VALIDATION

VERSION 2.50

-

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PREFACE

During the past 15 years, PORFLOW has evolved into a comprehensive software tool for analysis of a wide range of environmental applications in flow, heat and mass transport in geologic media. It provides for coupled transport of flow, heat and multiple chemical species in complex three-dimensional geometry, transient or steady-state flow, confined or unconfined aquifers, fully or partially saturated media, single or multiple phase systems, and phase change between liquid and solid and liquid and gaseous phases.

PORFLOW has been used to analyze problems as diverse as salinity intrusion into fresh water aquifers and remediation of hazardous waste sites. It has been used to evaluate pumping of an aquifer over a period of days, remediation of waste sites over a period of years, corrosion of waste canisters over tens of years, and transport of contaminants from nuclear waste over a time span of hundreds of thousands of years.

PORFLOW is distinguished from other computer models by the diversity of its users. It is being used by commercial, research and educational organizations in 10 countries. Among its users are: U.S. Department of Energy, U.S. Geological Survey, U.S. Nuclear Regulatory Commission, U.S. Department of the Army, Southwest Research Institute, Westinghouse Hanford Company, Idaho National Engineering Laboratory, Oak Ridge National Laboratory, Savannah River Laboratory, Battelle Pacific Northwest Laboratory, and a large number of commercial organizations. Over 100 publications and project reports on the benchmarking, verification and application of PORFLOW are currently available. In this process, PORFLOW has been extensively peer-reviewed.

In view of the increasing use of PORFLOW for projects subject to regulatory or peer-review, a need exists to verify its predictions against known analytic and numerical solutions. This document is an attempt in that direction. It describes the results of verification and benchmark tests conducted by Analytic & Computational Research, Inc. (ACRi) to validate PORFLOW Version 2.50 and to test its capability to simulate a wide variety of flow conditions. Several test problems, for which analytic or numerical solutions are available in the published literature, were selected for this purpose. PORFLOW input and output for these problems is also available on electronic media for a nominal charge. For additional information, please contact:

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CHAPTER 1

INTRODUCTION AND OVERVIEW

This document describes the results of verification and benchmark tests to validate the mathematical and numerical formulation of PORFLOW Version 2.50. PORFLOW is a software tool for solution of multi-phase fluid flow, heat transfer, and mass transport problems in variably saturated porous or fractured media. The software employs the FREEFORM command language pre-processor to provide a flexible, simple to use, and format-free user-interface. It interfaces with the acrPLOT post-processor to display the computed results as a variety of graphical images. A detailed description of the test problems, PORFLOW results, and comparison of these results with analytic, semi-analytic or numerical solutions is given in the following chapters. This chapter provides an introduction and overview of the test problems.

1.1 INTRODUCTION

Analytic & Computational Research, Inc. has extensively tested PORFLOW Version 2.50 software (ACRi, 1994; Runchal and Sagar, 1993) to evaluate its operational status and its capability to accurately solve a wide range of problems under diverse flow conditions. Two types of problems were selected for these tests: verification problems and benchmark problems. Verification problems compare the results of PORFLOW simulations to published analytic or semi-analytic solutions. These provide confidence that, for the features tested, the software provides satisfactory approximation to the theoretical results. Benchmark problems have no known analytic solution. Therefore, the only way to evaluate the PORFLOW results is to compare them with the numerical predictions of other independently developed computer codes. These provide some confidence in the correctness of the physical, mathematical and numerical features of PORFLOW in that the results are similar to those obtained from other computer codes.

Eleven verification and six benchmark problems were selected to test the software. Most of these were previously used to test other computer codes or to test earlier versions of PORFLOW . A short description of each problem is given in the following section. Complete description of the test problems, PORFLOW results and their comparison with known analytic or numerical solutions are given in Chapters 2 and 3.

Previous versions of PORFLOW were extensively verified by comparisons with analytic solutions, experimental and field data, and other numerical models. The results of these comparisons are described in more than 100 publications; a partial list of which is given in Appendix A. Specific applications of PORFLOW have included:

- **Analysis of high- and low-level nuclear waste repositories**
- **Pollution of ground water by organic and inorganic chemicals**
- **Movement of contaminants out of grout-waste containers**
- **Contamination of ground water by hydrocarbons**
- **Ground water resource and pumping studies**
- **Flow, heat transfer and chemical reactions in porous geologic media**
- **Use of deep aquifers for storage and withdrawal of fluids**
- **Intrusion of seawater into coastal aquifers**
- **Thawing and freezing of ground due to buried oil and gas pipelines**
- **Propagation of freezing fronts in soils**
- **Analysis of under-sea oil pipelines**
- **Interaction of ground water systems with the atmosphere**
- **Corrosion of waste canisters and liners**
- **Analysis of hydrologic effects of reverse-circulation drilling**
- **Enhancement of oil well performance by optimization of casing perforation**

- **Consolidation of soils and analysis of lithification processes.**
- **Dewatering of mines**

1.2 OVERVIEW OF TEST PROBLEMS

1.2.1 *Verification Test Problems*

Problem V1: Transient One-Dimensional Diffusion: This problem simulates the diffusive transport of a contaminant in a homogeneous, semi-infinite slab. The contaminant concentration at the right edge of the slab is maintained at a constant value. The left edge is insulated so that no contaminant enters or leaves the boundary. An analytic solution for this problem is given by Carslaw and Jaeger (1959). This problem tests the diffusive transport component of the PORFLOW algorithm.

Problem V2: Heat Transfer in Unidirectional Flow: In this test, advective, diffusive and dispersive heat transfer in a saturated porous medium is simulated. The computational domain consists of a horizontal slab with unidirectional flow from left to right. Initially, the temperature is uniform throughout the domain. At time t=0, water with a higher temperature begins entering the computational domain from the left boundary. The analytic solution for this problem is given by Carslaw and Jaeger (1959). The problem, as formulated, is attributed to Avdonin (1964) and has been used previously for verification of computer codes by several authors. The primary objective of this problem is to test the ablility of PORFLOW to correctly simulate coupled advective and dispersive transport.

Problem V3: Theis Solution for Transient Drawdown: This classic problem (Theis, 1935) simulates the transient drawdown of pressure head due to pumping in a homogeneous, confined aquifer of constant thickness that is fully penetrated by a well. The problem was originally posed and solved by Theis with the assumption that the flow is radial. It tests the ability of PORFLOW to correctly propagate a pressure transient in a radial geometry.

Problem V4: Finite Cylinder with Heat Source: This problem involves a finite cylinder in which heat is generated at a constant rate while the surface of the cylinder is maintained at zero temperature. The purpose of this test is to determine the ability of PORFLOW to simulate heat sources. The analytic solution for this problem is described by Carslaw and Jaeger (1959).

Problem V5: Convective Heat Transfer in Regional Flow: This problem concerns a homogenous, isotropic, vertical cross-section of a region with a geothermal gradient. The geothermal heat flux enters the region from the bottom and leaves through a constant-temperature surface at the top. The region is bounded on its two vertical faces with topological divides such that there is no major lateral flow. A recirculating flow pattern is induced due to lateral variations in the water table. This problem was formulated and solved by Domenico and Palciauskas (1973). The objective of the problem is to test the capability of the PORFLOW algorithm to predict convective heat transfer in the presence of a non-uniform flow field.

Problem V6: Three-Dimensional Contaminant Transport: This problem simulates the transport of a contaminant in a three-dimensional domain. A finite source near the upper surface of the computational domain continuously releases a contaminant into an aquifer that initially is free of the contaminant. The flow within the aquifer is unidirectional. Advective transport moves the contaminant in the downstream direction, while dispersive movement causes spreading of the contaminant in all directions. An analytic solution for this problem was obtained by Codell et al. (1982). This problem tests the ability of PORFLOW to simulate three-dimensional advective and dispersive transport of a contaminant from a finite source.

Problem V7: Philip's Horizontal Unsaturated Flow: The physical setting for this problem is a horizontal slab of homogeneous, isotropic soil. The vertical extent of the slab is infinite. Initially, the soil is partially saturated with ground water. At time t=0, the saturation at the left boundary is increased to unity. This saturation front then migrates downstream. The objective of this problem is to test the ability of PORFLOW to correctly compute a propagating saturation front in the absence of gravitational effects. An analogous problem was first formulated and analytically solved by Philip (1957a).

Problem V8: Philip's Vertical Unsaturated Column: The physical setting for this problem is a vertical column of homogeneous, isotropic soil. The horizontal extent of the column is considered to be infinite. The soil is initially partially saturated. At time t=0, the saturation at the top boundary is increased to unity. Transient infiltration of moisture in the vertical direction results from capillary forces and gravity. An analytic solution for an analogous problem with a propagating front was obtained by Philip (1957b). This problem tests the ability of PORFLOW to correctly simulate a migrating saturation front in the presence of gravitational effects.

Problem V9: Infiltration from a Line Source: This problem describes the flow from a single subsurface irrigation pipe that is located in an unsaturated zone above a shallow water table. Due to the infinite extent of the problem along the direction of the porous pipe, this three-dimensional problem with a line source is mathematically equivalent to a two-dimensional problem with a point source. An approximate analytic solution for this problem is given by Warrick and Lomen (1977). The objective of this problem is to evaluate the ability of PORFLOW to correctly simulate flow and saturation distribution in a variably-saturated, two-dimensional domain.

Problem V10: Free-Surface Boussinesq Flow with Recharge: This problem concerns a semi-infinite, unconfined aquifer. Initially, the phreatic surface is horizontal everywhere. At time t=0, the water level at the left boundary is suddenly raised. A compression wave, consisting of an elevated phreatic surface, then propagates from left to right in a transient manner. This problem is often referred to as the Boussinesq problem. It is described in detail by Polubarinova-Kochina (1954). The objective of this test is to determine the ability of PORFLOW to correctly model a compression wave in an unconfined aquifer.

Problem V11: Free-Surface Boussinesq Flow with Seepage: This test problem is a variation of the previous Boussinesq problem. In this test case also, the initial phreatic surface is horizontal everywhere. At time t=0, the water level at the left boundary is suddenly lowered. An expansion wave, consisting of a lowered phreatic surface, then propagates from right to left in a transient manner. The objective of this test is to determine the ability of PORFLOW to correctly simulate an expansion wave in an unconfined aquifer.

1.2.2 *Benchmark Test Problems*

Problem B1: Two-Dimensional Transient Infiltration: This problem considers flow through a two dimensional, rectangular column of partially saturated soil. The right vertical face of the column is held at its initial pressure head, while the pressure in the upper part of the left vertical face is increased. The lower part of the left face is impermeable. This causes a two-dimensional saturation front to propagate from left to right. This problem was proposed by Ross et al. (1982) for benchmark testing of computer codes. Pruess (1987) has solved this problem numerically with the TOUGH computer code. It tests the ability of PORFLOW to correctly simulate saturation fronts propagating in two dimensions.

Problem B2: Two-Dimensional Steady-State Infiltration: This problem concerns the steady-state movement of moisture under variably saturated flow conditions. The physical setting for the problem is a vertical cross-section of an aquifer with a regional hydrologic gradient. The lateral extent of the aquifer is assumed to be infinite and only a unit width is considered. Recharge occurs at the left boundary and the flow discharges at the right boundary. Additional recharge occurs through infiltration at the surface. The problem is described by Magnuson et al. (1990) and has been used as a benchmark problem for several codes. The FEMWATER computer code by Yeh and Ward (1979) was used as a benchmark for comparing the PORFLOW results. This problem tests the ability of PORFLOW to compute two-dimensional, variably saturated flow with infiltration.

Problem B3: Jornada Test Trench Simulation: This problem is based on the field tests conducted at the Jornada Test Site near Las Cruces, New Mexico. The test involves transient, two-dimensional infiltration of water into an extremely dry heterogeneous soil. The physical setting and hydraulic properties of the soil are described by Smyth et al. (1989). The test area comprises three layers of soil which vary in material and hydrologic properties. Additionally, a small zone of high conductivity soil is contained within the lowermost soil layer. The experiment was conducted under the direction of Dr. Peter Wierenga of the University of Arizona. Smyth et al. (1989) numerically solved four problems of increasing complexity using the TRACER3D computer code. The problem considered here is the fourth and most complex of these problems. It was also numerically solved by Magnuson et al. (1990) using the TRACER3D, FLASH and PORFLOW (Version 1.00) computer codes. This problem tests the ability of PORFLOW to correctly simulate variably saturated flow with infiltration in inhomogeneous soil under extremely dry conditions.

Problem B4: Saltwater Intrusion into a Confined Aquifer: This problem deals with the intrusion of seawater into a confined fresh water aquifer. The problem was described by Henry (1964) who obtained a Fourier-Galerkin solution from an idealized mathematical model. Fresh water recharge occurs at a constant rate at the left boundary of an aquifer. The right boundary is a seawater interface with hydrostatic pressure. No fluid enters or leaves through the top and bottom boundaries. The fluid density varies as a linear function of salinity. A Ghyben-Herzberg lens is formed due to the interaction of the buoyancy forces, freshwater recharge and salinity dispersion. This problem has been used extensively for verification of computer models (Pinder and Cooper, 1970; Segol et al, 1975; Huyakorn and Taylor, 1976; Desai and Contractor, 1977; INTERA, 1979; Frind, 1982, Voss, 1984; Sanford and Konikow, 1985). This problem tests the ability of PORFLOW to simulate strongly coupled, density-driven, flow and solute transport.

Problem B5: Saturated Flow in a Fractured Porous Medium: This problem concerns steady-state flow in a saturated, geologic medium with discrete embedded fractures. The hydraulic properties of the medium are based on core test data on basalts from the Idaho National Engineering Laboratory. The physical setting and the boundary conditions are selected to assure hydraulic interaction between the discrete fractures and porous medium. The computational domain contains two vertically oriented discrete fractures. The fractures are separated from each other and from the boundaries of the computational domain. The hydraulic conductivity of each fracture is more than 5 orders of magnitude larger than that of the porous media. This problem was originally devised and numerically solved by Magnuson et al. (1990) using the FLASH and PORFLOW (Version 1.00) computer codes. It tests the ability of PORFLOW to simulate flow in a porous media with embedded fractures of very high hydraulic conductivity.

Problem B6: Flow to a Geothermal Well: The physical setting for this problem is a geothermal well with production at a constant rate. Initially the reservoir is in single phase conditions. As the well is produced, pressure drops to the saturated vapor pressure creating two-phase liquid-vapor conditions. This leads to a boiling front which propagates outward from the well into the reservoir. Garg (1978) developed a semi-analytic theory for radial flow to a geothermal well. A modified version of Garg's Problem was used at the Stanford Geothermal Program (1980) for a comparative study of reservoir simulators. Pruess (1987) obtained a numerical solution for this problem with the TOUGH computer code. It tests the ability of PORFLOW to simulate porous media flow with evaporation, and the propagation of a boiling front.

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CHAPTER 2

VERIFICATION CASES

This chapter describes the verification problems which were used to validate PORFLOW . In this context, a verification problem is defined to be one for which an analytic or semi-analytic solution is available. Often such solutions are available only for problems which are relatively simple such as those for homogeneous, isotropic, porous media flow. For verification, eleven problems of increasing complexity were selected. Many of these problems have previously been used for validation of other computer codes. Each of these tests the ability of PORFLOW to simulate one or more distinct features, such as pure diffusive transport, coupled advective and diffusive flow, variably saturated flow, or unconfined flow with moving phreatic surface. The PORFLOW predictions for these selected problems, along with the comparative analytic results are described below. These provide confidence that for the features tested, PORFLOW provides satisfactory approximation to the theoretical results.

2.1 PROBLEM V1: TRANSIENT ONE-DIMENSIONAL DIFFUSION

Problem Statement

This test simulates the diffusive transport of a contaminant in a homogeneous, semi-infinite slab. The schematic for the problem is shown in Figure 2.1.1. The contaminant concentration at the right edge of the slab is maintained at a constant value. The left edge is insulated so that no contaminant enters or leaves the boundary. An analytic solution for this problem is given by Carslaw and Jaeger (1959). The objective of this test is to determine the concentration profile across the slab at selected times. The length of the computational domain is unity.

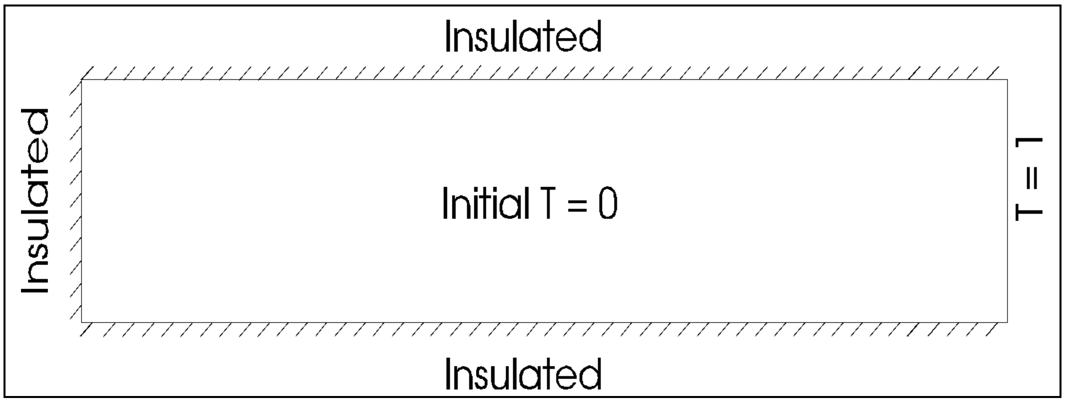

FIGURE 2.1.1: SCHEMATIC ILLUSTRATION OF PROBLEM V1

Initial Conditions Initial concentration is set to zero everywhere in the slab.

Boundary Conditions The concentration at the right boundary is set to unity. The left boundary is set to conditions of zero flux so that no contaminant enters or leaves through this boundary.

Properties For ease of comparison with the analytic solution, all properties are in non-dimensional units. The fluid and rock density, the molecular diffusivity and porosity are all set to unity. The distribution coefficient and the dispersivities are set to zero.

Computational Details A uniform grid consisting of 22 nodes in the x-direction is employed. The node spacing in the x-direction is 0.05. The total time of simulation is unity. The problem is solved in the transient mode with an initial steps of 0.00005 which is increased in a geometrical progression to 0.005. The progression ratio is 1.05. The PORFLOW input commands for this problem are shown in Table 2.1.1.

Comparison Solution The analytic solution for this problem is given by Carslaw and Jaeger (1959; p. 100-101).

PORFLOW Output Plots of concentration versus distance along the slab are generated at t = 0.02, 0.05, 0.10, 0.2, 0.5, and 1 for comparison with the analytic solution.

Results & Discussion Figure 2.1.2 shows plots of temperature for the analytic solution (solid line) and the PORFLOW simulations (symbols) at the selected times. The graphical comparison shows that the PORFLOW solution is in excellent agreement with the analytic solution.

TABLE 2.1.1: Input Commands for Problem V1

```
**********************************************************************
TITLe Transient One-Dimensional Diffusion
**********************************************************************
////  Carslaw, H.S. and J.C. Jaeger, 1959. Conduction of Heat in Solids
////  Oxford Press 2nd Ed.,  p. 101; Figure 11
**********************************************************************
/
GRID is 22 nodes in the X direction
COORdinate X  range 1
/
ROCK POROsity = 1
TRANsport kd 0 diffusivity 1
/
BOUNdary for C index -1: GRADient 0
BOUNdary for C index +1: INTErface value 1.
/
DIAGnostics at 20,1 every 10 steps
OUTPut C
SAVE C on file 'V1.ARC'
/
SOLVe .02   in steps of 0.00005   fac 1.05 max 0.005
SAVE NOW
SOLVe .03
SAVE NOW
SOLVe .05
SAVE NOW
SOLVe .10
SAVE NOW
SOLVe .30
SAVE NOW
SOLVe .50
/
END
```

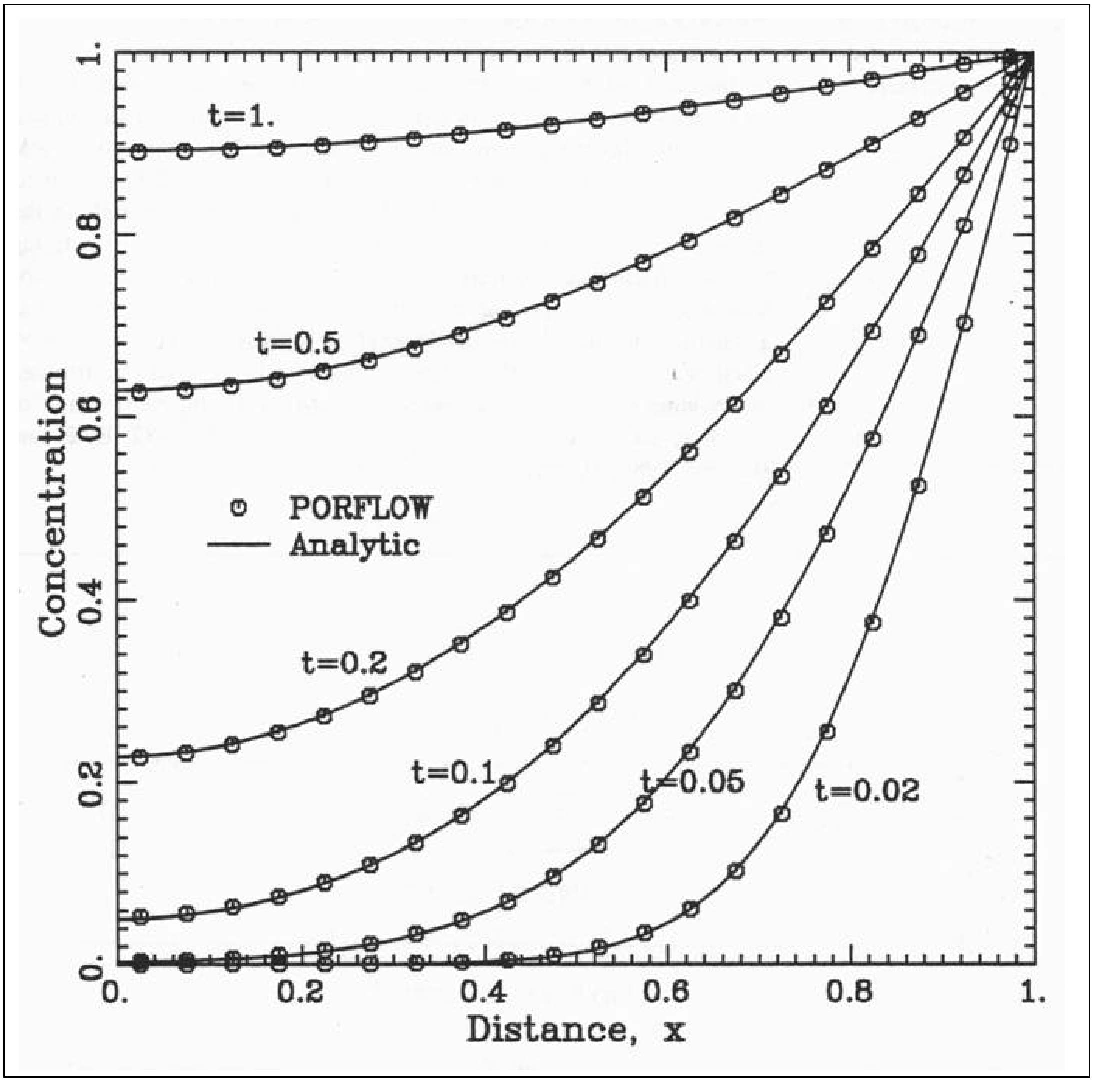

FIGURE 2.1.2: CONCENTRATION PROFILE AT SELECTED TIMES

2.2 PROBLEM V2: HEAT TRANSFER IN UNIDIRECTIONAL FLOW

Problem Statement

In this test advective, diffusive and dispersive heat transport in a saturated porous medium is simulated. The computational domain consists of a horizontal slab with unidirectional flow from left to right (Figure 2.2.1). The horizontal extent of the slab is 4,500 m and its width is unity. Initially, the temperature is uniform throughout the domain. At time t=0, water with a higher temperature begins entering the computational domain from the left boundary. The objective of the simulations is to determine the temperature distribution in the slab as a function of time. The analytic solution for this problem is given by Carslaw and Jaeger (1959). The problem as formulated is attributed to Avdonin (1964) and has been previously used for verification of computer codes by a number of authors (Ross et al., 1982; Eyler and Budden, 1984; Updegraff, 1989; Magnuson et al., 1990).

