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EVALUATION OF THE SWIFT CODE FOR USE IN BEDDED SALT

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ABSTRACT

In late 1975, Sandia Laboratories entered into an agreement with the NRC to develop a procedure to evaluate the risk of Nuclear Waste disposal. The Sandia Waste Isolation Flow and Transport (SWIFT) model is a development of the contract. The code is based on an earlier version which was developed for the USGS to which nuclide transport and decay was added.

The SWIFT code is a comprehensive three dimensional, transient, laminar flow, finite difference model for transport in a porous geologic media. It is the only code which deals simultaneously with 1) radioactive decay, 2) adsorption 3) concentration, 4) temperature dependent density and viscosity, and 5) pressure effects on enthalpy.

This report is an evaluation of the SWIFT code for bedded salt by the Interoffice Waste Management Modelling Group (IWMG). The limitations and capabilities of the code are discussed and major conclusions are as follows:

1. SWIFT is the most comprehensive model available to handle problems which are specific to salt, such as variable density solute transport and salt dissolutioning.
2. Limitations of Fick's law and Darcy's law are presently being researched and future modelling efforts will be effected by these research results.
3. Sandia staff and NRC staff plan to use SWIFT on media other than salt.
4. IWMG plans to develop experience with other codes such as the Network Flow and Transport (NWFT), Distributed Velocity Method (DVM), and Dynamic Network Flow and Transport (DNET).

EVALUATION OF THE SWIFT CODE FOR USE IN BEDDED SALT

EXECUTIVE SUMMARY

I. BACKGROUND

In late 1975, Sandia Laboratories (SL) entered into an agreement with the Nuclear Regulatory Commission (NRC) to develop a procedure to evaluate the risk of nuclear waste disposal facilities. The primary objective of this program was the development of a procedure (or methodology) to be used for the analysis of the performance of nuclear waste disposal facilities. This objective involved both the development of a workable conceptual approach and the construction of appropriate building blocks to support the conceptual approach. The objective of the work described in this report was the development of a mathematical model for the building block "Radionuclide Transport by Groundwater."

The first phase in the evolution of this code began independently of NRC's work in 1975 when the U.S. Geological Survey (USGS) awarded a contract to INTERCOMP Resource Development and Engineering, Inc., the parent company of INTERA, a company with international experience in oil reservoir simulation. The objective of this contract was the development of a general model to simulate non-radioactive waste injection in deep saline aquifers. The result of this effort was a simulator for three processes; single phase fluid flow, heat transport both through the rock and the fluid media, and fluid composition changes for a miscible component. The program was titled the Survey Waste Injection Program (SWIP). This work is discussed in the reference INTERCOMP (1976).

The second phase was the development of the Sandia Waste Isolation Flow and Transport (SWIFT) model which began in 1977 at Sandia Laboratories in Albuquerque, New Mexico. This organization, under contract to the NRC, sought to acquire, in the form of a computer simulation, a waste-isolation analysis methodology. For storage in salt such a methodology must treat coupled three dimensional transport of fluid, brine in nondilute concentrations, heat, and chains of radionuclides in dilute concentrations, for periods of time approaching one million years. After examining the existing technology at several national laboratories in the U.S. and within the USGS, Sandia scientists concluded that no computer model existed which included all the necessary features for a nuclear waste-isolation model. They also concluded that, among the available models, INTERA's waste-injection program represented the state of the art for geosphere simulation. Consequently, INTERA was engaged under subcontract to Sandia to add the transport of radionuclide chains to the SWIFT code. The resulting computer model, SWIFT, is discussed in the document Dillon, Lantz, and Phawa (1978).

II. CAPABILITIES AND LIMITATIONS OF SWIFT

SWIFT is a comprehensive three-dimensional, transient, laminar flow, finite difference model for transport in porous geologic media. Of the 250 international numerical models assessed by the Holcomb Research Institute of Butler University, Indiana, SWIFT is the only model which deals simultaneously with all the following: 1) radioactive decay, 2) adsorption, 3) concentration, 4) temperature dependent density and viscosity and 5) pressure effects on enthalphy.

Application

SWIFT can be used in four major types of transport simulation. They are transport of radionuclides, groundwater, brine, and heat. SWIFT has demonstrated its usefulness in practical water related studies as follows:

Radionuclide Transport

Waste Isolation in Various Geologic Media

Near-Field Waste Repository Evaluation

Reactor Safety Assessment

Simultaneous Transport of Reacting Species

Determination of Aquifer Parameters from Tracer Tests

Groundwater Transport

Water Supply

Regional Aquifer Analysis

Wellbore Performance

Groundwater/Surface Water Interactions

Dewatering Operations

Injection of Industrial Wastes

Determination of Aquifer Parameters

Brine Transport

Salt-Water Intrusion in Coastal Regions

Brine Disposal from Petroleum Product Production

Disposal/Holding Ponds

Aquifer Contamination

In-Situ Solution Mining

Salt Solutioning of Geologic Formations

Injection of Wastes in Saline Aquifers

Heat Transport

Thermal Storage in Aquifers

Thermal Pollution

Nuclear Waste Isolation

The SWIFT model has proven useful in actual field situations. Some of the applications of SWIP, the original form of SWIFT, are as follows:

- Professor Fred Molz of Auburn University considered the summer storage of hot water in aquifers for removal in the winter months as a heat source. Flow and temperature conditions were simulated by the INTERA code. The project was under the direction of the USGS and the results are described in "Groundwater," July/August 1978, Vol. 16, #4 (Contact: S. Larson, USGS, Reston, VA).

- At the Canadian Air Force Base, Borden, data on cadmium concentrations in an exposed landfill were collected. The code was applied to compare predictions of leaching and adsorption to the data collected. The project was under direction of Environmental Canada. (Contact: John Sikes, University of Waterloo; INTERA Environmental Consultants Ltd.).

- In the 1960's under the name of Project Gnome, the enhancement of permeability by nuclear explosion was studied near the WIPP site. Data from a tracer test taken at that time compared favorably to code

predictions. The DOE plans to conduct another tracer test (with an inert, non-adsorbing tracer) whose results are to be analyzed by INTERA as a subcontractor to Sandia) (Contact: Saresh Pahwa, INTERA/Environmental Consultants).

- The Electric Power Research Institute conducted a feasibility study for methane production from geopressure aquifers, in the Lousiana Gulf Coast. The project was subcontracted to Southwest Research Institute and the code was applied to predict methane flow. (Contact: Bob Swanson, Southwest Research Institute, Texas).

- The DOE funded a project to study the storage of petroleum in the Gulf salt domes (Bryan Mound, Weeks Island, Bayou Choctau). Initially water was pumped in; then data on flow and salt concentrations were compared with code predictions. Subcontractors were Jacobs Engineering and D'Appolonia.

- The USGS applied the code for flow simulation for a deep well waste injection problem in Florida in a fractured limestone aquifer. The program is FL 154 "Subsurface Waste Storage Statewide - Hydrologic and Geologic Aspects." (Contact: John Vecchiolo, USGS - Tallahassee).

- The USGS applied the flow and contaminant mass portions of the code and successfully predicted the movement of dissolved solids in groundwater in the Fallon area (near Carson City). The project was entitled, "Fallon Aquifer Systems" 4732-05800. (Contact: Tim Durbin, USGS - Denver).

- The USGS in Oklahoma applied the code to predict the movement of chloride in groundwater. The project is underway and is entitled "Great Salt Plains Project." (Contact: Joseph Reed, USGS, Oklahoma).

- The USGS applied the code to the storage of fresh water in salt water aquifers (instead of surface storage) to determine the feasibility of retrieval during periods of low water supply. Flow, temperature and contaminant conservation portions of the code were used. Some use has been made of the code to model the movement of uranium deposits and to consider their decay and adsorption. (Contact: Leonard Konikow, USGS - Reston).

A. Capabilities of SWIFT

SWIFT is a powerful numerical model because of the numerous options available to a user. Before discussing these options, the following are the general capabilities of SWIFT.

1. 3-D - The model is three dimensional and can be coded as a one- or two-dimensional model depending on specific applications. In addition to the three dimensional rectangular cartesian grid, SWIFT also provides a two-dimensional cylindrical coordinate system.

2. Fully Coupled Flow, Heat and Brine Equation

SWIFT can solve three fully coupled partial differential equations simultaneously. These equations represent fluid flow, heat transport and brine transport. In general, problems involving saline water require consideration of density changes. Density changes can become significant in situations where chloride concentrations are high, and therefore, the flow and transport equations must be solved simultaneously.

The equations involves.

- o Conservation of total liquid mass
- o Conservation of specific brine (contaminant) mass dissolved in the injection fluid
- o Conservation of energy (heat).

These three equations are coupled through the density and viscosity terms, and they provide the velocity field on which radionuclide transport depends. The radionuclide transport equation need not be coupled to the first three equations, because it is assumed that the contamination is in trace amounts and will not effect the flow field. The radionuclide equation conserves the mass of the species dissolved in the fluid phase and adsorbed on the rock medium. It also considers radioactive decay and generation from other constituents.

3. Density and Viscosity as Variables - Fluid density and viscosity are variables computed in SWIFT. Fluid density is computed as a function of composition, temperature and pressure. Viscosity is computed as a function of brine concentration and temperature.

4. Steady State Solution of Flow Equation - SWIFT can solve a steady state solution of flow without first solving the transient solution, eliminating many time steps and large amounts of computer time.

5. Salt Dissolution Simulations - SWIFT can simulate the salt dissolution process by two parameters namely a rate constant (Ks) and a mass fraction (fs) of solubles to total solid mass. These terms are included in the source terms of the brine transport and the flow equations. The resulting changes in porosity and intrinsic permeability are included in the equations. This formulation of salt dissolutioning is similar to that of Nolen, et al. (1974) where salt cavern formation for storage of crude oil was considered.

6. Waste Leach Simulation - SWIFT can simulate the source rate at which the waste is dissolved into solution. The code considers each radioactive component to be in one of three distinct phases characterized as being either:

a) unleached from the waste matrix

b) leached but undissolved

c) dissolved.

Some of the options available in the SWIFT code are listed below:

1. Problem Size - There is no upper limit placed on the actual problem size as long as the total core storage required is available on the computer.

2. Dynamic Core Allocation - SWIFT uses available dimensioning schemes for all large arrays which are made available on most CDC machines. After the program dimensions have been specified, by the user, the dimensions on arrays and total array storage required are calculated. Dynamic core allocation is cost effective since you use only the core space that is needed rather than some predetermined amount.

3. Decay Chains - There are no restrictions on the total number of components in a decay chain or on the number of parents or daughters that a component in the decay chain may have.

4. Heterogeneities - An option is available to describe different horizontal and vertical permeabilities, porosity and rock heat capacity in each grid block.

5. Geometry - Variable geometries can be obtained by setting pore volumes to zero in appropriate grid blocks. Individual grid block thicknesses and depths can be adjusted. If a cartesian coordinate system has been selected, dip angles in x and y directions can be specified.

6. Adsorption Coefficients - The user may enter a regional description of formation type. The numerical grid system may encompass a number of rock or formation types and adsorption coefficients for each isotope may be different for each rock type.

7. Aquifer Influence Functions - Aquifer influence functions are a mechanism treating both external and internal boundaries. They are used to characterize an external boundary of the system which is pressure controlled. They are simply pressures set up outside the grid boundaries. Additionally, another use of the functions is to characterize an internal boundary when going from far-field to near-field analyses. Through the use of aquifer influence functions, fluid, energy and contaminant transport across numerical grid boundaries may be permitted.

8. Solution Options - SWIFT offers the user an option to select a direct or an iterative method of solution for solving the difference equations. The direct method includes an ordered Gaussian elimination scheme and the iterative method is a two-line overrelaxation (L2SOR) method. The amount of computer storage space required for the direct solution is always larger than for the indirect method.

9. Automatic Time Step - This option is very useful in minimizing computer processing time. Optimum time steps are automatically calculated based on user-specified maximum pressure, temperature and concentration changes desired per grid block per time step.

10. Well Sepcification - The well specification option is very useful in expressing various types of pressure and flux boundary conditions by specifying wells at those grid block locations. The user may specify an injection well or a withdrawal well.

11. Restart Capability - SWIFT has an optional restart feature which will reduce the total computing time and expense. By retaining intermediate results and data on a magnetic tape or disc area, a problem may be interrupted and restarted at specified convenient times in the simulation run. This capability is cost effective for sensitivity and risk analyses.

12. Contour Mapping - To make the visualization of multidimensional results more comprehensible, two-dimensional contour maps can be prepared on the line printer of pressure, temperature or inert component concentration. These maps can be presented at any time during the calculation. The mapping program presents a diagram of up to 20 contours of the dependent variable. Each contour is described with a different mapping character.

13. Plotting Calculated Versus Observed Results - This option enables the user to plot comparative values of observed (measured) pressure, temperature or inert component concentration with calculated values of the same variable as a function of time for any specified well. Since the wellbore is made an integral part of the calculation, the user can compare these variables at surface conditions, at bottom-hole conditions or both.

B. Limitations of SWIFT

1. Numerical Dispersion and Oscillatory Instability - The major limitations of SWIFT, as of any finite difference models, are numerical dispersion and oscillatory instability. Numerical dispersion has the same effect as physical dispersion in that it results in a smearing or smoothing of a contaminant front.

Oscillatory instability results in solutions which exceed, or overshoot maximum possible concentrations and undershoot minimum concentrations. The user would be aware of this because the solutions would oscillate back and forth from very high values to very low values.
Fortunately the user can select various schemes which are inherently stable and those which produce only a small amount of numerical dispersion. The code offers certain criteria which must be followed regarding time and space increments which help to insure a stable solution.

2. Core Space and Time Requirements - Because of its comprehensiveness and numerous internal iterative processes, SWIFT requires large computer core space and run times for execution. For example, a one dimensional problem using the less restrictive "centered in space" approach uses the criterion $\Delta x \leq 2\alpha$. As α, the dispersivity, decreases, Δx, the required block size, becomes finer, increasing computer time and storage requirements, which means the cost of computer runs increases. This problem is most acute in the case of sensitivity and risk analyses where many computations are necessary. The solution to this problem is to run either the 1-D version of SWIFT or the Network Flow and Transport (NWFT) to conduct sensitivity or risk analyses.

3. Simplified Chemistry - SWIFT in its present form does not contain any reactive chemistry other than that which is associated with radioactive decay and the adsorption-desorption processes. The code uses k_d's to represent sorption. The geochemistry in the code is simplified by assuming constant distribution coefficeints, k_d's for each rock type although k_d's are permitted to vary for different rock types. It may be desirable to make k_d a function of salinity and to make the solubility of the radionuclides a function of both salinity and temperature.

4. Demands Upon User - Another limitation of SWIFT is its large demand on the user. Because of its comprehensiveness, the user should have some background in mathematics, geology, hydrology, and physics. It is also a big task for the user to learn all the different options provided in the code. Coding the input is also a big task because of the code's numerous input variables. These variables must be coded in the specified format. Future development should consider free format input.

5. English Units - In its present form, SWIFT uses the english units. Conversion to a more accepted set of units such as SI system is desirable since the subsequent model, Pathways To Man, uses SI units.

6. Output Format - The present output of the code is presented primarily in tabular form. Because this results in large quantities of printout, more efficient methods of displaying output need to be developed. Plots, especially

in three dimensions should be able to be displayed on a cathode ray tube (CRT) terminal with 3-D capability.

III. OBSERVATIONS OF PROBLEMS

This section will address several key problems which have been discussed within the IWMG. These problems are currently being addressed both by the DOE and the NRC under ongoing contracts. These issues are: 1) the errors involved in numerical modeling; 2) the limits of Darcy's law; and 3) the validity of Fick's law.

A. Errors

The following discussion of errors in mathematical models is taken from Mercer (unpublished).

> A mathematical model is simply a set of equations which, subject to certain assumptions, describes the physical processes active in the aquifer. While the model itself obviously lacks the reality of the groundwater system, the behavior of a valid model approximates (assumes the appearance of) that of the aquifer.
>
> The mathematical model discussed here consists of a partial differential equation which expresses conservation of mass. In addition, the model entails various phenomenological "laws" describing the rate processes active in the aquifer. Example laws are those due to Darcy (fluid flow), Fourier (heat conduction), and Fick (solute transport by diffusion or dispersion). Finally, various assumptions may be invoked such as those

of one- or two-dimensional flow, confined or unconfined, negligible dispersion, etc.

The model equations generally require numerical solution. A computer program is written to utilize some numerical technique in solving the equation. Required program input data include aquifer properties such as storage coefficients, and transmissibilities. Computed results generally consist of hydraulic heads at each of several grid points throughout the aquifer. In problems involving heat or solute flow, the model will also entail calculation of temperature or concentration at each grid point. These spatial distributions of hydraulic head, etc. are determined at each of a sequence of time levels covering the period of interest.

