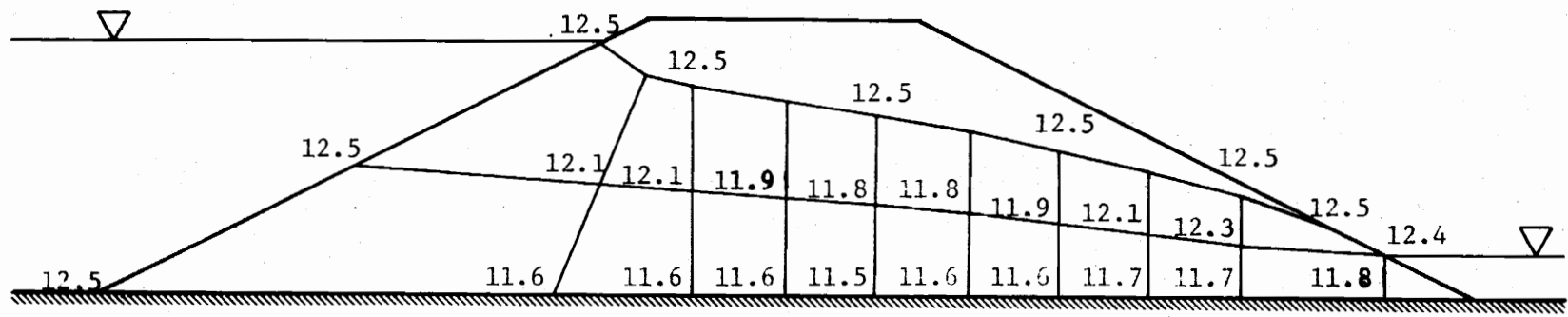


Figure 17 Nodal dissolved oxygen concentrations in mg/l for anisotropic soil permeability ($k_x = 5 \times 10^{-5}$ cm/sec and $K_y = 5 \times 10^{-6}$ cm/sec) and specified oxygen reaction coefficient (1×10^{-6} sec $^{-1}$)

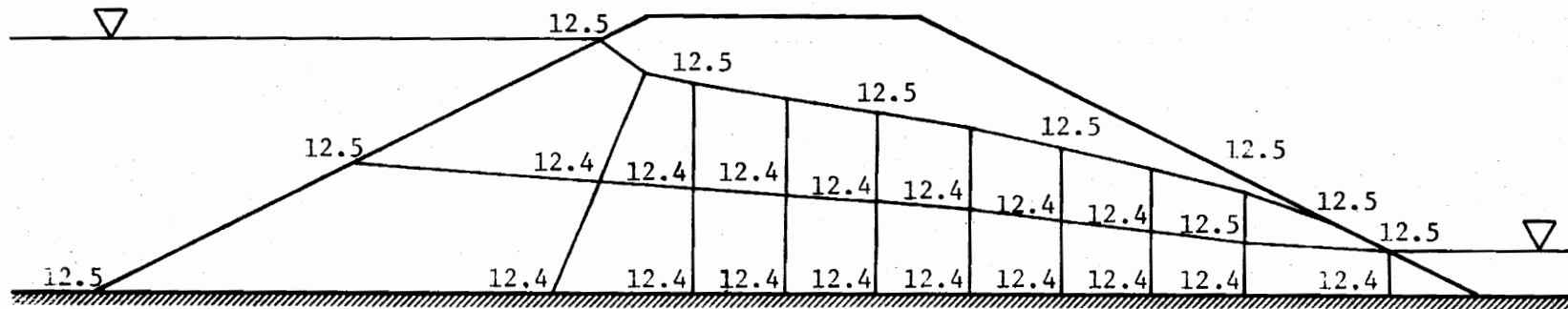


Figure 18 Nodal dissolved oxygen concentrations in mg/l for anisotropic soil permeability ($K_x = 5 \times 10^{-5}$ cm/sec and $K_y = 5 \times 10^{-6}$ cm/sec) and specified oxygen reaction coefficient (1×10^{-7} sec $^{-1}$)

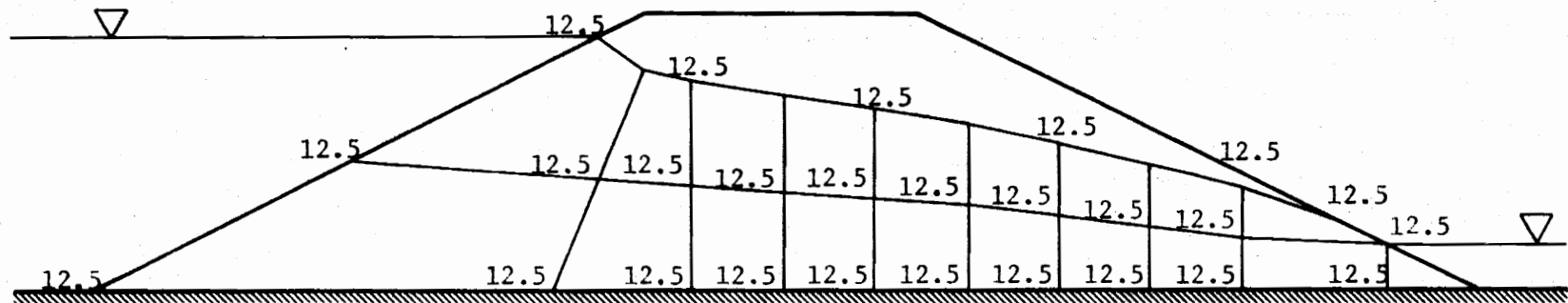


Figure 19 Nodal dissolved oxygen concentrations in mg/l for anisotropic soil permeability ($K_x = 5 \times 10^{-5}$ cm/sec and $K_y = 5 \times 10^{-6}$ cm/sec) and specified oxygen reaction coefficient (1×10^{-8} sec $^{-1}$)

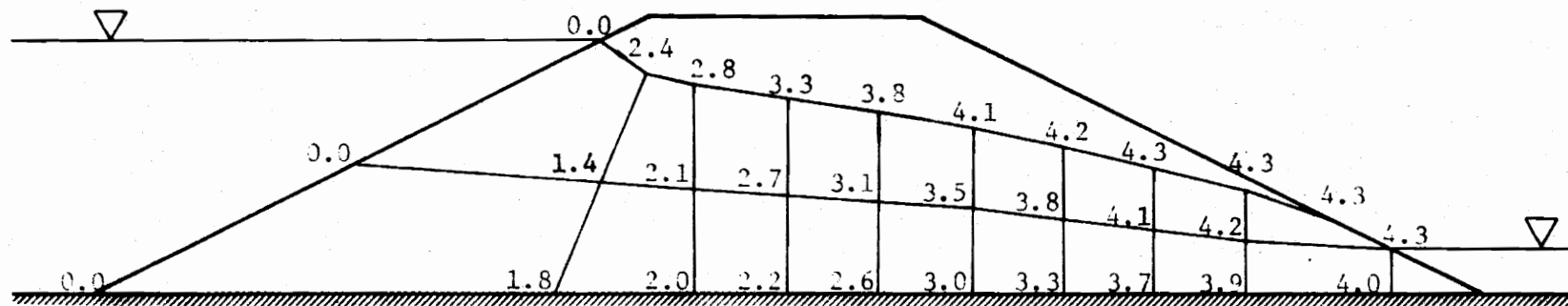


Figure 20 Nodal dissolved sulfate concentrations in mg/l for anisotropic soil permeability ($K_x = 5 \times 10^{-5}$ cm/sec and $K_y = 5 \times 10^{-6}$ cm/sec) and specified oxygen reaction coefficient (1×10^{-4} sec $^{-1}$)

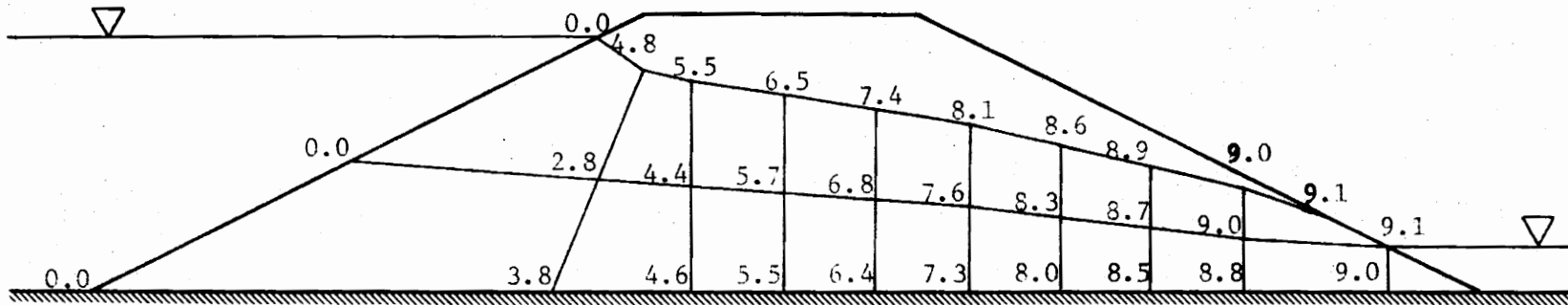


Figure 21 Nodal dissolved sulfate concentrations in mg/l for anisotropic soil permeability ($K_x = 5 \times 10^{-5}$ cm/sec and $K_y = 5 \times 10^{-6}$ cm/sec) and specified oxygen reaction coefficient (1×10^{-5} sec $^{-1}$)

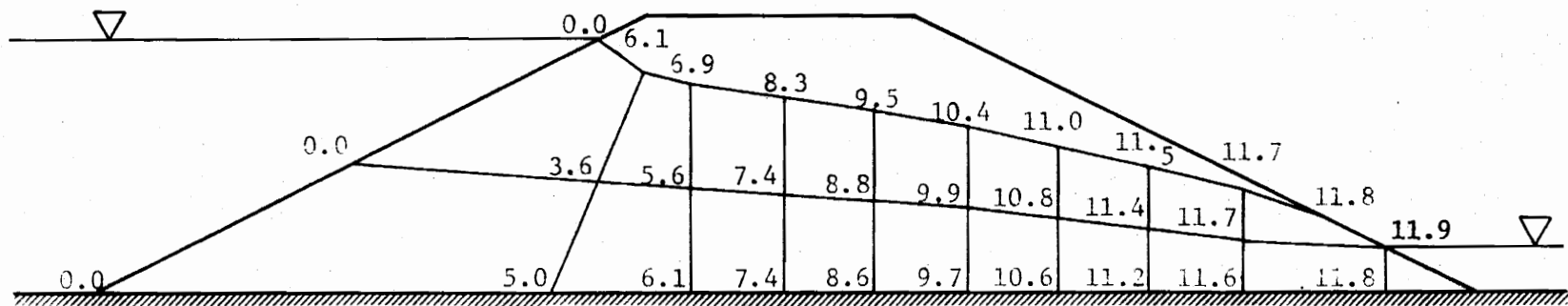


Figure 22 Nodal dissolved sulfate concentrations in mg/l for anisotropic soil permeability ($K_x = 5 \times 10^{-5}$ cm/sec and $K_y = 5 \times 10^{-6}$ cm/sec) and specified oxygen reaction coefficient (1×10^{-6} sec $^{-1}$)

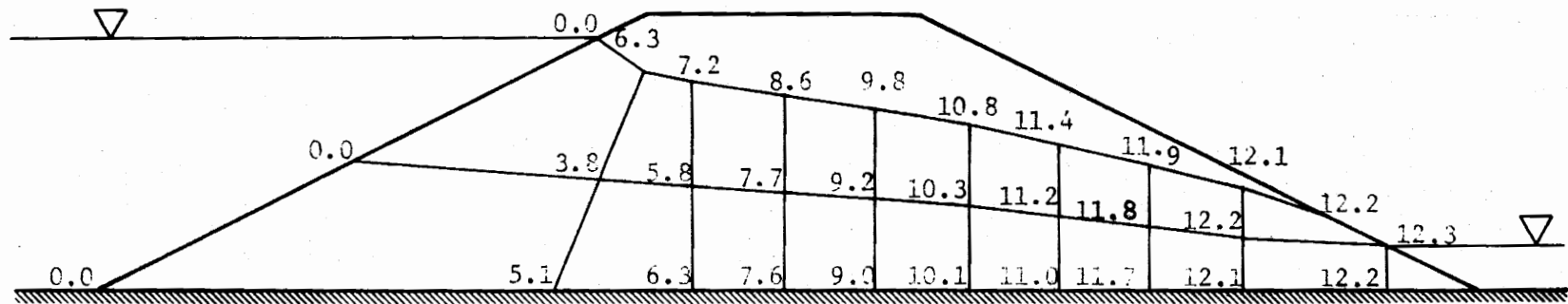


Figure 23 Nodal dissolved sulfate concentrations in mg/l for anisotropic soil permeability ($K_x = 5 \times 10^{-5}$ cm/sec and $K_y = 5 \times 10^{-6}$ cm/sec) and specified oxygen reaction coefficient (1×10^{-7} sec $^{-1}$)

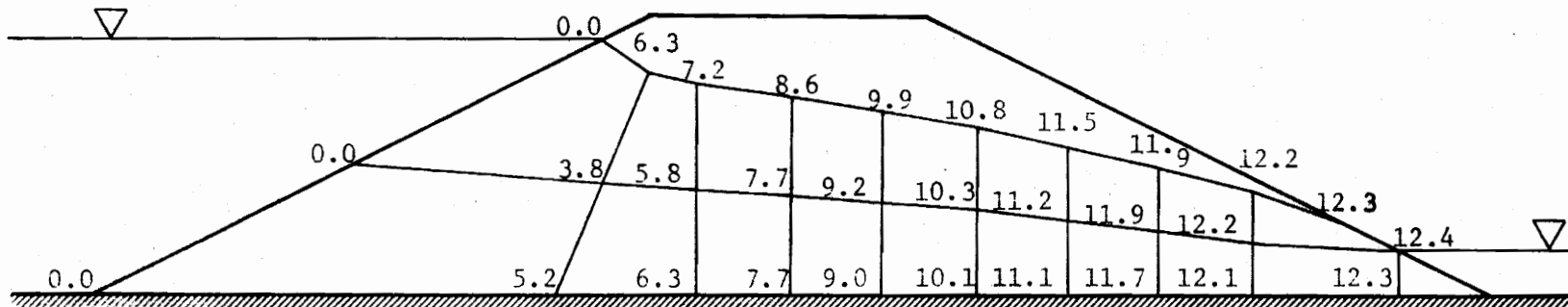


Figure 24 Nodal dissolved sulfate concentrations in mg/l for anisotropic soil permeability ($K_x = 5 \times 10^{-5}$ cm/sec and $K_y = 5 \times 10^{-6}$ cm/sec) and specified oxygen reaction coefficient (1×10^{-8} sec $^{-1}$)

Figure 25 is a plot of the dissolved oxygen deficit production versus isotropic permeability at node 30 of the mesh for various values of the oxygen reaction coefficient.