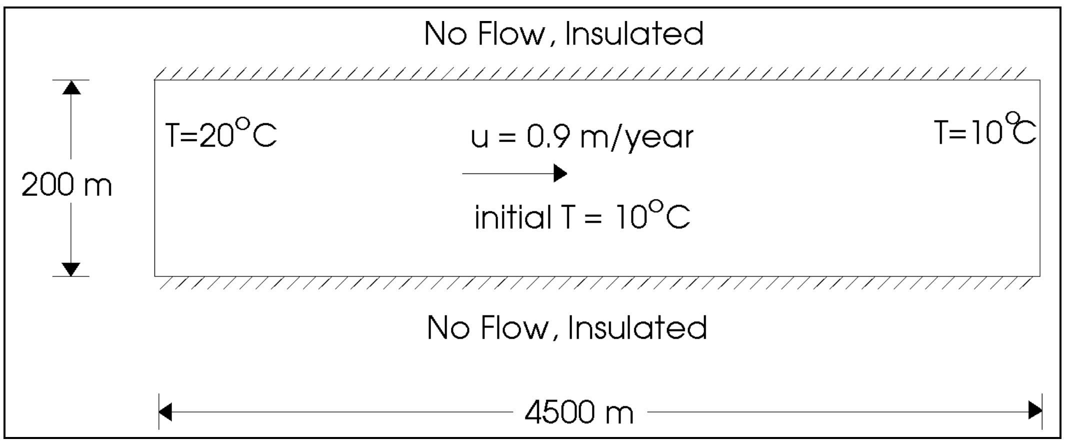

FIGURE 2.2.1: SCHEMATIC ILLUSTRATION OF PROBLEM V2

Initial Conditions Horizontal flow velocity is uniform and constant at 0.90 m/yr and the initial temperature is 10 C everywhere.

Boundary Conditions Both the boundaries are at fixed temperature. The temperature at the left (x=0) boundary is fixed at 20 C and that at the right (x=4500) boundary is at 10 C.

Properties The hydraulic and thermal properties for this problem are summarized in Table 2.2.1 below.

TABLE 2.2.1: Hydraulic and Thermal Properties for Problem V2

Property	Value
Fluid density (kg/m^3)	1,000
Specific heat of fluid (J/kg-K)	4,185
Thermal conductivity of fluid (J/m-yr)	2.05×10^7
Rock density (kg/m^3)	2,780
Specific heat of rock (J/kg-K)	850
Thermal conductivity of rock (J/m-yr)	5.00×10^7
Porosity	0.001
Longitudinal dispersivity (m)	2.0
Transverse dispersivity (m)	0.0

Computational Details A uniform grid consisting of 181 nodes in the x-direction is used. The node spacing is 25 m. The problem is one-dimensional and therefore independent of node spacing in the y-direction; a grid size of unity is assumed by default. The simulations are performed for a time period of 2,000 years in steps of 0.25 years. The PORFLOW input commands for this problem are shown in Table 2.2.2.

TABLE 2.2.2: Input Commands for Problem V2

```
***********************************************************************
TITLe One-Dimensional Heat Transport by Unidirectional Flow
***********************************************************************
////  Carslaw, H.S. and J.C. Jaeger, 1959. Conduction of Heat in Solids
////  Oxford Press 2nd Ed.,  pp. 387-389
***********************************************************************
/
GRID 181 nodes in the X direction
COORdinate X  minimum = 0.0  max = 4500.0
/
DENSity = 1000.0
FLUId: SPECific heat = 4185.0
FLUId: thermal CONDuctivity = 2.05E+07
/
ROCK density = 2780
ROCK porosity = 0.001
THERmal Ce = 850.0  Ke = 5.0E+07  L.D. = 2.0  T.D. = 0.0
/
SET U = 0.90 everywhere
SET T = 10.0
/
BOUNdary conditions for T: index -1, value = 20.0
BOUNdary conditions for T: index +1, value = 10.0
/
MATRix sweep X direction for T; method = ADI
/
DIAGnostic node (20,1) every 10 steps
SELEct window from (1,1) to (181,1) interval (2,1)
OUTPut for SELEcted window
SAVE T on 'V2.ARC'
/
SOLVe for  500 years in steps of 0.25 years
SAVE NOW
/
SOLVe for  500 more years in steps of 0.25 years
SAVE NOW
/
SOLVe for 1000 more years in steps of 0.25 years
/
END
```

Comparison Solution The analytic solution for this boundary-value problem is given by Carslaw and Jaeger (1959; p. 388). A subroutine published by van Genuchten and Alves (1982, p. 115) is used to compute the product of the exponential and complimentary error functions which are required to evaluate the solution.

PORFLOW™ Output The temperature at 500, 1000, and 2000 years is generated for comparison with the analytic solution.

Results & Discussion The PORFLOW simulation results and the analytic solution are shown in Figure 2.2.2 in a comparative format. This figure shows that the PORFLOW results (symbols) are nearly identical to the analytic solution (solid line). For the grid size and time step used in this problem, the maximum grid Peclet and Courant numbers are 1.6 and 0.3, respectively. Based on these results, PORFLOW does an excellent job of simulating advection and dispersion of thermal energy.

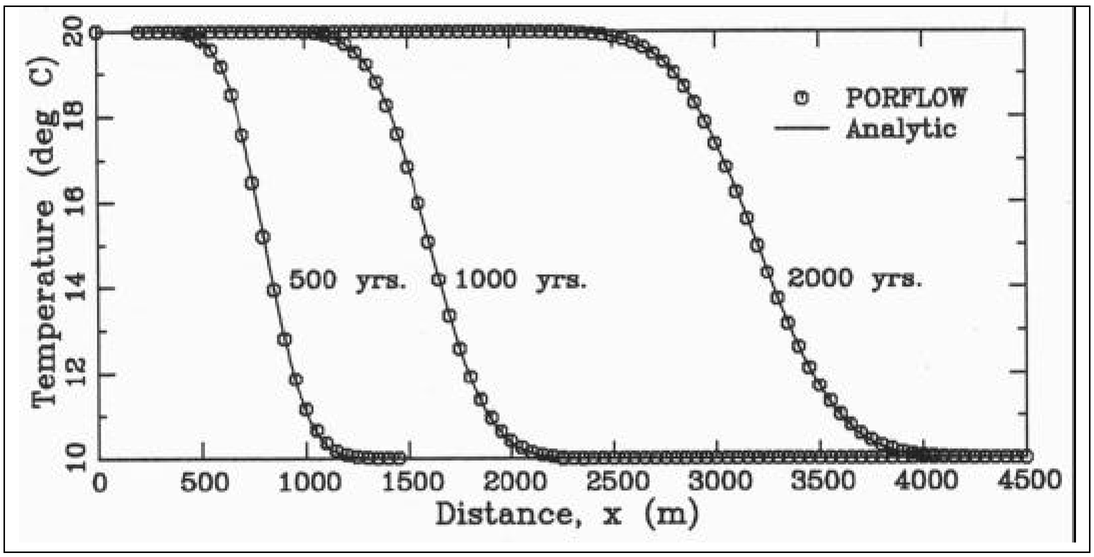

FIGURE 2.2.2: TEMPERATURE PROFILE AT SELECTED TIMES

2.3 PROBLEM V3: THEIS SOLUTION FOR TRANSIENT DRAWDOWN

Problem Statement

This classic problem simulates the transient drawdown of pressure head due to pumping in a confined aquifer of constant thickness that is fully penetrated by a well (Figure 2.3.1). The problem was originally posed and solved by Theis (1935). The objective of this test is to determine the pressure head as a function of distance from the well. In accordance with Theis's solution, the flow is assumed to be purely radial. The thickness of the well is taken to be unity. The computational domain stretches to a radius of 2,000 m, a distance adequate to prevent the effects of pumping from reaching the outer boundary of the cylinder during the period of simulation.

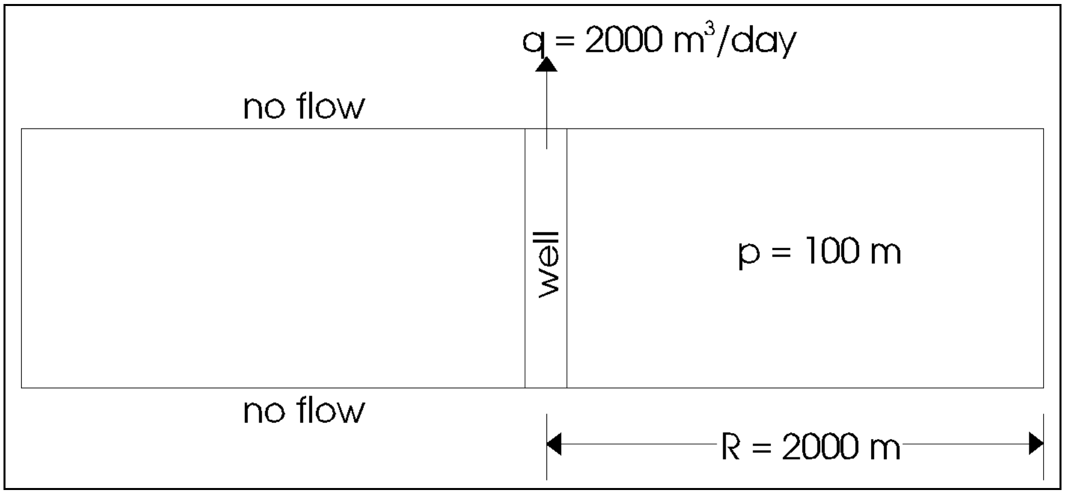

FIGURE 2.3.1: SCHEMATIC ILLUSTRATION OF PROBLEM V3

Initial Conditions

Initially the pressure is uniform everywhere at a value is 100 m.

Boundary Conditions

The pressure is held at its initial value of 100 m at the right boundary (r=2000). The well is producing at a rate of 2,000 m^3/day. Since the well radius is set at 0.25 m, this results in a constant flux of 1273.24 m^3/day per unit radian per square meter of the well surface at the left boundary of the computational domain.

Properties

The soil is isotropic and homogeneous. The hydraulic conductivity is 300 m/day and the specific storage is 0.002 m^{-1}.

Computational Details

The solution method implemented used a radial symmetry configuration around a vertical well. An arc of one radian through the entire aquifer thickness is simulated. In the radial (r) direction, 69 grids with variable grid spacing are used. The grid spacing near the center of the well is 0.5 m and it gradually increases to 200 m near the outer periphery. In the axial (x) direction only one grid element is used; by default, its thickness is unity. The problem is solved in the transient mode for 0.5 days in steps of 0.001 day. The PORFLOW input commands for this problem are shown in Table 2.3.1.

Comparison Solution

The analytic solution for the transient flow in response to pumping a horizontal, confined aquifer is well known and consists of a simple mathematical expression. It was derived by Theis (1935). The solution assumes a purely radial flow in an aquifer of infinite lateral extent with a constant thickness.

PORFLOW™ Output

The pressure head profile versus distance is compared after 12 hours of pumping.

Results & Discussion

The PORFLOW pressure head results (symbols) are compared to those from the Theis analytic solution (solid line) in Figure 2.3.2. The results show good agreement. Qualitatively, the two sets of results are indistinguishable from each other.

TABLE 2.3.1: Input Commands for Problem V3

```
*********************************************************************
TITLe Theis Solution for Transient Drawdown
*********************************************************************
////  Theis, C.V., 1935. The Relation Between the Lowering of the
////  Piezometric Surface and the Rate and Duration of Discharge of a
////  Well Using Groundwater Storage, Trans. Amer. Geophys. Union, 2,
////  p. 519-524.
*********************************************************************
/
GRID 1 by 69
COORdinate R
      0.0     .50     1.0      2.0    3.5    5.0     7.5
     10.0    15.0    20.0     25.0   30.0   35.0    40.0
     45.0    50.0    55.0     60.0   65.0   70.0    75.0
     80.0    85.0    90.0     95.0  100.0  110.0   120.0
    130.0   140.0   150.0    160.0  170.0  180.0   190.0
    200.0   220.0   240.0    260.0  280.0  300.0   320.0
    340.0   360.0   380.0    400.0  440.0  480.0   520.0
    560.0   600.0   640.0    680.0  720.0  760.0   800.0
    850.0   900.0   950.0   1000.0 1100.0 1200.0  1300.0
   1400.0 1500.0 1600.0    1700.0 1800.0 2000.0
/
HYDRaulic properties  S = 0.002, kx = 300 m/day, Ky = 300 m/day
/
SET P = 100.0 everywhere initially
/
BOUNdary conditions for P: index -2, FLUX  = -1273.24
/
MATRix sweep Y direction
/
DIAGnostic node (1,26) every 50 steps
OUTPut V, P, H
SAVE on 'V3.ARC' H only
/
SOLVe for 0.5 days in steps of 0.001 days
/
END
```

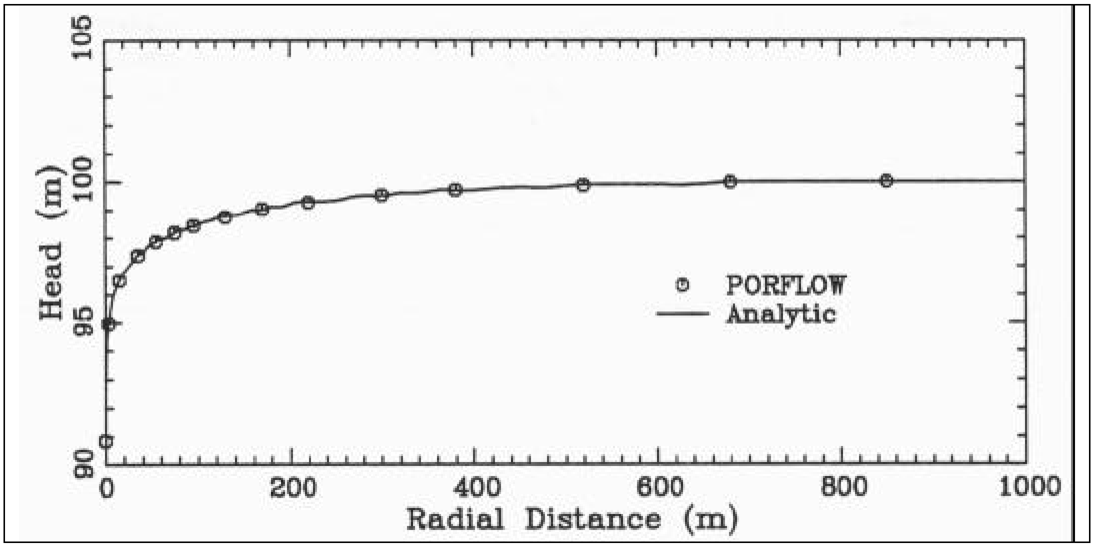

FIGURE 2.3.2: PROFILE OF PRESSURE HEAD

2.4 PROBLEM V4: FINITE CYLINDER WITH HEAT SOURCE

Problem Statement

This problem concerns a finite cylinder with heat production at a constant rate per unit time per unit volume. The schematic for the problem is shown in Figure 2.4.1. Both the axial length and the radius of the cylinder are unity. The surface of the cylinder is kept at zero temperature. The objective of this test is to determine the steady state distribution of temperature throughout the cylinder. The problem is described and solved in Carslaw and Jaeger (1959).

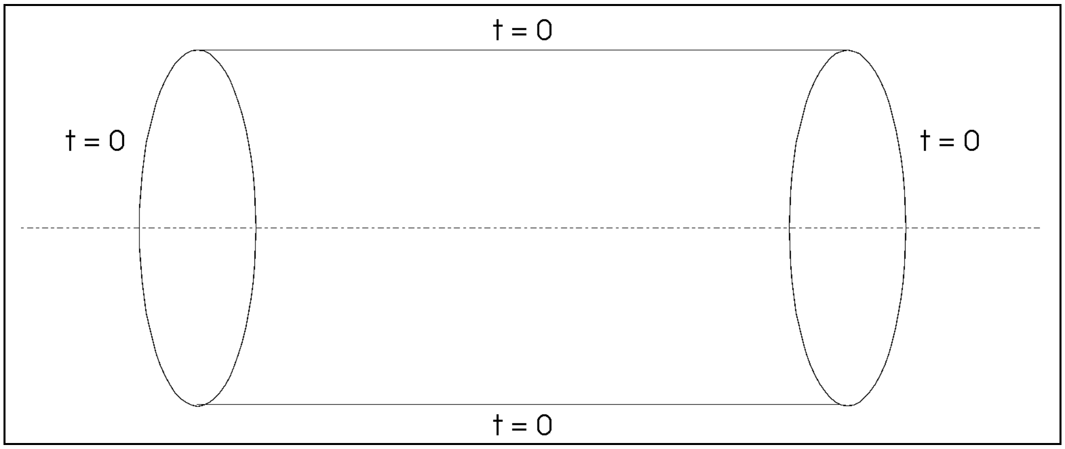

FIGURE 2.4.1: SCHEMATIC ILLUSTRATION OF PROBLEM V4

Initial Conditions

No initial conditions are required since the problem is a steady state problem. The computational procedure starts with the default initial value of zero temperature.

Boundary Conditions

The temperature of the exterior surfaces of the cylinder is kept at 0. The left boundary (at r=0) is adiabatic due to conditions of symmetry.

Properties

For ease of comparison with the analytic solution, all properties are in non-dimensional units. The density, specific heat and thermal conductivity of the fluid are all set to unity. The rock porosity is set to unity.

Sources

The heat is generated throughout the bulk of the cylinder. The rate of heat generation is constant at a rate of 4 non-dimensional units.

Computational Details

A 22 by 22 grid is used in the axial (x) and the radial (r) directions. The grid spacing is uniform and equal to 0.05 in both directions. The problem is solved in the steady state mode for a total of 200 iterative steps. The PORFLOW input commands for this problem are shown in Table 2.4.1.

Comparison Solution

The analytic solution for this problem is given by Carslaw and Jaeger (1959, p. 223-224).

PORFLOW™ Output

A contour plot of temperature after steady state has been reached is produced for comparison with the analytic solution.

Results & Discussion

Figure 2.4.2 shows steady state temperature contours for the analytic solution (solid line) and PORFLOW (symbols). The graphical comparison shows that the PORFLOW solution is in excellent agreement with the analytic solution.

TABLE 2.4.1: Input Commands for Problem V4

```
**********************************************************************
TITLe Finite Cylinder with Heat Source
**********************************************************************
////  Carslaw, H.S. and J.C. Jaeger. 1959. Conduction of Heat in Solids
////  Oxford Press 2nd Ed.,  p. 223-224
**********************************************************************
/
GRID 22 by 22
COORdinate R range = 1
/
BOUNdary conditions for T ib=-1, INTErface value = 0.
BOUNdary conditions for T ib= 1, INTErface value = 0.
BOUNdary conditions for T ib=-2, GRAD=0.
BOUNdary conditions for T ib= 2, INTErface value = 0.
/
SOURce for T: constant at 4 per unit VOLUme everywhere
/
DENSity 1
ROCK DENSity = 1
ROCK POROsity = 1
THERmal props cp = 1, kt = 1
FLUId SPECific heat = 1
FLUId thermal CONDuctivity = 1
/
DIAGnostic node at 12,2 print every 20 steps
OUTPut in NARRow mode
SAVE on 'V4.ARC' T only
/
SOLVE in steady mode max 200 steps min 200
/
END
```

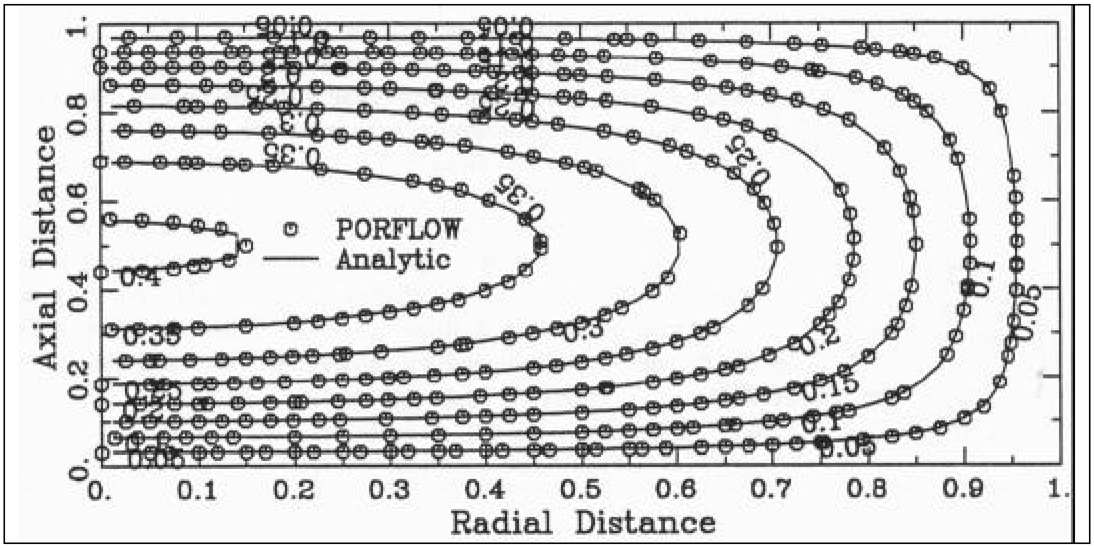

FIGURE 2.4.2: CONTOURS OF TEMPERATURE

2.5 PROBLEM V5: CONVECTIVE HEAT TRANSFER IN REGIONAL FLOW

Problem Statement

The schematic for this problem is shown in Figure 2.5.1. It represents a homogenous, isotropic region with a geothermal gradient. The geothermal heat flux enters the region from the bottom and leaves through a constant temperature surface at the top. The region is bounded on both vertical faces with topological divides so that there is no major lateral flow. A recirculating flow pattern is induced due to lateral variations in the water table. The problem is solved in a non-dimensional mode, and the computational domain is 100 units in each direction. The objective of the problem is to determine the steady state pressure and temperature distributions in the domain of interest. This problem was formulated and solved by Domenico and Palciauskas (1973).