There are several potential sources of error in computed results. First, the mathematical model itself is usually approximate since it involves certain assumptions which are only partially valid. Second, replacement of the model differential equations by difference equations introduces truncation error; that is, the exact solution of the difference equations differs somewhat from the solution to the original differential equations. Third, the exact solution of the difference equations is not obtained due to round-off error, incurred by the finite word length of the computer. Finally, and perhaps

most important, aquifer description data (e.g., permeability, porosity distributions) seldom are accurately known.

The level of truncation error in computed results may be estimated by repeating runs or portions of runs with smaller space and/or time increments. Significant sensitivity of computer results to change in these increment sizes indicates a significant level of truncation error and the corresponding need for smaller spatial and/or time steps. Compared to the other error sources, round-off error is generally negligible.

Error caused by erroneous aquifer description data is difficult to determine since the true aquifer description is never known. A combination of geologic core analysis, well tests, and geological studies often gives valid insight into the nature of permeability and porosity distributions and aquifer geometry. The best method of obtaining a valid aquifer description is to determine (in some manner) that description which results in best agreement between calculated and observed field performance over a period of available aquifer history.

The user of the SWIFT code should be aware of the inherent errors in any numerical simulation. Care should be taken to select options in the SWIFT code which summarize these numerical errors. Detailed analysis of both input and output data should be an important part of the simulation process.

B. Upper and Lower Limits of Darcy's Law

The following discussion of the limitations of Darcy's law is taken from Freeze and Cherry (1978).

Even if we limit ourselves to the consideration of specific discharge on a macroscopic scale through the Darcian continuum, there may be limitations on the applicability of Darcy's law. Darcy's law is a linear law. If it were universally valid, a plot of the specific discharge versus the hydraulic gradient would reveal a straight-line relationship for all

gradients between 0 and ∞. For flow through granular materials there are at least two situations where the validity of this linear relationship is in question. The first concerns flow through low-permeability sediments under very low gradients and the second concerns large flows through very high permeability sediments. In other words, there may be both a lower limit and an upper limit to the range of validity of Darcy's law.

For fine-grained materials of low permeability, it has been suggested on the basis of laboratory evidence that there may be a threshold hydraulic gradient below which flow does not take place. Swartzendruber (1962) and Bolt and Groenevelt (1969) review the evidence and summarize the various hypotheses that have been put forward to explain the phenomenon. As yet, there is no agreement on the mechanism, and the experimental evidence is still open to some doubt. In any event, the phenomenon is of very little practical importance; at the gradients being considered as possible threshold gradients, flow rates will be exceedingly small in any case.

Of greater practical importance is the upper limit on the range of validity of Darcy's law. It has been recognized and accepted for many years that at very high rates of flow, Darcy's law breaks down. The upper limit is usually identified with the aid of the Reynolds number R_e, a dimensionless number that expresses the ratio of inertial to viscous forces during flow. It is widely used in fluid mechanics to distinguish between laminar flow at low velocities and turbulent flow at high velocities. The Reynolds number for flow through porous media is defined as

$$R_e = \frac{pvd}{\mu}$$

where ρ and μ are the fluid density and viscosity, v the specific discharge, and d a representative length dimension for the porous medium, variously taken as a mean pore dimension, a mean grain diameter, or some function of the square root of the permeability k. Bear (1972) summarizes the experimental evidence with the statement that "Darcy's law is valid as long as the Reynolds number based on average grain diameter does not exceed some value between 1 and 10." For this range of Reynolds numbers, all flow through granular media is laminar.

Flow rates that exceed the upper limit of Darcy's law are common in such important rock formations as karstic limestones and dolomites, and cavernous volcanics. Darcian flow rates are almost never exceeded in nonindurated rocks and granular materials. Fractured rocks (and we will use this term to refer to rocks rendered more permeable by joints, fissures, cracks, or partings of any genetic origin) constitute a special case that deserves separate attention.

The user of SWIFT should be aware of the limitations of Darcy's law. The use of SWIFT in a fractured medium requires the application of various assumptions. It can be assumed that over a very large area, fractured media flow may be approximated by Darcy flow provided fractures are numerous. The user should also be aware of the double porosity option in SWIFT which approximates 2-D fracture flow by equivalent porous media techniques.

Field verified fracture flow codes are currently unavailable but are under development by NRC, DOE and various universities.

C. Fickian Transport Model

The following discussion of dispersion is taken from Freeze and Cherry (1979).

The process by which solutes are transported by the bulk motion of flowing groundwater is known as advection. Owing to advection, nonreactive solutes are carried at an average rate equal to the average linear velocity of the groundwater. There is a tendency, however, for the solute to spread out from the path that would be expected according to the simple advective hydraulics of the flow system. This spreading phenomenon causes dilution of the solute and is called hydrodynamic dispersion. It occurs as a result of mechanical mixing during fluid advection, and molecular diffusion due to the thermal kinetic energy of the solute particles. Diffusion is a dispersive process which dominates at low velocities; conversely, mechanical mixing predominates at high velocities.

On the microscopic scale, mechanical dispersion is caused by three main mechanisms, which result in a variation of molecular velocity in the individual pore channels. The first process is caused by drag exerted on the transport fluid by the roughness of the pore surfaces. The second process is caused by variations in pore size along the flow path. The third mechanism is related to tortuosity, i.e., the branching and interfingering of the pore channels. The spreading of the solute in the direction of bulk flow is known as longitudinal dispersion and spreading perpendicular to the flow is known as transverse dispersion. Longitudinal dispersion is normally much greater than lateral or transverse dispersion.

On the macroscopic scale, dispersion is caused by large scale heterogenieties in the rock mass causing velocity variations.

Diffusion in solutions is the process whereby ionic or molecular constituents move under the influence of their own kinetic activity in the direction of their concentration gradient. Diffusion is therefore independent of flow rate and may occur in the absence of any bulk hydraulic movement of the transport fluid. The mass of diffusing substance passing through a given cross section per unit time is proportional to the concentration gradient and is evaluated using Fick's law.

The SWIFT code combines the effects of both hydrodynamic dispersion and molecular diffusion in one term, the dispersivity tensor.

If dispersion were not accounted for, a concentration front, after injection into an aquifer would look sharp. The effect of dispersion is to smear the sharp edges of the front into a curve.

Recent developments have led several researchers to question the validity of Fick's law, among them are LBL, University of Arizona, and Camp Dresser and McKee. Enenoon and Detinger (1980) of Camp Dresser and McKee have found the dispersion coefficient to be crucially dependent on 1) the model being applied and 2) the scale of the transport that is being modelled.

University of Arizona (1979) has reached similar conclusions and additionally has problems with assuming a constant dispersion coefficient because it leads

to the conclusion that solute molecules may travel upstream in the absence of molecular diffusion, which is physically impossible.

The user of SWIFT should be aware of the controversy regarding Fick's law. The NRC has attempted to address this problem by entering into a research contract with University of Arizona to answer the following questions:

1) To what extent do existing governing equations for subsurface transport correctly describe the process?
2) If the process is not correctly described, what alternate methods of analysis should be adopted?
3) To what extent may the equations be extrapolated to fractured media?

Additionally, NRC has an ongoing contract with ORNL to investigate the transport process.

Future use or modifications to the SWIFT code will be resolved based upon the findings of these contracts.

IV. NRC STAFF EFFORTS

Once the SWIFT code development became complete, the next phase concerned the transfer of this technology from Sandia to the NRC. This phase necessitated the formation of a model user group among the NRC offices that would be involved in licensing and regulating high level waste repositories. The participating offices are Office of Nuclear Regulatory Research, Office of Nuclear Material Safety and Safeguards and Office of Standards Development. The group was entitled IWMG for Interoffice Waste Management Modeling Group.

The goals of the IWMG are to:

1. Develop expertise in using the waste isolation computer codes and apply the expertise to the licensing and rule-making processes.
2. Acquire an understanding of the capabilities and limitations of each code.
3. Identify the needs and to make recommendations regarding further research on nuclear waste isolation.

The objectives of the IWMG are to:

1. Provide insight into:
   a. Identification of desirable site characteristics
   b. Evaluation of alternate site and/or media
   c. Site/media performance specifications
   d. Monitoring requirements
   e. Identification of important technical criteria
2. Provide information to develop regulatory guidance (technical positions, regulatory guides, license review plans, environmental equations, and PSAR format and content guides).
3. Publish NUREGs on the work of the IWMG for future reference.
4. Provide waste isolation and statistical models and procedures for coordinating safety and environmental assessments in reviewing repository applications.
5. Identify key parameters that affect radionuclide release and migration and their relative importance.

6. Provide a better understanding of the sensitivity of the calculated consequences and their attendant uncertainties as a function of the variability of input parameters.

The group set out in 1979 to actually transfer the code to the Brookhaven National Laboratory computer and run six sample problems which had been designed to familiarize the user with the code. These six example problems were completed the first week in June 1980, and are included as Appendix A of this document.

On June 9-13, 1980, a seminar was conducted in Crystal City, Virginia, for the IWMG, under a contract entitled "Technology Transfer" issued to Sandia through NMSS. This seminar was conducted by Mark Reeves of INTERA and John Sykes, University of Waterloo, and was designed to discuss the six problems in detail and to explain the basic mathematic formulation of the SWIFT code.

Following this seminar, on June 27 a presentation of the six problems was given to the IWMG Oversight Group and a list of technical questions was developed to be answered by INTERA. These questions are included in Appendix B. The questions were given to INTERA through Sandia for response in August of 1980. Response is expected by November 1980. A preliminary advanced seminar for four more example problems on the SWIFT code was held at Sandia in August 1980.

V. FUTURE WORK ON SWIFT

An advanced seminar for the IWMG is planned for Silver Spring in December 1980. The advanced problems will address:

- o two-dimensional near-field heat transport
- o thermal convection
- o salt dissolution
- o two-dimensional flow and brine transport
- o Five-member decay chains.

Also expected to be covered at this seminar is the double porosity flow model to simulate fracture flow.

SWIFT will play a major part in the IWMG Work Plan for the next year and a half. Problems 7, 8, 9, and 10 of the Bedded Salt Reference Repository Site (BSRRS) will be analyzed and presented to the oversight group. Variation of the input will also be performed for problems 1 through 10. After the analysis of the BSRRS, SWIFT will be used to model the Hanford Site (basalt). For more information on future work of SWIFT and other codes, refer to the IWMG Program Plan.

CONCLUSIONS

- It is the opinion of the IWMG that the advantages of SWIFT outweigh the disadvantages. The code is the most comprehensive model available presently and has the capability to handle problems which are specific to salt domes and bedded salt, such as variable density solute transport and salt dissolutioning.

- Problems raised as to the validity of Fick's law and Darcy's law are currently being researched under DOE and NRC contracts. Decisions regarding how to proceed with modelling efforts will be affected by the conclusions reached in these research efforts.

- The IWMG plans to continue running example problems developed by INTERA and SLA to understand all aspects of the SWIFT code applicable to repository siting in Bedded Salt.

- Sandia staff and NRC staff plan to continue evaluating the SWIFT code for media other than Bedded Salt. Present plans include using the double porosity version of SWIFT, with certain simplifying assumptions, on basalt until better fracture flow models become available.

- Future IWMG work includes developing the capability to exercise other codes such as Network Flow and Transport (NWFT), Distributed Velocity Method (DVM), and Dynamic Network Flow and Transport (DNET). These codes are being transferred to us under the Technology Transfer and Reference Repository Contract between NMSS and SLA.

BIBLIOGRAPHY

1. Bear, J. (1972), Dynamics of Fluids in Porous Media, Elsever, New York.

2. Bolt, G.H., and P.H. Groenevelt, (1969), Coupling Phenomena as a Possible Cause for Non-Darcian Behavior of Water in Soil, Bull, Intern., Assoc. Sci. Hydrol., 14, no. 2, pp. 17-26.

3. Dillon, R.T., R. B. Lantz, and S. B. Pahwa, (1978) Risk Methodology for Geologic Disposal of Radioactive Waste. The Sandia Waste Isolation Flow and Transport (SWIFT) Model."

4. Enenoon, D.E., and M.D. Dettinger (May 1980), UCRL 15251 "Dispersive Processes in Models of Regional Radionuclide Migrations, for LLL by Camp Dresser and McKee, Inc.

5. Freeze and Cherry (1979), Groundwater, Prentice-Hall, Inc., Englewood Cliffs, New Jersey.

6. INTERCOMP, June 1976, "A Model for Calculating Effects of Liquid Waste Disposal in Deep Saline Aquifers Part I--Development Part II--Documentation."

7. Mercer, James (Unpublished), Class lecture notes, Finite Difference Analysis - Errors.

8. Nolen, J.S., Van Hartlemann, G., Meister, S., Kleinitz, W., and Heiblinger, J., (1924), Numerical Simulation of the Solution Mining Process, Soc. Pet. Eng., Paper No. SPE 4850.

9. Swartzendruber, D. (1962), Non-Darcy Flow Behavior in Liquid-Saturated Porous Media., J. Geophys. Res., 67, pp. 5205-5213.

10. University of Arizona (1979), Progress and Problems in the Analysis of Subsurface Mass Transport, A topical report to the NRC Contract No. NRC-04-78-275, University of Arizona, Tucson, AZ, pp. 141.

APPENDICES

APPENDIX A

APPENDIX B

TECHNICAL QUESTIONS

1. Please have the contractor or subcontractor justify using the SWIFT version with top-centered nodes and not block centered node points. Does this affect the dispersion and convective transport in problem 6?

2. For problem 4, how can the contractor prove that the pressure profile and Dancian velocity distribution is correct when the mass balance remaining and temperature profile is obviously incorrect?

3. Can the units be changed to the SI system?

4. Why are temperature changes calculated when the equation scheme option in the main program does not involve the temperature equation?

5. When the well index is calculated, what values do you chose for K_s?

6. How can a well change from a production to an injection well for a steady state solution when the program was told it was a production well (problem 4)?

7. Explain the book keeping mechanism for the mass balance and well summaries at the end of each time step.

8. Explain in detail the flow distribution development at the end of problem 5, and why the repository and bore hole are not included.

9. Has the contractor or subcontractor used this model to develop boundaries on the time required to resaturate the repository? (i.e., can an unsaturated flow subroutine be developed for this problem?)

IWMG ANALYSIS OF TEST PROBLEMS 1 THROUGH 6 OF THE "SWIFT" COMPUTER CODE

CONTENTS

1.0 PROBLEM 1

1.1 1-D FLOW WITH AQUIFER INFLUENCE BOUNDARY CONDITIONS

Boundary conditions for the three primary equations, i.e., for total mass conservation, for inert component conservation, and for energy conservation, may be one of two types; i.e., either a prescribed constant value of the dependent variable or a prescribed derivative, typically a flux. The former is imposed by means of both aquifer influence functions and "wells" (through a bottom-hole pressure limitation), and the latter is imposed only by means of "wells." This example illustrates the use of aquifer influence functions, the input for which appears on R1-27 and R1-28 cards (see SWIFT documentation).

For purposes of this example, the middle sandstone aquifer of the NRC reference site is approximated by a system having the following basic characteristics:

length = L = 305,000 ft (1)

width = 1 ft (2)

thickness = 1000 ft (3)

sine (dip angle) = SINX = -0.0129 (4)

hydraulic conductivity = K = 50 ft/da (5)

porosity = $\emptyset$ = 0.3 (6)

rock density = ρ_S = 170 lb/ft^3 (7)

compressibility of water = $c_w = 3.2 \times 10^{-6}$ psi^{-1} (8)

compressibility of rock = $c_r = 3.0 \times 10^{-6}$ psi^{-1} (9)

Assuming the boundary pressures to be

$$p(x=0) = p(x=L) = 0 \qquad (10)$$

corresponding to a saturated phreatic surface at both recharge and discharge ends, the pressure profile at steady-state may be determined. The final solution is, of course, trivial. However, familiarity with both input and output is of concern here. The input data listing (Appendix 1) should be compared with both the computer output of input data and with the input data description in the SWIFT user's guide. Also, each table of calculated initial data should be verified for accuracy. Note especially the following: (1) the pressure conditions in the aquifer-influence functions are given in the R1-28-2 cards as P1 = $\pm$2.8 psi. Why? (2) Transmissibilities are printed in units of ft^3 cp/psi.da. (3) Time-step summaries are discussed in the documentation of the SWIP code,[1] (Part II, pp. 4-19). (4) The final values of the calculated aquifer influx rates should be verified for accuracy.