Figure 26 is a plot of sulfate production versus isotropic permeability at node 30 of the mesh for various values of the oxygen reaction coefficient.

Figure 27 is a plot of dissolved oxygen concentration versus mixing factor at node 30 of the mesh for the isotropic permeability 5×10^{-5} cm/sec and an oxygen reaction coefficient of 1×10^{-4} sec⁻¹.

Figure 28 is a plot of sulfate concentration versus mixing factor at node 30 of the mesh for the isotropic permeability 5×10^{-5} cm/sec and an oxygen reaction coefficient of 1×10^{-4} sec⁻¹.

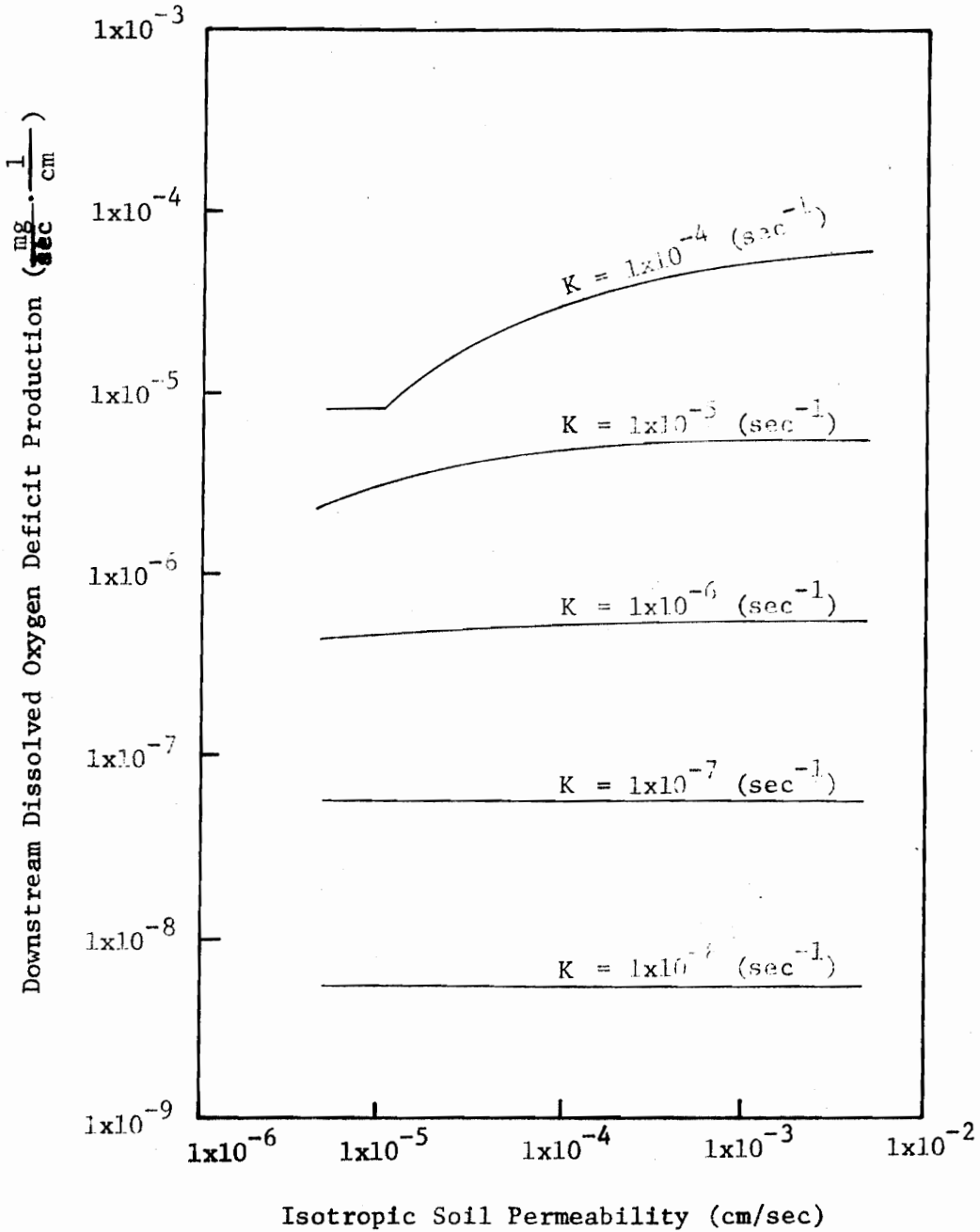


Figure 25 Plot of downstream (node 30) dissolved oxygen deficit production versus isotropic soil permeability for various values of dissolved oxygen reaction coefficient (K)

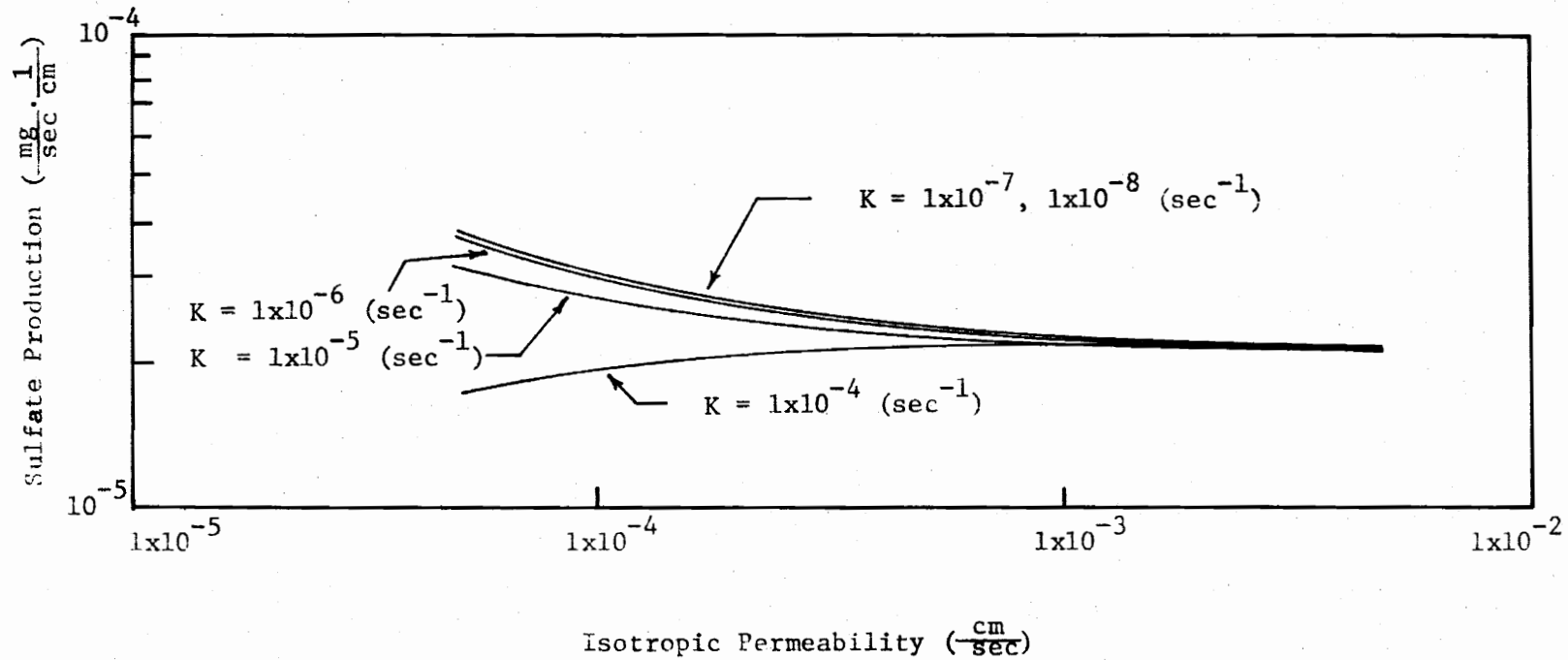


Figure 26 Plot of downstream (node 30) sulfate production versus isotropic soil permeability for various values of the dissolved oxygen reaction coefficient (K)

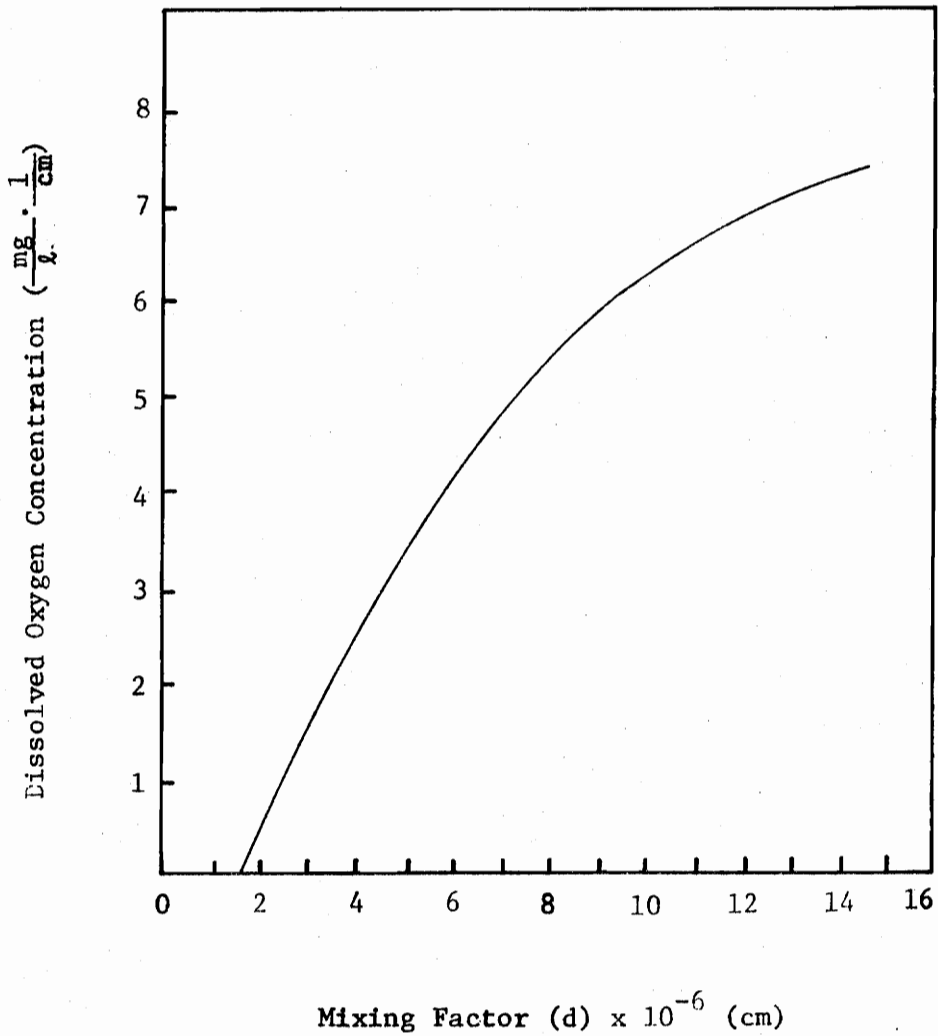


Figure 27 Plot of downstream (node 30) dissolved oxygen concentration versus mixing factor for an isotropic soil permeability = 5×10^{-5} (cm/sec) and a dissolved oxygen reaction coefficient = 1×10^{-4} (sec⁻¹)

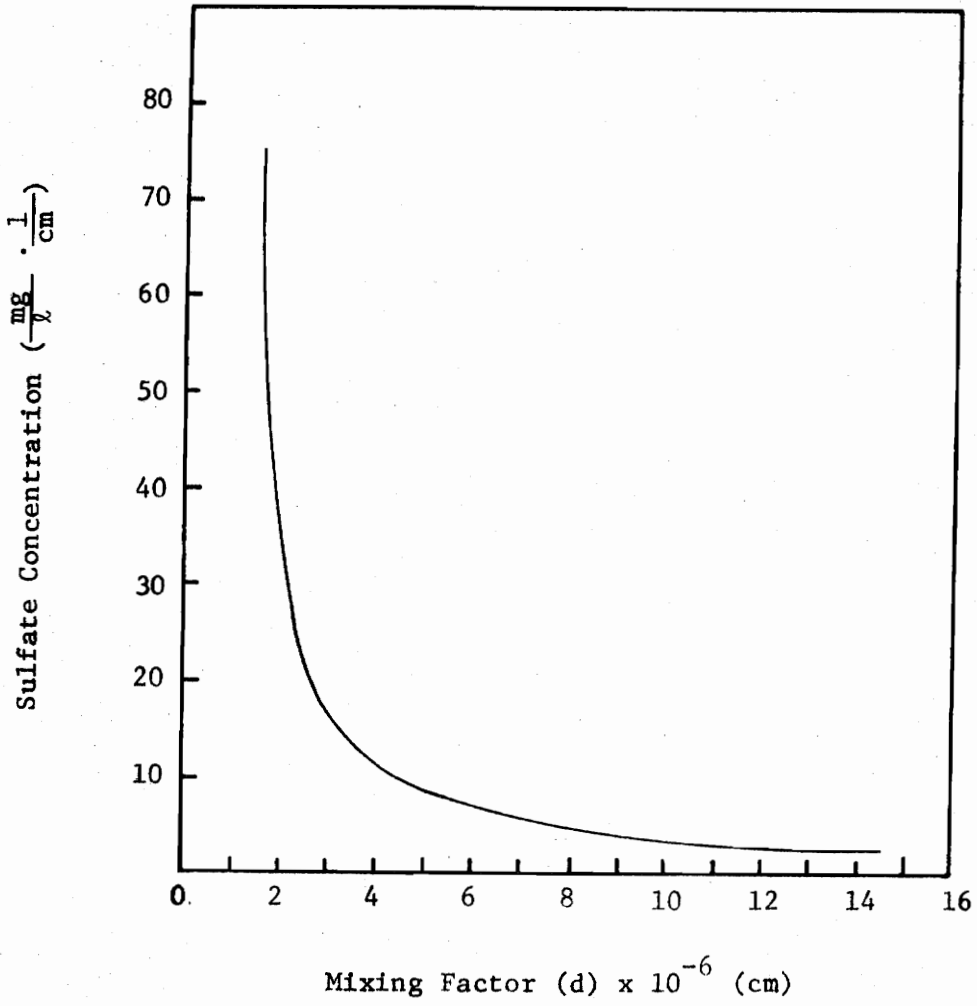


Figure 28 Plot of downstream (node 30) sulfate concentration versus mixing factor for an isotropic soil permeability = 5×10^{-5} (cm/sec) and dissolved oxygen reaction coefficient = 1×10^{-4} (sec⁻¹)

CHAPTER FIVE
DISCUSSION OF RESULTS

For all examples studied there was an increase in the DOC as the dissolved oxygen reaction coefficient decreased. This is clearly shown in Figures 5 - 9 and 15 - 19. These results are to be expected, for decreasing the oxygen reaction coefficient decreases the rate at which the chemical reaction occurs resulting in a lower amount of oxygen being used in the reaction.