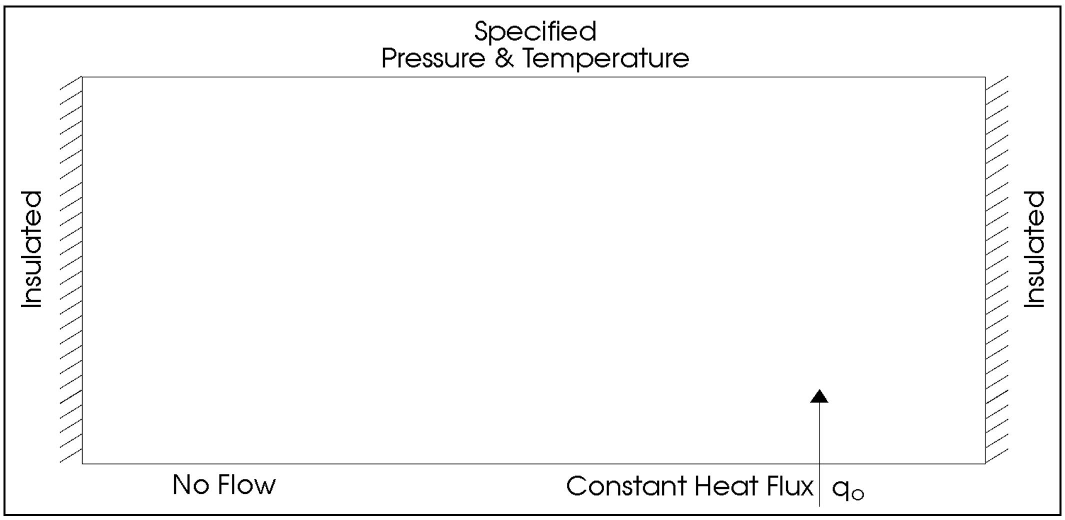

FIGURE 2.5.1: SCHEMATIC ILLUSTRATION OF PROBLEM V5

Initial Conditions

No initial conditions are required since the problem is a steady state problem. The computational procedure starts with the default initial value of zero for the state variables.

Boundary Conditions

The pressure at the upper (y=100) boundary is specified as the cosine function of distance:

$$P = -\cosh(\pi)\cos\left(\frac{\pi x}{100}\right) . \qquad (2.5.1)$$

All other boundaries are no-flow boundaries. The temperature at the upper boundary is fixed at zero. A temperature gradient of -0.0002 is specified at the lower boundary (y=0) to simulate the incoming geothermal heat flux. The left (x=0) and the right (x=100) boundaries are adiabatic.

Properties

For ease of comparison with the analytic solution, all properties are in non-dimensional units. The fluid and soil density, specific heat and thermal conductivity, and the soil porosity are all set to unity. The dispersivities are zero. The soil is isotropic and the hydraulic conductivity is set to 0.01. The specific storage is set to unity; since the problem is solved in the steady state mode, this parameter has no effect on the solution.

Computational Details

The problem is simulated using a grid of 41 by 41. The grid spacing in both direction is 2.5 units. In the horizontal (x) direction the grid is set in such a manner that the outer boundaries of the extreme elements are located at 0 and 100. In the vertical (y) direction the element boundary for the first element is located at 0 whereas the last grid node is located at 100. The problem is solved in the steady state mode for 2000 steps. The PORFLOW input commands for this problem are shown in Table 2.5.1.

TABLE 2.5.1: Input Commands for Problem V5

```
****************************************************************************
TITLe Coupled Flow and Heat Transfer in Regional Flow
****************************************************************************
////  Domenico, P.A. and V.V. Palciauskas, 1973. Theoretical Analysis
////  of Forced Convective Heat Transfer in Regional Ground-Water Flow,
////  Geological Society of America Bulletin, Vol. 84, p. 3803-3814,
////  December 1973.
****************************************************************************
/
GRID is 41 by 41
/
COORdinate X
   -2.5    2.5    5.0    7.5   10.0   12.5   15.0   17.5   20.0   22.5   25.0
          27.5   30.0   32.5   35.0   37.5   40.0   42.5   45.0   47.5   50.0
          52.5   55.0   57.5   60.0   62.5   65.0   67.5   70.0   72.5   75.0
          77.5   80.0   82.5   85.0   87.5   90.0   92.5   95.0   97.5          102.5

/
COORdinate Y
   -2.5    2.5    5.0    7.5   10.0   12.5   15.0   17.5   20.0   22.5   25.0
          27.5   30.0   32.5   35.0   37.5   40.0   42.5   45.0   47.5   50.0
          52.5   55.0   57.5   60.0   62.5   65.0   67.5   70.0   72.5   75.0
          77.5   80.0   82.5   85.0   87.5   90.0   92.5   95.0   97.5  100.0
/
/**************** Rock properties
ROCK DENSity = 1
ROCK POROsity = 1
THERmal properties: specific heat = 1, thermal conductivity = 1
HYDRaulic properties: ss = 1, hydraulic conductivity = 2*0.01
/
/**************** Fluid properties
DENSity = 1
FLUId SPECific heat = 1
FLUId thermal CONDuctivity = 1
/
/**************** Boundary for pressure
BOUNdary for P index -1: GRADient 0
BOUNdary for P index +1: GRADient 0
BOUNdary for P index -2: GRADient 0
BOUNdary for P index +2: P =  -11.591957 * COS ( 0.0314159 * X )
/
/**************** Boundary for temperature
BOUNdary for T index -1: GRADient 0
BOUNdary for T index +1: GRADient 0
BOUNdary for T index -2: GRADient -0.0002
/
DIAGnostics at 11,11 every 10 steps
Output P and T only
SAVE on file 'V5.ARC' T and H
/
SOLVe in STEAdy mode for 2000 minimum of 2000
/
END
```

Comparison Solution

An approximate analytic solution for this problem has been derived by Domenico and Palciauskas (1973). The solution relies upon a series expansion which is obtained by a perturbation method. It should be noted that (Equation 15 of Domenico and Palciauskas) has some typographical errors. Also the results shown in Figure 3 of their paper are in error because the terms in the series solution which are ignored as being negligible, in fact grow and become dominant for the selected parameter values. Hence the PORFLOW solution could be compared with the analytic solution only for a small enough ratio of the hydraulic conductivity to thermal diffusivity (=0.01).

PORFLOW™ Output

The steady-state total pressure and temperature distributions are generated for comparison with the approximate analytic solution.

Results & Discussion

Figures 2.5.2 and 2.5.3 show plots of the steady state analytic solution (solid line) versus the PORFLOW results (symbols) for both total head and temperature, respectively. They indicate an excellent agreement in the results.

FIGURE 2.5.2: CONTOURS OF HYDRAULIC POTENTIAL

FIGURE 2.5.3: CONTOURS OF TEMPERATURE

2.6 PROBLEM V6: THREE-DIMENSIONAL CONTAMINANT TRANSPORT

Problem Statement

This test case simulates the transport of a contaminant in a three-dimensional domain. The physical setting is a homogeneous and isotropic confined aquifer shown in Figure 2.6.1. A horizontal source area on the upper surface of the computational domain continuously releases a contaminant into the aquifer which is initially free of the contaminant. The amount of water brought in with the contaminant is negligible compared to the amount of water flowing through the aquifer. The flow within the aquifer is unidirectional and parallel to the longitudinal (x) axis. Advective transport moves the contaminant in the downstream direction, while dispersive movement causes spreading of the contaminant in all directions. The problem is symmetric in the lateral (y) direction therefore only half of the total domain is simulated. The depth of the aquifer is 56 m. The computational domain extends 3,700 m in the longitudinal and 800 m in the lateral direction. The source zone is located just below the surface and its center is 700 m downstream at the plane of symmetry.

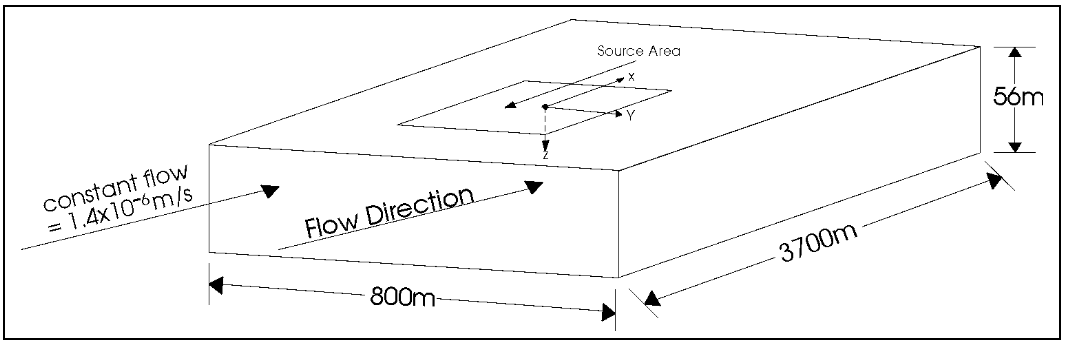

FIGURE 2.6.1: SCHEMATIC ILLUSTRATION OF PROBLEM V6

Initial Conditions The velocity component in the x-direction is 1.4×10^{-6} m/s everywhere. The initial contaminant concentration is 0 by default.

Boundary Conditions The flow entering the recharge boundary at left (x=-700) is free of any contaminant; thus the concentration at that boundary is zero. All other boundaries are set to conditions of zero flux.

Properties The transport properties for this problem are summarized in Table 2.6.1. The soil and fluid density do not affect the simulations since the distribution coefficient is zero and the fluid density is constant.

TABLE 2.6.1: Transport Properties for Problem V6

Property	Value
Porosity	0.10
Distribution coefficient (m^3/kg)	0.0
Molecular diffusivity (m^2/s)	0.0
Longitudinal dispersivity (m)	91.0
Transverse dispersivity (m)	20.0

Sources The source is located just below the top surface. Since the problem is symmetric in the y-direction, only half of the problem domain is simulated. The center of the source is located 700 m downstream (x=0) and at the plane of symmetry (y=0). The source zone is 0.10 m in depth and is 200 m in the x- and 100 m in the y-direction. The rate of contaminant release is constant at 2.5×10^{-4} kg/(m^3 s).

Computational Details A grid of 65x26x20 (33,800 nodes) in the x-, y- and z- directions, respectively, is used. Variable node spacing is used in each direction to provide finer resolution near the source area. The minimum and maximum node spacings in the x, y, and z directions are: 10 and 300, 20 and 110, and 0.1 and 8 m, respectively. The higher-order CONDIF scheme is used to provide better accuracy. The test problem is solved in the transient mode for 1.5768×10^{8} seconds (5 years) in constant steps of 3.1536×10^{4} seconds (0.001 year). The PORFLOW input commands for this problem are shown in Table 2.6.2.

TABLE 2.6.2: Input Commands for Problem V6

```
**************************************************************************
TITLe Three-Dimensional Transport of a Contaminant
**************************************************************************
////  Codell, R.B., T.K. Key and G. Whelan, 1982. A Collection of
////  Mathematical Models for Dispersion in Surface Water and
////  Groundwater, NUREG-0868, Division of Engineering, Office of
////  Nuclear Reactor Regulation, Washington, D.C.
**************************************************************************
/
GRID  65 by 26 by 20
/
COORdinate X user specifiied values:
  -700.  -500.  -370.  -280.  -220.  -180.  -150.  -130.  -110.   -90.
   -70.   -50.   -40.   -30.   -20.   -10.     0.    10.    20.    30.
    40.    50.    70.    90.   110.   130.   150.   170.   190.   210.
   240.   270.   300.   330.   360.   400.   440.   480.   520.   560.
   600.   650.   700.   750.   800.   850.   900.   950.  1000.  1075.
  1150.  1225.  1300.  1375.  1450.  1525.  1600.  1700.  1800.  1900.
  2050.  2200.  2400.  2700.  3000.
/
COORdinate Y user specifiied values:
   -10.    10.    30.    50.    70.    90.   110.   130.   150.   170.
   190.   210.   230.   250.   275.   300.   325.   360.   400.   440.
   480.   520.   570.   620.   690.   800.
/
COORdinate Z user specified values:
   -56.   -44.   -36.   -29.    -22.   -17.    -12.    -9.     -6.     -4.
   -3.    -2.   -1.5   -1.0   -0.75  -0.50  -0.25  -0.15   -0.05   0.05
/
ROCK POROsity = 0.1
TRANsport  kd = 0., md = 0, Ld = 91.0, Td = 20.0
/
LOCATE (10,1,19) to (24,6,19)   $ Represents the Contaminant Source
SOURce C is constant at 2.5E-4 VOLUmetric g/sec/cu m in SELEcted area
/
SET U to 1.4E-06
/
BOUNdary conditions for C: all boundaries at zero FLUX = 0.
BOUNdary conditions for C: -1: value = 0.0
/
PROPerty GEOMetric
/
INTEgration for C by CONDIF
/
Diagnostic node (27,4,19) output every 5 steps
HISTory at (27,4,19)  (27,4,2)  (27,16,19)
HISTory of C only on 'V6.HIS' every 5 steps
OUTPut OFF
SAVE only C on 'V6.ARC'
/
SOLVe for C for 1.5768E+8 seconds in steps of 3.1536E+4
/
END
```

Comparison Solution

A quasi-analytic solution for this problem is available in a collection of mathematical models published by Codell et al. (1982). One of these, GRDFLX, was modified by Rood et al. (1989) to solve the specific problem described here. This modified code was used to generate the comparative solution for verification of the PORFLOW results.

PORFLOW™ Output

The output consists of contaminant concentration everywhere in the computational domain 5 years after the start of the contaminant release. Additionally, time histories of contaminant concentration are generated at three locations with (x,y,z) coordinates: (150, 50, 0.05), (150, 50, 44) and (150, 300, 0.05) meters.

Results & Discussion

The contaminant distributions at the surface at the end of the 5 years, for both PORFLOW and the quasi-analytic solution, are shown in Figure 2.6.2. The results from the half-domain are mirrored across the y-axis to create the complete plume. As can be seen by the contours in Figure 2.6.2, the results are qualitatively and quantitatively in good accord.

The time histories of contaminant concentration at three selected locations are shown in Figure 2.6.3. For this three-dimensional, transient problem, the PORFLOW results compare well with the analytic solution. However, some differences between the two are noticed. For the two locations close to the centerline, near the top and the bottom of the aquifer, the two sets of results show extremely good agreement. The history for the location laterally away from the centerline shows a very slight deviation between the PORFLOW results and the analytic solution.

The maximum Peclet number for the grid employed is 5.5 and the maximum Courant number is 0.04. Since the Peclet number is almost three times the desired value of 2, some numerical errors may be present. These results could be improved by smaller grid size. However, the results are sufficiently accurate for verification purposes, and it was not considered necessary to do so.

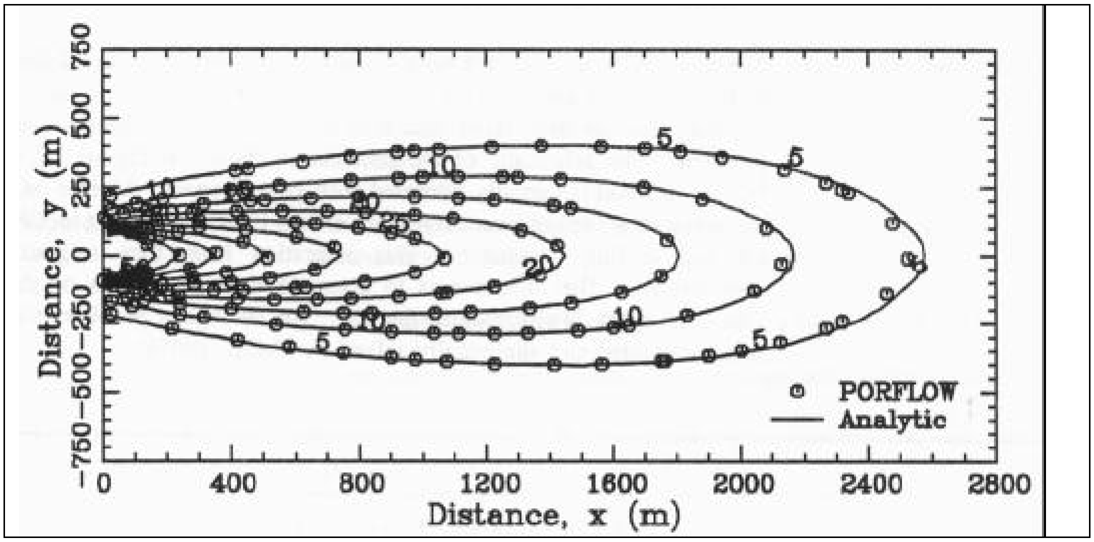

FIGURE 2.6.2: CONTOURS OF CONCENTRATION AT 5 YEARS

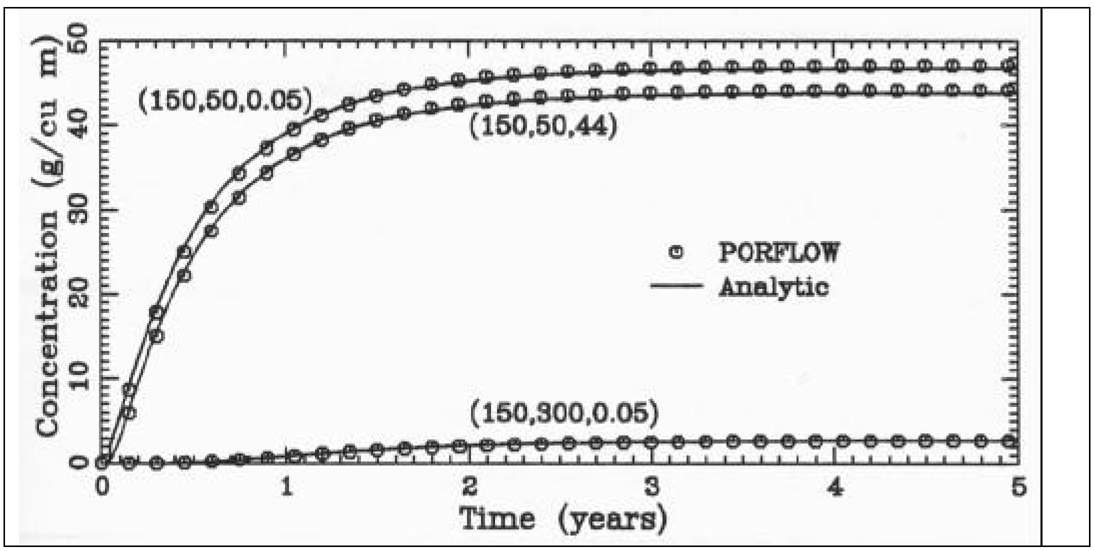

FIGURE 2.6.3: TIME HISTORY OF CONCENTRATIONS AT 3 POINTS

2.7 PROBLEM V7: PHILIP'S HORIZONTAL UNSATURATED FLOW

Problem Statement

The physical setting for this problem is a 20 cm long, horizontal slab of homogeneous and isotropic soil. The vertical extent of the slab is considered to be infinite so that it is essentially a one-dimensional problem. The schematic of the problem is shown in Figure 2.7.1. Initially the soil is partially saturated with ground water. At time t=0, the pressure at the left boundary of the slab is increased so that locally the soil is fully saturated. This saturation front then migrates downstream. The objective is to compute the propagation of the saturation front downstream in the soil. An analogous problem was first formulated and analytically solved by Philip (1957a).

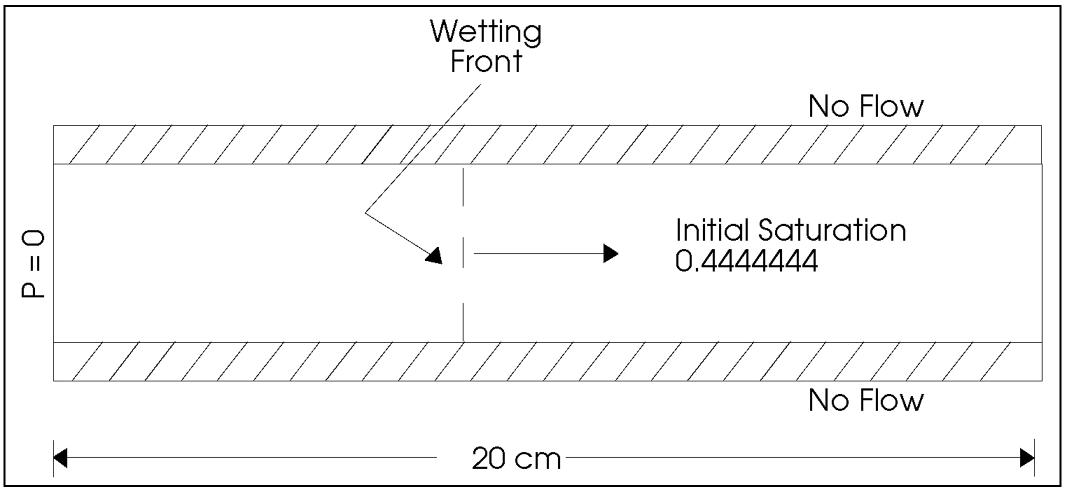

FIGURE 2.7.1: SCHEMATIC ILLUSTRATION OF PROBLEM V7

Initial Conditions

Initial saturation is set to 0.444444 everywhere.