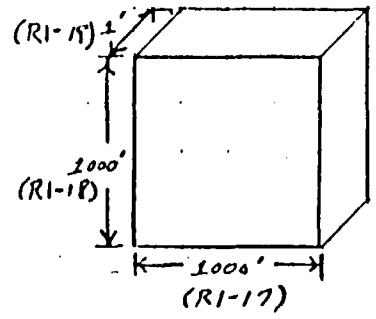
1.2 DISCUSSION

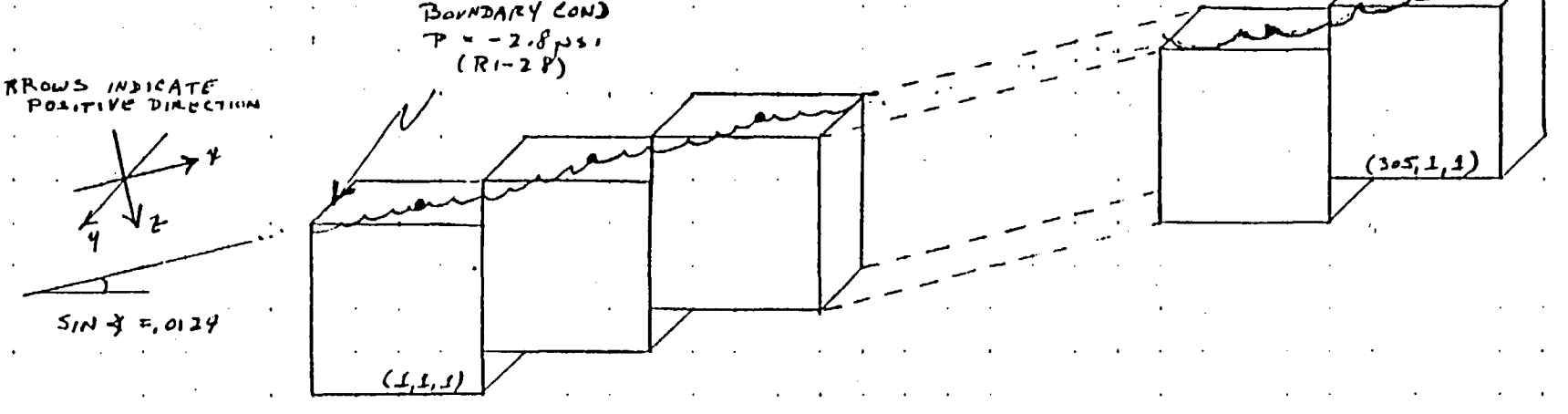
In this first problem, close attention should be given to the input for the problem and the calculation of parameters found in the program output. Below is a discussion of how the program interprets the input physical geometry parameters. Following that are the bases for other program output which are not readily understandable.

Figure 1 relates the code's approximation of the problem to a physical situation. One should particularly note: (1) the locations of the boundary conditions which are applied to the edges of the "aquifer influence blocks" specifically blocks # 1 and 305, (2) the locations of the printed values of the initial condition in the system (time=0) and of the output values printed at time greater than 0; these are denoted by '•', (3) the orientation of the input angle with the horizontal, whose sine was input as -0.0129, (4) the initial conditions in the system, i.e., P=0 (guage pressure) at elevation -6420.2 ft.; these conditions were input as variables PINIT and HINIT respectively and are denoted by the dashed line, and (5) the steady state conditions reached by the code, this is denoted by the wavy line.

Some other program output may be explained as follows:
"REFERENCE WATER INTERNAL ENERGY...UWO" (ref. subroutine "READ1")

FIGURE 1 - ILLUSTRATION OF PROBLEM 1





INDICATE POINTS AT WHICH OUTPUT VALUES ARE CALCULATED

From thermodynamics, the internal energy (UWO) = H-pv where p = PINIT and v = 1/(fluid density). The program uses this relationship and references its own internal enthalpy tables for values of H. For this problem, referring to standard enthalpy tables, the saturated liquid enthalpy, H, at the reference temperature, TO, is 36.04 Btu/lbm. The program calculates a value of 36.58 Btu/lbm. According to INTERA personnel, this 1.5 percent difference from the table value can be attributed to a difference in numerical interpolation. The density is calculated at TO and PINIT based on an interpolation from the input density at the "reference pressure for fluid density," BWR, and "reference temperature for fluid density," TBWR.

For other temperatures (T), the internal energy is calculated from the reference energy as UWO + c_p (T-TO), where c_p, the specific heat, of the fluid is also input.

"ELEVATIONS FEET" TABLE (ref. subroutine "READ1")

These are the elevations at the top centers of each of the grid blocks. They are calculated from the problem geometry by the use of the depth of grid block (1,1,1), the sines of the grid dip angles with the axes, and the dimensions of each grid block. All of these variables are input. The sign convention is elevations above HDATUM are negative and below HDATUM are positive.

"INITIAL AVERAGE PRESSURE," "AVERAGE PRESS" (ref. subroutines "PRINT1" and PRINT2")

This is the average pressure at HDATUM. Thus, it will be greater than any grid block pressure if HDATUM lies below the grid network.

"INITIAL PRESSURE AT ELEVATION H(PSI)" TABLE (ref. subroutine "INIT")

This table provides water pressure based on the elevation difference between HINIT and the elevations given in the "ELEVATIONS FEET" table. In the calculation, an average density (BWO) between HINIT and the grid block elevation is used. Thus, the pressure at each elevation, P(H), is calculated as:

$$P(H) = PINIT - BWO * (HINIT-H)$$

where BWO = BWRN/(1.0 + CW* (PBWR-PINIT) + CTW*(TBWR-TO)) and all variables on the right side of the equation are input.

"INITIAL WATER IN PLACE," "TOTAL IN PLACE, FLUID (LBM)" (ref. subroutine "PRINT1")

Calculates volume and mass of fluid in area being modeled from the geometry and the input porosity (ϕ_e); saturated conditions are assumed. Thus, for this problem, the total water in the system is =

(# of grid blocks) (ϕ_e) (Vol. per block) ( )

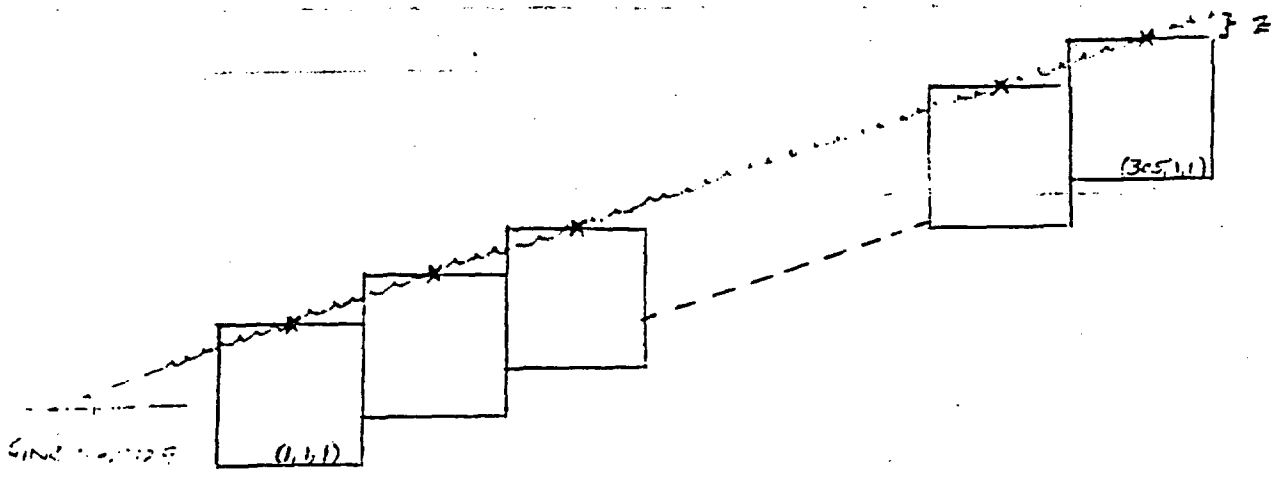
= (305) (.3) (1000x1000x1 ft^3) (62.4 lbm/ft^3)

= 5.7×10^9 lbm.

1.3 INTERPRETATION

As mentioned in Section 1.1, boundary conditions are applied at the aquifer influence blocks by the input of a constant value of the dependent variable(s) (only pressure was used in this problem). Initial conditions specify P=0 at the depth of -6420.2 feet which in Figure 1 coincides with the top of grid block 305. Thus, initially other grid blocks are under the water pressure indicated by the "INITIAL PRESSURE AT ELEVATION H (PSI)" Table.

The input boundary pressures were calculated by hand to induce the code output pressure to equal zero for all grid blocks, i.e., once steady state had been reached the water table would run through the top centers of the blocks in Figure 1. To do this, consider the following diagram:



Remembering that the points 'x' represent the average pressure in the block, we see that, for block 305, the application of a positive pressure on the top right corner to simulate the weight of water at that point, will be combined with the pressure on the left top corner to produce the printed pressure at the block center. It will be seen in problem 2 that "negative" pressures occur at elevations above the P=0 elevation. In this case, the negative pressure at the left top corner of block 305 just balances the input boundary condition to produce P=0 at the block center.

The numerical value of the boundary pressure for block 305 is determined from the head of water at the right boundary. From the geometry, z = 6.468 ft. Therefore, the appropriate pressure = (6.468 ft.) (62.4 $lb/ft^3/144\ in^2/ft^2$) = 2.80 psi. Similarly, the boundary pressure at block 1 was calculated. Water flow is into block 305 and out of block 1. This can be seen by the "AQUIFER INFLUX RATES" table. For this table, a negative sign indicates flow out of the aquifer influence block, a positive sign indicates flow into the block (N.B. This differs from the sign convention used for well flow, as will be seen in problem 2). Until steady state is reached, the water flow out of block 1 is greater than that into block 305 because of additional flow induced by the ΔP between block 1 center (originally 1704. psi) and the boundary condition applied at the edge of block 1 (-2.8 psi). However, by 10,000 days, the system has

reached steady state, as indicated by the "AQUIFER INFLUX RATES" Table. From the "1-D AQUIFER PROFILES" Tables, which print values at the top centers of the grid blocks, we see that the water table (P=0) now runs through the top surfaces of each grid block, as shown in Figure 1. By this time, flow through the system has equilibrated at 4.033×10^4 lbm/day.

It should also be noted that, transmissibilities for water flow are in units of (ft^3-cp/psi-d) because they are used in the model to represent water flux across block edges. Therefore, it is a parameter developed from the water flux across the block edge divided by the distance between two block centers, taking into account the density and viscosity of the resident fluid and the hydraulic conductivity of the material. Specifically (see page 52 of NUREG/CR-0424), the transmissibility (T) is calculated as

$$T = K(ft/d) \times \frac{\mu_o(cp)}{\rho_0(lb/ft^3)} \times \frac{A(ft^2)}{\Delta x\ (ft)} \times 143.8\ \left(\frac{lb}{psi\text{-}ft^2}\right)$$

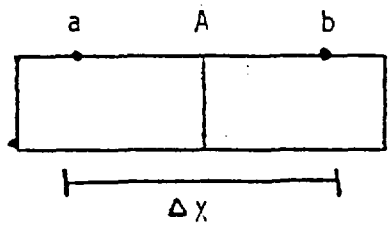
Time step summaries (described on page 4.18 - 4.22 in part II of the SWIP document) were as follows:

Time Step	Real Time (days)
1	1.00 E-05
6	10.0
11	25.75
16	68.08
21	181.4
26	590.3
31	3533
34	9999
35	10000

These time-step summary printouts were determined by the input parameters of cards R2-12, and R2-13 where TCHG, DT AND IO1 are specified. TCHG identifies times at which new data is read. Initially, this is at 10^{-5} days. To go from time = 0 to TCHG, the single time step, DT, was specified 10^{-5} days. Following the first time step, each subsequent printout was at the fifth additional time step (i.e., #6, #11, #16, etc.) according to the value of 5 for parameter IO1 until 9999 days are reached. Then at 10,000 days, a final printout is specified.

1.4 ADDITIONAL COMMENTS

1. To understand how the values in the table entitled "X-DIRECTION TRANSMISSIBILITY" were calculated, the figure below is helpful:



The code solves for the transmissibility across block edges by using the average values of K, μ_o, and ρ_o between two adjacent blocks. Specifically, to calculate the transmissibility across edge A, the averaged parameter from points a and b are used. However, for block 1, it was necessary for the code to set the transmissibility equal to zero at that edge because there was no previous block to average values with.

The calculation of the transmissibility across all other edges is verified by the following:

$$T = 50 \frac{ft}{d} \times \frac{1.0cp}{62.4\ lb/ft^3} \times \frac{1000\ ft^2}{1000\ ft} \times 143.8 \frac{lb}{psi\text{-}ft^2} = 115.3 \frac{ft^2}{d}$$

2. When the printout lists the input values of card R1-20 as x, y, and z direction transmissivities, this is incorrect. they are really hydraulic conductivities.

2.0 PROBLEM 2

2.1 1-D FLOW WITH "WELL" BOUNDARY CONDITION

Here the application of both flux and pressure boundary conditions is illustrated. This is done by using the data cards R2-4 through R2-7. Although the SWIFT documentation describes these cards as "well" data, the injection or production process to which they refer may not have any resemblance to a well, per se. The following two problems illustrate how wells are used to simulate both recharge and discharge.

Subcase 2.1. The physical system is defined by Eqs. (1)-(9) in Section 1.1. Figure 1 also depicts the geometry for this problem. Boundary conditions are a constant recharge flux of

$$q(x=L) = -600 \text{ ft}^3/\text{da} \qquad \text{(at block \#305)} \qquad (11)$$

and a discharge pressure

$$p(x=0) = 0 \qquad \text{(at block \#1)} \qquad (12)$$

For this demonstration it is assumed that recharge results from a rainfall rate of 2 ft/yr distributed over 140,000 ft^2 with 78% of the total discharging through the middle sandstone aquifer. It is desired to determine the pressure profile at steady state.

Both boundary conditions are simulated by means of injection and production wells. The injection well is the easiest to understand. Its specification option, IINDW1 = 1, causes the specified injection rate of -600 ft^3/da to be maintained regardless of conditions

within the aquifer. The production well is more of a challenge. There, a high specified flow rate, $Q=10^{10}$ ft^3/da, in conjunction with a specification option IINDW1 = -3 forces the well to go to pressure limitation BHP = 0. This circumstance then yields the desired pressure boundary condition. The descriptions of well characterization given in both the SWIFT document (pp. 64-65) and in the SWIP document (Part I, pp. B.1-B.4)[1] should be carefully reviewed. Also, one should understand the well summaries of the computer output. They are described in the SWIP documentation (Part II, p. 4.21-4.22).

Subcase 2.2. In the previous example, the presence of an unsaturated zone at the top of the aquifer was indicated by the presence of negative pressures. Thus, the aquifer could transmit the full 600 ft^3/da with no surface runoff from the recharge regions. In this case conductivity is reduced, i.e.,

$$K = 25 \text{ ft/da} \tag{13}$$

This means, as the calculation will show, that the system is not sufficiently conductive to transmit the entire 600 ft^3/da and that some runoff must occur.

The physically appropriate boundary condition is given by the following inequalitites;

$$q(x=L) \geq -600 \text{ ft}^3/\text{da} \tag{14}$$

and

$$p(x=L) \leq 0 \tag{15}$$

These conditions are imposed during a specific time step by choosing one of the two possible equalities. Equations (14) and (15) are applied in this problem in the following manner. The full recharge rate of 600 ft^3/da is used for the first 160 da. At this point, it is obvious that the pressure relation of Eq. (15) will soon be violated, and therefore the specification option is changed to IINDW1=-3, which imposes both Eq. (14) and Eq. (15). Thus, when the calculated "bottom-hole" pressure exceeds the specified "bottom-hole" pressure (BHP=0), the latter is applied as a boundary condition. Actually, the specification option IINDW1=-3 could have been used throughout this simulation; however, convergence would have been quite slow.

The necessary input data are listed in Appendix 2. In the resulting output, however, note that the steady-state grid-block pressure in block 305 is p = -5.59 psi, i.e., $p \neq 0$. Why? Hint: examine the well index, the achieved flow rate and the grid-block-to-well pressure drop to see if they are consistent.

2.2 DISCUSSION

The program output should be studied particularly for the indication of unsaturated flow and the modeling of the "wells." Since the version of the program with which these problems were run is designed to treat only saturated flow, it is important when interpreting results to be able to recognize when unsaturated conditions may have been inadvertantly included in the problem. The use of "wells" can be important in the modeling of such features as unsealed boreholes or permeable fractures and for monitoring flow at a particular grid block.

