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FERNALD RI/FS GROUND WATER MODELING FLOW AND SOLUTE TRANSPORT COMPUTER CODE VERIFICATION FINAL REPORT FEBRUARY 1990

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REPORT

Fernald RI/FS
Ground Water Modeling

Flow and Solute Transport Computer Code Verification

Final Report

For The

U. S. DEPARTMENT OF ENERGY
OAK RIDGE OPERATIONS

Prepared By

IT Corporation
Monroeville, Pennsylvania

February 1990

INTERNATIONAL TECHNOLOGY CORPORATION

February 27, 1990

Mr. H. Windecker
Advanced Sciences, Inc.
11002 Hamilton-Cleves Rd.
Ross, OH 45061

Transmittal of Flow and Solute
Transport Computer Code Verification Final Report

Dear Mr. Windecker:

Enclosed are eight (8) copies of the Flow and Solute Transport Computer Code Verification Final Report. Enclosed also is one unbound copy.

If you have any questions, please do not hesitate to contact us.

Sincerely,

Sirous H. Djafari, Ph.D., P.E.
Task Manager
Corporate Director

John E. Razor
Project Director

SHD/JER:mdp

Enclosures

cc: J. Yeasted

Regional Office
William Penn Plaza • 2790 Mosside Boulevard • Monroeville, Pennsylvania 15146-2792 • 412-372-7701

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FERNALD RI/FS
GROUND WATER MODELING

FLOW AND SOLUTE TRANSPORT
COMPUTER CODE VERIFICATION

PREPARED BY:

IT CORPORATION
MONROEVILLE, PENNSYLVANIA 15146

PREPARED FOR:

U.S. DEPARTMENT OF ENERGY
OAK RIDGE OPERATIONS

FEBRUARY 1990

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EXECUTIVE SUMMARY

Ground water flow and solute transport modeling are being performed for the U.S. Department of Energy (DOE) Feed Materials Production Center (FMPC) in Fernald, Ohio, to support the ongoing, sitewide remedial investigation/feasibility study (RI/FS). The purpose of the modeling during the remedial investigation (RI) is to assess the nature and extent of the contamination and to support the evaluation of potential public health and environmental risks. In particular, the evaluation of the no-action alternative requires the prediction of future conditions for both on-site and off-site receptors.

A similar application of the ground water flow and solute transport models will be made in support of the feasibility study (FS). In this case, however, the focus will be on the short- and long-term effects of various remedial action alternatives on contaminant source release rates and on contaminant migration rates. The temporal and spatial variations of contaminant concentration resulting from the different remedial actions will also be predicted.

The ground water flow model could also be used as a tool for the conceptual design phase of the FS. Therefore, ground water modeling plays an important role throughout the RI/FS process and a dependable, verified computer code is critical for reaching sound and defendable conclusions. The code verification is also a requirement of International Technology Corporation's (IT's) Quality Assurance (QA) Program.

To satisfy project and QA requirements, an extensive and independent verification study was performed for Version 2.25 of the Sandia Waste-Isolation Flow and Transport (SWIFT III) code. This code had been selected to evaluate ground water flow and solute transport for the overall sitewide RI/FS.

The objectives of the verification study were to:

- Determine if SWIFT III functions satisfactorily with respect to well-established ground water flow/solute transport codes and with respect to analytical solutions
- Verify the code's capability to model the complex, sitewide conditions at the FMPC study area
- Establish a high level of confidence in the code capabilities
- Correlate with the verification process performed by GeoTrans to show that the computer code was fully operational on IT's computer system
- Document the procedures and findings of the verification process

To make the verification program responsive to the project needs while minimizing duplication of previous verification efforts, several guidelines were devised. These guidelines were based on FMPC site modeling considerations, code capability requirements, and previous SWIFT III verification activities.

To verify the SWIFT III code, a series of verification problems were established. The verification process was divided into two parts, namely ground water flow and solute transport. For each part, several problems were chosen. The results of the SWIFT III code were compared with analytical solutions and with results of well-established computer codes.

The verification study proceeded from simple and idealized problems that have some relationship with intended model use at the FMPC to more complex problems representing the FMPC environment. Important features and characteristics of the site were selected and modeled throughout the verification process.

Based on the extensive verification studies performed on SWIFT III by IT and GeoTrans, it was concluded that the code has been tested thoroughly, and will adequately model ground water flow and solute transport conditions at the FMPC site. Because SWIFT III performs satisfactorily in relation to other well-established codes, it can be used with a high degree of reliability and confidence in the sitewide RI/FS modeling studies.

1.0

1.0 INTRODUCTION

Ground water flow and solute transport modeling are being performed for the U.S. Department of Energy (DOE) Feed Materials Production Center (FMPC) in Fernald, Ohio, to support the ongoing, sitewide remedial investigation/ feasibility study (RI/FS). The purpose of the modeling during the remedial investigation (RI) is to assess the nature and extent of the contamination and to support the evaluation of potential public health and environmental risks. In particular, the evaluation of the no-action alternative requires the prediction of future conditions for both on-site and off-site receptors.

A similar application of the ground water flow and solute transport models will be made in support of the feasibility study (FS). In this case, however, the focus will be on the short- and long-term effects of various remedial action alternatives of contaminant source release and migration rates. The temporal and spatial variations of contaminant concentration resulting from the different remedial actions will also be predicted. The ground water flow model could also be used as a tool for the conceptual design phase of the FS. Therefore, ground water modeling plays an important role throughout the RI/FS process and a dependable verified computer code is critical for reaching sound and defendable conclusions. The code verification is also a requirement of International Technology Corporation's (IT's) Quality Assurance (QA) Program.

1.1 OVERALL OBJECTIVES OF THE VERIFICATION STUDY

The SWIFT III computer code was selected to evaluate ground water flow and solute transport for the overall, sitewide RI/FS. At the time of computer code selection and preliminary application to the hydrogeologic study of FMPC discharges to the Great Miami River in August 1987, no verification of the SWIFT III computer code had been documented. GeoTrans subsequently completed a formal verification of SWIFT III with

the results published in March 1988. IT initiated an independent verification study of SWIFT III, with the results published in November 1987. Generally, the purpose of the verification study was to validate the accuracy of the computational algorithms used to solve the governing equations and to determine that the computer code was fully operational on the IT computer system. The most important purpose, however, was to test the code capabilities to model FMPC sitewide features such as site dimensions, and the hydrologic and geochemical diversities.

Specifically, the objectives of the computer code verification study were to:

- Determine if SWIFT III functions satisfactorily with respect to well-established ground water flow/solute transport codes and with respect to analytical solutions
- Verify the capability of the code to solve complex, large-scale problems and to model the sitewide conditions at the FMPC
- Establish a high level of confidence in the code capabilities
- Correlate with the verification process performed by GeoTrans to show that the computer code was fully operational on IT's computer system
- Document the procedures and findings of the verification process

In summary, the overall objective of the verification study was to document that the SWIFT III code could accurately model the ground water flow/solute transport processes at the FMPC site.

1.2 VERIFICATION METHODOLOGY

Various methods are used to verify a computer code. One method by which a computer code can be checked for the accuracy of its theoretical principles and of its computational algorithms is by executing selected

problems for which analytical (closed-form) solutions exist. In this method, a model of a problem is developed for simulation by the computer code. To the extent possible, input data to the analytical and numerical simulations are made identical. Comparison of results is a reliable means of verifying the accuracy of the computational method of the computer code.

Verifying complex numerical computer codes with analytical solutions has limitations, however. The limitations exist because analytical solutions are only available for simplified conditions. To overcome these limitations, the results of the computer code which is being verified are compared with results of other widely accepted and well-verified codes. Such comparisons assist in verifying the computer code's capabilities to simulate conditions such as domain heterogeneity and hydrogeologic stratification, partially penetrating wells, and differing boundary conditions.

Another method of verification is to compare field data with model simulated results. In this case, a site-specific model is developed which includes site hydrogeologic and geochemical properties, and other existing features such as extraction wells. Computer results, e.g., ground water (potentiometric) levels, are compared with field data. A good correlation of field measurements and computer results is indicative of acceptable code performance.

All three methods of verification, namely analytical, numerical, and field comparisons, were used to verify the SWIFT III computer code. Use of the methods and the rationale for their selection are discussed in Chapter 2.0. In Chapter 3.0, the details of ground water flow verification are presented, and Chapter 4.0 contains details of radionuclide and solute transport verification. Summary and conclusions are presented in Chapter 5.0.

2.0

2.0 VERIFICATION PROCESS

Ground water modeling (flow and solute transport) is a significant part of the RI/FS program. The model results are used in site characterization, risk assessment, and remedial action analysis. Because of the importance of model results in reaching conclusions, RI/FS modeling should be performed using a well-verified and documented computer code. To satisfy this requirement, several verification guidelines were established. The SWIFT III code verification program was implemented according to these guidelines.

2.1 CODE VERIFICATION GUIDELINES

The guidelines were devised to be responsive to the project needs while minimizing duplication of previous verification efforts. The guidelines for the verification process were the following:

- FMPC site modeling considerations
- Code capability requirements
- Previous SWIFT III verification activities

These guidelines are discussed in detail in the following sections.

2.1.1 FMPC Site Modeling Considerations

The RI/FS model study area is about 20 square miles. This area encompasses the FMPC site and adjacent areas which are affected by pumping wells and Great Miami River. The ground water flow modeling area is shown in Figure 2-1.

The hydrogeologic setting in the model study area is composed of a buried channel aquifer which is deeply incised into bedrock. The buried channel varies in width from about one-half mile to over two miles and has a U-shaped cross section with a broad, relatively flat bottom and steep valley walls (Figure 2-2). Bedrock is predominantly flat-lying shales with thin interbedded layers of limestone. Thick deposits (exceeding 200 feet) of glacial outwash material composed of coarse

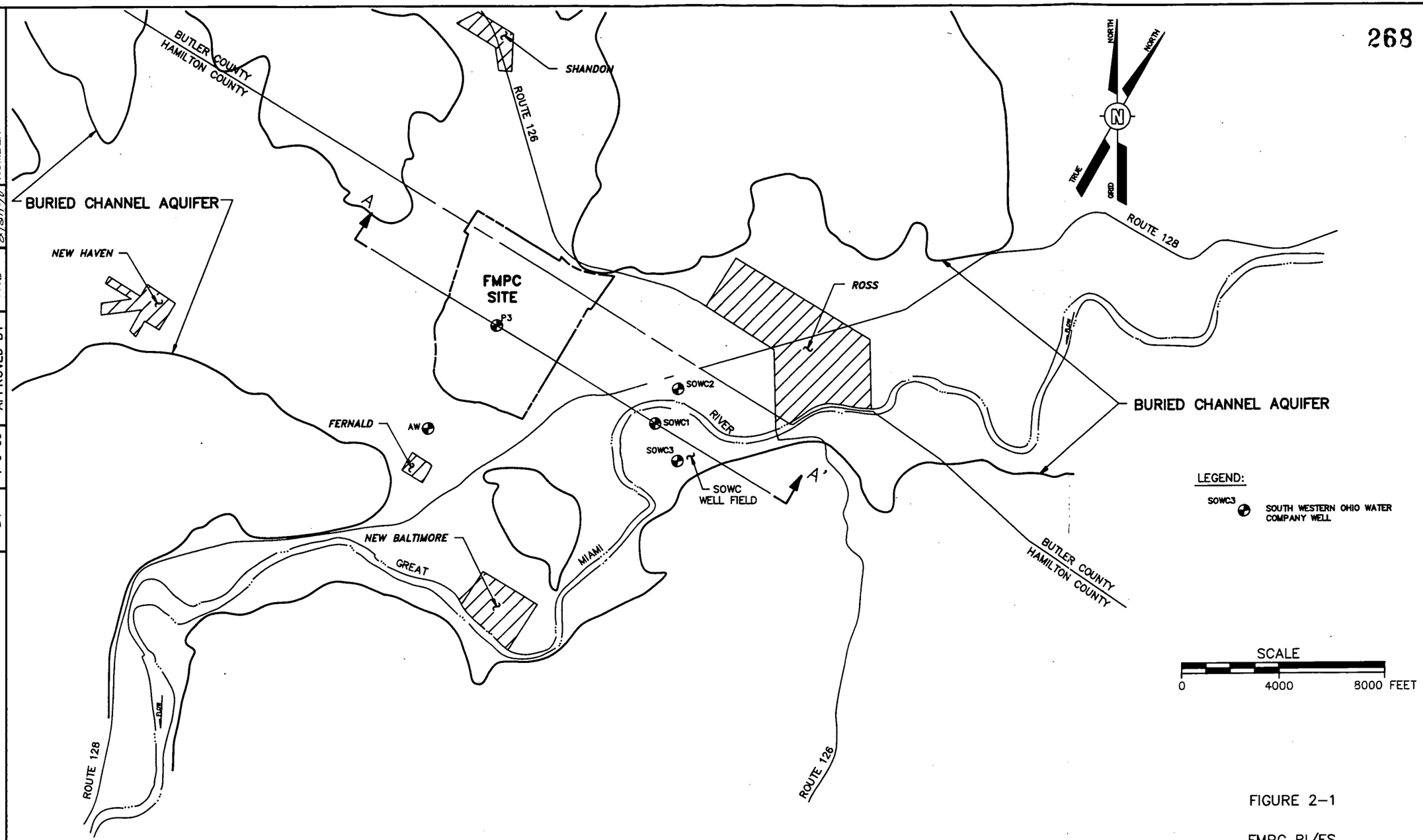

FIGURE 2–1

FMPC RI/FS
STUDY AREA AND VICINITY

PREPARED FOR

FERNALD RI/FS
U.S. DEPARTMENT OF ENERGY
OAK RIDGE OPERATIONS

INTERNATIONAL TECHNOLOGY CORPORATION

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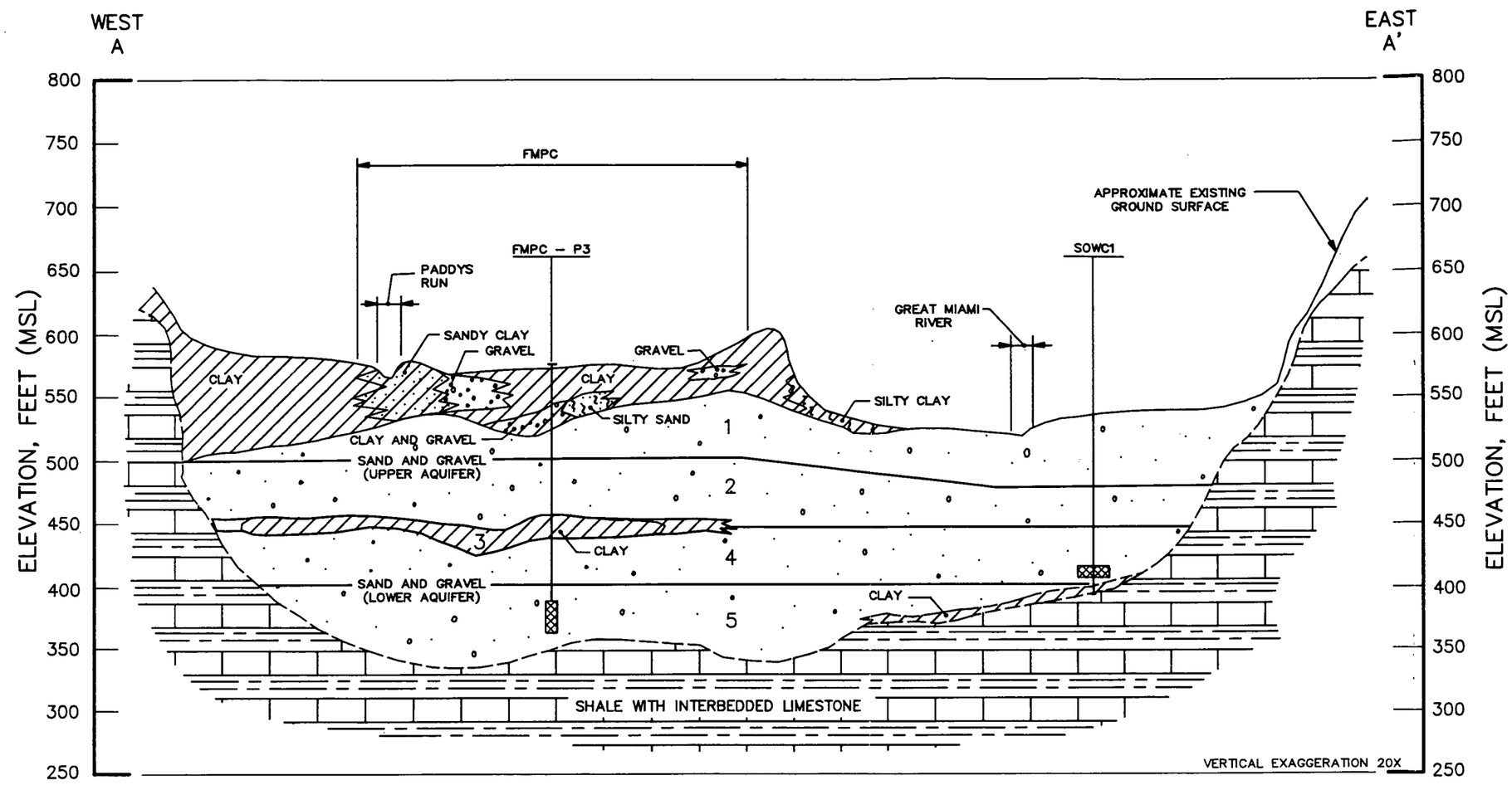

LEGEND:

OPEN INTERVAL

2 — HYDROGEOLOGIC LAYER USED IN SWIFT III MODELS

NOTES:

1. FOR LOCATION OF CROSS SECTION A–A' SEE FIGURE 2–1
2. SOWC1 IS A SOUTH WESTERN OHIO WATER COMPANY WELL.

REFERENCE:

MODIFIED FROM U.S.G.S. PROFESSIONAL PAPER 605–A USING AVAILABLE OHIO STATE WATER WELL RECORDS, SOWC WATER WELL DATA, DAMES & MOORE FEED MATERIALS PRODUCTION CENTER GROUND WATER STUDY TASK A & C REPORTS AND IT BORING LOGS.

CROSS SECTION A–A'

(LOOKING NORTH)

VERTICAL SCALE

0 100 200 FEET

HORIZONTAL SCALE

0 2000 4000 FEET

THE BORING LOGS AND RELATED INFORMATION DEPICT SUBSURFACE CONDITIONS ONLY AT THE SPECIFIC LOCATIONS AND DATES INDICATED. SOIL CONDITIONS AND WATER LEVELS AT OTHER LOCATIONS MAY DIFFER FROM CONDITIONS OCCURRING AT THESE BORING LOCATIONS. ALSO THE PASSAGE OF TIME MAY RESULT IN A CHANGE IN THE CONDITIONS AT THESE BORING LOCATIONS.

THE DEPTH AND THICKNESS OF THE SUBSURFACE STRATA INDICATED ON THE SECTIONS WERE FROM AND INTERPOLATED BETWEEN THE TEST BORINGS. INFORMATION ON ACTUAL SUBSURFACE CONDITIONS EXISTS ONLY AT THE LOCATION OF THE TEST BORINGS AND IT IS POSSIBLE THAT SUBSURFACE CONDITIONS BETWEEN THE TEST BORINGS MAY VARY FROM THOSE INDICATED.

FIGURE 2–2

GENERALIZED HYDROGEOLOGIC CROSS SECTION OF THE GREAT MIAMI AQUIFER

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sands and gravels with interbeds of silts and clays fill the buried channel. Overlying the aquifer in places are variable thicknesses of glacial overburden material which consists of clays and silty clay (Figure 2-2).

Site conditions considered important in the development of ground water flow and solute transport models for the RI/FS process are:

- Location of the site over a large, irregularly shaped buried channel aquifer
- Thick, highly permeable aquifer with complex variations in horizontal and vertical hydraulic conductivities
- Location of major pumping centers in the model study area which influence the aquifer potentiometric level over large areas
- Pumping at depth (partially penetrating wells) within the sand and gravel aquifer
- Large changes in horizontal hydraulic gradients across the study area
- The presence of vertical hydraulic gradients within the study area, possibly induced by local pumping
- Complex river and aquifer interactions
- Uncertainties of areal recharge through varying hydrogeologic zones composed of till, floodplain, and alluvial deposits
- Presence of several potential contaminant source areas with different strengths and periods of release as well as several types of potential receptors

Chemical and radiological contaminants associated with the FMPC site most likely would have been introduced to the aquifer from one or more of the following:

- Leaky waste pits in the waste storage area
- Discharges to and leakage from Paddys Run
- Discharges to and leakage from the storm sewer outfall ditch
- Leakage from the main effluent line
- Waste or product spills in the Production Area and other potential waste disposal areas within the FMPC site
- Any facility in the Production Area used for the storage, containment, or transfer of radiological or chemical material

Based on these site conditions, it was necessary to develop three-dimensional ground water and solute transport models.

2.1.2 Code Capability Requirements

To satisfy the site modeling considerations presented above, it was necessary to verify that the SWIFT III code had the capability to simulate the specific site features and study requirements, including:

- The capability to incorporate complex site hydrogeology including variable aquifer thickness, hydraulic conductivity, different stratigraphic units, and partially penetrating wells.
- The capability to model simultaneously an unconfined aquifer and a river, in case unsaturated flow beneath the river or waste storage units is eventually found to be a critical process.
- The capability to model decay chains. Although the radionuclides of most concern do not require the consideration of daughter products, this would become a consideration if other radionuclides are found to be important.
- The capability to accurately represent attenuation/retardation (e.g., adsorption) and decay processes so as to provide flexibility in the range of constituents that can be modeled.

- The capability to handle a wide variety of boundary conditions so as not to limit the available options for best representing actual site conditions.

In addition to verifying the SWIFT III capabilities to satisfy the above requirements, an appreciation was developed for the usage convenience of the code. The elements considered in this process were the code postprocessing capabilities, user documentation, mesh generation, solution method, restart capability, and applicability to available computer systems.

2.1.3 Previous SWIFT III Verification Activities

The SWIFT model code was originally developed by Sandia National Laboratories (SNL) for the Nuclear Regulatory Commission (NRC) for use in the high-level nuclear waste isolation program. The first extension of the SWIFT code was made by GeoTrans and was given the title SWIFT II.

Comparisons of results from the SWIFT II code and analytical solutions appear in many documents. Results of the SWIFT II model applications have also been compared with data collected in numerous field studies. The comparisons provide evidence that the equations solved in the model properly simulate observed hydrogeologic behavior. Applications of the code to actual sites have also appeared in several reports, the most noteworthy are those appearing in Ward, et al. (1984) and Reeves, et al. (1986), which are summaries of the model verification process and field comparisons.

Modifications to the SWIFT II code were made by GeoTrans in 1987. A primary modification consisted of changing the code from FORTRAN IV to FORTRAN 77 to make the code more generally usable. Modifications were also made for data input and output simplification. The resultant code was called SWIFT III and is the subject of the verification study being reported herein.

GeoTrans and IT concurrently were conducting verification work to test the validity of several features of the SWIFT III code. In late February 1988, IT was notified of the SWIFT III (Version 2.25) verification work being performed by GeoTrans. The results of GeoTrans' work have been published and were made available to IT (GeoTrans, Inc., 1988). With this information, IT reevaluated its verification program. The purpose of this reevaluation was to minimize the duplication of effort while satisfying the previously established verification requirements.

2.2 OVERVIEW OF IT'S VERIFICATION PROCESS

The SWIFT III code is a three-dimensional finite-difference computer code that solves the coupled equations for the following four processes: (1) fluid flow, (2) heat transport, (3) dominant-species (brine) miscible displacement, and (4) trace-species (radionuclides) miscible displacement. The first three processes are coupled via fluid density and viscosity. These coupled processes provide the velocity field required in the fourth process. The code has Cartesian and cylindrical coordinate options.

To verify the SWIFT III code, a series of verification problems were established. A "verification problem" is defined as a set of conditions and features for which analytical or numerical solutions exist that can be used to check the SWIFT III model results. Each problem has been uniquely named and that name has been used throughout the text, tables, and figures. The ground water flow problems are identified by "GWF" and the solute transport problems by "ST".

The verification study proceeded from simple and idealized problems that have some relationship with intended model use at the FMPC to more complex problems representing the FMPC environment. Important features and characteristics of the site were selected and modeled throughout the verification process. Among the criteria used to select the problems were the following:

- The problem must use Cartesian coordinates consistent with the geometric system of the sitewide model
- The problem must represent some important characteristic or feature of the site, including:
  - Constant head boundary condition
  - Anisotropic media
  - Constant recharge
  - Extraction and injection wells with full and partial penetration
  - Multiple layer aquifers
  - River leakage and recharge
  - Radionuclide decay and generation of daughter products

The remainder of this section discusses the rationale for the verification process. The process used for verifying the ground water flow model and that used for the radionuclide and solute transport mode are presented separately.

2.2.1 Ground Water Flow Verification

The problems selected for ground water flow verification were based on analytical solutions, numerical simulations, and field data comparisons.

2.2.1.1 Selection of Problems With Analytical Solutions

To correlate the results of IT's verification study with the verification work previously performed by GeoTrans, a replication of some of GeoTrans' verification problems was made. Among the problems chosen from the GeoTrans verification manual (Ward, et al., 1984) were two two-dimensional problems for which analytical solutions exist. The first problem (GWF-1) is the well-known Theis solution (Theis, 1935) for a fully penetrating well in a homogeneous and isotropic confined

aquifer. The second problem (GWF-2) is for a fully penetrating well in an anisotropic confined aquifer (Papadopulos, 1965). The solutions to these problems assume that the flow is transient and the aquifer is confined with constant transmissivity.

To check the features of the code for an unconfined aquifer condition, two additional two-dimensional problems for which analytical solutions exist were selected from the set provided by GeoTrans. The first problem (GWF-3) was the Dupuit-Forchheimer solution for a steady-state unconfined aquifer with recharge (Bear, 1972). The second problem (GWF-4) was the Boussinesq solution (Bear, 1972) for an unconfined aquifer for a transient condition. These problems were selected because unconfined conditions are significant to the FMPC modeling activities.

2.2.1.2 Selection of 2-D and 3-D Numerical Problems

Code-to-code comparisons, independent from the GeoTrans verification study, were made to check some additional capabilities of the SWIFT III code. These comparisons were made on a two-dimensional (2-D) FMPC sitewide ground water flow model and on a three-dimensional (3-D) hypothetical grid system given by Finley and Reeves (1982). The verification study was based on comparisons with the results of other well-verified and widely-accepted ground water codes, namely: the U.S. Geological Survey's modular three-dimensional ground water flow code, MODFLOW (McDonald & Harbaugh, 1984); IT's proprietary quasi-three-dimensional ground water flow and solute transport code, GEOFLOW (IT Corporation, 1986); and the three-dimensional ground water flow and solute transport code, Princeton Transport Code (PTC), developed at Princeton University (Babu, et al., 1987). A brief description of these codes is presented in Appendix A. By appropriate use of these three codes, comparisons were made to determine the capability of the SWIFT III code in simulating the following features:

- Model domain heterogeneity
- Hydrogeologic stratification
- Partially penetrating wells

- Nonuniform recharge rates
- Aquifer-river interactions

A sitewide 2-D flow problem, GWF-5, was developed for the verification study to include all the specified features for ground water flow comparisons except partial penetration. These features include:

- Varying hydraulic conductivity distribution
- Nonuniform recharge
- Meandering of the Great Miami River
- Nonuniform aquifer base elevations
- Constant-head and no-flow boundary conditions
- Spatial variation of extraction wells

In this verification step, comparisons were made of potentiometric levels, Darcy velocity components, and river leakages between the results of SWIFT III and the results of GEOFLOW and MODFLOW.

A hypothetical three-dimensional problem was selected to supplement the two-dimensional sitewide example problem discussed above. This problem, GWF-6, consisted of three model layers and included partially penetrating wells. The significant characteristics of this problem are as follow:

- Partially penetrating extraction and injection wells
- Confined and unconfined aquifer conditions
- A river in the uppermost layer
- Constant-head and no-flow boundary conditions at the boundaries of different layers
- Constant recharge at the uppermost layer

Comparisons of potentiometric levels, Darcy velocity components, and river leakages were made between the results of SWIFT III and the results of MODFLOW and PTC.

2.2.1.3 Field Comparisons

The calibration process used during the sitewide modeling constitutes a form of field verification (Heijde, 1987). The ground water flow calibration has been successfully performed as part of RI/FS modeling activities and will be reported upon in the RI/FS model documentation.

2.2.2 Radionuclide and Solute Transport Verification

The following subsections discuss the rationale for selecting the problems for solute transport verification of the SWIFT III code.

2.2.2.1 Selection of Problems With Analytical Solutions

The analytical solutions for solute transport available in the literature are limited to uniform ground water flow velocity. These analytical solutions are based on either the constant concentration (first-type or Dirichlet) boundary condition or constant solute flux (third-type or Cauchy) boundary condition. For the Fernald site, the solute flux boundary condition is appropriate; therefore, in the verification process, analytical solute transport models with the solute flux boundary conditions were used to validate the SWIFT III code.

Two analytical solutions with the solute flux boundary condition with uniform ground water flow velocity were used. To correlate with the verification work previously performed, a one-dimensional problem of radionuclide transport with the chain-decay (Ward, et al., 1984) was selected from the GeoTrans verification manual. This solution was developed by Coats and Smith (1964). The verification problem in this study is named ST-1. The second problem, ST-2, consists of solute transport from a strip solute source located between two impervious boundaries in a uniform ground water flow field with a constant solute flux (third-type) boundary condition. The analytical solution to this problem and its related computer program (STRIP1B-FBC-G) were developed by IT (1987). The program has been previously verified against both analytical cases and numerical codes. The solution and its associated

initial and boundary conditions, as well as comparisons with GEOFLOW, are documented in the GEOFLOW manual (IT, 1986).

The SWIFT III code was also checked against GEOFLOW with the conditions of Problem ST-2. This comparison constituted an independent numerical verification.

2.2.2.2 Selection of Problem With Numerical Solutions

The performance of the SWIFT III code in three-dimensional solute transport simulation was evaluated against a GEOFLOW vertical model. By assigning appropriate input data and boundary conditions in the SWIFT III 3-D model, it was possible to produce conditions such that vertical slices of that 3-D model would be identical. One vertical slice was made then simulated using a GEOFLOW vertical model. This procedure enabled the examination of the accuracy of the SWIFT III solute transport predictions in the vertical direction, which is an important consideration at the FMPC site. The problem which utilized this procedure was named ST-3.

2.3 SUMMARY OF VERIFICATION STUDY PROBLEMS

A summary of the ground water flow and solute transport problems used in the IT verification program is presented in Tables 2.1 and 2.2. The verification work by GeoTrans is also shown in these tables. A review of these tables indicates that the SWIFT III code has undergone comprehensive testing in various modes applicable to its use at the FMPC site.

It is concluded that the code can be used with a high degree of reliability and confidence in the sitewide RI/FS modeling studies. The efficiency of code usage could benefit from improvement of the user's manual and of pre- and post-processing features.

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SWIFT III CODE GROUND WATER FLOW VERIFICATION

	GEOTRANS			IT		
PROBLEM TYPE	ANALYTICAL SOLUTIONS	NUMERICAL SOLUTIONS	FIELD COMPARISON	ANALYTICAL SOLUTIONS	NUMERICAL SOLUTIONS	FIELD COMPARISON
TWO DIMENSIONAL	• FULLY PENETRATING WELL CONSTANT DISCHARGE HOMOGENEOUS ISOTROPIC CONFINED AQUIFER, CARTESIAN COORDINATES • FULLY PENETRATING WELL CONSTANT DRAWDOWN HOMOGENEOUS, ISOTROPIC AQUIFER CONFINED RADIAL COORDINATES • FULLY PENETRATING WELL HORIZONTAL ANISOTROPIC CONFINED AQUIFER, CARTESIAN COORDINATES • FULLY PENETRATING WELL, LEAKY HOMOGENEOUS ISOTROPIC CONFINED AQUIFER, RADIAL COORDINATES	NOT DOCUMENTED IN THE AVAILABLE USER MANUALS OR VERIFICATION REPORTS	• HYDRAULIC TESTING FOR THERMAL ENERGY STORAGE IN AN AQUIFER TO COMPARE – PRESSURE SOLUTIONS – ANISOTROPIC AQUIFER CHARACTERISTICS – INJECTION AND OBSERVATION WELL RESPONSES – FLOW FROM AQUITARDS – EFFECTS OF AQUIFER BOUNDARIES	GWF–1 • FULLY PENETRATING WELL, CONSTANT DISCHARGE, HOMOGENEOUS ISOTROPIC CONFINED AQUIFER, CARTESIAN COORDINATES GWF–2 • FULLY PENETRATING WELL CONSTANT DISCHARGE, ANISOTROPIC CONFINED AQUIFER, CARTESIAN COORDINATES GWF–3 • DUPUIT–FORCHHEIMER STEADY STATE PROBLEM – TO SIMULATE FLOW FROM A FREE–WATER SURFACE GWF–4 • BOUSSINESQ TRANSIENT DRAWDOWN	GWF–5 • COMPARISON OF ACTUAL SITE DATA WITH GEOFLOW AND MODFOLW CODES FOR FLOW IN AN UNCONFINED AQUIFER WITH IRREGULAR BOUNDARIES AND STEADY–STATE FLOW	NOT NECESSARY
THREE DIMENSIONAL	NOT DOCUMENTED IN THE AVAILABLE USER MANUALS OR VERIFICATION REPORTS	NOT DOCUMENTED IN THE AVAILABLE USER MANUALS OR VERIFICATION REPORTS	NOT DOCUMENTED IN THE AVAILABLE USER MANUALS OR VERIFICATION REPORTS	NOT NECESSARY	GWF–6a, 6b, 6c, 6d • COMPARISON OF SWIFT III RESULTS WITH RESULTS FROM MODFLOW AND PTC CODES	• CALIBRATION OF SITE–SPECIFIC MODEL TO FIELD DATA

TABLE 2.1

SWIFT III GROUND WATER FLOW VERIFICATION

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SWIFT III CODE SOLUTE TRANSPORT VERIFICATION

	GEOTRANS			IT		
PROBLEM TYPE	ANALYTICAL	NUMERICAL	FIELD	ANALYTICAL	NUMERICAL	FIELD
ONE DIMENSIONAL	• TRANSPORT WITH CHAIN DECAY AND EQUAL RETARDATION IN AN ISOTROPIC HOMOGENEOUS AQUIFER. CARTESIAN COORDINATES • TRANSPORT WITH CHAIN DECAY AND UNEQUAL RETARDATION IN AN ISOTROPIC HOMOGENEOUS AQUIFER. CARTESIAN COORDINATES	NOT DOCUMENTED IN THE AVAILABLE USER MANUALS OR VERIFICATION REPORTS	NOT DOCUMENTED IN THE AVAILABLE USER MANUALS OR VERIFICATION REPORTS	ST-1 • TRANSPORT WITH CHAIN DECAY AND EQUAL RETARDATION IN AN ISOTROPIC HOMOGENEOUS AQUIFER. CARTESIAN COORDINATES	NOT NECESSARY	NOT NECESSARY
TWO DIMENSIONAL	NOT DOCUMENTED IN THE AVAILABLE USERS MANUALS OR VERIFICATION REPORT	NOT DOCUMENTED IN THE AVAILABLE USER MANUALS OR VERIFICATION REPORTS	• CONTAMINANT MIGRATION FROM A LANDFILL TO TEST CODE FOR – SOLUTE CONVECTION AND HYDRODYNAMIC DISPERSION – STEADY STATE VELOCITY – TIME AND SPACE DEPENDENT CONTAMINANT SOURCE TERMS – AQUIFER INFLUENCE FUNCTIONS	ST-2a, 2b • TRANSIENT TRANSPORT IN UNIDIRECTIONAL FLOW FIELD BETWEEN TWO IMPERVIOUS BOUNDARIES NOTE: STRIP1B-FBC-G USED FOR ANALYTICAL SOLUTION	ST-2a, 2b • TRANSIENT TRANSPORT IN UNIDIRECTIONAL FLOW FIELD BETWEEN TWO IMPERVIOUS BOUNDARIES NOTE: GEOFLOW USED FOR NUMERICAL SOLUTION COMPARISON	• CALIBRATION OF SITE-SPECIFIC MODEL WITH FIELD DATA
THREE DIMENSIONAL	NOT DOCUMENTED IN THE AVAILABLE USER MANUALS OR VERIFICATION REPORTS	NOT DOCUMENTED IN THE AVAILABLE USER MANUALS OR VERIFICATION REPORTS	NOT DOCUMENTED IN THE AVAILABLE USER MANUALS OR VERIFICATION REPORTS	NOT NECESSARY	ST-3a, 3b • 3-D SOLUTE TRANSPORT FOR – ANISOTROPIC UNCONFINED AQUIFER – FLUX BOUNDARY CONDITION – VARIABLE HYDRAULIC CONDUCTIVITY – FMPC GRID DIMENSIONS – NUMERICAL STABILITY CRITERIA NOTE: COMPARISON MADE WITH GEOFLOW SOLUTION FOR TRANSPORT IN A VERTICAL SLICE OF A 3-D MODEL	• CALIBRATION OF SITE-SPECIFIC MODEL WITH FIELD DATA

TABLE 2.2

SWIFT III CODE SOLUTE TRANSPORT VERIFICATION

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3.0

3.0 GROUND WATER FLOW VERIFICATION

In this chapter the technical details of the ground water verification problems are presented. As discussed in Chapter 2.0, each problem has been selected to examine a combination of SWIFT III features relevant to the FMPC site. The SWIFT III simulations are checked against analytical and/or numerical solutions. In addition, model calibration has been used as a basis for examining the performance of the code against field data.

The following format is used to present the methodology and results of each verification problem:

- Problem name
- Purpose of problem selection
- Problem description
- Assumptions
- Analytical solution (where applicable)
- SWIFT III numerical simulation
- Input specifications
- Output specifications
- Results

Table 3.1 has been prepared to summarize the features of the verification problems and it includes problem name, model features to be tested, and figure and table references related to each problem. The computer file names associated with each verification problem are presented in Table B.1 of Appendix B.

Either English or Standard International (SI) units are used to maintain consistency of units used by the originators of the verification problems. To assist the reader, data are generally presented in both units.

3.1 VERIFICATION PROBLEMS - ANALYTICAL SOLUTIONS

The following four two-dimensional problems with analytical solutions were selected for use in verifying the SWIFT III ground water flow model:

TABLE 3.1

SWIFT III CODE GROUNDWATER FLOW VERIFICATION SUMMARY

GROUNDWATER FLOW PROBLEMS	GWF-1	GWF-2	GWF-3	GWF-4	GWF-5	GWF-6a	GWF-6b	GWF-6c	GWF-6d
SWIFT III FEATURES / CHARACTERISTICS									
CONFINED AQUIFER	X	X				X			
UNCONFINED AQUIFER			X	X	X		X	X	X
ISOTROPIC AQUIFER	X								
STEADY STATE PRESSURE SOLUTIONS			X		X	X	X	X	X
TRANSIENT STATE PRESSURE SOLUTIONS	X	X		X					
CARTESIAN COORDINATES	X	X	X	X	X	X	X	X	X
TWO-DIMENSIONAL CARTESIAN COORDINATES	X	X	X	X	X				
THREE-DIMENSIONAL CARTESIAN COORDINATES						X	X	X	X
CONSTANT PUMPING RATE	X	X			X	X	X	X	X
AQUIFER INFLUENCE FUNCTION	X	X	X	X	X	X	X	X	X
ANISOTROPIC HYDRAULIC CONDUCTIVITY DISTRIBUTION		X				X	X	X	X
CONSTANT-HEAD BOUNDARY CONDITION			X	X	X	X	X	X	X
NO-FLOW BOUNDARY CONDITION					X	X	X	X	X
RECHARGE			X		X		X	X	X
NON-UNIFORM RECHARGE					X				
IRREGULAR BOUNDARIES & BOTTOM ELEVATIONS OF THE AQUIFER					X				
VARIABLE HYDRAULIC CONDUCTIVITY					X				
RIVER HAVING AN IRREGULAR CURVED FORM					X				
RIVER AT THE UPPERMOST LAYER								X	X
INJECTION WELLS						X	X	X	
EXTRACTION WELLS					X	X	X	X	X
PARTIALLY PENETRATING WELLS						X	X	X	X
DARCY VELOCITY COMPONENTS					X	X	X	X	X
REFERENCES									
VERIFICATION PROBLEM DETAILS: SEE VERIFICATION REPORT	SECTION 3.1.1	SECTION 3.1.2	SECTION 3.1.3	SECTION 3.1.4	SECTION 3.2.1	SECTION 3.2.2	SECTION 3.2.2	SECTION 3.2.2	SECTION 3.2.2
RELEVANT TABLES	TABLE 2.1	TABLE 2.1	TABLE 2.1	TABLE 2.1	TABLE 2.1	TABLE 2.1	TABLE 2.1	TABLE 2.1	TABLE 2.1
	TABLE B.1	TABLE B.1	TABLE B.1	TABLE B.1	TABLE B.1	TABLE B.1	TABLE B.1	TABLE B.1	TABLE B.1
	TABLE 3.2	TABLE 3.2	TABLE 3.2	TABLE 3.2	TABLE 3.3	TABLE 3.8	TABLE 3.8	TABLE 3.8	TABLE 3.8
					TABLE 3.4	TABLE 3.9	TABLE 3.9		TABLE 3.12
					TABLE 3.5	TABLE 3.10	TABLE 3.11		TABLE 3.13
					TABLE 3.6				
					TABLE 3.7				
RELEVANT FIGURES	FIGURE 3 - 1	FIGURE 3 - 1	FIGURE 3 - 6	FIGURE 3 - 8	FIGURE 3 - 10	FIGURE 3 - 15	FIGURE 3 - 15	FIGURE 3 - 15	FIGURE 3 - 15
	FIGURE 3 - 2	FIGURE 3 - 4	FIGURE 3 - 7	FIGURE 3 - 9	FIGURE 3 - 11	FIGURE 3 - 16	FIGURE 3 - 16	FIGURE 3 - 16	FIGURE 3 - 16
	FIGURE 3 - 3	FIGURE 3 - 5			FIGURE 3 - 12	FIGURE 3 - 17	FIGURE 3 - 17	FIGURE 3 - 23	FIGURE 3 - 26
					FIGURE 3 - 13	FIGURE 3 - 18	FIGURE 3 - 22	FIGURE 3 - 24	FIGURE 3 - 27
					FIGURE 3 - 14	FIGURE 3 - 19		FIGURE 3 - 25	FIGURE 3 - 28
						FIGURE 3 - 20			
						FIGURE 3 - 21			

- Fully penetrating well with constant discharge (Problem GWF-1)
- Fully penetrating well in a horizontal anisotropic aquifer (Problem GWF-2)
- The Dupuit-Forchheimer Steady State Problem (Problem GWF-3)
- The Boussinesq Transient Problem (Problem GWF-4)

Problems GWF-1 and GWF-2 were selected from the document "Verification and Field Comparison of the Sandia Waste-Isolation Flow and Transport (SWIFT) Model" (Ward et al., 1984). Problems GWF-3 and GWF-4 were chosen from the "SWIFT II Self-Teaching Curriculum" (Reeves et al., 1986). The input data for these problems are exactly the same as the input data given in "SWIFT III Quality Assurance Benchmark Problem Execution Fiche" (GeoTrans, 1988). These problems were executed on IT's PRIME 750 and PRIME 316 EXL computers. Details of these problems and results are discussed in the following sections. Input parameters for these problems are given in Table 3.2.

3.1.1 Problem GWF-1: Fully Penetrating Well with Constant Discharge

3.1.1.1 Purpose of Problem Selection

Problem GWF-1 was selected to test the following aspects of the SWIFT III code:

- Confined aquifer
- Transient pressure solutions
- Cartesian coordinates
- Constant pumping rate

3.1.1.2 Problem Description

A description of this problem is given in Ward et al. (1984, pp. 2-1 to 2-3). The same description can also be found in Bear (1979, pp. 320 to 321) or Freeze and Cherry (1979, pp. 315 to 318).

TABLE 3.2

INPUT PARAMETERS FOR TWO-DIMENSIONAL ANALYTICAL GROUND WATER FLOW PROBLEMS

INPUT PARAMETER		PROBLEM GWF-1 THEIS SOLUTION (Theis, 1935)[b]		PROBLEM GWF-2 PAPADOPULOS SOLUTION (Papadopulos, 1965)[b]		PROBLEM GWF-3 DUPUIT-FORCHHEIMER SOLUTION (Bear, 1972)[b]		PROBLEM GWF-4 BOUSSINESQ SOLUTION (Bear, 1972)[b]	
	SYMBOL[a]	SI[b]	ENGLISH	SI	ENGLISH	SI	ENGLISH	SI	ENGLISH
Porosity	d	0.2	0.2	0.2	0.2	0.5	0.5	0.5	0.5
Hydraulic Conductivities:									
Horizontal	K_x, K_y	3.28 x 10^{-4} m/s	93.0 ft/d	3.28 x 10^{-4} m/s	93.0, 9.3 ft/d	0.03 m/s	8,503.1 ft/d	0.01 m/s	2,834.4 ft/d
Vertical	K_z	3.28 x 10^{-4} m/s	93.0 ft/d	3.28 x 10^{-4} m/s	93.0 ft/d	0.03 m/s	8,503.1 ft/d	100 m/s	2.83E+07 ft/d
Pumping rate	Q	0.003 m^3/s	9,153 ft^3/d	0.003 m^3/s	9,154 ft^3/d	N/A	N/A	N/A	N/A
Thickness	b	3.05 m	10.0 ft	3.05 m	10.0 ft	N/A	N/A	N/A	N/A
Aquifer radius	r_e	8,197 m	26,893 ft	8,197 m	26,893 ft	N/A	N/A	N/A	N/A
Storativity	S	99.67 x 10-4	99.67 x 10-4	99.67 x 10-4	99.67 x 10-4	N/A	N/A	N/A	N/A
Transmissivity	T	0.001 m^2/s	930 ft^2/d	0.001 m^2/s	930 ft^2/d	N/A[d]	N/A[d]	N/A[d]	N/A[d]
Wellbore radius	rw	0.1143 m	0.375 ft	0.1143 m	0.375 ft	N/A	N/A	N/A	N/A
Viscosity	)	0.001 Pa-s	1 cp	0.001 Pa-s	1cp	0.001 Pa-s	1 cp	0.001 Pa-s	1 cp
Water Density	P	1,000 kg/m^3	62.4 lb/ft^3	1,000 kg/m^3	62.4 lb/ft^3	1,000 kg/m^3	62.4 lb/ft^3	1,000 kg/m^3	62.4 lb/ft^3
Water Compressibility	C	0 1/Pa	0 1/psi	0 1/Pa	0 1/psi	0 1/Pa	0 1/psi	4.00E-10 1/Pa	2.76E-06 1/psi
Rock Compressibility	C_r	1.67E-07 1/Pa	0.00115 1/psi	1.67E-07 1/Pa	0.00115 1/psi	0 1/Pa	0 1/psi	0 1/Pa	0 1/psi
Height of Water Surface at:									
x = 0 meters (0-feet)	h_0	N/A	N/A	N/A	N/A	0.75 m	2.46 ft	0.5 m[f]	1.64 ft[f]
x = 20 meters (65.6-feet)	h_L	N/A	N/A	N/A	N/A	0.25 m	0.82 ft	N/A	N/A
t = 0 seconds (0-days)	h_{init}	N/A	N/A	N/A	N/A	N/A	N/A	1 m	3.28 ft
Surface Recharge	-	N/A	N/A	N/A	N/A	7.50E-05 m/s	21.27 ft/d	N/A	N/A

Notes:

[a] Symbols follow the convention adopted in SWIFT III manuals.

[b] See List of References for more information on the cited solutions.

[c] SI stands for Systeme Internationale or Metric System.

[d] N/A stands for Not Applicable.

[e] Transmissivity is a function of potentiometric head.

[f] For t > = 0.