Boundary Conditions

The pressure head at the left boundary is held fixed at zero; this corresponds to full saturation. By default, the pressure at the right boundary is held at its initial value corresponding to the initial saturation.

Properties

The hydraulic properties and the soil-moisture characteristic are summarized in Tables 2.7.1 and 2.7.2, respectively.

TABLE 2.7.1: Hydraulic Properties for Problem V7

Property	Value
Porosity	0.45
Hydraulic Conductivity (cm/s)	1.157×10^{-5}
Specific storage (cm^{-1})	0.0

TABLE 2.7.2: Soil Moisture Characteristic for Problem V7

Saturation	Capillary Pressure (cm)	Relative Conductivity
0.3333	100.	0.0
1.0000	0.0	1.0

Computational Details

The problem is simulated using a non-uniform grid distribution. The number of nodes in the horizontal (x) direction is 62. The minimum grid node spacing is 0.074 cm and the maximum is 1 cm. Since the problem is one-dimensional, one grid element, with a default thickness of unity, is used in the y-direction. The propagating front is simulated for a time period of 9,504 seconds (0.11 days). Initial time step is 0.1 seconds which, in two stages, is increased to 10 seconds in a geometric progression with a progression ratio of 1.1. The PORFLOW input commands for this problem are shown in Table 2.7.3.

TABLE 2.7.3: Input Commands for Problem V7

```
***********************************************************************
TITLe Philip's Solution for Horizontal Unsaturated Flow
***********************************************************************
////  Philip, J.R., 1957. Numerical Solution of Equations of the
////  Diffusion Type with Diffusivity Concentration-Dependent,
////  Transactions, Faraday Society 51:885-892.
***********************************************************************
/
GRID 52 in the X direction
COORdinate X
  0.       0.302   0.376   0.509   0.726   0.741   1.003   1.249
  1.440    1.483   1.744   1.950   2.107   2.237   2.406   2.780
  2.852    3.059   3.290   3.403   3.719   3.972   4.141   4.558
  4.572    4.970   5.173   5.379   5.479   5.785   6.112   6.190
  7.004    7.211   7.418   7.840   8.276   8.334   8.733   9.221
  9.764   10.407  11.285  12.0    13.0    14.0    15.0    16.0
 17.0     18.0    19.0    20.0
/
GRAVity is 0, 0
/
ROCK POROsity = 0.45
HYDRaulic properties: effective storativity = 0.;  2*1.157e-5 cm/sec
MULTiphase CONDuctivity, 2 sets in TABLe (S1,Kr): (0.3333,0)    (1,1)
MULTiphase with 2 sets in TABLe format (S1,Pcap): (0.3333,100) (1,0)
/
SET initial S to 0.444444 everywhere
/
BOUNdary for P  at NODE boundary -1  head = 0. cm
/
CONVergence of P is LOCAl criteria = 1.0e-5, iterations = 100
/
PROPerties at interfaces determined by ARIThmetic mean
/
DIAGnostic P and S at (3,1) every 10 steps
/
SOLVe for  864 sec in steps of 0.1, multiplier = 1.1, max time step = 5
OUTPut P and S NOW
SAVE   S NOW on file 'V7.ARC'
/
SOLVe for 4320 sec in steps of 5.0, multiplier = 1.1, max time step = 10
OUTPut NOW
SAVE NOW
/
SOLVe for 4320 sec
/
END
```

Comparison Solution

A semi-analytic solution for this problem was derived by Philip (1957a); this solution is available in the INFIL computer code by El-Kadi (1987).

PORFLOW™ Output

The saturation profiles at 864, 5,184 and 9,504 seconds are obtained for comparison against the analytic solution. These times correspond, respectively, to 0.01, 0.06 and 0.11 days.

Results & Discussion

Figure 2.7.2 shows plots of saturation for Philip's solution (solid line) versus the PORFLOW results (symbols) at three selected times. As is clear from this figure, there is an excellent match between the two sets of results.

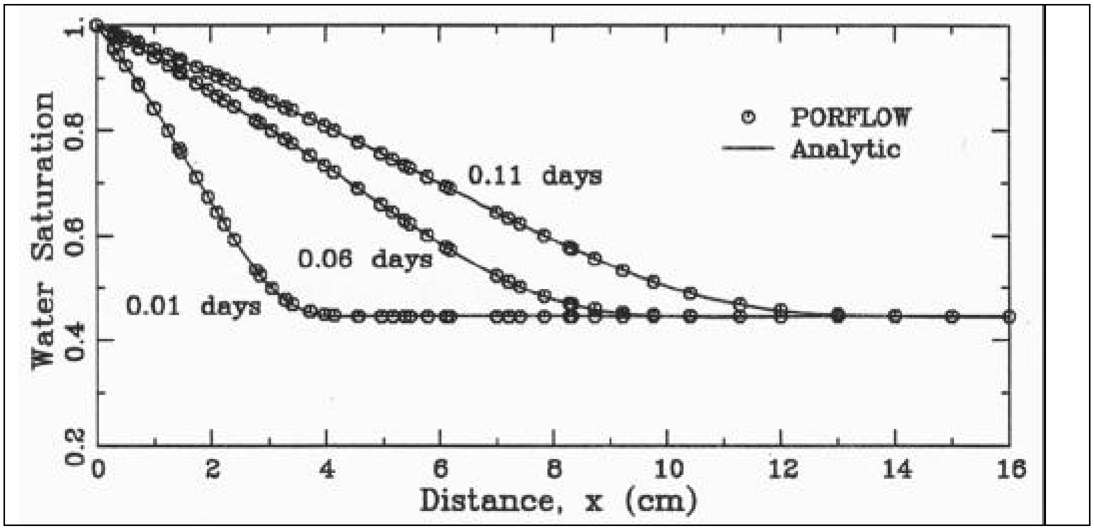

FIGURE 2.7.2: SATURATION PROFILE AT SELECTED TIMES

2.8 PROBLEM V8: PHILIP'S VERTICAL UNSATURATED COLUMN

Problem Statement

The physical setting for this problem is a 15 cm-long, vertical, homogeneous soil column which is shown in Figure 2.8.1. The horizontal extent of the column is considered to be infinite so that it is essentially a one-dimensional problem. The soil is initially partially saturated. At time t=0, the pressure head at the surface is increased so that the soil is fully saturated. Transient infiltration of moisture in the vertical direction results from capillary forces and gravity. The objective of this test problem is to determine the position of the wetting front during vertical infiltration of moisture into an unsaturated soil. An analytic solution for an analogous problem with a propagating front was obtained by Philip (1957b).

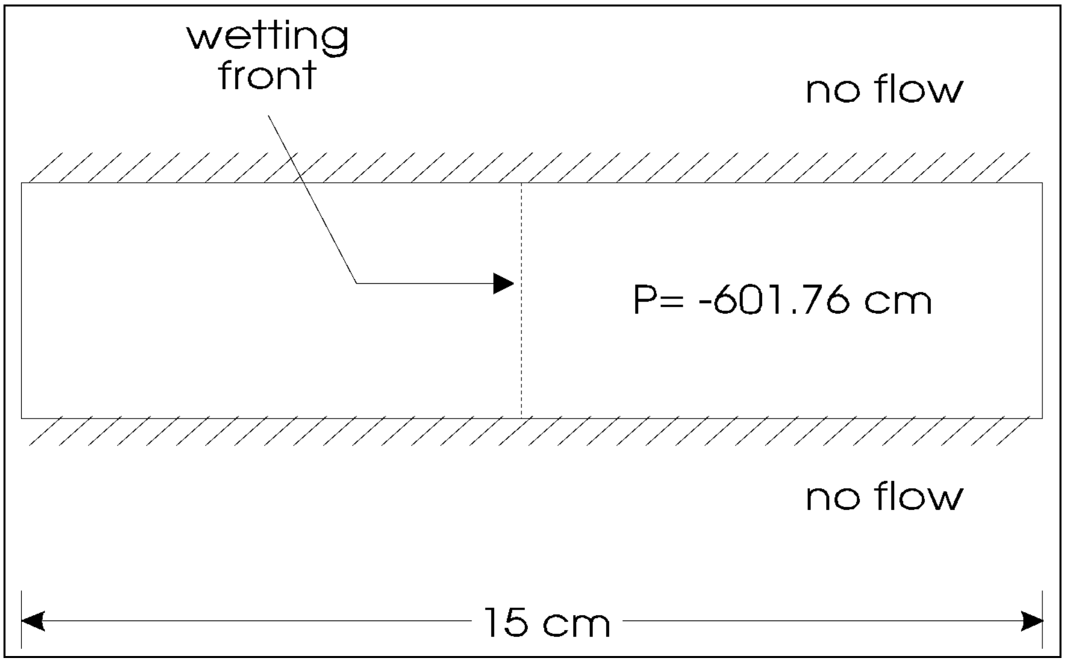

FIGURE 2.8.1: SCHEMATIC ILLUSTRATION OF PROBLEM V8

Initial Conditions

Initial pressure head everywhere is -601.76 cm; this corresponds to an initial saturation of 0.306.

Boundary Conditions

The upper boundary is set to a pressure head of -1 cm which corresponds to a saturation of unity. The pressure at the lower boundary is fixed at its initial value of -601.76 cm.

Properties

The hydraulic properties are given in Table 2.8.1. The soil moisture-characteristic is specified by Equations 2.8.1 and 2.8.2.

TABLE 2.8.1: Hydraulic Properties for Problem V8

Property	Value
Porosity	0.371
Hydraulic Conductivity (cm/hr)	0.04428
Specific Storage (cm^{-1})	10^{-7}

$$S = \frac{739}{739 + [\ln(\psi)]^4} \qquad (2.8.1)$$

$$k_r = \frac{124.6}{124.6 + \psi^{1.77}} \qquad (2.8.2)$$

Computational Details

This problem is simulated with 201 nodes in the vertical (y) direction. The nodes are uniformly distributed and the grid size is 0.075 cm. In the horizontal direction only one element is used; by default, its thickness is unity. The propagating moisture front is simulated for a time period of 2 hours. Initial time step is 0.01 hours which is increased to 0.1 hour in a geometric progression with a progression ratio of 1.001. The convergence criterion is set at 10^{-5} and the maximum number of iterations per time step is set to 200. The PORFLOW input commands for this problem are shown in Table 2.8.2.

TABLE 2.8.2: Input Commands for Problem V8

Comparison Solution

A quasi-analytic solution for this problem was derived by Philip (1957b). This solution is available in the INFIL computer code (El-Kadi, 1987).

PORFLOW™ Output

The output from this test consists of pressure head profile at 2 hours from the start of moisture infiltration.

Results & Discussion

The PORFLOW solution (symbols) is compared with the quasi-analytic solution (solid line) in Figure 2.8.2. The graphical comparison shows that the two are in excellent agreement with each other.

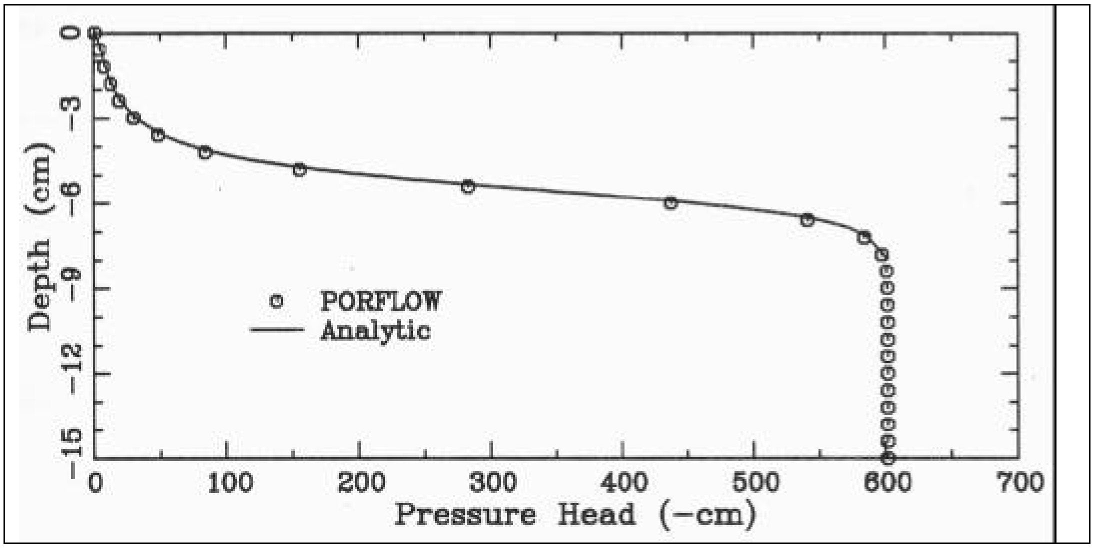

FIGURE 2.8.2: PROFILE OF PRESSURE HEAD

2.9 PROBLEM V9: INFILTRATION FROM A LINE SOURCE

Problem Statement

This test case describes the flow from a single subsurface irrigation pipe that is placed above a shallow water table. Figure 2.9.1 illustrates the physical setting for this problem. Due to the infinite extent of the problem along the direction of the porous pipe, the three-dimensional problem with a line source, illustrated in Figure 2.9.1, is mathematically equivalent to a two-dimensional (2D) problem with a point source. Further, due to symmetry in the lateral (horizontal) direction normal to axis of the pipe, only one-half of the 2D problem needs to be solved. The computational domain for this 2D problem is shown in Figure 2.9.2. The flux from the irrigation system now appears as a point source at the top left corner of the 2D domain. The lateral extent of the computational domain is 61 cm and the depth is 122 cm. The objective is to determine the resulting steady state flow distribution from the pipe into the surrounding soil. An approximate analytic solution for this case is given by Warrick and Lomen (1977).

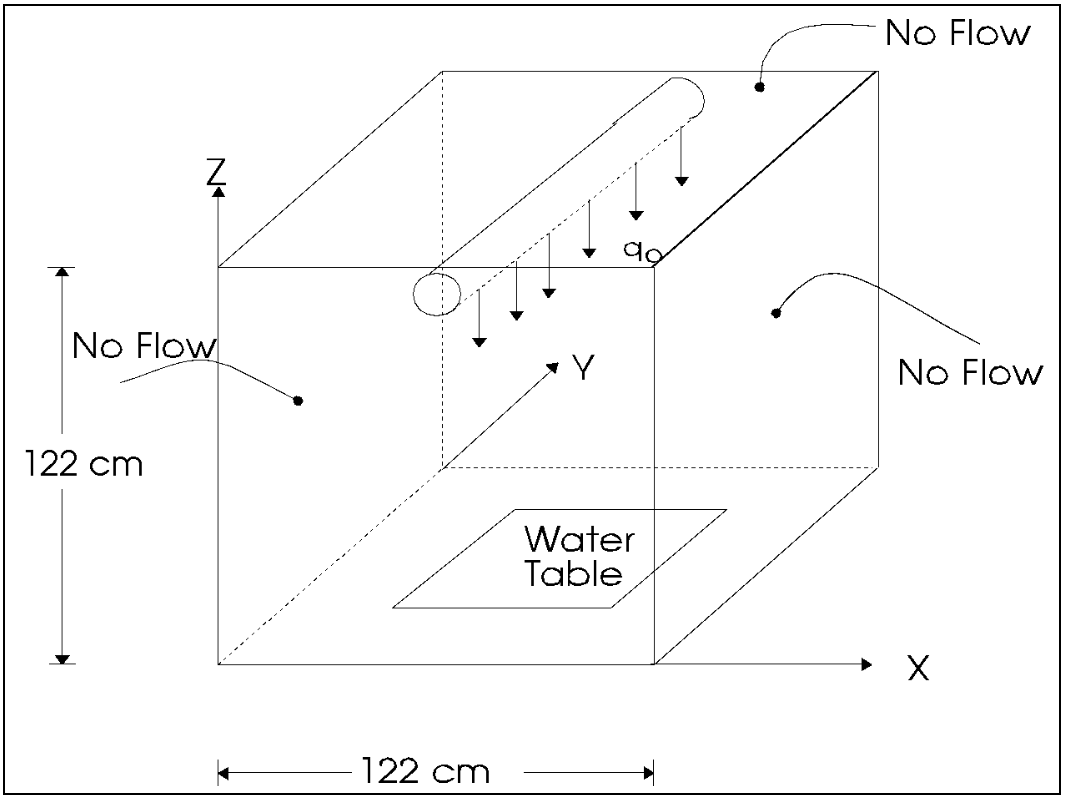

FIGURE 2.9.1: THE 3D PHYSICAL DOMAIN FOR PROBLEM V9

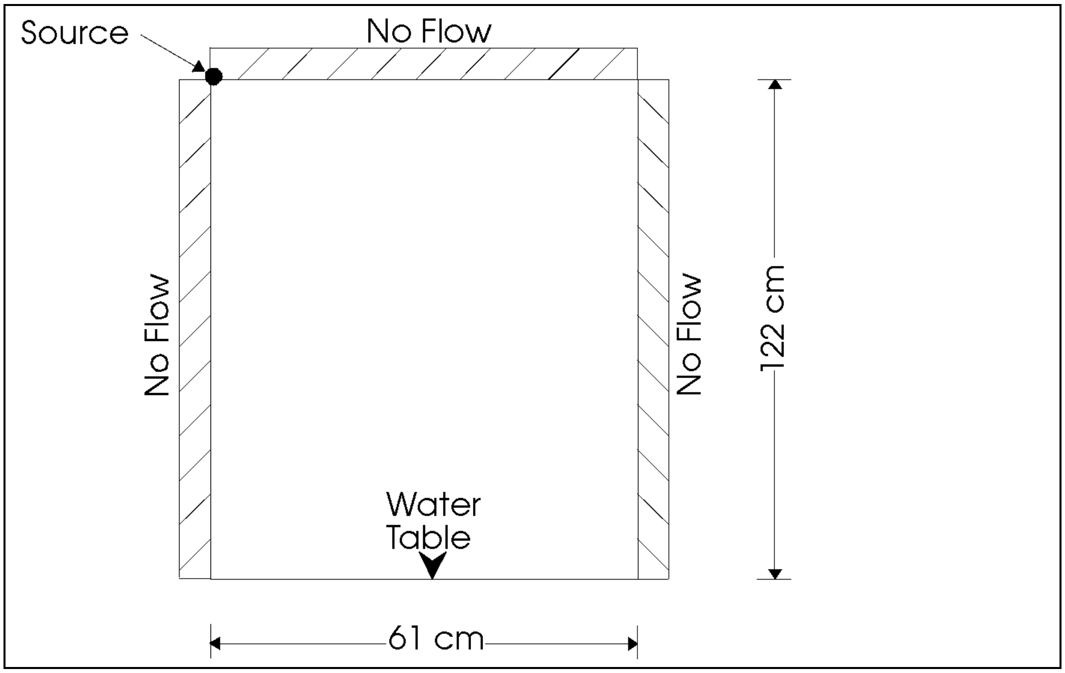

FIGURE 2.9.2: SCHEMATIC ILLUSTRATION OF THE 2D DOMAIN FOR PROBLEM V9

Initial Conditions

This problem is a steady state problem. The final solution is independent of any initial conditions. To provide starting values for the problem, the initial pressure is set to be a linear function of y:

$$P = -\frac{y}{2} \quad . \qquad (2.9.1)$$

Boundary Conditions

The top, the left and the right boundary are all set to be no-flow boundaries. The bottom boundary condition of zero pressure corresponds to the presence of a water table at the bottom of the computational domain.

Properties

The soil is isotropic and homogeneous. Its hydraulic conductivity is 0.00112 cm/s. The specific storage is taken to be zero. The relative conductivity is given by the exponential relation:

$$k_r = \exp(-0.1258 y) ; y > 0 . \tag{2.9.2}$$

The problem, as formulated, is independent of the soil moisture characteristics since it is a steady state problem and the relative conductivity is a direct function of the capillary pressure. For computational purposes, the moisture characteristic is assumed to be given by the Brooks & Corey relation:

$$S = y^{-4} ; y > 1 \tag{2.9.3}$$

Source

The discharge from the irrigation pipe is simulated by a source located at the top left node just inside the computational domain. The discharge rate from the source is set at 0.000525 $cm^3/(cm^3\ s)$; this corresponds to a total discharge rate of 0.00115 $cm^3/(cm^3\ s)$ since only the symmetric half of the problem is being simulated.

Computational Details

This problem is simulated using a uniform grid spacing of 1 cm in the x direction and 2 cm in the y direction. This results in a grid of 63 by 63 nodes. A steady state solution option is used with a specified number of 800 iterative steps. The PORFLOW input commands for this problem are shown in Table 2.9.1.

TABLE 2.9.1: Input Commands for Problem V9

```
************************************************************************
TITLe Infiltration from a Line Source to a Water Table
************************************************************************
////  Warrick, A.W. and D.O. Lomen, 1977. Flow from a Line Source above
////  a Shallow Water Table, Soil Sci. Soc. Am. J., 41, p. 849-852.
************************************************************************
/
GRID 63 by 63
COORdinate X: range 61
COORdinate Y: range 122
/
GRAVity 0, -1 normalized values
/
PROPerty mode for P GEOMetric
HYDRaulic properties ss = 0., kx = 0.00112 ky = 0.00112 cm_per_sec
/
MULTiphase BROOks & Corey option: lambda = 4, alpha = 1
MULTiphase CONDuctivity; EXPOnential n=1, alpha=0.1258
/
SET P as a LINEar function: 0 -0.5 Y
BOUNdary for P ib = -1 FLUX  = 0       $ No flow at left boundary
BOUNdary for P ib = +1 FLUX  = 0       $ No flow at right boundary
BOUNdary for P ib = -2 interface = 0   $ water table
BOUNdary for P ib = +2 FLUX  = 0.
LOCAte (2,999) source at the top
SOURce for P = 0.000525  in SELEcted zone
DIAGnostic node at (20,80) every 100 steps
/
SOLVe in STEAdy mode maximum steps 800 minimum 800
OUTPut U, V, P  in Narrow tabular format
SAVE P on 'V9.ARC'
/
END
```

Comparison Solution	An approximate analytic solution for this problem is given by Warrick and Lomen (1977). The solution is obtained by superposition of an infinite series.
PORFLOW™ Output	The steady state pressure head throughout the domain is produced for comparison with the analytic solution.
Results & Discussion	Figure 2.9.3 shows pressure contours for the analytic solution (solid line) and PORFLOW (symbols) at steady state. The graphical comparison shows that the PORFLOW solution is in excellent agreement with the analytic solution.