Initial conditions were set up with P=0 at -4500.0 feet (see card R1-16). Since P=0 indicates the pressure at the water table surface, we could conjecture that, in reality, below this level, saturated conditions exist and above this level, unsaturated conditions exist. In terms of the grid block network, -4500.0 feet lies somewhere between the centers of blocks 156 and 157, as can be seen from the "ELEVATIONS FEET" Table. Referring to the "INITIAL PRESSURE AT ELEVATION H (PSI)" Table, we note that the pressures in grid block 157 to 305, which lie above -4500.0 feet, are negative. Negative pressures in nature are found in rock or soil above the water-table, or induced by man through groundwater pumping. Reference to the tables entitled "1-D Aquifer Profiles" show the distribution of the negative and positive pressures. A further indication that the program treats only saturated conditions is the calculation for "INITIAL WATER IN PLACE" and the mass of fluid in place at a given

time step, "TOTAL IN PLACE." Even though one can logically deduce that unsaturated conditions exist in some or all of the grid blocks at varying times, saturated flow is assumed and the in place fluid is calculated as described in the discussion of problem 1 to be 5.7×10^9 lbm.

In problem 2, boundary conditions are imposed by specifying boundary flows instead of boundary pressures as was done in problem 1. The specification of boundary flows is done by use of wells. Well #1 located at block 305 is an injection well with a flow of 600 ft^3/day. For this well, the "well specification option," IINDW1, is specified as 1 which forces a flow of 600 ft^3/day into the well. By contrast, a production flow of 10^{10} ft^3/day is input for well #2 located at block 1 but a well specification option of -3 is chosen. This option allows a production well flow rate based either on the specified flow or the difference in pressure between the well bottom (BHP) and the grid block center, whichever is less. The parameter WI is input as a measure of the potential flow between these two points. The parameter WI can be interpreted as a transmissibility. For block 1 WI is 1000 ft^2/day, and for block 305 WI is 25 ft^2/day. Thus, as an example, at time 10^{-5} days, the flow from well #2 will be the lesser of 6.24×10^{11} lb/day (from the specified 10^{10} ft^3/day) or the quantity $WI\Delta P$ = (1000 ft^2/day) (861.58-.0001 lb/in^2)(144 in^2/ft^2) = 1.24×10^8 lb/day. As indicated by the output, the lesser flow is used.

2.3.1 INTERPRETATION (Subcase 2.1)

Initial conditions specify a partially unsaturated aquifer (area above -4500.0 feet) with an injection well having a constant flow of 600 ft^3/day at the upgradient end and a production well having a variable flow with a maximum rate of 10^{10} ft^3/day at the down-gradient end. The wells could simulate recharge and discharge or other physical conditions, as appropriate.

Because the initial flow from the production well is greater than that specified for the injection well, one might expect that the aquifer eventually would be drained to the point where the water table (P=0) surface would lie at the bottom of the production well (well #2). However, the flow from well #2 will be constantly decreasing flow due to the constantly decreasing pressure difference (of which the well #2 flow is a function) between block #1 center and the bottom of well #2 as the aquifer is drained. This decreasing flow would continue until the time is reached when well #2 produces exactly what is injected via well #1. These results can be seen by reviewing the "1-D AQUIFER PROFILES" tables and the well flow rates at varying time steps.

2.3.2 INTERPRETATION (Subcase 2.2)

In subcase 2.1, the physical parameters in the aquifer were specified such that the entire injection well flow was transmitted through the aquifer to the production well. Further, drawdown of the original partially saturated aquifer occurred resulting in what could be interpreted as a completely unsaturated region. The existence of this unsaturated region was made apparent by the presence of negative grid block pressures.

In subcase 2.2, the hydraulic conductivity of the aquifer was reduced to produce a runoff situation at well #1. From time = 0 to 160 days IINDW1 was set at 1 for well #1. This had the effect of forcing 600 ft^3/day into the aquifer and recharging it (because of the lower conductivity) until the aquifer became nearly saturated causing puddling to occur at the well. In other words, P(x=L) was approaching a positive value which would exceed the boundary conditions. At 160 days, the well specification option for well #1 was changed to -3 to allow either the specified 600 ft^3/day flow or a flow based on the ΔP between the grid block center and the well bottom. By reviewing the items "GRID BLOCK PRESS" and "FLWG BHP PSIA" printed after selected time steps, one can see that the ΔP will be the determining factor for the flow rate after about 160 days. For example, by 5000 days, WI P = (25 ft^2/day) x (5.59 lb/in^2)(144 in^2/ft^2) = 2.01×10^4 lb/day; which is less than the specified flow. As noted in Section 2.1, IINDW1 could

have been specified as -3 from time = 0, but convergence would have been slow. Since ΔP between the block center and well bottom was not controlling until about 160 days, IINOW1 was specified as 1 until then.

2.4 ADDITIONAL COMMENTS

1. The following can be considered as general guidance for the use of the parameter IINDW1:

   i) If natural recharge is to be simulated, the ±3 option should be selected over the ±1 option since pressure may be the controlling influence,

   ii) The ±1 option should be reserved for simulation of actual pumping and/or injection wells,

   iii) The ±2 option should be used for passive dewatering or recharging (man-related) systems?

2. When the printout lists the input values of card R1-20 as x, y and z direction transmissivities, this is incorrect. They are really hydraulic conductivities.

3. For an explanation of how well flow is calculated from the well index, WI, refer to "Lecture Notes for the Geosphere Transport Simulator SWIFT," Workshop for the Geosphere Transport Simulator SWIFT, Intera Environmental Consultants, Inc., June 9-13, 1980.

3.0 PROBLEM-3

3.1 1-D TRANSPORT OF A RADIONUCLIDE

In this group of simulations, a radionuclide is introduced such that the pressure equation and the radionuclide equations are solved simultaneously. The object is to exhibit the effects of hydrodynamic dispersion and radioactive decay and to show the necessity for considering two important numerical phenomena, namely numerical dispersion and overshoot. Failing to consider these two artifacts of numerical results can invalidate results and conclusions drawn therefrom.

The system characterization here is similar to that used previously with the following changes: The length is reduced to

$$L = 5000 \text{ ft} \tag{16}$$

and the flow is maintained at

$$q = 646.3 \text{ ft}^3/\text{da} \tag{17}$$

In addition, a radionuclide is introduced through an injection-well boundary condition with an arbitrarily chosen concentration of

$$C(x=L) = C_o = 1 \text{ ppm} = 10^{-6} \tag{18}$$

Transport of the radionuclide is characterized by three parameters, which nominally have the values

$$\text{dispersivity} = \quad = 100 \text{ ft} \tag{19}$$

$$\text{half-life} = T_{\frac{1}{2}} = 0 \tag{20}$$

$$\text{distribution coefficient} = k_d = 0 \tag{21}$$

The time of simulation is chosen to be

$$T = 1161 \text{ days} \tag{22}$$

in which time the radionuclide front should travel 2500 feet.

Subcase 3.1. This example is intended to exemplify dispersion phenomena. To do this, we apply the centered-in-space and backward-in-time criteria (see SWIP document, Part I, p. 5.5)[1] for the space increment Δx and the time increment Δt:

$$\Delta x = 100 \text{ ft} \leq 2\alpha \tag{23}$$

and

$$\Delta t \leq 10 \text{ da} << 2\alpha/V \tag{24}$$

where $V = 2.15$ ft/da is the interstitial velocity.

The results obtained should be compared with the approximate analytic solution [see Coats and Smith, 1964]

$$C/C_o = \frac{1}{2} \operatorname{erfc}\left[\frac{1}{2\sqrt{Dt}}(L-x-Vt)\right] \tag{25}$$

where the dispersion is

$$D = \alpha V, \; V = \text{interstitial velocity} \tag{26}$$

This may be done by looking at the standard-deviation points at time T, which should have the values

$$C/C_o = 0.16 \text{ at } x = x_o - \sqrt{2DT} \tag{27}$$

and

$$C/C_0 = 0.84 \text{ at } x-x_0 + \sqrt{2DT} \tag{28}$$

where x_0 is defined by

$$C/C_0 = 0.50 \text{ at } x=x_0 \tag{29}$$

Subcase 3.2. The object of this case is to demonstrate numerical disperison. Here we take

$$\Delta t = 100 \text{ da} \tag{30}$$

with all other parameters remaining the same as in Subcase 3.1. Calculated concentrations should be interpreted by Eqs. (27) and (28), this time with both numerical and physical dispersion, i.e.

$$D = (\alpha+\alpha_N)V \tag{31}$$

where the numerical dispersivity is

$$\alpha_N = V\Delta t/2 \tag{32}$$

Quantity V is again the interstitial velocity rather than the Darcy flux. Note that the width of the front is increased by over 40% and that the resulting prediction of concentrations $C/C_0 > 1/2$ is nonconservative.

Subcase 3.3. The desire in this case is to exhibit numerical overshoot. Consequently, the physical dispersion is reduced to

$$\alpha = 1.0 \text{ ft} \tag{33}$$

in violation of the centered-in-space restriction of Eq. (23). All other parameters are set to their values of Subcase 3.1. The resulting concentration profile at time T = 1161 da reveals the oscillatory behavior characteristic of the numerical overshoot phenomenon.

Subcase 3.4. In this, the last subcase of Problem 3, the effect of radioactive decay upon the concentration profile is exhibited. All parameters are reset to their values in Subcase 3.1, with the exception of half-life, which is arbitrarily set to be the same as the simulation time T:

$$T_{1/2} = 1161 \text{ da} = 3.18 \text{ yr} \tag{34}$$

The output may be compared with the approximate solution

$$C/C_o \approx \frac{1}{2} \exp\left[-\frac{x}{2D}(W-V)\right] \operatorname{erfc}\left[\frac{1}{2\sqrt{Dt}}(x-Wt)\right] \tag{35}$$

where the modified interstitial velocity is given by

$$W = \sqrt{V^2 + 4D\lambda} \tag{36}$$

with decay constant

$$= 0.693/T_{\frac{1}{2}} \tag{37}$$

As a rough check, however, one should note that the concentration at 2500 ft here is approximately one half its value in Subcase 3.1.

3.2.1 DISCUSSION (Subcase 3.1)

The purpose of subcase 3.1 is to introduce the dispersion phenomena. Central to this issue is the concept of concentration fronts. A concentration front is a result of a change in concentration either upward or downward. The types of concentration changes of concern to us are pulses and steps. An analogy used to demonstrate the types of concentration changes and concentration fronts is that of water flowing through a pipe supplied by two reservoirs. One reservoir contains clear water and the other reservoir contains water colored by immiscible blue dye (Figure 3.A). Initially, clear water is flowing through the pipe. At time, T, blue water is fed to the pipe and at at later time, T + DT, clear water is again fed to the pipe. This situation results in a pulse of blue water moving down the pipe (Figure 3.B) with a pulse width of (DT)(FLOW VELOCITY). For the step change assume at time, T, the feed is switched to reservoir 2 and not switched back to reservoir 1. This situation would result in replacing the clear water in the pipe with blue water. The interface of the two colors of water is the concentration front (Figure 3.C). Problem three is concerned with a step type concentration change.

The effect of dispersion on a concentration front is to "FUZZ" it up. Instead of having a clear step change, the concentration will change in a smooth continuous manner (see Figure 3.D). The characterization of a concentration front and its movement