A well fully penetrates an infinite confined aquifer and water is extracted at a constant rate, as depicted in Figure 3-1. The partial differential equation describing saturated flow in a confined aquifer in radial coordinates is given by Equation 3.1:

$$T \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial s}{\partial r}\right) = S \frac{\partial s}{\partial t} \qquad (3.1)$$

where

T = transmissivity [L^2/t]

S = storativity [dimensionless]

s = drawdown [L]

r = radial distance [L]

t = time [t]

The boundary and initial conditions are as follows:

$$s\ (r,\ t = 0) = 0, \qquad r \geq 0 \qquad (3.2)$$

$$s\ (r = \infty,\ t) = 0, \qquad t \geq 0 \qquad (3.3)$$

$$Q = 0, \qquad t = 0 \qquad (3.4a)$$

$$Q = \text{constant} > 0, \qquad t > 0 \qquad (3.4b)$$

where

Q = extraction rate [L^3/t]

3.1.1.3 Assumptions

The following assumptions are made:

- The aquifer is of infinite areal extent
- The aquifer is confined with no leakage
- The aquifer is homogeneous, horizontal, isotropic, and of uniform thickness

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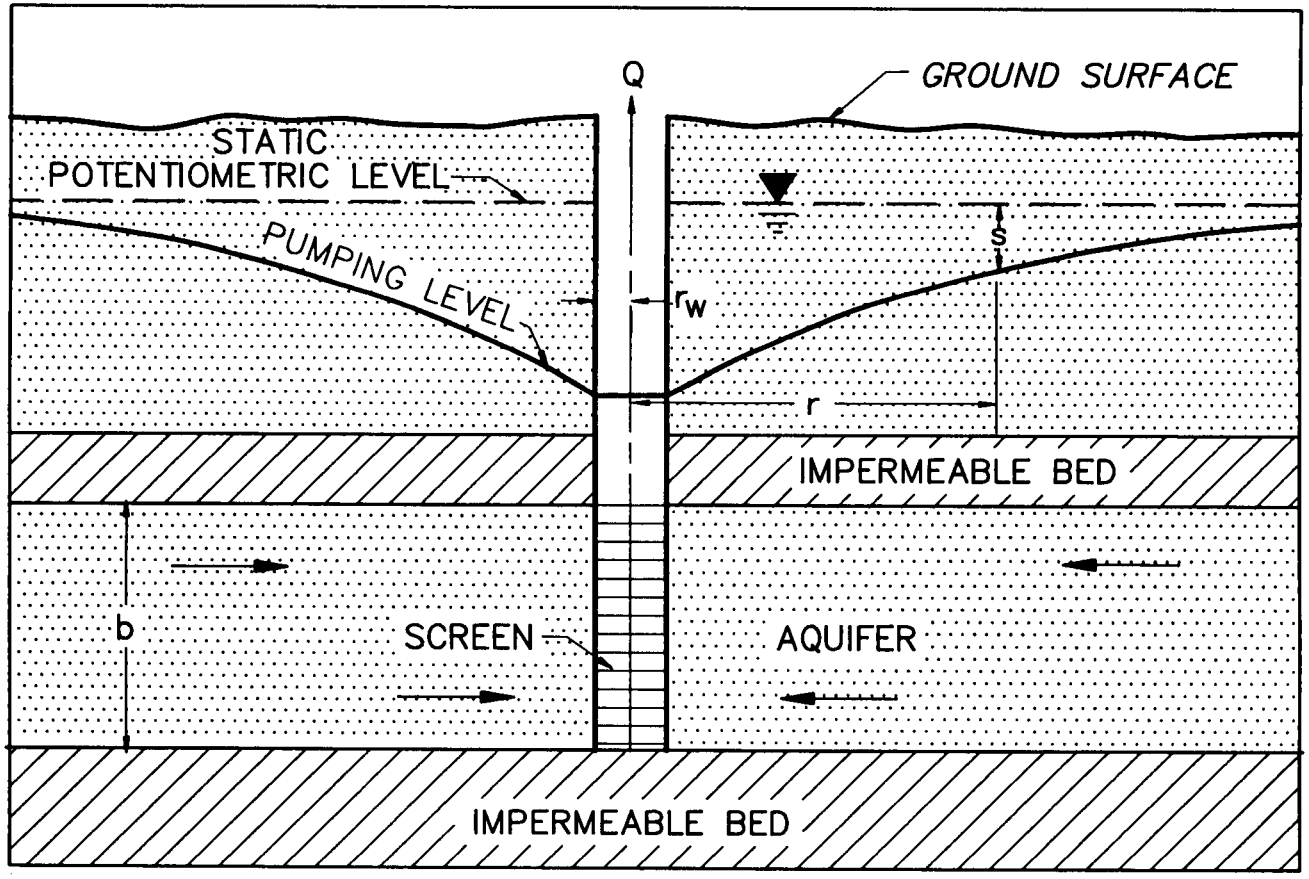

FIGURE 3-1

SCHEMATIC OF A FULLY PENETRATING WELL IN A CONFINED AQUIFER

PROBLEMS GWF-1 AND GWF-2

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- The static potentiometric surface is horizontal
- Water is extracted at a constant rate
- The extraction well penetrates the entire aquifer
- The diameter of the extraction well is sufficiently small that its internal storage may be neglected
- Darcy's law applies throughout the system, and nonlaminar flow near the well may be neglected

3.1.1.4 Analytical Solution

The analytical solution to this problem is given in Ward et al. (1984, pp. 2-3 to 2-4). The same solution can also be found in Bear (1979, pp. 320 to 321) and Freeze and Cherry (1979, pp. 315 to 318).

To solve Equation 3.1 for an aquifer of infinite areal extent, it is assumed that the well radius is infinitesimally small. The following boundary condition is, therefore, applicable:

$$\lim_{r \to 0} \left(r \frac{\partial s}{\partial r}\right) = -\frac{Q}{2\pi T}, \qquad t > 0 \qquad (3.5)$$

The solution of Equation 3.1, subject to the conditions of Equations 3.2, 3.3, 3.4, and 3.5, is the Theis solution:

$$s = \frac{Q}{4\pi T} W(u) \qquad (3.6)$$

where the dimensionless variable, u, is defined by:

$$u = \frac{r^2 s}{4Tt} \qquad (3.7)$$

and W(u) is the familiar well function (see Reed [1980] for numerical values of this function):

$$W(u) = \int_u^\infty \frac{e^{-u}}{u} du \qquad (3.8)$$

3.1.1.5 SWIFT III Simulation

Significant aspects of the numerical simulation of Problem GWF-1 are presented in Ward, et al. (1984, pp. 2-7 through 2-9), and are partly restated below.

The SWIFT III code solves the ground water equation (Equation 3.1) both in Cartesian and radial coordinates. For this verification problem, the Cartesian option was selected. The SWIFT III program solves for pressure as the dependent variable. The pressure must then be converted to potentiometric level and drawdown by separate calculations external to the SWIFT III code.

In the SWIFT III simulation, a finite well bore of radius r_w is considered at the inner model boundary. The effect of this finite radius is confined to a region of several well bore radii surrounding the origin, and therefore does not discredit the comparison of results with an analytical solution for which the well is infinitesimally narrow. The value used for the well radius is given in Table 3.2.

By taking advantage of mode symmetry within a Cartesian coordinate system, efficiency was gained through the use of only a quarter segment of the entire area as defined in the analytical solution. A 15-by-15-block grid was utilized with block dimensions ranging in size from 1 m (3.28 feet) at the well to 4,096 m (13,435 feet) at the outer extremity of the grid. No-flow symmetry conditions were applied along the coordinate axes and a Carter-Tracy condition was used at the outer extremity of the system.

3.1.1.6 Input Specifications

The input parameters for this example are given in Table 3.2. These data were taken from the "SWIFT III Quality Assurance Benchmark Problem Execution Fiche" (GeoTrans, 1988, File Name: VFC1), and were used directly in the verification process. The simulation period was 100 days.

3.1.1.7 Output Specifications

The output for this problem consists of pressure as a function of time and distance. By separate calculations, the resultant pressure was converted to hydraulic head, from which the drawdown was then derived.

3.1.1.8 Results

Drawdown as a function of time at 100 meters (328.0 feet) and as a function of distance at 100 days are given in Figures 3-2 and 3-3, respectively. The comparison of the SWIFT III results with the analytical solution is also depicted in these figures. Review of Figures 3-2 and 3-3 indicates that SWIFT III slightly overestimates drawdown when Cartesian coordinates are used. This overestimation is well within acceptable tolerance limits and is common to all other codes when Cartesian coordinates are used. The same results are also presented by Ward et al. (1984, pp. 2-10 to 2-11), thereby demonstrating that the SWIFT III code performs on the IT computer system in a manner comparable to other computer systems on which the code has been tested.

3.1.2 Problem GWF-2: Fully Penetrating Well in a Horizontally Anisotropic Aquifer

3.1.2.1 Purpose of Problem Selection

Problem GWF-2 was selected to test the following aspects of the SWIFT III code:

- Confined aquifer
- Transient pressure solution
- Two-dimensional Cartesian coordinates

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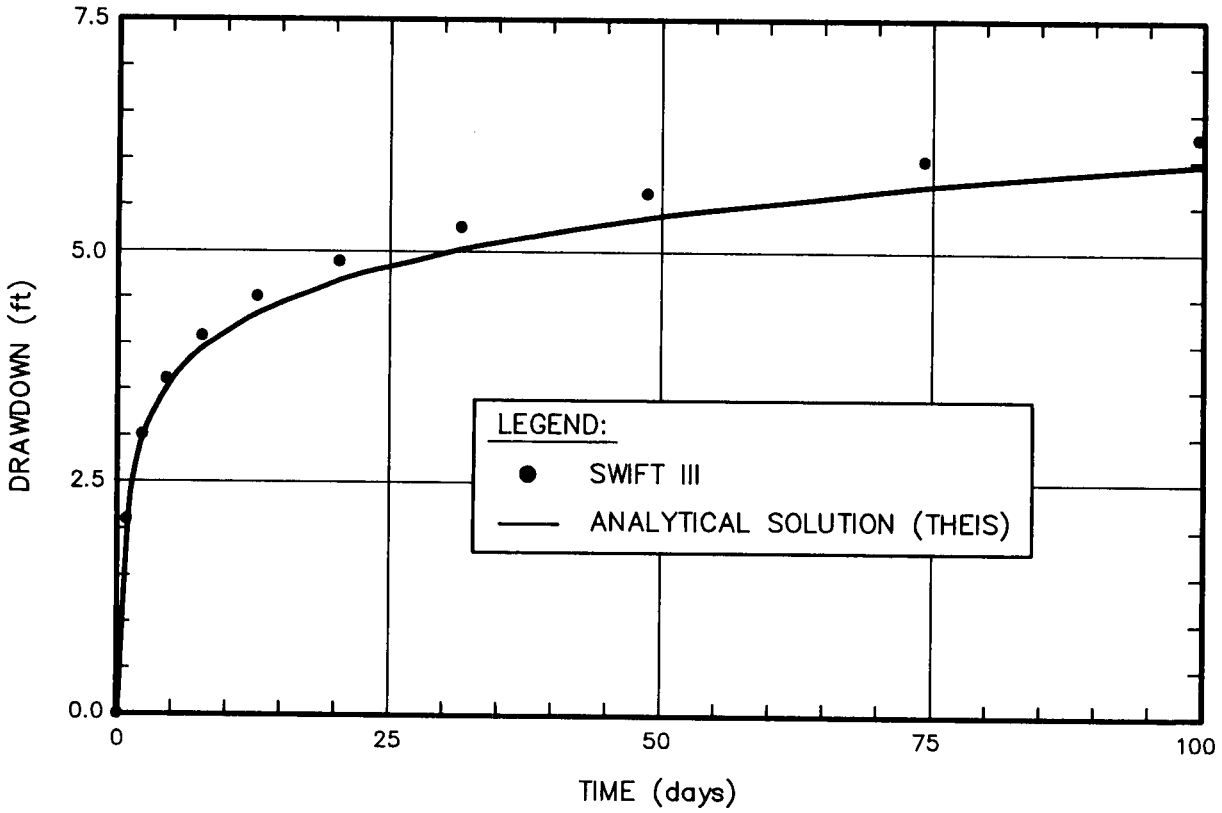

NOTE:

COMPARISON MADE AT A RADIUS OF 333.0 FEET.

FIGURE 3-2

COMPARISON OF DRAWDOWN VERSUS TIME

PROBLEM GWF-1

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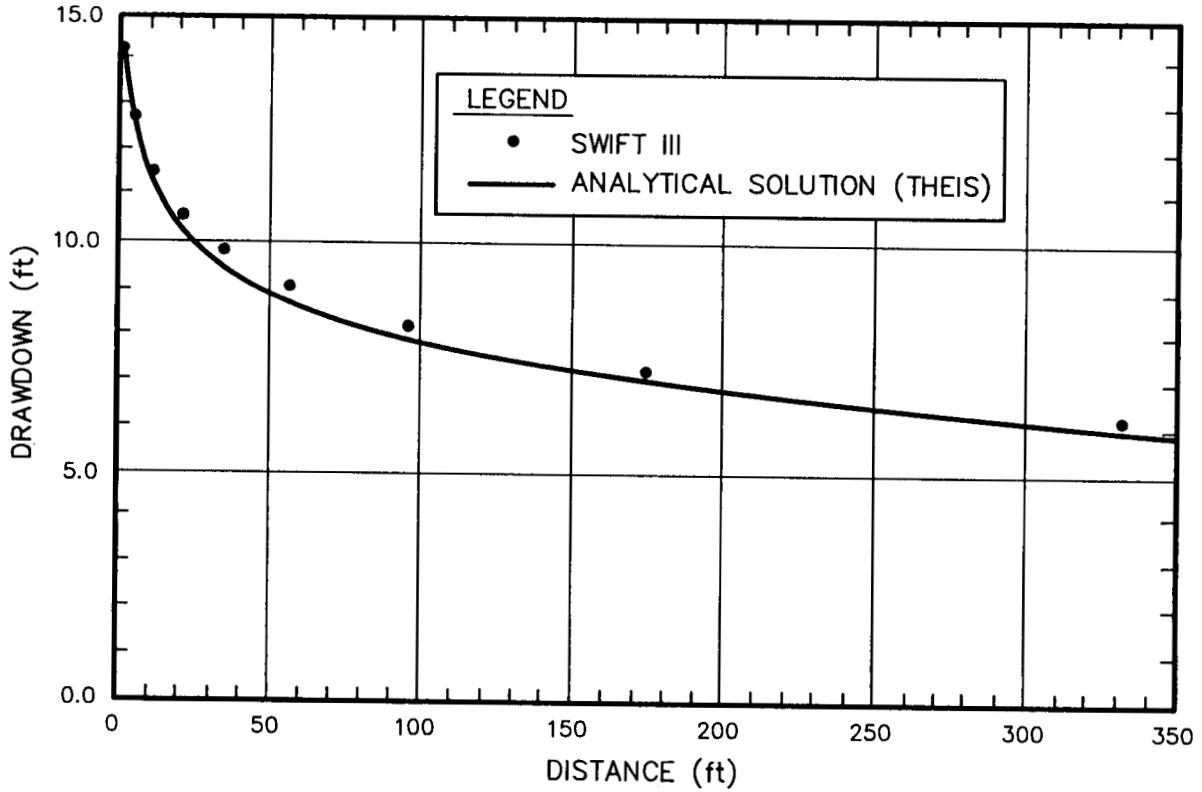

NOTE:

COMPARISON MADE AT 100 DAYS.

FIGURE 3-3

COMPARISON OF DRAWDOWN VERSUS DISTANCE

PROBLEM GWF-1

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- Constant pumping rate
- Anisotropic hydraulic conductivity distribution

3.1.2.2 Problem Description

A description of this problem is given in Ward, et al. (1984, pp. 2-19 and 2-20). The same description can also be found in Papadopulos (1965).

A well fully penetrates an infinite confined aquifer and water is extracted at a constant rate, as shown schematically in Figure 3-1. The aquifer is anisotropic and is parallel to the horizontal plane. If the coordinate axes (x and y) are aligned with the principal axes of the transmissivity tensor, the equation to be solved can be written as:

$$T_x \frac{\partial^2 s}{\partial x^2} + T_y \frac{\partial^2 s}{\partial y^2} + Q\ \delta(x)\ \delta(y) = S \frac{\partial s}{\partial t} \qquad (3.9)$$

where

T_x = transmissivity in the x-direction $[L^2/t]$

T_y = transmissivity in the y-direction $[L^2/t]$

s = drawdown $[L]$

S = storativity [dimensionless]

Q = pumping rate $[L^3/t]$

δ = Dirac delta function $[1/L]$

A coordinate transformation could be performed to facilitate the solution of this equation, namely:

$$\bar{x} = x \quad \text{and} \quad \bar{y} = (T_x/T_y)^{1/2} y \qquad (3.10)$$

This would, in effect, reduce the problem to the isotropic case, with the well-known Theis solution. This transformation is not considered further because the primary objective of this verification problem is to test the anisotropic simulation capabilities of the SWIFT III code.

The boundary and initial conditions are:

$$s(x, y, t = 0) = 0 , \quad x \geq 0 \quad \text{and} \quad y \geq 0 \tag{3.11}$$

$$s(x = \pm \infty, y, t) = 0 , \quad t > 0 \tag{3.12}$$

$$s(x, y = \pm \infty, t) = 0 , \quad t > 0 \tag{3.13}$$

$$Q = 0, \quad t = 0 \tag{3.14}$$

$$Q = \text{constant} > 0 \quad t > 0 \tag{3.15}$$

3.1.2.3 Assumptions

The assumptions in Section 3.1.1.3 are also valid for this problem, with the exception that the aquifer is anisotropic, in the current case.

3.1.2.4 Analytical Solution

The analytical solution for this problem was developed by Papadopulos (1965) and is also given in Ward et al. (1984, p. 2-20) and Reed (1980).

The solution of Equation 3.9, subject to the conditions of Equations 3.11 through 3.15, is as follows (Reed, 1980):

$$s = \frac{Q}{4\pi \, (T_x T_y)^{1/2}} W(u_{xy}) \tag{3.16}$$

where the dimensionless variable, u, is given by:

$$u_{xy} = \frac{S}{4t} \frac{T_x x^2 + T_y y^2}{T_x T_y} \tag{3.17}$$

and W (u_{xy}) is the familiar well function.

3.1.2.5 SWIFT III Simulation

The numerical simulation is discussed in Ward et al. (1984, pp. 2-21 and 2-22) and is summarized below.

The grid system for this simulation is similar to that used for Problem GWF-1, except that three additional rows of elements were added in the x-direction, thus extending the system length from 8,147.5 to 65,542 meters (26,730.6 to 21,5032.8 feet). The reason for this addition is that the cone of depression of an anisotropic aquifer is elliptical, thus requiring a larger domain in the direction of the major axis, in this case the x-direction. This is not an exact symmetric section of the areal plane surrounding the well. However, because of the small geometric discrepancy, the effects are expected to be negligible.

The infinite boundary condition of Equations 3.12 and 3.13 are approximated by no-flow conditions at the outer periphery of the system. This selection of these boundary conditions is valid because the cone of depression is not likely to extend to the finite boundaries during the maximum simulation period of 100 days. That is, the cone of depression should be well contained in the 65.5 km x 8.1 km region being modeled.

3.1.2.6 Input Specifications

The input data parameters for this problem are given in Table 3.2. The input data for this problem were taken directly from the "SWIFT III Quality Assurance Benchmark Problem Execution Fiche" (GeoTrans, 1988, File Name: VFC7), and was used directly in the verification process. The total simulation period, as indicated earlier, was 100 days.

3.1.2.7 Output Specifications

The output for this problem consists of pressure as a function of time and distance. Again, the pressure values were converted to hydraulic head and drawdown in a procedure external to the SWIFT III code.

3.1.2.8 Results

The same results found by Ward et al. (1984, pp. 2-23 and 2-24) were obtained by IT. The values of drawdown versus time and distance for this problem are presented in Figures 3-4 and 3-5, respectively. The drawdown as a function of time was determined at the point x = 332.9 feet, y = 1.6 feet (Figure 3-4). Drawdown along both the x and y axes as a function of distance were plotted at 100 days (Figure 3-5). These drawdown curves again indicate that the SWIFT III results compare well with the analytical solution of Papadopulos.

3.1.3 Problem GWF-3: The Dupuit-Forchheimer Steady-State Problem

3.1.3.1 Purpose of Problem Selection

Problem GWF-3 was selected to test the following aspects of the SWIFT III code:

- Unconfined aquifer
- Steady-state pressure solution
- Two-dimensional Cartesian coordinates
- Recharge
- Constant-head boundary condition

3.1.3.2 Problem Description

A description of this problem is given in Reeves et al. (1986, p. 70). The same description can also be found in Bear (1972, pp. 366 to 367).

A phreatic aquifer of length, L (Figure 3-6) with constant ground water elevations:

$$h(x = 0,t) = h_o \tag{3.18}$$

and

$$h(x = L,t) = h_L \tag{3.19}$$

is subjected to surface recharge at a rate, q. The ground water elevations, h_o and h_L, are defined as the height of the water table

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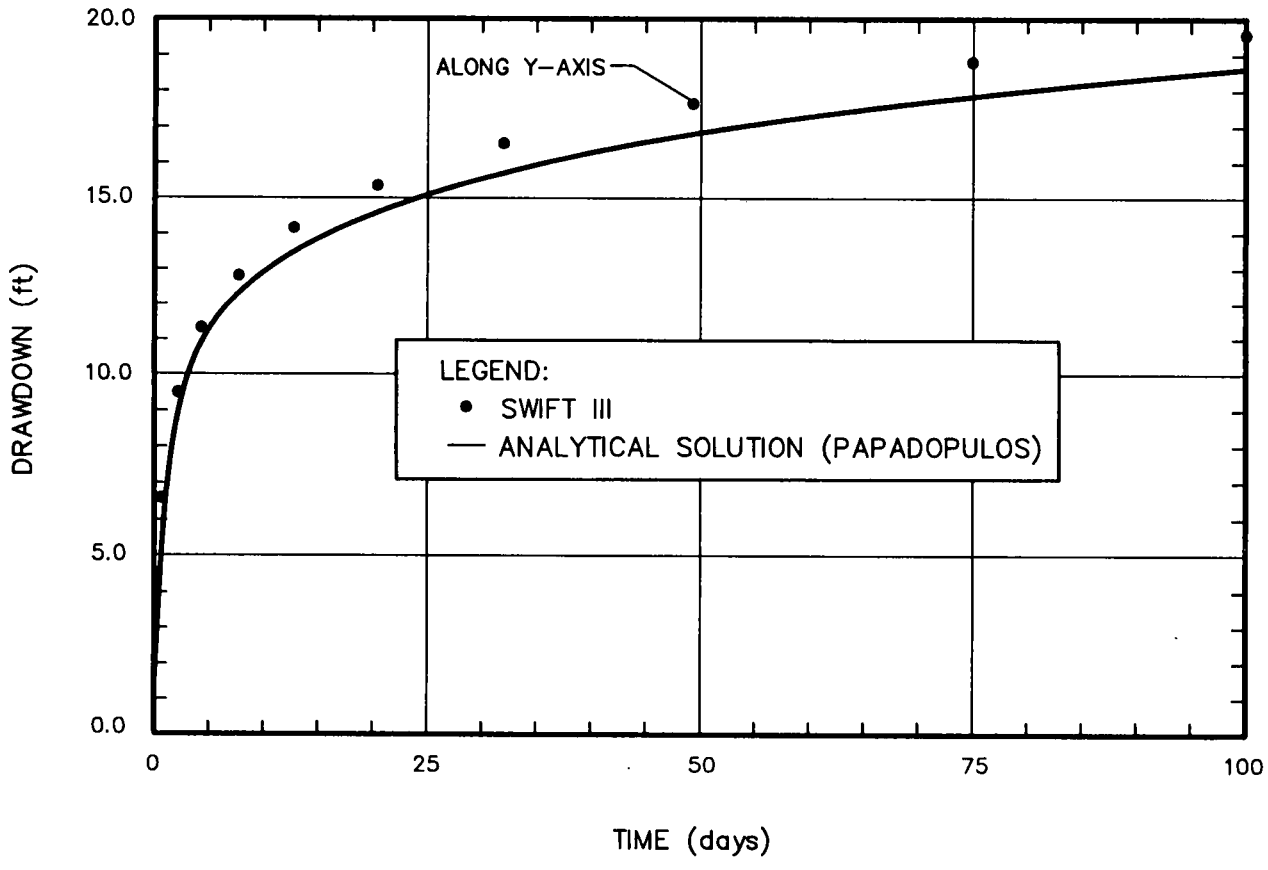

NOTE:

COMPARISON MADE AT WELL LOCATION: (9,1)
X = 332.863 FEET, Y = 1.64 FEET.

FIGURE 3-4

COMPARISON OF DRAWDOWN VERSUS TIME

PROBLEM GWF-2

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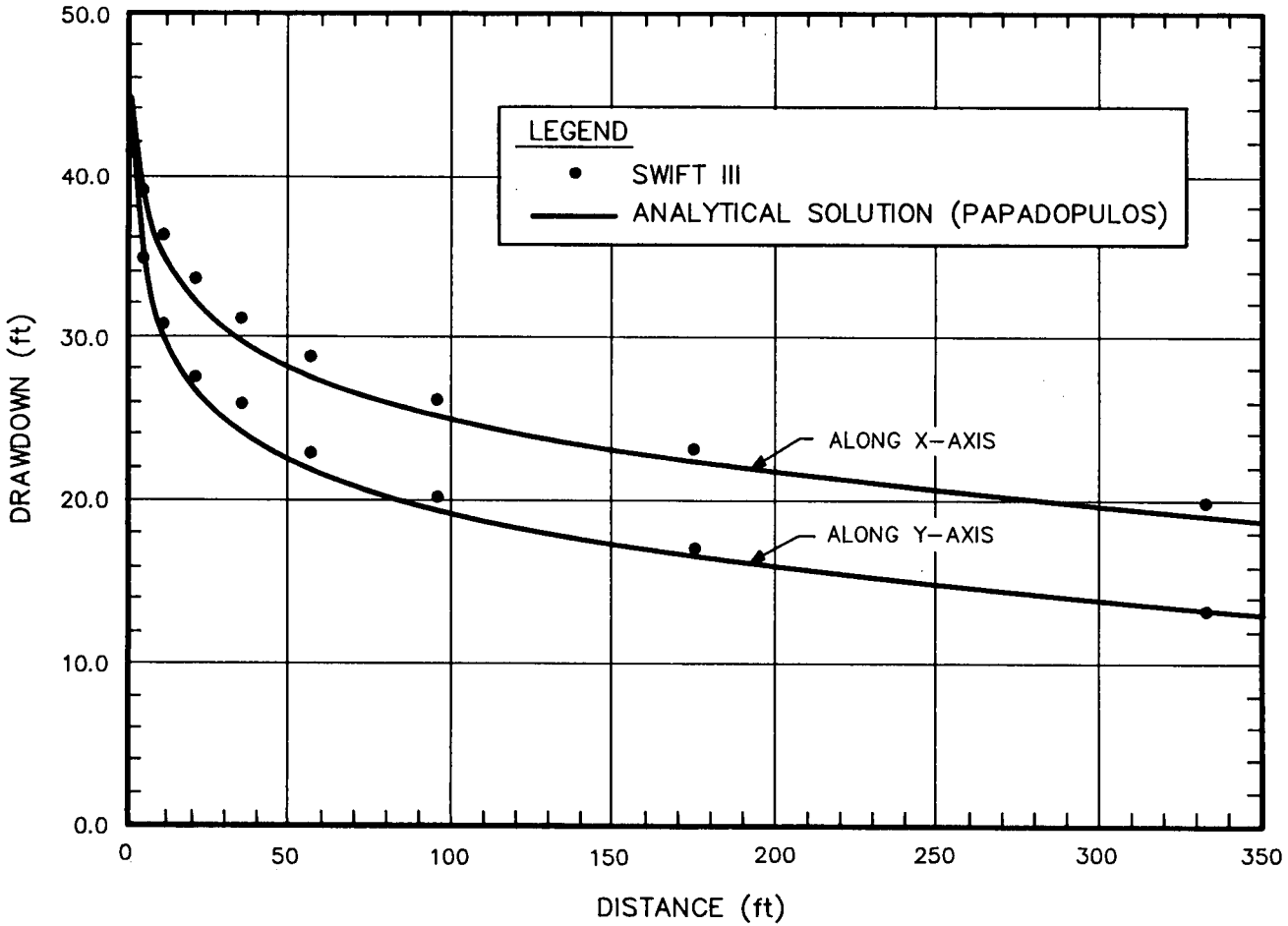

NOTE:

COMPARISON MADE AT 100 DAYS.

FIGURE 3-5

COMPARISON OF DRAWDOWN VERSUS DISTANCE

PROBLEM GWF-2

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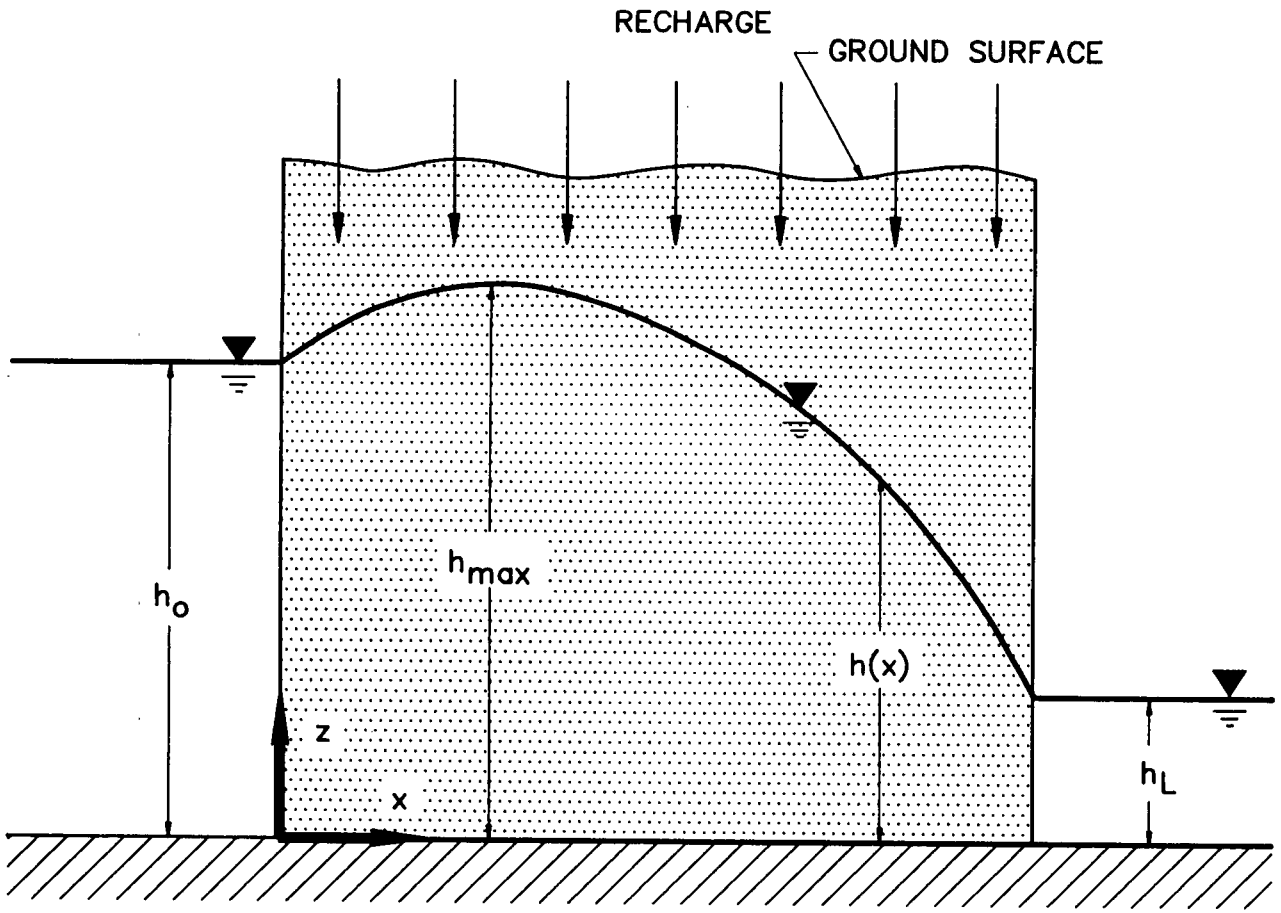

FIGURE 3-6

SCHEMATIC OF UNCONFINED AQUIFER WITH RECHARGE

PROBLEM GWF-3

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above an impervious bottom, and thus represents the saturated thickness at x = 0 and x = L (Figure 3-6). The objective of this problem is to determine the steady-state ground water elevation, h(x), at any distance x between x = 0 and x = L.

The governing equation for this problem for the steady state condition is (Bear, 1972):

$$\frac{\partial}{\partial x}\left(K_x h \frac{\partial h}{\partial x}\right) + q = 0 \qquad (3.18)$$

where

q = recharge [L/t]

The above is known as the Forchheimer equation.

3.1.3.3 Assumptions

The assumptions are the following:

- The aquifer is unconfined with no leakage at the bottom
- The aquifer is homogeneous and isotropic
- Darcy's law applies throughout the system
- Constant recharge

3.1.3.4 Analytical Solution

The analytical solution of Equation 3.18 is the Dupuit-Forchheimer parabola:

$$h^2 - h_o^2 = (h_L^2 - h_o^2)\frac{x}{L} + \frac{q}{K_x}(L-x)x \qquad (3.19)$$

in which h_o and h_L are the saturated thicknesses at x=o and x=L, respectively.

The analytical solution is given in Reeves et al. (1986, pp. 70 to 73). The same solution is also given in Bear (1972, pp. 366 to 367). Because the analytical solution neglects the vertical component of flow, a one-dimensional solution along the x-coordinate results (Equation 3.21).

The flow rates at the boundaries are given by:

$$u_o = \frac{K_x}{2L} (h_o^2 - h_L^2) - \frac{qL}{2} \qquad (3.22a)$$

$$u_L = \frac{K_x}{2L} (h_o^2 - h_L^2) + \frac{qL}{2} \qquad (3.22b)$$

The first term on the right-hand side of the equations represents the flow resulting from the difference in heads across the system. This rate is the same for both ends. The second term arises from the surface recharge.

3.1.3.5 SWIFT III Simulation

A two-dimensional vertical cross-section with a 20 by 20 grid was used to simulate Problem GWF-3. Constant ground water elevations of 0.75 and 0.25 meters were assigned at the boundaries. The distance between these boundaries was 20 meters. Additional discussions on the numerical solution can be found in Reeves et al. (1986, p. 73).

3.1.3.6 Input Specifications

The input data for this problem are given in Table 3.2. The input data are identical with the "SWIFT III Quality Assurance Benchmark Problem Execution Fiche" (GeoTrans, 1988, File Name: STC2-8).

3.1.3.7 Output Specifications

The output for this problem consisted of steady state pressures, which have been converted to ground water surface elevations.

3.1.3.8 Results

The values of ground water elevation versus distance for both the analytical solution and the model are depicted in Figure 3-7. The same results are also presented in Reeves et al. (1986, p. 77). The results indicate very good agreement between the analytical and numerical solutions.

3.1.4 Problem GWF-4: The Boussinesq Transient Problem

3.1.4.1 Purpose of Problem Selection

Problem GWF-4 was selected to test the following aspects of the SWIFT III code:

- Unconfined aquifer
- Transient pressure solution
- Two-dimensional Cartesian coordinates
- Constant-head boundary condition

3.1.4.2 Problem Description

Description of this problem is given in Reeves et al. (1986, p. 79). The same description can also be found in Polubarinova-Kochina (1962, pp. 508 to 512) and Bear (1972, pp. 381 to 384).

The problem considered is a semi-infinite phreatic aquifer (Figure 3-8), which is initially saturated such that:

$$h(x,0) = h_o \qquad (3.23)$$

where h is the elevation of the ground water table above an impervious bottom (equivalent to saturated thickness) as defined in Figure 3-8.

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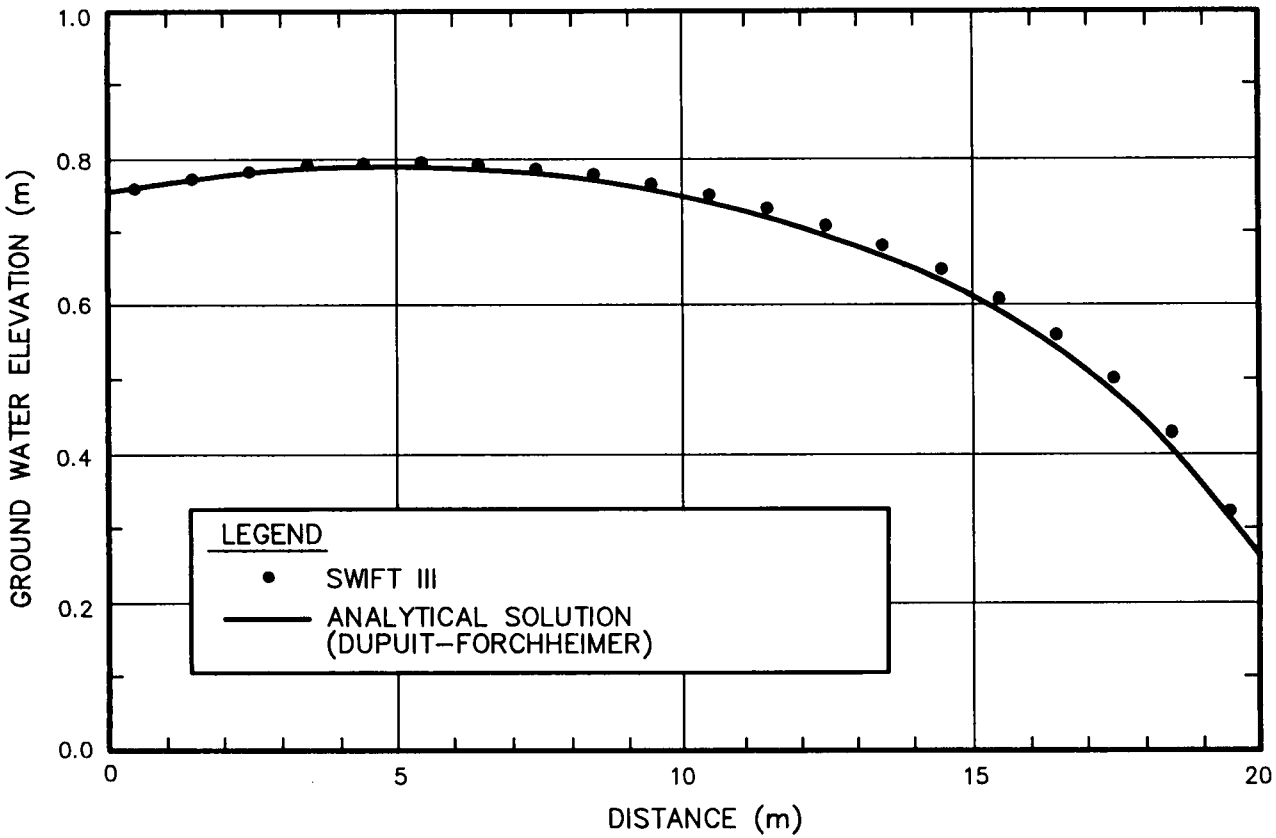

FIGURE 3-7

COMPARISON OF
GROUND WATER ELEVATION
VERSUS
DISTANCE

PROBLEM GWF-3

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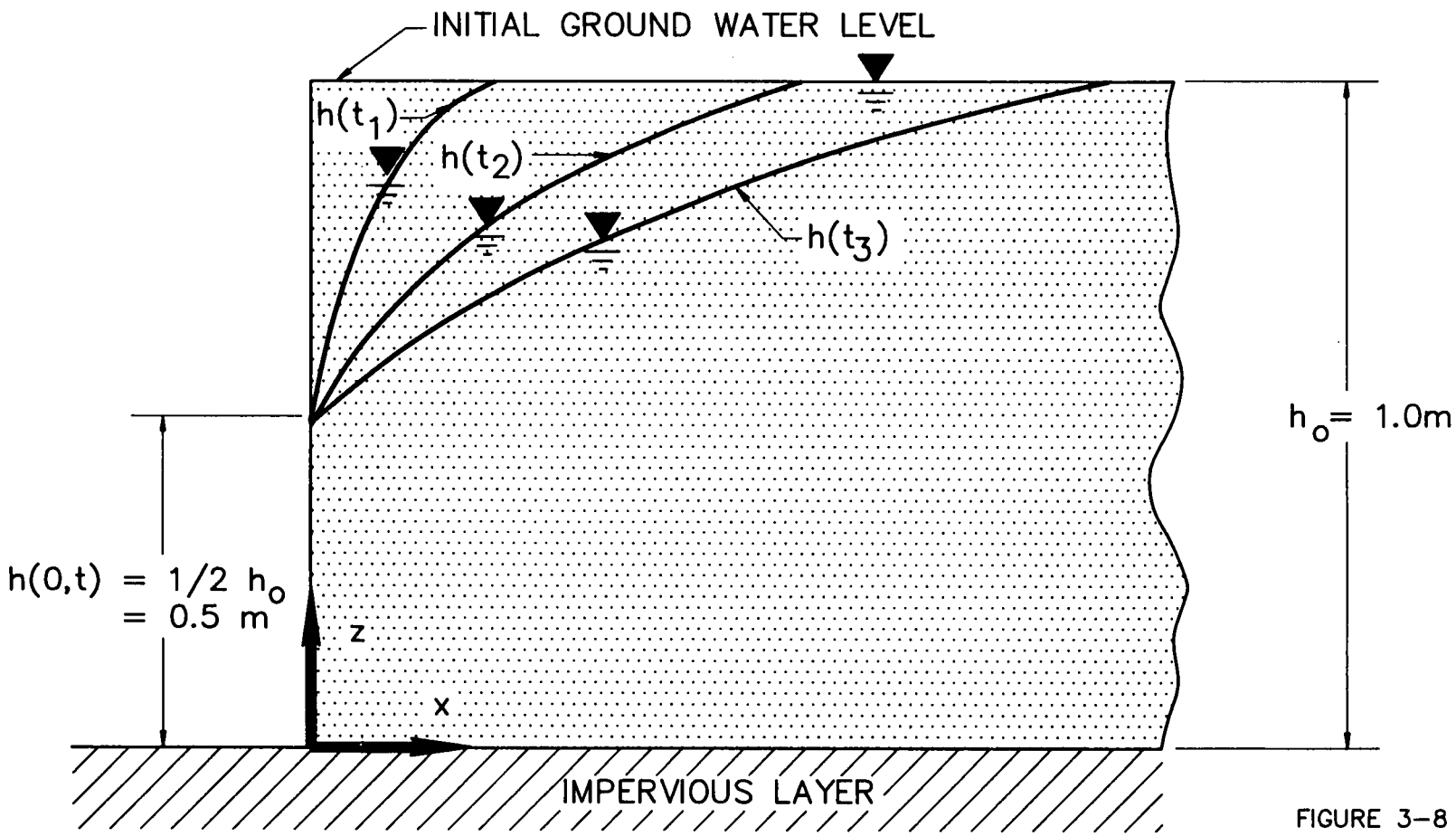

FIGURE 3-8

SCHEMATIC OF TRANSIENT DRAWDOWN IN AN UNCONFINED AQUIFER

PROBLEM GWF-4

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For t > 0, the saturated thickness at x = o end is reduced to half of its original value, i.e.

$$h(0,t) = \frac{h_o}{2} \tag{3.24}$$

No recharge occurs through the upper surface. The objective is to determine the ground water surface elevation, h(x, t), as a function of position and time.

3.1.4.3 Assumptions

The assumptions are the following:

- The aquifer is unconfined with no leakage
- The aquifer is homogeneous and isotropic
- Darcy's law applies throughout the system

3.1.4.4 Analytical Solution

The analytical solution is given in Polubarinova-Kochina (1962, p. 511) and Bear (1972, p. 384).

Transmissivity is taken to be proportional to the saturated thickness, h, and flow is assumed to be horizontal. The equation of continuity (Bear, 1972) is:

$$\frac{\partial}{\partial x}\left(K_x h \frac{\partial h}{\partial x}\right) = \phi \frac{\partial h}{\partial t} \tag{3.25}$$

where

K_x = horizontal hydraulic conductivity [L/t]

h = saturated thickness [L]

ϕ = porosity [dimensionless]

Equation 3.25 is the Boussinesq equation. The Polubarinova-Kochina general solution for this nonlinear equation is presented in Bear (1972, p. 384). A dimensionless form of this solution is presented in Figure 3-9 using normalized ground water elevation versus normalized time coordinates.

3.1.4.5 SWIFT III Simulation

A two-dimensional grid is used in the numerical simulation of the problem. The grid length is 5.8 meters and the initial ground water elevation is 1.0 meters. To approximate the assumption of one-dimensional flow in the analytical solution, a relatively high vertical hydraulic conductivity, K_z, was chosen for the numerical solution. By this approach, flow in the x-direction dominated the numerical solution. Other aspects of the numerical solution are discussed in Reeves et al. (1986, pp. 79 to 87).

3.1.4.6 Input Specifications

The input data for this problem are given in Table 3.2. The input data for this problem are identical to the "SWIFT III Quality Assurance Benchmark Problem Execution Fiche" (GeoTrans, 1988, File Name: STC2-9).

3.1.4.7 Output Specifications

The output for this problem was the transient pressure distribution, which has been converted to ground water elevations for purposes of direct comparison with analytical results.

3.1.4.8 Results

The normalized ground water elevation versus normalized time values for two different locations along the x-axis are plotted in Figure 3-9. These locations are at 0.25 meters and 0.125 meters from the origin, as shown in Figure 3-8. Similar results have been obtained by Reeves et al. (1986, p. 82). Review of Figure 3-9 indicates that for small elapsed times i.e., when the value of the term $\xi/\sqrt{2h(0)}$ is large, the SWIFT III computed ground water surface declines more rapidly than that of the analytical solution. Even in this case, however, the relative difference between the analytical and model results is only a few percent. As time increases the agreement improves and the discrepancy becomes very small.

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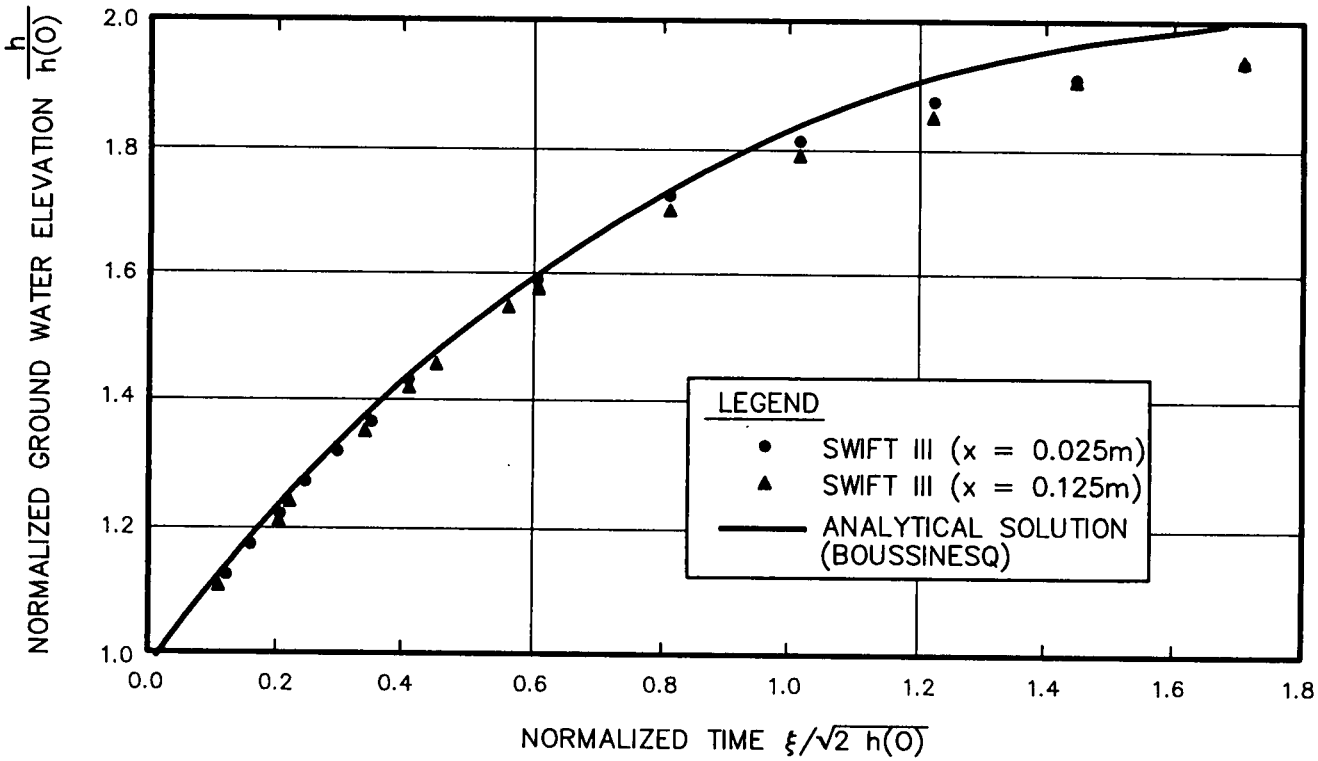

LEGEND:

$\xi = \left(\frac{\phi}{2Kt}\right)^{1/2} x$

ϕ = POROSITY

K_x = HYDRAULIC CONDUCTIVITY (0.01 m/sec.)

$h_o/h(o,t) = 2.0$

K_z = 100m/sec

FIGURE 3-9

COMPARISON OF
NORMALIZED GROUND WATER ELEVATION
VERSUS
NORMALIZED TIME

PROBLEM GWF-4

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3.2 VERIFICATION PROBLEMS - NUMERICAL SOLUTIONS

As discussed in Chapter 2.0, comparisons were made of two- and three-dimensional numerical ground water flow simulations using different codes to further verify the performance of the SWIFT III code. For a two-dimensional simulation, the GEOFLOW and MODFLOW computer codes were used as the basis for comparison with the SWIFT III Code. A grid system previously established by IT for a separate study at the FMPC (IT 1988) was used for this simulation. This verification exercise is defined as Problem GWF-5.

Three-dimensional ground water flow simulations were also made with SWIFT III, MODFLOW, and PTC. These simulations were made using Problem GWF-6. The SWIFT III results were compared with those of MODFLOW and PTC. A three-dimensional hypothetical grid, given in Finley and Reeves (1982, p. 4), was selected for this simulation. Several code features relevant to the FMPC site were tested with Problem GWF-6.

Details of the numerical simulations and results are discussed in the following sections.