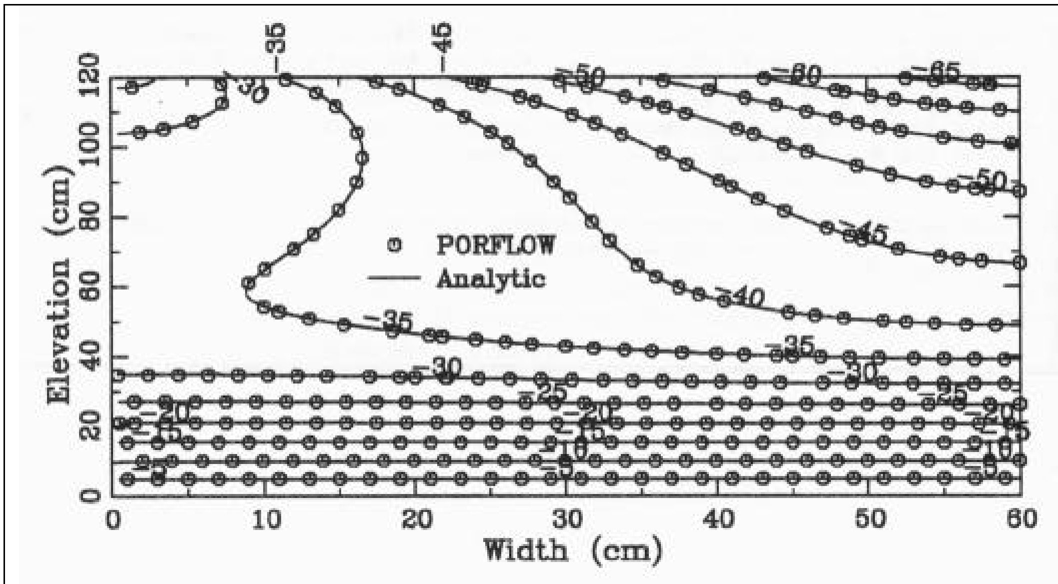

FIGURE 2.9.3: CONTOURS OF PRESSURE

2.10 PROBLEM V10: FREE-SURFACE BOUSSINESQ FLOW WITH RECHARGE

Problem Statement

This test case concerns a semi-infinite, unconfined aquifer. Initially the phreatic surface is at 10 meters everywhere. At time t=0, the water level at the left boundary is suddenly raised to 11 meters. The schematic is shown in Figure 2.10.1. The horizontal extent of the computational domain is set at 200 meters and the vertical extent at 11 meters. The objective is to determine the phreatic surface at selected times. This problem is often referred to as the Boussinesq problem. It is described in detail by Polubarinova-Kochina (1954).

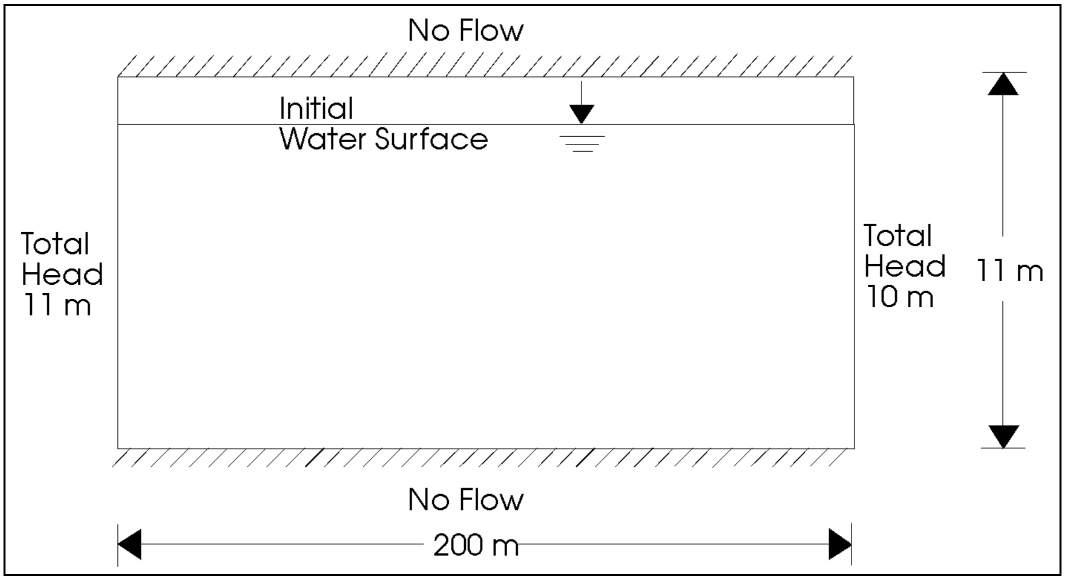

FIGURE 2.10.1: SCHEMATIC ILLUSTRATION OF PROBLEM V10

Initial Conditions

The initial total head is 10 m everywhere except at the recharge boundary (x=0) where the total head is set to 11 meters.

Boundary Conditions

The left and right boundaries are maintained at their initial specified head. The top and bottom boundaries are defined to be no-flow boundaries.

Properties

The soil properties are summarized in Table 2.10.1. The analytic solution for this problem is based on the assumptions that the flow is horizontal; that is, the vertical component of velocity is negligible. To approximate this condition, the vertical component of the hydraulic conductivity is set to be 10 times the value of the horizontal component.

TABLE 2.10.1: Hydraulic Properties for Problem V10

Property	Value
Horizontal hydraulic conductivity (m/day)	0.10
Vertical hydraulic conductivity (m/day)	1.00
Specific storage (m^{-1})	0.0
Porosity	0.25

Computational Details

The problem is simulated with a grid of 44 nodes in the horizontal and 23 in the vertical direction. The grid spacing in the horizontal direction increases in a geometric ratio of 1.1. The minimum grid spacing is 0.37 m and the maximum is 16.95 m. The grid spacing in the vertical direction varies from 0.1 m at the top to 2 m at the bottom. The grid spacing near the top is smaller to allow better resolution near the phreatic surface. The total time of simulation is 324 days. In the first 9 days of the simulation, the time step is increased from an initial value of 0.02 days to 1 day in a geometric ratio of 1.01; thereafter the time step is kept constant at 1 day. The convergence criterion is specified as 10^{-6} and the maximum number of iterations is set at a large number (1,000) to assure that the transient solution is accurate. The PORFLOW input commands for this problem are shown in Table 2.10.2.

TABLE 2.10.2: Input Commands for Problem V10

```
*********************************************************************
TITLe Transient Free-Surface Boussinesq Flow - Recharge
*********************************************************************
////  Polubarinova-Kochina, P.Ya., 1954. Theory of Groundwater Movement,
////  Translated from Russian to English by J.M. Roger de Weist, 1962,
////  Princeton University Press, N.J.
*********************************************************************
/
PROB WITH FREE SURFACE
/
GRID 44 BY 23
COOR X:  MIN=0  MAX=200  ratio=1.1
COOR Y:    0.    2.0   4.0   5.5   7.0   8.0   8.5   9.0   9.25  9.5
           9.7   9.9  10.0  10.1  10.2  10.3  10.4  10.5  10.6  10.7
          10.8  10.9  11.1
/
ROCK POROsity = 0.25
HYDRAULIC S=0., Kx=0.1, Ky=1.0
/
INITial H = 10 everywhere
INITial H = 11 from (1,1) to (1,99)
BOUNDARY FOR P AT -2 FLUX = 0     $ No-flow bottom boundary
BOUNDARY FOR P AT +2 FLUX = 0     $ No-flow top boundary
/
CONVergence for FLOW as a reference: 1.E-6, 1000 iter
/
DIAGNOSITC NODE AT (2,6)
SAVE H on file 'V10.ARC'
OUTPUT U, V, P, H, and S in NARROW format
/
SOLVE FOR  9 days, ini step=0.02, incr by 1.01, max step=1.
SAVE NOW
SOLVe for 27 days
SAVE NOW
SOLVe for 45 days
SAVE NOW
SOLVe for 63 days
SAVE NOW
SOLVe for 81 days
SAVE NOW
SOLVe for 99 days
/
END
```

Comparison Solution The analytic solution for this problem is available in Polubarinova-Kochina (1954).

PORFLOW™ Output The pressure head at 9, 36, 81, 144, and 324 days is obtained for comparison against the analytic solution.

Results & Discussion Figure 2.10.2 shows a comparison of the phreatic surface at the specified times for the analytic solution (solid line) and for PORFLOW (symbols). Qualitatively the two sets of results are in good agreement. There are some departures between the two sets of results. It is possible that the differences between the two could be decreased with a smaller grid size and a smaller time step. It is also possible, that these differences are, at least, partly due to the limiting assumption of a horizontal flow which is inherent in the analytic solution. Within the framework of the present verification effort, the agreement is considered acceptable. Therefore no attempt was made to improve the PORFLOW result.

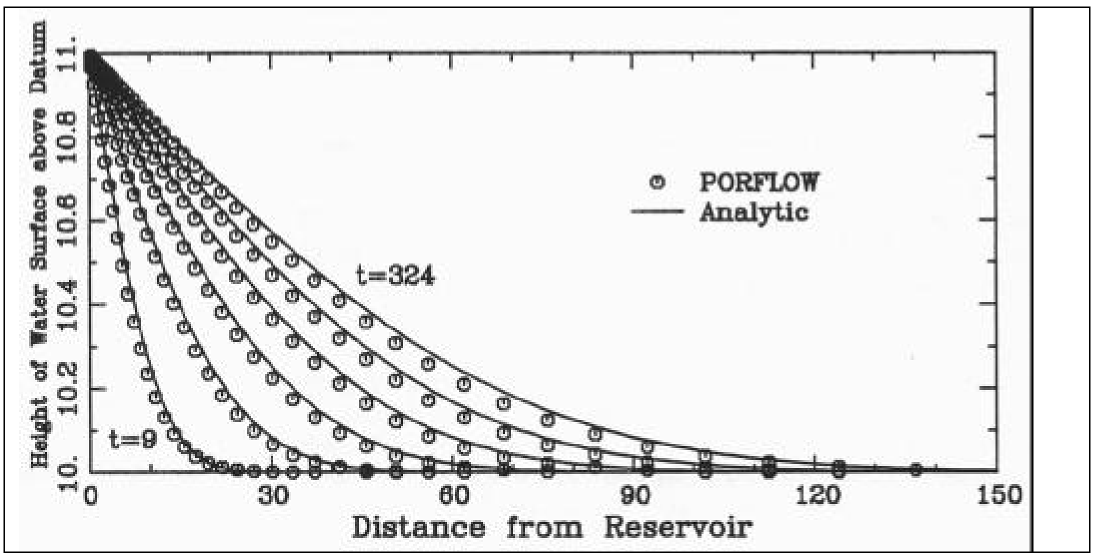

FIGURE 2.10.2: TIME-HISTORY OF PHREATIC SURFACE DUE TO RECHARGE

2.11 PROBLEM V11: FREE-SURFACE BOUSSINESQ FLOW WITH SEEPAGE

Problem Statement

This test problem is variation on the previous Boussinesq problem. In this case, the initial phreatic surface is at 10 meters. At time t=0, the water level at the left boundary is suddenly lowered to 9 meters. The schematic is shown in Figure 2.11.1. The horizontal extent of the problem is 200 meters and the vertical extent is 10 meters. The objective is to determine the phreatic surface at selected times. This problem is described in detail by Polubarinova-Kochina (1954).

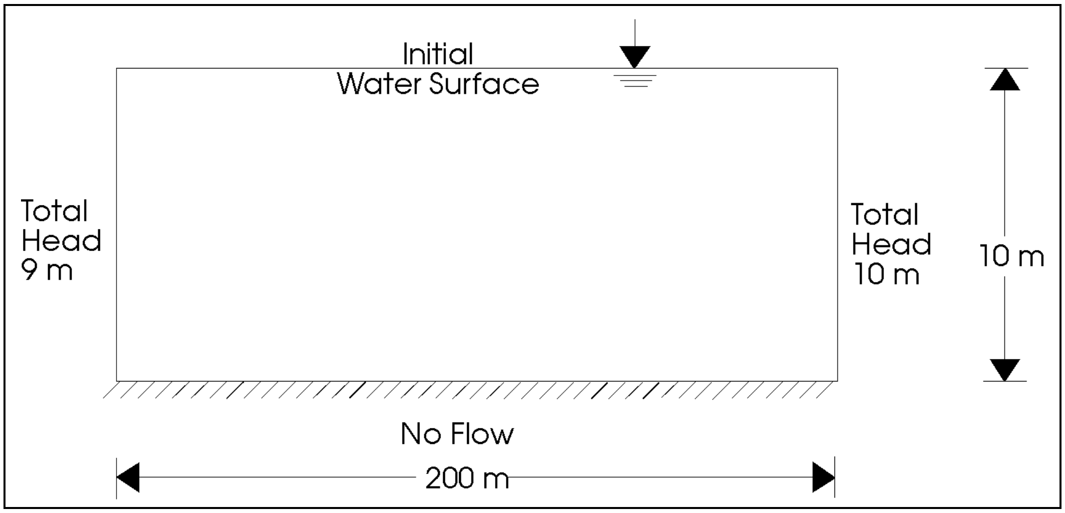

FIGURE 2.11.1: SCHEMATIC ILLUSTRATION OF PROBLEM V11

Initial Conditions

The initial total head is 10 m everywhere except at the left boundary (x=0) where the total head is 9 meters.

Boundary Conditions

The left, the right and the top boundaries are all maintained at their initially specified head. The bottom boundary is defined to be a no-flow boundary.

Properties

The soil hydraulic properties are summarized in Table 2.11.1. The analytic solution for this problem is based on the assumptions that the flow is horizontal; that is, the vertical component of velocity is negligible. To approximate this condition, the vertical component of the hydraulic conductivity is set to be 10 times the value of the horizontal component.

TABLE 2.11.1: Hydraulic Properties for Problem V11

Property	Value
Horizontal Hydraulic Conductivity (m/s)	0.10
Vertical Hydraulic Conductivity (m/s)	1.0
Specific Storage (cm^{-1})	0.0
Porosity	0.25

Computational Details

The problem is simulated with a grid of 44 nodes in the horizontal and 23 in the vertical direction. The grid spacing in the horizontal direction increases in a geometric ratio of 1.1. The minimum grid spacing is 0.37 m and the maximum is 16.95 m. The grid spacing in the vertical direction varies from 0.1 m at the top to 2 m at the bottom. The grid spacing near the top is smaller to allow better resolution near the phreatic surface. The total time of simulation is 324 days. In the first 9 days of the simulation, the time step is increased from an initial value of 0.02 days to 1 day in a geometric ratio of 1.01; thereafter the time step is kept constant at 1 day. The convergence criterion is specified as 10^{-6} and the maximum number of iterations is set at a large number (1,000) to assure that the transient solution is accurate. The PORFLOW input commands for this problem are shown in Table 2.11.2.

TABLE 2.11.2: Input Commands for Problem V11

```
***********************************************************************
TITLe Transient Free-Surface Boussinesq Flow - Seepage
***********************************************************************
////  Polubarinova-Kochina, P.Ya., 1954. Theory of Groundwater Movement,
////  Translated from Russian to English by J.M. Roger de Weist, 1962,
////  Princeton University Press, N.J.
***********************************************************************
/
PROB WITH FREE SURFACE
/
GRID 44 BY 23
COOR X:  MIN=0  MAX=200  ratio=1.1
COOR Y:    0.    1.5   3.0   4.5   6.0   7.0   7.5   8.0   8.25  8.5
           8.7   8.9   9.0   9.1   9.2   9.3   9.4   9.5   9.6   9.7
           9.8   9.9  10.1
/
ROCK POROsity = 0.25
HYDRAULIC S=0., Kx=0.1, Ky=1.0
/
INITial H = 10 everywhere
INITial H =  9 from (1,1) to (1,99)
/
BOUNDARY FOR P AT -2 FLUX = 0      $ No-flow bottom boundary
/
CONVergence for FLOW as a reference: 1.E-6, 1000 iter
/
DIAGNOSITC NODE AT (2,6)
SAVE H on file 'V11.ARC'
OUTPUT U, V, P, H, and S in NARROW format
/
SOLVE FOR  9 days, ini step=0.02, incr by 1.01, max step=1.
SAVE NOW
SOLVe for 27 days
SAVE NOW
SOLVe for 45 days
SAVE NOW
SOLVe for 63 days
SAVE NOW
SOLVe for 81 days
SAVE NOW
SOLVe for 99 days
/
END
```

Comparison Solution The analytic solution for this problem is available in Polubarinova-Kochina (1954).

PORFLOW™ Output The pressure head at 9, 36, 81, 144, and 324 days is obtained for comparison against the analytic solution.

Results & Discussion Figure 2.11.2 shows a comparison of the free water surface at the specified times for the analytic solution (solid line) and for PORFLOW (symbols). Qualitatively the two sets of results are in good agreement. There are some departures between the two sets of results as the time progresses. It is possible that the differences between the two could be decreased with smaller grid size and time. It is also possible, that these differences are, at least, partly due to the limiting assumption of a one-dimensional horizontal flow which is inherent in the analytic solution. Since, in reality, the flow must have a small vertical component, it is possible that the differences accumulate with time. With the framework of the present verification effort, the agreement is considered acceptable.

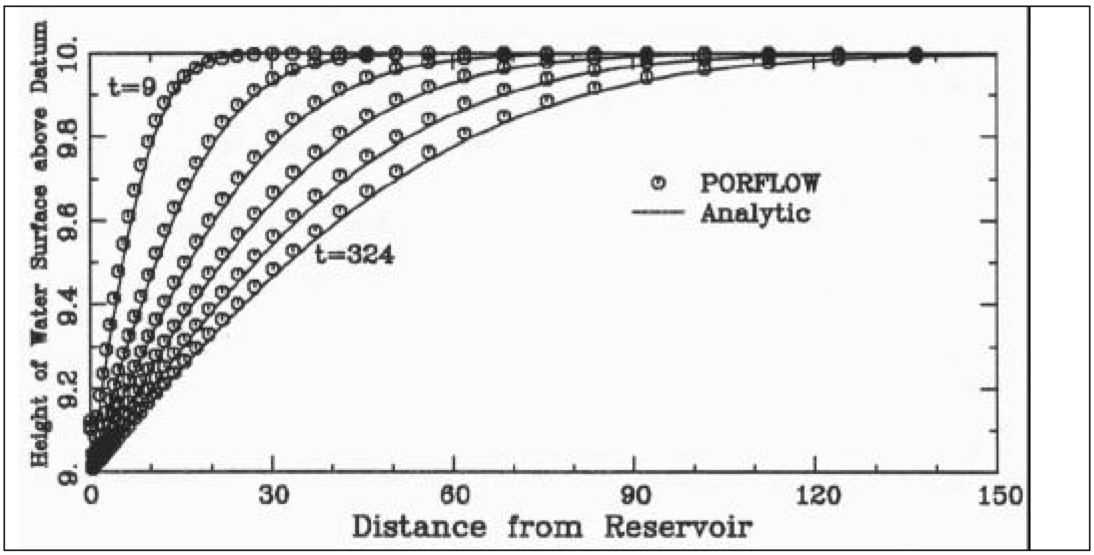

FIGURE 2.11.2: TIME-HISTORY OF PHREATIC SURFACE DUE TO SEEPAGE

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CHAPTER 3

BENCHMARK CASES

This chapter describes the benchmark problems which were used to validate PORFLOW . In this context, a benchmark problem is defined to be one for which a numerical solution from another computer code is available. The problems selected are of such complexity that often no analytic solution is available. The only option then is to compare the PORFLOW predictions against those from another computer code. For benchmark testing, six problems of increasing complexity were selected. All of these problems have been used previously for validation of other computer codes. The PORFLOW predictions for these problems, along with the comparative numerical results are described below. These provide some validation of the correctness of the physical, mathematical and numerical features of PORFLOW in that the results are similar to those obtained from other computer codes.

3.1 PROBLEM B1: TWO-DIMENSIONAL TRANSIENT INFILTRATION

Problem Statement

This test case considers flow through a two dimensional, rectangular, column of soil which is 10 cm high and 15 cm long. The soil is partially saturated with an initial pressure of 0.9 m. The right vertical face of the column is held at its initial pressure head, while the pressure in the upper part of the left vertical face is increased. The lower part of the left face is impermeable. This causes a two-dimensional saturation front to propagate from left to right. The schematic of the problem is shown in Figure 3.1.1. This problem was proposed by Ross et al. (1982) for benchmark testing of computer codes. Pruess (1987) has solved this problem numerically with the TOUGH computer code.

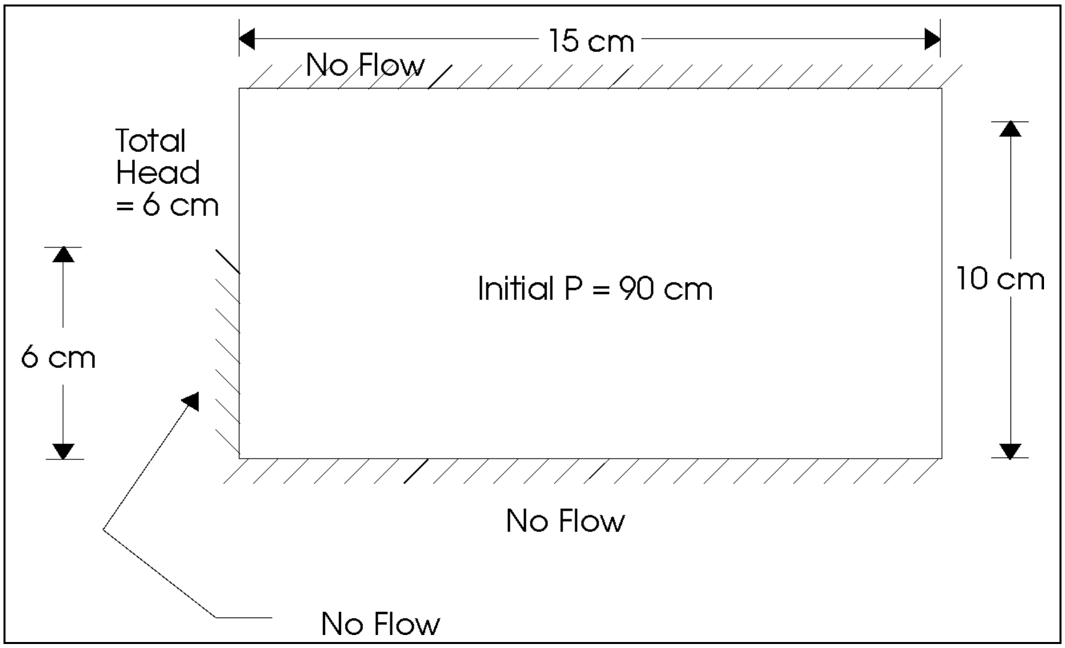

FIGURE 3.1.1: SCHEMATIC ILLUSTRATION OF PROBLEM B1

Initial Conditions The entire rectangular section of soil is initially at a pressure head of 0.9 m; the corresponding saturation is 0.4.