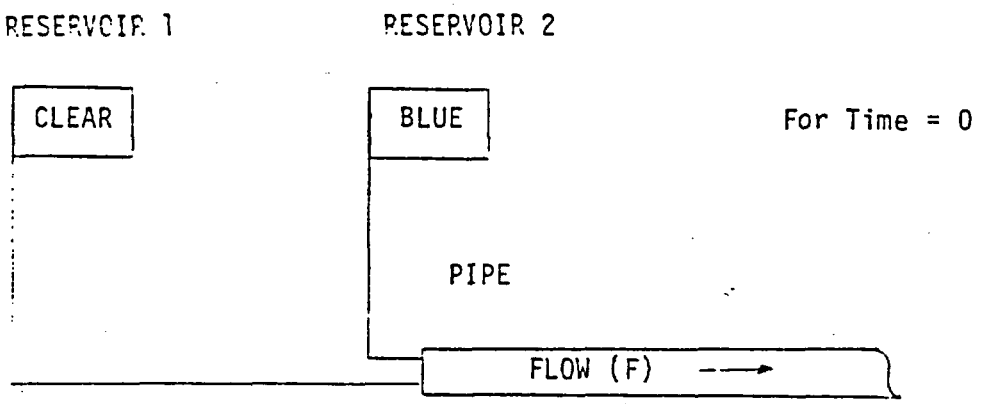


FIGURE 3.A

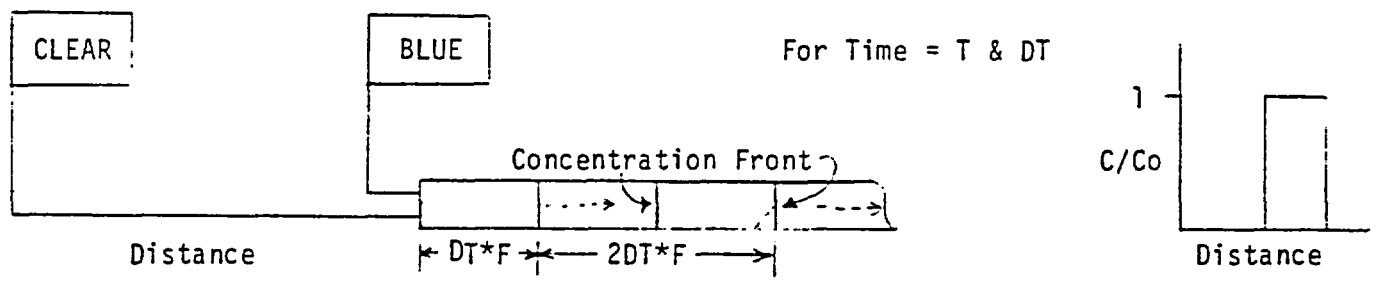


FIGURE 3.B Pulse

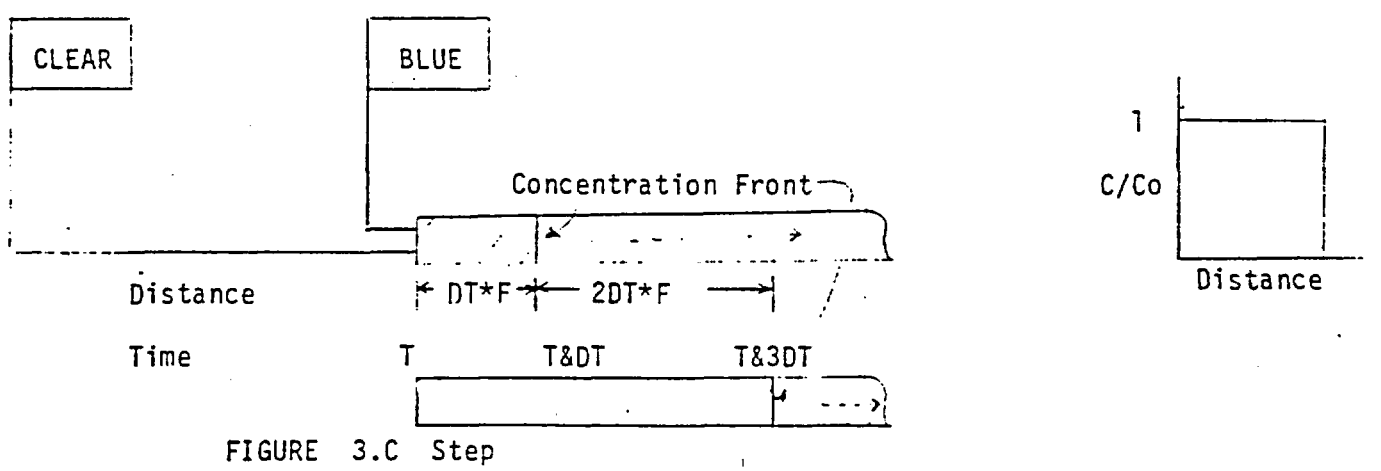


FIGURE 3.C Step

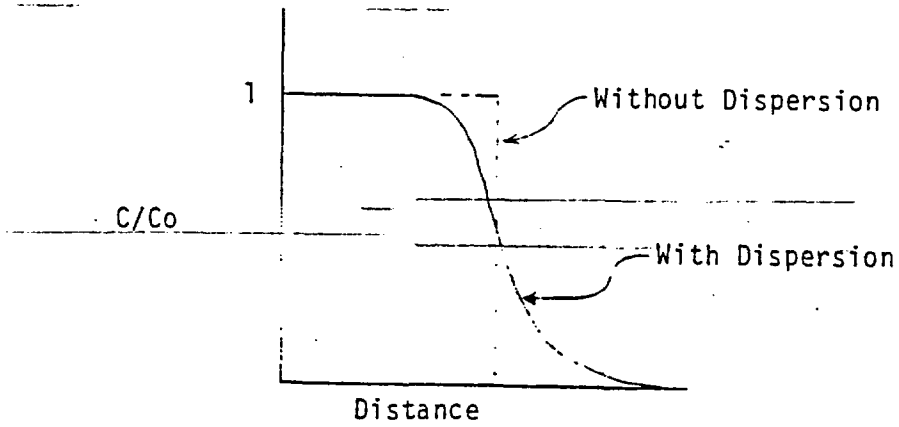
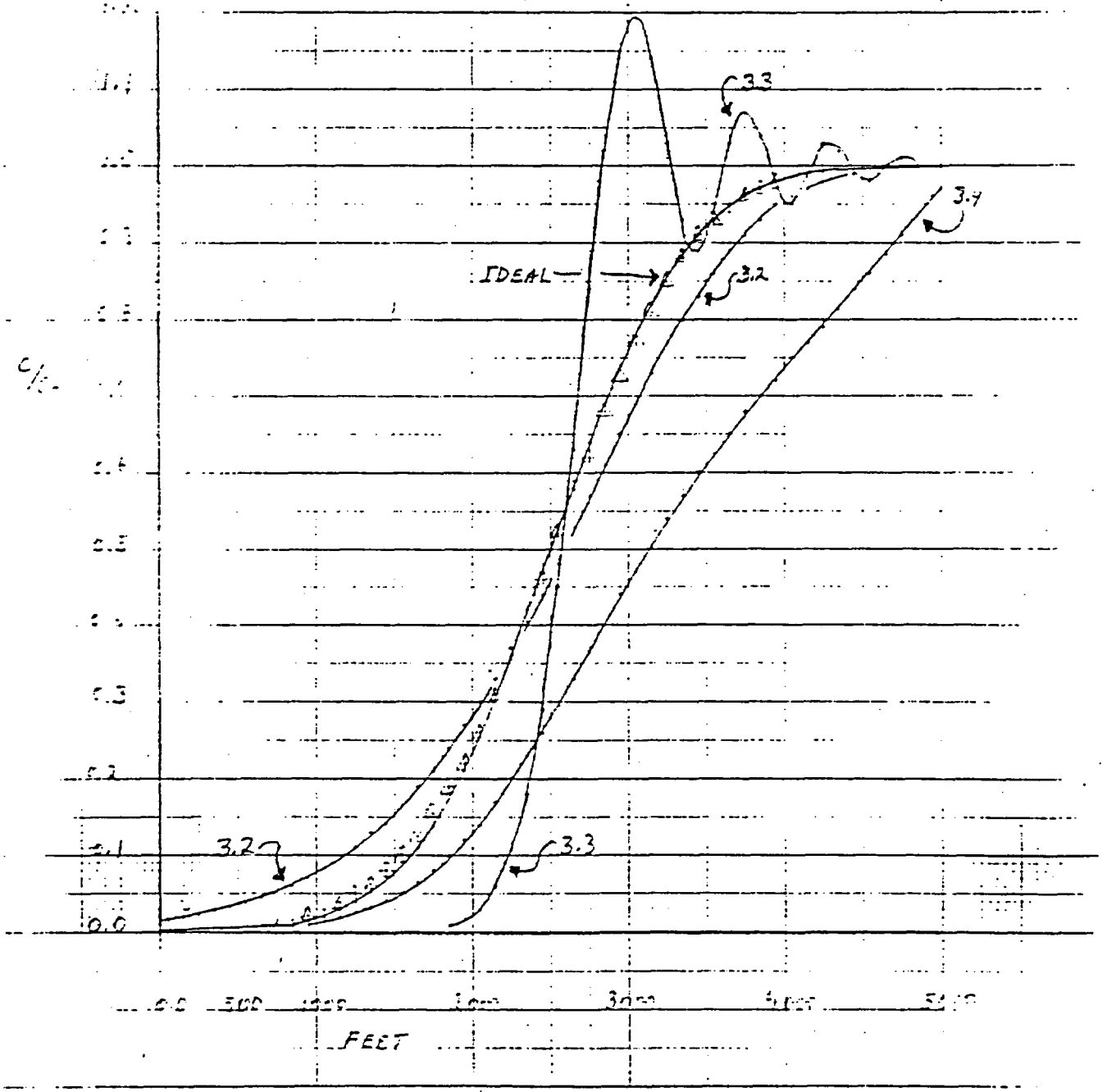


FIGURE 3.D

becomes more difficult when dispersion is taken into account. The ratio of concentration at a position (C) to the concentration of the input (C_0) is used to help characterize a concentration front. A measure of dispersion is the distance between two values of C/C_0. A measure of position of the front is usually given by the position of a selected C/C_0 value. The leading and trailing edges of the front are disregarded in our case and only the linear portion of the front is used. The C/C_0 values chosen to measure dispersion are .16 and .84 and the position value used is $C/C_0 = 0.5$. The analytical solution indicates that $C/C_0 = 0.16$ is at x = 1800 feet, $C/C_0 = .84$ is at x = 3200 feet and $C/C_0 = .5$ is at x = 2500 feet. Thus, the dispersion is 3200 - 1800 or 1400 feet and the front location is 2500 feet. The computed results of subcase 3.1 indicate that $C/C_0 = .16$ is at x = 1820 feet, $C/C_0 = .84$ is at x = 3280 feet, and $C/C_0 = .5$ is at x = 2519 feet. Thus, the dispersion is 3280 - 1820 or 1460 feet and the front is located at 2570 feet. The error between the analytical solution and subcase 3.1 is small (i.e., dispersion = 4.3 percent, position = 2.8 percent). The dispersion and position errors lead to maximum concentration errors of approximately 2.2 percent. The errors were conservative for 0 to 2050 feet and 3750 to 5000 feet and non-conservative for 2150 to 3650 feet (see Figure 3.E).

FIGURE 3.E

CONCENTRATION RATIO V.S. DISTANCE



For subcase 3.1, the DARCY VELOCITY = -0.646 ft/da (since q = -646.3 ft^3/da divided by cross section AREA = 1000 ft x 1 ft). The interstitial velocity is -0.646 ft/da divided by effective porosity of 0.30 leads to -2.15 ft/day. The dispersion coefficient is dispersivity (α = 100 ft) x interstitial velocity (2.15 ft/da) and leads to 215 ft^2/da. The time step was 10 days (see card R2-12).

3.2.2 DISCUSSION (Subcase 3.2)

Since the objective of subcase 3.2 is to show the effects of numerical dispersion, the reader may wish to review Section 3 and Section 5.2.1 of the SWIP document.[1] The Taylor series expansion truncation produces a numerical error which is identical in form to physical dispersion. For subcase 3.2 the physical dispersion is $\alpha\overline{V}$, where α = dispersivity constant and $\overline{V}$ = interstitial velocity and the numerical dispersion is $(DT/2)V^2$ where DT is the time step size. Thus, the total dispersion expected is $(\alpha + \overline{V}DT/2)\overline{V}$. For subcase 3.1, $\overline{V}DT/2$ maximum is 2.15 ft/da (10 da/2) or 10.75 feet and α is 100 feet which results in a 3.5 percent error in dispersion. For subcase 3.2, the ΔT is specified as 100 days, thus the numerical dispersivity is constant throughout the calculation (except for the initial transient V) at (2.15)(100)/2 or 107.5 feet. The physical dispersivity and the numerical dispersivity are approximately equal for subcase 3.2. Thus, the error for subcase 3.2 is expected to be large. The computed results of subcase 3.2 indicate that C/C_0 = .16 is at 1580 feet, C/C_0 = .84 is at 3520 feet and C/C_0 = .5 is at 2640 feet. The dispersion is 3520 - 1580 or 1940 feet and the front location is at 2640 feet. Comparing these results with the analytical results gives a dispersion error of 39 percent and a position error of 6 percent. The dispersion errors and the position error lead to a maximum concentration error of approximately 12 percent. Thus, a large error in choice of the time step (i.e., 100 vs. 10) produces a relatively small error ($<$12 percent) in concentrations. The errors in concentration are now conservative from 2350 feet to

5000 feet (Figure 3.E). The reader should note that the pressure profile, the Darcy velocity and the total flow are correct (check with subcase 3.1) for subcase 3.2 (i.e., only dispersion is affected).

3.2.3 DISCUSSION (Subcase 3.3)

Since the object of this problem is to demonstrate numerical overshoot (i.e., instability due to violations in finite-difference grid spacing), the reader should review Section 3 and 5.2.2 of the SWIP document[1] (Note: E in SWIP document = $U\alpha$). To avoid oscillations, the criteria $DX/2 < \alpha$ should be met. For subcase 3.3, Δx = 100 feet and α is set at 1.0 feet (see R1-2 card), thus (100)/2 or 50 feet is not smaller than 1.0 feet and oscillations will occur. The output of subcase 3.3 shows that oscillations do occur (Figure 3.E) and that the concentration information is of no use. The reader should note that only concentrations were affected for this problem; the pressure profiles, the Darcy velocities and the total flow are unaffected.

3.2.4 DISCUSSION (Subcase 3.4)

The input values for this problem are identical to those of subcase 3.1 except that the nuclide half life is set to 1161 days. Thus, in 1161 days (the time of the run) 1/2 of the initial inventory has decayed away. If no dispersion were taking place, the concentration front would have moved to 2500 feet in 1161 days and would be 1/2 the initial concentration. The effect of dispersion is essential to reduce the concentration at the point where the front would have been if no dispersion were present. Thus, to use the 3.1 value at 2500 feet to estimate the 3.2 value at 2500 feet multiply the 3.1 value by 0.5. A similar proceeding could be used to estimate all of the 3.2 values from the 3.1 values. The fact to note here is that for a given period of time, the concentration profile will be most affected by the distance from the radioactive source and the radionuclide decay time. Figure 3.E shows the effect of decay on the concentration front. Not all concentration ratios will be reduced equally but range from 1 to 0.25 based upon the time the radionuclide has been in the system. For distances from 0 to 2500 ft from the radionuclide the concentration mass ratio, C/C_o, varies from 1 at x = 0 to slightly less than 0.5 times the 3.1 value at x = 2500 ft.

For distances from 2500 ft to 5000 ft from the radionuclide source the value range from slightly less than 0.5 time the

value at x = 2500 to slightly more than 0.25 at x = 5000 ft and may be approximated by the function C/C_o = (3.1 value)(exp $[-\frac{x}{2D}(W-V)]$)

3.3 ADDITIONAL COMMENTS

1. At time equal to 1161 days, in Problem 3.1, the total well production is 4.6818E+07 and the total well injection is 4.6822E+07. This difference implies that 4000 lbs of fluid have been stored in the aquifer. This storage is apparently due to differences in rock and water compressibilities, but we were unable to approximate this number by hand. Conversations with INTERA personnel indicate that this difference may simply be due to numerical error. While this difference is small in comparison with the magnitude of total flow through the aquifer, an understanding of whether it is due to numerical error or has some physical basis may prove important to a user for other applications.

4.0 PROBLEM 4

4.1 2-D FLOW WITHIN NRC REFERENCE SITE

This example is intended to demonstrate the simulation of two-dimensional steady-state ground water movement within the hypothetical NRC reference site. By incorporation of the entire flow domain one is able to compute the steady-state pressure distribution in the vicinity of the site. Subsequently, one can then compute the velocity field essential to the simulation of radionuclide transport. This example illustrates the use of heterogeneous block specification, R1-20 cards; zero pore volume block modification, R1-26 cards; and two-dimensional contour-printer maps, R2-14, 15 cards.

The geology of the site is shown in vertical cross section in Figure 4.1. The valley is underlain by crystalline bedrock which crops out over a narrow width at the ridge crest surrounding the valley. This bedrock is assumed to be impermeable to ground water flow. Above the bedrock a sequence of sedimentary layers form the flow domain of interest. The hydraulic properties are tabulated below. For complete details concerning the inherent assumptions the reader is referred to the interim report describing this NRC project, NUREG-0458.[2]

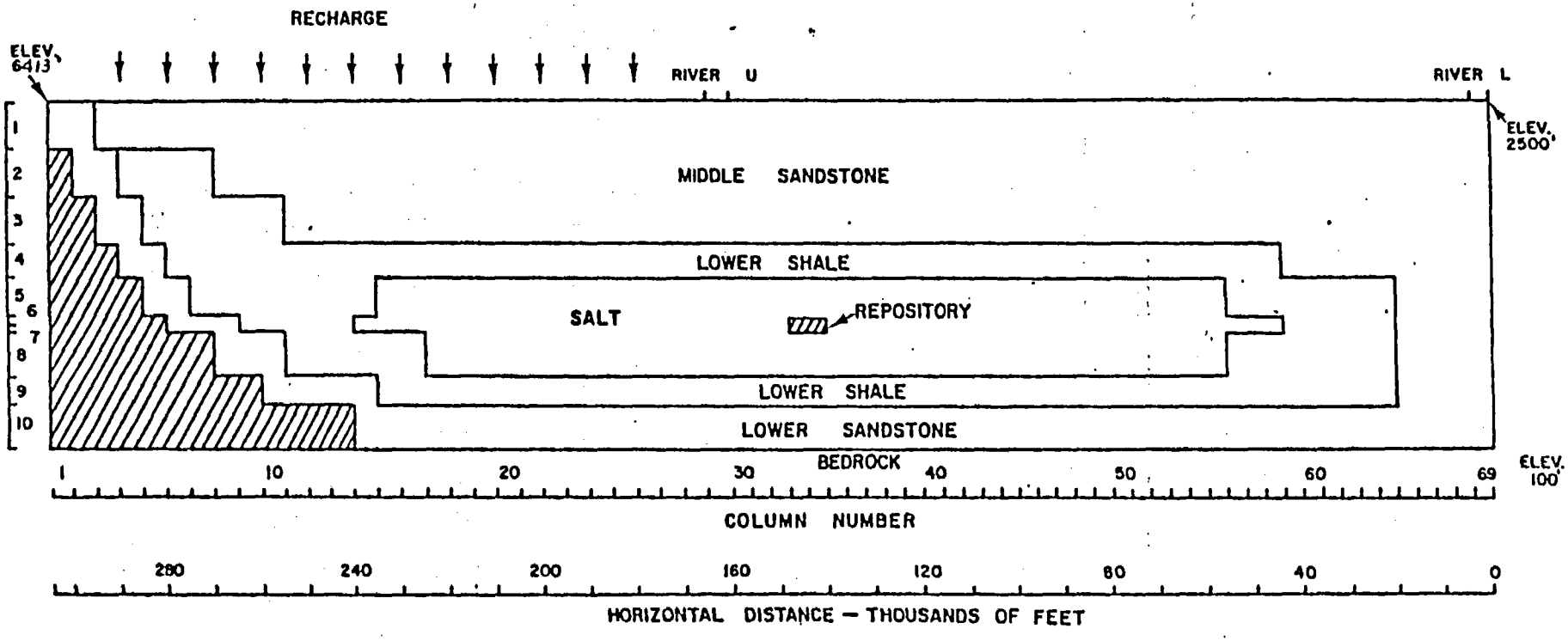


FIGURE 4.1 Radioactive waste repository reference site cross-section.

Aquifer Hydraulic Properties

	Hydraulic Conductivity		Porosity
	Horizontal (ft/day)	Vertical (ft/day)	(fractional)
Middle Sandstone	50.	1.4	0.3
Lower Shale	10^{-2}	10^{-3}	0.3
Salt	10^{-5}	10^{-6}	0.03
Lower Sandstone	40.	7.	0.3

Boundary conditions were applied through a combination of "wells" in an attempt to simulate the natural system. "No flow" boundaries were assumed (1) along the crystalline bedrock interface; (2) along the vertical boundary at River L where flow is assumed to be vertical; and (3) between River U and L to represent a non-leaky aquitard (upper shale). This last assumption is valid for the unperturbed system as computed pressure isopleths were nearly vertical in this area (i.e., no vertical pressure gradient). From the ridge crest to River U, wells were imposed under a flux controlling condition (IINDW1=1). These 18 wells were distributed over the region to impose a steady influx of 24 inch/yr of net precipitation (total precipitation less evapotranspirative losses). At Rivers U and L pressures were controlled at bottom hole pressure = 0. psi, thus allowing all flow to the rivers to be discharged. The proportional flux to each river is dependent upon the geologic strata and the assumed dip angle.

The SWIFT code requires the solution of all blocks within a given rectangular domain. In this example, the crystalline bedrock underlying the lower sandstone in the ridge crest region was assigned zero pore volume. The numerical efficiencies gained in solving the entire set of blocks vastly outweighs the losses in solving for a few additional zero pore-volume blocks. Zero pore assignment is preferred over zero conductivity as additional numerical savings are gained.

The pressure distribution is readily interpreted through the use of contour mapping. For this example it was chosen to plot the pressure at datum (psi) on two separate pages. The 20 contour intervals, defined in the map legend, are computed from the minimum and maximum dependent variable values specified on the R2-15 cards.