3.2.1. Problem GWF-5: Two-Dimensional Comparisons

3.2.1.1 Purpose of Problem Selection

Problem GWF-5 was selected to test the combination of the following capabilities of the SWIFT III code:

- Unconfined aquifer
- Steady-state pressure solution
- Two-dimensional Cartesian coordinates
- Irregular boundaries and variable aquifer thickness
- Variable hydraulic conductivity
- Constant-head and no-flow boundary conditions

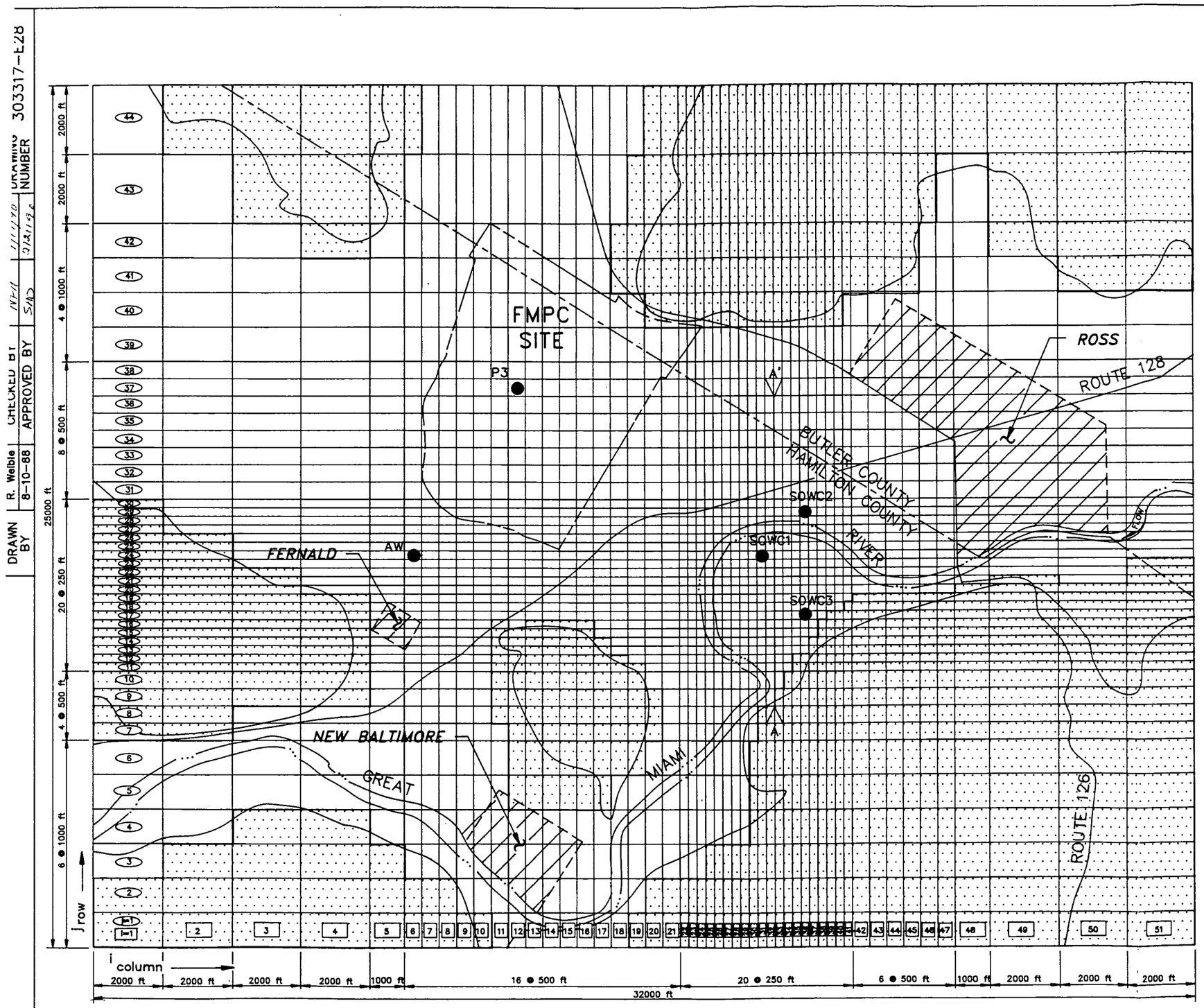
- Nonuniform recharge
- Irregular river curvature
- Constant rate pumping of wells

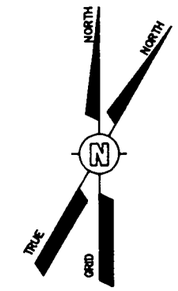
3.2.1.2 Problem Description

The sitewide simulation area for Problem GWF-5 is shown in Figures 3-10 or 3-11. This area was used in the Zone of Influence Study and includes the area under the possible influence of the Southwestern Ohio Water Company (SOWC) extraction (collector) wells, located within and near the major bend in the river east of the FMPC.

The aquifer in the study area is comprised of highly permeable, well-sorted sands and gravels and was modeled as an unconfined aquifer. The model area has basically three zones. The presence or absence of a till layer over the sand and gravel aquifer differentiates two of these zones. Bedrock outcrops form the third zone. The aquifer has the potential to receive recharge from the land surface and from the Great Miami River. Four active extraction (collector) wells exist in the study area and were included in the model. One additional well, SOWC 3, is shown on the figures but is used on a standby basis only and, therefore, it was not used in the modeling.

Because of certain characteristics of the codes used in this verification problem, and because of the need for accurate comparisons between the codes, two different grids were used in the problem solution. SWIFT III and MODFLOW are block-centered finite-difference codes. The two-dimensional grid system for the SWIFT III and MODFLOW models is shown in Figure 3-10. GEOFLOW is a node-centered finite element code. The two-dimensional grid system for the GEOFLOW model is shown in Figure 3-11. The nodes on the finite element (GEOFLOW) grid correspond to the corners of the block-centered finite-difference (SWIFT III and MODFLOW) grid. Similarly, the element centers of the finite element grid correspond to the centers of the finite-difference blocks. This permits a one-to-one





LEGEND

- MODEL CELL
- 39 MODEL CELL J-(ROWS) NUMBER
- BEDROCK CELL (LOW HYDRAULIC CONDUCTIVITY)
- 5 MODEL CELL I-(COLUMN) NUMBER
- ● PRODUCTION WELLS

NOTE:

1. SECTION A-A' WAS USED TO COMPARE DARCY VELOCITIES BETWEEN MODELS
2. SOWC1, SOWC2 AND SOWC3 ARE SOUTH WESTERN OHIO WATER COMPANY WELLS.

SCALE

0 2000 4000 6000 FEET

FIGURE 3-10

SWIFT III AND MODFLOW GRID SYSTEM FOR TWO-DIMENSIONAL FINITE-DIFFERENCE MODEL PROBLEM GWF-5

PREPARED FOR

FERNALD RI/FS
U.S. DEPARTMENT OF ENERGY
OAK RIDGE OPERATIONS

INTERNATIONAL TECHNOLOGY CORPORATION

DRAWN BY R. Weible 8-10-88
CHECKED BY
APPROVED BY
DRAWING NUMBER 303317-E28

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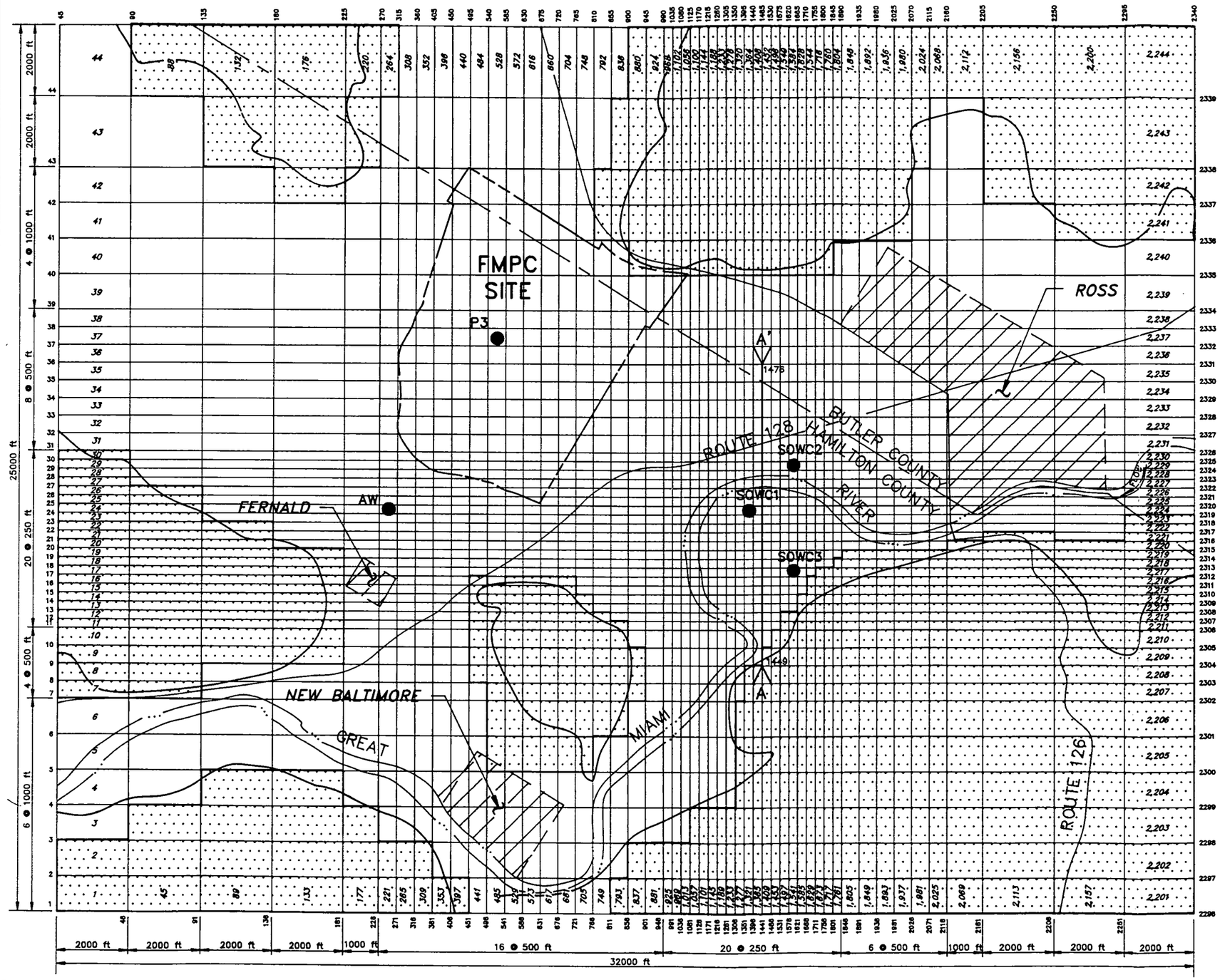

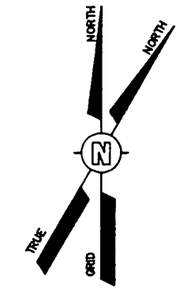

LEGEND

- MODEL FINITE ELEMENT
- FINITE ELEMENT NUMBER
- BEDROCK ELEMENT (LOW HYDRAULIC CONDUCTIVITY)
- PRODUCTION WELLS

NOTES:

1. SECTION A–A' WAS USED TO COMPARE DARCY VELOCITIES BETWEEN MODELS
2. SOWC1, SOWC2 AND SOWC3 ARE THE SOUTH WESTERN OHIO WATER COMPANY WELLS.

SCALE

0 2000 4000 6000 FEET

FIGURE 3–11

GEOFLOW GRID SYSTEM FOR TWO–DIMENSIONAL FINITE ELEMENT MODEL PROBLEM GWF–5

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correlation between cells and elements, and facilitates the transfer of information between finite-difference and finite element models.

A rectangular finite difference grid system consisting of 44 rows and 51 columns was used to model the study area. At the outer limit of the model area, where less detail is required, elements are 2,000 by 2,000 feet (609.6 by 609.6 meters). The grid size becomes gradually smaller inward and reaches a minimum size of 250 by 250 feet (76.2 by 76.2 meters) in the area surrounding the SOWC extraction wells and the meander loop on the Great Miami River.

The finite element grid system has an identical configuration to the finite-difference grid. It consists of 2244 elements and 2340 nodes.

3.2.1.3 Assumptions

The following assumptions are made in the simulations:

- The aquifer is unconfined with no base leakage
- Extraction is performed at a constant rate at each well, although rates vary from well to well
- The extraction wells penetrate the entire aquifer
- Darcy's law applies throughout the system, and nonlaminar flow near the wells may be neglected

3.2.1.4 Numerical Simulations

All three codes, SWIFT III, GEOFLOW, and MODFLOW, solve the same ground water flow equation. However, the numerical algorithm of each code is different. The differences can be summarized in the following manner:

- The three codes handle boundary conditions differently. The constant head boundary condition is treated in SWIFT III by assigning the head to the outer face of the boundary blocks. In the MODFLOW code, the constant heads are assigned at the center of boundary blocks. In GEOFLOW, constant heads are assigned at the boundary nodes.

- The SWIFT III uses a well submodel to calculate pressures near well bores. This formulation assumes that a skin surrounds the well bore and that the pressure drop across this "skin" is proportional to the flow rate. GEOFLOW and MODFLOW do not have well submodels.

- In the SWIFT III code, the well submodel is also used to simulate aquifer discharge into rivers and streams (Finley and Reeves, 1982, p. 29). In GEOFLOW, the river is simulated using its "recharge and thickness data" subset (IT, 1986, p. 2-8). MODFLOW has a separate river package to simulate river effects (McDonald & Harbaugh, 1984, p. 209).

3.2.1.5 Input Specifications

Input parameters for this example were initially taken from the Zone of Influence Study report (IT, 1988a). However, to better incorporate the verification study objectives, some changes were made to the initial input data. These changes did not compromise the types of aquifer conditions forming the underlying purpose of this verification problem (Section 3.2.1.1). The input parameters for SWIFT III, MODFLOW, and GEOFLOW models are given in Tables 3.3, 3.4, and 3.5, respectively.

3.2.1.6 Output Specifications

The output for SWIFT III consists of the pressure distribution, river leakage values, and Darcy velocity components. The output for GEOFLOW includes hydraulic head, river leakages, and Darcy velocity components. The output for MODFLOW consists of hydraulic head, river leakages, and flow rates for the front, right, and bottom faces of each block. In comparing the results of the three different codes, the following factors must be accounted for:

- The pressure and Darcy velocity components for SWIFT III are given at the center of each block. SWIFT III provides Darcy velocity components assuming a fully saturated cell. Thus, a correction factor has to be applied to those cells that are not fully saturated to allow a direct comparison of Darcy velocity components.

TABLE 3.3

INPUT PARAMETERS
FOR TWO-DIMENSIONAL NUMERICAL
GROUND WATER FLOW
SWIFT III MODEL
PROBLEM GWF-5

I. Finite-Difference Grid System[a]

Length: (i-direction)	32,000 feet
Width: (j-direction)	25,000 feet
Number of cells:	2,244
Number of layers:	1

II. Hydrogeologic Parameters

Base of aquifer:	From 350 to 525 feet MSL[b]
Precipitation recharge:	
Zone 1 (river flood plain):	14 inches/year
Zone 2 (bedrock elements):	0
Zone 3 (aquifer covered by till):	6 inches/year
Note: River elements lack precipitation recharge	
Hydraulic conductivities:	
Zone 1:	400 feet/day
Zone 2:	3×10^{-3} feet/day
Zone 3:	400 feet/day
Note: Hydraulic conductivity is assumed isotropic within each zone	
Porosities:	
Zone 1:	0.25
Zone 2:	0.10
Zone 3:	0.25
Type of aquifer:	Unconfined
Flow regime:	Steady state

See footnotes at end of table.

TABLE 3.3
(Continued)

II. Hydrogeologic Parameters (cont'd)

Boundary conditions:

Grid lower west boundary:	492 feet MSL[b]
Grid upper west boundary:	535 feet MSL
Grid north boundary:	540 feet MSL
Grid south boundary:	504 feet MSL
Grid east boundary:	530 feet MSL

Extraction wells production schedule:

WELL	CELL i, j[a]	PUMPING RATE
SOWC 1	32, 24	1,644,000 $feet^3$/day
SOWC 2	36, 30	822,000 $feet^3$/day
FMPC-P3	12, 37[c]	64,000 $feet^3$/day
Albright and Wilson	7, 25	19,000 $feet^3$/day

River bed leakage factor: 0.42 day^{-1}

[a]Refer to Figure 3-10 for cell locations.

[b]MSL = above mean sea level.

[c]The correct coordinates for Well P3 are i = 12, j = 37; however, for the verification study, this well was located in the same cell as in the other models.

TABLE 3.4

INPUT PARAMETERS
FOR TWO-DIMENSIONAL NUMERICAL
GROUND WATER FLOW
MODFLOW PROBLEM GWF-5

I. Finite-Difference Grid System[a]

Length: (i-direction)	32,000 feet
Width: (j-direction)	25,000 feet
Number of cells:	2,244
Number of layers:	1

II. Hydrogeologic Parameters

Base of aquifer:	From 350 to 525 feet MSL[b]
Precipitation recharge:	
Zone 1 (river flood plain):	14 inches/year
Zone 2 (bedrock elements):	0
Zone 3 (aquifer covered by till):	6 inches/year
Note: River elements have precipitation recharge	
Hydraulic conductivities:	
Zone 1:	400 feet/day
Zone 2:	3×10^{-3} feet/day
Zone 3:	400 feet/day
Note: Hydraulic conductivity is assumed isotropic within each zone	
Porosities:	
Zone 1:	0.25
Zone 2:	0.10
Zone 3:	0.25
Type of aquifer:	Unconfined
Flow regime:	Steady state

See footnotes at end of table.

TABLE 3.4
(Continued)

II. Hydrogeologic Parameters (cont'd)

Boundary conditions:

Grid lower west boundary:	492 feet MSL[b]
Grid upper west boundary:	535 feet MSL
Grid north boundary:	540 feet MSL
Grid south boundary:	504 feet MSL
Grid east boundary:	530 feet MSL

Extraction wells production schedule:

WELL	CELL i, j[a]	PUMPING RATE
COLL 1	32, 24	1,644,000 $feet^3$/day
COLL 2	36, 30	822,000 $feet^3$/day
FMPC-P3	12, 37[c]	64,000 $feet^3$/day
Albright and Wilson	7, 25	19,000 $feet^3$/day

River bed leakage factor: 0.42 day^{-1}

[a]Refer to Figure 3-10 for cell locations.

[b]MSL = above mean sea level.

[c]The correct coordinates for Well P3 are i = 12, j = 37; however, for the verification study, this well was located in the same cell in the other models.

TABLE 3.5

INPUT PARAMETERS
FOR TWO-DIMENSIONAL NUMERICAL
GROUND WATER FLOW
GEOFLOW MODEL
PROBLEM GWF-5

I. Finite Element Grid System[a]

Length: (x-direction)	32,000 feet
Width: (y-direction)	25,000 feet
Number of elements:	2,244
Number of nodes:	2,340

II. Hydrogeologic Parameters

Base of aquifer:	From 350 to 525 feet MSL[b]
Precipitation recharge:	
Zone 1 (river flood plain):	14 inches/year
Zone 2 (bedrock elements):	0
Zone 3 (aquifer covered by till):	6 inches/year
Note: River elements have precipitation recharge	
Hydraulic conductivities (K):	
Zone 1:	400 feet/day
Zone 2:	0.003 feet/day
Zone 3:	400 feet/day
Note: Hydraulic conductivity is assumed isotropic within each zone	
Porosities:	
Zone 1:	0.25
Zone 2:	0.1
Zone 3:	0.25
Type of aquifer:	Unconfined
Flow regime:	Steady state

See footnotes at end of table.

TABLE 3.5
(Continued)

II. Hydrogeologic Parameters (cont'd)

Boundary conditions:

Grid lower west boundary:	492 feet MSL[b]
Grid upper west boundary:	535 feet MSL
Grid north boundary:	540 feet MSL
Grid south boundary:	504 feet MSL
Grid east boundary:	530 feet MSL

WELL	CELL i, j[a]	EXTRACTION RATE
SOWC 1	32, 24	1,644,000 $feet^3$/day
SOWC 2	36, 30	822,000 $feet^3$/day
FMPC-P3	13, 40[c]	64,000 $feet^3$/day
Albright and Wilson	6, 23	19,000 $feet^3$/day

River bed leakage factor: 0.42 day^{-1}

[a]Refer to Figure 3-11 for grid element locations.

[b]MSL = above mean sea level.

[c]The correct coordinates for Well P3 are i = 12, j = 37; however, for the verification study, this well was located in the same cell in the other models

- The hydraulic head for MODFLOW are given at the center of each block. However, this code does not give the Darcy velocity components as output. To obtain the Darcy velocity components, additional calculations are needed based on the flow rates provided.

- GEOFLOW gives the hydraulic head at each node and provides the Darcy velocity components at the center of the elements.

3.2.1.7 Results

The potentiometric levels at selected wells, as computed by SWIFT III, GEOFLOW, and MODFLOW, are compared in Table 3.6. The wells selected as the basis for comparison of these models are the same as those used for the calibration of the Zone of Influence study model (IT, 1988a)

The analysis of Table 3.7 shows that SWIFT III and MODFLOW compute ground water levels with great relative precision as evidenced by the high degree of correlation between the two outputs (0.99981). The average value of the relative differences between the results of the two models is only -0.01 feet (0.003 m), indicating no bias in the respective model results. The maximum difference of -0.5 feet (0.15m) occurs at a relatively large cell that is close to the boundaries (i = 13, j = 40). This difference occurs because the boundary conditions in SWIFT III and MODFLOW are handled differently, as mentioned earlier.

The relative differences between SWIFT III and GEOFLOW potentiometric levels are within plus or minus 2 feet (0.61 m), with the exception of three values (Wells H-126, H-129, and SW-3A) that can be explained by the differences in the location of wells in the grid configurations. In GEOFLOW, wells are assigned to nodes, whereas in SWIFT III, wells are assigned at block centers. In GEOFLOW, to obtain the ground water elevation at the center of a finite element, nodal values of the element were averaged. In many cases, the value obtained was not representative

TABLE 3.6

COMPARISON OF POTENTIOMETRIC LEVELS COMPUTED BY SWIFT III, MODFLOW, AND GEOFLOW TWO-DIMENSIONAL GROUND WATER FLOW MODELS
PROBLEM GWF-5

WELL ID[a]	SWIFT III AND MODFLOW I	J[b]	SWIFT III GROUND WATER LEVEL (ft, MSL)[c]	MODFLOW GROUND WATER LEVEL (ft, MSL)[c]	GEOFLOW ELEMENT NUMBER[d]	GEOFLOW GROUND WATER LEVEL (ft, MSL)[e]	SWIFT III - MODFLOW RELATIVE DIFFERENCE (ft)	SWIFT III - MODFLOW ABSOLUTE DIFFERENCE (ft)	SWIFT III - GEOFLOW RELATIVE DIFFERENCE (ft)	SWIFT III - GEOFLOW ABSOLUTE DIFFERENCE (ft)
12-7A	2	32	532.4	532.4	76	532.3	0.0	0.1	0.1	0.1
STATE16	4	41	530.9	530.9	173	531.1	0.0	0.0	-0.2	0.2
H-124	5	8	507.0	507.4	186	505.7	-0.4	0.4	1.3	1.3
H-122	5	25	524.8	524.9	201	524.9	-0.1	0.1	-0.1	0.1
RE	6	16	517.4	517.6	236	517.3	-0.2	0.2	0.1	0.1
H-115	5	17	518.3	518.5	193	518.4	-0.2	0.2	-0.1	0.1
7-8A	6	24	523.5	523.6	244	523.5	-0.1	0.1	0	0
H-105	6	31	526.4	526.4	251	526.4	0.0	0.0	0	0
BPH	6	35	528.0	528.0	255	528.0	0.0	0.0	0	0
FMPC-17-D	7	31	526.1	526.1	295	526.1	0.0	0.0	0	0
H-129	8	6	504.8	504.9	314	504.3	-0.1	0.1	0.5	0.5
H-126	8	10	511.9	512.1	318	511.3	-0.2	0.2	0.6	0.6
HK-	8	28	524.8	524.8	336	524.8	0.0	0.0	0	0
FMPC-16-S	8	34	527.0	527.0	342	527.1	0.0	0.0	-0.1	0.1
FMPC-9	9	38	528.1	528.1	390	528.2	0.0	0.0	-0.1	0.1
DE	10	16	519.3	519.4	412	519.1	-0.1	0.1	0.2	0.2
FMPC-18-S	9	37	527.8	527.7	389	527.8	0.1	0.1	0	0
PALLETCO	9	41	530.3	530.3	393	530.3	0.0	0.0	0	0
16-1-S	9	3	503.8	503.8	355	503.6	0.0	0.0	0.2	0.2
FMPC-3	13	40	528.2	528.7	568	528.1	-0.5	0.5	0.1	0.1
FMPC-14-D	8	32	526.3	526.2	340	526.3	0.1	0.1	0	0
IT-5	13	27	524.0	524.0	555	524.0	0.0	0.0	0	0
IT-1	14	33	525.2	525.1	605	525.2	0.1	0.1	0	0
FMPC-10	14	39	527.3	527.3	611	527.3	0.0	0.0	0	0
BLK	16	34	523.2	523.2	684	523.2	0.0	0.0	0	0

See footnotes at end of table

TABLE 3.6
(Continued)

WELL ID[a]	SWIFT III AND MODFLOW I	SWIFT III AND MODFLOW J[b]	SWIFT III GROUND WATER LEVEL (ft, MSL)[c]	MODFLOW GROUND WATER LEVEL (ft, MSL)[c]	GEOFLOW ELEMENT NUMBER[d]	GEOFLOW GROUND WATER LEVEL (ft, MSL)[e]	SWIFT III - MODFLOW RELATIVE DIFFERENCE (ft)	SWIFT III - MODFLOW ABSOLUTE DIFFERENCE (ft)	SWIFT III - GEOFLOW RELATIVE DIFFERENCE (ft)	SWIFT III - GEOFLOW ABSOLUTE DIFFERENCE (ft)
IT-2	17	33	524.4	524.3	737	524.5	0.1	0.1	-0.1	0.1
FMPC-13-s	18	37	524.9	524.9	785	525.0	0.0	0.0	-0.1	0.1
02-E	18	26	523.0	522.9	774	523.0	0.1	0.1	0	0
IT-3	20	36	524.1	524.0	872	524.2	0.1	0.1	-0.1	0.1
W-127	21	29	522.6	522.5	909	522.6	0.1	0.1	0	0
IT-4	24	34	523.0	522.9	1046	523.1	0.1	0.1	-0.1	0.1
B-3	24	34	523.0	522.9	1046	523.1	0.1	0.1	-0.1	0.1
B-2	27	32	522.1	522.0	1176	522.2	0.1	0.1	-0.1	0.1
SW-4A	28	25	519.4	519.4	1213	519.6	0.0	0.0	-0.2	0.2
B-1	29	31	521.5	521.4	1263	521.6	0.1	0.1	-0.1	0.1
SW-3A	30	24	514.9	514.9	1300	515.3	0.0	0.0	-0.4	0.4
R-7	34	26	517.6	517.7	1478	517.8	-0.1	0	-0.2	0.2
B-4	32	28	520.4	520.4	1392	520.3	0.0	0.0	0.1	0.1
K-4	40	27	521.8	521.7	1743	521.9	0.1	0.1	-0.1	0.1
EL-1	42	30	522.2	522.2	1834	522.3	0.0	0.0	-0.1	0.1
03	42	38	523.7	523.7	1842	523.8	0.0	0.0	-0.1	0.1
ER-1	45	21	523.8	523.8	1957	523.8	0.0	0.0	0	0
LB-1	47	30	524.2	524.2	2054	524.2	0.0	0.0	0	0
WK1	48	24	524.1	524.2	2092	524.2	-0.1	-0.1	-0.1	-0.1
WW-1	48	35	525.2	525.1	2103	525.2	0.1	0.1	0	0

[a]These wells were obtained from the "Hydrogeologic Study of FMPC Discharge to the Great Miami River" (IT, 1988).

[b]Refer to Figure 3-10 for cell locations.

[c]MSL means above mean sea level.

[d]Refer to Figure 3-11 for grid element locations.

[e]GEOFLOW's ground water elevations were calculated as the average of the node values corresponding to a cell.

TABLE 3.7

STATISTICS FOR THE TWO-DIMENSIONAL
GROUND WATER FLOW NUMERICAL MODEL COMPARISONS
PROBLEM GWF-5

	SWIFT III - MODFLOW	SWIFT III - GEOFLOW
SUM OF DIFFERENCES[a] DIVIDED BY NUMBER OF OBSERVATIONS	-0.01	0.03
SUM OF ABSOLUTE DIFFERENCES DIVIDED BY NUMBER OF OBSERVATIONS	0.07	0.12
STANDARD DEVIATION OF DIFFERENCES	0.12	0.25
DEGREE OF CORRELATION BETWEEN MODELS[b]	0.99981	0.99943

SWIFT III - MODFLOW

Regression Output:

Constant	3.2355035
Std Err of Y Est	0.1202181
R Squared	0.9996197
No. of Observations	45
Degrees of Freedom	43
X Coefficient(s)	0.99382
Std Err of Coef.	0.00295

X = SWIFT III
Y = MODFLOW

SWIFT III - GEOFLOW

Regression Output:

Constant	-11.950
Std Err of Y Est	0.21385
R Squared	0.99886
No. of Observations	45
Degrees of Freedom	43
X Coefficient(s)	1.0228
Std Err of Coef.	0.0052

X = SWIFT III
Y = GEOF

[a]The relative and absolute differences are presented in Table 3.6.
[b]The correlation coefficient was used as the degree of correlation between computed ground water level

of the element because of an abrupt change in hydraulic gradient, or because of the proximity of the element to a feature such as the river or a pumping well.

The statistics in Table 3.7 show that, although both models have good agreement with SWIFT III, the match between SWIFT III and MODFLOW (degree of correlation = 0.99981) is slightly better than the match between SWIFT III and GEOFLOW (degree of correlation = 0.99943). This is expected because SWIFT III and GEOFLOW differ in: 1) the treatment of boundary conditions; 2) the location of the assignment of features (cell centers or nodes); 3) the simulation of the river; and 4) the location of extraction wells within the corresponding cell. As will be discussed in Section 3.2.2, greater agreement was obtained when the center of each cell of the finite-difference model corresponded to the nodes of the finite element model.

The horizontal Darcy velocities (specific discharges) were compared for a cross section of the model. The Cross Section A-A' (shown in Figures 3-10 and 3-11) was selected to compare Darcy velocities for the three different computer simulations. The criteria used for the selection of the cross section included intersection of a river, intersection of an Extraction Well (SOWC-1), and the spanning of the effective model boundaries.

The comparisons of Darcy velocity components in the x- and y-directions are given in Figures 3-12 and 3-13, respectively. The values for the three wells are generally in good agreement. As shown in Figure 3-12, the specific discharges in the x-direction (Cells 9 through 35) vary between 0.6 feet/day (0.18 m/day) close to the influence of Extraction Well SOWC-2 and -15.5 feet/day (-4.72 m/day) at Extraction Well SOWC-1. The maximum variation, which represents an approximate 20 percent discrepancy, can be explained by the fact that the SWIFT III code computes specific discharges assuming a fully saturated cell. This

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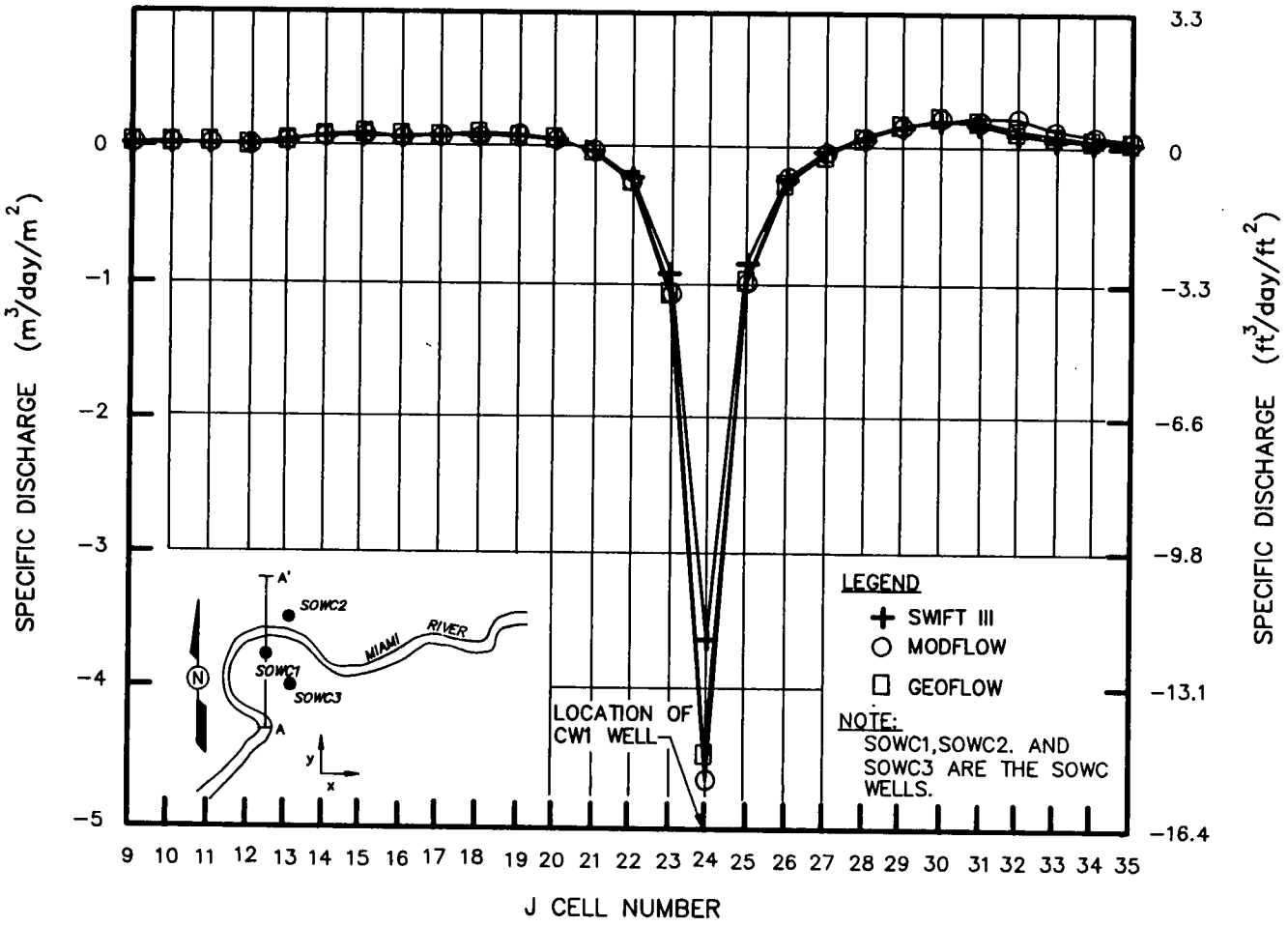

NOTES:

1. REFER TO FIGURE 3-10 (CROSS-SECTION A-A') FOR i- AND j-CELL NUMBERS. THE CELLS IDENTIFIED IN FIGURE 3-10 CORRELATE TO THE NODES AT CROSS-SECTION A-A' ON FIGURE 3-11.

2. SPECIFIC DISCHARGE IS EQUIVALENT TO DARCY VELOCITY.

FIGURE 3-12

COMPARISON OF SPECIFIC DISCHARGE (x-COMPONENT) VERSUS DISTANCE

PROBLEM GWF-5

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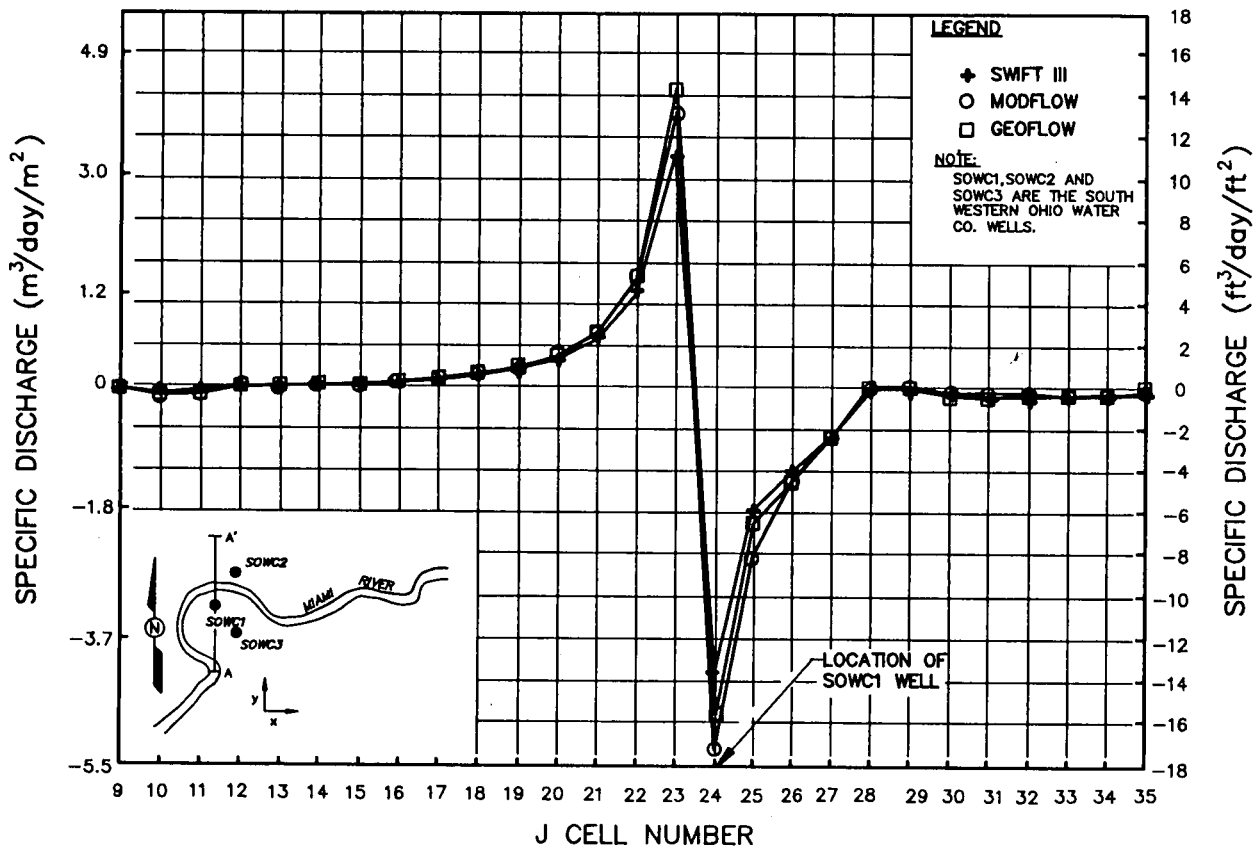

NOTES:

1. REFER TO FIGURE 3-10 (CROSS-SECTION A-A') FOR i- AND j-CELL NUMBERS. THE CELLS IDENTIFIED IN FIGURE 3-10 CORRELATE TO THE NODES AT CROSS-SECTION A-A' ON FIGURE 3-11.

2. SPECIFIC DISCHARGE IS EQUIVALENT TO DARCY VELOCITY.

FIGURE 3-13

COMPARISON OF SPECIFIC DISCHARGE (y-COMPONENT) VERSUS DISTANCE

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condition is likely not well satisfied at a cell with a major pumping well. If a correction factor is applied to the unsaturated cell at Well SOWC-1, the difference decreases to four percent. As shown in Figure 3-13, the specific discharges in the y-direction display very small values except around the extraction well, where an abrupt change of sign occurs. The agreement is good, except for the two extremes where the aforementioned effect of a saturated cell used to compute specific discharges artificially reduces the values computed by SWIFT III.

Leakage rates per unit area at selected points along the Great Miami River, as computed from the results of the SWIFT III, MODFLOW, and GEOFLOW models, are compared in Figure 3-14. The area represented is an approximate 5,000-foot reach of river, starting about 2,000 feet upstream from Extraction Well SOWC-1. This figure shows that the river recharges the aquifer throughout this reach. Recharge rates within the selected reach as computed by all three models, range between -2.0 and -0.2 cubic feet per day per square foot. The negative sign indicates that recharge from the river to the aquifer is occurring. The maximum values of recharge rates coincide with the overlapping influence of Extraction Wells SOWC-1 and SOWC-2. The differences in the predicted values from the three models are within seven percent. Considering the fact that each model used a different method of simulating the river, this agreement in model predictions is very good.

In summary, the results of verification Problem GWF-5 indicate that there is a good agreement among the results obtained by sitewide modeling with the SWIFT III, MODFLOW, and GEOFLOW codes. This agreement was obtained even through the models differ in grid configuration and solution algorithms.

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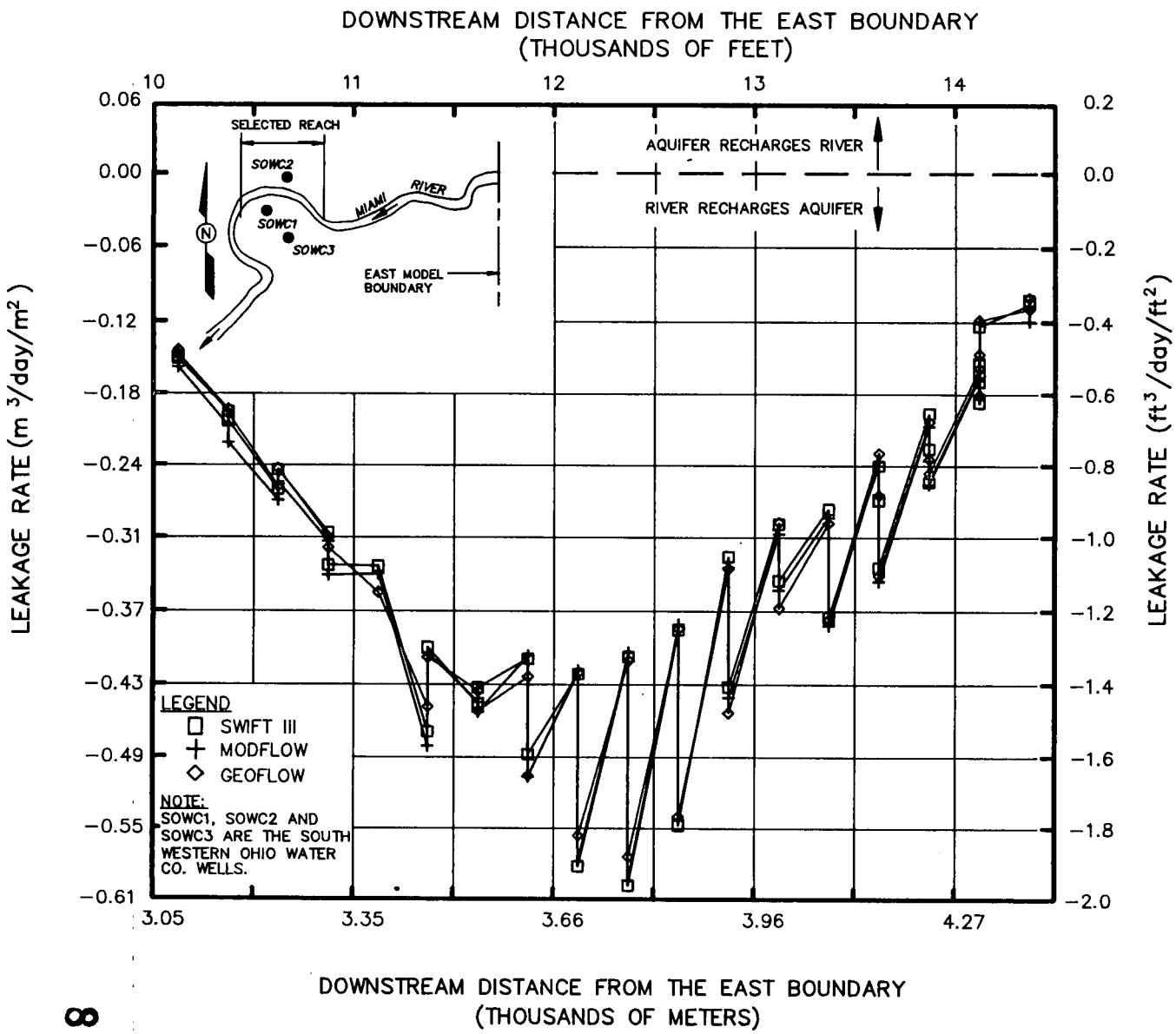

FIGURE 3-14

COMPARISON OF
THE GREAT MIAMI RIVER
LEAKAGE RATE
VERSUS
DISTANCE

PROBLEM GWF-5

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3.2.2 Problems GWF-6a, 6b, 6c, and 6d: Three-Dimensional Comparisons

To verify the site specific, three-dimensional simulation capabilities of the SWIFT III code, a series of problems were simulated using the SWIFT III and MODFLOW programs. The PTC program was also used in some of these problems, as appropriate.

To systematically test the SWIFT III code capabilities, a baseline verification problem was first established. Variations were then made to the baseline problem to test new combinations of features.

3.2.2.1 Purpose of Problem Selection

The series of three-dimensional ground water flow problems was selected to test the modeling of various combinations of capabilities of the SWIFT III code. Aquifer complexity was increased with each successive problem. The features of Problem GWF-6a (the baseline problem) are as follows:

- Confined aquifer
- Anisotropic aquifer
- Steady-state pressure solution
- Three-dimensional Cartesian coordinates
- Constant-head boundary condition
- No-flow boundary condition
- Extraction well
- Injection well
- Partially penetrating wells
- Darcy velocity components
- Constant well pumping rate
- Aquifer influence function

In the second problem of the GWF-6 sequence (Problem GWF-6b), the aquifer was changed to an unconfined condition and a natural recharge was added as a hydrologic input. To verify the computational accuracy of the SWIFT III code when simulating a river system potentially affected by nearby pumping wells, a river was added and the injection well deleted in Problem GWF-6c. The final problem in the series, Problem GWF-6d, introduced a larger extraction well system to simulate a more significant hydrologic stress on steady-state aquifer conditions.

3.2.2.2 Problem Description

The input data of the example problem in Finley and Reeves (1982, p. 94, Problem 6.2) was modified to establish Problem GWF-6a. The isometric grid system used for the three-dimensional ground water flow verification is shown in Figure 3-15. Because of model symmetry, only one-half of the grid system was used. The symmetry plane is the front face parallel to the x-z plane in Figure 3-15. The horizontal grid system used in the finite-difference models (SWIFT III and MODFLOW) is shown in Figure 3-16. Because PTC is node-centered, a revised grid was developed for the purpose of obtaining nodal results at the center of the finite-difference model blocks. The finite element grid system for PTC is shown in Figure 3-17. The vertical grid has three layers and was the same for the three models. The uppermost face on the x-z plane (the first layer) was simulated as a constant-head boundary. All of the other faces were simulated as no-flow boundaries.