Boundary Conditions The domain is bounded by no flow boundaries at the top and bottom. The right vertical boundary is maintained at a constant pressure head of 0.9 m. The left vertical side has dual boundary conditions: for the lower 6 cm of the boundary ($0 \leq z < 6$) there is no flow; for the upper 4 cm ($6 \leq z \leq 10$), the total hydraulic head is maintained at 6 cm.

Properties The hydraulic properties and the soil-moisture characteristic are summarized in Tables 3.1.1 and 3.1.2, respectively.

TABLE 3.1.1: Hydraulic Properties for Problem B1

Property	Value
Porosity	0.45
Hydraulic Conductivity (m/s)	1.157×10^{-7}
Specific storage (m^{-1})	0.0

TABLE 3.1.2: Soil Moisture Characteristic for Problem B1

Saturation	Capillary Pressure (m)	Relative Conductivity
0.3333	1.0	0.0
1.0000	0.0	1.0

Computational Details A uniform grid of 16 horizontal and 12 vertical nodes with a node spacing of 1 cm is used. This case is solved in the transient mode for 43891 seconds (0.508 days). The **AUTO**matic mode of the **SOLV**e command with a starting time step of 0.1 s is used. The time step is increased in a geometric progression with the built-in default options. No maximum is imposed on the time step size. The convergence tolerance is set at 10^{-5} in the GLOBal mode and a maximum of 30 iterations per time step is specified. The PORFLOW input commands for this problem are shown in Table 3.1.3.

TABLE 3.1.3: Input Commands for Problem B1

```
************************************************************************
TITLe Two-Dimensional Transient Infiltration
************************************************************************
////  Ross, B., J.W. Mercer, S.D. Thomas, and B.H. Lester, 1982.
////  Benchmark Problems for Repository Siting Models, NRC-report
////  NUREG/CR-3097, December, 1982.
************************************************************************
/
USER ACRi - August 29, 1993
/
GRID  16 by 12
COORDINATE  X MINIMUM 0 MAX 0.15
COORDINATE  Y RANGE 0.10
GRAVITY constants 0,  -1 relative value
/
ROCK density = 2385 kg_per_m_cubed, Por = 0.45
PROPERTY averages by UPWIND
HYDRaulic properties for P:  ss=0.,  kx=1.157e-7,   ky=1.157e-7
/
MULTiphase CONDuctivity TABLe of 2 sets
/* sl        krl  */
  0.333333    0.
  1.000000    1.
/
MULTiphase TABLe of 2 sets
/* sl         Pcap  */
  0.333333    1 m
  1.000000    0.
/
SET initial P = -.90 m
/
BOUNDary P at -2: FLUX = 0
BOUNDary P at  2: FLUX = 0
LOCAte from (1, 1) to (1, 7)
BOUNDary P at -1: FLUX = 0 in SELEcted region
LOCAte from (1, 8) to (1,12)
BOUNdary P at -1: LINEar function 0.06 -1. Y in SELEcted region
/
CONVergence of P GLOBAL criterian=1.E-5, iterations=30
/
DIAGNOSTIC P, U, S  at (3,18) every 10 steps
/
SAVE H, P, S on 'B1.ARC'
OUTPut U, V, H, P, S in NARROW tabular format
/
SOLVE for P to 43891 sec in steps of .1 sec in AUTO mode
/
END
```

Comparison Solution

The PORFLOW solution is compared to a solution using the TOUGH computer code (Pruess, 1987).

PORFLOW™ Output

The outputs required for this problem are pressure profile at the top and bottom base of the domain and liquid saturation throughout the domain at time t = 0.508 days.

Results & Discussion

The PORFLOW solution is shown alongside the TOUGH solution in Figure 3.1.2. This figure shows the capillary pressure at the top and the bottom of the column as a function of the horizontal distance. The two solutions are seen to be in excellent agreement with each other.

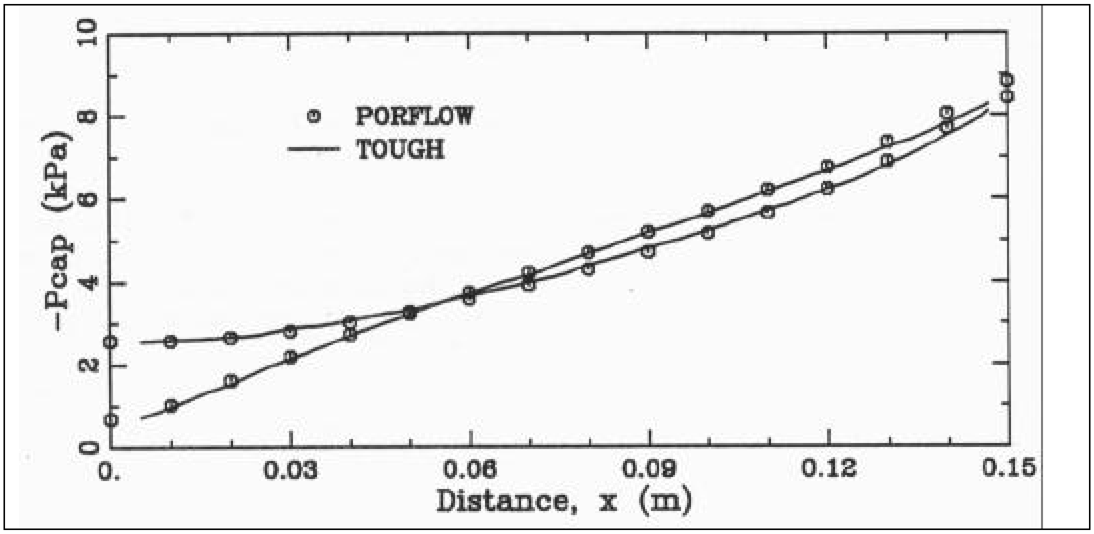

FIGURE 3.1.2: CAPILLARY PRESSURE PROFILES AFTER 0.508 DAYS

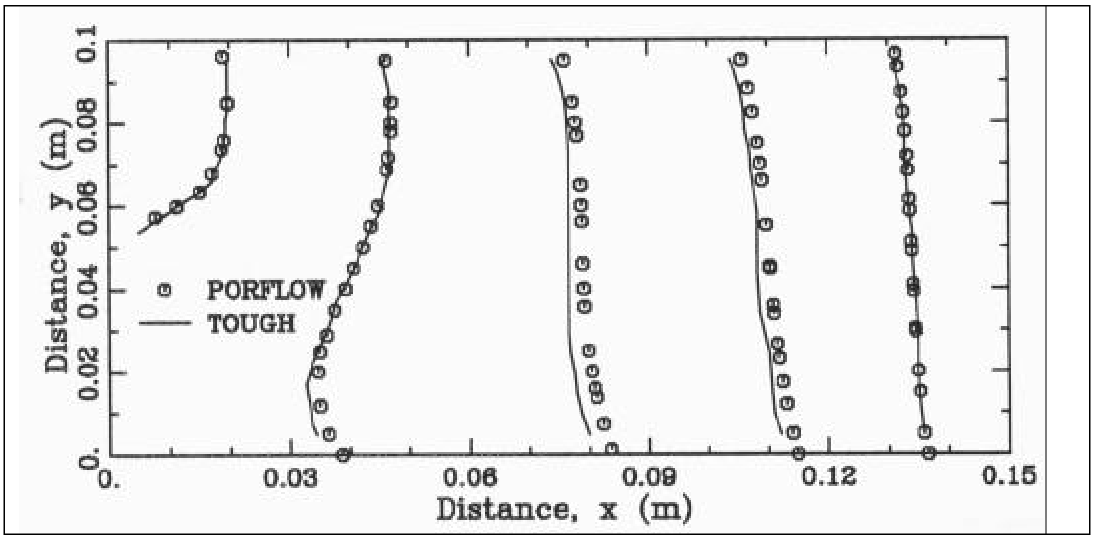

FIGURE 3.1.3: LIQUID SATURATIONS AFTER 0.508 DAYS

3.2 PROBLEM B2: TWO-DIMENSIONAL STEADY-STATE INFILTRATION

Problem Statement

This test case considers the steady-state movement of moisture in variably saturated flow conditions. The physical setting for the problem is a vertical cross-section of an aquifer with a regional hydrological gradient of 1 in 75. The depth of the aquifer is 35 m and a horizontal extent of 150 m is simulated. The lateral extent of the aquifer is assumed to be infinite and only a unit width is considered. Recharge occurs at the left boundary where the water table is at 21 m and the flow discharges at the right with the water table at 19 m. Additional recharge occurs through infiltration at the surface at a rate of 1 m/yr. The schematic of the problem is shown in Figure 3.2.1. The problem is described by Magnuson et al. (1990) and has been used as a benchmark problem for a number of codes (Huyakorn et al., 1989). The FEMWATER computer code by Yeh and Ward (1979) was used as a benchmark for comparing the PORFLOW results.

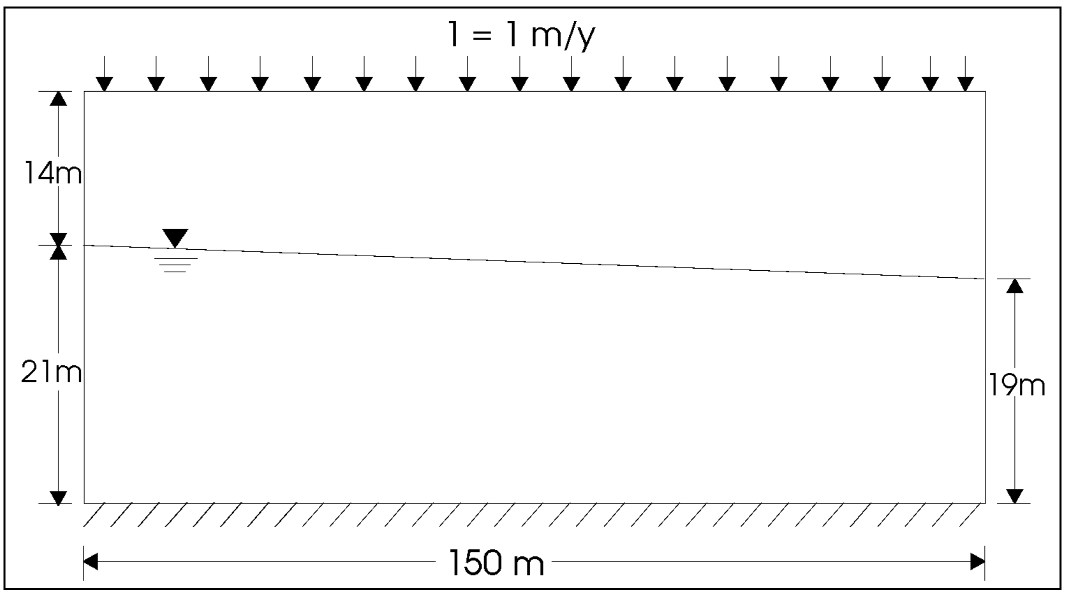

FIGURE 3.2.1: SCHEMATIC ILLUSTRATION OF PROBLEM B2

Initial Conditions

No initial conditions are required since it is a steady state problem. To assist the model in converging more rapidly initial pressure head is set to -10 m everywhere.

Boundary Conditions

The bottom of the aquifer is set to be a no-flow boundary. An infiltration rate of 1 m/yr is specified at the top. The water table at the recharge (left) boundary is at 21 m and, at the discharge (right) boundary it is at 19 m. This implies that the pressure head below the water table decreases linearly with distance (y) from the bottom. The soil above the water table is set to conditions of no flow.

Properties

The hydraulic properties are given in Table 3.2.1. The soil moisture-characteristic is specified by Equation set 3.2.1.

TABLE 3.2.1: Hydraulic Properties for Problem B2

Property	Value
Porosity	0.1875
Hydraulic Conductivity (m/yr)	750
Specific Storage (m^{-1})	10^{-7}
Residual liquid saturation, S_r	0.25

$$\hat{S} = \frac{S - S_r}{1 - S_r} = \frac{1}{1 + [0.2\,y]^2} \; ,$$

(3.2.1)

$$k_r = \hat{S}^{\,4} \; .$$

Computational Details

A 31 by 33 grid is used. The grid spacing in the horizontal (x) direction is uniform and equal to 5 m. In the vertical (y) direction, the grid spacing varies from a minimum of 0.2 m to a maximum of 2 m. The density of grid nodes is higher near the phreatic surface to provide better resolution in this area. The simulation is carried on for 5 years in steps of 0.025 years. A relaxation factor of 0.2 is used for the saturation variable. Though the solution method converges without relaxation, the convergence behavior is smoother with relaxation. The PORFLOW input commands are shown in Table

3.2.2.

TABLE 3.2.2: Input Commands for Problem B2

```
**********************************************************************
TITLe Two-Dimensional Steady-State Infiltration
**********************************************************************
////  Magnuson S.W., R.G. Baca & A.J. Sondrup, August 1990.  Independent
////  Verification and Benchmark Testing of The PORFLO-3 Computer Code,
////  Version 1.0, EGG-BG-9175; INEL, Idaho Falls, ID 83415.
**********************************************************************
/
GRID 31 by 33
COORdinate X
   0.0     5      10     15     20     25     30     35
   40     45      50     55     60     65     70     75     80     85
   90     95     100    105    110    115    120    125    130    135
  140    145     150.
COORdinate Y
   -0.1    0.1    2.     4.     6.     8.     10.    12.    14.    16.
   18.    18.5   18.9   19.1   19.5   20.5   20.9   21.1   21.5   22.
   23.    24.    25.    26.    27.    28.    29.    30.    31.    32.
   33.    34.    36.
/
DATUM 0., 0.
/
GRAVity 0., -1 (normalized; absolute value not required for
single-phase)
/
ROCK density 1.0, porosity = 0.1875, 0.25, 0.1852
HYDRaulic properties: ss = 1.E-7, (kx,ky,kz) --> 3*750
PROPerty averages by GEOMetric mean option
/
SET initial P  -10. everywhere
/
SELEct  subdomain (1,1) to (1,17)
BOUNdary P: index -1 LINEar function: 21 -1 Y for SELEcted segment
SELEct  subdomain (1,18) to (1,99)
BOUNdary P: index -1 FLUX = 0. for SELEcted segment
/
SELEct  subdomain from (31,1) to (31,13)
BOUNdary P: index +1 LINEar function: 19 -1 Y for SELEcted segment
SELEct  subdomain from (31,14) to (31,99)
BOUNdary P: index +1 FLUX = 0. for SELEcted segment
/
BOUNdary P: index +2 FLUX =-1. m/yr EVERywhere
BOUNdary P: index -2 FLUX = 0.      EVERywhere
/
MULTifluid VAN Genuchten GENEral form: 2, 0.2, 0.25, 0, 1
MULTifluid CONDuctivity POWEr law: 4, 1, 0, 0, 0.25
/
CONVergence REFErence variable P: local mode; e=1.0E-5
/
DIAGnostic NODE (9, 25) EVERY 10 STEPS
/
SAVE on 'B2.ARC' P S M
SOLVE for 5 years in 0.025 yr steps
/
OUTPut U, V, P, H, S, MOIS
/
END
```

Comparison Solution

The computer code FEMWATER (Yeh and Ward, 1979) was used for comparison with PORFLOW . The FEMWATER simulations were performed by Magnuson et al. (1990) and the comparative data was supplied by Magnuson (1993).

PORFLOW™ Output

Two types of output are required for comparative tests. The first output is a contour plot of pressure head for the whole of the computational domain. The second is a profile of the moisture content with depth from the surface to the bottom of the aquifer at a distance of 30 meters from the left boundary of the domain.

Results & Discussion

Figure 3.2.2 shows a comparison of pressure heads for PORFLOW and FEMWATER. The two sets of results are nearly identical except near the top and bottom boundaries where a slight departure is noticed. These differences are attributed to the different methods for imposing boundary conditions in PORFLOW and FEMWATER.

The moisture content profile at the required location is shown in Figure 3.2.3. The PORFLOW and FEMWATER results are in very good agreement with each other throughout the depth of the aquifer.

FIGURE 3.2.2: CONTOURS OF PRESSURE HEAD

FIGURE 3.2.3: PROFILES OF MOISTURE CONTENT

3.3 PROBLEM B3: JORNADA TEST TRENCH SIMULATION

Problem Statement

This problem is based on the field tests conducted at the Jornada Test Site near Las Cruces, New Mexico. The test involves transient, two-dimensional infiltration of water into an extremely dry heterogeneous soil. The physical setting and soil-hydraulic properties of the soil system are described by Smyth et al. (1989). The test area comprises three layers of soil which vary in material and hydrological properties. Additionally a small zone of high conductivity soil is contained within the lowermost soil layer. The physical extent of the domain is 800 cm horizontally and 650 cm vertically. The schematic is shown in Figure 3.3.1. The experiment was conducted under the direction of Dr. Peter Wierenga of the University of Arizona. Smyth et al. (1989) numerically solved four problems of increasing complexity using the TRACER3D computer code. The problem considered here is the fourth and most complex of these problems. This problem was also numerically solved by Magnuson et al. (1990) using the TRACER3D, FLASH and PORFLOW (Version 1.00) computer codes.

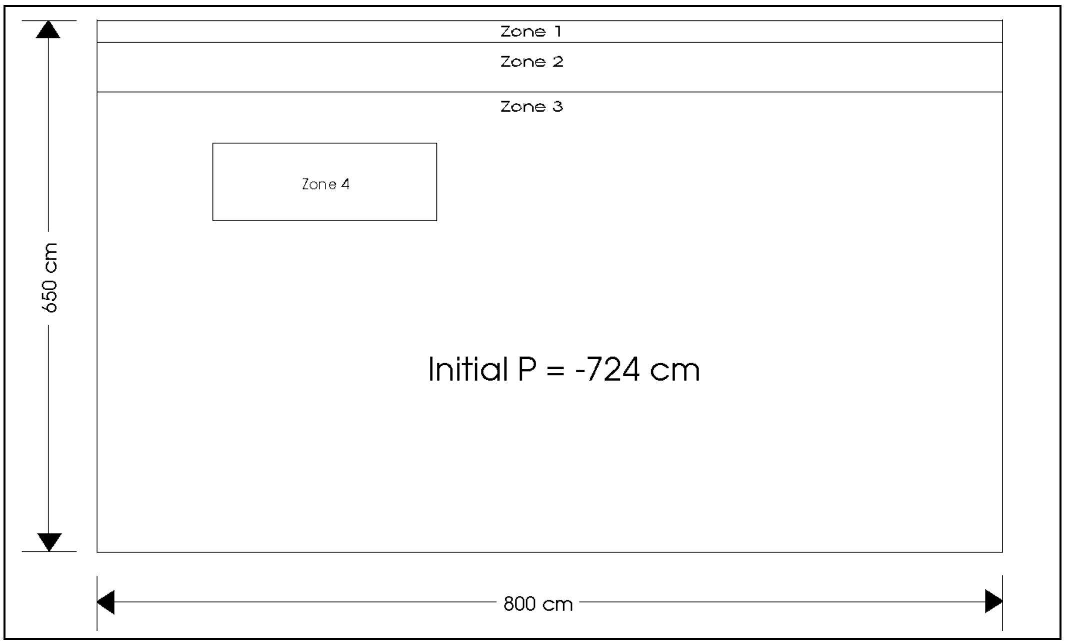

FIGURE 3.3.1: SCHEMATIC ILLUSTRATION OF PROBLEM B3

Initial Conditions Initial pressure head in the soil is uniform and equal to -724 cm. This corresponds to a relative saturation which varies from 0.309 in the top layer to 0.380 in the lower-most layer. Since the soil porosity is between 0.325 and 0.368, the initial soil moisture content is on the order of 0.1

Boundary Conditions Uniform infiltration at the rate of 2 cm/day occurs for an area of the top boundary extending 225 cm from the left of the domain. The boundary at the bottom of the trench is held at its initial pressure. The rest of the top boundary, and the vertical faces at the left and right of the domain are treated as no flow boundaries.

Properties The hydraulic properties of the soil are summarized in Table 3.3.1. The soil moisture-characteristics are specified by the van Genuchten and Mualem relations given in the Equation set 3.3.1; the constants for these relations, for the four different soil types which are present, are given in Table 3.3.1.

TABLE 3.3.1: Hydraulic Properties for Problem B3

Property	Value			
	Zone 1	Zone 2	Zone 3	Zone 4
Porosity	0.368	0.351	0.325	0.325
Hydraulic Conductivity (cm/day)	790.9	469.9	415.0	4150.0
Specific Storage (cm^{-1})	0.0	0.0	0.0	0.0
van Genuchten Exponent, N	1.982	1.632	1.573	1.573
van Genuchten Coefficient, α (cm^{-1})	0.0334	0.0363	0.0345	0.0345
Residual Saturation, S_r	0.2772	0.2806	0.2643	0.2643

$$\hat{S} = \frac{S - S_r}{1 - S_r} = \frac{1}{[1 + (\alpha\psi)^N]^M} \; ; \psi > 0 \; ;$$

$$= 1 \qquad ; \psi \leq 0 \, , \tag{3.3.1}$$

$$k_r = \hat{S}^{0.5} \left[1 - \left(1 - \hat{S}^{1/M} \right)^M \right]^2$$

Computational Details

A computational grid of 56 by 47 nodes in the horizontal and vertical directions respectively, is superimposed on the domain of interest. In the x direction the node spacing varies from a minimum of 6 to a maximum of 25 cm. In the y direction the node spacing varies from 10 to 25 cm. The computational domain is subdivided into four regions representing the four soil types. The problem is solved for a time period of 30 days. The initial time step is 0.0005 day which is increased to 0.02 day in a geometric ratio of 1.02.