In examining the computed printout, one should take note of several points:

1. Was a steady-state continuity achieved? (hint: check mass balance and well summary totals.)

2. What is the magnitude of flow achieved in each river? Are they influent or effluent streams?

3. Where is the approximate location of the predicted "water table?"

4. What is direction and magnitude of ground water flow through the repository zone?

The last question deserves special attention. Let us consider the pressure differential between rows 5 and 8 along column 33. Remembering that the finite-difference approximations are written centered in the x- and y-directions and at the top (z) of each block, the pressure differential through the salt is computed as

P (Row 5, col. 33; upper salt lay - P (Row 9, col. 33; lower shale)

The vertical flow rate per unit areal (x-y) cross section area is computed as

$$q = \frac{K\nabla P}{\nabla z} = \left[\frac{M}{L^2}\right]$$

where ∇z is the thickness of the salt layer. What would be the total flow through a repository of dimensions x = 1000 ft by y = 400 ft during a one-year period? (Watch units! 1 psi = 2.31 ft water pressure).

4.2 DISCUSSION

Problem 4 introduces the use of the code for solving two dimensional problems. In this particular example, the reference repository site developed for the NRC is being modelled. The physical characteristics of the site, the method of depicting impermeable regions and the basis for the well selection were described in Section 4.1. As implied in Section 5.1, this problem is a prelude to Problem 5 in that the boundary conditions for Problem 5, which will model the local region around the depository, are to be determined from the output of this problem.

Like previous problems, problem 4 does not involve the solution of the temperature or inert component conservation equations. Further, no radioactive or "trace" components are considered in this problem. However, the solution of the remaining pressure equation differs from previous solutions in that a "steady state" solution (invoked by setting NCALL = 4) will be used. With the solution technique, the pressure equation is solved once based on the assumption of time invariant boundary conditions. This results in a time invariant pressure distribution and velocity field. This type of output has the advantage of considerable savings in computer time over that required for a transient solution. It is of particular interest in the transport of radionuclides from a repository where the physical system may be expected to be stable for extremely long periods of time. It may also be of use for the solution of systems with zones of low permeability, where the computation times are characteristically

long. The derivation of the steady state solution from the full transient solution can be found in the Intera Environmental Consultants, Inc. (draft) report, describing SWIFT code modifications.[3]

4.3 INTERPRETATION

Boundary conditions were applied with the use of 20 wells; 1 through 18 are injection wells simulating natural recharge, 19 and 20 are production wells located at what can be interpreted as the physical locations of potential system discharge, i.e., Rivers U and L. Wells 1 through 18 have IINDW1 specified as 1 with the corresponding constant input flow rates printed in the "Well Number" vs. "Rate" table. Wells 19 and 20 are variable flow rate wells as allowed by specifying IINDW1 as -3. (The difference in the specification of IINDW1 as 1 or -3 was discussed in Section 2 of this report.)

A "steady state" solution as discussed in Section 4.2, rather than the transient solution used in Problem 1, was implemented for this problem. Of course, for both solution methods, conservation of mass must be conserved. For the "steady state" solution, the output pressure distributions and velocity fields do not vary overtime; for the transient solution, output varies depending on the variation of the boundary conditions with time. However, when Problem 4 was run with the version of the SWIFT code presently in-house, a number of anomalies in the output appeared. Conversations with INTERA personnel revealed that there is an apparent error in the programming of the "steady state" solution method (utilized by setting NCALL = 4) which is being corrected. It is believed that the error affected the predicted velocity fields and flow rates, but that the pressure distribution was accurately depicted.

The symptoms of this program error are noted below to highlight the need for the user to have a good understanding of both the physical problem being modelled and the code being used for that purpose.

1. Mass balance, the ratio of system influx to efflux differed from 1.000; it was .0029.

2. Well 19 showed the injection of a component (1.0000 lb/day) when the number of radioactive components (NCP) was specified as 0.

3. Well 19, specified initially as a production well with a 10^{20} ft^3/day flow limit, became an <u>injection</u> well of time = 10^{-2} days with a flow of .144 lb/day (as indicated by the negative sign).

4. The bottom hole temperatures for wells 19 and 20 changed from the specified $68^{o}F$. These should not have been affected since the conservation of energy equation was not to have been solved when specifying NCALL = 4.

Since the pressure distribution is unaffected by the errors in the program, the "2-D PRESSURE MAP" is still correct, except it depicts the x-z plane and not the x-y plane as indicated. The "MAP LEGEND" printed before the pressure map gives the ranges of pressure (N.B. DATUM pressures are used) associated with each symbol used on the map. These ranges can be either input by the user or determined by the program according to the values input on card R2-15 for parameters

AMAXP and AMINP. When reviewing the pressure maps, it should then be remembered that flow is perpendicular to the pressure contours and from higher pressure to lower pressure.

Finally, to answer the question of vertical flow through a depository of given dimensions ($A = 400000\ ft^2$), it is assumed that the depository is located in column 33. There the ΔP across the salt strata (i.e., from the top of layer 5 to the top of layer 9, measured from DATUM) is 196.9 lb/in^2. Therefore, the flow through the depository over a year is:

$$q = \frac{AK\Delta P}{\Delta z} = (400000\ ft^2)\ \frac{(10^{-6}\ ft/d)(196.9\ lb/in^2)(144\ in^2/ft^2)\ 365\ d/y}{700\ ft}$$

$$= 5.91 \times 10^3\ lbm$$

This flow is in the downward direction according to the pressure gradient.

4.4 ADDITIONAL COMMENTS

1. The 2-D pressure maps give a visual display of the pressure distribution. The general flow direction can also be determined from these maps by assuming it is perpendicular to the pressure contours. Local flow interpretation from the map may be questionable. For example, in the region of Well 20, a discharge well, where flow must proceed vertically upward, the flow direction was not apparent. The map does not cover the area directly under the well, and the grid blocks are large. Further, each symbol used in the mapping represents a range of values. Therefore, some care should be used when using the map to interpret local flow rates as perturbations.

5.0 PROBLEM 5

5.1 2-D NEAR-FIELD TRANSPORT

With knowledge of the steady-state hydraulic potentials at the reference site from the previous example, one is able to extract boundary conditions for more detailed near-field radionuclide transport calculations. In this example, potentials from the previous simulation of the entire flow system are used as prescribed aquifer influence function in the simulation of near-field migration as shown in Figure 5.1.

A region of high permeability extending from the middle to lower sandstone, representative of what might be an undetected bore hole or vertical thrust or fault, was imposed on the system. Simulation of the site similar to Problem 4 provided the potentials on the left and right edge grid blocks. A judicious choice was made such that interference from the boundary conditions on interior fluid flows was minimal.

The waste repository, located in row 6, if filled with low-level radioactive waste. Leaching of the contents was initiated at 10^{-5} days and continued for 3.6×10^{6} days. The initial concentration of waste was 10 lb/cu. ft. An unrestrictive nuclide solubility 10 (mass of solubles/fluid mass) was imposed.

After 10 years one can see the waste being leached, unrestricted by solubility limits and migrating downward towards the lower sandstone. After 100 years the concentration within the repository has further increased.

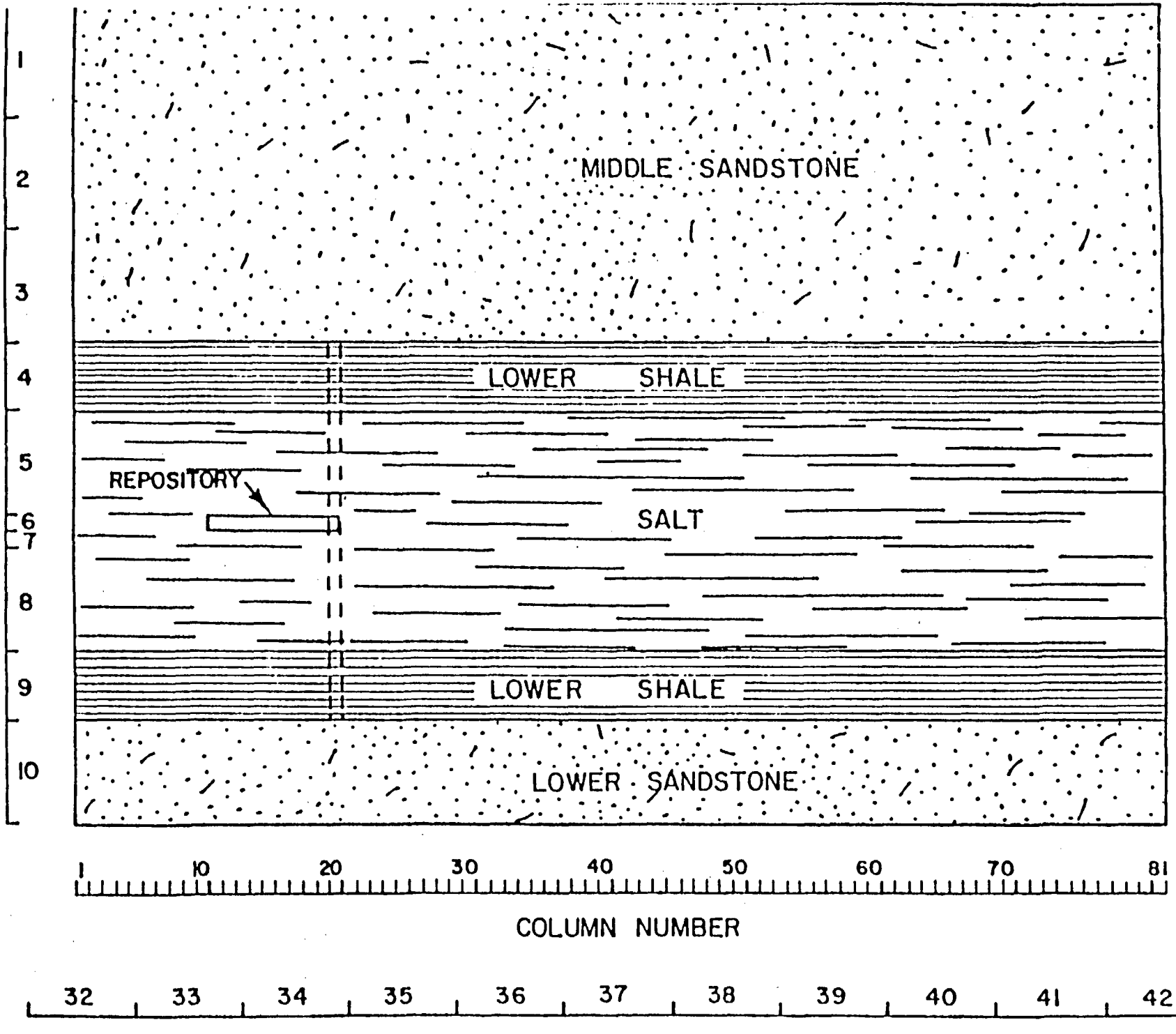


FIGURE 5.1. Radioactive waste repository cross-section

In examining the output there are a multitude of "what if" questions one could ask. What if

1. the distribution coefficients were increased?
2. a shorter half-life radionuclide were introduced?
3. salt-dissolution and solution to the brine equation were performed? Density gradients?
4. more realistic restrictive solubility limits were imposed?
5. liquid waste were someday disposed of by injection into the lower sandstone? (The direction of flow in the shaft could possibly be reversed!)

The list could go on for pages, but of importance is the interpretation of this single scenario. The input should be carefully examined. The stability criteria for centered-in-time and centered-in-space should be examined. ($V_x$max = .75 ft/day; $V_z$max = .02 ft/day). For the case presented the criteria are met.

This example introduces the concepts of multimedia, salt-dissolution and waste-leach as specified on the R1A cards. At present, the rock type specification (R1A-1) controls the (1) distribution coefficients, (2) thermal conductivities, and (3) salt-dissolution coefficient. Salt-dissolution and waste-leach data are entered on cards R1A-2 to R1A-9.

5.2 DISCUSSION

The emphasis in Problem 5 is near field transport of a radionuclide. In Problem 4, the distribution of the influx and efflux of water flow in a large physical system was used to solve the conservation of total mass equation. That solution was represented, in part, by the pressure distribution at each grid block in the system. Problem 5 will be concerned with a smaller part of the system modelled in Problem 4 and, as in Problem 1, aquifer influence blocks will be used as boundary conditions. The values for the pressure at each of the aquifer influence blocks is simply read from the blocks with x coordinates 32 and 42 in Problem 4. There are 10 blocks in the z direction for each of the x coordinates. The 10 block values with the x coordinate of 32 will become the left side boundary for Problem 5; the 10 block values with the x coordinate of 42 will become the right side boundary.

The method of simulating a waste depository should be noted. In general, radionuclides may be introduced to the system via wells as was done in Problem 3 or in specific blocks with the I-1 and I-4 cards.* However, in Problem 5, a third method of inputting radionuclides, which is particularly well suited to simulating a waste depository, is introduced. Use of this method requires inputs (NTIME, NCOMP

*In this problem, an initial radionuclide concentration was put in each block of the system via card I-4. This concentration is indicated early in the printout as "TRACE COMPONENT 1 INITIAL COMP IN PLACE = .939233 E-90 LBM."

and NREPB) in the M-3 card and the R1A series of cards. This method is required if solubility or leaching of radionuclides is to be considered. Account of radionuclide solubility is made in the R1A card series, while radionuclide leaching (and the time until leaching begins) is modelled in the R1A series and the R10-5 card.

The SWIFT code does have the capability to consider salt dissolution due to the water flow in the region, although that was not considered in this problem because it is not expected to occur to a significant extent. However, if it need be modelled, perhaps as a check on predicted flows through a region, the R1A-2 can be utilized. For further information on the salt dissolutioning portion of the SWIFT code, refer to the (draft) INTERA report.[3]

5.3 INTERPRETATION

Of particular interest in Problem 5 is the movement of radionuclides from the depository under the pressure gradient derived from Problem 4. A similar determination would be essential to the placement of an actual waste depository.

In the one-dimensional Problem 3, the phenomenon of dispersion, both physical and numerical, was discussed. The need to understand the effect of numerical dispersion (as a function of solution technique), on the predicted radionuclide concentrations was highlighted. In this problem, the effects of dispersion can be seen in the "2-D Concentration Maps." In those maps, radionuclide concentrations appear upstream of the flow around the depository. However, of more importance in Problem 5 is the actual direction of radionuclide flow. Radionuclide concentrations are quantitatively printed out for each grid block, but the concentration maps show the flow more dramatically. Essentially, they show the radionuclide flow moving toward the lower aquifer through the high permeability region in column 20. The importance of this can be seen from another perspective. That is, when siting a depository, the stable and disrupted conditions of that site must be considered. Under the conditions of this problem, a disrupted condition actually caused radionuclide movement away from the biosphere. Of course, the introduction of radionuclides into the lower aquifer could eventually lead to intrusion into the biosphere, but this should be validated by further flow calculations. In any event, the radionuclide flow path to the environment is lengthened by entering the lower, rather than the upper, aquifer.

Other factors besides the dispersion and the hydraulic potential have effects on the radionuclide movement. Their importance can vary according to the radionuclide, the media through which transport occurs or the physical geometry. Thus, further investigation should be made of the effects on radionuclide movement of:

1. adsorption coefficients,
2. diffusivity,
3. leachability of the radionuclide from the waste form,
4. solubility of the radionuclide in the transport media, and
5. the stability of the salt layer itself, as modelled with the salt dissolution coefficient.

5.4 ADDITIONAL COMMENTS

1. When problem 5 was run with the version of the SWIFT code presently inhouse, an anomaly concerning the Darcy-velocities appeared. At various grid blocks printed in the Darcy velocity table, the velocity vectors were predicted to be directions not explainable for this problem. This apparent anomaly could be due to the error in the programming of the "steady state" solution method, as discussed in problem 4. It also, however, could be attributed to an error in geometry. That is, problem 5 was a near field simulation of grid blocks 32 to 42 of problem 4--which models 40,000 feet. The geometric setup for problem 5, however, covers only 20,250 ft and the boundary pressures used for the edges were those from columns 32 and 42 of problem 4. Also, there is an inconsistency in the reservoir dip angle. In problem 4, sin x = -0.129379, in problem 5, sin x = .01321875.

2. In the "REPOSITORY DATA" table, it should be noted that if a low level waste form is being analyzed (i.e., ILEVEL = 0) then the units of DENSTR are not feet as indicated, rather DENSTR is unitless. This is derived from the fact that low level waste is input as ft^3WASTE/ft^3BULK.