Figures 15 - 19 also show the effect of decreasing the vertical soil permeability on the DOC. Lower values for the DOC are found because the ease of free surface oxygen recharge has been reduced. Compared to the isotropic soil permeability results previously discussed, the free surface oxygen recharge effects are not as pronounced.

The DOC data illustrates the mechanism of free surface oxygen recharge. In all cases studied, the DOC rebounds from the minimum value that occurs internally in the dam to the values on the downstream end of the flow field. Under certain conditions, relatively high permeabilities and low dissolved oxygen reaction coefficients, the downstream DOC values can closely approximate the saturated upstream conditions. This is the case in Figure 9.

The sulfate concentration results are somewhat more difficult to analyze. Besides being a function of soil permeability and the sulfate reaction coefficient, the sulfate concentration is also a

function of the DOC. This relation is shown by Equation 2.7.

From Figures 10 - 14 and 20 - 24 it can be seen that the sulfate concentration effects are cumulative. The further the water flows through the dam the more sulfate that is produced. Unlike the DOC analysis where the dissolved oxygen deficit can be recharged at the free surface, the sulfates are produced and their concentration will increase as the water flows toward the downstream end of the flow field.

As the dissolved oxygen reaction coefficient decreases, there is a corresponding increase in the sulfate concentration. The lower the dissolved reaction coefficient, the higher the DOC and the higher the sulfate reaction coefficient and sulfate concentration.

Figure 25 shows that for constant values of the dissolved oxygen coefficient greater than or equal to $1 \times 10^{-6} \text{ sec}^{-1}$, a decrease in the soil permeability will result in a corresponding decrease in the dissolved oxygen deficit production. At values of the reaction coefficient less than $1 \times 10^{-6} \text{ sec}^{-1}$ the dissolved oxygen deficit production is independent of the soil permeability and is a function of the oxygen reaction coefficient only.

The horizontal part of the $\text{ORC} = 1 \times 10^{-4} \text{ sec}^{-1}$ curve in Figure 26 results from complete oxygen depletion of lower soil permeabilities. When all the dissolved oxygen has been removed from the water, the maximum deficit production at a given permeability occurs. This causes the bottoming out effect shown in the curve. Complete dissolved oxygen depletion would be unlikely to occur in nature because

the dissolved oxygen reaction coefficients will be much lower.

Figure 26 shows that the downstream sulfate production falls into a narrow range regardless of the value of the oxygen reaction coefficient. It is interesting to note that the sulfate production is confined to a small range of values even though the oxygen reaction coefficient takes on such widely varying values. This would indicate that a certain amount of sulfate will be produced regardless of the DOC values of the flow field.

The $ORC = 1 \times 10^{-4} \text{ sec}^{-1}$ curve has a reverse curvature when compared to the other curves in Figure 26. At the lower permeabilities, the dissolved oxygen has been completely depleted and, consequently, the sulfate reaction coefficient, as seen from Equation 2.7, and the sulfate concentration would be predictably lower.

Figure 26 also indicates that at higher permeabilities, the sulfate production is a constant $2.2 \times 10^{-5} \text{ mg/sec/cm}$. This indicates that increasing the soil permeability will decrease the sulfate production.

The oxygen reaction coefficient was chosen as the independent variable because the sulfate reaction coefficient is uniquely defined once the oxygen reaction coefficient has been chosen.

The sulfate portion of this analysis was found to be numerically unstable for values of the isotropic permeability less than $5 \times 10^{-5} \text{ cm/sec}$. In actual field problems the soil permeabilities should be higher and, therefore, this instability would not affect the solution process.

Figure 27 shows that as the mixing factor increases, the DOC

also increases. An increase in the mixing factor implies an increase in the dispersion coefficient, making it easier to recharge the oxygen deficit from the free surface.

Figure 28 shows that as the mixing factor increases the sulfate production decreases. Increasing the mixing factor will increase the dispersion coefficient. This can also be accomplished by increasing the soil permeability. This, in turn, increases the fluid velocity which will increase the dispersion coefficient. A higher permeability implies the water will remain in the dam a shorter amount of time, reducing the amount of sulfate produced.

Unfortunately, no data exists with which to correlate these results. However, the element material property matrix generation is similar for the seepage and DOC models. The only differences are the exponential and sink terms in Equation 3.4. In light of the results obtained from the seepage model, it is felt that the DOC and sulfate models are reasonable.

If data were available, parameters such as the oxygen reaction coefficient K and the mixing factor d would be varied until a good comparison between the measured and computed values was obtained.

CHAPTER SIX
CLOSING REMARKS AND RECOMMENDATIONS
FOR FURTHER STUDY

The purpose of this thesis was to develop a mathematical model for the determination of oxygen drawdown and sulfate production due to chemical reactions of pyrite assuming steady state conditions and no internal oxygen sources. This purpose has been accomplished. The finite element solution is straight forward and permits material properties to vary throughout the continuum.

Any analysis will suggest new avenues of investigation. The main areas of investigation suggested by this problem are the further study of transient conditions that could exist, time dependent material properties, a thorough investigation of non-uniform dispersion coefficients, and additional experimental effort to understand and narrow down the variation of reaction rate coefficients. Also, experimental data on dissolved oxygen and sulfate levels from actual strip mine spoil dams is needed. And finally, modification of this model should be considered to determine the dissolved oxygen and sulfate concentrations when rainfall infiltration and surface runoff effects are considered.

BIBLIOGRAPHY

1. Abramowitz, M. and I. A. Stegun. Handbook of Mathematical Functions. New York: Dover Publications, 1970.
2. Braley, S. A. Summary Report to Commonwealth of Pennsylvania, Department of Health, Industrial Fellowship 326-B. 1954.
3. Clark, C. S. "Oxidation of Coal Mine Pyrite", Journal of the Sanitary Engineering Division, American Society of Civil Engineers. V. 92, SA 2, 1966, pp. 127-148.
4. Desai, C. S. "Seepage Analysis of Earth Banks Under Drawdown", Journal of the Soil Mechanics and Foundations Division, American Society of Civil Engineers. V. 98, SM 11, 1972, pp. 1143-1161.
5. Desai, C. S. and J. F. Abel. Introduction to the Finite Element Method. New York: Van Nostrand Rheinhold Company, 1972.
6. Guymon, G. L. Irvine, California. Telephone Interview, April 4, 1975.
7. Guymon, G. L. "Mathematical Modeling of Dissolved Constituents in Ground Water Aquifers by the Finite Element Method". Ph.D. dissertation, University of California, Davis, 1970.
8. Guymon, G. L., V. H. Scott, and C. R. Hermann. "A General Numerical Solution of the Two Dimensional Diffusion-Convection Equation by the Finite Element Method", Water Resources Research. V. 6, #6, 1970, pp. 1611-1617.
9. Harleman, D. R. F., P. F. Mehlhorn, and R. R. Rumer. "Dispersion-Permeability Correlation in Porous Media", Journal of the Hydraulics Division, American Society of Civil Engineers. V. 89, HY 2, 1963, pp. 67-85.
10. Harleman, D. R. F. and R. R. Rumer. "Longitudinal and Lateral Dispersion in an Isotropic Porous Media", Journal of Fluid Mechanics. V. 16, Pt. 3, 1963, pp. 385-394.
11. "Identification of Factors Affecting Water Quality From Strip Mine Sites", Progress Report A-055-Va, Virginia Water Resources Center, V.P.I. & S.U., Blacksburg, Virginia, Winter Quarter, 1974.
12. Kim, A. G. "An Experimental Study of Ferrous Iron Oxidation in Acid Mine Water", 2nd Symposium on Coal Mine Drainage Research. Pittsburgh, Pennsylvania, 1968, pp. 40-45.

13. Marino, M. A. "Longitudinal Dispersion in Porous Media", Journal of the Hydraulics Division, American Society of Civil Engineers. V. 100, HY 1, 1974, pp. 151-157.
14. Martel, C. J. "Dispersion in Non-Uniform Porous Media", Civil Engineering Department, University of Massachusetts, Amherst, Massachusetts, December, 1972.
15. Melosh, R. J. Unpublished Lecture Notes, CE 631, Advanced Engineering Analysis. Department of Civil Engineering, V.P.I. & S.U., Blacksburg, Virginia, Spring Quarter, 1973.
16. Neumann, S. P. and P. A. Witherspoon. "Finite Element Method of Analyzing Steady Seepage with a Free Surface", Water Resources Research. V. 6, #3, 1970, pp. 889-897.
17. Ogata, A. "A Theory of Dispersion in Porous Media", United States Geological Service Professional Paper 411-I. United States Government Printing Office, 1961.
18. Reese, R. D. "A Study of Reactions Between Coal and Coal Mine Drainage" Masters Thesis. The Pennsylvania State University, December, 1965.
19. Singer, P. C. and W. Stumm. "Kinetics of the Oxidation of Ferrous Iron", 2nd Symposium on Coal Mine Drainage Research. Pittsburgh, Pennsylvania, 1968, pp. 12-34.
20. Stauffer, T. E. and H. L. Levell. "The Oxygenation of Iron (II) in Relation to Coal Mine Drainage Treatment", Special Report Number SR-69, Conducted in the Department of Mining, The Pennsylvania State University, 1968.
21. Steel, E. W. Water Supply and Sewerage. New York: McGraw-Hill, 1960.
22. Tagamets, T. and V. M. Sturnberg. "A Predictor-Corrector Method for Solving the Convection-Dispersion Equation for Adsorption in Porous Media", Department of Civil Engineering, University of Maryland, College Park, Maryland, 1974.
23. Taylor, R. C. "Darcy Flow Solutions With a Free Surface", Journal of the Hydraulics Division, American Society of Civil Engineers. V. 93, HY 2, 1962, pp. 25-33.
24. Zienkiewicz, O., P. Mayer, and V. K. Cheung. "Solution of Anisotropic Seepage by Finite Elements", Journal of the Engineering Mechanics Division, American Society of Civil Engineers. V. 92, EM 1, 1966, pp. 111-120.

APPENDIX

APPENDIX A

DEFINITION OF TERMS

The following terms are defined as they pertain to this analysis.

{c}	State variable vector
c	State variable
c_i	State variable at i^{th} elemental node
D_{ik}	Positive dispersion tensor
d_x	Mixing factor in the x direction
d_y	Mixing factor in the y direction
D_x	Dispersion coefficient in the X direction
D_y	Dispersion coefficient in the Y direction
DOC	Dissolved oxygen concentration
[J]	Jacobian matrix
K	Dissolved oxygen reaction coefficient
[k]	Elemental material property matrix
K_x	Coefficient of permeability in the x direction
K_y	Coefficient of permeability in the y direction
N_i	Shape function for the i^{th} node
Q	Source term
{r}	Right hand side of elemental matrix equation
s	Natural coordinate
s_i	Natural coordinate of the i^{th} node
t	Time

t	Natural coordinate
t_i	Natural coordinate of the i^{th} node
u_i	Convection parameter in the i^{th} direction
V_x	Elemental velocity in the x direction
V_y	Elemental velocity in the y direction
X	General cartesian coordinate
x_i	Coordinate direction ($i = X, Y, X$)
x_n	x coordinate of n^{th} elemental node
Y	General cartesian coordinate
y_n	y coordinate of n^{th} elemental node
Z	Elemental displacement function

APPENDIX B
DESCRIPTION OF THE COMPUTER PROGRAM
USED IN THE ANALYSIS

The solution of Equation 3.11 was performed at the Virginia Polytechnic Institute and State University Computer Center in Blacksburg, Virginia by use of twin IBM System/370 Model 158 Digital Computers. The program was written in FORTRAN IV Level G computer language.

The program is designed to operate with no internal modifications and will generate the seepage solution and determine the dissolved oxygen and sulfate concentration solutions. If the user desires, the program can terminate after the calculation of the seepage solution.

Data Input

Data for the program is read in in three sections all of which are found in SUBROUTINE ASEMBL. Refer to Appendix C for all program references.

Section 1 This section inputs all the general information that is required in the program. One data card is needed for this segment. Table 2 presents all pertinent information required for the data input. The numbers in parenthesis at the end of the variable description are the numbers used to produce the solution that is presented in Figure 5.