Comparison Solution

The FLASH computer code (Baca and Magnuson, 1992) was used for comparison with PORFLOW . The comparative data for FLASH simulations was supplied by Magnuson (1993). A comparison of the TRACER3D (Travis, 1984) and PORFLOW simulations has also been published by Magnuson et al. (1990).

PORFLOW™ Output

The relative soil saturation for the entire cross-section is obtained at 30 days after the start of moisture infiltration. This time period is sufficient for steady-state conditions to be achieved. For this test, pressure head distribution does not show the influence of the high conductivity zone as readily as the soil saturation; hence pressure data is not used for comparison with the FLASH solution.

Results & Discussion

The soil saturation for PORFLOW is compares with that from FLASH in Figure 3.3.2. The effect of the embedded high-conductivity zone of soil is clearly seen in the manner in which the moisture contours deflect towards the this zone. The two sets of data compare very well with each other both qualitatively and quantitatively. Except for small departures for the outermost contours, the two data are near-identical.

TABLE 3.3.2: Input Commands for Problem B3

```
*************************************************************************
TITLe Jornada Test Trench Simulation
*************************************************************************
////  Magnuson S.W., R.G. Baca & A.J. Sondrup, August 1990.  Independent
////  Verification and Benchmark Testing of The PORFLO-3 Computer Code,
////  Version 1.0, EGG-BG-9175; INEL, Idaho Falls, ID 83415.
*************************************************************************
/
GRID 56 by 47
/
COORdinate X
   -5.    5.   15.   25.   35.   45.   55.   65.   75.   85.   95.  105.
  115.  125.  135.  145.  155.  165.  175.  185.  195.  205.  215.  222.
  228.  235.  245.  255.  265.  275.  285.  295.  305.  315.  325.  335.
  345.  355.  380.  405.  430.  455.  480.  505.  530.  555.  580.  605.
  630.  655.  680.  705.  730.  755.  780.  820.
/
COORdinate Y
 -655. -645. -630. -605. -580. -555. -530. -505. -480. -455. -430. -405.
 -380. -355. -330. -305. -295. -285. -275. -265. -255. -245. -235. -225.
 -215. -205. -195. -185. -175. -165. -155. -145. -135. -125. -115. -105.
  -95.  -85.  -75.  -65.  -55.  -45.  -35.  -25.  -15.   -5.    5.
/
ZONE  1 from ( 1,44) to (56,47)
ZONE  2 from ( 1,38) to (56,43)
ZONE  3 from ( 1, 1) to (56,37)
ZONE  4 from (12,22) to (32,30)
/
GRAVity vector: 0., -1. (only relative value required)
/
FOR zone 1
HYDRaulic props S=0.0, kx=790.9, ky=790.9, kz=790.9 cm/day
ROCK POROsity eff = 0.368, total = 0.368, diffusive = 0.266
MULTiphase: VAN genuchten+MUALem n=1.982 alpha=0.0334, sr=0.2772
/
FOR zone 2
HYDRaulic props S=0.0, kx=469.9, ky=469.9, kz=469.9 cm/day
ROCK POROsity eff = 0.351, total = 0.351, diffusive = 0.2525
MULTiphase: VAN genuchten+MUALem n=1.632 alpha=0.0363, sr=0.2806
/
FOR zone 3
HYDRaulic props S=0.0, kx=415.0, ky=415.0, kz=415.0 cm/day
ROCK POROsity eff = 0.325, total = 0.325, diffusive = 0.2391
MULTiphase: VAN genuchten+MUALem n=1.573 alpha=0.0345, sr=0.2643
/
FOR zone 4
HYDRaulic props S=0.0, kx=4150., ky=4150., kz=4150. cm/day
ROCK POROsity eff = 0.325, total = 0.325, diffusive = 0.2391
MULTiphase: VAN genuchten+MUALem n=1.573 alpha=0.0345, sr=0.2643
/
PROPerty averages using GEOMetric mean option
/
SET initial P = -724. cm everywhere
/
BOUNdary cond P: index -1, FLUX = 0. everywhere
BOUNdary cond P: index +1, FLUX = 0. everywhere
SELEct (1,47) to (24,47)
BOUNdary cond P: index +2, FLUX =-2. cm/day SELEct
SELEct (25,47) to (56,47)
BOUNdary cond P: index +2, FLUX = 0. SELEct
/
DIAGnostic node at (4,46) every 10 steps
SAVE on 'B3.ARC' S
/
SOLVe for 30. days in steps of 0.0005 days factor = 1.02 max 0.02
/
END
```

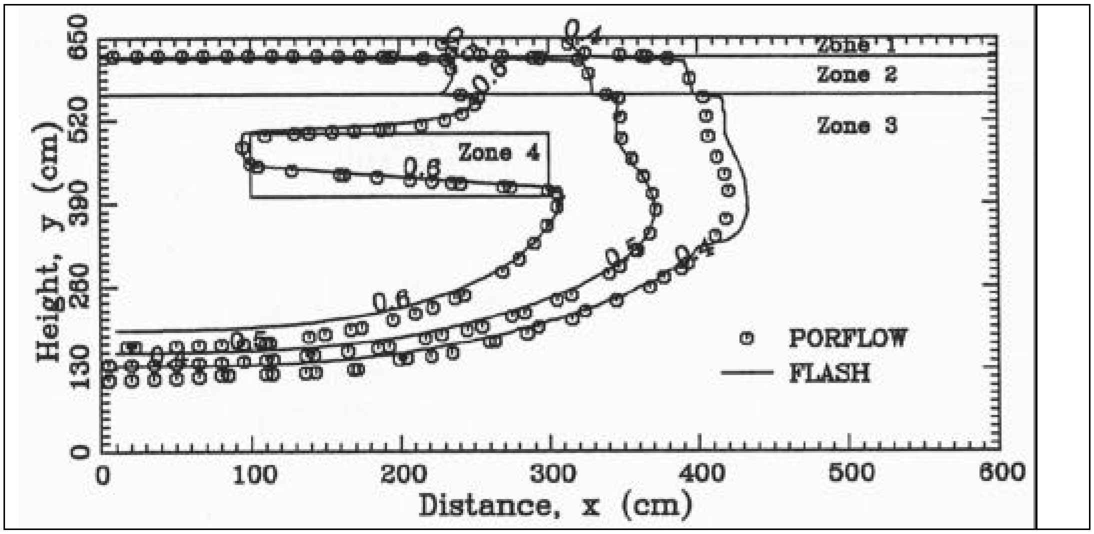

FIGURE 3.3.2: CONTOURS OF MOISTURE CONTENT

3.4 PROBLEM B4: SALTWATER INTRUSION INTO A CONFINED AQUIFER

Problem Statement

This case deals with the intrusion of seawater into a confined fresh water aquifer. The problem was described by Henry (1964) who used an idealized mathematical model and obtained a Fourier-Galerkin solution for this problem. A constant and steady recharge of fresh water occurs at the left boundary of the aquifer. The right boundary is a seawater interface with hydrostatic pressure. No fluid enters or leaves through the top and bottom boundaries. The computation domain is a rectangle with a length of 2 and a depth of 1. The schematic is shown in Figure 3.4.1. The fluid density varies as a linear function of salinity. A Ghyben-Herzberg lens is formed due to the interaction of the buoyancy forces, freshwater recharge and salinity dispersion. This problem has been used extensively as a test case for verification of computer models (Pinder and Cooper, 1970; Segol et al, 1975; Huyakorn and Taylor, 1976; Desai and Contractor, 1977; INTERA, 1979; Frind, 1982, Voss, 1984; Sanford and Konikow, 1985)

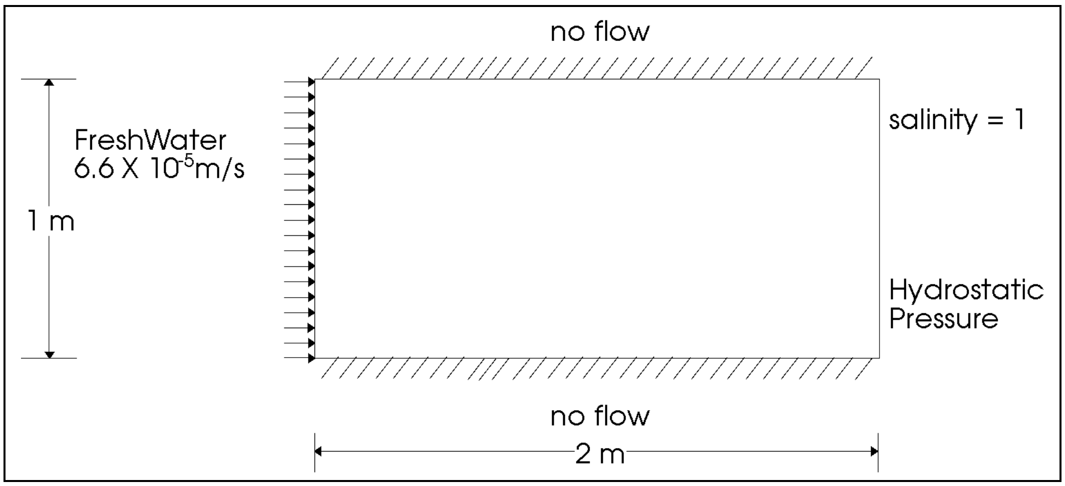

FIGURE 3.4.1: SCHEMATIC ILLUSTRATION OF PROBLEM B4

Initial Conditions

This is a steady state problem. Therefore no initial conditions are required. For computational purposes, the total head is set at zero. The initial concentration is zero by default.

Boundary Conditions

The left boundary is specified to have a steady recharge of fresh water at the rate of 6.6×10^{-5} m/s. At the right boundary, the pressure is hydrostatic. Since the ratio of the salt water to fresh water density is 1.025, this implies that the head is zero at the bottom (y=0) and decreases linearly with y at a rate of 1.025 m/m. The normalized salt concentration is fixed at 0 at the recharge (x=0) boundary and at 1 at the sea water (x=2) boundary. The top and the bottom are no-flow, zero salinity flux boundaries.

Properties

The hydraulic and transport properties for this problem are summarized in Table 3.4.1 below. The fluid density is given as a function of the salt concentration, C, by the linear relation:

TABLE 3.4.1: Hydraulic and Transport Properties for Problem B4

$$\rho = 1. - 0.025\ C \qquad (3.4.1)$$

Property	Value
Fluid density	Equation 3.4.1
Porosity	0.35
Specific storage	0.0
Hydraulic conductivity (m/s)	0.01
Distribution coefficient (m^3/kg)	0.0
Molecular diffusivity (m^2/s)	1.88571×10^{-5}

Computational Details

A uniform grid consisting of 41 by 21 nodes in the x and y directions, respectively, is used. The node spacing is uniform at 1 m in both directions. The problem is solved in steady state mode for 5000 steps. The PORFLOW input commands for this problem are shown in Table 3.4.2.

TABLE 3.4.2: Input Commands for Problem B4

```
***********************************************************************
TITLe Saltwater Intrusion into a Confined Aquifer
***********************************************************************
////  Henry, H.R., 1964. Effects of Dispersion on Salt Encroachment in
////  Coastal Aquifers, Sea Water in Coastal Aquifers, U.S. Geological
////  Survey Water Supply Paper 1613-C, p. C71-C84.
***********************************************************************
/
GRID 41 by 21
COORdinate x: min=0.0, max=2.0
COORdinate y: min=0.0, max=1.0
/
GRAVity  0, -1. nomalized value
/
SET initial H to 0. everywhere
/
/top and bottom no flow boundary
BOUNdary for P IB=+2, flux=0.0
BOUNdary for P IB=-2, flux=0.0
BOUNdary for P IB=-1, flux=6.60E-5
BOUNdary for P IB=+1, LINEar function 0.  -1.025 * Y
/
BOUNdary for C IB=+2, flux = 0.
BOUNdary for C IB=-2, flux = 0.
BOUNdary for C IB=-1, value= 0.
BOUNdary for C IB=+1, value= 1.
/
DENSity LINEar rho=1, a1=0., c*=0., a2=-0.025
/
ROCK POROsity = 0.35
HYDRaulic ss = 0.0, kx=0.01, ky=0.01
TRANsport C kd=0, Dm = 1.88571E-5
/
DIAGnostic node at 11,2 every 10 steps
/
OUTPut U,V,P,H,C
SOLVe STEAdy state mode for P,C  max = 5000, min= 5000
SAVE U,V,H,C 'B4.ARC'
/
END
```

Comparison Solution

The Fourier-Galerkin solution of Henry (1964) and the numerical solutions of SUTRA (Voss, 1984) and INTERA (1979) are used for comparison. The Henry's solution is limited by the small number of terms retained in the numerical solution and by the idealization that the effect of changes in density in the Darcy equation can be ignored.

PORFLOW™ Output

The salinity distribution is obtained throughout the domain after steady state is reached.

Results & Discussion

Figure 3.4.2 compares the 0.5 isochlor for the PORFLOW solution with the solutions of Henry (1964), SUTRA (Voss, 1984) and INTERA (1979). The normalized salinity at the bottom of the aquifer as a function of distance is shown in Figure 3.4.3 for numerical solutions from PORFLOW and SUTRA. All, except Henry's solution, are in qualitative agreement with each other; all other solutions differ from Henry's solution for the lower two-thirds of the aquifer. This may be partly attributed to the neglect of the density differences in the analytic solution. Also, Henry (1964) states that his numerical solution had probable errors due to computational limitations.

Only the PORFLOW results are in reasonable quantitative agreement with Henry's solution for the upper third of the aquifer. The solutions from SUTRA and INTERA have two major discrepancies. First, these show that the salinity interface terminates at the right boundary about one-third distance below the top. This implies that fresh water intrudes into sea water at that interface, which is incompatible with the conditions of hydrostatic pressure. Second, for these solutions neither end of the isochlor intersects the boundary with a zero normal gradient as required at a no-flux boundary. These discrepancies seem to result from either incorrect imposition of boundary conditions or numerical inaccuracies. The same discrepancies are also present in the numerical results published by Huyakorn and Taylor (1976), Segol et al. (1975) and other authors. In contrast, the results from PORFLOW show the correct trends at the upper and lower boundaries.

Another feature to note is that the salinity interface predicted by PORFLOW is closer to Henry's solution, and it penetrates farther upstream than the interface from other numerical models. Considering that all models used the same grid, these observations point to the fact that PORFLOW has lower numerical diffusion, and therefore higher numerical accuracy, than the other models.

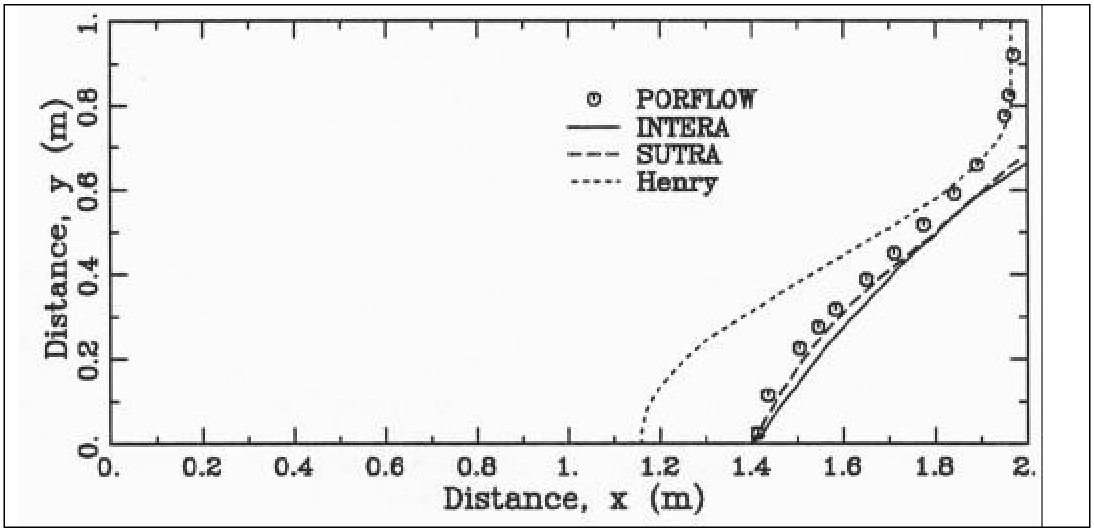

FIGURE 3.4.2: ISOCHLORS

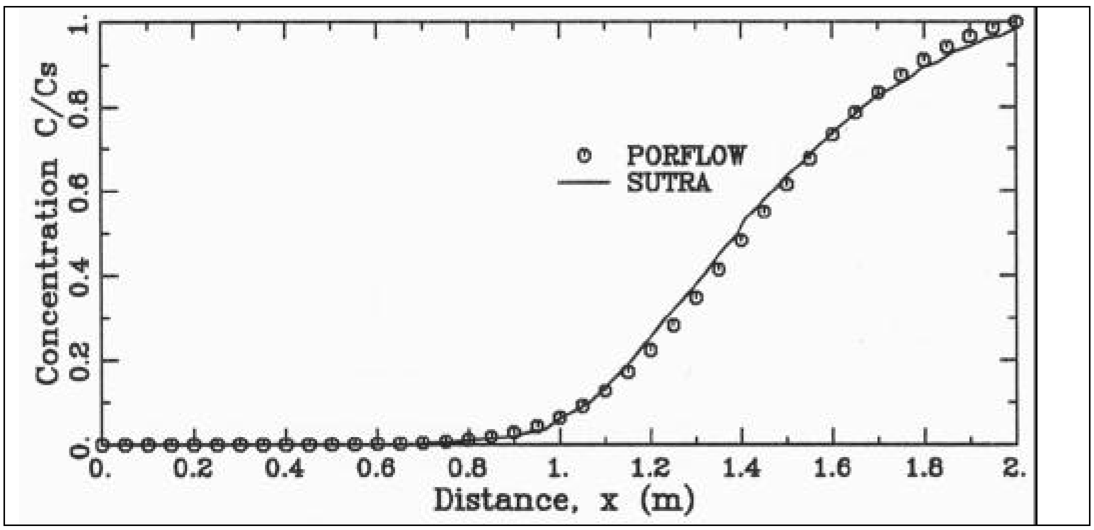

FIGURE 3.4.3: CONCENTRATION ALONG THE BOTTOM

3.5 PROBLEM B5: SATURATED FLOW IN A FRACTURED POROUS MEDIUM

Problem Statement

This test problem concerns a steady-state flow in a saturated, geologic medium with discrete embedded fractures. The hydraulic properties of the medium are based on core test data on basalts from the Idaho National Engineering Laboratory. The physical setting and the boundary conditions are selected to assure hydraulic interaction between the discrete fractures and porous medium. The computational domain, which is 30 cm long and 80 cm in depth, contains two vertically oriented discrete fractures. Each fracture is 20 cm long and its width is 0.03 cm. The fractures are separated by a horizontal distance of 10 from each other and from the boundaries of the computational domain. The hydraulic permeability of each fracture is more than 5 orders of magnitude greater than that of the porous media. The schematic is shown in Figure 3.5.1. This problem was originally devised, and numerically solved, by Magnuson et al. (1990) using the FLASH and PORFLOW (Version 1.00) computer codes.

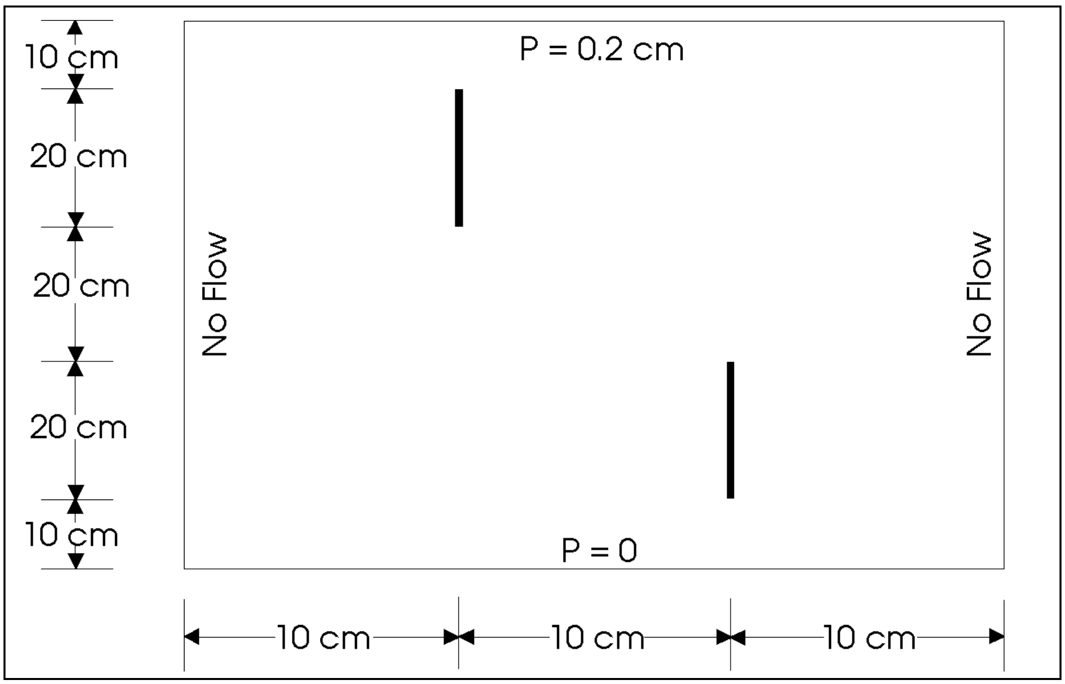

FIGURE 3.5.1: SCHEMATIC ILLUSTRATION OF PROBLEM B5

Initial Conditions

This is a steady state problem; therefore, the final solution is independent of the initial conditions. To start the computational process, the pressure head is specified as a linear function of the vertical distance, y, according to the relation:

$$P = 0.0025 \ y \ . \qquad (3.5.1)$$

Boundary Conditions

Pressure head at the bottom of the computational domain is fixed at 0; that at the top is 0.2 cm. The vertical sides are specified as no-flow boundaries.

Properties

The hydraulic properties of the rock matrix and the fractures are given in Table 3.5.1. The porosity for the fractures is set to unity and the hydraulic permeability of the fractures is more than six orders of magnitude greater than that of the rock matrix.