3. NTIME: In this problem equals 2, this represents the values that must be input into the "Interpolation Table for Unleached Radionuclide Concentration in Repository (LB/CU.FT.WASTE)." For values of NTIME = 1, the program uses a logarithm interpolation

to get repository concentrations of the value of NTIME = 1, the program uses a numerical solution to calculate radionuclide concentrations at later times, given the initial conditions.

4. When modelling a given grid network, the program assumes that the entire network has the characteristics given in the table "HOMOGENEOUS RESERVOIR" unless modifications are made. Modifications can be made via:

   a. specification of rock types which allow modification of thermal conductivities and adsorption coefficients. The specification of the rock type is also necessary when the dissolution of the material is to be considered,

   b. the specification of heterogeneous blocks or regions as noted in the "HETERGENEOUS RESERVOIR" table. The system properties that can be modified in this manner are listed in the "HETERGENEOUS RESERVOIR" table, and

   c. the specification of heterogeneous blocks or regions as noted in the "RESERVOIR DESCRIPTION MODIFICATIONS" table.

5. There is an apparent anomaly in the calculation "TRACE COMPONENT 1 INITIAL COMP IN PLACE," calculated as .939233 E-90 LBM. Card I-4 specified an initial concentration of 1.00 E-99 for the entire grid and the "INITIAL WATER IN PLACE" was calculated as 6.819144 E+08. Thus it would appear that the radionuclide concentration should be .6819144 E-90.

6. The "Material Balance Summary" table tracks radionuclide concentrations by noting that all radionuclides must fit into one of three categoreis: (1) unleached, (2) leached but undissolved, and (3) leached and dissolved or sorbed. Category 1 refers to radionuclide concentration in the waste form; category 2 refers to radionuclides which may have been leached from the waste form, but have not been dissolved in the transporting fluid; and category 3 refers to radionuclides which are dissolved in the transporting fluid or have been adsorbed onto the surrounding media. Categories 1 and 2 refer only to radionuclide concentrations in the depository. Category 3 takes into account not only radionuclides leached from the depository, but also any other radionuclide concentrations in the entire repository region. Thus, the "SINK" for category 1 is the source for category 2 and the "SINK" for category 2 is the source for category 3. "In place" is the mass of radioactive components present in that category by the end of that time step. The "Balance" is a mass balance integrated over all the grid blocks at each time step.

7. It appears that the "grid vectors" for the 2-D concentration maps represent the midpoints of each of the grid blocks. However, there is an inconsistency in our version of the code in the z direction. There are only nine vertical grid vectors, corresponding to what appears to be the centers of z coordinate blocks 2 through 10.

6.0 PROBLEM 6

6.1 AQUIFER PARAMETER CALIBRATION FROM WELL TEST DATA

The following two examples typify the use of the model in the calibration of aquifer transport parameters. The determination of permeability and dispersivity by calibration with historical data is essential to the prediction of future water and contaminant transport at a particular site. While analytical tools exist for simple geometries, the calibration of an aquifer possessing pronounced heterogeneity and anisotropy of complex geometries is possible only with numerical models.

Subcase 6.1. Determination of permeability from a single-well test.

The permeability of an aquifer can be calculated through a trial-and-error procedure of matching observed field data (historical) and the computed potentials from the model (calculated). The general approach is to

1. start with a homogeneous formation permeability and porosity,
2. add a skin (high or low permeability) zone around the well, and
3. examine a two-layer representation of other heterogeneous descriptions of the aquifer consistent with the geological interpretation.

In this example, an injectivity test was performed along an isolated interval of the well. The static water level in the well prior to

injection was 973 feet below ground surface (BGS). Approximately 24.9 cubic feet of water was injected over the interval from 3205 to 3308 feet BGS. After 240 minutes, injection was stopped and the tubing was allowed to drain. An example calibration of the pressure build-up and fall-off at the 3205 foot level is shown in Figure 4.

The numerical representation of the aquifer is a cylinder of 2000 feet radius and 103 feet thickness. The nine-inch diameter well, centrally located, imposes a flux boundary condition (IINDW1 = 1). The pressure drop between the well screen and the first grid block is achieved through the use of the well index (See SWIP documentation, Part 1, Appendix B).

Included in the data are the historical bottom-hole pressures observed during pressure build-up and fall-off (Symbol "O"). At the end of the simulation these are superimposed on a plot of the computed results (Symbol "X"). By altering the homogeneous data set listed in the Appendix, one can calibrate the model for a best fit. It is important to note the effect of the well index in a single-well calibration. Without additional drilling or well completion information it is advisable to maintain a well index consistent with the first grid-block conductivity. The influence of this parameter decreases with increasing distance from the injection well; thus, a calibration at an observation well located far from the injection well would be less sensitive to the well index. While an observation well(s) would provide more information for a better calibration of the formation permeability, the additional data are not always available.

In the initial calibration of the formation, the observed maximum pressure build-up is less than the observed. By changing the permeability a better match can be obtained. The magnitude of the reduction necessary is based on previous calibration runs and experience. What effect would changing the porosity have?

Subcase 6.2. Determination of dispersivity from a two-well test. The transport of a dissolved constituent is governed by convection of the carrier fluid and hydrodynamic dispersion. For an inert tracer used in ground water studies adsorption and chemical changes are negligible. With knowledge of the formation permeability and by maintaining sufficient flow that molecular diffusive processes are small, one is able to reduce the calibration parameters to two: namely longitudinal and transversal dispersivity.

In this example a tracer is introduced into a three-dimensional flow field at one well. While both wells are pumped continuously, samples are collected at the collection well. The concentration break-through is used to match the computer model output for calibration.

Only half of the flow field is simulated in the model by taking advantage of the symmetry with respect to both wells (Figure 6.1). Constant potential boundaries are applied at the periphery of the aquifer and a steady-state velocity field is computed.

If the observed peak concentrations were smaller and appeared at the collection well at a later time, should the dispersivities be

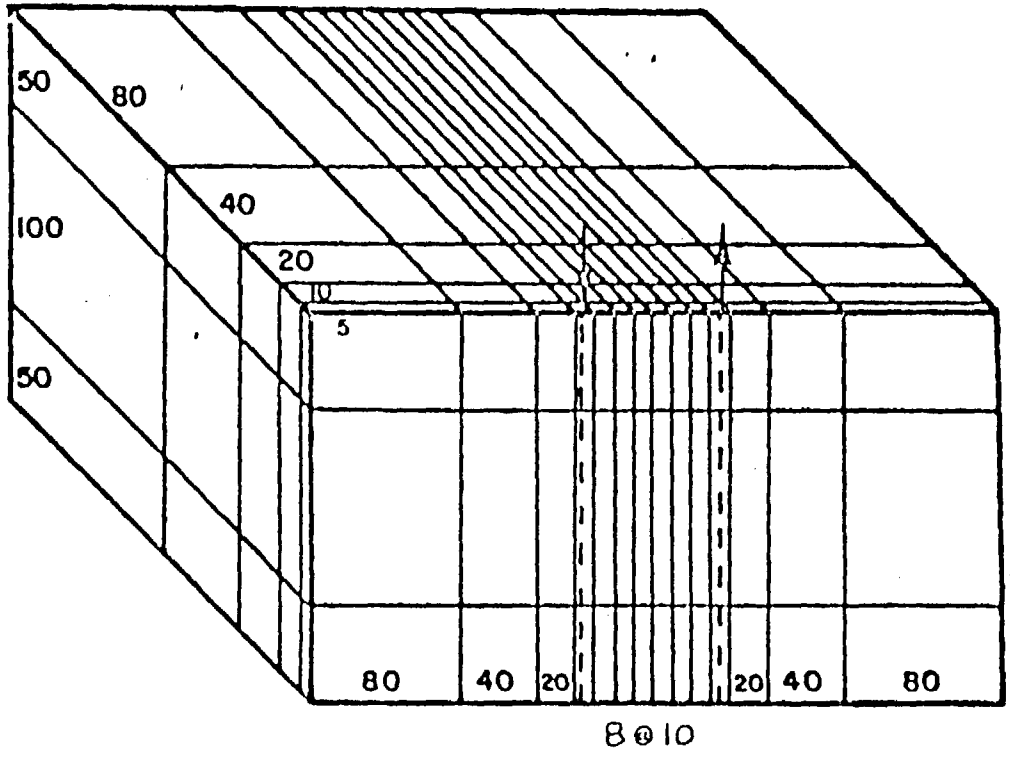


Figure 6.1 Two-well tracer test grid.

increased or decreased? What is the effect of longitudinal to transversal dispersivity ratio? Hint: Execute the model and examine with the two-dimensional contour maps.

6.2 DISCUSSION

The purpose of Problem 6 is to demonstrate the use of the SWIFT code to determine aquifer (host rock) transport properties. Subcase 6.1 deals with permeability. Subcase 6.2 works with dispersivity. Problem 6 also demonstrates the use of output plots and output contour maps.

6.2.1 DISCUSSION (Subcase 6.1)

Determination of permeability from a single well test. The purpose of Subcase 6.1 is to show how to use the SWIFT code to determine the permeability of a rock mass around a single well. The text of the problem outlined an iterative procedure for using the code to fit the data of a field test. Subcase 6.1 presents only the last iteration. The two main factors to be varied are the permeability of the surrounding medium and the permeability of a skin around the well. A homogeneous aquifer is being used for this problem. Figure 6.1.1 is a schematic of the system being characterized.

When a comparison was made between the statement of the problem and the input to the code, we found that the code input could not be generated from information provided by the problem. A discussion of this comparison will be provided later. To proceed with the problem, the input was accepted as fact and a comparison of the input to the output was made. The desired output is a comparison of the calculated pressure profile with the test pressure profile. The comparison of the profiles is given by a print-plot of bottom hole pressure vs. time provided in the output. Figure 6.1.2 is a replot of the significant portion of the print-plot. The print-plot was generated by using the R2 and the P2-P4 data cards.

The recurring sets of data; cards R2-1, R2-4, RR-5, R2-12 and R2-13; represent the discretization of the field data and generate the calculated pressure curve. The P4 cards are the field generated pressure results. Two facts seem to be obvious from Figure 6.1.2. First, the calculated pressures are all below the field pressures, thus, the permeability used is too large and another run should be executed using a smaller permeability. Second, either the field data has a spurious value or there was a state change of the rock surrounding the well. Figure 6.1.2 may be misleading about the importance of the above two facts. When the percent difference between the two curves is calculated, the average difference is 4% with a maximum value of 10% and a minimum value of 1% (see insert on Figure 6.1.2). The decision to perform another computer calculation is dependent on how sensitive the pressure profile is to changes in permeability. If the other iterations (previous to the one presented in Subcase 6.1) were available, the sensitivity would be known and the decision could be made. The anomalous value in pressure was investigated in two ways. First, the actual input field data was plotted on Figure 6.1.2 which provided more data points on the curve. Second, the curve was smoothed with a french curve and the maximum percent difference was found to be 4%. The conclusions drawn are that the low data point is not spurious but resulted from minor hydrofracturing of the rock and that the overall effect on the accuracy of the

permeability test is negligible. Another computer calculation was not executed because of the low percent difference between the curves. A good way to investigate the flexibility and the sensitivity of the SWIFT code would be to try to simulate they hydrofracturing effects using the well index, the grid block spacing and the heterogeneous aquifer specifications (the fracture zone being more permeable).

The well summary tables and the aquifer pressure profile tables were used in two ways. The well summary tables were used to show the effects of the recurring well input data (i.e., volume of water entering the rock formation and bottom hole pressure). The aquifer pressure profiles were used to determine the extent (distance) of influence of the well.

Recommendations

Four recommendations are made.

1. The statement of the problem should always provide the necessary and sufficient information to generate the input to the computer run. For example, the problem should explain the test procedure since the recurring well input is dependent on the test procedure.

2. A table of plot point values should accompany a print-plot to facilitate the use of the print-plot.

3. One should always check for the percent difference between the two pressure profiles. If the SWIFT code is to be used to determine transport properties very often, perhaps the percent difference calculation should be added to the code output.

4. More than one iteration should be presented in subcase 6.1. The usefullnes of subcase 6.1 would be considerably enhanced by the addition of one or more consecutive iterations.

6.2.2 DISCUSSION (Subcase 6.2)

Determination of dispersivity from a two-well test. Subcase 6.2 can be used to familiarize a SWIFT user with the set-up of a three dimensional geometry and with the contour map output. Subcase 6.2 uses a homogeneous aquifer with two wells 70 feet apart. The centerline axis of the wells is used as an axis of symmetry for the problem. The grid blocks are of unequal size to allow more detailed representation around the wells. The longitudinal, transverse and vertical dispersivities are equal. The tracer fraction for the injection well is one. The initial tracer fraction in the aquifer fluid is zero. The movement of the tracer through the aquifer can be followed by determining its concentration in the grid blocks. Figure 6.2.1 is a sketch of the problem geometry showing the well location and grid numbering.

For the initial study of this problem, the input will be accepted as a given. The pressure gradients were looked at first since the tracer movement is dictated by water flow. The wells provide the only driving force for water flow (no dip angle or boundary pressure driving force). The injection well should set-up flow away from the well. The production well should set-up flow toward the well. The wells are isolated in the middle vertical layer (i.e., z=2). Thus, the vertical flow around the injection well is up to the surface and down

to the aquifer bottom. The vertical flow around the production well is down from the surface and up from the bottom of the aquifer (see Figure 6.2.2). The aquifer pressure profiles were checked and concurred with the above expectations (see Figure 6.2.3). In a similar manner, the concentration contours were predicted and confirmed. Subcase 6.2 needs more work which is expected to occur during the first SWIFT code seminar.