3.2.2.3 Assumptions

The assumptions are the following:

- The aquifer is ideally confined or unconfined, according to the problem being studied
- Extraction and injection rates are constant at each well
- The extraction and injection wells are assumed to be screened in the second layer, and thus receive or contribute water from or to the entire thickness of the aquifer by horizontal flow
- Darcy's law applies throughout the system

3.2.2.4 Numerical Simulations

As mentioned before, a revised horizontal grid (Figure 3-17) was used for PTC to produce results that can be correlated to the center of the finite-difference model blocks. As outlined in Section 3.2.1.4, the constant-head boundary condition is treated by SWIFT III by assigning the value of the hydraulic head to the outer face of the boundary

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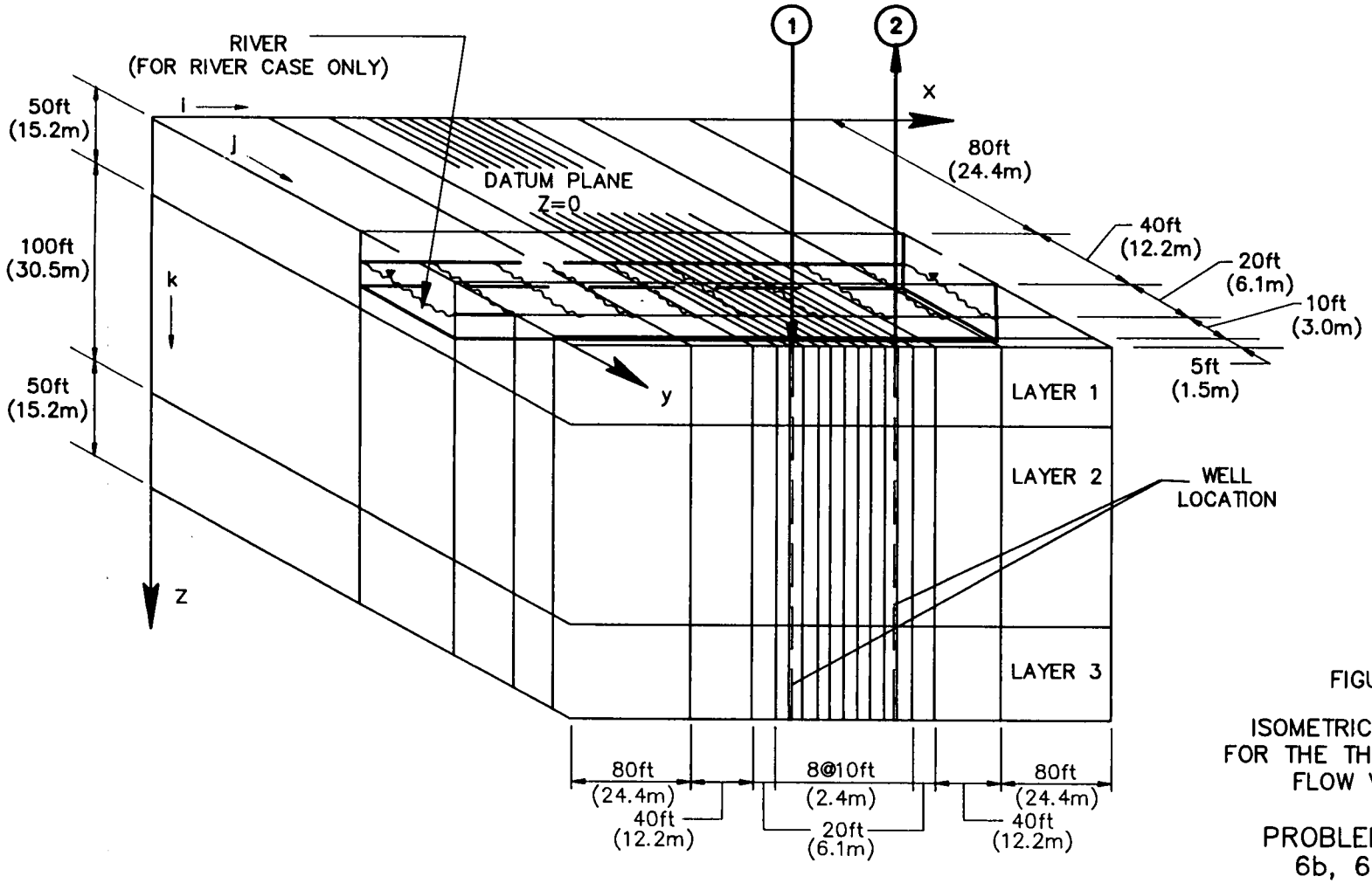

FIGURE 3-15

ISOMETRIC GRID SYSTEM
FOR THE THREE-DIMENSIONAL
FLOW VERIFICATION

PROBLEMS GWF-6a,
6b, 6c AND 6d

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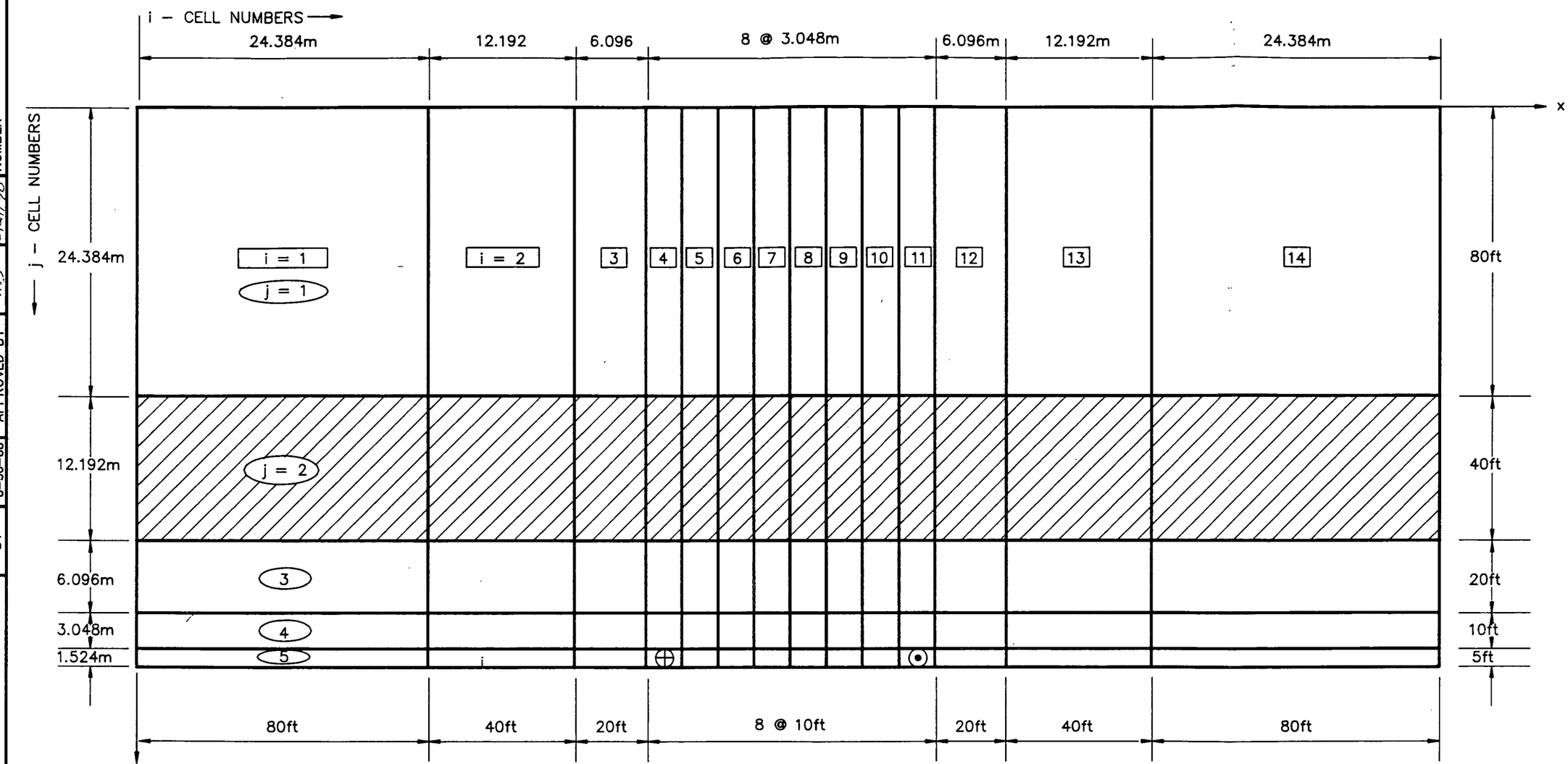

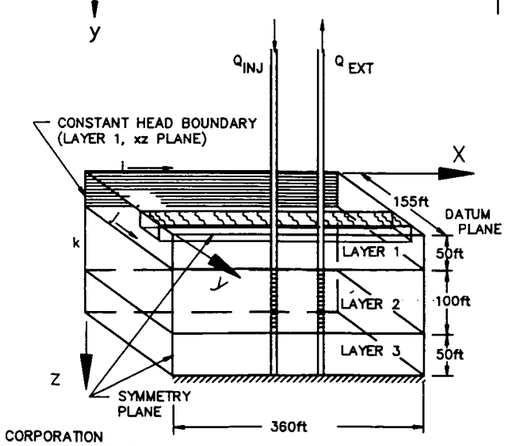

LEGEND

- 3 — i – CELL NUMBER
- 3 — j – CELL NUMBER
- ⊕ — INJECTION WELL
- ⊙ — EXTRACTION WELL
- LOCATION OF RIVER FOR MODELS THAT INCLUDED A RIVER IN LAYER 1

NOTE:

INJECTION AND EXTRACTION WELLS WERE ASSIGNED ONLY IN LAYER 2.

SCALE

0 30 60 FEET

FIGURE 3–16

HORIZONTAL GRID SYSTEM FOR THE FINITE–DIFFERENCE SOLUTION

PROBLEMS GWF–6a, 6b, 6c, AND 6d

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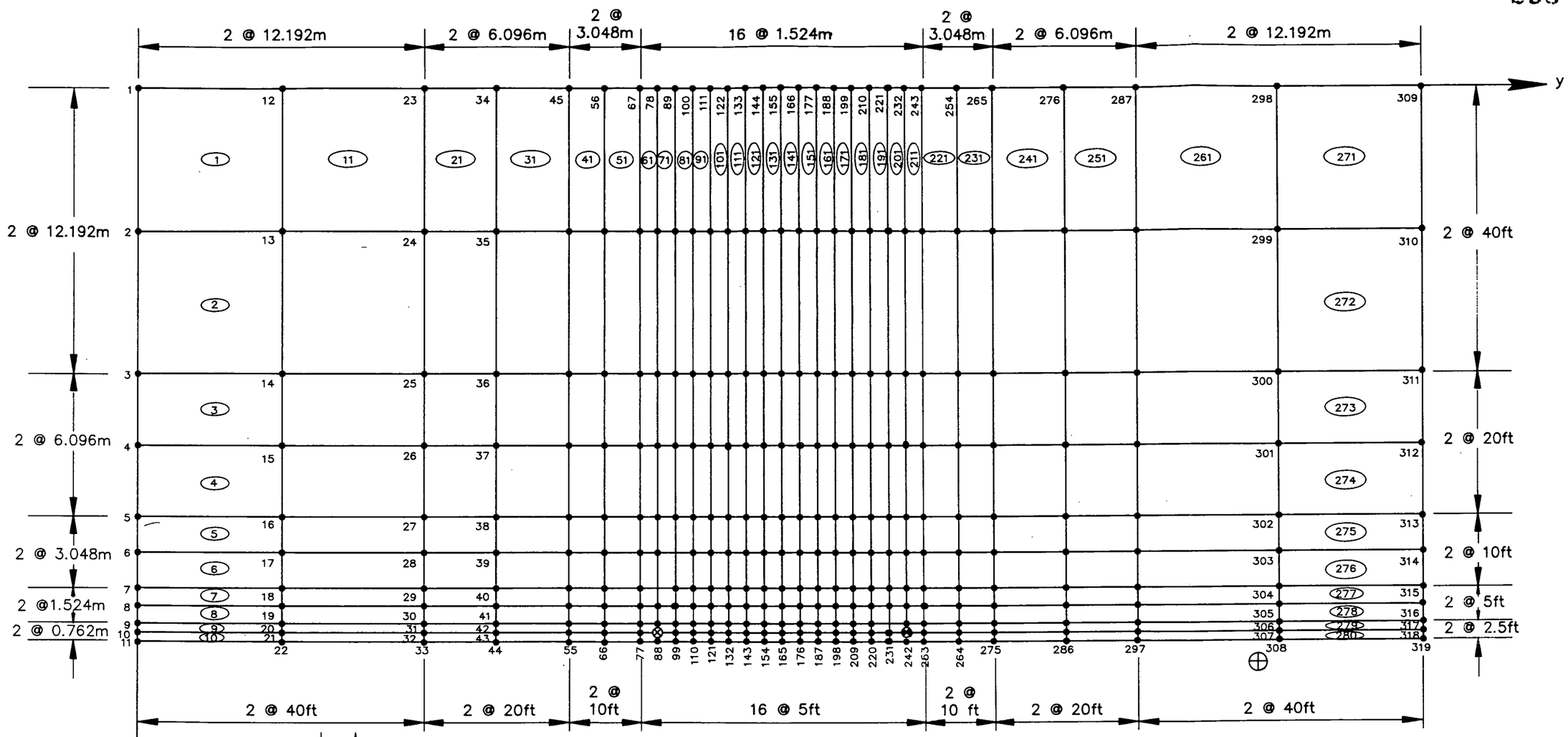

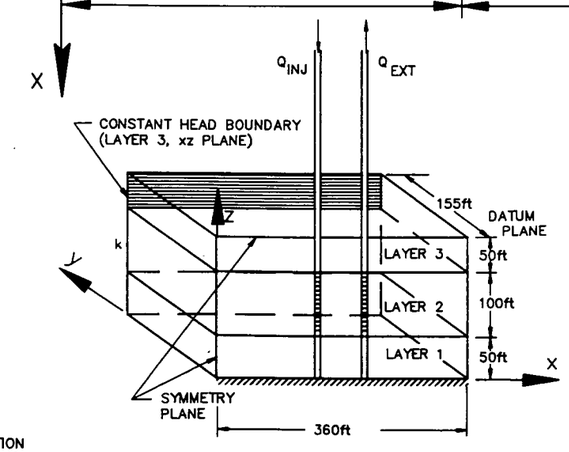

LEGEND

- FINITE ELEMENT NODE NUMBER
- FINITE ELEMENT NUMBER
- INJECTION WELL
- EXTRACTION WELL

NOTE:

INJECTION AND EXTRACTION WELLS WERE ASSIGNED ONLY IN LAYER 2.

SCALE

0 30 60 FEET

FIGURE 3-17

FINITE ELEMENT HORIZONTAL GRID SYSTEM FOR PRINCETON TRANSPORT CODE (PTC) MODEL

PROBLEMS GWF-6a AND 6b

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blocks. However, the MODFLOW model assigns constant-head values to the center of the boundary blocks. This situation became a complicating issue for the river leakage comparisons, but was overcome by simulating the constant-head cells with wells (Finley and Reeves, 1982, p. 31). The other aspects of the SWIFT III and MODFLOW models are as specified in Section 3.2.1.4.

3.2.2.5 Input Specifications

The input parameters for SWIFT III/MODFLOW and PTC are given in Tables 3.8 and 3.9, respectively. The hydrogeologic parameters given in these tables are representative of values at the FMPC site, with the exception that actual well rates are twice the values given in Tables 3.8 and 3.9.

3.2.2.6 Output Specifications

For the GWF-6 sequence of problems, the output from SWIFT III consisted of pressure, river leakage values, and Darcy velocity components. The output from MODFLOW consisted of hydraulic head, river leakages, and flow rates for the front, right, and bottom faces of each block. The output of PTC was limited to hydraulic head and Darcy velocity components because the river was not included in the PTC simulations.

3.2.2.7 Results - Problem GWF-6a

The steady-state potentiometric levels computed by SWIFT III, MODFLOW, and PTC for a confined aquifer with an injection well and an extraction well are presented in Figure 3-18. Table 3.10 lists the differences in potentiometric levels between SWIFT III and MODFLOW and between SWIFT III and PTC, respectively. Table 3.10 and Figure 3-18 indicate that the maximum difference in results among the models occurs at the cells containing wells. This is expected because of differences in the algorithms used to simulate wells in the respective codes. SWIFT III results match the MODFLOW results more closely than the match to PTC results because of the similar numerical technique used in the SWIFT III and MODFLOW code.

TABLE 3.8

INPUT PARAMETERS FOR THE
THREE-DIMENSIONAL SWIFT III AND MODFLOW
GROUND WATER FLOW MODELS
PROBLEMS GWF-6a, 6b, 6c, and 6d

I. Finite-Difference Grid System[a]	
Length: (i-direction)	109.728 m (360 ft)
Width: (j-direction)	47.244 m (155 ft)
Number of cells:	70
Number of layers:	3
Elevation of datum plane:	0 m (0 ft)
II. Hydrogeologic Parameters	
Thickness of first layer:	15.240 m (50 ft)
Thickness of second layer:	30.480 m (100 ft)
Thickness of third layer:	15.240 m (50 ft)
Precipitation recharge:[b]	6.443×10^{-7} cm/s (8 inches/year)
Hydraulic conductivities:	
Horizontal:	1.41×10^{-1} cm/s (400 ft/day)
Transversal:	1.41×10^{-1} cm/s (400 ft/day)
Vertical:	4.70×10^{-2} cm/s (133.33 ft/day)
Porosity:	0.25
Types of aquifers simulated:	Confined/Unconfined/ Unconfined with recharge and river
Flow regime:	Steady state
Boundary conditions (cells i = 1 through 14, j = 1, and k = 1):[c]	
Confined case:	30.48 m (100 ft)
Unconfined case:	0 m (0 ft)

See footnotes at end of table.

TABLE 3.8
(Continued)

II. Hydrogeologic Parameters (cont'd)

Injection and extraction wells production schedule:

Problem	Well Type	Well Location i	Well Location j	Rates
Confined	Injection	4	5	15,000 m^3/day (529,720 ft^3/day)
	Extraction	11	5	15,000 m^3/day (529,720 ft^3/day)
Unconfined with recharge	Injection	4	5	35,396 m^3/day (1,250,000 ft^3/day)
	Extraction	11	5	35,396 m^3/day (1,250,000 ft^3/day)
Unconfined with river and recharge	Extraction	11	5	35,396 m^3/day (1,250,000 ft^3/day)
Unconfined with river and recharge	Extraction	4	5	35,396 m^3/day (1,250,000 ft^3/day)
	Extraction	11	5	35,396 m^3/day (1,250,000 ft^3/day)

[a]Refer to Figure 3-15 for isometric model and Figure 3-16 for horizontal grid system.

[b]Precipitation recharge is applicable to Problems GWF-6b, GWF-6c, and GWF-6d.

[c]MODFLOW boundary values were assigned to the center of the cells and SWIFT III's to the center of the outer face.

TABLE 3.9

INPUT PARAMETERS FOR THE
THREE-DIMENSIONAL PRINCETON TRANSPORT CODE (PTC) MODEL
PROBLEMS GWF-6a, AND 6b

I. Finite Element Grid System[a]

Length: (x-direction)	47.244 m (155 ft)
Width: (y-direction)	109.728 m (360 ft)
Number of elements:	280
Number of nodes:	319
Number of layers:	3
Elevation of datum plane:	0 m (0 ft)

II. Hydrogeologic Parameters

Thickness of first layer:	15.240 m (50 ft)
Thickness of second layer:	30.480 m (100 ft)
Thickness of third layer:	15.240 m (50 ft)
Precipitation recharge:	6.443×10^{-7} cm/s (8 inches/year)
Hydraulic conductivities:	
Horizontal:	1.41×10^{-1} cm/s (400 ft/day)
Vertical:	4.70×10^{-2} cm/s (133.33 ft/day)
Porosity:	0.25
Types of aquifers simulated:	Confined/Unconfined with recharge
Flow regime:	Steady state
Boundary conditions:	
Layer:	3 (Top)[b]
Node numbers: (Constant Head)	1, 12, 23, 34, 45, 56, 67, 78, 89, 100, 111, 122, 133, 144, 155, 166, 177, 188, 199, 210, 221, 232, 243, 254, 265, 276, 287, 298, and 309
Confined case value:	30.48 m (100 ft)
Unconfined case value:	0 m (0 ft)

See footnote at end of table.

TABLE 3.9
(Continued)

II. Hydrogeologic Parameters (cont'd)

Injection and extraction wells production schedule:

Case	Well Type	Well Location i*	Well Location j*	Rates
Confined	Injection	4	5	15,000 m^3/day (529,720 ft^3/day)
	Extraction	11	5	15,000 m^3/day (529,720 ft^3/day)
Unconfined	Injection	4	4	35,396 m^3/day (1,250,000 ft^3/day)
	Extraction	11	5	35,396 m^3/day (1,250,000 ft^3/day)

[a]Refer to Figure 3-17 for Finite Element Grid.

[b]PTC model reverses the order of the layers; thus,

SWIFT III Layer No.	Corresponding PTC Layer No.
1	3
2	2
3	1

*The location of the injection and extraction well defined as above applies to the SWIFT III grid.

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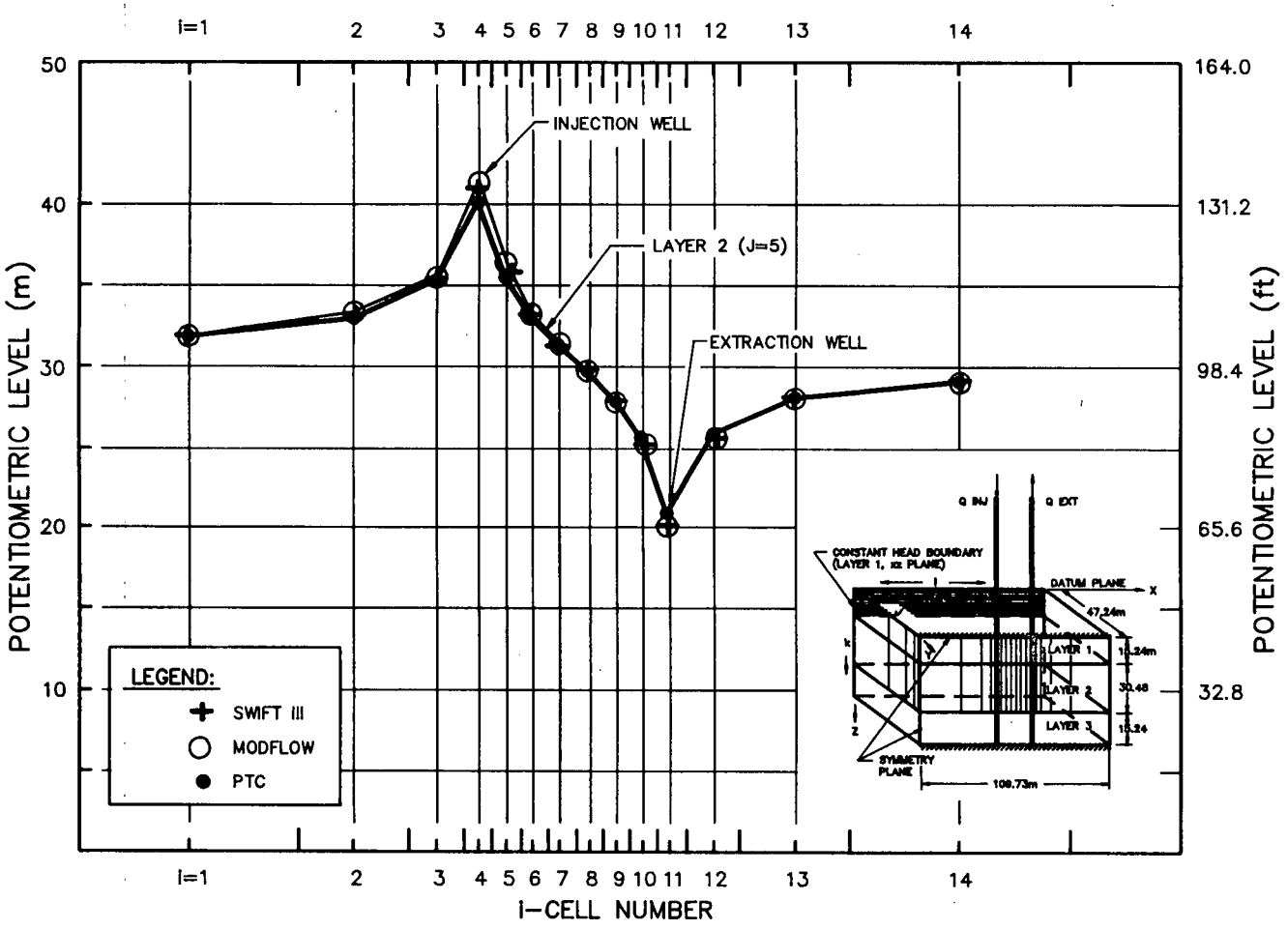

NOTES:

1. REFER TO FIGURE 3-16 FOR LOCATION OF i- AND j-CELLS.
2. REFER TO TABLE 3.10 FOR CORRELATION BETWEEN PTC NODES. AND SWIFT III CELL NUMBERS.
3. INPUT DATA FOR PROBLEM GWF-6a ARE IDENTICAL TO THAT SHOWN IN TABLES 3.8 AND 3.9 EXCEPT THAT FOR THIS FIGURE INJECTION AND EXTRACTION RATES ARE 35,396 m^3/day

FIGURE 3-18

COMPARISON OF STEADY-STATE POTENTIOMETRIC LEVEL VERSUS DISTANCE

PROBLEM GWF-6a

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TABLE 3.10

COMPARISON OF POTENTIOMETRIC LEVELS
FOR THE SECOND LAYER OF SWIFT III, MODFLOW AND PTC
GROUND WATER FLOW MODELS CONFINED CASE[a]
PROBLEM GWF-6a

SWIFT III				MODFLOW	PRINCETON TRANSPORT CODE		DIFFERENCE SWIFT III	
COORDINATES[b] I	J	K	POTENTIOMETRIC LEVEL (meters)	POTENTIOMETRIC LEVEL (meters)	NODE[c] NUMBER	POTENTIOMETRIC LEVEL (meters)	MINUS MODFLOW (meters)	MINUS PTC (meters)
1	5	2	33.11	31.89	11	31.94	-0.01	-0.06
2	5	2	32.94	33.04	33	32.97	-0.10	-0.03
3	5	2	35.20	35.49	55	35.24	-0.29	-0.04
4	5	2	40.09	40.73	77	41.75	-0.64	-1.66
5	5	2	35.42	35.74	99	35.49	-0.32	-0.07
6	5	2	33.02	33.19	121	33.06	-0.17	-0.04
7	5	2	31.27	31.33	143	31.31	-0.06	-0.04
8	5	2	29.67	29.63	165	29.71	0.04	-0.04
9	5	2	27.92	27.77	187	27.95	0.15	-0.03
10	5	2	25.51	25.22	209	25.53	0.29	-0.02
11	5	2	20.83	20.24	231	19.26	0.59	1.57
12	5	2	25.73	25.48	253	25.77	0.25	-0.04
13	5	2	28.01	27.92	275	28.04	0.09	-0.03
14	5	2	29.06	29.08	297	29.06	0.02	-0.00

[a]The potentiomeric levels have been plotted in Figure 18.
[b]Refer to Figures 3-15 and 3-16 for cell locations.
[c]Refer to Figure 3-17 for node locations.

To further investigate the accuracy of computations among the three codes, a comparison of Darcy velocities or specific discharges was performed for the confined aquifer case. The codes provided Darcy velocities in different ways. SWIFT III assumed a fully saturated cell in the computations of specific discharges, MODFLOW produced flow rates across three faces of each cell, and PTC produced Darcy velocities only in the z-direction and disregarded the sign in the middle layers. Moreover, PTC gives the horizontal velocities at the center of the elements, which made it necessary to average the velocities of four elements to obtain the required Darcy velocity at the center node of a block. These differences in output structure made it necessary to perform certain computations to obtain equivalent Darcy velocities.

In addition to the computational procedures, each code calculated Darcy velocities at different locations on a given block. For example, in calculating the x-component of Darcy velocity, SWIFT III provided the result at the rear face of the block, MODFLOW provided the result at the front face of the block, and the PTC four-element average was calculated at the center of the block.

Figures 3-19, 3-20, and 3-21 present comparisons for the steady-state Darcy velocity components in the x-, y-, and z-directions, respectively, for SWIFT III, MODFLOW, and PTC models for Problem GWF-6a. The cells selected for comparison were those with coordinates j=5 and i=1 through i = 14 for the second layer (refer to Figures 3-15 and 3-16). These cells were selected because of their proximity to the wells, where the largest velocities, and thus model discrepancies, are likely to be found. Figure 3-19 confirms the expected symmetry of Darcy velocities (specific discharges) in the x-direction about the center of the grid. The symmetry is particularly apparent from the PTC data which were calculated and plotted at the center of blocks. Darcy velocity components for SWIFT III and MODFLOW were calculated and plotted at the back and front faces, respectively, of grid blocks, the faces of the

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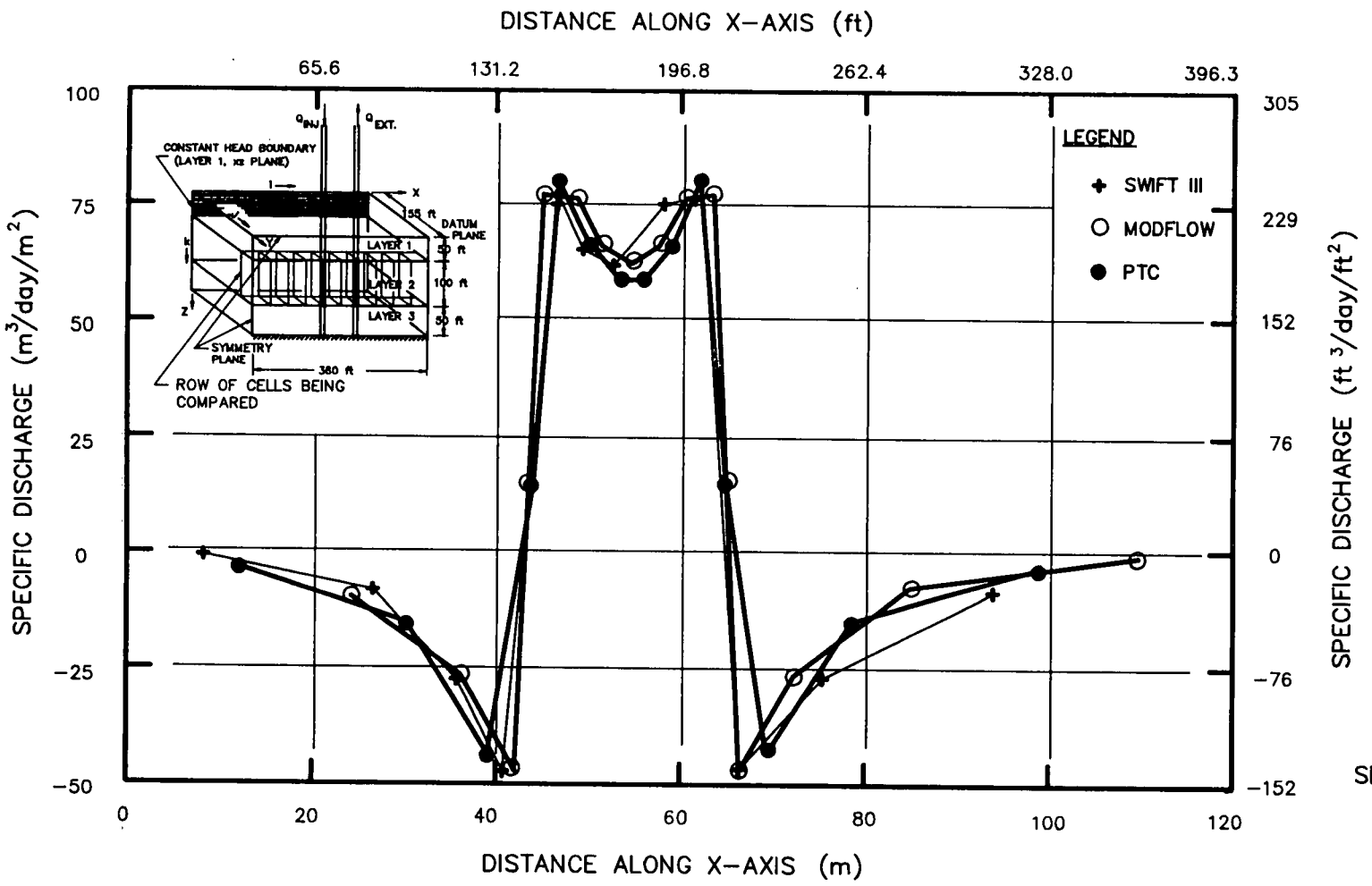

NOTE:

SPECIFIC DISCHARGE IS EQUIVALENT TO DARCY VELOCITY.

FIGURE 3-19

COMPARISON OF STEADY-STATE SPECIFIC DISCHARGE (X-COMPONENT) VERSUS DISTANCE

PROBLEM GWF-6a

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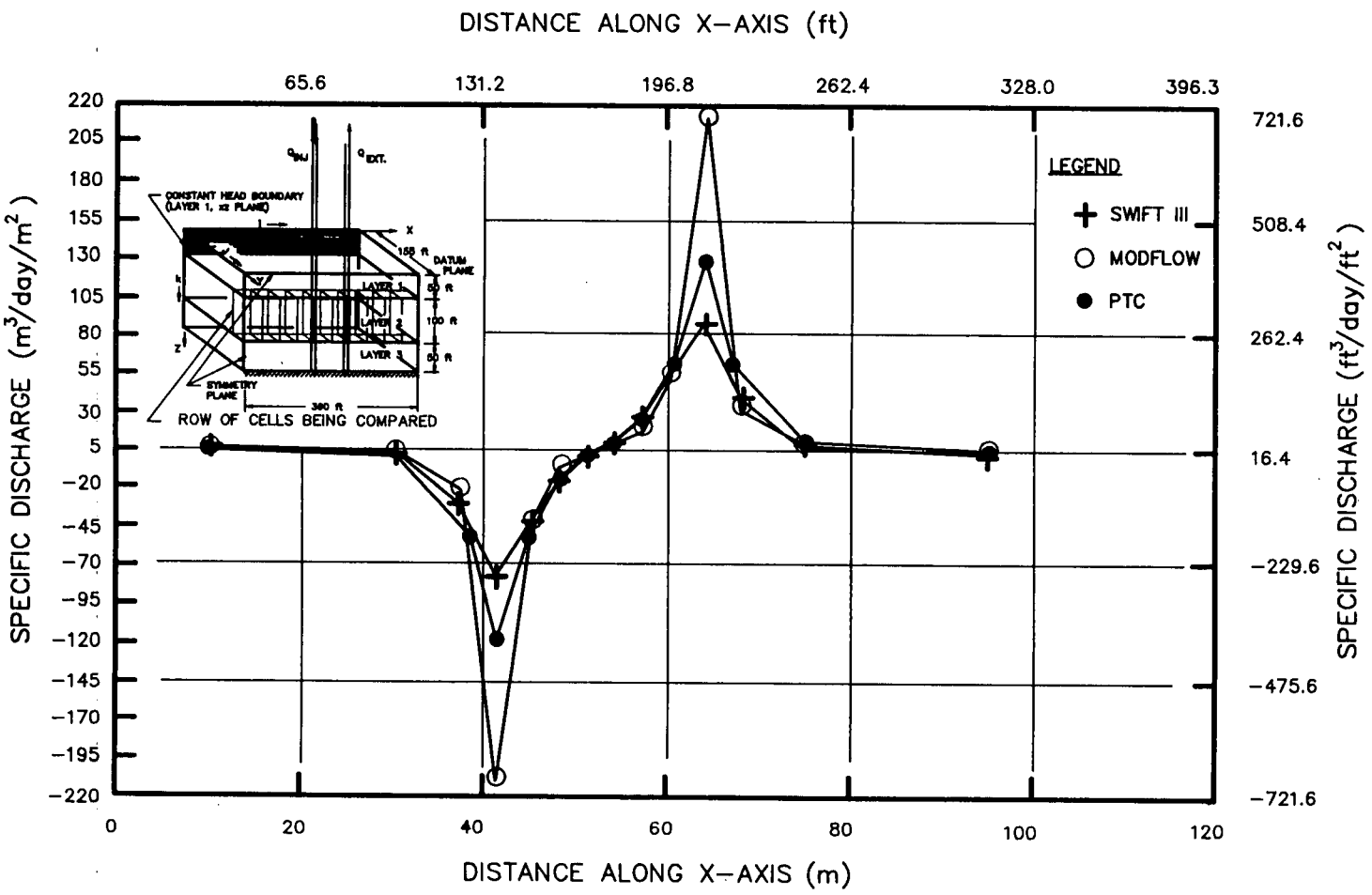

NOTE:

SPECIFIC DISCHARGE IS EQUIVALENT TO DARCY VELOCITY.

FIGURE 3-20

COMPARISON OF STEADY-STATE SPECIFIC DISCHARGE (y-COMPONENT) VERSUS DISTANCE

PROBLEM GWF-6a

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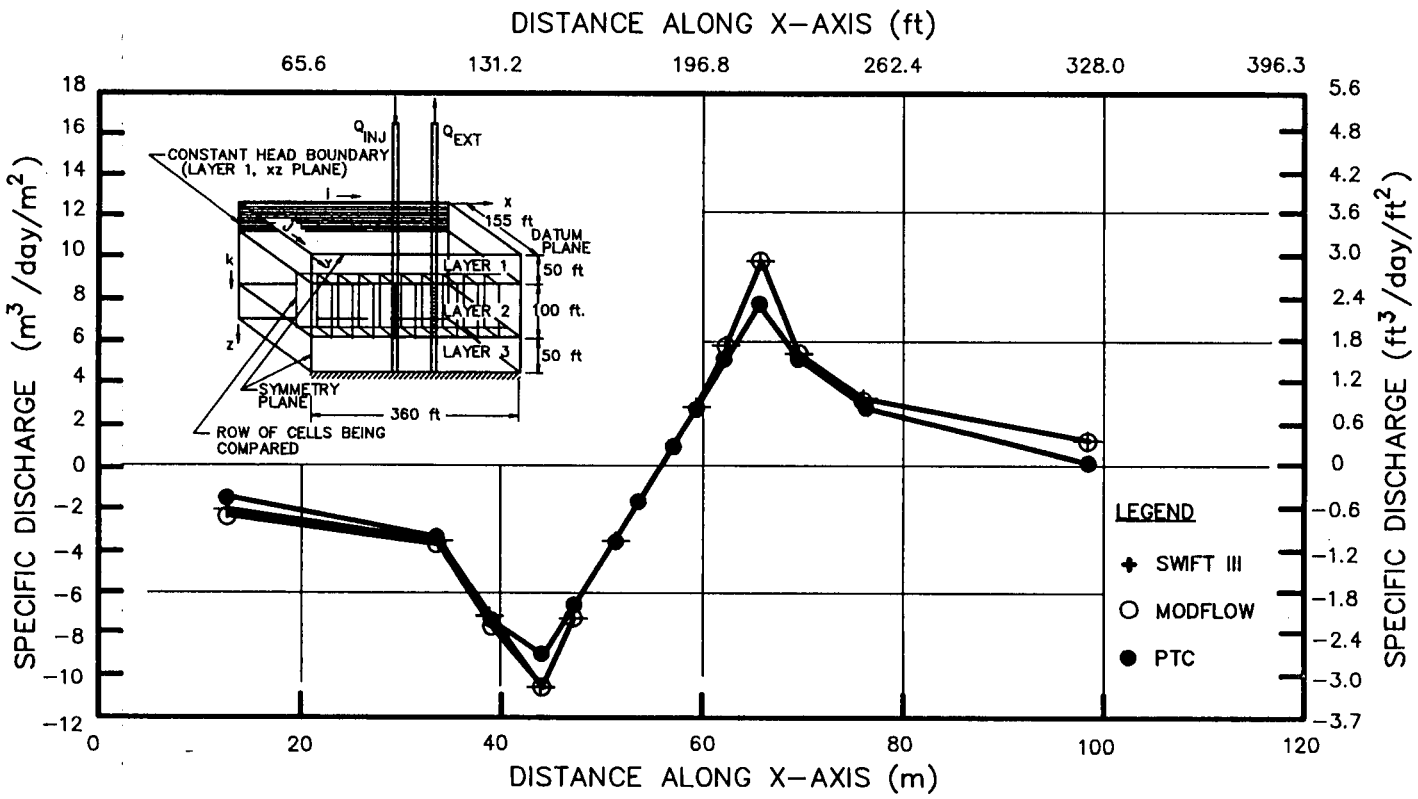

FIGURE 3-21

COMPARISON OF
STEADY-STATE SPECIFIC DISCHARGE
(Z-COMPONENT)
VERSUS
DISTANCE

PROBLEM GWF-6a

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NOTE:

SPECIFIC DISCHARGE IS EQUIVALENT TO DARCY VELOCITY.

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blocks being defined by the positive direction of the Darcy velocity component.

The maximum discrepancy in specific discharge (7.5 $m^3/day/m^2$, 23 $ft^3/day/ft^2$) occurred at the location of the wells. Figures 3-20 and 3-21 exhibit similar characteristics, except for the expected asymmetry about the center of the grid in the x-direction. The comparison between SWIFT III and MODFLOW is excellent in the three vertical directions, except in the cells at the wells. PTC results were closer to SWIFT III results at the well cells in the y-direction because of the aforementioned averaging of velocities in PTC. These differences are expected at the well locations because of the grid size and methods of computation. However, because excellent agreements were obtained in areas away from the well locations, the SWIFT III code is performing ground water flow simulations satisfactorily.

Problem GWF-6b

In Problem GWF-6, the aquifer is unconfined and natural recharge is added to the system. The steady-state potentiometric levels computed by the SWIFT III, MODFLOW, and PTC models are shown in Table 3.11 and Figure 3-22. As both the table and figure indicate, the computed potentiometric levels compare favorably except at the well locations. These differences are basically attributed to differences in code algorithms, and to the necessary extrapolation of output results. The significance of these differences is exactly as discussed in Problem GWF-6a previously.

Problem GWF-6c

Simulations with a river and an extraction well were performed in Problem GWF-6c. The river was located in the top layer (k=1) along the x-axis (i=1 through i=14) and between the boundary and the wells (j=2). A sketch of the model system, including the river, is presented as an insert in Figures 3-23 through 3-25. Because SWIFT III lacks a

TABLE 3.11

COMPARISON OF POTENTIOMETRIC LEVELS
FOR THE SECOND LAYER OF SWIFT III, MODFLOW AND PTC
GROUND WATER FLOW MODELS UNCONFINED CASE[a]
PROBLEM GWF-6b

SWIFT III				MODFLOW	PRINCETON TRANSPORT CODE		DIFFERENCE SWIFT III	
COORDINATES[b] I	J	K	POTENTIOMETRIC LEVEL (meters)	POTENTIOMETRIC LEVEL (meters)	NODE[c] NUMBER	POTENTIOMETRIC LEVEL (meters)	MINUS MODFLOW (meters)	MINUS PTC (meters)
1	5	2	1.45	1.41	11	1.57	-0.04	-0.13
2	5	2	2.49	2.56	33	2.59	-0.07	-0.10
3	5	2	4.75	5.00	55	4.84	-0.25	-0.09
4	5	2	9.65	10.26	77	11.33	-0.61	-1.68
5	5	2	4.96	5.26	99	5.05	-0.30	-0.09
6	5	2	2.55	2.71	121	2.60	-0.16	-0.05
7	5	2	0.78	0.85	143	0.82	-0.07	-0.04
8	5	2	-0.84	-0.85	165	-0.80	0.01	-0.03
9	5	2	-2.61	-2.71	187	-2.58	0.10	-0.03
10	5	2	-5.04	-5.26	209	-5.03	0.23	-0.02
11	5	2	-9.93	-10.25	231	-11.31	0.32	1.39
12	5	2	-4.85	-5.00	253	-4.82	0.15	-0.03
13	5	2	-2.57	-2.56	275	-2.57	-0.01	0.00
14	5	2	-1.51	-1.41	297	-1.58	-0.10	0.07

[a]The potentiomeric levels have been plotted in Figure 3-22.

[b]Refer to Figures 3-15 and 3-16 for cell locations.

[c]Refer to Figure 3-17 for node locations.

[d]MODFLOW.

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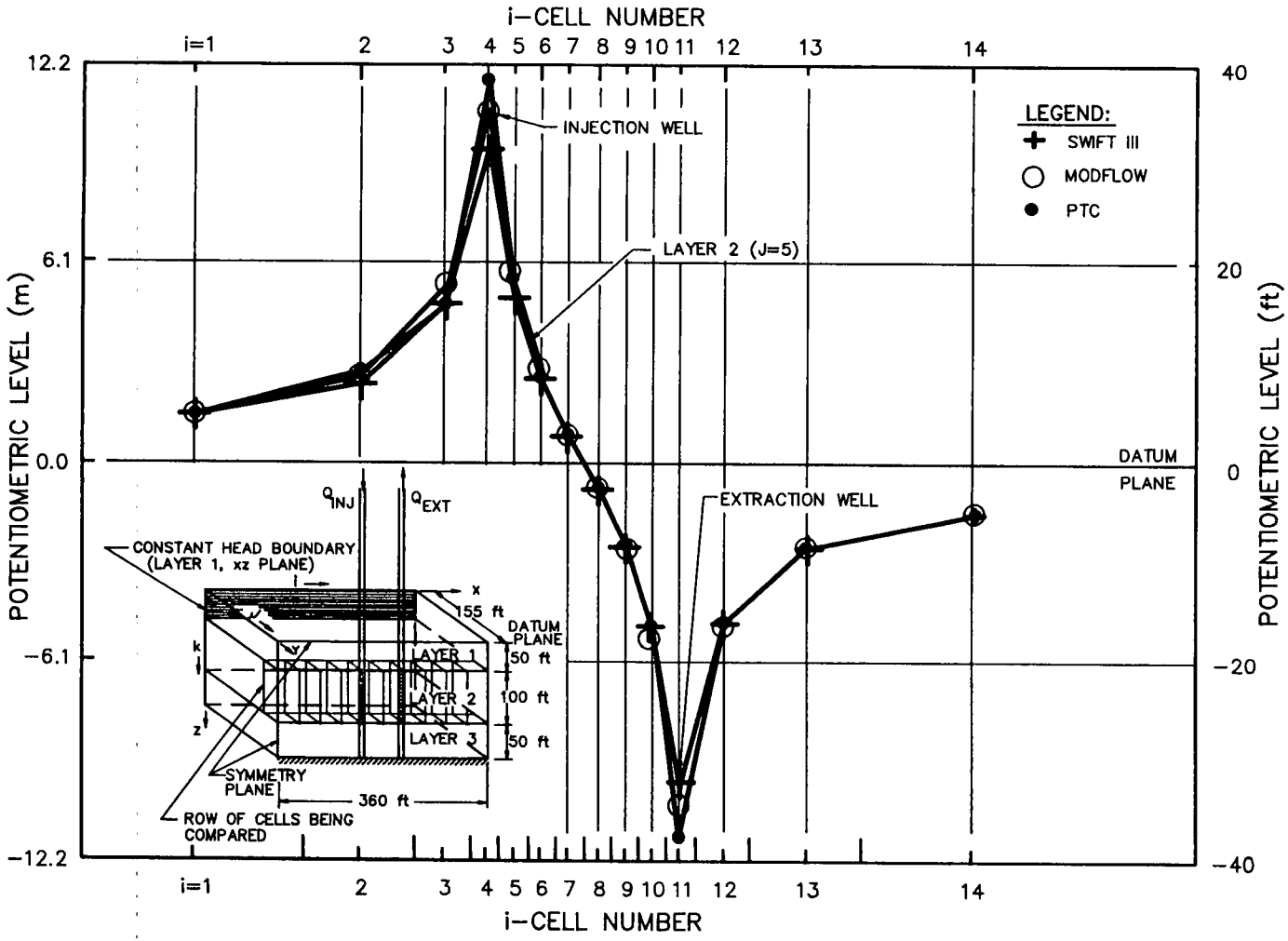

NOTE:

1. REFER TO FIGURE 3-16 FOR LOCATION OF i- AND j-CELLS.
2. REFER TO TABLE 3.10 FOR CORRELATION BETWEEN PTC NODES AND SWIFT III CELL NUMBERS.