TABLE 3.5.1: Hydraulic Properties for Problem B5

Property	Value	
	Rock	Fractures
Porosity	0.24	1.0
Hydraulic Conductivity (cm/s)	0.004	600.00
Specific Storage (cm^{-1})	0.0	0.0

Computational Details

A grid of 49 horizontal and 93 vertical nodes is used for numerical simulations. Two line elements (defined as zone 2 and 3) are superimposed on the background rock matrix (defined as Zone 1) at the fracture locations. The node spacing is variable in both the vertical and horizontal directions in order to increase the numerical resolution near the fractures. The minimum and maximum node spacing in the horizontal direction is 0.125 and 1.25 cm, respectively; the corresponding numbers in the vertical direction are 0.2 and 1.0 cm. This case was solved in steady mode for a specified maximum of 1000 and a minimum of 500 steps. In actual simulations, the solution converged to the specified convergence in less than 500 steps.

TABLE 3.5.2: Input Commands for Problem B5

```
************************************************************************
TITLe Saturated Flow in a Fractured Porous Medium
************************************************************************
////  Magnuson S.W., R.G. Baca & A.J. Sondrup, August 1990.  Independent
////  Verification and Benchmark Testing of The PORFLO-3 Computer Code,
////  Version 1.0, EGG-BG-9175; INEL, Idaho Falls, ID 83415.
************************************************************************
/
GRID 49 by 93
/
COORdinate X
    -1.250  1.250  2.500  3.750  5.000  6.250  7.500  8.125  8.750  9.062
     9.375  9.562  9.750  9.875 10.000 10.125 10.250 10.438 10.625 10.937
    11.250 11.875 12.500 13.750 15.000 16.250 17.500 18.125 18.750 19.062
    19.375 19.562 19.750 19.875 20.000 20.125 20.250 20.438 20.625 20.937
    21.250 21.875 22.500 23.750 25.000 26.250 27.500 28.750 31.250
/
COORdinate y
            0.0    1.0    2.0    3.0    4.0    5.0    6.0    7.0    8.0
     9.0    9.5    9.9   10.1   10.5   11.0   12.0   13.0   14.0   15.0
    16.0   17.0   18.0   19.0   20.0   21.0   22.0   23.0   24.0   25.0
    26.0   27.0   28.0   29.0   29.5   29.9   30.1   30.5   31.0   32.0
    33.0   34.0   35.0   36.0   37.0   38.0   39.0   40.0   41.0   42.0
    43.0   44.0   45.0   46.0   47.0   48.0   49.0   49.5   49.9   50.1
    50.5   51.0   52.0   53.0   54.0   55.0   56.0   57.0   58.0   59.0
    60.0   61.0   62.0   63.0   64.0   65.0   66.0   67.0   68.0   69.0
    69.5   69.9   70.1   70.5   71.0   72.0   73.0   74.0   75.0   76.0
    77.0   78.0   79.0   80.0
/
ZONE  1 from  (1, 1)  to  (49,93)
ZONE  2 from (15,59)  to  (15,81)  FRACture width=0.030 cm
ZONE  3 from (35,13)  to  (35,35)  FRACture width=0.030 cm
/
FOR zone 1     $the basalt matrix
HYDRaulic props S=0.0, kx=4.e-3, ky=4.e-3, kz=4.e-3 cm/sec
ROCK rho=1 eff porosity=0.24, total porosity=0.24, diffusive por=0.24
PROP for P using GEOMetric mean option
/
FOR zone 2 and 3      $fractures
HYDRaulic porps S=0.0 K=(3*6.E2) cm/sec
/HYDRaulic porps S=0.0 K=(3*6.E3) cm/sec
ROCK rho=1 porosity = (3*1.0)
/
SET LINEar function P = 0. + 0.0025 Y
/
BOUNdary cond for P: index -1, grad  = 0.
BOUNdary cond for P: index +1, grad  = 0.
BOUNdary cond for P: index -2, value = 0.
BOUNdary cond for P: index +2, value = .2
/
DIAGnostic node at (13,69) every 10 steps
SELEct window from (13,1) to (13,93)
SAVE on 'B5.ARC' P and H only
/
MATRix for P X and Y directions
CONVERGENCE CRITERION 1.E-7
/
SOLVe for STEAdy state  max 1000 min 500
OUTPut P for SELEcted window
/
END
```

Comparison Solution

The FLASH computer code (Baca and Magnuson, 1992) was used for comparison with PORFLOW . The comparative data for FLASH simulations was supplied by Magnuson (1993).

PORFLOW™ Output

The output requirement for this test is the steady-state pressure distribution for the computational domain.

Results & Discussion

The steady-state pressure distribution for PORFLOW is compared with that from FLASH in Figure 3.5.2. The effect of the embedded fractures is clearly seen in that the pressure drop through the fracture is smaller than in the corresponding length of the rock. The pressure contours therefore "bow out" in the vicinity of the fractures. Since the fluid pathlines are orthogonal to the pressure contours, this implies that the fluid is preferentially channelled through these fractures. In general, the two sets of results from PORFLOW and FLASH compare very well. Small differences that exist reflect the two different methodologies used by the two models.

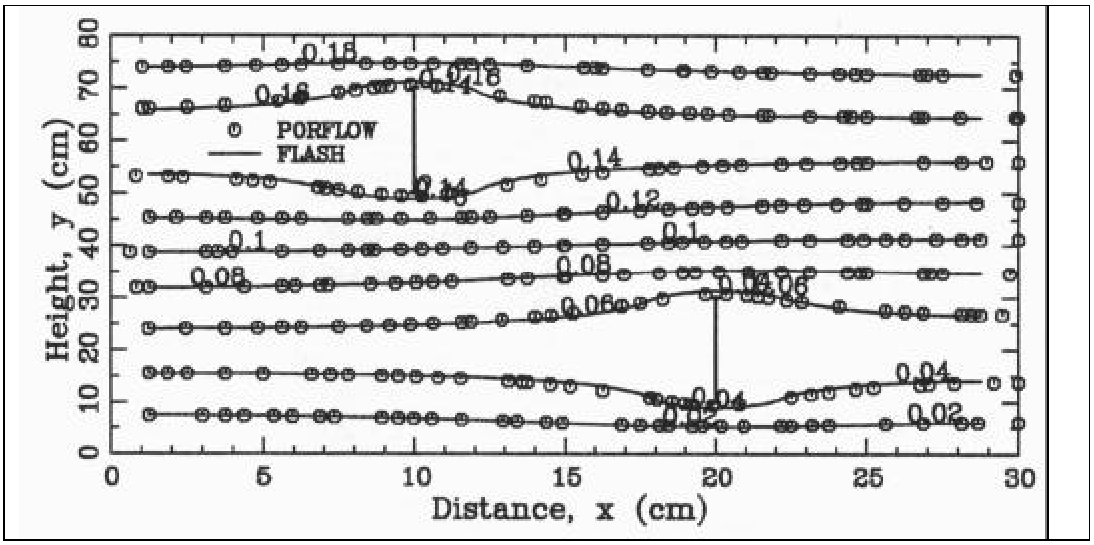

FIGURE 3.5.2: CONTOURS OF PRESSURE HEAD

3.6 PROBLEM B6: FLOW TO A GEOTHERMAL WELL

Problem Statement

The physical setting for this test problem is a geothermal well with production at a constant rate of 0.14 kg/s per meter thickness of the reservoir. Initially the reservoir is in single phase thermodynamic conditions. As the well is produced, pressure drops to the saturated vapor pressure creating two-phase liquid-vapor conditions. This leads to a boiling front which propagates outward from the well into the reservoir. Garg (1978) developed a semi-analytic theory for radial flow to a geothermal well. A modified version of Garg's problem was used at the Stanford Geothermal Program (1980) for a comparative study of reservoir simulators. Pruess (1987) obtained a numerical solution for this problem with the TOUGH computer code. The schematic of the problem is shown in Figure 3.6.1. The problem is essentially a one-dimensional problem with radial symmetry. The outer radius of the reservoir is set at 2000 m.

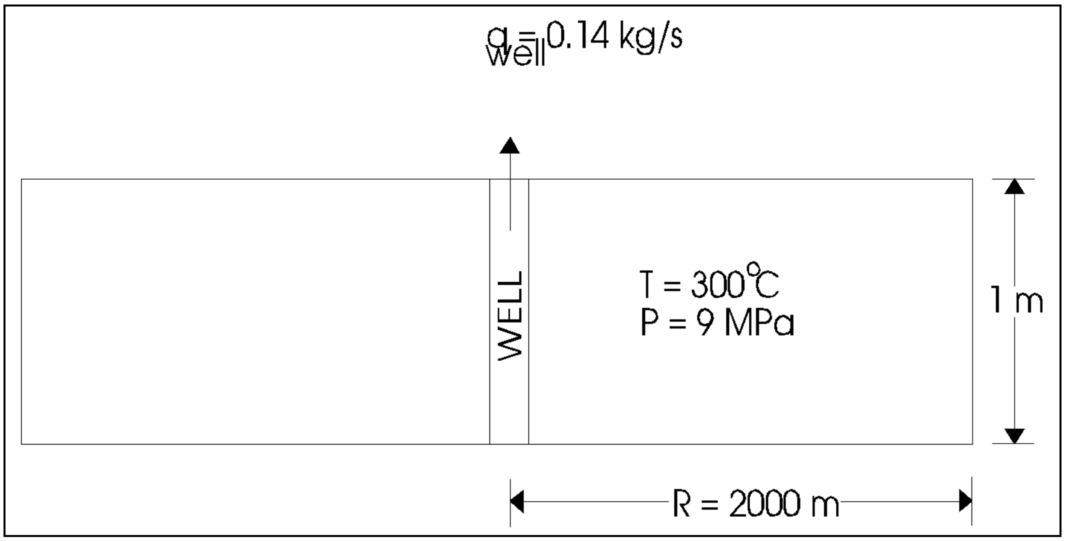

FIGURE 3.6.1: SCHEMATIC ILLUSTRATION OF PROBLEM B6

Initial Conditions

Initially, the entire reservoir is at a uniform temperature of 300 °C. The reference gas pressure is 9.0 mega-pascal (MPa) and the initial pressure head (relative to the gas pressure) is set to 0.0 m by default.

Boundary Conditions

The left boundary of the reservoir (at the well) is set to conditions of zero flux for both the liquid and gas pressures, and the temperature. The right boundary, by default, is maintained at conditions of fixed pressure and temperature at the corresponding initial value.

Properties

The fluid properties are summarized in Table 3.6.1. The reference fluid properties correspond to the initial temperature and pressure of the fluid. The actual density of the gas is computed from the gas law; the value given in Table 3.6.1 is for reference purposes only. The hydraulic properties are summarized in Table 3.6.2. The capillary pressure between the liquid and gas phases is identically zero; relative saturations of the two phases are obtained from the requirement of thermal equilibrium between the liquid and the gas. The relative hydraulic conductivity for the liquid and gas phases is computed from Equation set 3.6.1.

TABLE 3.6.1: Fluid Properties for Problem B6

Property	Liquid	Vapor
Density (kg/m^3)	712.22	46.19
Viscosity (kg/m-s)	8.60x10^{-5}	1.60x10^{-5}
Specific Heat (J/kg-K)	5741	5538
Thermal Conductivity (W/m-K)	0.545	0.0718
Compressibility (1/pascal)	3.00x10^{-9}	Gas Law
Heat of vaporization (J/kg)	---	1.51x10^6
Molecular Weight (kg/kg-mole)	---	18

TABLE 3.6.2: Hydraulic Properties for Problem B6

Property	Value
Rock density (kg/m^3)	2650
Porosity	0.20
Hydraulic Conductivity (m/s)	8.02x10^{-7}
Specific storage (m^{-1})	0.00
Specific heat of rock (J/kg-K)	1000
Thermal conductivity of rock (W/m-K)	5.25
Capillary pressure, ψ (m)	0.00
Residual liquid saturation, S_r	0.30
Residual liquid saturation, S_g	0.05

$$k_{rl} = \hat{S}^4 \ ,$$

$$k_{rg} = 1 - 2\ \hat{S} + 2\ \hat{S}^3 - \hat{S}^4 \ ,$$

$$\hat{S} = \frac{S - S_r}{1 - S_r - S_g} \ , \qquad (3.6.1)$$

where k_{rl} and k_{rg} are the relative conductivities for the liquid and gas phases, respectively, and S is the saturation of the liquid phase. S_r and S_g are the residual liquid and gas saturations, respectively.

Source

The producing well is simulated as a source just inside the left boundary. The strength of the source is 3.1285x10^{-5} m^3/m^3-s per radian. With the reference density of 712.22 kg/m^3, this corresponds to a production rate of 0.14 kg/s from the well.

Computational Details

A total of 42 nodes in the radial direction are used. The first 10 nodes from the well are placed at a uniform interval of 1 m. Thereafter, the grid size is gradually increased outward from the well to a maximum of 200 m near the outer radius of the reservoir. The problem is simulated for a total of 100,000 seconds. The starting time step of 1 second is increased in a geometric ratio of 1.02 to a maximum value of 100 seconds. Due to the very high pressure in the flow system, the gravitational effects are negligible. The interface hydraulic conductivities are evaluated by the maximum option in which the interface value is set to be the larger of the values at the two nearest neighboring nodes. The convergence tolerance for the flow is 10^{-4} and the maximum number of inner iterations is 299. The PORFLOW input commands for this problem are shown in Table 3.6.3.

Comparison Solution

The PORFLOW solution is compared to a solution using the TOUGH computer code (Pruess, 1987).

PORFLOW™ Output

The output required for this problem is well pressure as a function of time over the period of the simulation.

Results & Discussion

The PORFLOW results are shown along with those from the TOUGH computer code in Figure 3.6.2. The solid line in this figure shows the solution obtained from PORFLOW with the fluid properties as listed in Table 3.6.1. This PORFLOW solution compares well with the results from TOUGH both at the initial and the final stages of the simulations. In the time interval, $10 < t < 1000$, PORFLOW results indicate a lower pressure than that given by TOUGH. The differences between the two are largely attributed to the fluid property algorithms used in PORFLOW . TOUGH simulations employed the empirical water and steam properties as listed by the International Formulation Committee (1967). The current version of PORFLOW provides for simple polynomial relations for fluid properties; it does not provide for tabulated fluid properties. For these simulations, all fluid properties, except gas density, are set to a constant value. To explore the effect of changes in fluid properties, one simulation was performed where the liquid reference density was increased to 1,000 kg/m^3 and the vapor viscosity was decreased to 1.0×10^{-5} kg/m-s. The results for this case, shown by a dotted line in Figure 3.6.2, match the TOUGH results very well throughout the period of simulation.

TABLE 3.6.3: Input Commands for Problem B6

```
*****************************************************************************
TITLe Flow to a Geothermal Well
*****************************************************************************
////  Pruess, K., 1987.  TOUGH Users Guide. NUREG/CR-4645. U.S. Nuclear
////  Regulatory Commission (NRC), Washington, D.C. (Problem 4)
*****************************************************************************
/
PROBLEM     with EVAPoration in EQUIlibrium mode
/
GRID is     1 by 44
/
COORDINATE  r [m] are:
    -0.5    0.5    1.5    2.5  3.5  4.5  5.5   6.5   7.5   8.5
    10     12     15     20    25   30   37.5  45    55    65
    75     90     105    120   140  165  195   230   270   320
   380    450    550    650   750  850  975  1100  1200  1350
  1500  1700  1900  2100
/
GRAVITY constant 0, 0, 0, 9.81
/
REFErence T = 300                                             deg_centigrade
DENSity primary fluid: uniform  rho* =  712.22                kg_per_m^3
DENSity SECOnd fluid:  GAS law  rho* =   46.19                kg_per_m^3
VISCosity for primary fluid: 8.60E-5                          kg_per_s_m
VISCosity for SECOnd fluid:  1.60E-5                          kg_per_s_m
/
FLUId SPECific heat = 5741                                    J/kg_K
FLUId SPECific heat for SECOnd phase = 5538                   J/kg_K
FLUId second phase ENTHalphy: h0 = 1.51E6; a = 5538           J/kg
FLUId thermal CONDuctivity = 5.45E-1                          W/m_K
FLUId thermal CONDuctivity SECOnd phase = 7.18E-2             W/m_K
FLUId COMPressibility = 3.00E-9                               pascal^-1
/
GAS molecular weight: H2O = 18
GAS PRESsure  = 9.00E6                                        pascal
/
ROCK DENSity  = 2650                                          kg/m^3
ROCK POROsity = 0.20
HYDRaulic ss= 0.;  k_x = 8.02E-7, k_y = 8.02E-7               m^-1; m/s
THERmal property cp_s = 1000;  Kt_s = 5.25                    J/kg_K; W/m_K
/
MULTiphase POLYnomial: a=0, b=0, c=0, d=0, e=0, sr=0.3
MULTiphase CONDuctivity POWEr law: n=4., a=1., b=0., c=0., sr=0.3, sg=0.05
MULTiphase CONDuctivity SECOnd phase POLYnomial COMPlimentary
   a=0., b=2., c=0., d=-2., e=1., sr=0.3, sg=0.05
/
PROPerty P, P2, T  MAXimum option
/
SET T initially to 300                                        deg_centigrade
BOUNdary for P  ib = -2   FLUX =  0
BOUNdary for P2 ib = -2   FLUX =  0
BOUNdary for T  ib = -2   FLUX =  0
/
LOCAte source at (2,2)
SOURce FLOW: strength = -3.13E-5  in SELEcted region          m^3/m^3_s
/
CONVergence for FLOW criterian=1.E-4, max iter = 999
/
SAVE OFF
HISTory at (2,2)
HISTory every 2 steps on 'B6A.HIS'
DIAGnostic P, T, S  at (2,2) every 5 steps
/
SOLVe for 1E5 sec in steps of 1  1.02 100
/
END
```

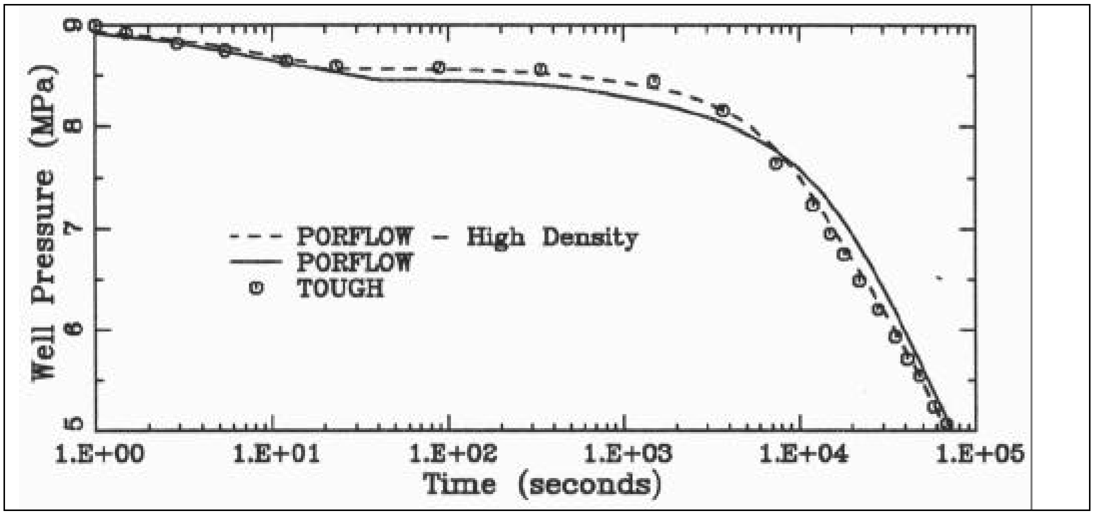

FIGURE 3.6.2: TIME HISTORY OF WELL PRESSURE

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CHAPTER 4

CONCLUSIONS

Detailed computational testing of PORFLOW Version 2.50 was conducted to determine the operational status of the software and its ability to accurately solve a wide range of problems under diverse flow conditions. For this purpose, eleven verification and six benchmark test problems were selected. PORFLOW predictions for these were compared with known analytic, semi-analytic and numerical solutions. For all test problems, the results from PORFLOW compare well, qualitatively and quantitatively, with those published in the literature. This demonstrates that PORFLOW is able to simulate all of the test problems in a satisfactory manner.

The results from PORFLOW are in very good to excellent agreement with the known analytic or semi-analytic solutions of the eleven verification problems. For the two Boussinesq problems, the PORFLOW solution initially compares very well with the semi-analytic solution; at later simulation times, minor differences exist between the two solutions. These differences may be due to the fact that the analytic solution assumes a purely horizontal flow which is theoretically, but not practically, possible.

The results from PORFLOW , for the six benchmark problems, are comparable to those produced by other computer codes. The codes used for these comparisons were TOUGH (Pruess, 1987), FEMWATER (Yeh and Ward, 1979), TRACER3D (Travis, 1984), FLASH (Baca and Magnuson, 1992), SUTRA (Voss, 1984) and INTERA (1979). These codes differ from each other significantly either in the numerical method adopted or in their mathematical formulation. Where possible, the same grid size and time step were used in PORFLOW as by the code used for comparison. In each case, the PORFLOW results compare well, both qualitatively and quantitatively, with the solution from the comparative code.

The primary purpose of the verification and benchmark testing was to demonstrate the capability of PORFLOW to produce solutions which compare well with the other known solutions rather than to achieve any specific level of accuracy. It is possible that refinements in grid size and time step may bring even closer agreement between the PORFLOW predictions and the known analytic or numerical solutions. For the benchmark case 6, PORFLOW results can be improved by incorporating fluid property algorithms more suitable for the very high pressure and temperature conditions prevailing in a geothermal reservoir. It is also to be noted that, as far as the benchmark problems are concerned, it is possible that numerical solutions from other computer codes may suffer from their own approximations and inaccuracies. For example, for the Henry's problem (Problem B4), it is quite likely that the numerical solution from PORFLOW is more accurate than those from the other codes. Consequently, no sensitivity studies were undertaken to refine the PORFLOW results or to achieve closer agreements with the results from the other codes.

Based on the results for these verification and benchmark problems, and the results from the applications of PORFLOW to a diverse range of problems over the previous 15 years (Appendix A), it can be concluded that PORFLOW is able to adequately simulate a wide range of problems in fluid flow, heat transfer and mass transport in geologic media under a diverse range of flow conditions.

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APPENDIX A

PARTIAL LIST OF PUBLICATIONS

PORFLOW has been extensively used over the last 15 years. Approximately 100 publications and project reports on the benchmarking, verification and application of PORFLOW are currently available. This appendix presents a partial list of these publications.

ACRi, 1994. PORFLOW: A Software Tool for Multiphase Fluid Flow, Heat and Mass Transport in Fractured Porous Media - Validation, Version 2.50. *Analytic & Computational Research, Inc, Los Angeles, CA.*

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