TABLE 2
DESCRIPTION OF GENERAL INPUT DATA

<u>Column</u>	<u>Format</u>	<u>Variable</u>	<u>Variable description</u>
1-5	I5	NE	Number of elements in the continuum (18)
6-10	I5	NN	Number of nodes in the continuum (30)
11-20	F10.3	TAIL	Downstream tailwater level in cm (100.0)
21-25	I5	IBBSAD	Node separating the seepage surface and downstream face of dam (28)
26-30	I5	NPSE	Number of elements adjoining the free surface (9)
31-40	F10.3	TOLH	Accuracy of the free surface determination in cm (0.1)
41-50	F10.3	SLOPE	Slope of the downstream face of the dam (-0.5)
51-55	I5	NSL	Number of rows of elements + 1 (3)
56-65	F10.3	CINIT	Initial dissolved oxygen concentration in mg/l (12.47)
65-74	F10.3	CONVRG	Convergence parameter for free surface iteration (1.0)
79	I1	IPRINT	Debut printer option (0)
80	I1	ICON	Flow option (0)

The IPRINT option is a programming debugging aid and should be used only for specific program sections. IPRINT = 1 will cause the debug printout, whereas IPRINT = 0 will suppress the debug printout. Indiscriminate use of this parameter can result in an excess of 50,000 lines of output.

The ICON option has two uses. In the seepage solution, it determines the type of flow problem. ICON = 0 indicates that the problem has a free surface. ICON = 1 indicates that the problem has no free surface.

In the DOC solution, ICON specifies whether oxygen recharge is permitted on the free surface. ICON = 0 permits oxygen recharge along the free surface. ICON = 1 indicates that there is no oxygen recharge on the free surface.

Section 2 This section inputs the nodal information. The data consists of the node numbers and their cartesian coordinates. The number of cards required in this section is equal to the number of nodes in the continuum discretization. The form of a typical data card for the i^{th} node is presented in Table 3. The numbers of parenthesis following the variable description are the nodal data for node 1 of the continuum discretization which is shown in Figure 4.

The node number values can be left blank, for they serve no purpose in the program execution. These numbers are of considerable value in organizing the sequence of the data. These cards must be read in starting with the first node and increasing consecutively to the last node.

TABLE 3

DESCRIPTION OF NODAL INPUT DATA FOR Ith NODE

<u>Column</u>	<u>Format</u>	<u>Variable</u>	<u>Variable description</u>
1-10	I10	NODE(I)	Node number (1)
11-20	F10.3	CORX(I)	X coordinate of i th node in meters (11.0)
21-30	F10.3	CORY(I)	Y coordinate of i th node in meters (5.5)

Section 3 This section inputs all the elemental data. The number of cards required in this section is equal to the number of elements in the continuum. Table 4 presents the form of the data input for the j^{th} element. The numbers in parenthesis after the variable description are the data for the first element of the example presented in Figure 5. There is no set order in which the elemental data need be read in. If only a seepage solution is desired, give the first value of the SF array a negative value.

The ICHECK variable defines the type of boundary condition to be imposed on an element. Table 5 presents the definitions of the various values of ICHECK. The elemental values of ICHECK are circled within the individual elements in Figure 29. These boundary conditions are imposed only on the nodes that are on the surface that the boundary condition describes.

The input data will consist of the following number of cards:

$$\text{Number of data cards} = 1 + \text{NN} + \text{NE} \quad \text{B.1}$$

NN and NE are determined by the continuum discretization and are defined in Table 2. In the example problem presented in Figure 5, 49 cards are required to input the data.

As a convenience to the user, all input data is automatically printed out. In addition, the appropriate seepage solution, elemental bulk fluid velocities, DOC solution, sulfate reaction coefficients, and sulfate production solution are also printed out. The initial seepage solution is the unadjusted free surface solution. The free surface

TABLE 4

DESCRIPTION OF ELEMENTAL DATA FOR Jth ELEMENT

<u>Column</u>	<u>Format</u>	<u>Variable</u>	<u>Variable description</u>
1-2	I2	ISAVE(J,1)	Upper left corner node for the j th element (1)
3-4	I2	ISAVE(J,2)	Lower left corner node for the j th element (2)
5-6	I2	ISAVE(J,3)	Lower right corner node for the j th element (5)
7-8	I2	ISAVE(J,4)	Upper right corner node for the j th element (4)
10-19	F10.7	PERMX(J)	Coefficient of permeability in the x direction for the j th element in cm/sec (0.00005)
20-29	F10.7	PERMY(J)	Coefficient of permeability in the y direction for the j th element in cm/sec (0.00005)
30-39	F10.7	SF(J)	Dissolved oxygen reaction coefficient in sec ⁻¹ (0.0001)
40-49	F10.7	D50(J)	Mean grain diameter in the j th element in cm (0.0075)
50-64	D14.7	FACTRX(J)	Mixing factor in the x direction for the j th element (0.805 D 6)
65-79	D14.7	FACTRY(J)	Mixing factor in the y direction for the j th element (0.805 D 6)
80	I1	ICHECK(J)	Boundary condition identifier for the j th element (1)

TABLE 5

DEFINITION OF BOUNDARY CONDITIONS

<u>ICHECK value</u>	<u>Type of element</u>	<u>Boundary condition</u>
1	Upstream	Seepage - Nodes defined to have specific head DOC - DOC = CINIT Sulfate - Sulfate concentration = 0
2	Seepage surface	Seepage - Total head = elevation head
3	Free surface	Seepage - No flow normal to free surface Total head = elevation head DOC - Oxygen recharge permitted, DOC = CINIT
4	Bottom	Seepage - No flow normal to base DOC - No DOC change normal to base Sulfate - No sulfate concentration change normal to base
5	Downstream surface	Seepage - Total head = downstream tailwater level

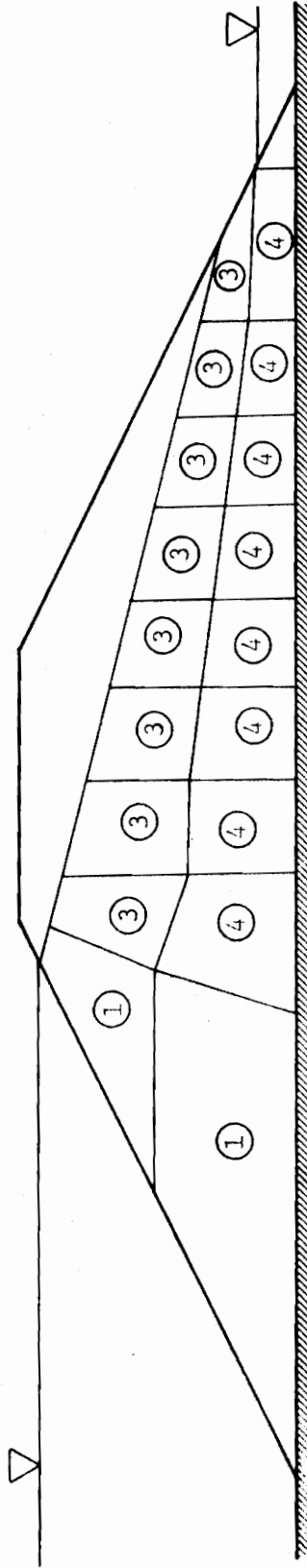


Figure 29 Continuum discretization with ICHECK values noted

solution is the solution in which the free surface has been located and it is accurate to the value of TOLH that is specified in Section 1 of the data input.

Error Messages Generated Within the Program

Two error messages have been inserted into the program to alert the user that the correct solution is unattainable. Any output that follows either of these messages should be ignored.

The first of these messages is

```
** ERROR RETURN **
```

```
IER = -1
```

This message is generated in SUBROUTINE DGELG and indicates that the constrained global material matrix is singular. The corrective action is to determine the position of this error with respect to the output data and use the IPRINT = 1 option in the section where the error occurs. The IPRINT option will output the element matrix generation and constrained global material property matrix. From this information, it can be determined where the singularity exists.

If the error message precedes the initial seepage solution printout, place the IPRINT = 1 card before the CALL ASEMBL (ICON) card in the main program. If the error is after the initial seepage solution but before the free surface solution, place the IPRINT = 1 card immediately before the CALL FREATC (IWARN) card in the main program.

If the error occurs after the free surface solution printout, place the IPRINT = 1 card immediately before the CALL CONCEN (ICON) card in the main program.

The second error message that terminates execution is

***** EXCESSIVE ITERATIONS *****

This statement is generated in SUBROUTINE FREATC and indicates that the number of iterations needed to find the position of the free surface has exceeded the number of free surface elements, NPSE from Table 2. Either the iterations are not converging to the correct solution fast enough or the convergence is too rapid and the solution is oscillating. The corrective action is to place an IPRINT = 1 card immediately before the CALL FREATC (IWARN) statement in the main program. By checking the successive iterations of the free surface nodes, it can be determined what caused the error.

Adjustments of the rate of convergence is made by varying the variable CONVRG read in in Section 1. Numbers less than the value of CONVRG (1.0 in this analysis) will accelerate the rate of convergence. Numbers greater than the present value of CONVRG will decelerate the convergence rate. Over acceleration of the rate of convergence will result in answers that seem to oscillate and possibly even diverge from the correct solution.

Solution of the System Matrix Equation

The actual solution of the system matrix equation is performed by the IBM Scientific Subroutine Package double precision linear simultaneous equation solver DGELG. DGELG uses a Gauss elimination procedure with complete row and column pivoting.

Program Execution

The entire program is executed in double precision to minimize round-off error in the Gauss elimination procedure. Of necessity, the real array storage space must be doubled. However, it is felt that the extra accuracy of the solution more than justifies the increased expense. The solution of the 30 node example problem used in the analysis required approximately 30 seconds of computer time and a storage area of 110^k bytes.

APPENDIX C
COMPUTER PROGRAM

```

      IMPLICIT REAL*8(A-H,O-Z)
      COMMON  ELEMT(4,4),STIFF(33,33),SI(4),TI(4),RHS(33),TOLH,TAIL,
1          UPSTRM,CORX(33),CORDY(33),COLUMN(1089),SF(20),D50(20),SLOPE,
2          VX(20),VY(20),PERMX(20),PERMY(20),EPS,CINIT,HEAD(33),
3          FACTRX(20),FACTRY(20),CONVRG
      COMMON  NE,NN,KCUNT,ICHECK(20),IPRINT,JOE,ISAVE(20,4),IBBSAD,INUM,
2          IER,NPSE,NSL

```

C
C
C
C
C
C
C

```

      THIS PROGRAM CALCULATES THE STEADY STATE OXYGEN DRAWDOWN AND
      SULFATE PRODUCTION IN EARTH DAMS DUE TO PYRITIC CHEMICAL
      REACTIONS.  THE DIFFUSION-CONVECTION EQUATION IS USED.  THE
      METHOD USED IS A FINITE ELEMENT ANALYSIS UTILIZING LINEAR
      ISOPARAMETRIC QUADRILATERAL ELEMENTS AND NATURAL COORDINATES.

```

```

      JOE = -1
      IWARN = 0
      IWRITE = 1
      INUM = 1
      EPS = 1.0 D -16
      CALL ASEMBL(ICON)
      NPSN = NPSE + 1
      CALL ARANGE (IVPI,IVPISU)
      CALL DGELG (RHS,COLUMN,NN,INUM,EPS,IER,IVPI,IVPISU)
      IF(IER.EQ.0) GO TO 706
      CALL OUTPUT(IWRITE)
      IF(IER.LT.0) GO TO 999
706 CONTINUE
      IF(ICON.EQ.1) GO TO 4975
      CALL FREATC (NPSN,IWARN)
      IWRITE = 5
      CALL OUTPUT(IWRITE)
      IF(IWARN.EQ.1) GO TO 999

```

```
4975 CONTINUE
      CALL VELCTY
      IF(SF(1).LT.0.0) GO TO 999
      CALL CONCNEN (JCON)
999  CONTINUE
      RETURN
      END
```

```

SUBROUTINE ASEMBL(ICCN)
  IMPLICIT REAL*8 (A-H,O-Z)
  COMMON ELEM(4,4),STIFF(33,33),SI(4),TI(4),RHS(33),TOLH,TAIL,
1      UPSTRM,CDRX(33),CDRY(33),COLUMN(1089),SF(20),D50(20),SLOPE,
2      VX(20),VY(20),PERMX(20),PERMY(20),EPS,CINIT,HEAD(33),
3      FACTRX(20),FACTRY(20),CONVRG
  COMMON NE,NN,KCOUNT,ICHECK(20),IPRINT,JOE,ISAVE(20,4),IBBSAD,INUM,
2      IER,NPSE,NSL
  DIMENSION NODE(50),IEX(110),SSI(4),TTI(4)

C
C   SUBROUTINE ASEMBL RECEIVES THE ELEMENT MATRICES, APPLIES APPROPRIATE
C   BOUNDARY CONDITIONS, CONSTRAINS THE ELEMENT EQUATIONS, AND
C   ASSEMBLES THEM INTO THE CONSTRAINED GLOBAL MATERIAL PROPERTY
C   MATRIX FOR THE SEEPAGE PART OF THE PROBLEM.
C
      IF(JOE) 8000,8000,9011
8000 CONTINUE
      READ(5,1000)NE,NN,TAIL,IBBSAD,NPSE,TOLH,SLOPE,NSL,CINIT,CONVRG
1      ,IPRINT,ICCN
1000 FORMAT(2I5,F10.3,2I5,2F10.3,I5,F10.3,F10.3,T79,I1,I1)

C
C   THE PRECEEDING VARIABLES IN THE READ STATEMENT ARE DEFINED AS FOLLOWS
C
C   NN = NUMBER OF NODES IN THE PROBLEM
C   NE = NUMBER OF ELEMENT IN THE PROBLEM
C   TAIL = HEAD AT THE DOWNSTREAM FACE OF THE DAM (CM)
C   IBBSAD = NODE ON THE BOUNDARY BETWEEN THE SEEPAGE AND DOWN STREAM SURFACES
C   NPSE = NUMBER OF PHREATIC SURFACE ELEMENTS
C   TOLH = ACCURACY OF PHREATIC SURFACE DETERMINATION
C   SLOPE = AMOUNT OF RUN OF THE SLOPE FOR ONE UNIT RISE ON THE
C           DOWNSTREAM DAM FACE
C   NSL = NUMBER OF STREAMLINES