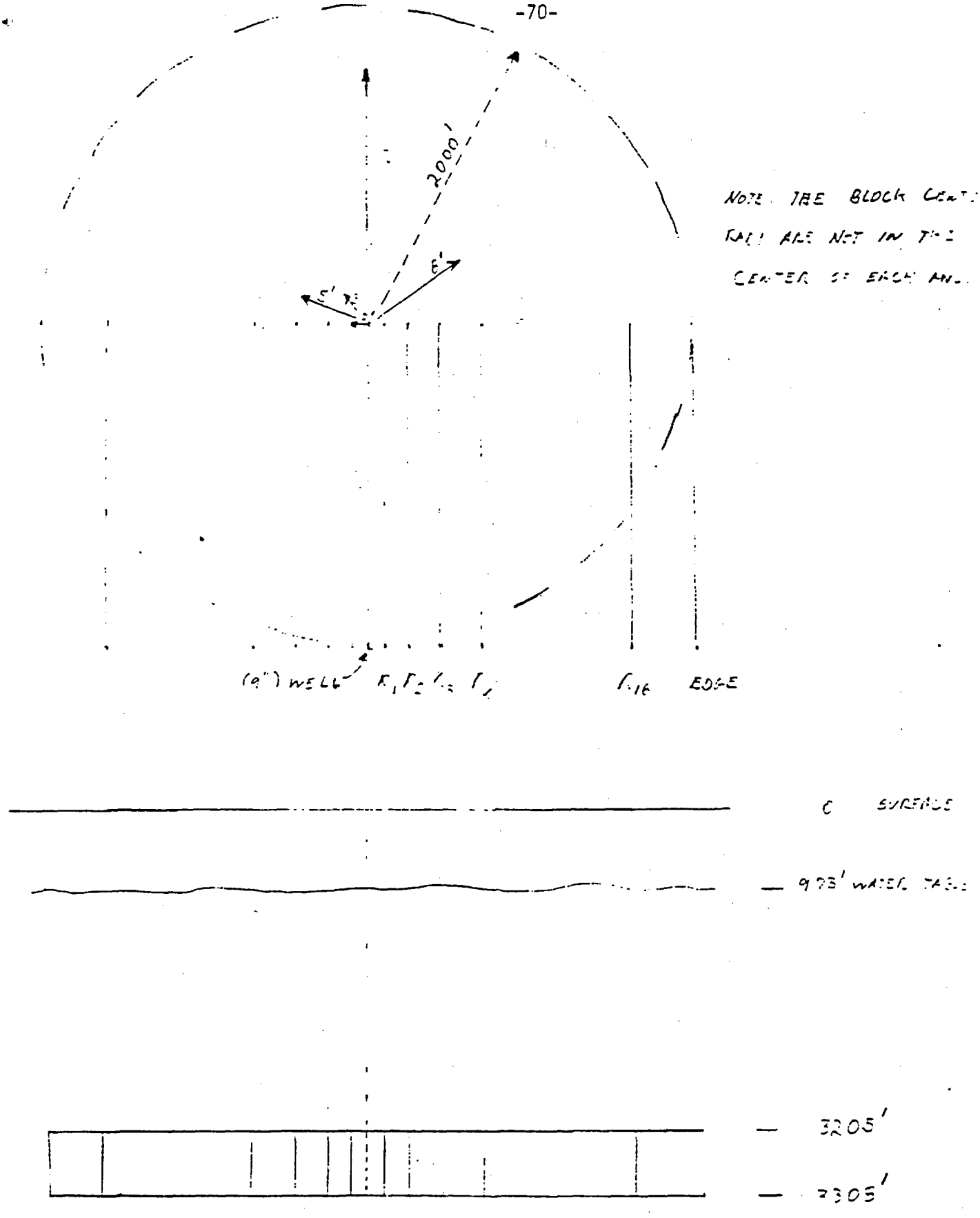


FIGURE 6.1.1 GEOMETRY FOR PROBLEM 6.1

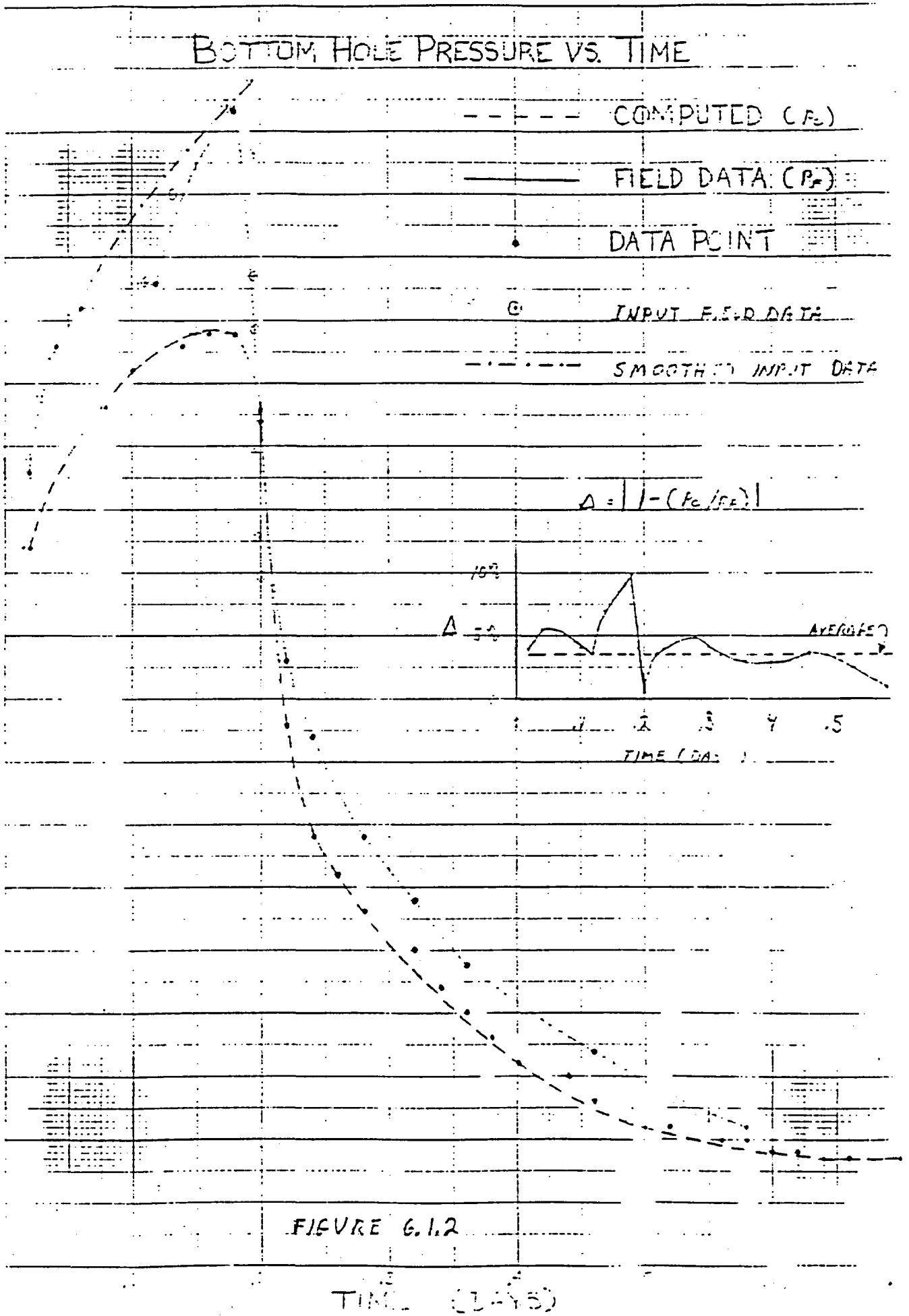

BOTTOM HOLE PRESSURE VS. TIME
COMPUTED (P_c)
FIELD DATA (P_f)
DATA POINT
INPUT FIELD DATA
SMOOTHED INPUT DATA
$\Delta = |1-(P_c/P_f)|$
10%
$\Delta = 0$
AVERAGE
1
2
3
4
5
TIME (DAYS)
TIME (DAYS)

FIGURE 6.1.2

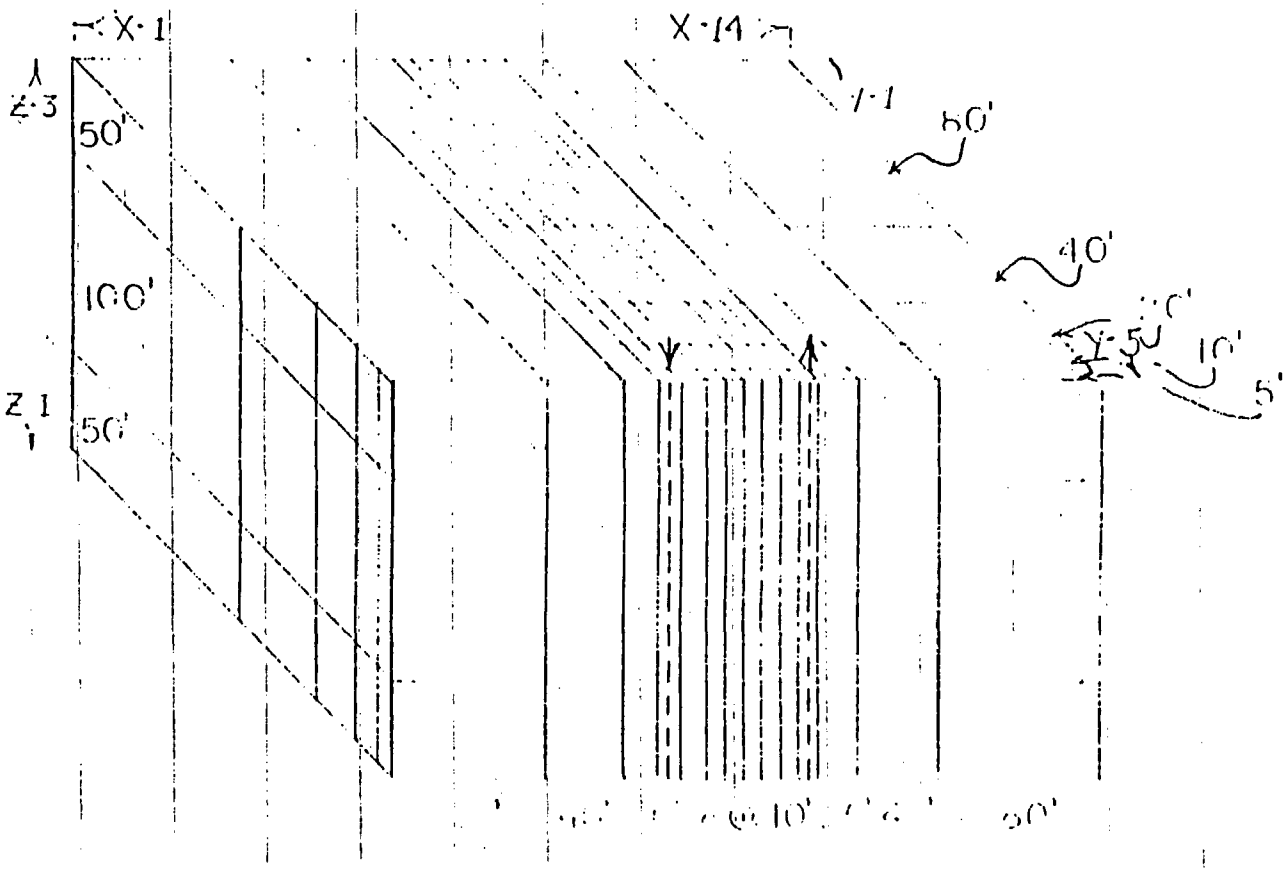
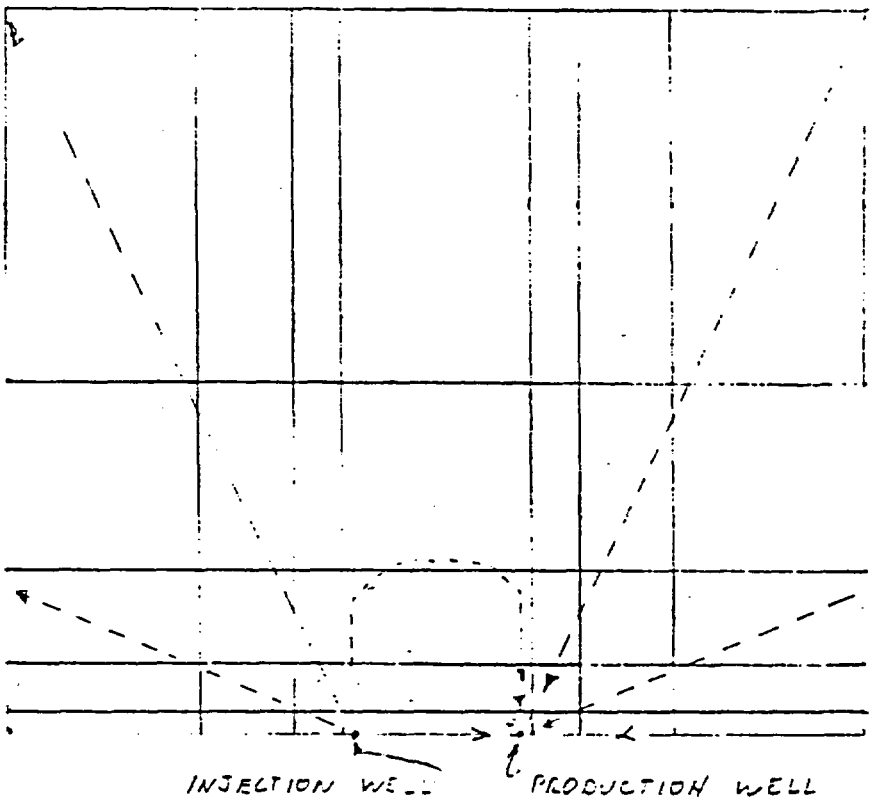
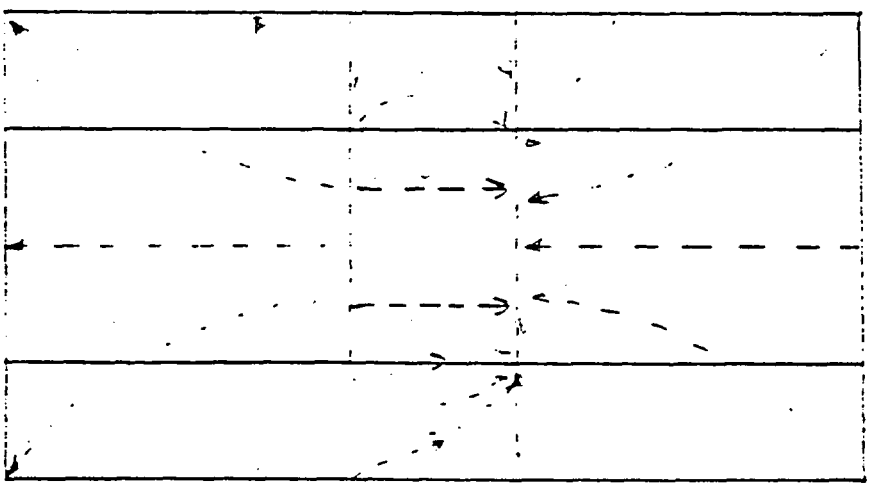


Figure 6.2.1

[illegible] Tracer Test Grid With Wells



X-Y PLANE



X-Z PLANE

FIGURE 6.2.2

PRESSURE GRADIENTS FOR PROBLEM 6.2

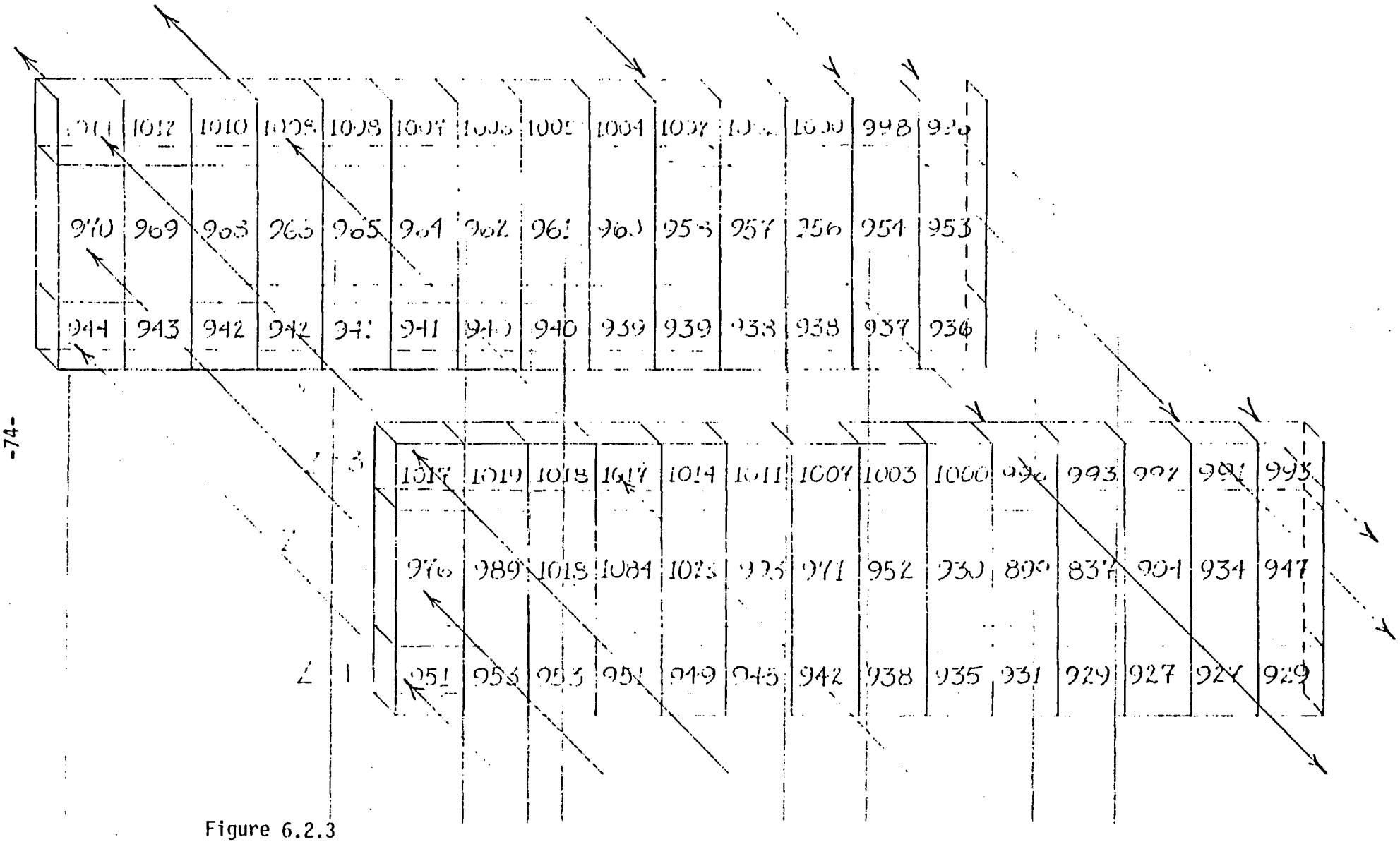


Figure 6.2.3

PRESSURE CROSS SECTION AT Y = 1 and Y = 5 * X SCALE EXAGGERATED

Arrows represent Y component of potential flow.

REFERENCES

1. "A Model for Calculating Effects of Liquid Waste Disposal in Deep Saline Aquifer: Part I--Development, Part II--Documentation," INTERCOMP Resource Development Engineering, Inc.

2. "Risk Methodology for Geologic Disposal of Radioactive Waste: Interim Report," NUREG/CR-0458, J. E. Campbell et al, October 1978.

3. "Risk Methodology for Geologic Disposal of Radioactive Waste: Final Report on Contract 13-3269," INTERA Environmental Consultants, Inc., August 1978. (Draft Report)