FIGURE 3-22

COMPARISON OF STEADY-STATE POTENTIOMETRIC LEVEL VERSUS DISTANCE

PROBLEM GWF-6b

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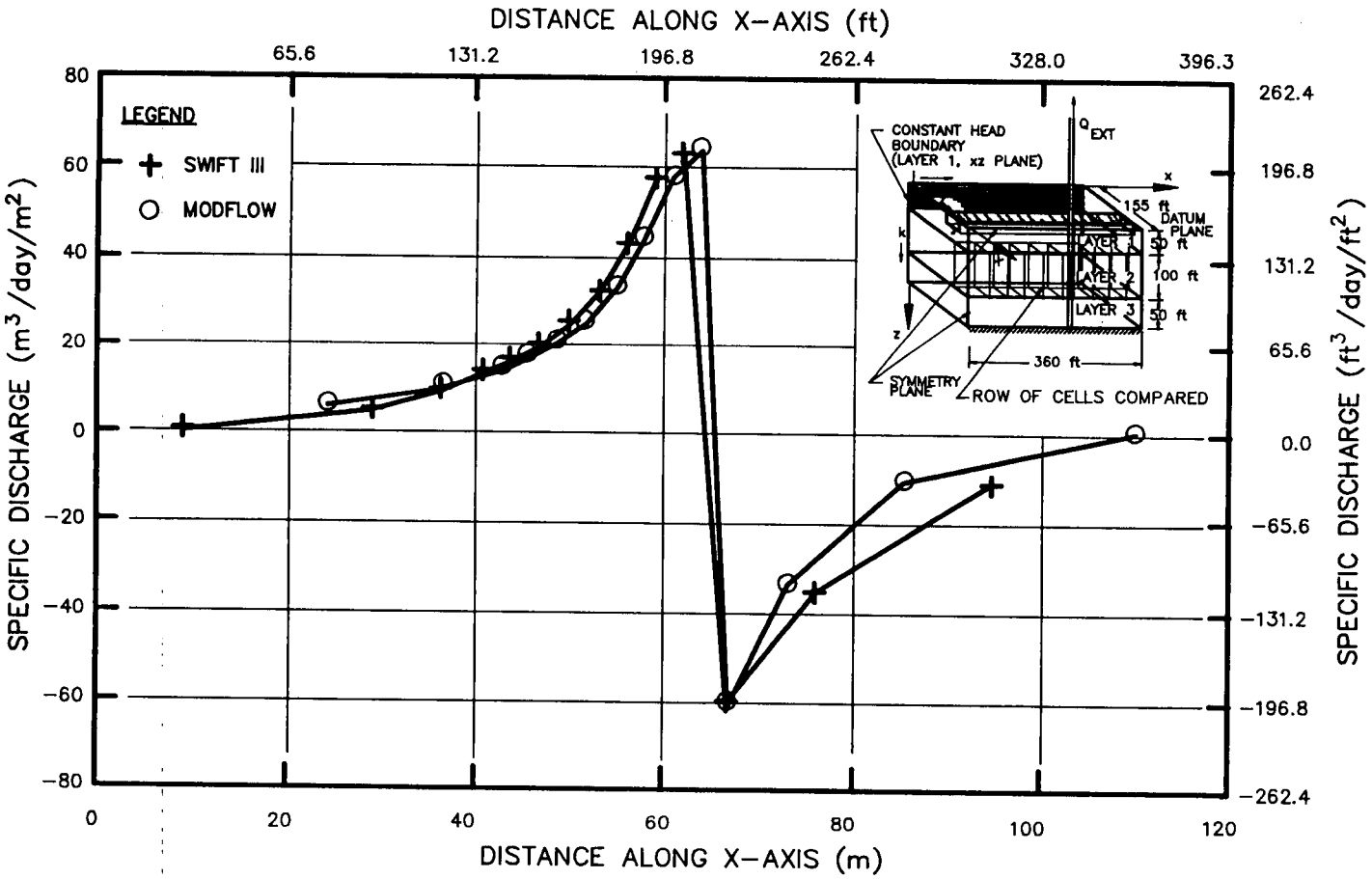

NOTE:

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FIGURE 3-23

COMPARISON OF STEADY-STATE SPECIFIC DISCHARGE (x-COMPONENT) VERSUS DISTANCE

PROBLEM GWF-6c

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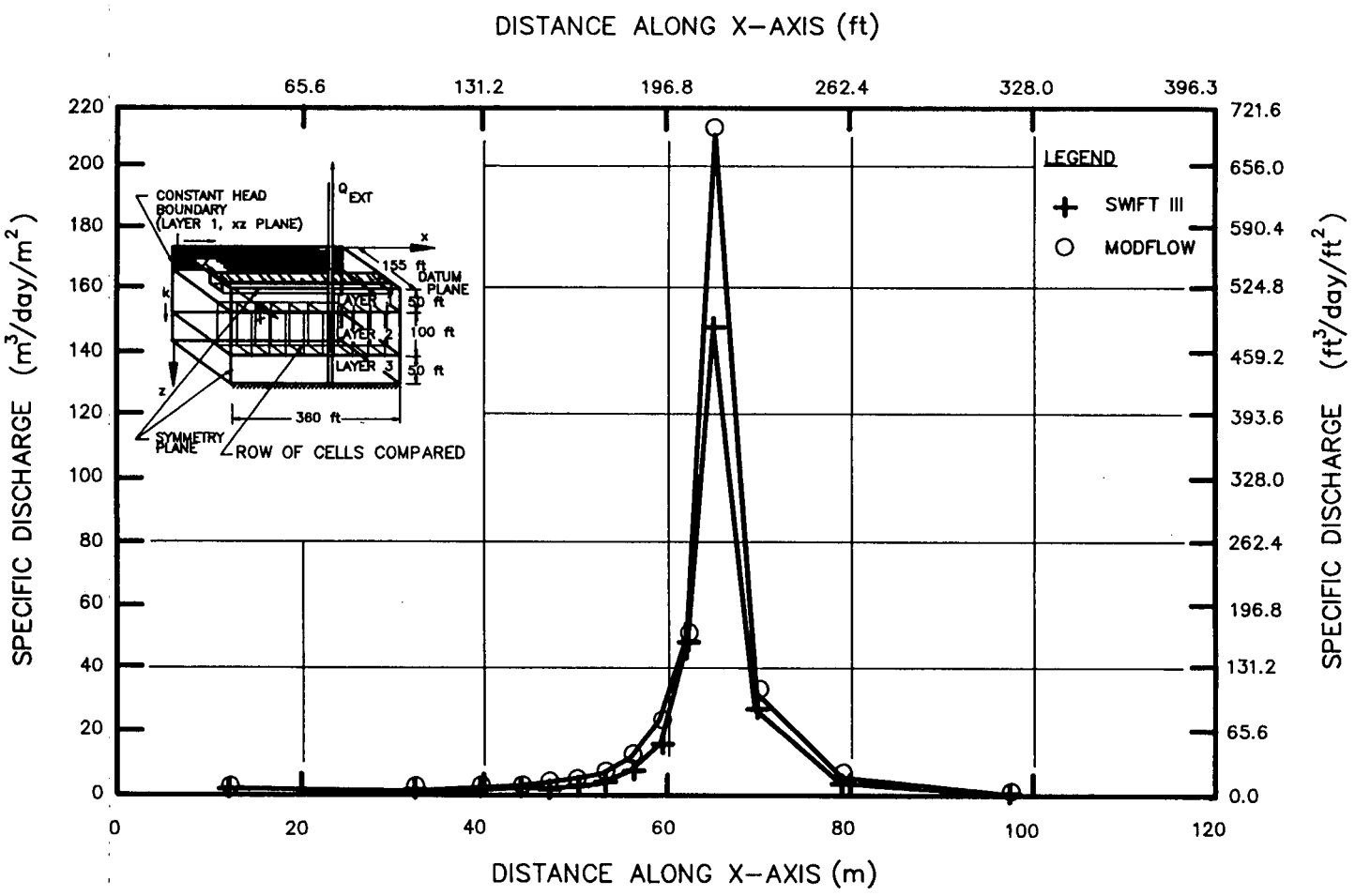

NOTE:

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FIGURE 3-24

COMPARISON OF STEADY-STATE SPECIFIC DISCHARGE (y-COMPONENT) VERSUS DISTANCE

PROBLEM GWF-6c

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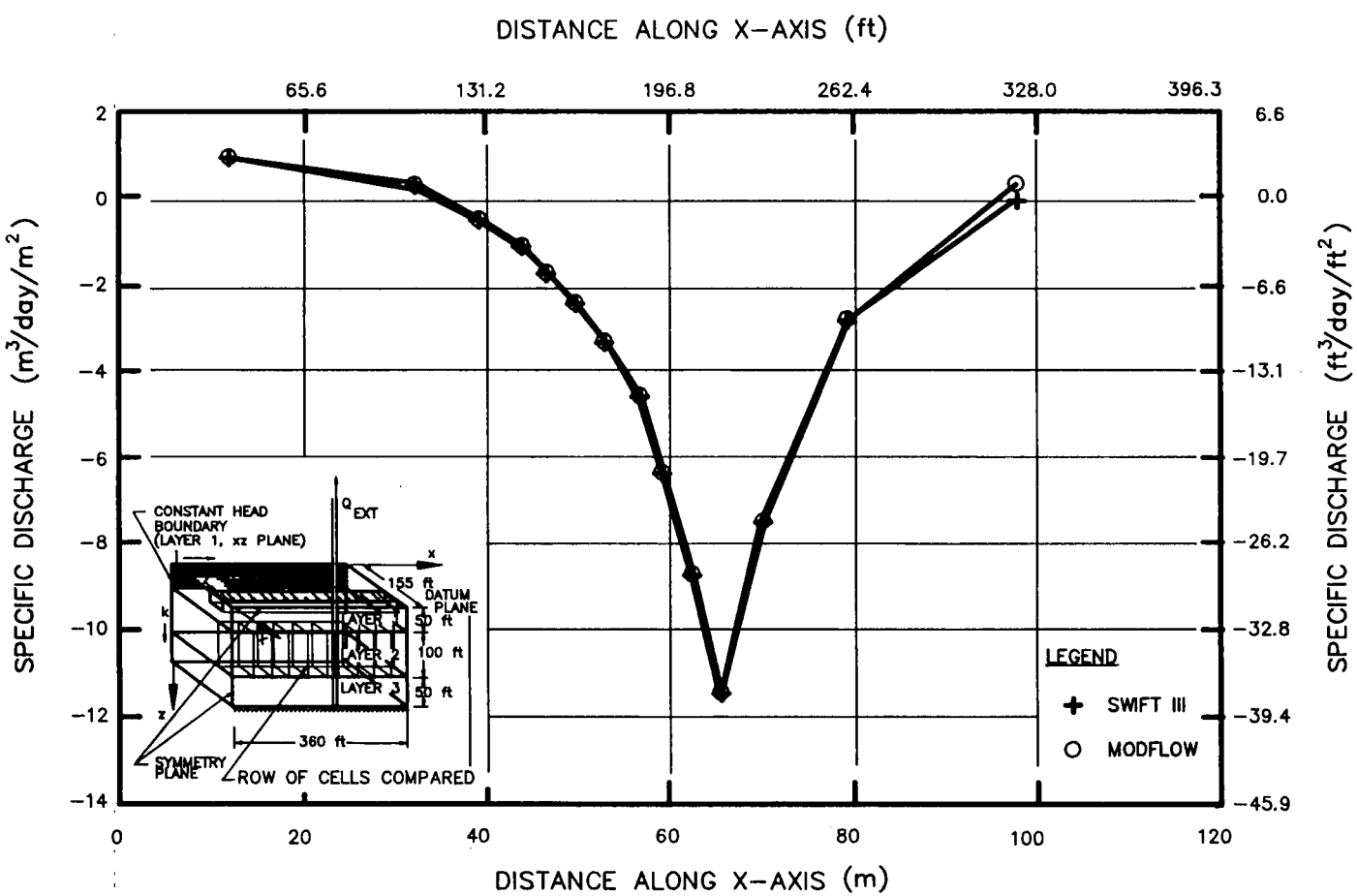

NOTE:

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FIGURE 3-25

COMPARISON OF STEADY-STATE SPECIFIC DISCHARGE (z-COMPONENT) VERSUS DISTANCE

PROBLEM GWF-6c

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submodel to simulate a river, the well submodel was used to simulate the aquifer recharge/discharge to or from a river system. The feature of the well submodel that assigns either a variable recharge/discharge rate or a pressure limitation was exercised to simulate seepage to or from the river. To account for an upper bound on river leakages, the flow rate limitation option was specified for each one of the wells used for river simulation. Such limiting flows were computed using the difference between the river stage and river bottom as the hydraulic head, the planar area of the river as the seepage face, and the river bed conductance as the river bed vertical hydraulic conductivity. These input variables were common to SWIFT III and MODFLOW.

The MODFLOW model simulates seepage to or from a river by adding one of two sets of terms to the ground water flow equations. One set, involving a river bed which is in contact with the aquifer, assumes that leakage varies as a function of the difference in heads between the river and the aquifer. The other set, accounting for unsaturated material below the river bed, assumes that leakage is only a function of the head in the river. The choice of which set to use is made internal to the model at the beginning of each iteration by comparing the most recent value of the head in the cell with the elevation of the riverbed bottom.

The input data for Problem GWF-6c are given in Table 3.8. Steady-state simulations were made with the SWIFT III and MODFLOW models. The steady-state specific discharge (Darcy velocity) components in the x-, y-, and z-directions are shown in Figures 3-23, 3-24, and 3-25, respectively. The specific discharge computed from these two models compare favorably except near the extraction well, where SWIFT III appears to slightly underestimate the y-component of Darcy velocities (Figure 3-24). These differences are not significant to the model application for the FMPC site as discussed previously.

Problem GWF-6d

To enhance verification of the ground water flow models, it was necessary to evaluate the accuracy of the SWIFT III code's leakage rate computations under a significant drawdown condition. The reliable computation of leakage rates is critical because of the prominent river-aquifer interface at the FMPC site. To compare leakage rates, the SWIFT III and MODFLOW models were used to study the effect of large pumping wells in an area close to the river. Extraction wells pumping at a combined rate of 70,850 cubic meters per day (13,000 gpm) were assigned to two cells (Cell i=4, j=5, k=2 and Cell i=11, j=5, and k=2). Leakage rates through the river bed were calculated in Layer 1. The grid system and model layers are shown in Figures 3-15 and 3-16.

The river leakage rates per cell computed from the results of the SWIFT III and MODFLOW models are presented in Figure 3-26. The leakage rates are plotted in gallons per minute (gpm). The plot follows the symmetry of the model, with the largest rates appearing at the boundaries where the cells are large. Figure 3-26 shows that the SWIFT III code yielded somewhat larger leakage rates than MODFLOW. This observation is confirmed in Table 3.12 and Figure 3-27 in which leakage rates per unit area are presented. This deviation can be attributed to the subtle differences in the boundary conditions of the models. SWIFT III draws more water from the river because the boundary conditions are face-centered instead of block-centered. To overcome this situation, special boundary conditions had to be used in SWIFT III in an attempt to match the results of the MODFLOW model. Because the MODFLOW code has a river package, the results obtained from this package were regarded as being more reliable. This greater reliability is demonstrated in Figure 3-27 which shows, consistent to expectations, that river leakage as calculated by MODFLOW is constant whenever the potentiometric level of the aquifer is below the river bottom (compare Figure 3-28). If differences in leakage rates arising from boundary effects are neglected, the computed leakage rates by the two codes will

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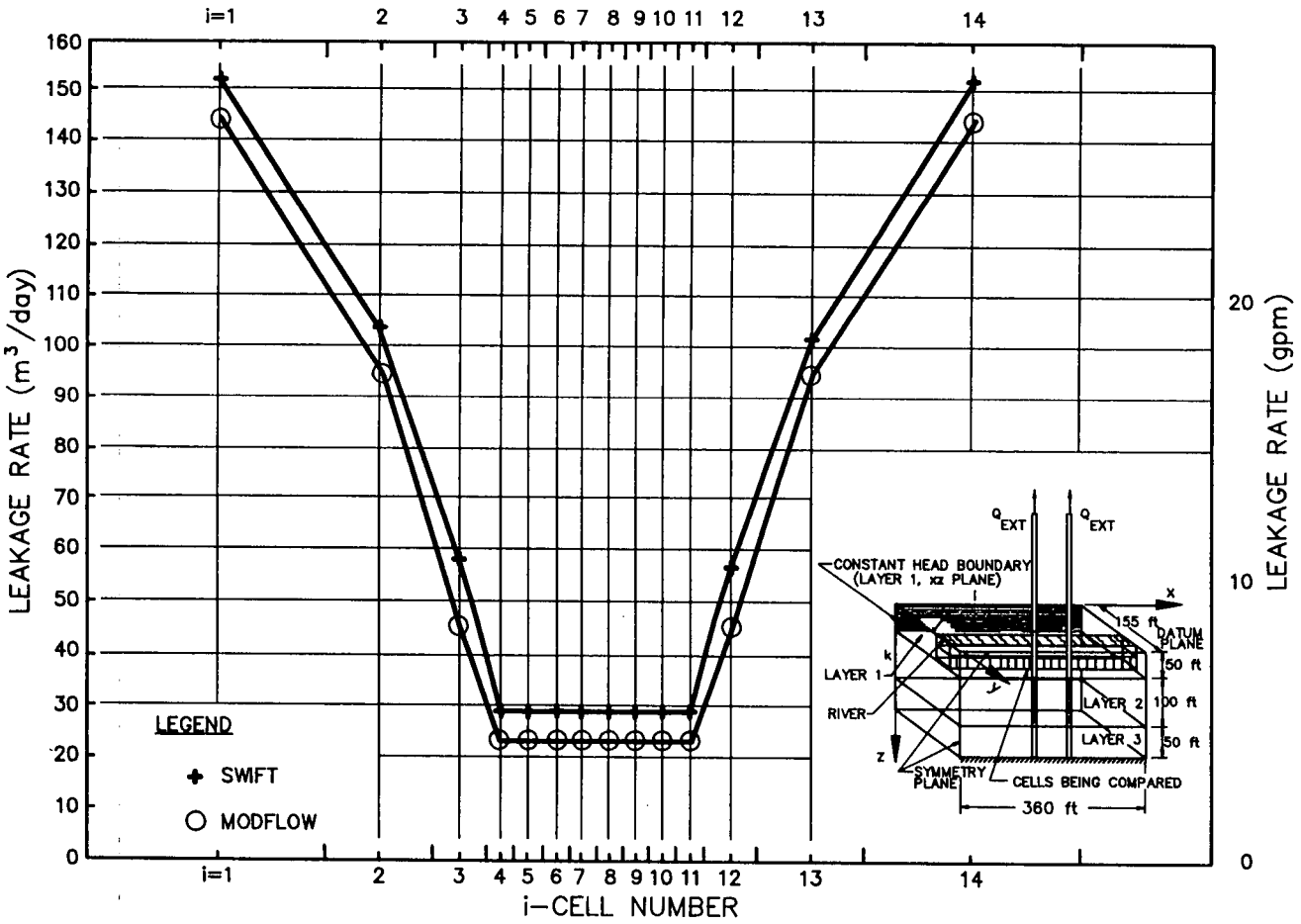

NOTES:

1. REFER TO FIGURE 3-16 FOR LOCATION OF i- AND j-CELLS.
2. REFER TO TABLE 3.10 FOR CORRELATION BETWEEN PTC NODES AND SWIFT III CELL NUMBERS.

FIGURE 3-26

COMPARISON OF RIVER LEAKAGE RATE VERSUS DISTANCE

PROBLEM GWF-6d

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TABLE 3.12

COMPARISON OF RIVER LEAKAGE RATES FOR SWIFT III AND MODFLOW GROUND WATER FLOW MODELS FOR THE FIRST LAYER BENEATH THE RIVER[a] PROBLEM GWF-6d

COORDINATES[b] I	J	K	CELL AREA (m^2)	CELL FLOW SWIFT III m^3/day	CELL FLOW MODFLOW m^3/day	CELL FLOW SWIFT III $m^3/day/m^2$	CELL FLOW MODFLOW $m^3/day/m^3$
1	2	1	297.29	-154.66[c]	-146.2	-0.520	-0.49
2	2	1	148.64	-101.95	-95.14	-0.69	-0.64
3	2	1	74.32	-57.80	-47.58	-0.78	-0.64
4	2	1	37.16	-30.15	-23.79	-0.811	-0.64
5	2	1	37.16	-30.76	-23.79	-0.828	-0.64
6	2	1	37.16	-31.19	-23.79	-0.839	-0.64
7	2	1	37.16	-31.36	-23.79	-0.844	-0.64
8	2	1	37.16	-31.36	-23.79	-0.844	-0.64
9	2	1	37.16	-31.19	-23.79	-0.839	-0.64
10	2	1	37.16	-30.76	-23.79	-0.828	-0.64
11	2	1	37.16	-30.15	-23.74	-0.811	-0.64
12	2	1	74.32	-57.80	-47.58	-0.78	-0.64
13	2	1	148.64	-101.95	-95.14	-0.69	-0.64
14	2	1	297.29	-154.66	-146.2	-0.52	-0.49

[a]The leakage rates have been plotted in Figures 3-27 and 3-28.

[c]Refer to Figures 3-15 and 3-16 for cell locations.

[c]The negative values are a result of the location of the datum (Figure 3-15).

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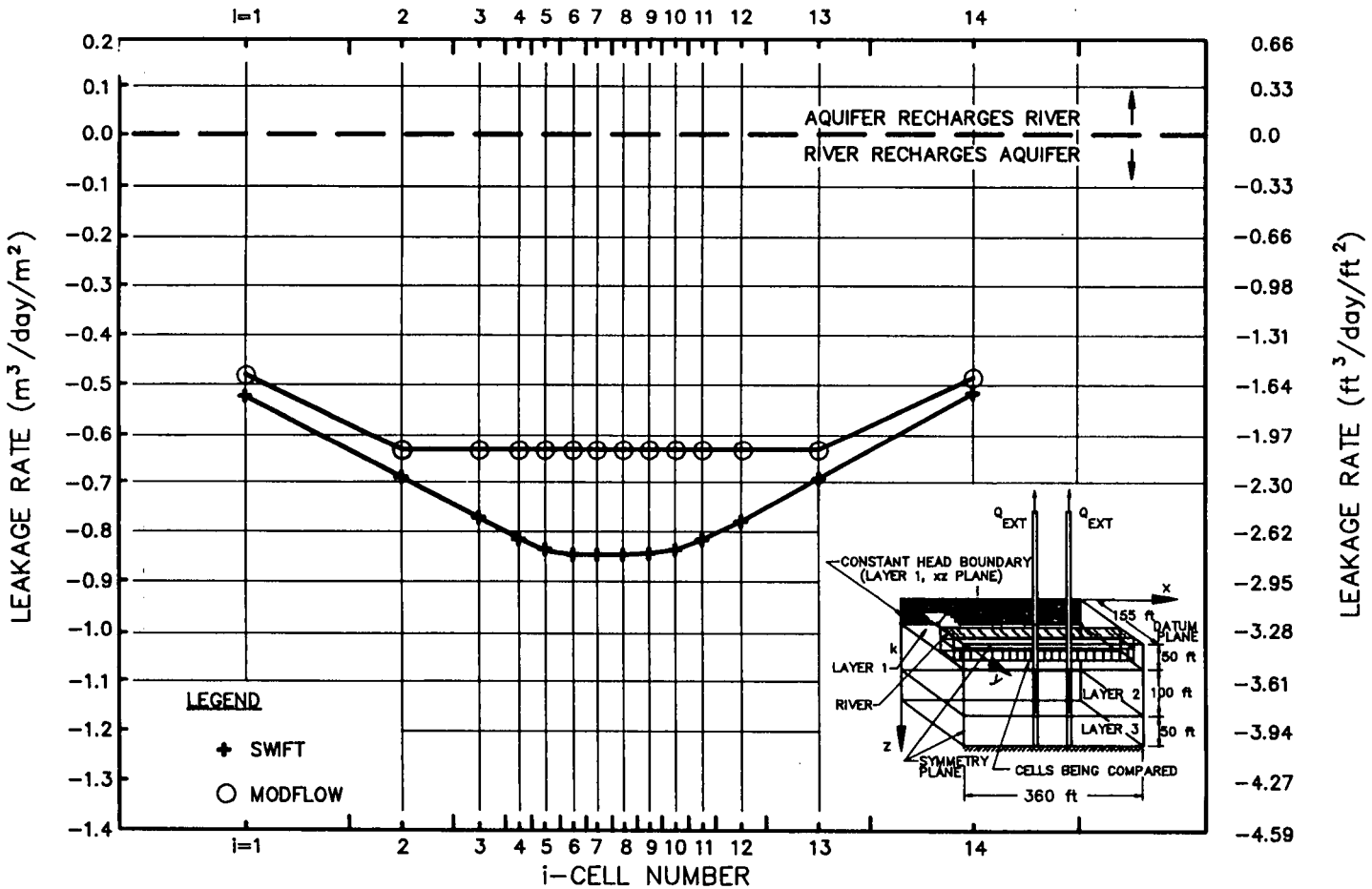

NOTES:

1. REFER TO FIGURE 3-16 FOR LOCATION OF i- AND j-CELLS.
2. REFER TO TABLE 3.10 FOR CORRELATION BETWEEN PTC NODES AND SWIFT III CELL NUMBERS.

FIGURE 3-27

COMPARISON OF RIVER LEAKAGE RATE VERSUS DISTANCE

PROBLEM GWF-6d

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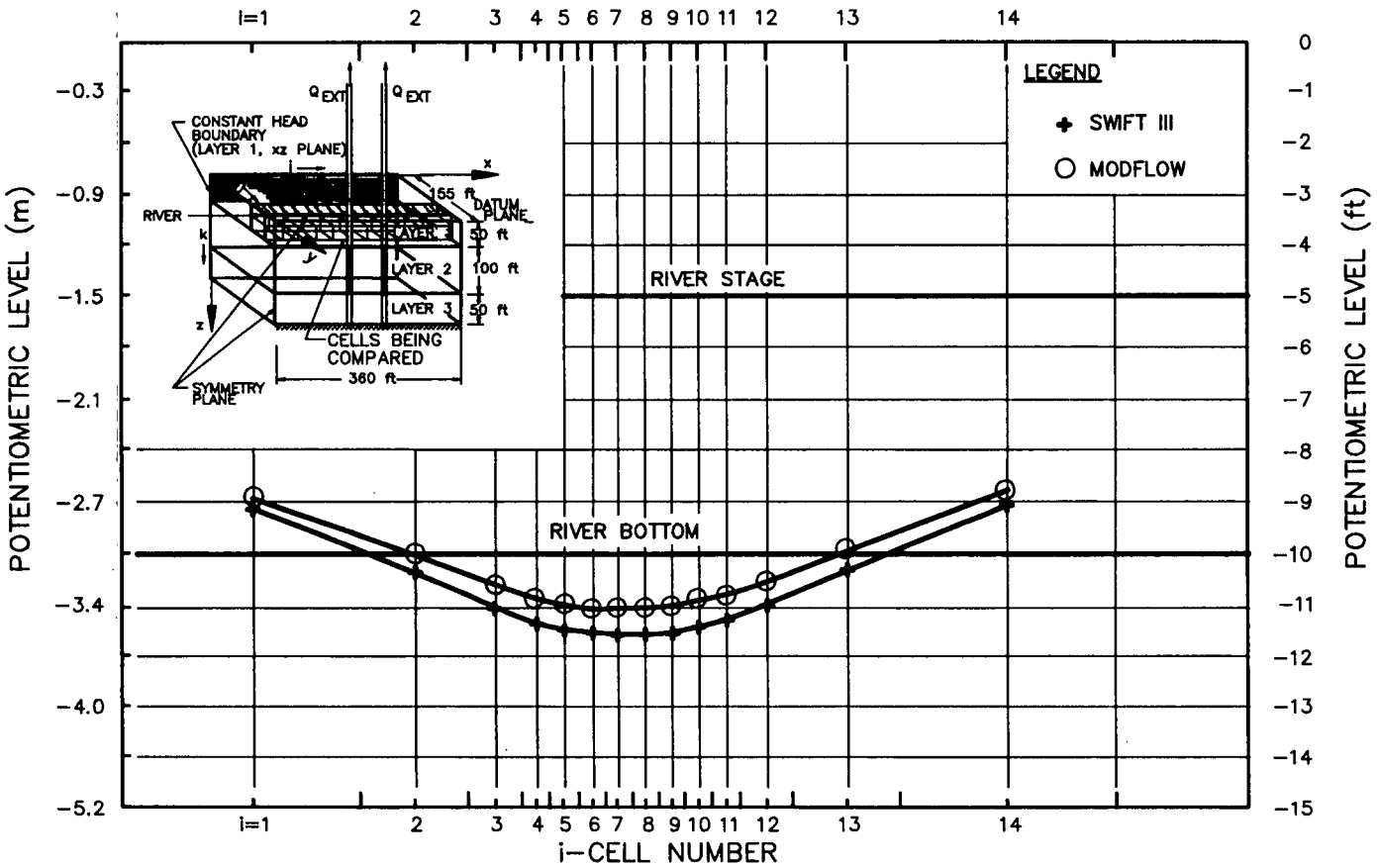

NOTES:

1. REFER TO FIGURE 3-16 FOR LOCATION OF i- and J-CELLS.
2. REFER TO TABLE 3.10 FOR CORRELATION BETWEEN PTC NODES AND SWIFT III CELL NUMBERS.

FIGURE 3-28

COMPARISON OF STEADY-STATE POTENTIOMETRIC LEVEL VERSUS DISTANCE

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be the same except where potentiometric level declines below the bottom of the river bed. In this case, as shown in Figure 3-27, the leakage rate calculated by SWIFT III is about 17 percent more than that calculated by MODFLOW.

It may be noted that the leakage rates calculated in Problem GWF-5 (Figure 3-14) are smaller than the rates for Problem GWF-6d. This is consistent with differences in pumping rates, because Problem GWF-6d has much larger pumping rates than the rates of pumping at wells near the FMPC.

The comparison of potentiometric levels below the river is plotted in Figure 3-28 and presented in Table 3.13. The SWIFT III model exhibits greater drawdown than the MODFLOW model. This is consistent with the larger leakage rates calculated by the SWIFT III model. It is relevant, however, to note that the differences in the potentiometric levels were of the order of one-percent. These differences fall well within the level of expected performance of the codes.

3.3 FIELD COMPARISONS

Field verification of a code is achieved by the development of a site-specific calibrated model which satisfies established calibration criteria. The calibration of the two- and three-dimensional flow models for the FMPC using the SWIFT III program has been successfully completed as part of the RI/FS modeling study. The results will be presented in a separate RI/FS modeling report.

TABLE 3.13

COMPARISON OF POTENTIOMETRIC LEVELS FOR SWIFT III AND MODFLOW GROUND WATER FLOW MODELS FOR THE FIRST LAYER BENEATH THE RIVER[a] PROBLEM GWF-6d

COORDINATES[b] I	J	K	SWIFT III POTENTIOMETRIC LEVEL (meters)	MODFLOW POTENTIOMETRIC LEVEL (meters)	SWIFT III MINUS MODFLOW (meters)	DIFFERENCE (%)
1	2	1	-2.76[c]	-2.69[c]	-0.06	-0.55
2	2	1	-3.16	-3.05	-0.11	-0.88
3	2	1	-3.37	-3.24	-0.13	-1.02
4	2	1	-3.45	-3.31	-0.14	-1.07
5	2	1	-3.49	-3.34	-0.15	-1.09
6	2	1	-3.52	-3.37	-0.15	-1.11
7	2	1	-3.53	-3.38	-0.15	-1.11
8	2	1	-3.53	-3.38	-0.15	-1.11
9	2	1	-3.52	-3.37	-0.15	-1.11
10	2	1	-3.49	-3.34	-0.15	-1.09
11	2	1	-3.45	-3.31	-0.14	-1.07
12	2	1	-3.37	-3.24	-0.13	-1.02
13	2	1	-3.16	-3.05	-0.11	-0.88
14	2	1	-2.76	-2.69	-0.07	-0.60

[a]The potentiometric levels have been plotted in Figure 3-28.

[b]Refer to Figures 3-15 and 3-16 for cell locations.

[c]The negative values are a result of the location of the datum (Figure 3-15).

4.0

4.0 RADIONUCLIDE AND SOLUTE TRANSPORT VERIFICATION

In this chapter, technical details for each of the solute transport verification problems are discussed. The details presented here are also intended to be a documentation and reference of the computer codes and files associated with the verification study. Verification results are presented in English units and/or Standard International (SI) units. The flexibility was provided to maintain consistency of units used by the originators of the comparison verification problems. Unit conversions are given in pertinent tables.

Table 4.1 has been prepared to summarize the application of each problem to the solute transport simulation capabilities of the SWIFT III code being verified. This table includes problem name, model features to be tested, and references to appropriate figures and tables. References to associated files for each solute transport verification problem are presented in Table B.2 of Appendix B.

The following three problems were selected for use in verifying the radionuclide and solute transport components of the SWIFT III code:

- One-dimensional analytical solute transport with chain decay and equal retardation parameters (Problem ST-1)
- Two-dimensional numerical and analytical solute transport (Problem ST-2)
- Three-dimensional numerical solute transport (Problem ST-3)

The above problems were selected to verify the performance of the SWIFT III code and are consistent with the verification process outlined in Table 2.2.

TABLE 4.1

SWIFT III CODE SOLUTE TRANSPORT VERIFICATION SUMMARY

SOLUTE TRANSPORT PROBLEMS	ST-1	ST-2a	ST-2b	ST-3a	ST-3b
		Retardation Factor=1.0	Retardation Factor=2.5	small grid	large grid
SWIFT III FEATURES / CHARACTERISTICS					
ONE-DIMENSIONAL SOLUTE TRANSPORT	X				
TWO-DIMENSIONAL SOLUTE TRANSPORT		X	X		
THREE-DIMENSIONAL SOLUTE TRANSPORT				X	X
RADIONUCLIDE DECAY & GENERATION OF DAUGHTER COMPONENTS	X			X	X
WASTE-LEACH RADIONUCLIDE-SOURCE MODEL	X	X	X	X	X
CARTESIAN COORDINATES	X	X	X	X	X
ENGLISH ENGINEERING UNITS	X			X	X
THE EFFECTS OF THE RETARDATION FACTOR		X	X	X	X
FINITE LENGTH OF SOLUTE SOURCE		X	X	X	X
ASYMMETRICAL SOLUTE SOURCE LOCATION		X	X		
REFERENCES					
VERIFICATION PROBLEM DETAILS	SECTION 4.1.1	SECTION 4.1.2	SECTION 4.1.2	SECTION 4.2	SECTION 4.2
RELEVANT TABLES	TABLE 2.2	TABLE 2.2	TABLE 2.2	TABLE 2.2	TABLE 2.2
	TABLE B.2	TABLE B.2	TABLE B.2	TABLE B.2	TABLE B.2
	TABLE 4.1	TABLE 4.4	TABLE 4.4	TABLE 4.7	TABLE 4.7
	TABLE 4.2	TABLE 4.5	TABLE 4.5	TABLE 4.4	TABLE 4.8
	TABLE 4.3	TABLE 4.6	TABLE 4.6		
RELEVANT FIGURES	FIGURE 4 - 1	FIGURE 4 - 2	FIGURE 4 - 2	FIGURE 4 - 13A	FIGURE 4 - 14A
		FIGURE 4 - 3	FIGURE 4 - 3	FIGURE 4 - 13B	FIGURE 4 - 14B
		FIGURE 4 - 4	FIGURE 4 - 4	FIGURE 4 - 15	FIGURE 4 - 18
		FIGURE 4 - 5	FIGURE 4 - 5	FIGURE 4 - 16	FIGURE 4 - 19
		FIGURE 4 - 6	FIGURE 4 - 10	FIGURE 4 - 17	FIGURE 4 - 20
		FIGURE 4 - 7	FIGURE 4 - 11		
		FIGURE 4 - 8	FIGURE 4 - 12		
		FIGURE 4 - 9			

4.1 VERIFICATION PROBLEMS - ANALYTICAL SOLUTIONS

One- and two-dimensional analytical solutions of solute transport in uniform ground water flow fields were used in the SWIFT III code verification process. The first problem (Problem ST-1) is one-dimensional and was reproduced from "Verification and Field Comparison of the Sandia Waste-Isolation Flow and Transport Model (SWIFT)" by Ward, et al. (1984). The second one (Problem ST-2) is a two-dimensional problem, the solution for which was developed by IT (1986).

4.1.1 Problem ST-1: One-Dimensional Transport with Chain Decay and Equal Retardation Parameters

4.1.1.1 Purpose of Problem Selection

Problem ST-1 was selected to test the combination of the following capabilities of the SWIFT III code:

- One-dimensional solute transport
- Radionuclide decay and generation of daughter products
- Waste-leach radionuclide source
- Cartesian coordinates

4.1.1.2 Problem Description

The problem has been selected from Ward, et al. (1984, pp. 4-1 to 4-2), and is partly reproduced here for the purpose of completeness of presentation. The problem was previously used by GeoTrans to verify the SWIFT III code. By selecting this problem and duplicating the GeoTrans results, it could be ascertained that the SWIFT III code is functioning on the IT computer system. A schematic of the problem is included as an insert in Figure 4-1. It represents a one-dimensional, constant velocity flow in a porous medium. An impervious boundary exists on both sides of the porous system, and a radionuclide source is located at the upgradient end.

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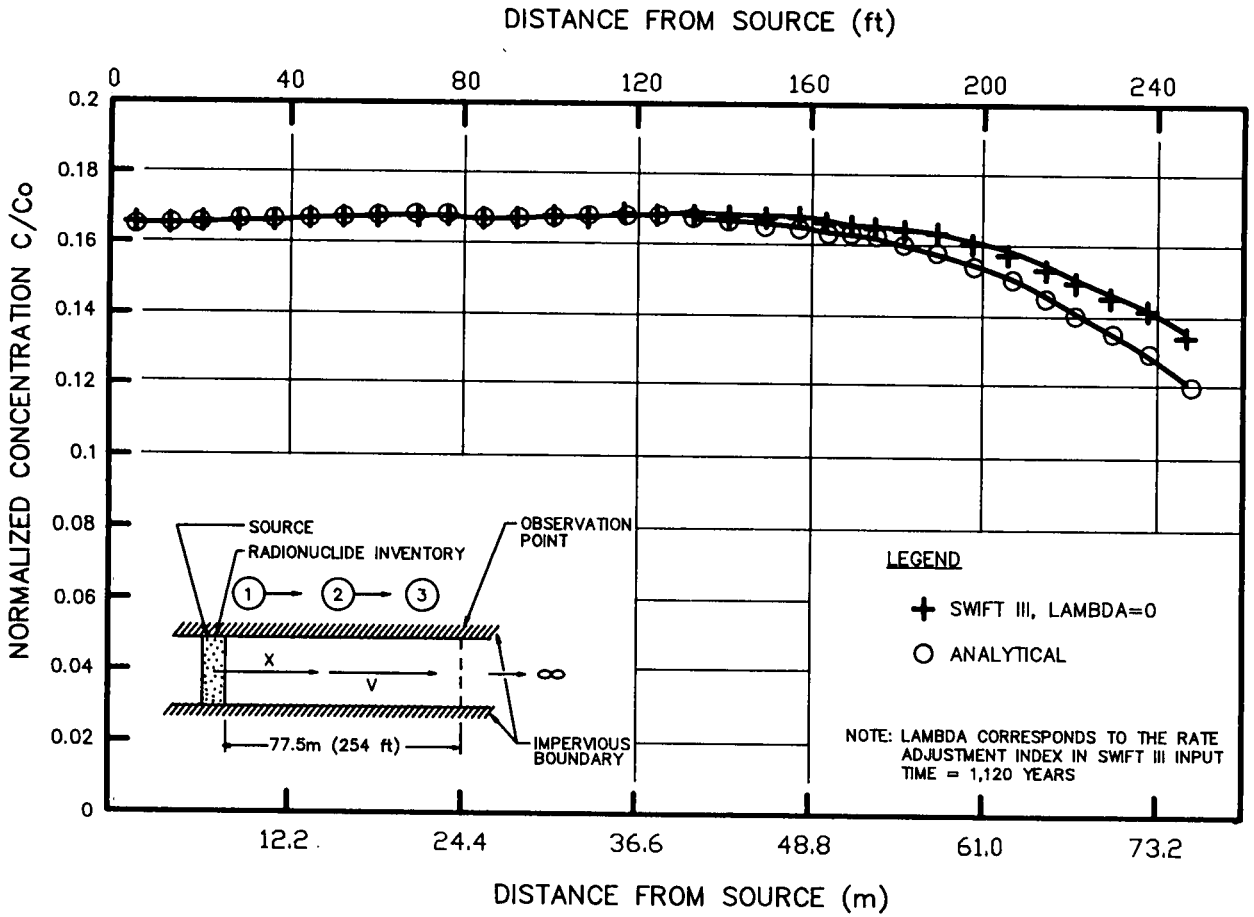

FIGURE 4-1

COMPARISON OF NORMALIZED CONCENTRATION OF COMPONENT 1 VERSUS DISTANCE

PROBLEM ST-1

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A three-component radionuclide chain is released into the porous medium, where it is subject to convection, dispersion, and sorption. The sorption is assumed to be represented by a single retardation factor which is constant in space and time and is the same for all three components. Assuming a one-dimensional transport system, the equation to be solved is (Ward, et al., 1984):

$$- \tilde{U} \frac{\partial C_r}{\partial x} + \frac{\partial^2 C_r}{\partial x^2} + k_{r,r-1}\nu_{r-1}C_{r-1} - \nu_r C_r = \frac{\partial C_r}{\partial t} \text{ , } r = 1,2,3 \quad (4.1)$$

where

$\tilde{U}$ = retarded interstitial velocity of radionuclide [L/t],

C_r = radionuclide concentration [M/L^3] for each daughter component,

$k_{r,s}$ = product of a branching ratio and a daughter-to-parent mass fraction (dimensionless),

ν = decay constant [1/t],

r = a subscript representing each daughter component;

The velocity appearing in Equation 4.1 is the retarded interstitial velocity, which is defined in terms of the Darcy velocity, v:

$$\tilde{U} = \frac{v}{\phi R_d} \quad (4.2a)$$

where R_d is the retardation factor. The dispersion coefficient is defined in terms of this velocity, i.e.,

$$D = \alpha_L \tilde{U} \quad (4.2b)$$

where

D = dispersion coefficient [L^2/t],

α_L = longitudinal dispersivity [L]

The initial concentration of the radionuclides in the porous medium is zero for each component:

$$C_r(x,t=0) = 0, \qquad x \geq 0 \tag{4.3a}$$

Furthermore, the infinite boundary is held at the initial condition for each component:

$$C_r(x = \infty,t) = 0, \qquad t \geq 0 \tag{4.3b}$$

However, a time-dependent flux, $\tilde{U}\tilde{C}_r$, enters the system through a third-type boundary condition:

$$\tilde{U}C_r - D\frac{\partial C_r}{\partial x} = \tilde{U}\tilde{C}_r, \qquad x = 0,\ t > 0 \tag{4.3c}$$

The time-dependent boundary value, $\tilde{C}_r(t)$, arises from a radionuclide inventory undergoing Bateman decay/production relative to the initial boundary values, i.e.

$$\tilde{C}_r(t=0) = \tilde{C}_{ro} \tag{4.4}$$

4.1.1.3 Assumptions

The following assumptions are made:

- Ground water flow and solute transport are one dimensional
- The domain is semi-infinite
- Hydrogeologic parameters are constant throughout the domain
- The inventory of radionuclides are infinite, and thus the period of leaching are infinite

- Radionuclides are present in trace quantities only, and as such they do not influence flow
- Diffusion is insignificant within the fluid field
- Adsorption may be approximated by a linear equilibrium isotherm
- Dispersivity and retardation factor are constant throughout the domain
- The radionuclide components have equal retardation factors

4.1.1.4 Analytical Solution

The analytical solution for this problem is derived in Coats and Smith (1964). The same solution is also reported in Ward et al. (1984, pp. 4-4 and 4-5).

Because of the assumption of equal retardations, the solution of Equation 4.1 may be written in the factored form:

$$C_r(x,t) = \tilde{C}_r(t)\Theta^{(3)}(x,t) \qquad (4.5)$$

where $\tilde{C}_r$ contains only decay/production terms, and $\Theta^{(3)}$, a dimensionless function, contains only transport terms. The function $\tilde{C}_r$ is given by:

$$\tilde{C}_r(t) = \tilde{C}_{10}e^{-\nu_r t}, \; r=1 \qquad (4.6a)$$

$$\tilde{C}_r(t) = \tilde{C}_{ro}e^{-\nu_r t} + \{\sum_{k=1}^{r-1}[\tilde{C}_{ko}\sum_{j=k}^{r-1} Y_{rj}(t)S_j \cdot \prod_{\substack{\ell=k \\ \ell\neq j}}^{r-1} S_\ell/(\nu_\ell - \nu_j)]\}, \quad r > 1 \qquad (4.6b)$$

where

$$S_j = k_{j+1,j}\nu_j \tag{4.7a}$$

$$\prod_{\substack{\ell=k \\ \ell\neq j}}^{r-1} S_\ell/(\nu_\ell-\nu_j) = 1, \qquad k = r-1 \tag{4.7b}$$

and

$$Y_{rj} = (e^{-\nu_j t} - e^{-\nu_r t})/(\nu_r - \nu_j) \tag{4.7c}$$

The solution to Equation 4.1 is in the form of a dimensionless function which contains the transport terms given in Coats and Smith (1964).

$$\begin{aligned}\Theta^{(3)} = \frac{1}{2}\{&\mathrm{erfc}[\frac{x - \tilde{U}t}{2(Dt)^{1/2}}] - \exp(\frac{\tilde{U}x}{D})\mathrm{erfc}[\frac{x + \tilde{U}t}{2(Dt)^{1/2}}]\} \\ &- \frac{\tilde{U}}{2D}(x + \tilde{U}t)\exp(\frac{\tilde{U}x}{D})\mathrm{erfc}[\frac{x + \tilde{U}t}{2(Dt)^{1/2}}] \\ &+ (\frac{\tilde{U}^2 t}{\pi D})^{1/2} \exp[-\frac{(x - \tilde{U}t)^2}{4Dt}]\end{aligned} \tag{4.8}$$

The Equations 4.5, 4.6, and 4.8 are used to calculate radionuclide concentrations for various daughter components as functions of time and distance.

4.1.1.5 Numerical Solution

Important aspects of the numerical solution are discussed in Ward et al. (1984, pp 4-5 to 4-9) and are restated below.

A finite-difference grid containing 32 one-dimensional blocks was constructed to simulate solute transport. The numerical model was 77.5m

(254 ft) in length. This length was sufficient to minimize the effect of placing the source at the first cell, rather than at the exact boundary, which is the case for the analytical solution (Equation 4.3c).

Centered-in-space differencing was selected, and the spatial increments were chosen to be consistent with the appropriate criterion ($\Delta x \leq 2\alpha_L$) for numerical stability. Centered differencing was also chosen for the time domain. The analyses were performed for a period up to 1,120 years.

After the breakthrough occurs at about 640 years, the concentration gradient within the system for Component 1 dissipates and the concentration becomes virtually uniform over the length of the system. In the absence of sharp concentration gradients, numerical dispersion does not appear in the solution because the convection term causing the numerical dispersion disappears. Thus, after 640 years it was necessary only to observe constraints arising from the half-life of Component 1 (433 years). As this component became insignificant it was necessary only to track Component 3, which had a considerably longer half-life (6,540 years).

4.1.1.6 Input Specifications

Input parameters for this problem are given in Table 4.2.

4.1.1.7 Output Specifications

The output consists of curves of concentration versus distance for each of the three radionuclide components.

4.1.1.8 Results

A comparison of normalized concentrations as a function of distance for Component 1 of the three-component radionuclide chain decay is shown in Figure 4-1. Review of Figure 4-1 indicates that the normalized concentration of Component 1 resulting from the numerical model agrees

TABLE 4.2

INPUT PARAMETERS FOR THE THREE-COMPONENT RADIONUCLIDE CHAIN DECAY PROBLEM ST-1

PARAMETER	SYSTEM PARAMETERS SYMBOL[a]	VALUE SI	VALUE ENGLISH
System length	L	77.5 m	254 ft
Spatial increments	Δx	1.68 to 2.5 m	5.5 to 8.2 ft
Boundary pressure	ρ_0	3.33×10^5 Pa	48.3 psi
Boundary pressure	ρ_1	6.98×10^4 Pa	10 psi
Hydraulic conductivity	K_x	6.7×10^{-6} m/s	1.9 ft/day
Spatial differencing	CIS[b]	-	-
Time differencing	CIT[c]	-	-
Darcy velocity	μ	2.31×10^{-6} m/s	0.656 ft/day
Porosity	ϕ	0.1	0.1
Longitudinal dispersivity	α_L	2.59 m	8.5 ft
Retardation factor	R_d	9,352	9,352
Retarded interstitial velocity	$\tilde{U}$[d]	2.47×10^{-9} m/s	7.01×10^{-4} ft/day
Dispersion coefficient	D	6.39×10^{-9} m^2/s	5.96×10^{-3} ft^2/day

COMPONENT PARAMETERS

COMPONENT NUMBER	PARAMETER[e] $k_{r,r-1}$	HALF-LIFE (y)	DECAY CONSTANT, ν (y^{-1})	INITIAL CONCENTRATION, C_{ro}
1	0	433	1.60×10^{-3}	1
2	1	15	4.62×10^{-2}	0
3	1	6,540	1.06×10^{-4}	0

[a]Symbols follow the convention adopted in SWIFT's verification manual (Ward, et al., 1984).

[b]CIS = centered in space.

[c]CIT - centered in time.

[d]Retarded interstitial velocity is defined as $u/\phi R_d$.

[e]Product of branching ratio and mass fraction of daughter to parent.

well with the analytical solution up to 40 meters from the source. Thereafter the computed values diverge to some degree from the analytical values. Table 4.3 presents the comparison of analytical and SWIFT III results for Component 2 for t = 270 and 1,120 years. The comparison between analytical and numerical results of Component 2 in Table 4.3 indicate that at relatively low concentrations, the analytical and numerical model results do not agree well. This is of no consequence to future applications of the SWIFT III codes because it results from numerical inaccuracies introduced in either model via computations with very small numbers. A case in point is illustrated in Table 4.3, where at 273 years, the difference between numerical and analytical concentrations is one order of magnitude (10^{-5} to 10^{-6}) at 56.25 meters from the source. However, after 1,120 years, the agreement between numerical and analytical values is excellent throughout the length of the model.

4.1.2 Problems ST-2a and 2b: Two-Dimensional Solute Transport

Two-dimensional solute transport comparisons were made between SWIFT III and both analytical solutions and a second numerical code. For analytical solutions, the program STRIP1B-FBC-G developed by IT (1986) was chosen. For numerical solutions, the GEOFLOW code was used. Problems ST-2a and ST-2b are identical except for the retardation factor, which for Problem ST-2a is equal to 1 and for Problem ST-2b is equal to 2.5.

4.1.2.1 Purpose of Problem Selection

Problems ST-2a and ST-2b were selected to test the modeling behavior of the following aspects of the SWIFT III code:

- Two-dimensional solute transport
- Cartesian coordinates
- The effects of the retardation factor

TABLE 4.3

COMPARISON OF SWIFT III AND ANALYTICAL RESULTS FOR RADIONUCLIDE DECAY AND TRANSPORT FOR COMPONENT 2[a] PROBLEM ST-1

		t = 273 years		t = 1120 years	
ft	DISTANCE FROM SOURCE (meters)	SWIFT III	ANALYTICAL	SWIFT III	ANALYTICAL
4.1	1.25	2.36E-02[b]	2.28E-02	6.11E-03	5.97E-03
12.3	3.75	2.34E-02	2.24E-02	6.11E-03	5.97E-03
20.5	6.25	2.32E-02	2.17E-02	6.11E-03	5.97E-03
28.7	8.75	2.27E-02	2.08E-02	6.11E-03	5.97E-03
36.9	11.25	2.19E-02	1.95E-02	6.10E-03	5.97E-03
45.1	13.75	2.07E-02	1.75E-02	6.10E-03	5.97E-03
53.3	16.25	1.92E-02	1.59E-02	6.10E-03	5.97E-03
61.5	18.75	1.73E-02	1.37E-02	6.10E-03	5.97E-03
69.7	21.25	1.50E-02	1.14E-02	6.10E-03	5.97E-03
77.9	23.75	1.27E-02	9.18E-03	6.10E-03	5.97E-03
86.1	26.25	1.03E-02	7.08E-03	6.10E-03	5.96E-03
94.3	28.75	8.08E-03	5.23E-03	6.10E-03	5.96E-03
102.5	31.25	6.09E-03	3.70E-03	6.09E-03	5.95E-03
110.7	33.75	4.41E-03	2.50E-03	6.09E-03	5.94E-03
118.9	36.25	3.08E-03	1.61E-03	6.08E-03	5.93E-03
127.1	38.75	2.07E-03	9.91E-04	6.08E-03	5.91E-03
135.3	41.25	1.34E-03	5.79E-04	6.07E-03	5.89E-03
143.5	43.75	8.36E-04	3.22E-04	6.05E-03	5.86E-03
151.7	46.25	5.04E-04	1.70E-04	6.03E-03	5.83E-03
159.9	48.75	2.94E-04	8.54E-05	6.00E-03	5.78E-03
166.7	50.83	1.86E-04	4.62E-05	5.97E-03	5.73E-03
172.2	52.50	1.25E-04	2.76E-05	5.94E-03	5.69E-03
177.7	54.17	8.27E-05	1.61E-05	5.91E-03	5.64E-03
184.5	56.25	4.77E-05	7.91E-06	5.86E-03	5.56E-03
192.7	58.75	2.47E-05	3.22E-06	5.78E-03	5.46E-03
200.9	61.25	1.25E-05	1.24E-06	5.69E-03	5.34E-03
209.1	63.75	6.13E-05	64.54-E07	5.58E-03	5.19E-03
217.4	66.25	2.94E-06	1.57E-07	5.45E-03	5.03E-03
225.5	68.75	1.39E-06	5.16E-08	5.30E-03	4.85E-03
233.7	71.25	6.40E-06	1.60E-08	5.13E-03	4.65E-03
241.9	73.75	2.91E-06	4.71E-09	4.96E-03	4.42E-03
250.1	76.25	1.42E-07	1.32E-09	4.83E-03	4.18E-03

[a]Refer to Figure 4-1 for plot of Component 1 Concentrations.
Refer to Figure 4-1 for insert of schematic geometry of problem.
Refer to Table 4.2 for characteristics of Component 2.

[b]All values are given as the ratio of concentration at the given time to the initial concentration of the parent radionuclide: Component 1.