```

```

C      CINIT = INITIAL DISSOLVED OXYGEN CONCENTRATION (MG/L)
C      CONVRG = RATE OF CONVERGENCE IN FREE SURFACE ITERATIONS
C      IPRINT = DEBUG PRINTER OPTION.  IF(IPRINT.EQ.0) NO DEBUG PRINTOUT
C      ICON = FLOW OPTION
C          ICON = 0    UNCONFINED FLOW
C          ICON = 1    CONFINED FLOW
C
C      WRITE(6,1400) NE,NN,TAIL,IBBSAD,TOLH,SLOPE,NPSE,NSL,CINIT,CONVRG,
1      ICON
1400  FORMAT(IH1,T10,'NUMBER OF ELEMENTS = ',I4/
1      T10,'NUMBER OF NODES = ',I4/
*      T10,'TAILWATER HEAD = ',F10.3/
*      T10,'SEEPAGE-TAILWATER NODE = ',I3/
*      T10,'HEAD TOLERANCE = ',F10.3/
*      T10,'DOWNSTREAM SLOPE = ',F10.3/
7      T10,'NUMBER OF PHREATIC SURFACE ELEMENTS = ',I3/
*      T10,'NUMBER OF STREAMLINES = ',I2/
*      T10,'UPSTRM DISSOLVED OXYGEN CONC. (MG/L) = ',E14.7/
*      T10,'CONVERGENCE FACTOR = ',F10.3/
8      T10,'FLOW OPTION = ',I3)
      ISTOP = 0
      KCUNT = 1
      CALL ZERG
      DO 2 J1 = 1,NN
      READ(5,100) NCDE(J1),CORX(J1),CORY(J1)
100  FORMAT(I10,2F10.2)
      2  CONTINUE
C
C      THE PRECEEDING VARIABLES IN THE READ STATEMENT ARE DEFINED AS
C      FOLLOWS
C
C      NCDE = MATRIX OF NODE NUMBERS

```

```

C      CORX = MATRIX OF THE NODAL X COORDINATES
C      CORY = MATRIX OF THE NODAL Y COORDINATES
C
C      INPUT THE NODE COORDINATES IN METERS
C
      UPSTRM = CORY(1)*100.0
      WRITE(6,9033) UPSTRM
9033  FORMAT(T10,'UPSTREAM HEAD = ',F10.3//)
      WRITE(6,1550)
1550  FORMAT(///T8,'NODE',T16,'X-COR',T26,'Y-COR'//)
      DO 401 I=1,NA
      CORX(I) = CORX(I)*100.0
      CORY(I) = CORY(I)*100.0
      WRITE(6,100) NODE(I),CORX(I),CORY(I)
401  CONTINUE
      WRITE(6,8017)
8017  FORMAT(1H1,T40,'*** INPUT - ELEMENT DATA ***'//2X,'ELEMENT NODES',
      1T24,'KX',T39,'KY',T54,'SF',T69,'D50',T82,'FACTRX',T97,'FACTRY',
      1T113,'ICHECK'//)
      DO 901 J=1,NE
      READ(5,101) (ISAVE(J,II),II=1,4),PERMX(J),PERMY(J),SF(J),
      1      D50(J),FACTRX(J),FACTRY(J),ICHECK(J)
101  FORMAT(4I2,T10,4F10.7,2D14.7,T80,I1)
      WRITE(6,8018) (ISAVE(J,II),II=1,4),PERMX(J),PERMY(J),SF(J),D50(J),
      1FACTRX(J),FACTRY(J),ICHECK(J)
8018  FORMAT(2X,I2,'-',I2,'-',I2,'-',I2,T20,E10.3,T35,E10.3,T50,
      1E10.3,T65,E10.3,T80,D10.3,T95,D10.3,T116,I2//)
901  CONTINUE
C
C      THE PRECEEDING READ STATEMENT INPUTS ALL THE ELEMENT PROPERTIES.
C
C      THE PRECEEDING VARIABLES IN THE READ STATEMENT ARE DEFINED AS

```



```

C      FOLLOWS
C      ISAVE = MATRIX OF NODE NUMBERS FOR EACH ELEMENT
C      PERMX = ELEMENT PERMEABILITY IN THE X DIRECTION (CM/SEC)
C      PERMY = ELEMENT PERMEABILITY IN THE Y DIRECTION (CM/SEC)
C      FACTRX = MIXING FACTOR IN THE X DIRECTION (CM)
C      FACTRY = MIXING FACTOR IN THE Y DIRECTION (CM)
C      D50 = MEAN GRAIN SIZE IN EACH ELEMENT (CM)
C      SF = REACTION COEFFICIENT (1/SEC)
C      ICHECK DEFINES THE TYPE OF BOUNDARY CONDITIONS TO BE IMPOSED
C
C      ICHECK = 1 - UPSTREAM BOUNDARY ELEMENT
C      ICHECK = 2 - SEEPAGE SURFACE ELEMENT
C      ICHECK = 3 - PHREATIC SURFACE ELEMENT
C      ICHECK = 4 - BOTTEM BOUNDARY ELEMENT
C      ICHECK = 5 - DOWNSTREAM ELEMENT
C
C
C      SI AND T1 ARE THE NUMERICAL INTEGRATION POINTS USED IN
C      GENERATING THE ELEMENT STIFFNESS MATRICES FOR THE EARTH DAM
C      AND OXYGEN CONCENTRATION MODLES.
C
C      WRITE(6,66)
66  FORMAT(T10,'INTEGRATION PTS. IN NATURAL COORD.'//)
      SI(1) = (-0.577350269189626 D 0)
      SI(2) = (-0.577350269189626 D 0)
      SI(3) = 0.577350269189626 D 0
      SI(4) = 0.577350269189626 D 0
      T1(1) = 0.577350269189626 D 0
      T1(2) = (-0.577350269189626 D 0)
      T1(3) = (-0.577350269189626 D 0)
      T1(4) = 0.577350269189626 D 0
      DO 300 L=1,4

```

```

WRITE(6,102) SI(L),TI(L)
102 FORMAT(2D30.15)
300 CCNTINUE
9011 KCUNT = 1
CALL ZERO
DO 700 J=1,NE
NI = ISAVE(J,1)
NJ = ISAVE(J,2)
NK = ISAVE(J,3)
NL = ISAVE(J,4)
CALL QUAD4 (J)
IF(ICHECK(J).NE.1) GO TO 801
ELEVI = UPSTRM
ELEVJ = UPSTRM
RHS(NI) = ELEVI + RHS(NI)
RHS(NJ) = ELEVJ + RHS(NJ)
RHS(NK) = (-ELEM(3,1)* ELEVI - ELEM(3,2)* ELEVJ ) +RHS(NK)
RHS(NL) = (-ELEM(4,1)* ELEVI - ELEM(4,2)* ELEVJ ) +RHS(NL)
DO 461 JJ2=1,4
ELEM(1,JJ2) = 0.0
ELEM(2,JJ2) = 0.0
461 CCNTINUE
DO 433 KK=1,2
ELEM(3,KK) = 0.0
ELEM(4,KK) = 0.0
433 CCNTINUE
ELEM(1,1) = 1.0
ELEM(2,2) = 1.0
IF(IPRINT.EQ.0) GO TO 2003
WRITE(6,17)
17 FORMAT(//T30,'UPSTREAM B. C. '//)
WRITE(6,666) NI,RHS(NI),NJ,RHS(NJ),NK,RHS(NK),NL,RHS(NL)

```

```

666 FORMAT(T10,'RHS('',I2,') = ',D14.7/T10,'RHS('',I2,') = ',D14.7/
1T10,'RHS('',I2,') = ',D14.7/T10,'RHS('',I2,') = ',D14.7//)
DC 467 I=1,4
WRITE(6,667) (ELEM(I,JJ),JJ=1,4)
667 FORMAT(4E20.7/)
467 CONTINUE
2003 CONTINUE
801 CONTINUE
IF(ICHECK(J).NE.3) GO TO 822
IF(NK.NE.IBBSAD) GO TO 802
ELEVK = TAIL
IF(TAIL.EQ.0.0) ELEVK = CORY(NK)
RHS(NK) = ELEVK + RHS(NK)
RHS(NI) = (-ELEM(1,3)*ELEVK) + RHS(NI)
RHS(NJ) = (-ELEM(2,3)*ELEVK) + RHS(NJ)
RHS(NL) = (-ELEM(4,3)*ELEVK) + RHS(NL)
DC 875 JJ2 = 1,4
ELEM(JJ2,3) = 0.0
ELEM(3,JJ2) = 0.0
875 CONTINUE
ELEM(3,3) = 1.0
IF(IPRINT.EQ.0) GO TO 2004
WRITE(6,671)
671 FORMAT(T30,'SEEPAGE-DOWNSTREAM B. C.'//)
WRITE(6,666) NI,RHS(NI),NJ,RHS(NJ),NK,RHS(NK),NL,RHS(NL)
DC 672 JJ2=1,4
WRITE(6,673) (ELEM(JJ2,K),K=1,4)
673 FORMAT(4E20.7/)
672 CONTINUE
2004 CONTINUE
802 CONTINUE
822 CONTINUE

```

```

IF(ICHECK(J).NE.5) GO TO 1660
ELEVK = TAIL
IF(TAIL.EQ.0.0) ELEVK = CORY(NK)
ELEVEL = TAIL
RHS(NK) = ELEVK + RHS(NK)
RHS(NL) = ELEVEL + RHS(NL)
DO 1670 JJ=1,4
ELEM(3,JJ) = 0.0
ELEM(4,JJ) = 0.0
1670 CCONTINUE
RHS(NI) = (-ELEM(1,3)* ELEVK      - ELEM(1,4)* ELEVEL  ) + RHS(NI)
RHS(NJ) = (-ELEM(2,3)* ELEVK      - ELEM(2,4)* ELEVEL  ) + RHS(NJ)
DO 1680 JJ=1,4
ELEM(JJ,3) = 0.0
ELEM(JJ,4) = 0.0
1680 CCONTINUE
ELEM(3,3) = 1.0
ELEM(4,4) = 1.0
IF(IPRINT.EQ.0) GO TO 2015
WRITE(6,1690)
1690 FORMAT(//T30,'DOWNSTREAM B. C.'//)
WRITE(6,666) NI,RHS(NI),NJ,RHS(NJ),NK,RHS(NK),NL,RHS(NL)
DO 1700 JJ=1,4
WRITE(6,1710) (ELEM(JJ,KK),KK=1,4)
1710 FORMAT(4E20.7/)
1700 CONTINUE
2015 CONTINUE
1660 CONTINUE
DO 480 IR=1,4
DO 480 IC=1,4
X = ISAVE(J,IR)
Y = ISAVE(J,IC)

```

```

      STIFF(X,Y) = ELEM(IR,IC) + STIFF(X,Y)
480 CONTINUE
700 CONTINUE
      IF(IPRINT.EQ.0) GO TO 2007
      WRITE(6,221)
221  FORMAT(1H1,T10,'CONSTRAINED GLOBAL STIFFNESS MATRIX'//)
      NNN = NN/12 + 1
      DO 412 JJ=1,NNN
      LF = 12*(JJ-1) + 1
      LL = LF+11
      IF(LL.GE.NN) LL=NN
      DO 454 II=LF,LL
      IEX(II) = II
454 CONTINUE
      WRITE(6,222) (IEX(II),II=LF,LL)
222  FORMAT(T6,12I10//)
      DO 410 L=1,NN
      WRITE(6,105) L,(STIFF(L,K),K=LF,LL)
105  FORMAT(T2,I2,T6,12E10.3//)
410 CONTINUE
      WRITE(6,6)
      6  FORMAT(1H1)
412 CONTINUE
      DO 4726 I=1,NN
      WRITE(6,5521) I,RHS(I)
5521 FORMAT(T20,I2,F12.2//)
4726 CONTINUE
      WRITE(6,6)
2007 CONTINUE
      RETURN
      END

```

```

SUBROUTINE OUTPUT(IWRITE)
  IMPLICIT REAL*8(A-H,O-Z)
  COMMON /ELEM/ (4,4), STIFF(33,33), SI(4), TI(4), RHS(33), TOLH, TAIL,
1     UPSTRM, CORX(33), CORY(33), COLUMN(1089), SF(20), D50(20), SLOPE,
2     VX(20), VY(20), PERMX(20), PERMY(20), EPS, CINIT, HEAD(33),
3     FACTRX(20), FACTRY(20), CONVRG
  COMMON /CONV/ NE, NN, KOUNT, ICHECK(20), IPRINT, JOE, ISAVE(20,4), IRBSAD, INUM,
2     IER, NPSE, NSL

C
C   THIS SUBROUTINE OUTPUTS THE EARTH DAM, OXYGEN CONCENTRATION, AND
C   SULFATE PRODUCTION SOLUTIONS.
C

  IF(IWRITE.EQ.1) WRITE(6,600)
600  FORMAT(1H1,T10,'UNADJUSTED FREE SURFACE'//)
  IF(IWRITE.EQ.4) WRITE(6,601)
601  FORMAT(1H1,T10,'INTERMEDIATE FREE SURFACE SOLUTION'//)
  IF(IWRITE.EQ.5) WRITE(6,602)
602  FORMAT(1H1,T10,'FREE SURFACE SOLUTION'//)
  IF(IWRITE.EQ.2) GO TO 1111
  IF(IWRITE.EQ.3) GO TO 400
  WRITE(6,208)
208  FORMAT(
//T10,'NODE',T20,'X-COORD
1.' ,T35,'Y-COORD.',T50,'ELEV. HEAD',T70,'PRESS. HEAD',T90,'TOTAL H
2EAD'/T53,'(CM)',T74,'(CM)',T93,'(CM)'//)
  DO 471 JJ=1,NN
  Z = CORY(JJ)
  ZZ = RHS(JJ) - Z
  WRITE(6,253) JJ,CORX(JJ),CORY(JJ),Z,ZZ,RHS(JJ)
253  FORMAT(T11,I2,T21,F8.2,T36,F8.2,T52,F8.2,T70,F9.2,T93,F8.2//)
471  CONTINUE
  GO TO 20
1111 CONTINUE