- Finite length of solute source
- Asymmetrical solute source location

4.1.2.2 Problem Description

A schematic drawing of the general solute source problem is given in Figure 4-2. The problem considers transient two-dimensional solute transport in a unidirectional ground water flow field between two impervious boundaries with the third-type (Cauchy) flux boundary condition at the source. The solute source is located irregularly along the z-axis and flow is in the x-direction. The source concentrations are functions of distance along the z-axis. The porous medium extends to infinity in the x-direction and has a finite length, H_m, along the z-axis, as depicted in Figure 4-2. In this figure, C_{m_i} represents the source concentration at the ith strip.

With linear equilibrium adsorption and first-order decay, the two-dimensional hydrodynamic dispersion equation in a unidirectional flow field can be written as:

$$R_d \frac{\partial C}{\partial t} = D_x \frac{\partial^2 C}{\partial x^2} + D_z \frac{\partial^2 C}{\partial z^2} - U \frac{\partial C}{\partial x} - R_d \nu C \qquad (4.9)$$

where

C = mass of solute for unit volume of fluid $[M/L^3]$,
R_d = retardation factor [dimensionless],
ν = decay constant $[1/t]$,
U = seepage velocity $[L/t]$,
x,z = Cartesian coordinates $[L]$,
D_x, D_z = longitudinal and transverse dispersion coefficients, respectively $[L^2/t]$

The seepage velocity, U, appearing in Equation 4.9 is the ground water velocity which is defined in terms of the Darcy velocity, v, and porosity, ϕ, as:

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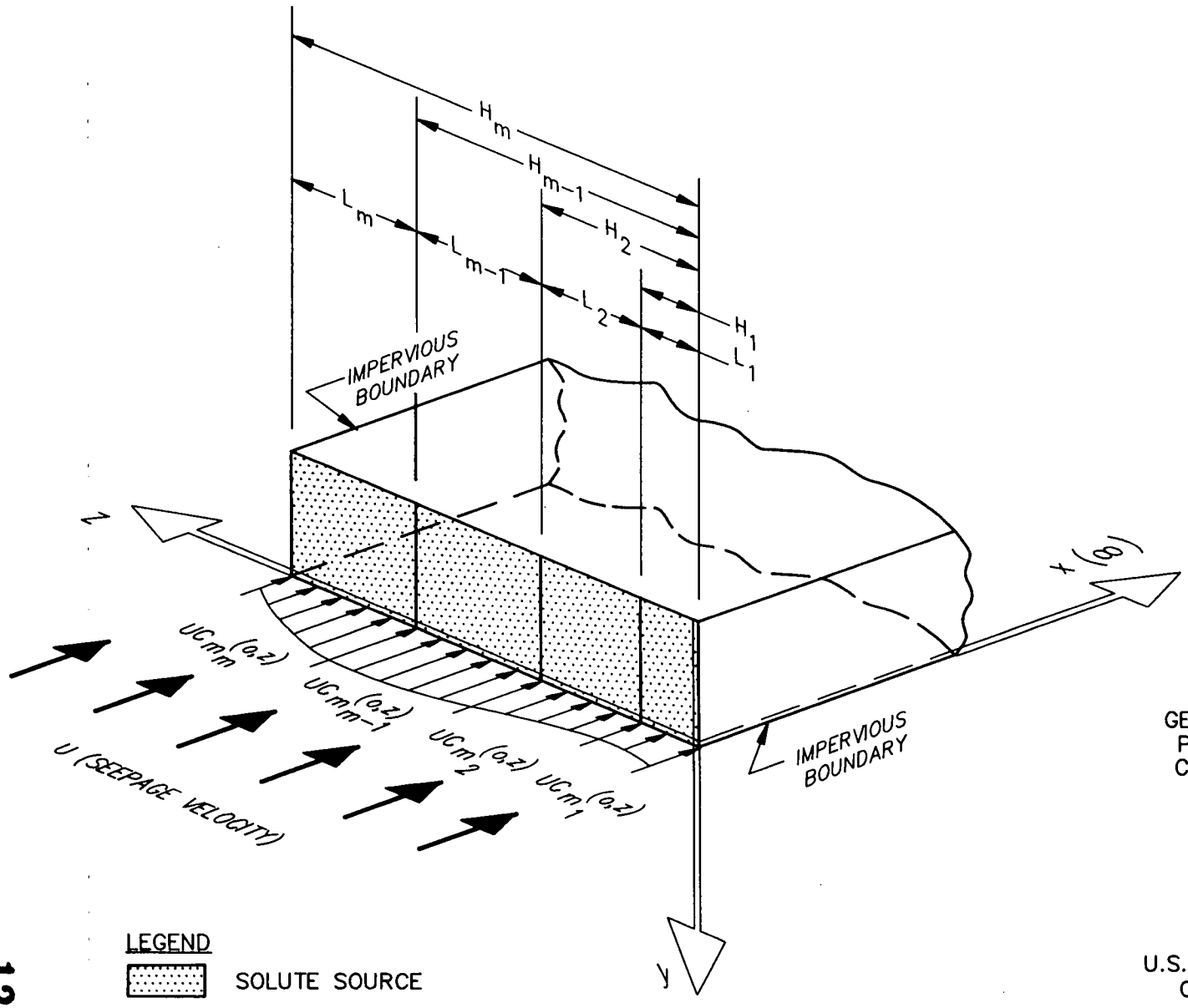

LEGEND

SOLUTE SOURCE

FIGURE 4-2

GENERAL SCHEMATIC OF A POROUS MEDIUM WITH A CONSTANT CONTAMINANT FLUX BOUNDARY

PROBLEM ST-2

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$$U = \frac{v}{\phi} \tag{4.10}$$

D_x and D_z are the longitudinal and transverse dispersion coefficients and are defined as:

$$D_x = \alpha_L U \tag{4.11}$$

$$D_z = \alpha_T U \tag{4.12}$$

where α_L [L] and α_T [L] are the longitudinal and transverse dispersivities, respectively.

Initially, the concentration in the porous medium is zero. Therefore, the initial condition for the transport field is:

$$C\ (x,\ z,\ t = 0) = 0 \tag{4.13}$$

The third-type (Cauchy) or flux-type boundary conditions at the sources (x = 0) is:

$$\frac{F_x(0,z,t)}{\phi} = UC_{m_1}(z) \qquad 0 < z < H_1 \tag{4.14a}$$

$$= UC_{m_{m-1}}(z) \qquad H_{m-2} < z < H_{m-1} \tag{4.14b}$$

$$= UC_{m_m}(z) \qquad H_{m-1} < z < H_m \tag{4.14c}$$

where

$$H_i = \sum_{j=1}^{i} L_j \tag{4.15}$$

where L_j is the length of the jth strip source.

$$U = \frac{v}{\phi} \tag{4.10}$$

D_x and D_z are the longitudinal and transverse dispersion coefficients and are defined as:

$$D_x = \alpha_L U \tag{4.11}$$

$$D_z = \alpha_T U \tag{4.12}$$

where α_L [L] and α_T [L] are the longitudinal and transverse dispersivities, respectively.

Initially, the concentration in the porous medium is zero. Therefore, the initial condition for the transport field is:

$$C\ (x,\ z,\ t = 0) = 0 \tag{4.13}$$

The third-type (Cauchy) or flux-type boundary conditions at the sources (x = 0) is:

$$\frac{F_x(0,z,t)}{\phi} = UC_{m_1}(z) \qquad 0 < z < H_1 \tag{4.14a}$$

$$= UC_{m_{m-1}}(z) \qquad H_{m-2} < z < H_{m-1} \tag{4.14b}$$

$$= UC_{m_m}(z) \qquad H_{m-1} < z < H_m \tag{4.14c}$$

where

$$H_i = \sum_{j=1}^{i} L_j \tag{4.15}$$

where L_j is the length of the jth strip source.

Conditions at the impervious boundaries are:

$$\frac{\partial C(x,z,t)}{\partial z} = 0 \qquad z = 0 \qquad 0 < x < \infty \qquad (4.16)$$

$$\frac{\partial C(x,z,t)}{\partial z} = 0 \qquad z = H_m \qquad 0 < x < \infty \qquad (4.17)$$

The boundary conditions at infinity are:

$$\lim_{x \to \infty} C\,(x,z,t) = 0 \qquad 0 < z < H_m \qquad (4.18)$$

$$\lim_{x \to \infty} \frac{\partial C(x,z,t)}{\partial x} = 0 \qquad 0 < z < H_m \qquad (4.19)$$

4.1.2.3 Assumptions

The following assumptions are made:

- Ground water flow is one-dimensional
- Solute transport is two-dimensional
- The transport domain is bounded by two impervious boundaries
- The transport domain goes to infinity in the x-direction
- Hydrogeological parameters are constant throughout the domain
- Diffusion is insignificant within the fluid field
- Adsorption may be approximated by a linear equilibrium isotherm
- Longitudinal and transverse dispersivities and retardation factor are constant throughout the transport domain

4.1.2.4 Analytical Solution

The general solution of Equation 4.1 with pertinent initial and boundary conditions was determined by IT (1986b). Using this general solution, a special solution was obtained for a single strip source whose geometry is shown in Figure 4-3. This special solution is reported in the GEOFLOW manual (IT, 1986, pp. 3-18 to 3-20).

For the special solution (Figure 4-3), the flux boundary at x = 0 is defined as:

$$\frac{F_x(0,z)}{\phi} = UC_m \qquad D_1 < z < D_1 + 2B \qquad (4.20)$$

$$= 0 \qquad \text{otherwise} \qquad (4.21)$$

where C_m is the source concentration and 2B is the width of the strip source.

The derivation of the general solution for Equation (4.1) is presented in Appendix C. The special solution of the general model for a strip source with boundary conditions defined in Equation (4.20) and (4.21) is:

$$\frac{C(x,z,t)}{C_m} = \frac{U}{D_x} \frac{2B}{(D_1+2B+D_2)} \int_0^t F_1(u)[F_2(u)$$

$$- F_3(u)\ F_4(u)]du + \frac{2}{\pi}\frac{U}{D_x} \sum_{n=1}^{\infty} \frac{1}{n} \{\sin[\lambda_n(D_1+2B)]$$

$$- \sin(\lambda_n D_1)\} \cos(\lambda_n z) \int_0^t F_1(u)\exp\left(-\frac{D_z}{R_d}\lambda_n^2 u\right)$$

$$\bullet\ [F_2(u) - F_3(u)\ F_4(u)]du \qquad (4.22)$$

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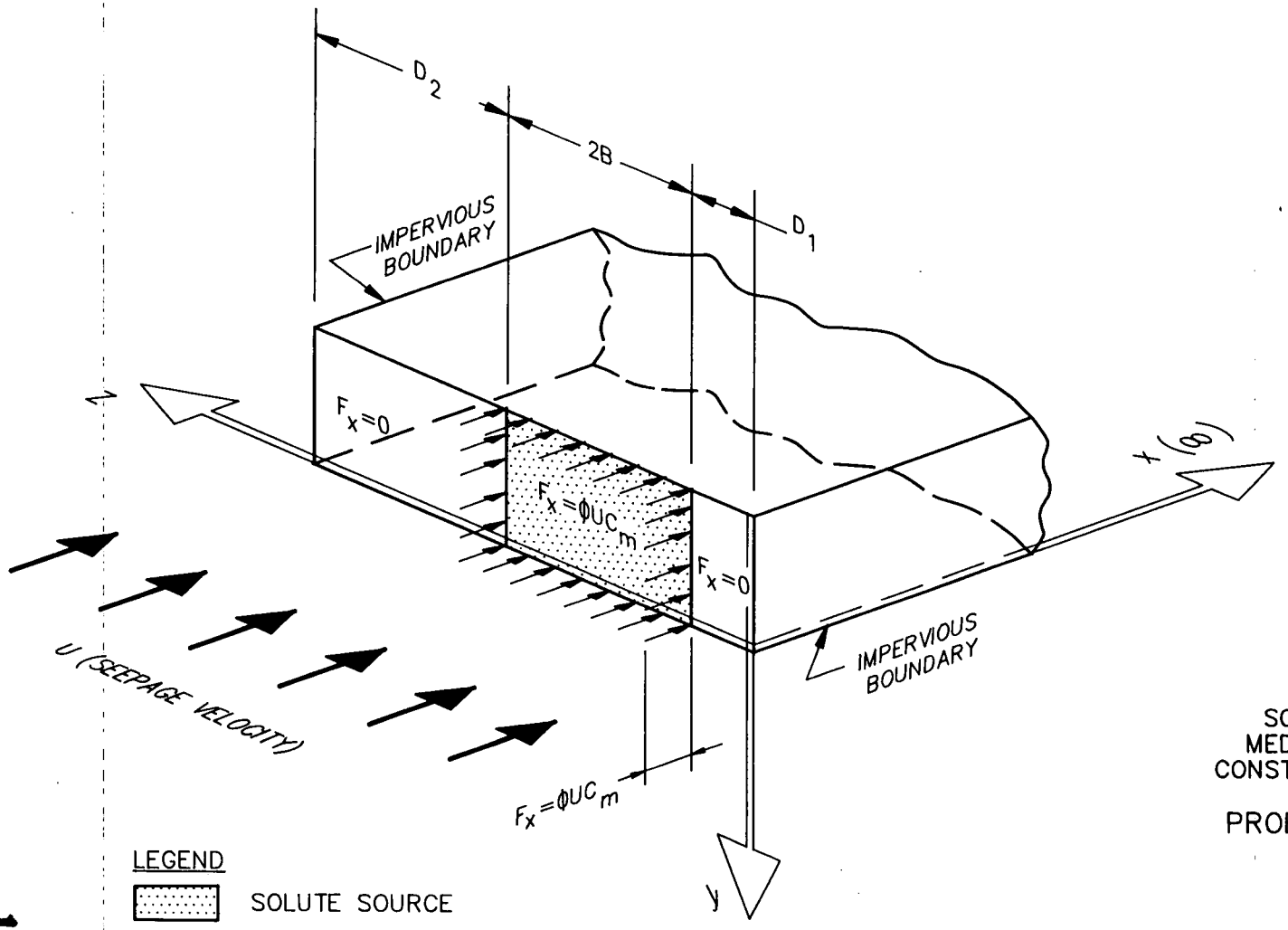

FIGURE 4-3

SCHEMATIC OF A POROUS MEDIUM WITH A FINITE STRIP CONSTANT CONTAMINANT SOURCE

PROBLEMS ST-2a AND 2b

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where

$$F_1(u) = \exp\left(\frac{Ux}{2D_x} - \nu u - \frac{U^2}{4D_xR_d}u\right) \tag{4.23}$$

$$F_2(u) = \left(\frac{D_x}{\pi R_d u}\right)^{1/2} \exp\left(-\frac{R_d x^2}{4D_x u}\right) \tag{4.24}$$

$$F_3(u) = \frac{U}{2R_d} \exp\left(\frac{Ux}{2D_x} + \frac{U^2 u}{4R_d D_x}\right) \tag{4.25}$$

$$F_4(u) = \mathrm{erfc}\left[\frac{R_d x}{2(D_x R_d u)^{1/2}} + \frac{U}{2}\left(\frac{u}{R_d D_x}\right)^{1/2}\right] \tag{4.26}$$

$$\lambda_n = \frac{n\pi}{H_m} \qquad n = 0,1,2,\ldots \tag{4.27}$$

The integrals in Equation 4.22 can only be evaluated numerically. For these integrals, the Gaussian integration procedure is appropriate and provides accurate results. The application of this methodology is included in Appendix C. A computer program called STRIPIB-FBC-G, was developed by IT to solve Equation 4.22 for the concentration distribution C(x,z,t).

4.1.2.5 Numerical Solutions

For the numerical solution, a finite modeling domain had to be chosen rather than the domain which extends to infinity in the x-direction for the analytical solution. The modeling area was chosen to be 75 x 50 m^2 (246.0 x 164.0 ft^2). The length of the modeling domain was selected such that the solute front with the minimum retardation factor and assigned hydrogeological parameters would not reach the boundary at x = 75 m (246 feet) at the end of 100 days.

The grid systems for GEOFLOW and SWIFT III are shown in Figure 4-4 and 4-5, respectively. Because GEOFLOW is node-centered and SWIFT III is block-centered, two different grids were created. The finite-element nodes of GEOFLOW coincide with the block centers of SWIFT III. Cartesian coordinates were used in both models (the z-coordinate in the analytical model is equivalent to the y-coordinate of the numerical models). For both models, the x-y plane was selected to be the datum plane. The boundaries at x = 0 and x = 75 m (246 feet) were simulated as constant-head and constant-pressure boundaries for GEOFLOW and SWIFT III, respectively. The other boundaries were simulated as no-flow boundaries for both models. These boundary conditions define a one-dimensional ground water flow field. Equal seepage velocities were used in all models. In the numerical models, the values of hydraulic heads, hydraulic conductivity, and porosity were selected such that the computed seepage velocity was equal to the seepage velocity specified in the analytical model. Spatial increments of the grids satisfied the appropriate criterion ($\Delta x \leq 2\alpha_L$) to reduce numerical oscillation (Huyakorn and Pinder, 1983, p. 206).

4.1.2.6 Input Specifications

The input data for these models are given in the following:

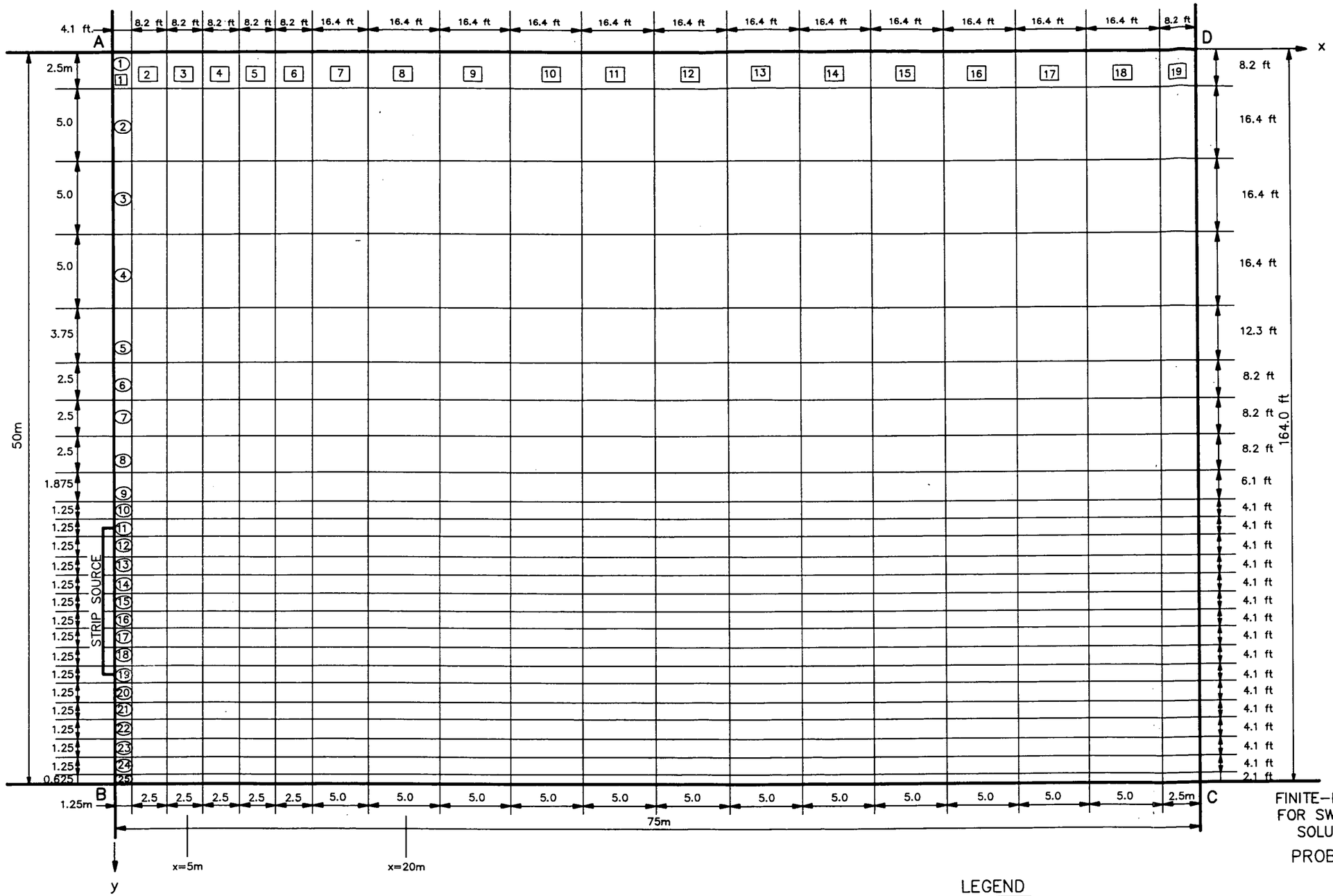
- Table 4.4 - STRIP1B-FBC-G model
- Table 4.5 - SWIFT III model
- Table 4.6 - GEOFLOW model

4.1.2.7 Output Specifications

The output consists of computed normalized concentrations as functions of distance and time for different retardation factors.

4.1.2.8 Results

The computed concentrations as functions of time and distance for Problems ST-2a and ST-2b are compared for STRIP1B-FBC-G, SWIFT III, and GEOFLOW. Normalized concentrations versus distance for Problem ST-2a are given in Figures 4-6 and 4-7. Figures 4-8 and 4-9 depict the



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6 i = CELL NUMBER

3 j = CELL NUMBER

FIGURE 4-4

FINITE-DIFFERENCE GRID SYSTEM FOR SWIFT III TWO-DIMENSIONAL SOLUTE TRANSPORT MODEL

PROBLEMS ST-2a AND 2b

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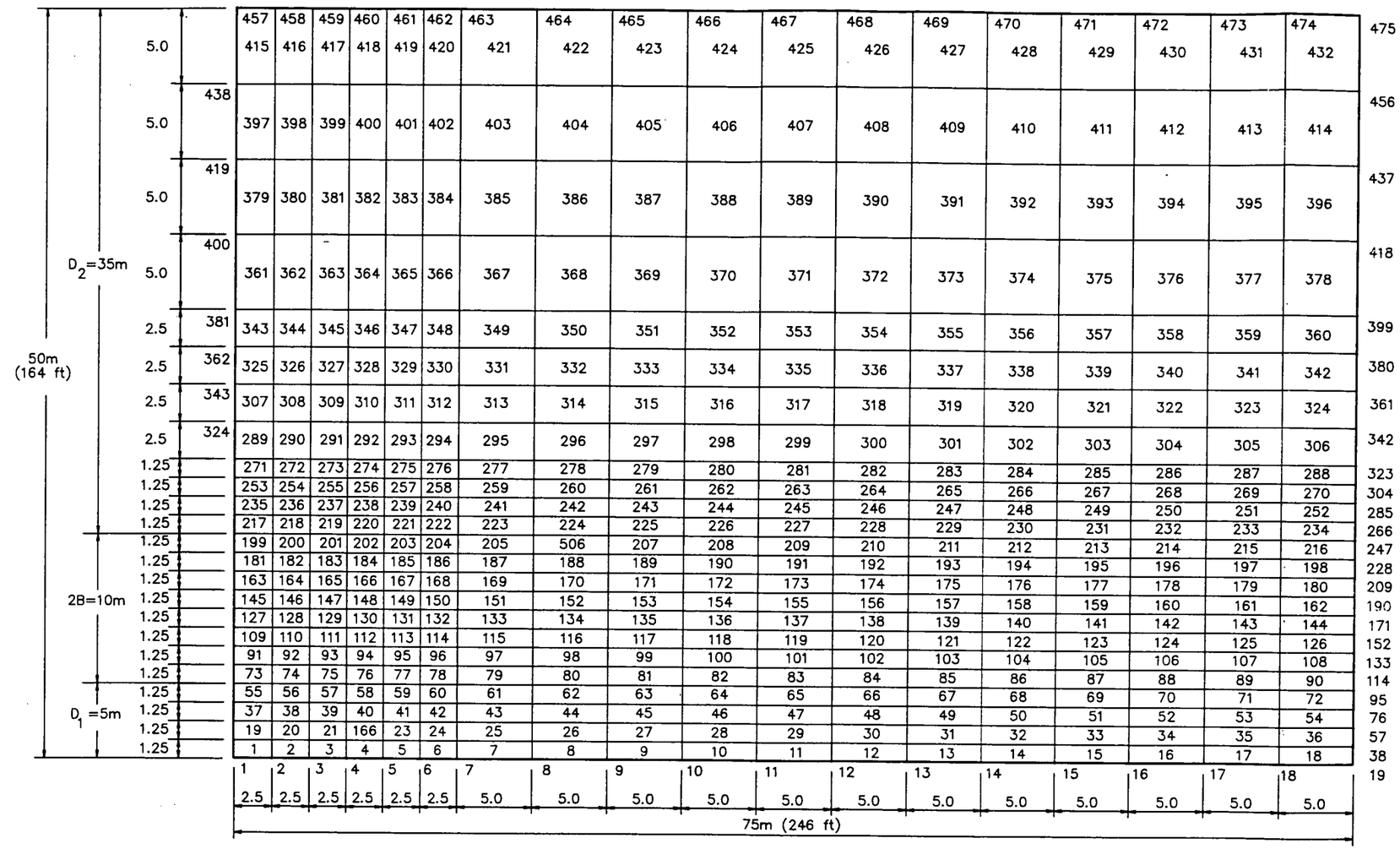

LEGEND

474 — NODE NUMBER

432 — ELEMENT NUMBER

FIGURE 4–5

FINITE ELEMENT GRID SYSTEM FOR GEOFLOW TWO–DIMENSIONAL SOLUTE TRANSPORT MODEL

PROBLEMS ST–2a AND 2b

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TABLE 4.4

INPUT PARAMETERS FOR TWO-DIMENSIONAL ANALYTICAL STRIP1B-FBC-G[a] MODEL PROBLEM ST-2a and 2b

PARAMETER	SYMBOL	VALUE SI	VALUE ENGLISH
Seepage velocity	U	0.1 m/day	0.328 ft/day
Longitudinal dispersion coefficient	D_x	1.0 m^2/day	10.76 ft^2/day
Transverse dispersion coefficient	D_z	0.1 m^2/day	1.08 ft^2/day
Retardation factor	R_d	1 and 2.5	1 and 2.5
The half width of the strip source	B	5 m	16.40 ft
Distance to the impervious boundary	D_1	5 m	16.40 ft
Distance to the impervious boundary	D_2	35 m	114.83 ft

[a]See Figure 4-3 for the schematic of the model. Refer to Figures 4-6 through 4-12 for plotted graphs from the model's results.

TABLE 4.5

INPUT PARAMETERS FOR TWO-DIMENSIONAL
NUMERICAL SOLUTE TRANSPORT SWIFT III MODEL
PROBLEM ST-2a and 2b

I. Finite-Difference Grid System[a]	
Length: (i-direction)	75 m (246.0 ft)
Width: (j-direction)	50 m (164.0 ft)
Number of cells:	475
Number of layers:	1
II. Water and Solute Transport Parameters	
Type of aquifer	Confined
Flow regime	Steady-state
Thickness of aquifer[b]	1 m (3.28 ft)
Hydraulic conductivity, in x- and y-directions (K_x and K_y)	1 m/day (3.28 ft/day)
Porosity (ϕ)	0.3
Longitudinal dispersivity (α_L)	10 m (32.8 ft)
Transverse dispersivity (α_T)	1 m (3.28 ft)
Retardation factor (R_d)	1 and 2.5
III. Boundary Conditions for Ground Water Flow (refer Figure 4-4)	
Grid AB boundary	Dirichlet condition 36,787.5 Pa (53342×10^{-4} psi)
Grid CD boundary	Dirichlet condition 14,715.0 Pa (21337×10^{-4} psi)
Grid AD boundary	No-flow condition
Grid BC boundary	No-flow condition
IV Initial and Boundary Conditions for Solute Transport (refer Figure 4-4)	
Initial Concentrations (all cells)	0
Grid AB (except the source), BC, CD, and AD boundaries	No-solute transport condition
Source concentration	1 unit

See footnotes at end of table.

TABLE 4.5
(Continued)

Solute flux of the source cells[b] (Cauchy boundary condition)	4.34×10^{-4} unit x kg/s (9.57×10^{-4} unit x lb/s)
Solute flux of the source edge cells[c] (Cauchy boundary condition)	2.17×10^{-4} kg/s (4.78×10^{-4} lb/s)

[a]Refer to Figure 4-4 for the finite difference grid.

[b]Solute flux at the source cells = $C_o \rho q A$

where

C_o = source concentration given in units,

ρ = density of water,

q = Darcy velocity, and

A = the area of cell at source in the y-z plane.

$$(\text{unit})\ (1{,}000\ \frac{\text{kg}}{\text{m}^3})\ (0.3 \times 0.1\ \frac{\text{m}}{\text{day}})\ (1.25\ \text{m})\ (1\ \text{m})$$

$$= 4.34 \times 10^{-4}\ \text{unit x kg/s}$$

[c]Solute flux at the source edge cells = $(1/2)\ (4.34 \times 10^{-4})$ unit x kg/s.

TABLE 4.6

INPUT PARAMETERS FOR TWO-DIMENSIONAL NUMERICAL SOLUTE TRANSPORT GEOFLOW MODEL PROBLEMS ST-2a and 2b

I. Finite Element Grid System[a]	
Length: (x-direction)	75 m (246.0 ft)
Width: (y-direction)	50 m (164.0 ft)
Number of elements:	432
Number of nodes:	475
Type of elements:	Quadrilateral
II. Water and Solute Transport Parameters	
Type of aquifer	Confined
Flow regime	Steady-state
Thickness of aquifer	1 m (3.28 ft)
Hydraulic conductivity, in x- and y-directions (K_x, K_y)	1 m/day (3.28 ft/day)
Porosity (ϕ)	0.3
Longitudinal dispersivity (α_L)	10 m (32.8 ft)
Transverse dispersivity (α_T)	1 m (3.28 ft)
Retardation factor (R_d)	1 and 2.5
III. Boundary Conditions for Ground Water Flow (refer Figure 4-5)	
Grid AB boundary (Dirichlet condition)	2.25 m (7.38 ft)
Grid CD boundary (Dirichlet condition)	0.0 m (0.0 ft)
Grid AD boundary (no-flow condition)	
Grid BC boundary (no-flow condition)	
IV Initial and Boundary Conditions for Solute Transport (refer Figure 4-5)	
Initial Concentrations (all elements)	0
Grid AB (except the source), BC, CD, and AD boundaries	No-solute transport condition
Source concentration	10 units
Solute flux at the source elements[b] (Cauchy boundary condition)	(0.375 unit x $\frac{m^3}{day}$) (13.24 unit x $\frac{ft^3}{day}$)
Solute flux of the source edge elements[c] (Cauchy boundary condition)	0.1875 unit x $\frac{m^3}{day}$ (6.22 unit x $\frac{ft^3}{day}$)

See footnotes at end of table.

TABLE 4.6
(Continued)

[a]Refer to Figure 4-5 for the finite element grid.

[b]Solute flux at the source cells = C_0qA = (10 units) $(0.3 \times 0.1 \frac{m}{day})$ (1.25 m)(1 m) =

$$= 0.375 \text{ unit } \frac{m^3}{day}$$

where

C_0 = source concentration given in units,

q = Darcy velocity, and

A = the area

[c]Solute flux at the source edge cells = $\frac{1}{2}$ (0.375) unit x $\frac{m^3}{day}$.

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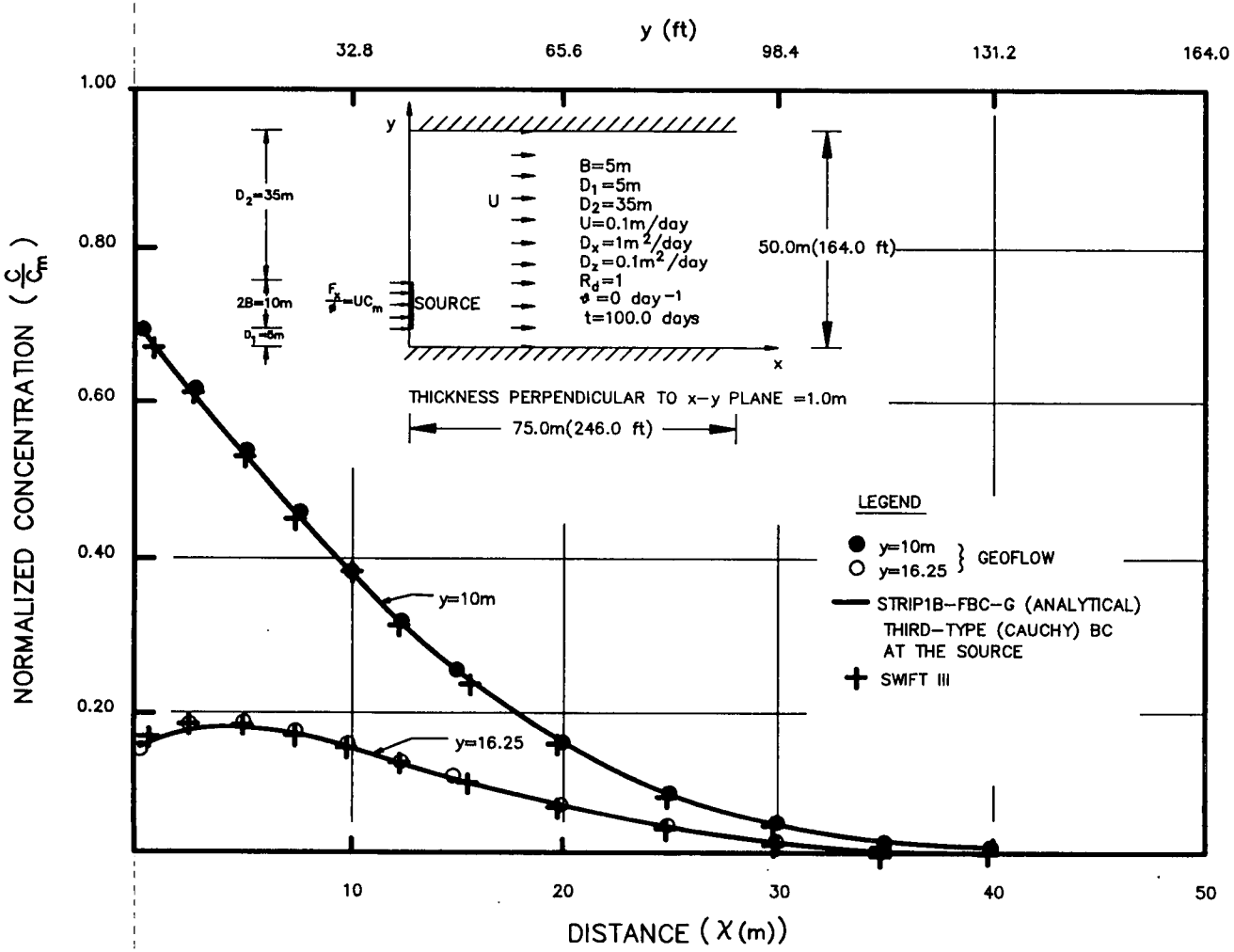

FIGURE 4-6

COMPARISON OF
NORMALIZED CONCENTRATION
VERSUS
DISTANCE ALONG x-AXIS

PROBLEM ST-2a

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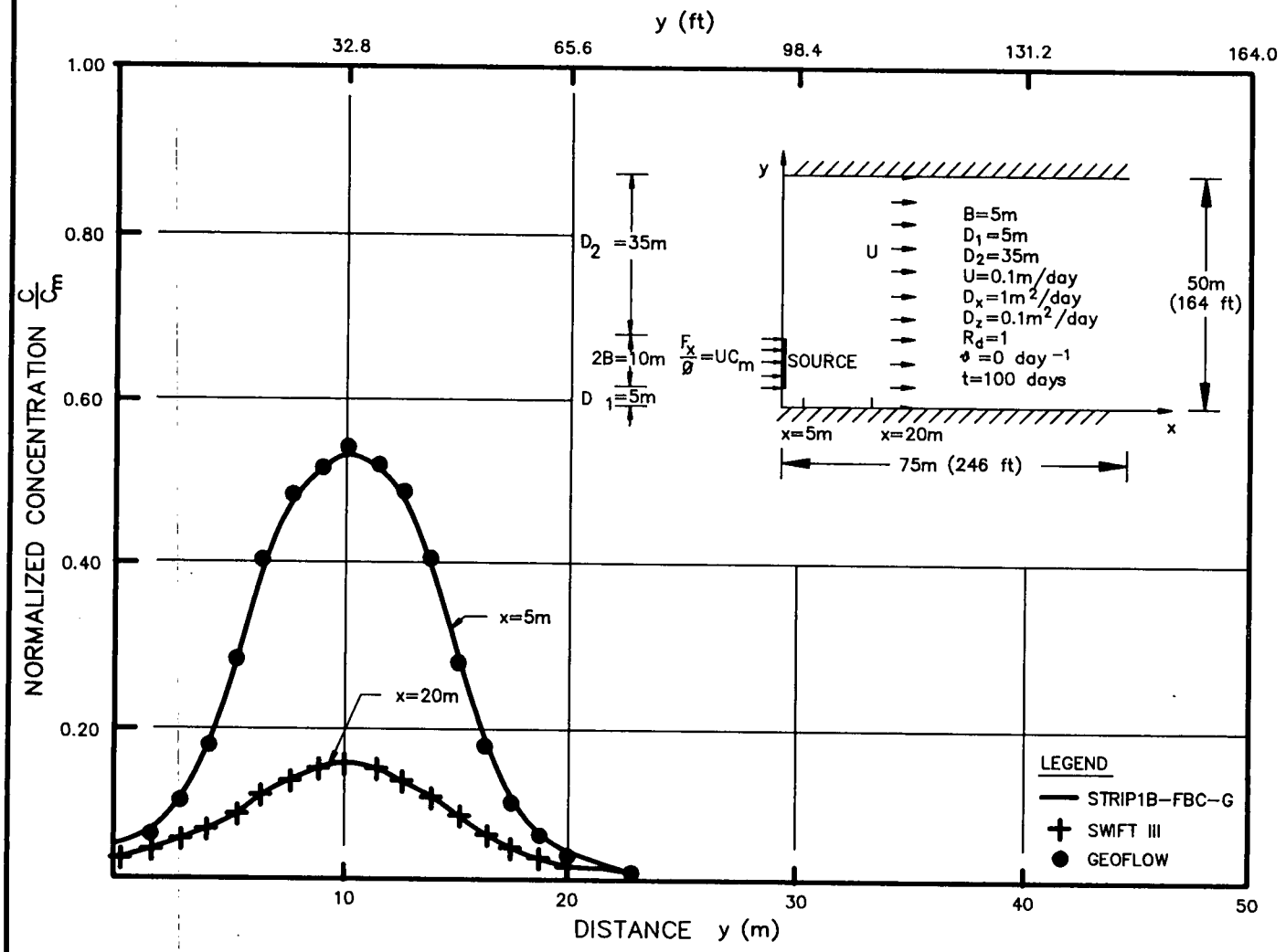

FIGURE 4-7

COMPARISON OF NORMALIZED CONCENTRATION VERSUS DISTANCE ALONG y-AXIS

PROBLEM ST-2a

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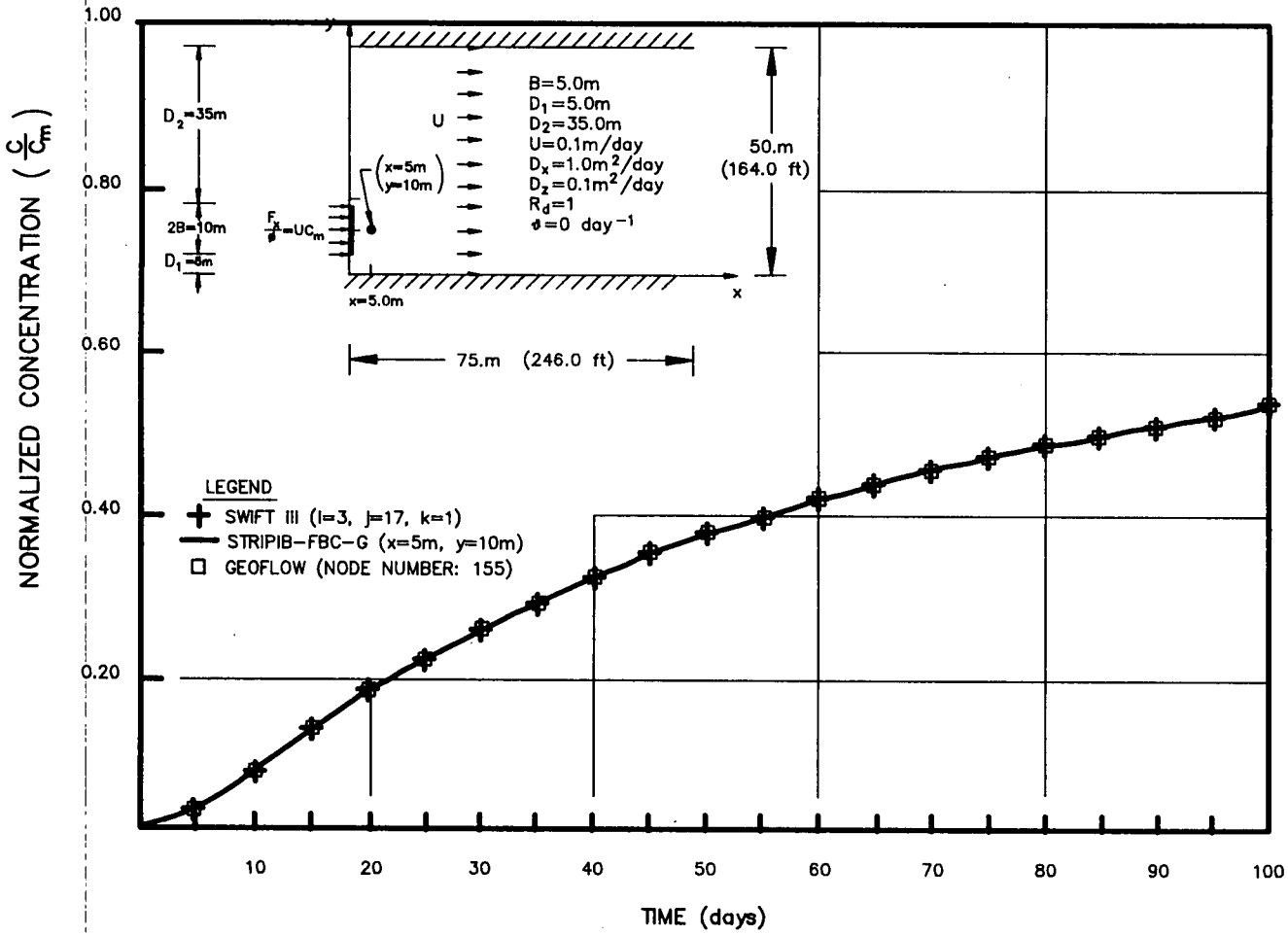

FIGURE 4-8

COMPARISON OF
NORMALIZED CONCENTRATION
VERSUS
TIME
AT LOCATION OF x=5m, y=10m

PROBLEM ST-2a

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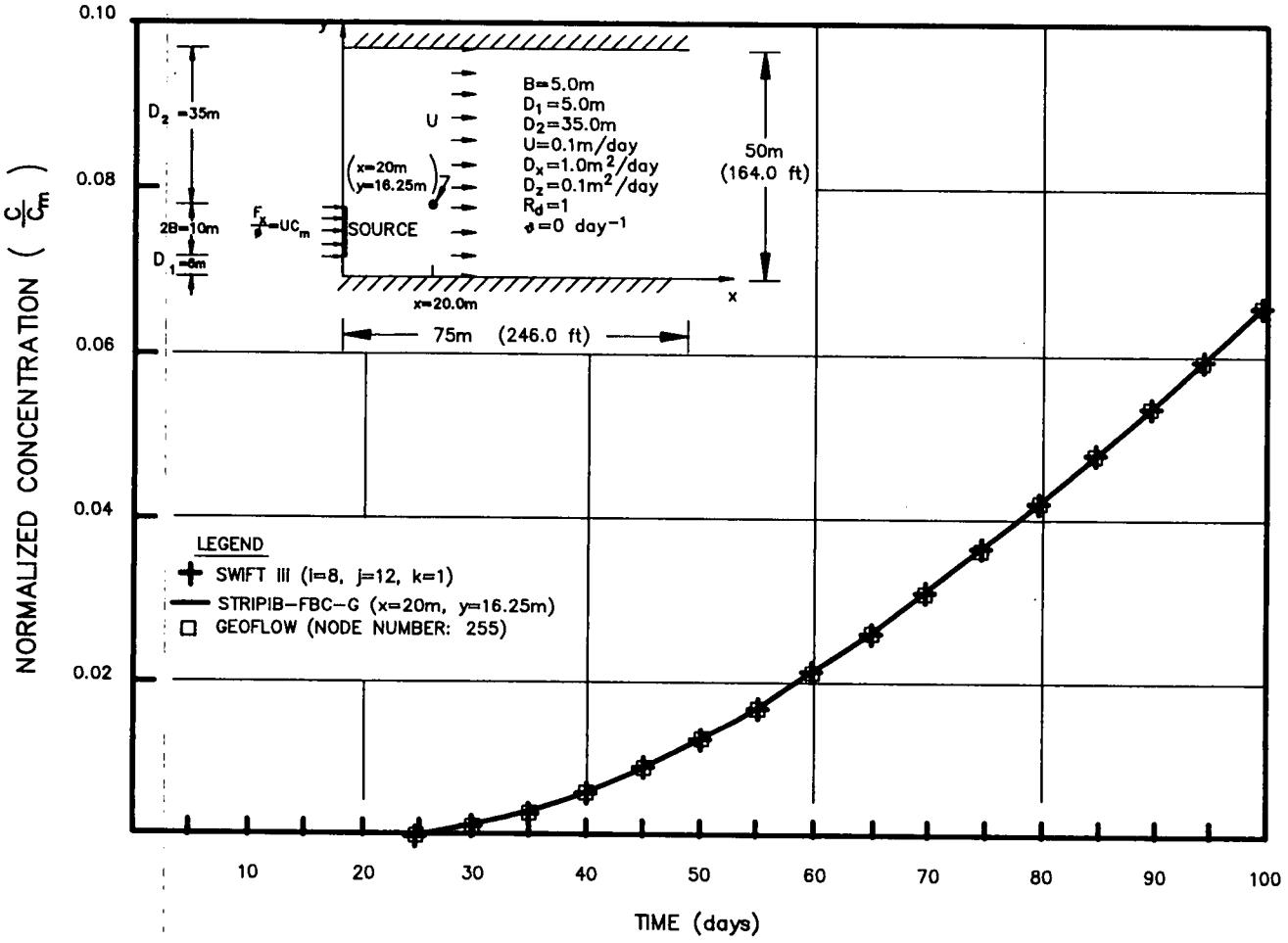

NOTE:

REFER TO FIGURES 4-4 AND 4-5 FOR LOCATION OF COMPARISON POINT IN NUMERICAL MODELS.

FIGURE 4-9

COMPARISON OF NORMALIZED CONCENTRATION VERSUS TIME AT LOCATION OF x=20m, y=16.15m

PROBLEM ST-2a

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normalized concentrations versus time for this problem. These two last curves correspond to the concentration at points x = 5 m (16.4 ft), y = 10 m (32.8 ft), and x = 20 m (65.65 ft), y = 16.25 m (53.31 ft). The corresponding curves for Problem ST-2b are given in Figures 4-10, 4-11, and 4-12, respectively. The normalized concentration at locations of x = 20 m are y = 16.25 are not plotted for Problem ST-2b because of their small values. Review of these figures indicates that excellent correlation exists among the three analytical and numerical models.

4.2 VERIFICATION PROBLEMS - NUMERICAL SOLUTIONS

The purpose of the three-dimensional solute transport verification was to test the SWIFT III code simulation capability in the vertical direction by comparison with other available codes. The Princeton Transport Code (PTC) was initially selected for this purpose. However, during the simulation, certain errors were encountered in the handling of vertical velocity components by the solute transport portion of the code. Therefore, it was decided to compare the SWIFT III three-dimensional solute transport results with a GEOFLOW vertical model.

Two different grid systems were used for these comparisons. The SWIFT III grid was three-dimensional, whereas the GEOFLOW grid was two-dimensional and corresponds to a vertical cross-section of the three-dimensional grid of SWIFT III. By assigning pertinent input data and boundary conditions to the three-dimensional SWIFT III model, it was possible to correlate the results of the models at any vertical slice.

Different grid sizes were used for Problems ST-3a and ST-3b. Initially, a grid with element lengths of 10 feet was used to maintain numerical stability. This verification problem is named ST-3a. In the second verification problem (ST-3b), the grid element length was increased by a factor of 10. The purpose of this increase was to test the SWIFT III numerical stability in field scale modeling.