```

```

WRITE(6,15)
15 FORMAT(////T10,'NODE',T22,'X',T32,'Y',T44,'HEAD',T61,'OXYGEN'
1,T80,'OXYGEN'/T20,'COORD.',T30,'COORD.',T44,'(CM)',T60,'DEFICIT',
2T77,'CONCENTRATION'/T61,'(MG/L)',T80,'(MG/L)',T21,'(CM)',T31,'(CM)
1'//)
DO 77 I=1,NN
WRITE(6,19) I,CORX(I),CORDY(I),HEAD(I),C COLUMN(I),RHS(I)
19 FORMAT(T11,I2,T26,F8.2,T30,F8.2,T43,F7.2,T57,D14.7,T77,D14.7//)
77 CONTINUE
GO TO 200
400 CONTINUE
WRITE(6,201)
201 FORMAT(T15,'SULFATE SOLUTION'//T10,'NODE',T20,'SULFATE CONC.'/
1T24,'(MG/L)'//)
DO 401 I=1,NN
WRITE(6,202) I,RHS(I)
202 FORMAT(T11,I2,T20,D14.7//)
401 CONTINUE
200 CONTINUE
20 CONTINUE
WRITE(6,6)
6 FORMAT(1H1)
RETURN
END

```

```

SUBROUTINE CHECK (KOLD,NOTPS,NPSN,PHEAD)
IMPLICIT REAL*8(A-H,O-Z)
COMMON  ELE(4,4),STIFF(33,33),SI(4),TI(4),RHS(33),TOLH,TAIL,
1      UPSTRM,CORX(33),CORY(33),COLUMN(1089),SF(20),D50(20),SLOPE,
2      VX(20),VY(20),PERMX(20),PERMY(20),EPS,CINIT,HEAD(33),
3      FACTRX(20),FACTRY(20),CONVRG
COMMON  NE,MN,KOUNT,ICHECK(20),IPRINT,JCE,ISAVE(20,4),IBBSAD,INUM,
2      IER,NPSE,NSL
DIMENSION NCTPS(11),PHEAD(11)

```

C
C
C
C

```

THIS SUBROUTINE CALCULATES THE PRESSURE HEADS OF THE PHREATIC
SURFACE NODES.

```

```

KEEP = 0
DO 401 I=1,NPSN
MY = NOTPS(I)
PHEAD(I) = RHS(MY) - CORY(MY)
APHEAD = DABS(PHEAD(I))
IF(APHEAD.LE.TOLH) KEEP = KEEP+1
401 CONTINUE
IF(KEEP.EQ.NPSN) KOLD = 1
RETURN
END

```



```

SUBROUTINE FREATC (NPSN, IWARN)
  IMPLICIT REAL*8(A-H, O-Z)
  COMMON ELEM(4,4), STIFF(33,33), SI(4), TI(4), RHS(33), TOLH, TAIL,
1      UPSTRM, CDRX(33), CDRY(33), COLUMN(1089), SF(20), D50(20), SLOPE,
2      VX(20), VY(20), PERMX(20), PERMY(20), EPS, CINIT, HEAD(33),
3      FACTRX(20), FACTRY(20), CONVRG
  COMMON NE, NN, KOUNT, ICHECK(20), IPRINT, JOE, ISAVE(20,4), IBSAD, INUM,
2      IER, NPSE, NSL
  DIMENSION NOTPS(11), PHEAD(11)

C
C   FREATC ADJUSTS THE FREATIC SURFACE TO SATISFY THE BOUNDARY
C   CONDITION OF ZERO PRESSURE HEAD.
C

  IHOLD = 0
  KOLD = 0
  JOE = 1
  J1 = 1
  NOTPS(1) = 1
  DO 401 I=2, NPSN
    J1 = J1+NSL
    NOTPS(I) = J1
401 CONTINUE
    IF(IPRINT.EQ.0) GO TO 1000
    WRITE(6,201)
201  FORMAT(1H1,T10,'PHREATIC SURFACE NODES'//)
    DO 402 I=1, NPSN
      WRITE(6,202) I, NOTPS(I)
202  FORMAT(T10,I2,T20,I2//)
402 CONTINUE
1000 CONTINUE
    1 IHOLD = IHOLD + 1
    CALL CHECK(KOLD, NOTPS, NPSN, PHEAD)

```

```

IF(IHOLD.GT.NPSN) IWARN = 1
IF(IHOLD.GT.NPSN) GO TO 998
IF(KOLD.EQ.1) GO TO 999
DO 403 I=1,NPSE
MY = NOTPS(I)
CORY(MY) = CCORY(MY) + PHEAD(1)/CONVRG
IF(CORY(MY).LT.0.0) CORY(MY) = 0.0
IF(NSL.NE.3) GO TO 403
CCRY(MY+1) = (CORY(MY+2)+CORY(MY))/2.0
CCRX(MY+1) = (CORX(MY+2)+CORX(MY))/2.0
403 CONTINUE
DELY = PHEAD(NPSN)/CONVRG
DELX = DELY/SLOPE
MY = NOTPS(NPSN)
CCRX(MY) = CORX(MY) + DELX
CORY(MY) = CCORY(MY) + DELY
IF(IPRINT.EQ.0) GO TO 1001
WRITE(6,6)
6 FORMAT(1H1)
WRITE(6,203) IHOLD
203 FORMAT(T10,'NEW PHREATIC SURFACE COORDINATES - ITERATION ',I4//)
DO 404 I=1,NPSN
MY = NOTPS(I)
WRITE(6,204) CORX(MY),CCRY(MY)
204 FORMAT(T20,F10.3,T35,F10.3/)
404 CONTINUE
1001 CONTINUE
CALL ASEMBL(ICCN)
CALL ARANGE(IVPI,IVPISU)
CALL DGELG(RHS,COLUMN,NN,INUM,EPS,IER,IVPI,IVPISU)
IWRITE = 4
IF(IPRINT.NE.0) CALL OUTPUT(IWRITE)

```

```
GO TO 1
998 WRITE(6,207)
207 FORMAT(1H1,T10,'****' EXCESSIVE ITERATIONS '*/)
999 CONTINUE
RETURN
END
```

```

SUBROUTINE VELCTY
  IMPLICIT REAL*8 (A-H,O-Z)
  COMMON ELEM(4,4),STIFF(33,33),SI(4),TI(4),RHS(33),TOLH,TAIL,
1      UPSTRM,CORX(33),CORY(33),COLUMN(1089),SF(20),D50(20),SLOPE,
2      VX(20),VY(20),PERMX(20),PERMY(20),EPS,CINIT,HEAD(33),
3      FACTRX(20),FACTRY(20),CONVRG
  COMMON NE,NN,KOUNT,ICHECK(20),IPRINT,JOE,ISAVE(20,4),IBBSAD,INUM,
2      IER,NPSE,NSL
  DIMENSION X(4),Y(4)

```

C
C
C

VELCTY CALCULATES THE AVERAGE X AND Y VELOCITY IN EACH ELEMENT.

```

DO 400 J=1,NE
DO 399 I=1,4
  N = ISAVE(J,I)
  X(I) = CORX(N)
  Y(I) = CORY(N)
399 CONTINUE
  M1 = ISAVE(J,1)
  M2 = ISAVE(J,2)
  M3 = ISAVE(J,3)
  M4 = ISAVE(J,4)
  XM12 = (X(1)+X(2))/2.0
  YM12 = (Y(1)+Y(2))/2.0
  XM23 = (X(2)+X(3))/2.0
  YM23 = (Y(2)+Y(3))/2.0
  XM34 = (X(3)+X(4))/2.0
  YM34 = (Y(3)+Y(4))/2.0
  XM41 = (X(4)+X(1))/2.0
  YM41 = (Y(4)+Y(1))/2.0
  SLOPEH = (YM12-YM34)/(XM12-XM34)
  IF(XM41-XM23) 10,20,10

```

```

10 SLOPEV = (YM41-YM23)/(XM41-XM23)
   GO TO 30
20 XINT = XM41
30 B1 = YM12 - SLOPEH*XM12
   IF(XM41.EQ.XM23) GO TO 50
   B2 = YM41 - SLOPEV*XM41
   XINT = (B2-B1)/(SLOPEH-SLOPEV)
50 CONTINUE
   YINT = SLOPEH*XINT + B1
   IF(IPRINT.EQ.0) GO TO 1000
   WRITE(6,200) J,SLOPEH,SLOPEV,B1,B2,XINT,YINT
200 FORMAT(1H1,T10,'ELEMENT -',I3//T15,'HORIZ. SLOPE - ',D14.7/T15,
1' VERT. SLOPE - ',D14.7/T15,'B1 - ',D14.7/T15,'B2 = ',D14.7//T15,
2'MEDIAN INTERSECTION - ',2D20.7//)
   WRITE(6,2001) XM12,YM12,XM23,YM23,XM34,YM34,XM41,YM41
2001 FORMAT(//4(2F10.4)//)
1000 CONTINUE
   HATOP = RHS(M1) - (X(1)-XINT)*(RHS(M1)-RHS(M4))/(X(1)-X(4))
   HABOT = RHS(M2) - (X(2)-XINT)*(RHS(M2)-RHS(M3))/(X(2)-X(3))
   YTOP = (Y(1)-Y(4))/(X(1)-X(4))*(XINT-X(4)) + Y(4)
   YBOT = (Y(2)-Y(3))/(X(2)-X(3))*(XINT-X(3)) + Y(3)
   PHRY = (HATOP-HABOT)/(YTOP-YBOT)
   IF(X(1).EQ.X(2)) GO TO 500
   XLS = (X(1)-X(2))/(Y(1)-Y(2))*(YINT-Y(2)) + X(2)
   GO TO 501
500 CONTINUE
   XLS = X(1)
501 HALS = (RHS(M1)-RHS(M2))/(Y(1)-Y(2))*(YINT-Y(2)) + RHS(M2)
   IF(X(3).EQ.X(4)) GO TO 502
   XRS = (X(4)-X(3))/(Y(4)-Y(3))*(YINT-Y(3)) + X(3)
   GO TO 503
502 CONTINUE

```

```

XRS = X(4)
503 HARS = (RHS(M4)-RHS(M3))/(Y(4)-Y(3))*(YINT-Y(3)) + RHS(M3)
PHRX = (HALS-HARS)/(XLS-XRS)
VX(J) = (-PERMX(J)*PHRX)
VY(J) = (-PERMY(J)*PHRY)
IF(IPRINT.EQ.0) GO TO 1001
WRITE(6,202)
202 FORMAT(//T10,'PHRY'//)
WRITE(6,201) HATOP,XINT,YTOP,HABCT,XINT,YBOT,PHRY
201 FORMAT(//T10,'HEAD = ',D14.7,' AT ',2D20.7//
1 T10,'HEAD = ',D14.7,' AT ',2D20.7//T10,'GRAD = ',D20.7//)
WRITE(6,203)
203 FORMAT(//T10,'PHRX'//)
WRITE(6,201) HALS,XLS,YINT,HARS,XRS,YINT,PHRX
1001 CONTINUE
400 CONTINUE
WRITE(6,701)
701 FORMAT(1H1,T10,'ELEMENTAL VELOCITIES (CM/SEC)'//T20,'ELEMENT',T40,
1'VX',T55,'VY'//)
DO 4006 J=1,NE
WRITE(6,702) J,VX(J),VY(J)
702 FORMAT(T23,I2,T36,D10.3,T51,D10.3//)
4006 CONTINUE
RETURN
END

```

```
SUBROUTINE ARANGE (IVPI,IVPISU)
  IMPLICIT REAL*8(A-H,O-Z)
  COMMON ELEM(4,4),STIFF(33,33),SI(4),TI(4),RHS(33),TDLH,TAIL,
1      UPSTRM,CDRX(33),CDRY(33),COLUMN(1089),SF(20),D50(20),SLOPE,
2      VX(20),VY(20),PERMX(20),PERMY(20),EPS,CINIT,HEAD(33),
3      FACTRX(20),FACTRY(20),CONVRG
  COMMON NE,NN,KCUNT,ICHECK(20),IPRINT,JOE,ISAVE(20,4),IBBSAD,INUM,
2      IER,NPSE,NSL
```

```
C
C
C
C
```

```
  SUBROUTINE ARANGE CONVERTS THE 2-D GLOBAL MATERIAL PROPERTY MATRIX
    INTO A 1-D VECTOR THAT IS NEEDED FOR SUBROUTINE DGELG.
```

```
  JKL = 0
  IVPISU = NN**2
  IVPISU = NN
  DO 475 JJ=1,NN
  DO 475 KK=1,NN
  JKL = JKL+1
  COLUMN(JKL) = STIFF(KK,JJ)
475 CONTINUE
  RETURN
  END
```

```
SUBROUTINE DGELG(R,A,M,N,EPS,IER,IVPI,IVPISU)
  IMPLICIT REAL*8 (A-H,O-Z)
  DIMENSION A(IVPI),R(IVPISU)
```

C
C
C
C
C

```
  DGELG IS THE IBM SCIENTIFIC SUBROUTINE PACKAGE DOUBLE PRECISION
  LINEAR SIMULTANEOUS EQUATION SOLVER. THE METHOD USED IS
  GAUSS ELIMINATION WITH COMPLETE PIVOTING.
```

```
  IF(M)23,23,1
1  IER=0
  PIV=0.D0
  MM=M*M
  NM=N*M
  DO 3 L=1,MM
  TB=DABS(A(L))
  IF(TB-PIV)3,3,2
2  PIV=TB
  I=L
3  CONTINUE
  TCL=EPS*PIV
  LST=1
  DO 17 K=1,M
  IF(PIV)23,23,4
4  IF(IER)7,5,7
5  IF(PIV-TCL)6,6,7
6  IER=K-1
7  PIVI=1.D0/A(I)
  J=(I-1)/M
  I=I-J*M-K
  J=J+1-K
  DO 8 L=K,MM,M
  LL=L+I
```