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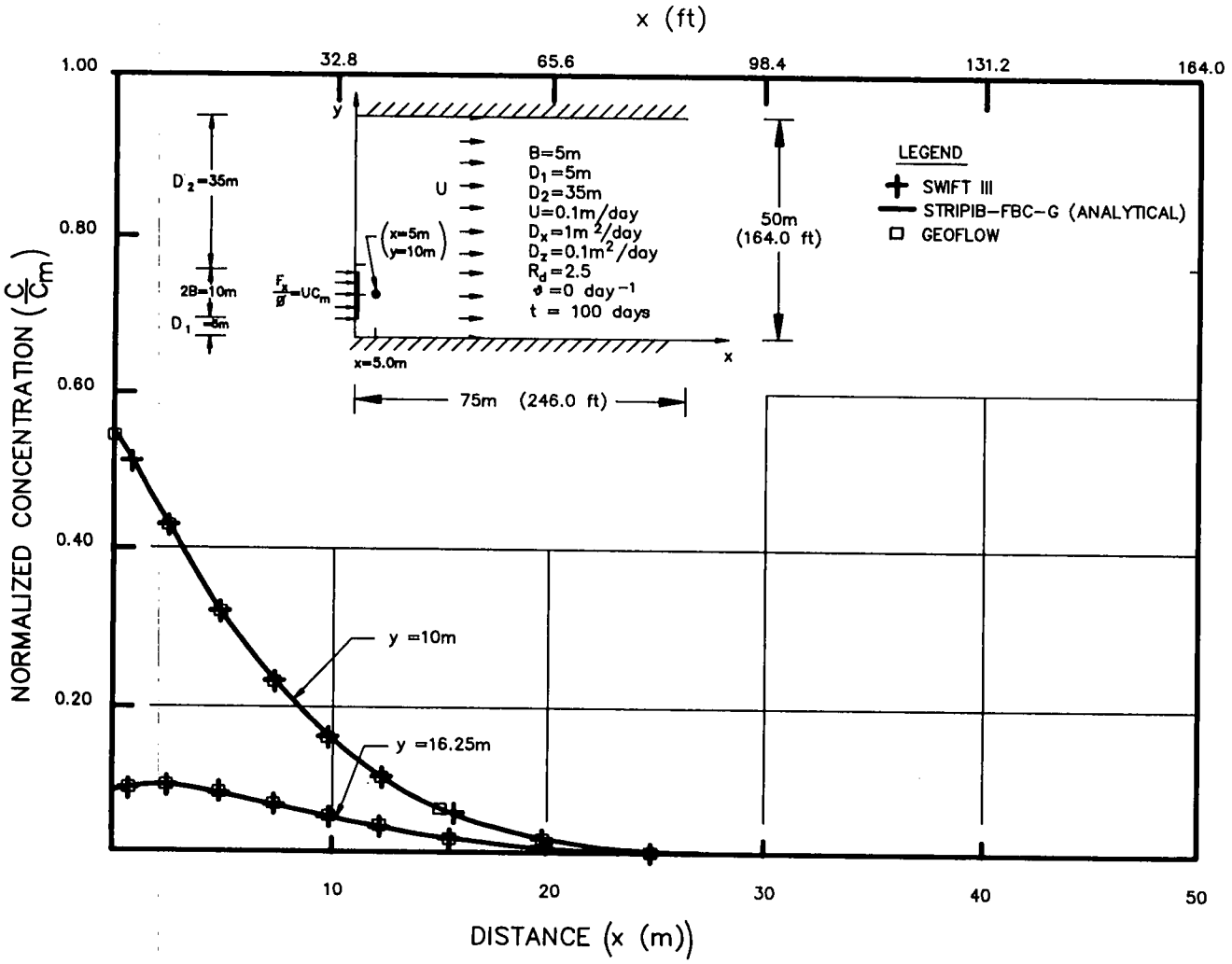

NOTE:

REFER TO FIGURES 4-4 AND 4-5 FOR LOCATION OF COMPARISON POINT IN NUMERICAL MODELS.

FIGURE 4-10

COMPARISON OF NORMALIZED CONCENTRATION VERSUS DISTANCE ALONG x-AXIS

PROBLEM ST-2b

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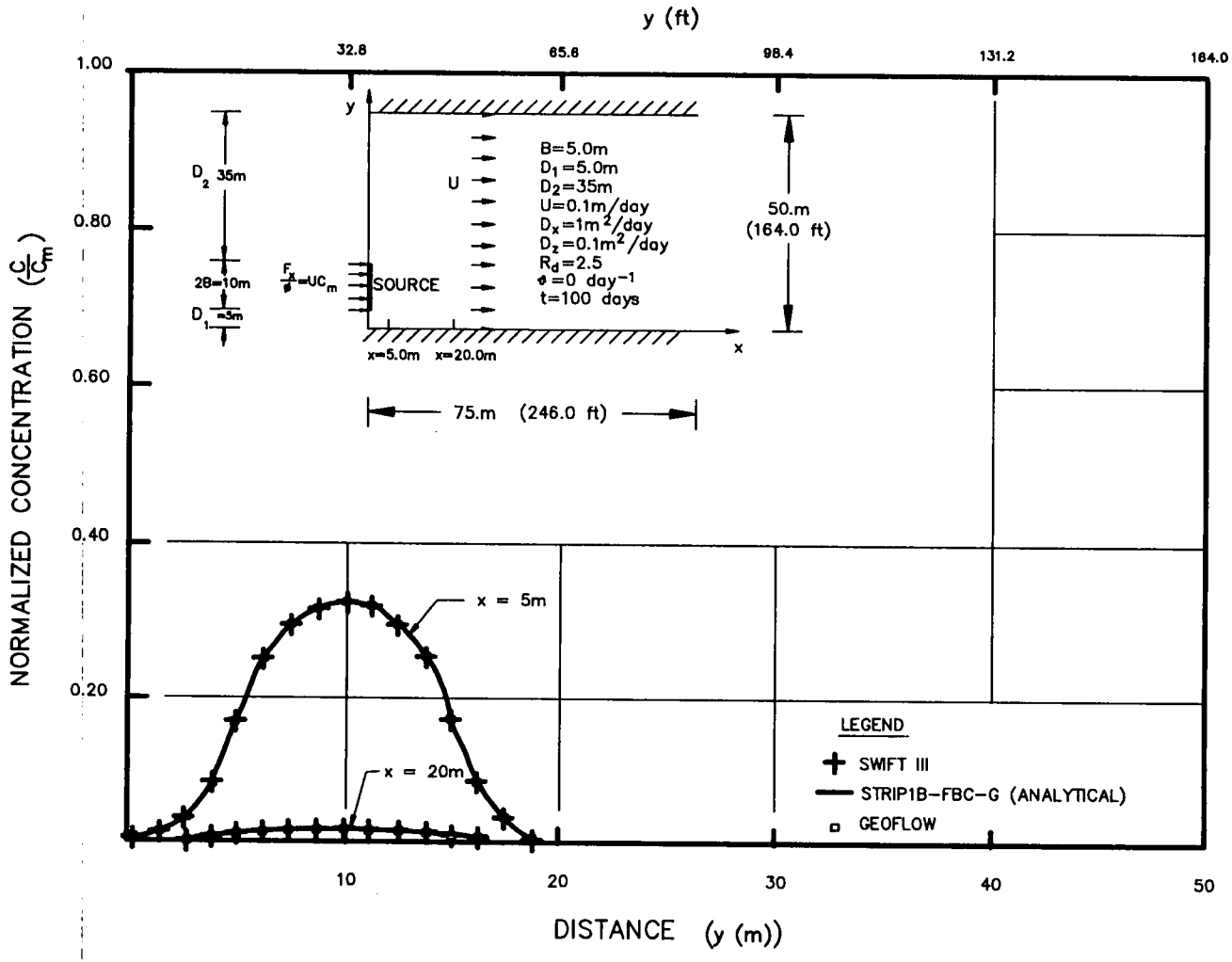

NOTE:

REFER TO FIGURES 4-4 AND 4-5 FOR LOCATION OF COMPARISON POINT IN NUMERICAL MODELS.

FIGURE 4-11

COMPARISON OF NORMALIZED CONCENTRATION VERSUS DISTANCE ALONG y-AXIS

PROBLEM ST-2b

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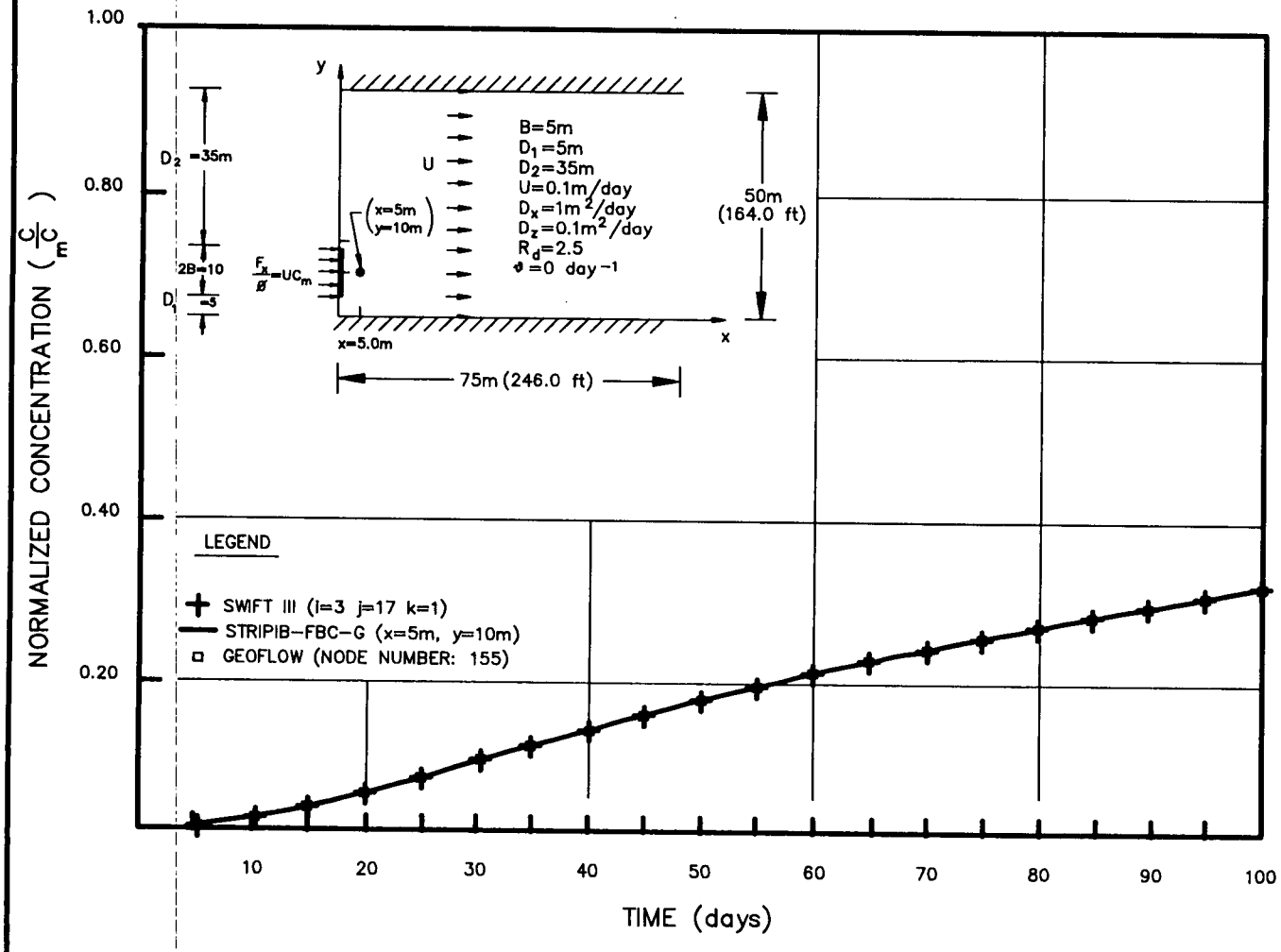

FIGURE 4-12

COMPARISON OF NORMALIZED CONCENTRATION VERSUS TIME AT LOCATION OF x=5m, y=10m

PROBLEM ST-2b

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NOTE:

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4.2.1 Problems ST-3a and 3B: Three-Dimensional Solute Transport

4.2.1.1 Purpose of Problem Selection

Problem ST-3a and ST-3b were selected to test the following capabilities of the SWIFT III code:

- Three-dimensional solute transport
- Anisotropic aquifer
- Three-dimensional Cartesian coordinates
- Variable hydraulic conductivity
- Grid dimensions appropriate to the FMPC site
- Flux source boundary condition
- Numerical stability criteria

4.2.1.2 Description of Problem

The selected problem set consists of constant head boundaries at both ends of the system. A constant line source is located at the upper left hand of the model. The objective is to simulate solute transport in the vertical plane under variable hydrogeologic properties.

4.2.1.3 Assumptions

The following assumptions are made:

- The aquifer is confined
- Darcy's law applies throughout the system
- Adsorption may be approximated by a linear equilibrium isotherm
- Longitudinal and transverse dispersivities and retardation factor are constant throughout the transport domain

4.2.1.4 Numerical Simulation

The grid system for the three-dimensional SWIFT III model for Problem ST-3a is shown in Figure 4-13A. The two-dimensional GEOFLOW grid system for this problem is depicted in Figure 4-13B. The GEOFLOW grid corresponds to vertical cross-sections of the SWIFT III grid, parallel to the x-axis. The internal nodes of the finite element (GEOFLOW)

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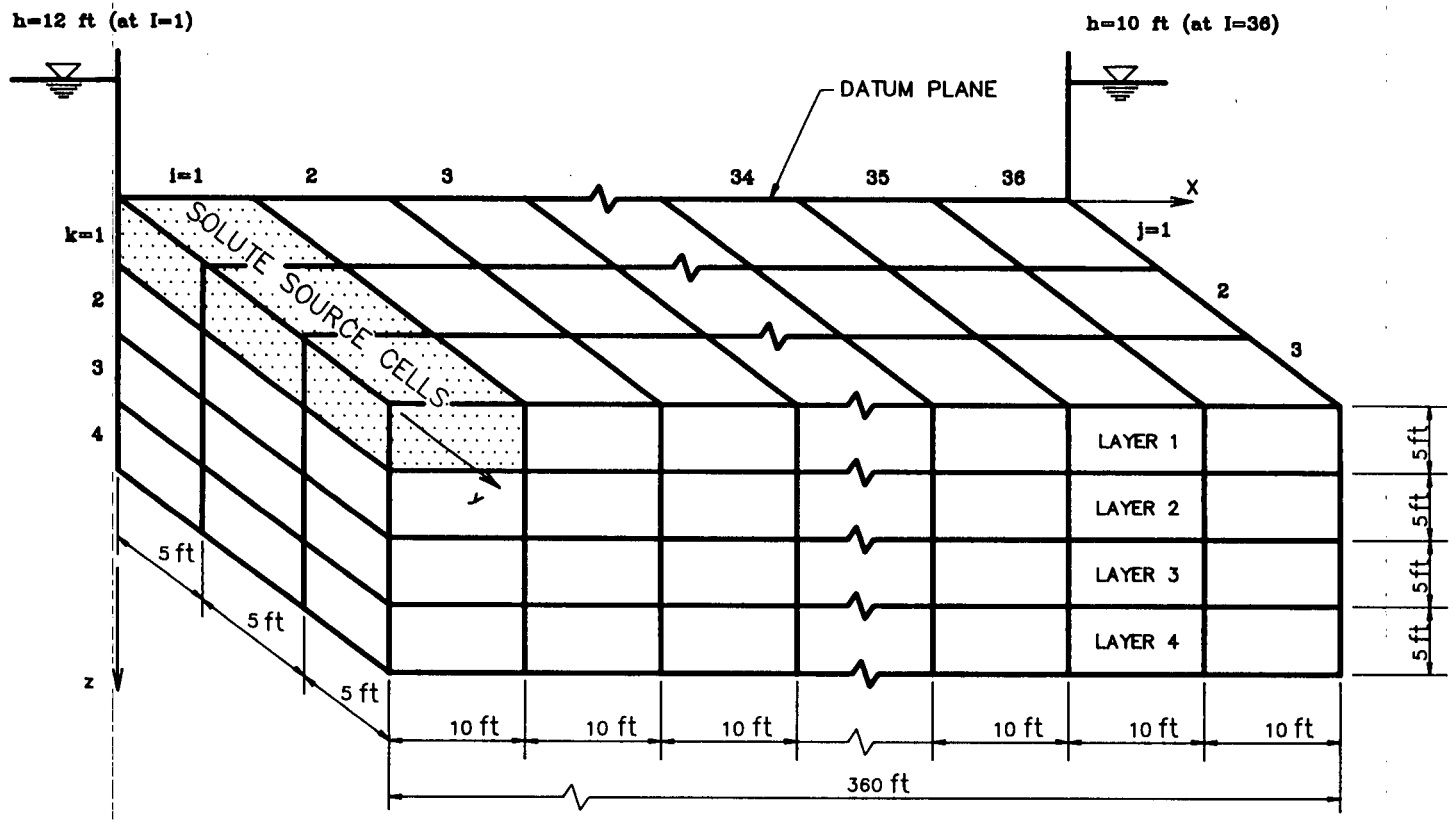

FIGURE 4-13A

ISOMETRIC GRID SYSTEM
FOR THREE-DIMENSIONAL SOLUTE
TRANSPORT VERIFICATION FOR SWIFT III

PROBLEM ST-3a

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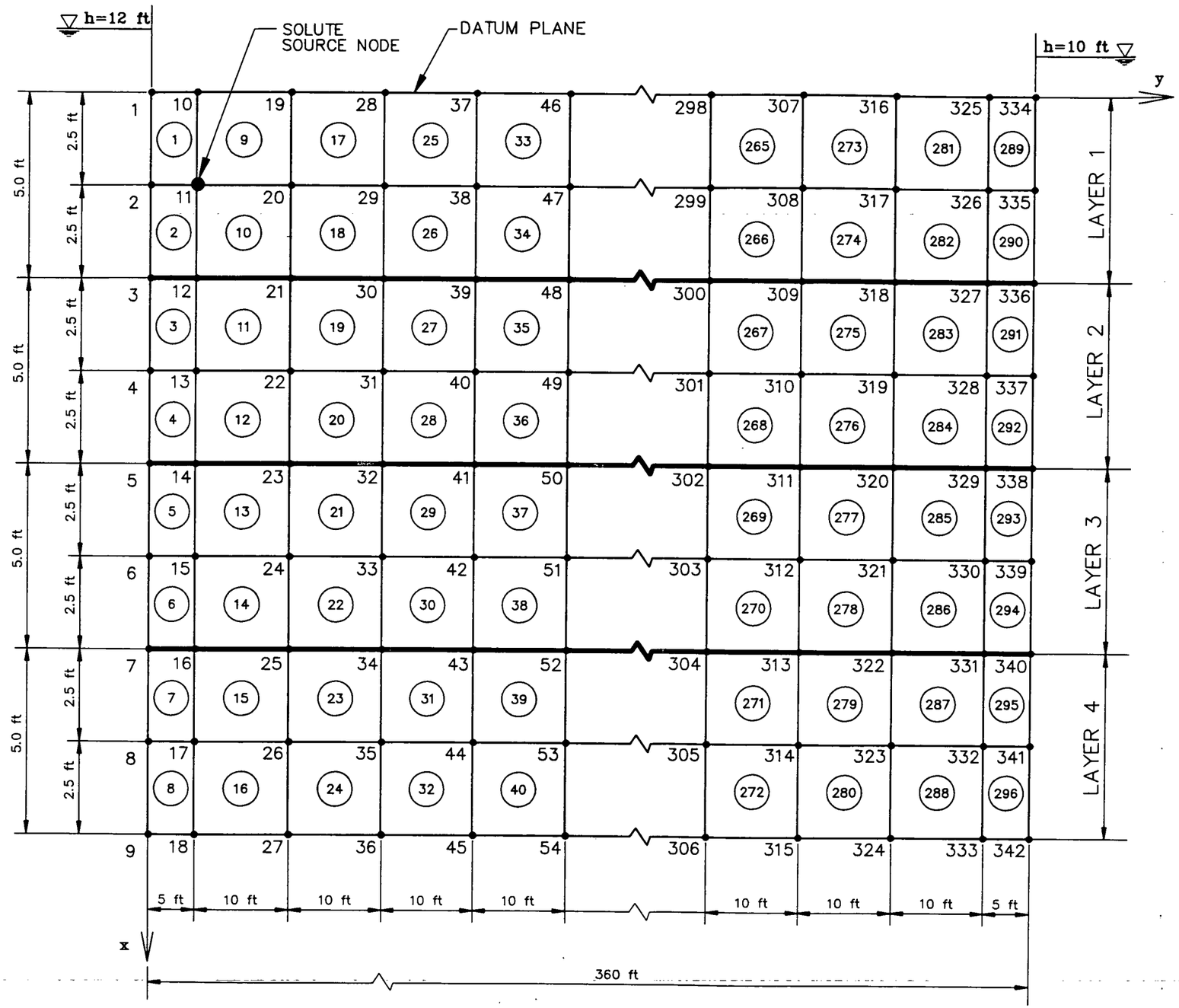

LEGEND

310 — NODE NUMBER

268 — ELEMENT NUMBER

FIGURE 4–13B

FINITE ELEMENT GRID SYSTEM FOR GEOFLOW

PROBLEM ST–3a

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grid correspond to the centers of the finite-difference (SWIFT III) blocks. This permits a one-to-one correlation between cells and nodes, and facilitates transfer of information between finite-difference and finite element models. The SWIFT III grid system has four layers and each layer has 108 blocks (Figure 4-13A). The GEOFLOW finite element grid system consists of 296 finite elements and 342 nodes (Figure 4-13B). Constant-head boundaries were maintained at the blocks with i=1 and i=36. All other faces of the grid system were simulated as no-flow boundaries. For GEOFLOW, the top and bottom boundaries were simulated as no-flow boundaries; the rest were simulated as constant-head boundaries. The solute sources for SWIFT III were assumed to be located at one of the edge blocks (i=1) of the uppermost layer. The solute source for GEOFLOW is located at Node 11 in Figure 4-13B.

The large size grid system was simulated by Problem ST-3b. The SWIFT III three-dimensional grid system for this problem is presented in Figure 4-14A. The corresponding two-dimensional GEOFLOW grid system is depicted in Figure 4-14B. As stated earlier, the grid length for Problem ST-3b is 10 times larger than for Problem ST-3a. Similar boundary conditions were used in Problem ST-3b.

4.2.1.5 Input Specifications

The input parameters for SWIFT III and GEOFLOW are given in Tables 4.7 and 4.8, respectively. Theoretical investigation and experience indicate that in a case where the dispersion coefficient is greater than zero, numerical oscillations can be virtually eliminated if the cell or element size is selected so that its local Peclet number does not exceed a value of 2 (Huyakorn and Pinder, 1983, p. 206). This means that $\Delta x \leq 2\alpha_L$ where Δx is the length of the cell or element and α_L is the longitudinal dispersivity. The value of α_L is 100 feet (Tables 4.7 and 4.8) and the longitudinal dimensions of the grids are 10 feet and 100 feet in Problem ST-3a and ST-3b, respectively. These values easily satisfy the condition given above.

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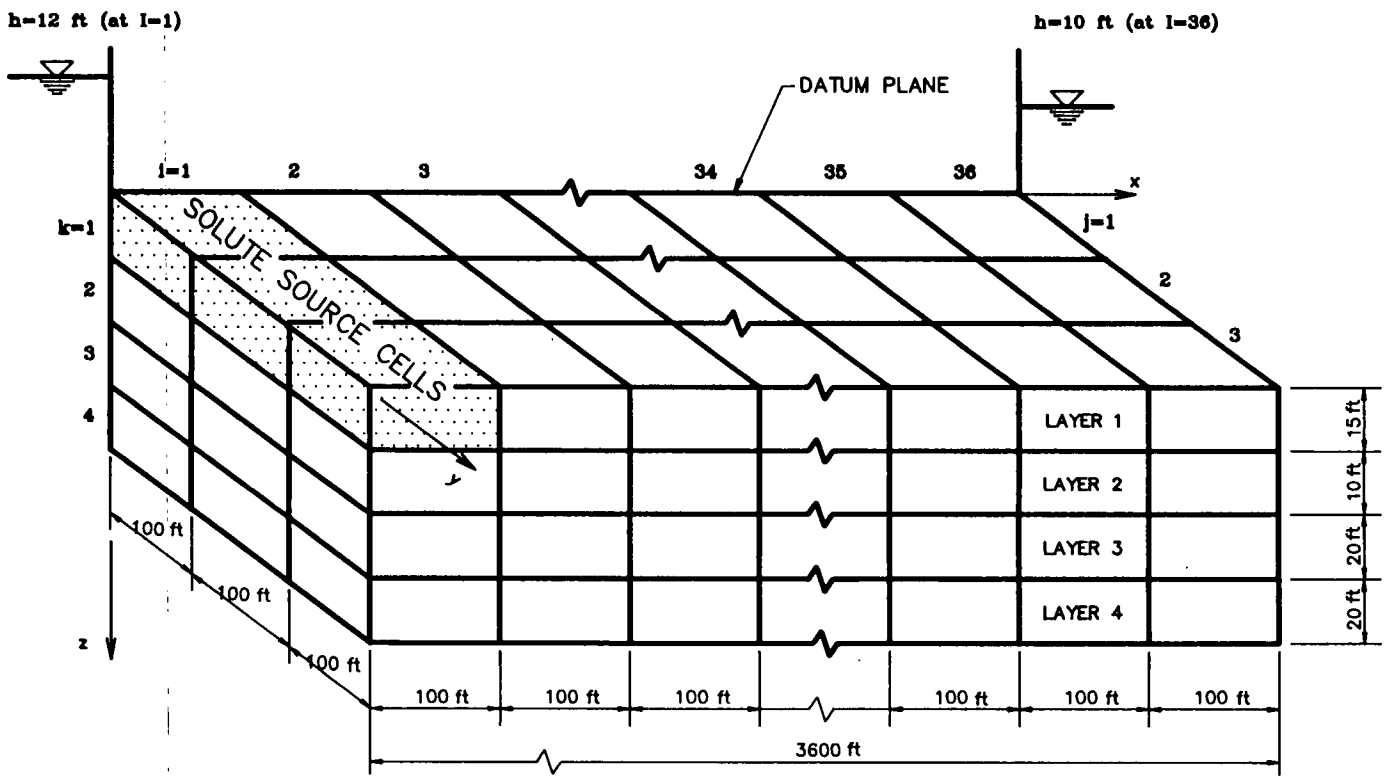

FIGURE 4-14A

ISOMETRIC GRID SYSTEM FOR
THREE-DIMENSIONAL SOLUTE TRANSPORT
VERIFICATION FOR SWIFT III

PROBLEM ST-3b

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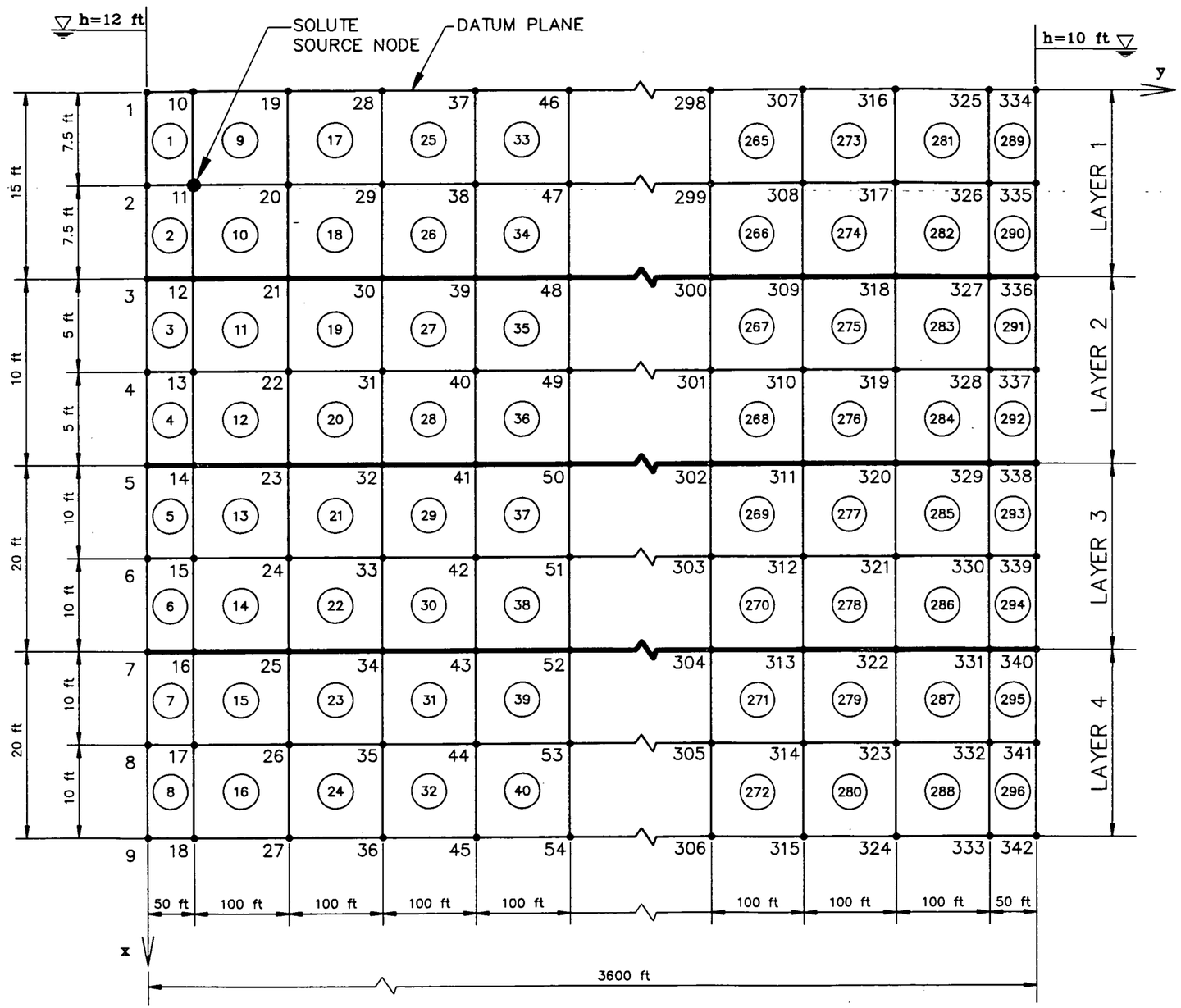

LEGEND

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(268) — ELEMENT NUMBER

FIGURE 4–14B

FINITE ELEMENT GRID SYSTEM FOR GEOFLOW

PROBLEM ST–3b

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TABLE 4.7

INPUT PARAMETERS FOR THE THREE-DIMENSIONAL
SOLUTE TRANSPORT SWIFT III MODEL
PROBLEM ST-3a and 3b

	PROBLEM ST-3a	PROBLEM ST-3b
I. FINITE-DIFFERENCE GRID SYSTEM		
Length: (i-direction)	360 feet	3,600 feet
Width: (j-direction)	15 feet	300 feet
Height: (k-direction)	20 feet	65 feet
Number of cells:	432	432
Elevation of datum plane:	0.0 feet	0.0 feet
II. HYDROGEOLOGIC PARAMETERS		
Thickness of each layer:	5 feet	15,10,20,20 feet
Hydraulic conductivities (Layers 1 and 4):		
Horizontal	400 ft/day	400 ft/day
Vertical	133.3 ft/day	133.3 ft/day
Hydraulic conductivities (Layer 2):		
Horizontal	200 ft/day	200 ft/day
Vertical	66.7 ft/day	66.7 ft/day
Hydraulic conductivities (Layer 3):		
Horizontal	100 ft/day	100 ft/day
Vertical	50 ft/day	50 ft/day
Type of aquifer simulated:	Confined	Confined
Flow regime:	Steady state	Steady state
Boundary conditions (Constant-head)		
Cells i=1, and j=1,2,3 and k=1,2,3	12 feet	12 feet
Cells i=36, and j=1,2,3 and k=1,2,3	10 feet	10 feet

TABLE 4.7
(Continued)

III. SOLUTE TRANSPORT PARAMETERS

Porosity:	0.25
Half-life of radioactive component:	0 years
Longitudinal dispersivity:	100 feet
Transverse dispersivity:	10 feet
Retardation factor:	1
Solute source cells[a]:	i=1, j=1,2,3, and k=1
Initial condition:	Zero concentrations
Boundary condition:	No-solute transport
Solute source boundary condition:	Third-type (Cauchy)
Total simulation times:	40 days (ST-3a) and 300 days (ST-3b)
Spatial differencing:	CIS[b]
Time differencing:	CIT[c]
Method of solution:	Two-line successive overrelaxation

[a]Solute flux at the source cells = $C_o \rho q A$ where

C_o = Source concentration given in units
ρ = Density of water
q = Darcy velocity (taken from the ground water flow model output), and
A = The area of cell at source in the y-z plane

$$(1 \text{ unit})(62.37 \frac{\text{lb}}{\text{ft}^3})(2.222 \frac{\text{ft}}{\text{day}})(5 \text{ ft} \times 5 \text{ ft}) = 3464.6535 \text{ (unit} \times \frac{\text{lb}}{\text{day}})$$

[b]CIS = Centered in space
[c]CIT = Centered in time

TABLE 4.8

INPUT PARAMETERS FOR THE TWO-DIMENSIONAL SOLUTE TRANSPORT GEOFLOW MODEL PROBLEMS ST-3a and ST-3b

	PROBLEM ST-3a	PROBLEM ST-3b
I. FINITE ELEMENT GRID SYSTEM		
Length: (y-direction)	360 feet	3,600
Width: (x-direction)	20 feet	65 feet
Number of elements:	296	296
Number of nodes:	342	342
Elevation of datum plane:	0.0 feet	0.0 feet
II. HYDROGEOLOGIC PARAMETERS		
Thickness of each layer:	5 feet	15,10,20,20 feet
Hydraulic conductivities (Layers 1 and 4):		
Horizontal	400 ft/day	400 ft/day
Vertical	133.3 ft/day	133.3 ft/day
Hydraulic conductivities (Layer 2):		
Horizontal	200 ft/day	200 ft/day
Vertical	66.7 ft/day	66.7 ft/day
Hydraulic conductivities (Layer 3):		
Horizontal	100 ft/day	100 ft/day
Vertical	50 ft/day	50 ft/day
Type of aquifers simulated:	Confined	Confined
Flow regime:	Steady state	Steady state
Boundary conditions (Constant-head)		
Nodes 1 through 9	12 feet	12 feet
Nodes 334 through 342	10 feet	10 feet

TABLE 4.8
(Continued)

III. SOLUTE TRANSPORT PARAMETERS

Porosity:	0.25
Half-life of radioactive component:	0 years
Longitudinal dispersivity:	100 feet
Transverse dispersivity:	10 feet
Retardation factor:	1
Solute source node No.[a]:	11
Initial condition:	Zero concentrations
Boundary condition:	No-solute transport
Solute source boundary condition:	Third-type (Cauchy)
Total simulation times:	40 days (ST-3a) and 300 days (ST-3b)

[a]Solute flux at the source cells = $C_o qA$ where

C_o = Source concentration given in units
q = Darcy velocity (taken from the ground water flow model output), and
A = The area of the element per unit thickness perpendicular to the figure

$$(1 \text{ unit})(2.222 \frac{\text{ft}}{\text{day}})(5 \text{ ft} \times 1 \text{ ft}) = 11.11 \ (\text{unit} \times \frac{\text{ft}^3}{\text{day}})$$

The Courant number, C, controls oscillations of the numerical solution arising from the temporal discretization. The governing criterion for numerical stability is $C = U\Delta t/\Delta x < 1$ (Huyakorn and Pinder, 1983, p. 206), where U is the ground water velocity and Δt is the time step. The time steps were selected in accordance with this criterion.

The solute sources were simulated with the third-type (Cauchy) flux boundary condition. The solute source cells for SWIFT III are located at i=1, j=1,2,3, and k=1 (Figures 4-13A and 4-14A). The concentration of the source was taken to be unity and the calculated solute source for each cell is given at the end of Table 4.7. The Darcy velocity (2.22 ft/day) was taken from the corresponding flow model. The calculated solute source flux is 3464 lb/day for SWIFT III. For GEOFLOW, the corresponding solute source is located at the Node 11 (Figures 4-13B and 4-14B) and the calculated solute source flux is 11.1 ft^3/day. The nodal Darcy velocity given by the GEOFLOW output is the same as the value given above (Table 4.8).

4.2.1.6 Output Specifications

The output for this problem consists of normalized concentrations as functions of distance and time for the finite-difference cells and finite element nodes.

4.2.1.7 Results

The normalized concentrations versus time in Layer 3 at a distance of 13.5 feet from the source is given in Figure 4-15 for Problem ST-3a. This figure compares the concentrations computed by SWIFT III and GEOFLOW in a vertical plane. For SWIFT III, the coordinates of this cell are i=14, j=1, and k=3 and the corresponding node number for GEOFLOW is 132. Figures 4-16 and 4-17 present the normalized concentrations versus distance at 20 days for two different locations. These three figures indicate an excellent comparison between GEOFLOW and SWIFT III model results.

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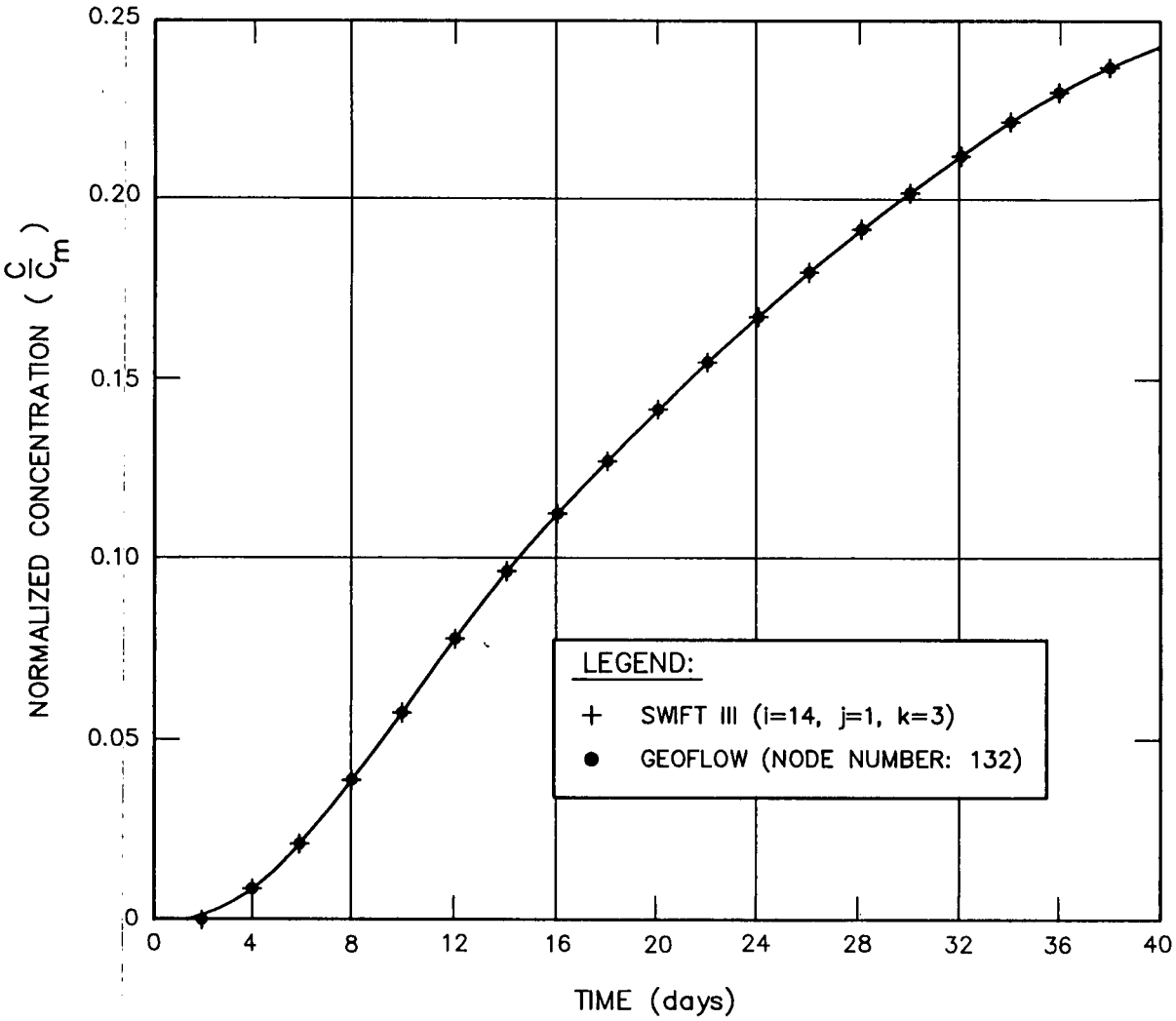

NOTE:

REFER TO FIGURES 4-13A AND 4-13B FOR LOCATIONS OF THE COMPARISON POINTS.

FIGURE 4-15

COMPARISON OF NORMALIZED CONCENTRATION VERSUS TIME AT 135 FT FROM THE SOURCE IN LAYER 3

PROBLEM ST-3a

PREPARED FOR

FERNALD RI/FS
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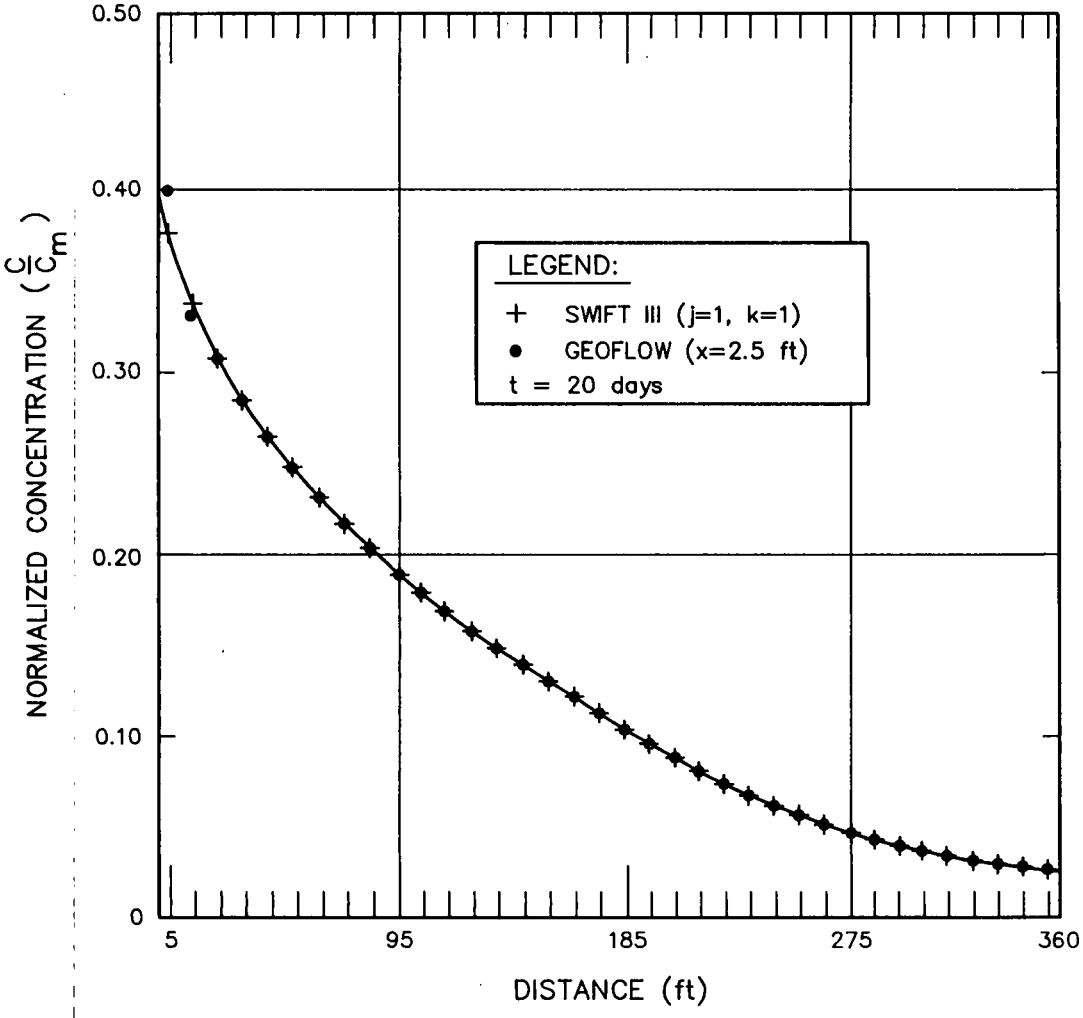

NOTES:

1. DISTANCE IS MEASURED FROM THE SOURCE IN THE FLOW DIRECTION.

2. REFER TO FIGURES 4-13A AND 4-13B FOR LOCATIONS OF COMPARISON POINTS.

FIGURE 4-16

COMPARISON OF
NORMALIZED CONCENTRATION
VERSUS
DISTANCE IN LAYER 1

PROBLEM ST-3a

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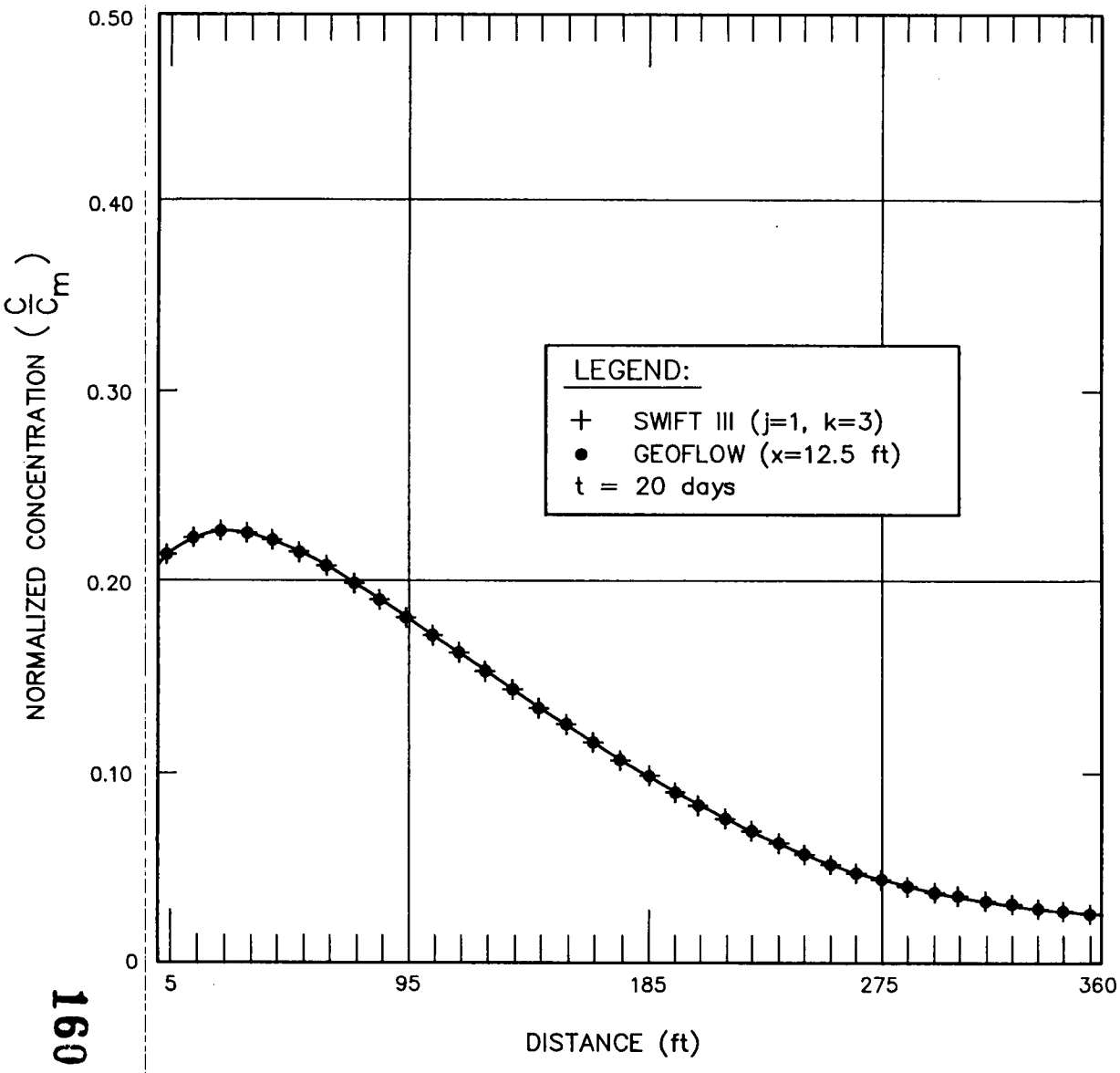

NOTES:

1. DISTANCE IS MEASURED FROM THE SOURCE IN THE FLOW DIRECTION.
2. REFER TO FIGURES 4-13A AND 4-13B FOR LOCATION OF COMPARISON POINTS.

FIGURE 4-17

COMPARISON OF NORMALIZED CONCENTRATION VERSUS DISTANCE IN LAYER 3

PROBLEM ST-3a

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Similar figures have been prepared for Problem ST-3b. Figure 4-18 shows the normalized concentrations versus time in Layer 3 at a distance of 135 feet from the source. The normalized concentrations versus distance at 250 days for different locations are depicted in Figures 4-19 and 4-20. Similar conclusions can be made with respect to the larger grid system used in Problem ST-3b. Excellent agreement is seen between the results of the two numerical models.