DELG 600
DELG 630
DELG 640
DELG 650
DELG 660
DELG 670
DELG 680
DELG 690
DELG 700
DELG 710
DELG 720
DELG 730
DELG 780
DELG 790
DELG 820
DELG 830
DELG 840
DELG 850
DELG 860
DELG 870
DELG 880
DELG 890
DELG 930
DELG 940

	TB=PIVI*R(LL)	DELG 950
	R(LL)=R(L)	DELG 960
8	R(L)=TB	DELG 970
	IF(K-M)9,18,18	DELG1000
9	LEND=LST+M-K	DELG1030
	IF(J)12,12,10	DELG1040
10	II=J*M	DELG1050
	DO 11 L=LST,LEND	DELG1060
	TB=A(L)	DELG1070
	LL=L+II	DELG1080
	A(L)=A(LL)	DELG1090
11	A(LL)=TB	DELG1100
12	DO 13 L=LST,MM,M	DELG1130
	LL=L+I	DELG1140
	TB=PIVI*A(LL)	DELG1150
	A(LL)=A(L)	DELG1160
13	A(L)=TB	DELG1170
	A(LST)=J	DELG1200
	PIV=0.D0	DELG1230
	LST=LST+1	DELG1240
	J=0	DELG1250
	DO 16 II=LST,LEND	DELG1260
	PIVI=-A(II)	DELG1270
	IST=II+M	DELG1280
	J=J+1	DELG1290
	DO 15 L=IST,MM,M	DELG1300
	LL=L-J	DELG1310
	A(L)=A(L)+PIVI*A(LL)	DELG1320
	TB=DABS(A(L))	DELG1330
	IF(TB-PIV)15,15,14	DELG1340
14	PIV=TB	DELG1350
	I=L	DELG1360

15	CONTINUE	DELG1370
	DO 16 L=K,NM,M	DELG1380
	LL=L+J	DELG1390
16	R(LL)=R(LL)+PIVI*R(L)	DELG1400
17	LST=LST+M	DELG1410
18	IF(M-1)23,22,19	DELG1460
19	IST=MM+M	DELG1470
	LST=M+1	DELG1480
	DO 21 I=2,M	DELG1490
	II=LST-I	DELG1500
	IST=IST-LST	DELG1510
	L=IST-M	DELG1520
	L=A(L)+.5D0	DELG1530
	DO 21 J=II,NM,M	DELG1540
	TB=R(J)	DELG1550
	LL=J	DELG1560
	DO 20 K=IST,MM,M	DELG1570
	LL=LL+1	DELG1580
20	TB=TB-A(K)*R(LL)	DELG1590
	K=J+L	DELG1600
	R(J)=R(K)	DELG1610
21	R(K)=TB	DELG1620
	IF(IER.EQ.0) GO TO 26	
	WRITE(6,25) IER	
25	FORMAT(1H1,T10,'DGELG SOLUTION'//T15,'IER = ',I3//)	
26	CONTINUE	
22	RETURN	DELG1630
23	IER=-1	DELG1670
	WRITE(6,24) IER	
24	FORMAT(1H1,T10,'** ERROR RETURN **'/// T20,'IER = ',I2///)	
	RETURN	DELG1680
	END	DELG1690

```

SUBROUTINE ZERO
  IMPLICIT REAL*8(A-H,D-Z)
  COMMON ELEM(4,4),STIFF(33,33),SI(4),TI(4),RHS(33),TOLH,TAIL,
1      UPSTRM,CDRX(33),CDRY(33),COLUMN(1089),SF(20),D50(20),SLOPE,
2      VX(20),VY(20),PERMX(20),PERMY(20),EPS,CINIT,HEAD(33),
3      FACTRX(20),FACTRY(20),CONVRC
  COMMON NE,NN,KCUNT,ICHECK(20),IPRINT,JOE,ISAVE(20,4),IBBSAD,INUM,
2      IER,NPSE,NSL

```

C
C
C
C

```

  THIS SUBROUTINE ZEROES ALL ARRAYS THAT ARE USED MORE THAN ONCE
  IN THE PROGRAM.

```

```

  IF(KCUNT.EQ.2) GO TO 530
  DO 450 JJ=1,NN
  DO 450 JK=1,NN
  STIFF(JJ,JK) = 0.0
450 CONTINUE
  DO 451 JJ = 1,NN
  RHS(JJ) = 0.0
451 CONTINUE
530 CONTINUE
  DO 452 KK=1,4
  DO 452 JJ=1,4
  ELEM(JJ,KK) = 0.0
452 CONTINUE
  KCUNT = 2
  RETURN
  END

```

```

SUBROUTINE QUAD4(J)
IMPLICIT REAL*8 (A-H,O-Z)
COMMON ELEM(4,4),STIFF(33,33),SI(4),TI(4),RHS(33),TCLH,TAIL,
1      UPSTRM,CORX(33),CORY(33),COLUMN(1089),SF(20),D50(20),SLOPE,
2      VX(20),VY(20),PERMX(20),PERMY(20),EPS,CINIT,HEAD(33),
3      FACTRX(20),FACTRY(20),CONVRG
COMMON NE,NN,KCOUNT,ICHECK(20),IPRINT,JCE,ISAVE(20,4),IBBSAD,INUM,
2      IER,NPSE,NSL
DIMENSION B(2,4),BT(4,2),XMULT(2,4),X(4),Y(4),JBAR(2,2),R(4,4)
DOUBLE PRECISION JBAR

```

C
C
C
C
C

```

QUAD4 GENERATES THE UNCONSTRAINED MATERIAL PROPERTY MATRIX THAT
IS REQUIRED IN THE EARTH DAM, OXYGEN CONCENTRATION, AND
SULFATE PRODUCTION MODELS.

```

```

DO 399 I=1,4
NUM = ISAVE(J,I)
X(I) = CORX(NUM)
Y(I) = CORY(NUM)
399 CONTINUE
DO 398 I=1,4
DO 398 K=1,4
ELEM(I,K) = 0.0
R(I,K) = 0.0
398 CONTINUE
DO 400 I=1,4
S = SI(I)
T = TI(I)
XMULT(1,1) = (-1-T)/4.0
XMULT(1,2) = (T-1)/4.0
XMULT(1,3) = (1-T)/4.0
XMULT(1,4) = (1+T)/4.0

```

```

XMULT(2,1) = (1-S)/4.0
XMULT(2,2) = (S-1)/4.0
XMULT(2,3) = (-S-1)/4.0
XMULT(2,4) = (1+S)/4.0
DET = 1.0/8.0*((X(1)-X(3))*(Y(2)-Y(4))-(X(2)-X(4))*(Y(1)-Y(3)) +
1S*((X(2)-X(3))*(Y(1)-Y(4))-(X(1)-X(4))*(Y(2)-Y(3))) +
2T*((X(1)-X(2))*(Y(3)-Y(4))-(X(3)-X(4))*(Y(1)-Y(2))))
JBAR(1,1) = (XMULT(1,1)*X(1) + XMULT(1,2)*X(2) + XMULT(1,3)*X(3) +
1XMULT(1,4)*X(4)) / DET
JBAR(1,2) = (-(XMULT(1,1)*Y(1) + XMULT(1,2)*Y(2) + XMULT(1,3)*Y(3)
1 + XMULT(1,4)*Y(4))) / DET
JBAR(2,1) = (-(XMULT(2,1)*X(1) + XMULT(2,2)*X(2) + XMULT(2,3)*X(3)
1 + XMULT(2,4)*X(4))) / DET
JBAR(2,2) = (XMULT(2,1)*Y(1) + XMULT(2,2)*Y(2) + XMULT(2,3)*Y(3) +
1XMULT(2,4)*Y(4)) / DET
DO 401 L=1,4
B(1,L) = JBAR(2,2)*XMULT(1,L) + JBAR(2,1)*XMULT(2,L)
B(2,L) = JBAR(1,2)*XMULT(1,L) + JBAR(1,1)*XMULT(2,L)
401 CONTINUE
IF(IPRINT.EQ.0) GO TO 3000
WRITE(6,5004)
5004 FORMAT(/////T10,'** B MATRIX **'///)
DO 5000 M=1,2
WRITE(6,5001) (B(M,L),L=1,4)
5001 FORMAT(T10,4D20.7/)
5000 CONTINUE
3000 CONTINUE
DO 402 L=1,4
DO 402 M=1,2
BT(L,M) = B(M,L)
402 CONTINUE
DO 403 L=1,4

```

```

      BT(L,1) = PERMX(J)*BT(L,1)
      BT(L,2) = PERMY(J)*BT(L,2)
403  CONTINUE
      DO 520 KK=1,4
      DO 520 KR=1,4
      TCT = 0.0
      DO 521 KC=1,2
      A = BT(KK,KC)*B(KC,KR)
      TCT = TCT + A
521  CONTINUE
      R(KK,KR) = TCT
520  CONTINUE
      IF(JDE.EQ.10) CALL CORNER(X,Y,I,J,R,S,T,DET)
      DO 406 L=1,4
      DO 406 M=1,4
      R(L,M) = DET*R(L,M)
406  CONTINUE
      DO 407 L=1,4
      DO 407 M=1,4
      ELEM(L,M) = ELEM(L,M) + R(L,M)
407  CONTINUE
400  CONTINUE
      IF(KCUNT.EQ.32249) IPRINT = 1
      IF(IPRINT.EQ.0) GO TO 2001
      IF(KCUNT.EQ.32249) IPRINT = 0
      WRITE(6,349) (ISAVE(J,M),M=1,4)
349  FORMAT(/T10,'UNCONSTRAINED STIFFNESS MATRIX FOR ELEMENT ',
14I4//)
      DO 405 K=1,4
      WRITE(6,350) (ELEM(K,L),L=1,4)
350  FORMAT(4E20.7//)
405  CONTINUE

```

2001 CCNTINUE
RETURN
END

```

SUBROUTINE CORNER (X,Y,I,J,R,S,T,DET)
  IMPLICIT REAL*8 (A-H,O-Z)
  COMMON ELEM(4,4),STIFF(33,33),S1(4),TI(4),RHS(33),TOLH,TAIL,
1      UPSTRM,CORX(33),CORY(33),COLUMN(1089),SF(20),D5G(20),SLOPE,
2      VX(20),VY(20),PERMX(20),PERMY(20),EPS,CINIT,HEAD(33),
3      FACTRX(20),FACTRY(20),CONVRG
  COMMON NE,NN,KCUNT,ICHECK(20),IPRINT,JCE,ISAVE(20,4),IBBSAD,INUM,
2      IFR,NPSE,NSL
  DIMENSION X(4),Y(4),R(4,4),P(4)

```

C
C
C
C

```

  THIS SUBROUTINE GENERATES THE EXPONENTIAL MULTIPLIER FOR THE
  OXYGEN CONCENTRATION AND SULFATE PRODUCTION MODELS.

```

```

  NI = ISAVE(J,1)
  NJ = ISAVE(J,2)
  NK = ISAVE(J,3)
  NL = ISAVE(J,4)
  P(1) = 1.0/4.0*(1.0+T-S-S*T)
  P(2) = 1.0/4.0*(1.0-T-S+S*T)
  P(3) = 1.0/4.0*(1.0-T+S-S*T)
  P(4) = 1.0/4.0*(1.0+T+S+S*T)
  XX = 0.0
  YY = 0.0
  DO 400 K=1,4
  XX = P(K)*X(K) + XX
  YY = P(K)*Y(K) + YY
400 CONTINUE
  BETA = (-VX(J)*XX/PERMX(J) - VY(J)*YY/PERMY(J))
  POWER = DEXP(BETA)
  DO 7865 LI=1,4
  DO 7865 LJ=1,4
  R(LI,LJ) = ( SF(J)*P(LI)*P(LJ)) + R(LI,LJ)

```



```

      R(LI,LJ) = R(LI,LJ)*DEXP(BETA)
7865 CONTINUE
      IF(KCUNT.EQ.32249) IPRINT = 1
      IF(IPRINT.EQ.0) GO TO 1000
      IF(KOUNT.EQ.32249) IPRINT = 0
      WRITE(6,6090) J,I
6090 FORMAT(/T10,'ELEMENT ',I3/T10,'RUN',I2//)
      WRITE(6,1066) XX,YY
1066 FORMAT(T10,'XX = ',D14.7,T40,'YY = ',D14.7)
      WRITE(6,667) DET,BETA,POWER,(P(K),K=1,4)
      667 FORMAT(/3D20.7/4D20.7/)
      WRITE(6,202) I
      202 FORMAT(///T10,'DELEM',I3//)
      DO 500 L=1,4
      WRITE(6,203) (R(L,LL),LL=1,4)
      203 FORMAT(T10,4D20.7/)
      500 CONTINUE
1000 CONTINUE
      RETURN
      END

```

```

SUBROUTINE CCNCEN (ICCN)
IMPLICIT REAL*8(A-H,O-Z)
COMMON  ELEM(4,4),STIFF(33,33),SI(4),TI(4),RHS(33),TOLH,TAIL,
1      UPSTRM,CDRX(33),CDRY(33),CCLUMN(1089),SF(20),D50(20),SLOPE,
2      VX(20),VY(20),PERMX(20),PERMY(20),EPS,CINIT,HEAD(33),
3      FACTRX(20),FACTRY(20),CONVRG
COMMON  NE,NN,KOUNT,ICHECK(20),IPRINT,JOE,ISAVE(20,4),IBBSAD,INUM,
2      IER,NPSE,NSL
DIMENSION IEX(50)
DIMENSION VLON(20),ANGLE(20)
DIMENSION E(4,4)

```

C
C
C
C
C
C
C

```

THIS SUBROUTINE CALCULATES THE STEADY STATE OXYGEN DRAWDOWN AND
SULFATE PRODUCTION IN AN EARTH DAM DUE TO CHEMICAL REACTION.
THE DIFFUSION-CONVECTION IS SOLVED ASSUMING NO UPSTREAM
OXYGEN CONCENTRATION VARIATION WITH TIME AND NO INTERNAL
OXYGEN SOURCES.