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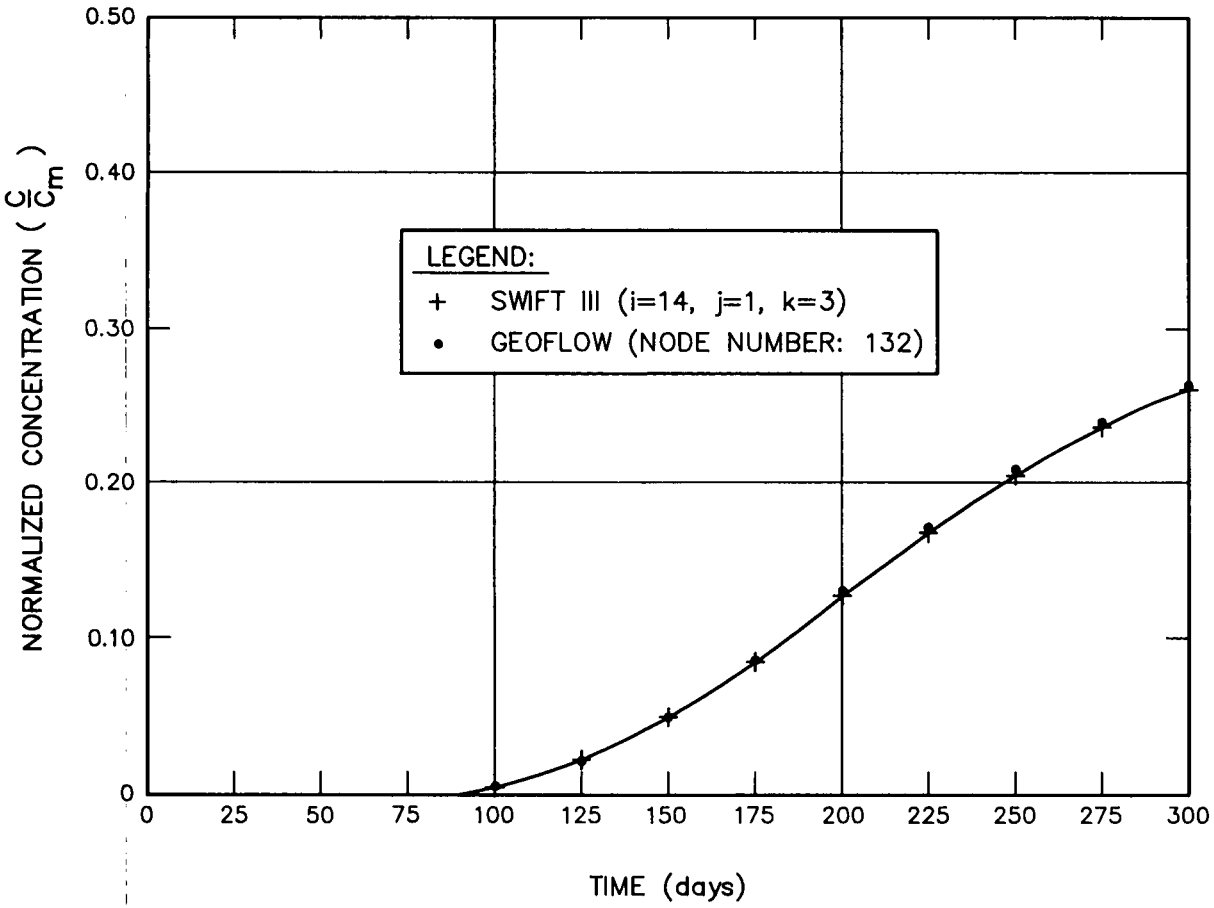
	27JULY89	APPROVED BY	SHD	2/21/90		



NOTE:

REFER TO FIGURE 4-14A AND 4-14B FOR LOCATION OF THE COMPARISON POINTS.

FIGURE 4-18

COMPARISON OF NORMALIZED CONCENTRATION VERSUS TIME AT 1350 FT FROM THE SOURCE IN LAYER 3

PROBLEM ST-3b

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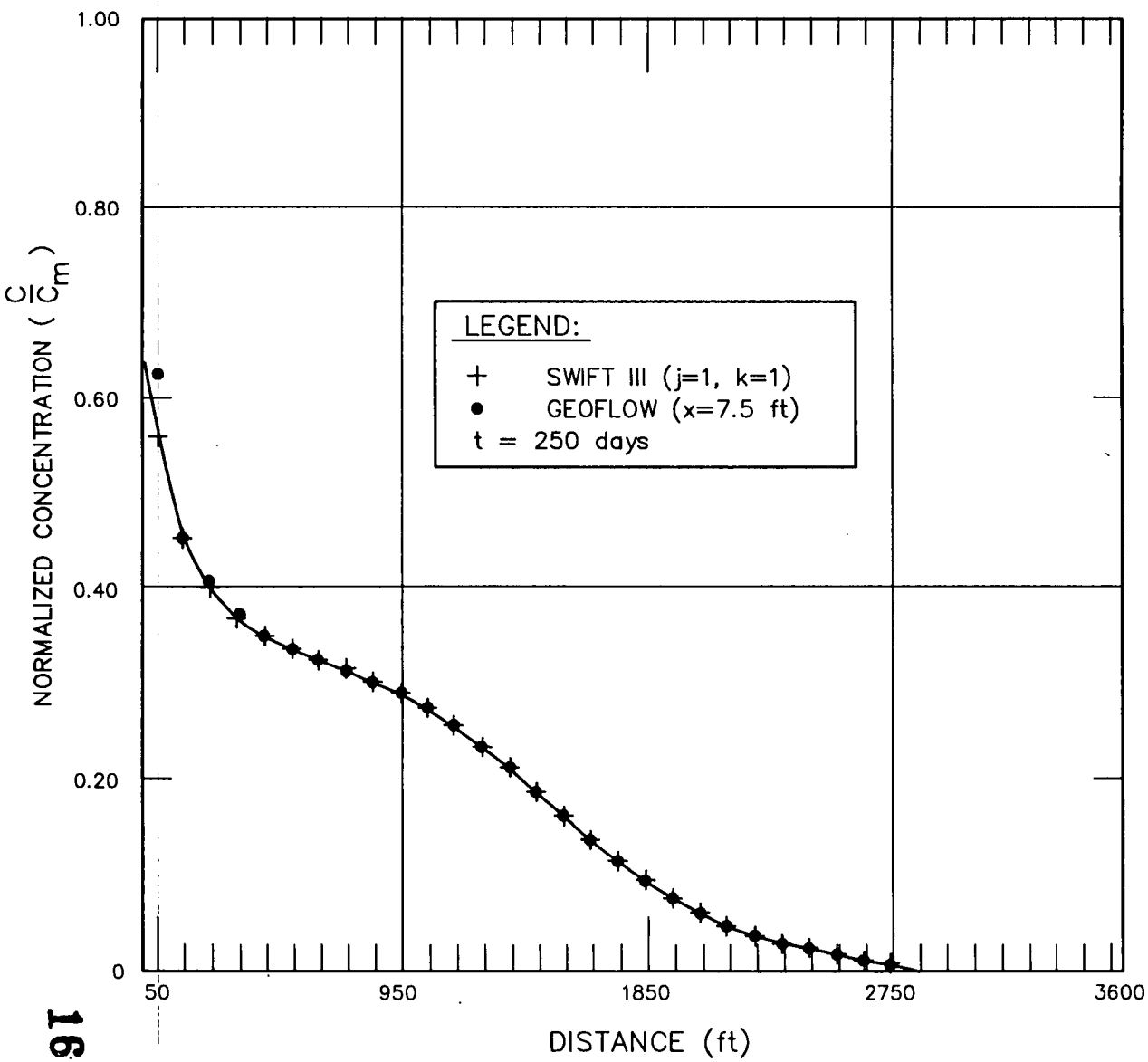

NOTES:

1. DISTANCE IS MEASURED FROM THE SOURCE IN THE FLOW DIRECTION.
2. REFER TO FIGURES 4-14A AND 4-14B FOR LOCATION OF COMPARISON POINTS.

FIGURE 4-19

COMPARISON OF NORMALIZED CONCENTRATION VERSUS DISTANCE IN LAYER 1

PROBLEM ST-3b

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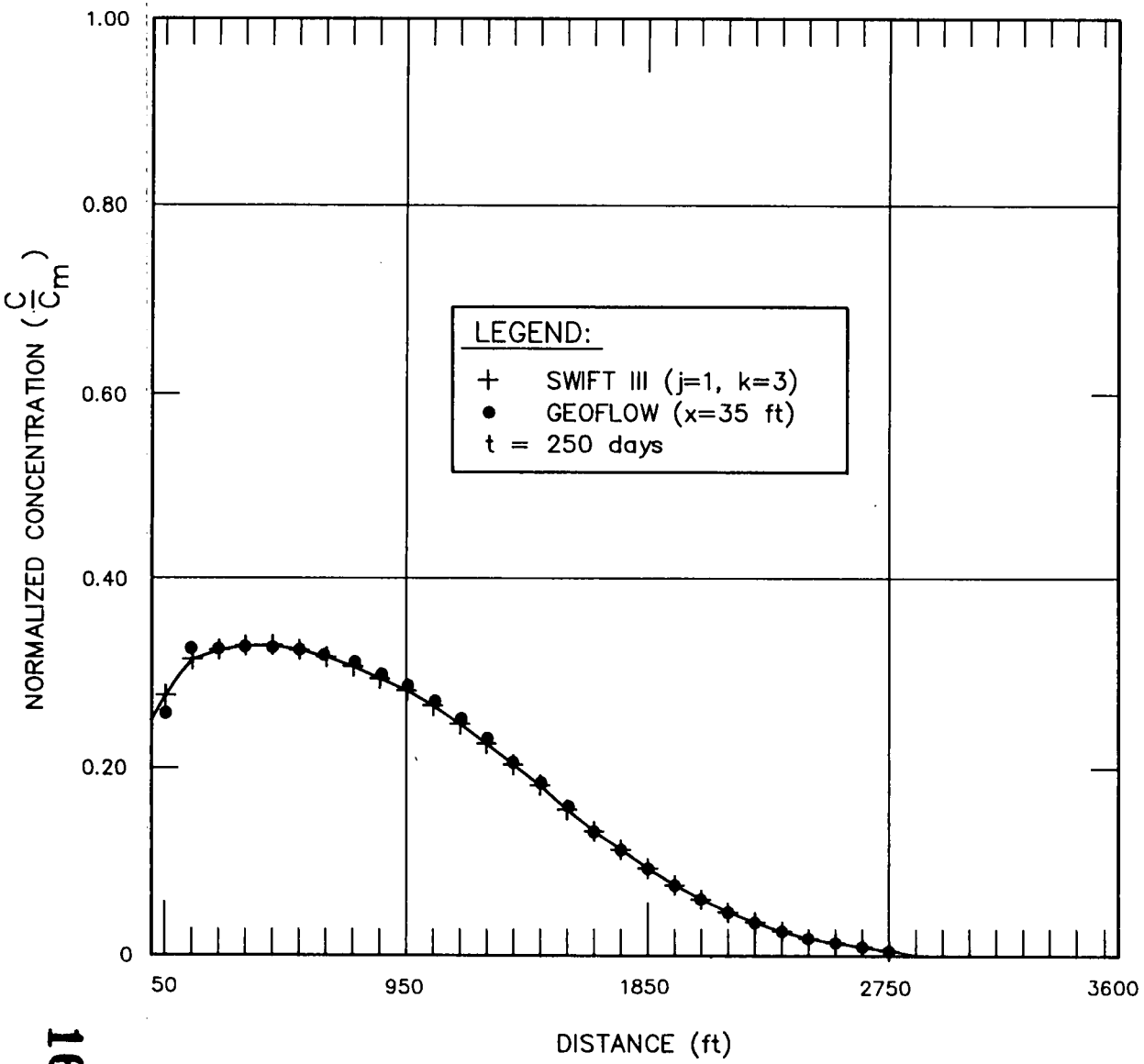

NOTES:

1. DISTANCE IS MEASURED FROM THE SOURCE IN THE FLOW DIRECTION.
2. REFER TO FIRURES 4-14A AND AND 4-14B FOR LOCATION OF COMPARISON POINTS.

FIGURE 4-20

COMPARISON OF NORMALIZED CONCENTRATION VERSUS DISTANCE IN LAYER 3

PROBLEM ST-3b

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5.0

5.0 SUMMARY AND CONCLUSIONS

The SWIFT III computer code was selected to evaluate ground water flow and solute transport for the sitewide RI/FS at the FMPC. An extensive and independent verification study was performed by IT for Version 2.25 of the computer code. The objectives of the computer code verification study were to:

- Determine if SWIFT III functions satisfactorily with respect to well-established ground water flow/solute transport codes and with respect to analytical solutions
- Verify the code's capability to model the complex, sitewide conditions at the FMPC
- Establish a high level of confidence in the code capabilities
- Correlate with the verification process performed by GeoTrans to show that the computer code was fully operational on IT's computer system
- Document the procedures and findings of the verification process

To verify the SWIFT III code, a series of verification problems were established. Each problem had either an analytical solution or a numerical simulation by a well-established computer code, or both.

Different analytical and numerical codes were used for the verification of the SWIFT III code. During this verification process, results of the SWIFT III code were compared with analytical ground water flow models (Table 2.1), and with a one-dimensional and two-dimensional analytical solute transport models (Table 2.2). The results of the SWIFT III code were also compared with the results of three different numerical ground water flow models, i.e., MODFLOW, PTC, and GEOFLOW (Table 2.1) and with the results of numerical solute transport models using GEOFLOW (Table 2.2). The verification problems were specifically selected to

test the capability of SWIFT III to model the hydrogeologic, geochemical, and radiological features present at the FMPC site. These features include pumping and injection wells, recharge, different types of boundary conditions, river leakages, different types of aquifers, various solute transport parameters, and radioactive decay.

This report documents the procedures and findings of the verification process. Based on the extensive verification tests performed on SWIFT III by GeoTrans and IT, it is concluded that the code has been thoroughly tested and will adequately simulate the features at the FMPC site. Because SWIFT III performs satisfactorily in relation to other well-established codes, it can be used with a high degree of reliability and confidence in the sitewide RI/FS modeling studies.

APPENDIX
A

APPENDIX A

SUMMARY DESCRIPTION OF COMPUTER CODES

This appendix contains a brief description of the computer programs which were used in the verification of the SWIFT III computer code. These codes are GEOFLOW, MODFLOW, and PTC.

A.1.0 GEOFLOW

The computer program GEOFLOW (IT, 1986) is a Galerkin finite element program capable of numerically simulating fluid flow and solute mass transport in a two-dimensional ground water system. The aquifer can be confined, semiconfined (leaky), or unconfined. Both transient and steady state models of fluid flow and solute transport can be solved. In the fluid flow simulations, the aquifer can be nonhomogeneous, anisotropic, and of nonuniform thickness. Multiple wells with time-dependent flow rates can also be specified in the model. In the solute transport simulations, the geochemical reactions such as adsorption, acid neutralization, and radioactive decay can be incorporated by specifying proper characteristic coefficients.

The main routine of GEOFLOW contains two mutually dependent finite element subprograms; one is the flow model which solves the ground water flow equations, and the other is the solute mass transport model which solves the hydrodynamic dispersion equation. Result output at user selected times in the simulation period include: piezometric heads, velocity and flow (discharge) vectors, concentrations, saturated thicknesses, and retardation factors for acid-front neutralization.

To supplement the numerical results produced by GEOFLOW, a graphical postprocessing program permits the plotting of potentiometric contours, velocity vectors, and isopachs of the other output.

GEOFLOW is also equipped with a "restart" option which enables the program to carry over necessary information from a previous execution and to continue the execution after pertinent data are modified according to the new simulation requirements.

GEOFLOW has been extensively verified and has a user friendly and well documented manual.

A.2.0 MODFLOW

MODFLOW is a finite-difference ground water flow model. The program has been developed by McDonald and Harbaugh (1984) and it is also known as USGS Modular 3-D computer program. This program has been recently augmented with pre- and postprocessor by TECSOFT, Inc., and renamed MODFLOW. The model simulates flow in three dimensions. Ground water flow within an aquifer is simulated using a block-centered finite-difference approach. Layers can be simulated as confined, unconfined, or a combination of confined and unconfined. Flow from external stresses, such as flow to wells, areal recharge, evapotranspiration, flow to drains, and flow through riverbeds, can also be simulated. The finite-difference equations can be solved using either the Strongly Implicit Procedure or Slice-Successive Overrelaxation.

The code structure consists of a Main Program and a series of highly independent subroutines called "modules." The modules are grouped into "packages." Each package deals with a specific feature of the hydrologic system which is to be simulated, such as flow from rivers or flow into drains, or with a specific method of solving linear equations which describe the flow system, such as the Strongly Implicit Procedure or Slice-Successive Overrelaxation.

The division of the program into modules permits examination of specific hydrologic features of the model independently. This also facilitates development of additional capabilities because new modules or packages can be added to the program without modifying the existing modules or packages. The input and output systems of the computer program are also designed to permit maximum flexibility.

A.3.0 PRINCETON TRANSPORT CODE (PTC)

The Princeton Transport Code (PTC) was developed by the staff of Princeton University, Princeton, New Jersey (Babu et al., 1987). PTC is a three-dimensional ground water flow and solute transport code. It takes advantage of the ability of two-dimensional finite elements to represent irregular shapes accurately. A finite element formulation is applied to the horizontal cross section and the finite difference methods to the vertical direction. It treats single-phase Darcy ground water flow in fully three dimensional space under nonisothermal conditions. The code has the capability to model layered aquifer systems. The code offers a wide choice of boundary conditions such as prescribed heads, nodal injection or withdrawal, constant or spatially varying infiltration rates, and elemental source/sink. The heterogeneity in aquifer hydraulic conductivity and porosity can be described by geologic unit or by explicit data for given elements.

PTC is written in standard FORTRAN 77. The program is divided into five groups of program units. The code is structured to do the following: The (nearly) steady state flow is either computed first, or is assumed to be known from previous runs of the model. Utilizing these known or given heads, the transport section of the code then computes the velocities and the chemical concentrations.

APPENDIX
B

APPENDIX B
REFERENCES FOR VERIFICATION PROBLEMS

This appendix contains references to input and output file names and figures and tables pertinent to the verification problems.

TABLE B.1

SWIFT III CODE GROUNDWATER FLOW VERIFICATION REFERENCE

GROUNDWATER FLOW PROBLEMS	GWF-1	GWF-2	GWF-3	GWF-4	GWF-5	GWF-6a	GWF-6b	GWF-6c	GWF-6d
REFERENCES									
SWIFT III RELATED INPUT FILENAMES	VFC1.DAT	VFC7.DAT	STC2-8.DAT	STC2-9.DAT	TRIAL3A.DAT	EXST-1.DAT	EXST-US1.DAT	EXSTRIV4.DAT	EXSTRIV5.DAT
						EXST-ANN.DAT			
SWIFT III RELATED OUTPUT FILENAMES	VFC1.OUT	VFC7.OUT	STC2-8.OUT	STC2-9.OUT	TRIAL3A.OUT	EXST-1.OUT	EXST-US1.OUT	EXSTRIV4.OUT	EXSTRIV5.OUT
	VFC1.FT12	VFC7.FT12				EXST-ANN.OUT			
GEOFLOW RELATED INPUT FILENAMES					IN.GEO.1A				
GEOFLOW RELATED OUTPUT FILENAMES					OUT.GEO.1A				
MODFLOW RELATED INPUT FILENAMES					IN.MCFER6C	IN.EXST-1	IN.EXST-US1	IN.EXST-US1RV	IN.EXST-US3RV
						IN.EXST-2S		IN.EXST-US2RV	IN.EXST-US4RV
MODFLOW RELATED OUTPUT FILENAMES					OUT.MCFER6C	OUT.EXST-1	OUT.EXST-US1	FILE14.OUT.EXST-US1RV	OUT.EXST-US3RV
					LUNIT14.OUT.MCFERC	OUT.EXST-1S		FILE14.OUT.EXST-US2RV	OUT.EXST-US4RV
						OUT.EXST-2		OUT.EXST-US1RV	F14OEXSTUS4RV
						OUT.EXST-2S		OUT.EXST-US2RV	
PTC RELATED INPUT FILENAMES						INITHD.IN.EXST-1			
						SAMPLE.IN.EXST-1			
PTC RELATED OUTPUT FILENAMES						PTC1.OUT			
						PTC1.LHD			
VERIFICATION PROBLEM DETAILS: SEE VERIFICATION REPORT	SECTION 3.1.1	SECTION 3.1.2	SECTION 3.1.3	SECTION 3.1.4	SECTION 3.2.1	SECTION 3.2.2	SECTION 3.2.2	SECTION 3.2.2	SECTION 3.2.2
RELEVANT TABLES	TABLE 2.1	TABLE 2.1	TABLE 2.1	TABLE 2.1	TABLE 2.1	TABLE 2.1	TABLE 2.1	TABLE 2.1	TABLE 2.1
	TABLE B.1	TABLE B.1	TABLE B.1	TABLE B.1	TABLE B.1	TABLE B.1	TABLE B.1	TABLE B.1	TABLE B.1
	TABLE 3.2	TABLE 3.2	TABLE 3.2	TABLE 3.2	TABLE 3.3	TABLE 3.8	TABLE 3.8	TABLE 3.8	TABLE 3.8
					TABLE 3.4	TABLE 3.9	TABLE 3.9		TABLE 3.12
					TABLE 3.5	TABLE 3.10	TABLE 3.11		TABLE 3.13
					TABLE 3.6				
					TABLE 3.7				
RELEVANT FIGURES	FIGURE 3 - 1	FIGURE 3 - 1	FIGURE 3 - 6	FIGURE 3 - 8	FIGURE 3 - 10	FIGURE 3 - 15	FIGURE 3 - 16	FIGURE 3 - 15	FIGURE 3 - 15
	FIGURE 3 - 2	FIGURE 3 - 4	FIGURE 3 - 7	FIGURE 3 - 9	FIGURE 3 - 11	FIGURE 3 - 16	FIGURE 3 - 16	FIGURE 3 - 16	FIGURE 3 - 16
	FIGURE 3 - 3	FIGURE 3 - 5			FIGURE 3 - 12	FIGURE 3 - 17	FIGURE 3 - 17	FIGURE 3 - 23	FIGURE 3 - 26
					FIGURE 3 - 13	FIGURE 3 - 18	FIGURE 3 - 22	FIGURE 3 - 24	FIGURE 3 - 27
					FIGURE 3 - 14	FIGURE 3 - 19		FIGURE 3 - 25	FIGURE 3 - 28
						FIGURE 3 - 20			
						FIGURE 3 - 21			

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TABLE B.2

SWIFT III CODE SOLUTE TRANSPORT VERIFICATION REFERENCE

SOLUTE TRANSPORT PROBLEMS	ST-1	ST-2a	ST-2b	ST-3a	ST-3b
		Retardation Factor=1.0	Retardation Factor=2.5	small grid	large grid
REFERENCES					
ANALYTICAL SOLUTION INPUT FILENAMES	ERRFUNCT.IN	IN.ST-5(T)	IN.STR-5(T)		
	ERRFUNCT.OUT				
ANALYTICAL SOLUTION OUTPUT FILENAMES		OUT.ST-5(T)	OUT.STR-5(T)		
SWIFT III RELATED INPUT FILENAMES	VFC19.DAT	STF1.DAT	STF1MR.DAT	SW3D1.DAT	SW3D2.DAT
	VFC19A.DAT	STF1M.DAT		SW3D1M.DAT	SW3D2F.DAT
					SW3DX.DAT
SWIFT III RELATED OUTPUT FILENAMES	VFC19.OUT	STF1.OUT	STF1MR.OUT	SW3D1.OUT	SW3D2.OUT
	VFC19A.OUT	STF1M.OUT		SW3D1M.OUT	SW3D2F.OUT
					SW3DX.OUT
GEOFLOW RELATED INPUT FILENAMES		IN.GEO.COM-5	IN.GEO.COM-5A	IN.GEO.SW3D1	IN.GEO.SW3D2
GEOFLOW RELATED OUTPUT FILENAMES		OUT.GEO.COM-5	OUT.GEO.COM-5A	OUT.GEO.SW3D1	OUT.GEO.SW3D2
VERIFICATION PROBLEM DETAILS: SEE VERIFICATION REPORT	SECTION 4.1.1	SECTION 4.1.2	SECTION 4.1.2	SECTION 4.2	SECTION 4.2
RELEVANT TABLES	TABLE 2.2	TABLE 2.2	TABLE 2.2	TABLE 2.2	TABLE 2.2
	TABLE B.2	TABLE B.2	TABLE B.2	TABLE B.2	TABLE B.2
	TABLE 4.1	TABLE 4.4	TABLE 4.4	TABLE 4.7	TABLE 4.7
	TABLE 4.2	TABLE 4.5	TABLE 4.5	TABLE 4.8	TABLE 4.8
	TABLE 4.3	TABLE 4.6	TABLE 4.6		
RELEVANT FIGURES	FIGURE 4 - 1	FIGURE 4 - 2	FIGURE 4 - 2	FIGURE 4 - 13A	FIGURE 4 - 14A
		FIGURE 4 - 3	FIGURE 4 - 3	FIGURE 4 - 13B	FIGURE 4 - 14B
		FIGURE 4 - 4	FIGURE 4 - 4	FIGURE 4 - 15	FIGURE 4 - 18
		FIGURE 4 - 5	FIGURE 4 - 5	FIGURE 4 - 16	FIGURE 4 - 19
		FIGURE 4 - 6	FIGURE 4 - 10	FIGURE 4 - 17	FIGURE 4 - 20
		FIGURE 4 - 7	FIGURE 4 - 11		
		FIGURE 4 - 8	FIGURE 4 - 12		
		FIGURE 4 - 9			

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FOOTNOTE :

For files associated with ST-2a and ST-2b, (T) indicates that a file name is typical of a number of runs ending with -5, -10, -15, TO 100

APPENDIX
C

APPENDIX C

ANALYTICAL SOLUTION OF TWO-DIMENSIONAL HYDRODYNAMIC DISPERSION EQUATIONS WITH FLUX SOURCE BOUNDARY

C.1.0 PROBLEM DESCRIPTION

The governing equation and the analytical solution of two-dimensional hydrodynamic dispersion equation with flux source boundary are given in Chapter 4.0 (Equation 4.22). The solution of this equation was used to verify the SWIFT III code, as part of Verification Problem ST-2. This appendix contains the derivation of Equation 4.22. A portion of the Chapter 4.0 is reproduced in this appendix to provide a completeness and continuity.

A schematic drawing of the general multiple solute sources problem is given in Figure C-1. The problem under consideration is transient two-dimensional solute transport in a unidirectional ground water flow field between two impervious boundaries with the third-type (Cauchy) or flux-type boundary condition at the sources. The solute sources are located irregularly along the z-axis in a unidirectional velocity field along the x-axis. The source concentrations are functions of the distance along the z-axis. The medium extends to infinity along the x-direction and has a finite length, H_m, along the z-axis. In Figure C-1, C_{m_i} represents the source concentration at the ith strip.

C.1.1 GOVERNING EQUATION

The two-dimensional hydrodynamic dispersion equation in a unidirectional flow field, with linear equilibrium adsorption and first-order decay, can be written as:

$$R_d \frac{\partial C}{\partial t} = D_x \frac{\partial^2 C}{\partial x^2} + D_z \frac{\partial^2 C}{\partial z^2} - U \frac{\partial C}{\partial x} - R_d \nu C \qquad (C.1)$$

where

C = mass of solute for unit volume of fluid $[M/L^3]$,
R_d = retardation factor [dimensionless],
ν = decay constant $[1/t]$,
U = seepage velocity $[L/t]$,

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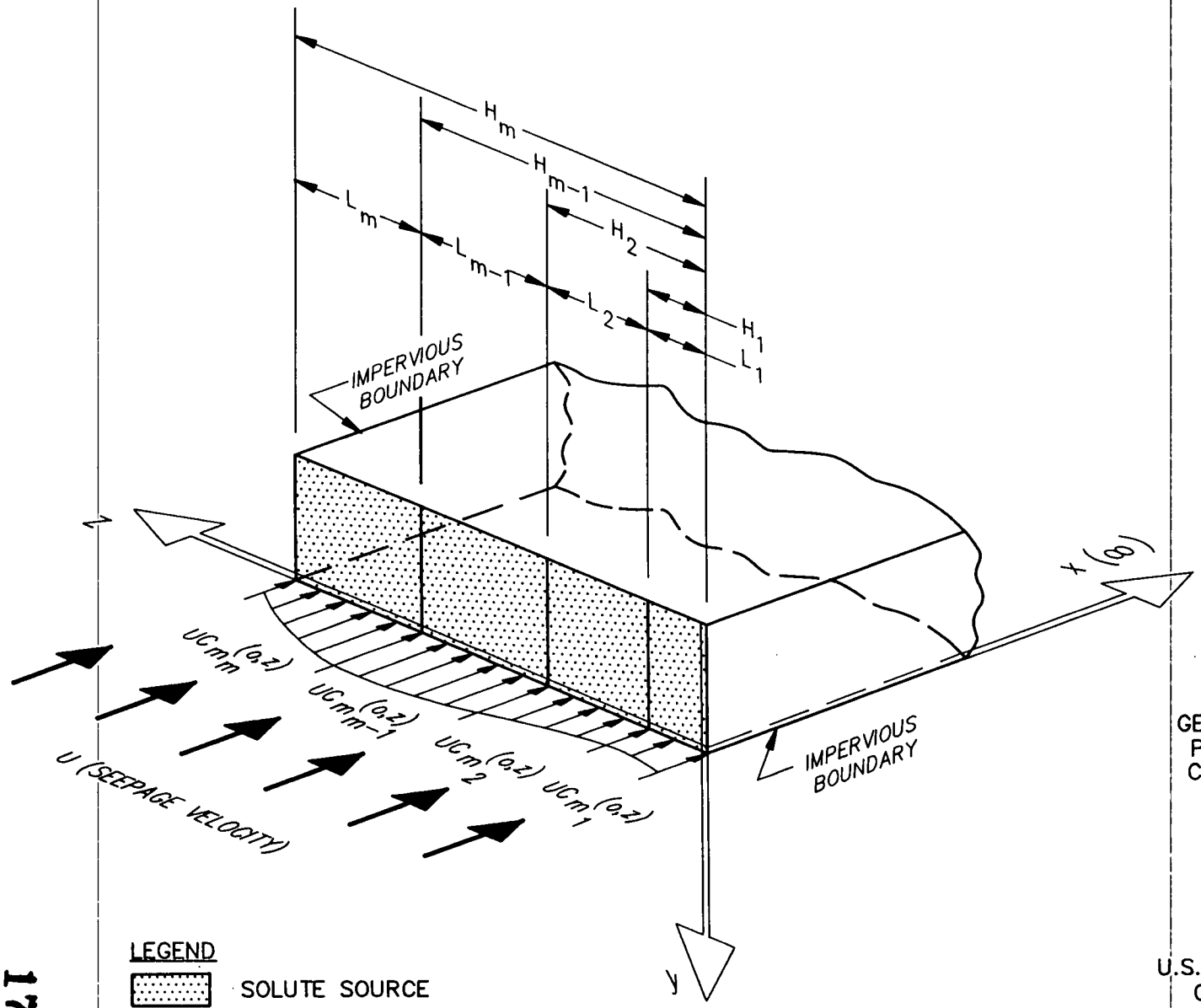
		APPROVED BY	SHD	8/31/90		



LEGEND

SOLUTE SOURCE

FIGURE C-1

GENERAL SCHEMATIC OF A POROUS MEDIUM WITH A CONSTANT CONTAMINANT FLUX BOUNDARY

PROBLEM ST-2

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x,z = Cartesian coordinates [L],

D_x, D_z = longitudinal and transverse dispersion coefficients, respectively [L^2/t]

The seepage velocity, U, appearing in Equation C.1 is the ground water velocity which is defined in terms of Darcy velocity, v, and porosity, ϕ, as:

$$U = \frac{v}{\phi} \tag{C.2}$$

The longitudinal and transverse dispersion coefficients and are defined as:

$$D_x = \alpha_L U \tag{C.3}$$

$$D_z = \alpha_T U \tag{C.4}$$

where α_L[L] and α_T[L] are the longitudinal and transverse dispersivities, respectively.

C.2.0 INITIAL AND BOUNDARY CONDITIONS

Initially, the concentration in the porous medium is zero. Therefore, the initial condition for the transport field is:

$$C\ (x,\ z,\ t = 0) = 0 \tag{C.5}$$

The flux-type or third-type (Cauchy) boundary conditions at the sources (x = 0) is:

$$\frac{F_x(0,z)}{\phi} = UC_{m_1}(z) \qquad 0 < z < H_1 \tag{C.6a}$$

$$= UC_{m_{m-1}}(z) \qquad H_{m-2} < z < H_{m-1} \tag{C.6b}$$

$$= UC_{m_m}(z) \qquad H_{m-1} < z < H_m \qquad (C.6c)$$

where

$$H_i = \sum_{j=1}^{i} L_j \qquad (C.7)$$

where L_j is the length of the jth strip source.

Conditions at the impervious boundaries are:

$$\frac{\partial C(x,z,t)}{\partial z} = 0 \qquad z = 0 \qquad 0 < x < \infty \qquad (C.8)$$

$$\frac{\partial C(x,z,t)}{\partial z} = 0 \qquad z = H_m \qquad 0 < x < \infty \qquad (C.9)$$

The boundary conditions at infinity are:

$$\lim_{x \to \infty} C(x,z,t) = 0 \qquad 0 < z < H_m \qquad (C.10)$$

$$\lim_{x \to \infty} \frac{\partial C(x,z,t)}{\partial x} = 0 \qquad 0 < z < H_m \qquad (C.11)$$

C.3.0 GENERAL SOLUTION FOR THE LAPLACE TRANSFORM FUNCTION

Taking the Laplace transform of Equation C.1 with respect to time and using the initial condition given by Equation C.5 yields (Batu, 1983):

$$R_d\,(s+\nu)u = D_x \frac{\partial^2 u}{\partial x^2} + D_z \frac{\partial^2 u}{\partial z^2} - U \frac{\partial u}{\partial x} \qquad (C.12)$$

in which u is the Laplace transform of C. By applying, the method of separation of variables with $u(x,z) = X(x)Z(z)$; the general solution can be obtained as [Batu, 1983; Equations 23 and 24]:

$$X(x) = A_1 \exp\left(\frac{Ux}{2D_x} - px\right) + B_1 \exp\left(\frac{Ux}{2D_x} + px\right) \qquad \text{(C.12a)}$$

$$Z(z) = A_2 \sin(\lambda z) + B_2 \cos(\lambda z) \qquad \text{(C.12b)}$$

where

$$p = \left[\frac{D_z}{D_x}\lambda^2 + \frac{R_d}{D_x}(s + \nu) + \frac{U^2}{4D_x^2}\right]^{1/2} \qquad \text{(C.13)}$$

in which A_1, B_1, A_2, and B_2 are constants. To satisfy the conditions given by Equations C.10 and C.11, B_1 and A_2 in Equation C.12 must vanish. Equation C.9 implies that the following equation is the condition for the values of λ:

$$\lambda_n = \frac{n\pi}{H_m} \qquad n = 0,1,2,\ldots \qquad \text{(C.14)}$$

Introducing the values in the $u(x,z)$ solution gives:

$$u(x,z) = \sum_{n=0}^{\infty} A_n \exp\left(\frac{Ux}{2D_x} - p_n x\right) \cos(\lambda_n z) \qquad \text{(C.15)}$$

where

$$p_n = \left[\frac{D_z}{D_x}\lambda_n^2 + \frac{R_d}{D_x}(s+\nu) + \frac{U^2}{4D_x^2}\right]^{1/2} \qquad \text{(C.16)}$$

The general solute flux equation along the x-axis can be written as:

$$\frac{F_x(0,z)}{\phi} = UC - D_x \frac{\partial C}{\partial x} \qquad \text{(C.17)}$$

Using the Laplace transform of Equation C.17 with the boundary condition stated by Equation C.6 can be written as:

$$\frac{F_x(0,z)}{\phi} = (Uu - D_x \frac{\partial u}{\partial x})s \qquad (C.18)$$

Taking the derivative of the solution u(x,z) given by Equation C.15 with respect to x, and substituting it in Equation C.18 gives:

$$\frac{F_x(0,z)}{\phi} = \sum_{n=0}^{\infty} B_n \cos(\lambda_n z) \qquad (C.19)$$

where

$$B_n = A_n \left(\frac{U}{2} + D_x p_n\right)s \qquad (C.20)$$

Consideration of the right hand side of Equation C.19 as a Fourier cosine series for the interval z = 0 to H_m yields (Churchill, 1941):

$$B_n = \frac{2}{H_m} \int_0^{H_m} \frac{F_x(0,z)}{\phi} \cos(\lambda_n z)dz \qquad (C.21)$$

Substituting Equation C.21 in Equation C.20 and solving for A_n yields:

$$A_n = \frac{2}{H_m(\frac{U}{2} + D_x p_n)s} \int_0^{H_m} \frac{F_x(0,z)}{\phi} \cos(\lambda_n z)dz \qquad (C.22)$$

Introducing Equation C.22 into Equation C.15 and using conditions of Equation C.14 gives:

$$u(x,z) = u_1(x,z) + u_2(x,z) \qquad (C.23)$$

where

$$u_1(x,z) = \frac{2}{H_m(\frac{U}{2} + D_x p_0)s} \left[\int_0^{H_m} \frac{F_x(0,z)}{\phi} dz\right] \exp\left(\frac{Ux}{2D_x} - P_0 x\right) \qquad (C.24)$$

$$u_2(x,z) = \sum_{n=1}^{\infty} \left\{ \frac{2}{H_m \left(\frac{U}{2} + D_x p_n\right) s} \int_0^{H_m} \frac{F_x(0,z)}{\phi} \cos(\lambda_n z) dz \right\}$$

$$\cdot \exp\left(\frac{Ux}{2D_x} - p_n x\right) \cos(\lambda_n z) \qquad (C.25)$$

In Equation C.24, p_0 is the value of p_n, given by Equation C.16, for $n = 0$.

Equation C.23 is the general solution for the Laplace transform function and is valid for any solute flux distribution at $x = 0$ (Figure C-1).

C.4.0 INVERSE LAPLACE TRANSFORM FOR THE GENERAL SOLUTION

To solve Equation C.23 and obtain concentration distribution it is necessary to perform inverse Laplace transformation. The inverse Laplace transform of Equation C.24 can be expressed as:

$$u_1(x,z,s-b) = \frac{f_1(s-b)}{s} \qquad (C.26)$$

where

$$b = -\nu - \frac{U^2}{4D_x R_d} \qquad (C.27)$$

Substituting for values of p_0 from Equation C.16, $f_1(s-b)$ can be written as:

$$f_1(s-b) = \frac{2}{H_m\left\{\frac{U}{2} + [R_d D_x (s-b)]^{1/2}\right\}} \left[\int_0^{H_m} \frac{F_x(0,z)}{\phi} dz\right]$$

$$\cdot \exp\left(\frac{Ux}{2D_x}\right) \exp\left\{-\left[\frac{R_d}{D_x}(s-b)\right]^{1/2} x\right\} \qquad (C.28)$$

Using the convolution (or Faltung) theorem, Equation C.26 can be expressed as (Spiegel, 1965):

$$C_1(x,z,t) = L^{-1}\{u_1(x,z,s-b)\} = L^{-1}\{\frac{f_1(s-b)}{s}\}$$

$$= \int_0^t F_1(u)du \qquad (C.29)$$

where L^{-1} is the symbol of the inverse Laplace transform.

Now, using the first translation or shifting property (Spiegel, 1965):

$$F_1(t) = L^{-1}\{f_1(s-b)\} = K_o\, e^{bt} G_1(t)\, \exp(\frac{Ux}{2D_x}) \qquad (C.30)$$

$$L^{-1}\{g_1(s)\} = G_1(t) \qquad (C.31)$$

where

$$K_0 = \frac{2}{H_m}\,[\int_0^{H_m} \frac{F_x(0,z)}{\phi}\, dz] \qquad (C.32)$$

where

$$g_1(s) = \frac{\exp[-(\frac{R_d s}{D_x})^{1/2} x]}{D_x\,[\frac{U}{2D_x} + (\frac{R_d s}{D_x})^{1/2}]} \qquad (C.33)$$

The inverse Laplace transform of Equation C.33 is [Carslaw and Jaeger, 1959, p. 494, Equation C.12]:

$$G_1(t) = \left(\frac{D_x}{\pi R_d t}\right)^{1/2} \exp\left(-\frac{R_d x^2}{4D_x t}\right) - \frac{U}{2R_d D_x} \exp\left(\frac{Ux}{2D_x} + \frac{U^2 t}{4R_d D_x}\right)$$

$$\operatorname{erfc}\left[\frac{R_d x}{2\,(D_x R_d t)^{1/2}} + \frac{U}{2}\left(\frac{t}{R_d D_x}\right)^{1/2}\right] \qquad (C.34)$$

From Equations C.29, C.30, C.32, and C.34, the following results:

$$C_1(x,z,t) = K_0 \int_0^t F_1(u)[F_2(u) - F_3(u)F_4(u)]du \qquad (C.35)$$

in which $F_1(u)$, $F_2(u)$, $F_3(u)$, and $F_4(u)$ are expressed by the following equations

$$F_1(u) = \exp\left(\frac{Ux}{2D_x} - \nu u - \frac{U^2}{4D_x R_d} u\right) \qquad (C.36)$$

$$F_2(u) = \left(\frac{D_x}{\pi R_d u}\right)^{1/2} \exp\left(-\frac{R_d x^2}{4D_x u}\right) \qquad (C.37)$$

$$F_3(u) = \frac{U}{2R_d} \exp\left(\frac{Ux}{2D_x} + \frac{U^2 u}{4F_d D_x}\right) \qquad (C.38)$$

$$F_4(u) = \operatorname{erfc}\left[\frac{R_d x}{2(D_x R_d u)^{1/2}} + \frac{U}{2}\left(\frac{u}{R_d D_x}\right)^{1/2}\right] \qquad (C.39)$$

The inverse Laplace transform of Equation C.25 can similarly be taken and expressed as:

$$C_2(x,z,t) = \sum_{n=1}^{\infty} K_n F_1(u) \exp\left(-\frac{D_z}{R_d}\lambda_n^2 u\right) \cdot [F_2(u) - F_3(u)\, F_4(u)]du \qquad (C.40)$$

where

$$K_n = \frac{2}{H_m} \int_0^{H_m} \frac{F_x(0,z)}{\phi} \cos(\lambda_n z)dz \qquad (C.41)$$

and λ_n, $F_1(u)$, $F_2(u)$, $F_3(u)$, and $F_4(u)$ are defined by Equations C.14 and C.36 through C.39.

The concentration at any point and time could be calculated by adding C_1 and C_2

$$C(x,z,t) = C_1(x,z,t) + C_2(x,z,t) \qquad (C.42)$$

which is the inverse Laplace transport Equation C.23.

C.4.0 SPECIAL SOLUTION FOR A STRIP SOLUTE SOURCE

The geometry of a solute strip source is shown in Figure C-2 which is a special case of Figure C-1. The boundary conditions at x = 0 are expressed by Equations 4.20 and 4.21. Using these equations in Equations C.32 and C.41 and after simplification, the solution for the normalized concentration distribution given by Equation (4.22) could be obtained.

C.6.0 NUMERICAL INTEGRATION PROCEDURE

The integrals in Equation 4.22 could only be evaluated numerically. For these integrals, the Gaussian integration procedure was used. Because

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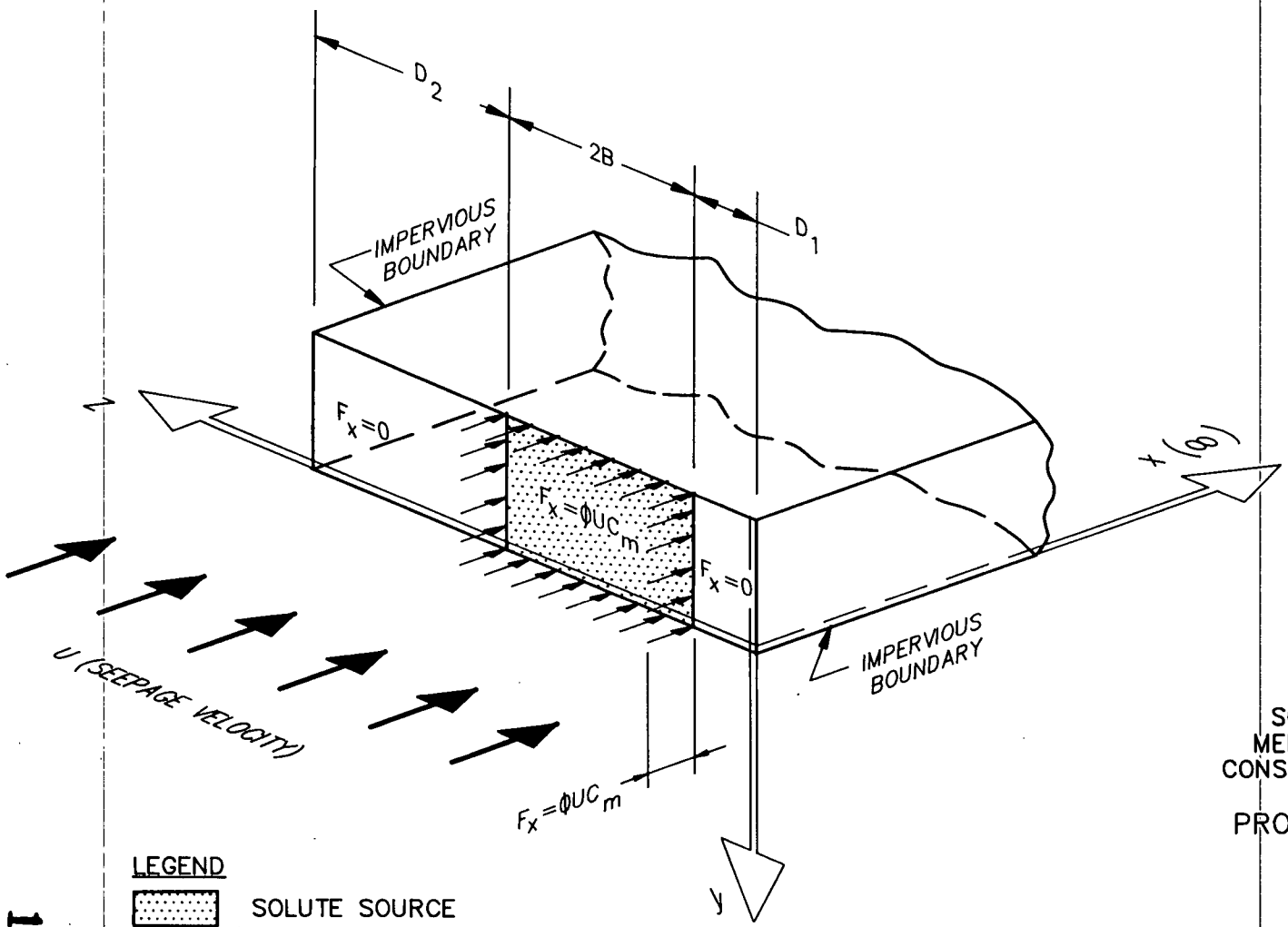

FIGURE C-2

SCHEMATIC OF A POROUS MEDIUM WITH A FINITE STRIP CONSTANT CONTAMINANT SOURCE

PROBLEMS ST-2a AND 2b

PREPARED FOR

FERNALD RI/FS
U.S. DEPARTMENT OF ENERGY
OAK RIDGE OPERATIONS

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the integrals in the aforementioned expression have the limits 0 and t, whereas the Gauss method requires limits of -1 and +1, a change of variables was performed, i.e.,:

$$u = \frac{t}{2}(u'+1) \qquad (C.43)$$

Thus, when u' is -1, u is 0; when u' = +1, u = t; and u' becomes the variable in the Gauss integration:

$$du = \frac{1}{2} t \, du' \qquad (C.44)$$

With the combination of Equations 4.22, C.43, and C.44, a computer program called STRIP1B-FBC-G, was developed to compute the normalized concentration. The computer program has the capability to use 4, 5, 10, 20, 60, 104, or 256 Gauss points.

APPENDIX D

APPENDIX D
NOMENCLATURE

This appendix contains the nomenclature for commonly referenced variables in the text and figures.

TABLE D.1

LIST OF ACRONYMS

GWF	Ground water flow
ST	Solute transport
PTC	Princeton Transport Code
MODFLOW	U.S. Geological Survey's three-dimensional finite-difference ground water flow code
SWIFT	Sandia Waste-Isolation Flow and Transport Code
GEOFLOW	International Technology Corporations ground water flow and solute transport code

TABLE D.2

NOMENCLATURE FOR COMMONLY USED VARIABLES

VARIABLE	DEFINITION	DIMENSION	FIRST SECTION DEFINED
B	Half-source width	L	4.1.2.4
C	Mass of solute for unit volume of fluid	M/L^3	4.1.1.2
C_r	Radionuclide concentration	M/L^3	4.1.1.2
D	Dispersion coefficient	L^2t	4.1.1.2
D_i	Distance	L	4.1.2.4
D_x	Logitudinal dispersion	L^2/t	4.1.2.2
D_z	Transverse dispersion coefficient	L^2/t	4.1.2.2
F_x	Solute flux in the x-direction	$M/(L^2t)$	4.1.2.2
H_m	Distance between the impervious boundaries	L	4.1.2.2
h	Hydraulic head	L	3.1.3.2
k_{rs}	Product of branching ration and a daughter-to-parent mass fraction	Dimensionless	4.1.1.2
Q	Extraction or flow rate	L^3/t	3.1.1.2
q	Recharge	L/t	3.1.3.2
r	Radial distance	L	3.1.1.2
R_d	Retardation factor	Dimensionless	4.1.1.2
S	Storativity	Dimensionless	3.1.1.2
s	Drawdown	L	3.1.1.2
T	Transmissivity	L^2/t	3.1.1.2
T_x	Transmissivity in the x-direction	L^2/t	3.1.1.2
T_y	Transmissivity in the y-direction	L^2/t	3.1.1.2
t	Time	t	3.1.1.2
U	Seepage velocity	L/t	4.1.2.2
$\bar{U}$	Retarded interstitial velocity of radionuclide	L/t	4.1.1.2
u	Variable	Dimensionless	3.1.1.2

TABLE D.2
(Continued)

VARIABLE	DEFINITION	DIMENSION	FIRST SECTION DEFINED
v	Darcy velocity	L/t	4.1.2.2
W	Well function	Dimensionless	3.1.1.2
x	Coordinate	L	3.1.2.2
y	Coordinate	L	3.1.2.2
z	Coordinate	L	4.1.2.2
α_L	Logitudinal dispersivity	L	4.1.1.2
α_T	Transverse dispersivity	L	4.1.2.2
δ	Dirac delta function	1/L	3.1.1.2
ϕ	Porosity	Dimensionless	3.1.4.4
ν	Decay constant	1/t	4.1.1.2