```

```

JOE = 10
DO 14 I=1,NN
HEAD(I) = RHS(I)
14 CONTINUE
SAVE = PERMX(1)
SAVE1 = PERMY(1)
IF(IPRINT.EQ.0) GO TO 6068
WRITE(6,5310)
5310 FORMAT(1H1,T10,'ELEMENT VELOCITY AND DISPERSION DATA'//T5,'ELEMENT
1',T20,'VX',T40,'VY',T60,'DX',T80,'DY',T100,'REYNOLDS',T120,
1'ANGLE'/T101,'NUMBER'//)
6068 CONTINUE
VND = 0.013098
DO 1792 I=1,NE

```

```

VLCN(I) = DSQRT(VX(I)**2+VY(I)**2)
V = VX(I)/VY(I)/2.0/DARCOB(-1.0D0)
IV = V
VA = IV
RADIAN = V-VA
ANGLE(I) = DATAN(RADIAN)*180.0/DARCOB(-1.0D0)
V1 = DABS(VLCN(I))
RYNLDS = V1*D50(I)/VNU
PERMX(I) = DABS(FACTRX(I)*VX(I))
PERMY(I) = DABS(FACTRY(I)*VY(I))
IF(IPRINT.EQ.0) GO TO 6078
WRITE(6,5311) I,VX(I),VY(I),PERMX(I),PERMY(I),RYNLDS,ANGLE(I)
5311 FORMAT(T8,I2,T14,D14.7,T34,D14.7,T54,D14.7,T74,D14.7,T97,
1D14.7,T115,D14.7/)
6078 CONTINUE
1792 CONTINUE
WRITE(6,201)
201 FORMAT(1H1,T10,'** OXYGEN CONCENTRATION **'//)
KOUNT = 1
CALL ZERC
ISULF = 0
913 DO 400 I=1,NE
NI = ISAVE(I,1)
NJ = ISAVE(I,2)
NK = ISAVE(I,3)
NL = ISAVE(I,4)
IF(IPRINT.EQ.0) GO TO 7443
WRITE(6,7441) I,NI,NJ,NK,NL
7441 FORMAT(1H1,T10,'ELEMENT NUMBER ',I2,' NODES - ',4I5/)
7443 CONTINUE
IF(IPRINT.NE.0) KOUNT = 32249
IPRINT = 0

```

```

      CALL QUAD4(I)
      IF(KCUNT.EQ.32249) IPRINT = 1
      DO 701 JJ=1,4
      DO 701 JK=1,4
      E(JJ,JK) = ELEM(JJ,JK)
701  CONTINUE
      CFAC11 = E(1,1)*(E(2,2)*E(3,3)*E(4,4) + E(2,3)*E(3,4)*E(4,2) +
1E(2,4)*E(3,2)*E(4,3) - (E(2,4)*E(3,3)*E(4,2) + E(2,3)*E(3,2)*E(4,4)
2+ E(2,2)*E(3,4)*E(4,3)))
      CFAC12 = (-E(1,2)*(E(2,1)*E(3,3)*E(4,4) + E(3,1)*E(4,3)*E(2,4) +
1E(4,1)*E(2,3)*E(3,4) - (E(2,4)*E(3,3)*E(4,1) + E(2,3)*E(3,1)*E(4,4)
2 + E(3,4)*E(4,3)*E(2,1))))
      CFAC13 = E(1,3)*(E(2,1)*E(3,2)*E(4,4) + E(2,2)*E(3,4)*E(4,1) +
1E(2,4)*E(3,1)*E(4,2) - (E(2,4)*E(3,2)*E(4,1) + E(2,2)*E(3,1)*E(4,4)
2+ E(2,1)*E(3,4)*E(4,2)))
      CFAC14 = (-E(1,4)*(E(2,1)*E(3,2)*E(4,3) + E(2,2)*E(3,3)*E(4,1) +
1E(2,3)*E(3,1)*E(4,2) - (E(2,3)*E(3,2)*E(4,1) + E(2,2)*E(3,1)*E(4,3)
2+ E(2,1)*E(3,3)*E(4,2))))
      DET4X4 = CFAC11 + CFAC12 + CFAC13 + CFAC14
      IF(IPRINT.EQ.0) GO TO 2005
      WRITE(6,2006) DET4X4
2006  FORMAT(/T10,'DET. OF UNCONSTRAINED STIFFNESS MATRIX = ',D14.7//)
2005  CONTINUE
      IF(ICHECK(I).NE.1) GO TO 801
      IF(ISULF.EQ.1) NSAVE = NSL
      IF(ISULF.EQ.1) NSL = 100
      ELEV I = CINIT
      ELEV J = CINIT
      IF(NL.EQ.NSL+1) ELEVEL = CINIT
      IF(NL.EQ.NSL+1) RHS(NL) = RHS(NL) + ELEVEL
      RHS(NI) = ELEV I + RHS(NI)
      RHS(NJ) = ELEV J + RHS(NJ)

```

```

      IF(NL.EQ.NSL+1) GO TO 7222
      RHS(NK) = (-ELEM(3,1)* ELEV1 - ELEM(3,2)* ELEVJ ) +RHS(NK)
      RHS(NL) = (-ELEM(4,1)* ELEV1 - ELEM(4,2)* ELEVJ ) +RHS(NL)
      GO TO 7223
7222 RHS(NK) = (-ELEM(3,1)*ELEV1-ELEM(3,2)*ELEVJ-ELEM(3,4)*ELEV1) +
1      RHS(NK)
7223 CONTINUE
      DO 461 JJ2=1,4
      ELEM(1,JJ2) = 0.0
      ELEM(2,JJ2) = 0.0
      IF(NL.EQ.NSL+1) ELEM(4,JJ2) = 0.0
461 CONTINUE
      DO 433 KK=1,2
      ELEM(3,KK) = 0.0
      IF(NL.EQ.NSL+1) GO TO 433
      ELEM(4,KK) = 0.0
433 CONTINUE
      ELEM(1,1) = 1.0
      ELEM(2,2) = 1.0
      IF(NL.EQ.NSL+1) ELEM(4,4) = 1.0
      IF(NL.EQ.NSL+1) ELEM(3,4) = 0.0
      IF(IPRINT.EQ.0) GO TO 2003
      WRITE(6,17)
17 FORMAT(//T30,'UPSTREAM B. C. '//)
      WRITE(6,666) NI,RHS(NI),NJ,RHS(NJ),NK,RHS(NK),NL,RHS(NL)
666 FORMAT(T10,'RHS(',I2,') = ',D14.7/T10,'RHS(',I2,') = ',D14.7/
1T10,'RHS(',I2,') = ',D14.7/T10,'RHS(',I2,') = ',D14.7//)
      DO 467 L=1,4
      WRITE(6,667) (ELEM(L,JJ),JJ=1,4)
667 FORMAT(4E20.7/)
467 CONTINUE
2003 CONTINUE

```

```

      IF(ISULF.EQ.1) NSL = NSAVE
801  CONTINUE
      IF(ISULF.GE.1) GO TO 802
      IF(ICDN.EQ.1) GO TO 802
      IF(ICHECK(I).NE.3) GO TO 802
      ELEVI = CINIT
      ELEVEL = CINIT
      RHS(NI) = ELEVI + RHS(NI)
      RHS(NL) = ELEVEL + RHS(NL)
      RHS(NJ) = (-ELEM(2,1)* ELEVI - ELEM(2,4)* ELEVEL ) +RHS(NJ)
      RHS(NK) = (-ELEM(3,1)* ELEVI - ELEM(3,4)* ELEVEL ) +RHS(NK)
      DC 462 JJ2=1,4
      ELEM(1,JJ2) = 0.0
      ELEM(4,JJ2) = 0.0
462  CONTINUE
      DC 443 KK=2,3
      ELEM(KK,1) = 0.0
      ELEM(KK,4) = 0.0
443  CONTINUE
      ELEM(1,1) = 1.0
      ELEM(4,4) = 1.0
      IF(IPRINT.EQ.0) GO TO 2004
      WRITE(6,671)
671  FORMAT(/T30,'FREE SURFACE B. C. '//)
      WRITE(6,666) NI,RHS(NI),NJ,RHS(NJ),NK,RHS(NK),NL,RHS(NL)
      DD 672 L=1,4
      WRITE(6,667) (ELEM(L,JJ),JJ=1,4)
672  CONTINUE
2004 CONTINUE
802  CONTINUE
      DC 404 L=1,4
      DD 404 LL=1,4

```

```

IX = ISAVE(I,L)
IY = ISAVE(I,LL)
STIFF(IX,IY) = STIFF(IX,IY) + ELEM(L,LL)
404 CONTINUE
400 CONTINUE
IF(IPRINT.EQ.0) GO TO 2007
DO 8120 KKK=1,NN
WRITE(6,8210) KKK,RHS(KKK)
8210 FORMAT(T10,I3, T20,E20.7/)
8120 CONTINUE
WRITE(6,221)
221 FORMAT(1H1,T10,'CONSTRAINED GLOBAL STIFFNESS MATRIX'//)
NNN = NN/12 + 1
DO 412 JJ=1,NNN
LF = 12*(JJ-1) + 1
LL = LF+11
IF(LL.GE.NN) LL=NN
DO 454 II=LF,LL
IEX(II) = II
454 CONTINUE
WRITE(6,222) (IEX(II),II=LF,LL)
222 FORMAT(T2,12I10//)
DO 410 L=1,NN
WRITE(6,105) L,(STIFF(L,K),K=LF,LL)
105 FORMAT(T2,I2,T6,12E13.3/)
410 CONTINUE
WRITE(6,6)
6 FORMAT(1H1)
412 CONTINUE
2007 CONTINUE
CALL ARANGE (IVPI,IVPISU)
CALL DGELG (RHS,COLUMN,NN,INUM,EPS,IER,IVPI,IVPISU)

```

```

      IF(ISULF.GE.1) GO TO 160
      DO 1236 I=1,NN
      IF(RHS(I).LT.0.0) RHS(I) = 0.0
1236 CONTINUE
      NI = 2 + NSL
      DO 1235 I=NI,NN,NSL
      IF(RHS(I).EQ.0.0) RHS(I+1) = 0.0
      IF(RHS(I+1).GT.RHS(I)) RHS(I+1) = 0.0
1235 CONTINUE
      DO 1234 I=1,NN
      CCOLUMN(I) = CINIT - RHS(I)
1234 CONTINUE
      GO TO 161
160 CONTINUE
      DO 163 I=1,NN
      RHS(I) = RHS(I) - CINIT
163 CONTINUE
161 CONTINUE
      WRITE(6,6)
      WRITE(6,37) SAVE,SAVE1,SF(1),FACTRX(1),FACTRY(1)
37 FORMAT(T10,'KX = ',D10.3/T10,'KY = ',D10.3/T10,'RC = ',D10.3/
1T10,'FACTRX = ',D10.3/T10,'FACTRY = ',D10.3//)
      IF(ISULF.GE.1) GO TO 910
      IWRITE = 2
      CALL OUTPUT(IWRITE)
      ISULF = 1
      WRITE(6,250)
250 FORMAT(1H1,T10,'SULFATE REACTION COEFFICIENTS'//T15,'ELEMENT',
1T30,'REACTION COEFFICIENT'//)
      CONST = 0.023/1000.0/60.0
      DO 911 I=1,NE
      MI = ISAVE(I,1)

```



```
M2 = ISAVE(I,2)
M3 = ISAVE(I,3)
M4 = ISAVE(I,4)
AVGCCN = (RHS(M1)+RHS(M2)+RHS(M3)+RHS(M4))/4.0
SF(1) = AVGCCN**(2.0/3.0)*CONST
SF(I) = (-AVGCCN**(2.0/3.0)*CONST)
WRITE(6,251) I,SF(I)
251 FORMAT(T17,I2,T32,D14.7/)
911 CONTINUE
KCUNT = 1
CALL ZERO
GO TO 913
910 CONTINUE
IWRITE = 3
CALL OUTPUT(IWRITE)
99999 CONTINUE
RETURN
END
```

VITA

Joseph H. Amend III was born in 1949 in Altoona, Pennsylvania. Upon graduating from Lower Merion High School in 1967, he entered Virginia Polytechnic Institute and was graduated with a Bachelor of Science Degree in Civil Engineering in 1971. In 1973 he received a Master of Science Degree in Civil Engineering specializing in Soil Mechanics. While in graduate school he was a Graduate Teaching Assistant from 1971 through the 1974 school year, teaching Construction Materials, Soil Mechanics, Construction Management, and FORTRAN IV Computer Programming. He is a 1st Lieutenant in the United States Air Force and a member of the following Engineering societies and honorary fraternities: American Society of Civil Engineers, Society of American Military Engineers, Chi Epsilon, Phi Kappa Phi, and Sigma Xi.

Joseph H. Amend III

A FINITE ELEMENT ANALYSIS OF DISSOLVED OXYGEN DRAWDOWN AND SULFATE
PRODUCTION IN STRIP MINE SPOIL DAMS DUE TO PYRITIC CHEMICAL REACTION

by

Joseph H. Amend III

(ABSTRACT)

The problem of dissolved oxygen drawdown and sulfate production in strip mine spoil dams due to chemical reaction between an excess of pyrite, water, and dissolved oxygen is investigated. A finite element analysis is used to solve the diffusion-convection equation assuming steady state conditions and no internal oxygen sources. Oxygen recharge along the free surface is permitted. The analysis is performed in three steps. Step one calculates the nodal piezometric heads and elemental bulk fluid velocities. Steps two and three determine the nodal dissolved oxygen and sulfate concentrations. Solutions are presented for a wide range of soil permeabilities and dissolved oxygen reaction coefficients.

It is found that as the dissolved oxygen reaction coefficient decreased, the dissolved oxygen deficit decreased and the sulfate concentration increased. From these results it was found that the maximum dissolved oxygen deficit occurs at an internal point in the dam and the maximum sulfate concentration occurs on the downstream face of the dam.

The computer program used in the analysis is written in FORTRAN IV computer language and requires a minimum of programming knowledge to implement.