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Sandia Implementation of the TRACR3D Flow and Transport Code

Nancy K. Prindle

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SANDIA IMPLEMENTATION OF THE TRACR3D FLOW AND TRANSPORT CODE

Nancy K. Prindle
NNWSI Repository Performance Assessments
Division 6312

and

Jeffery Foster
Technadyne Engineering Consultants, Inc.

ABSTRACT

TRACR3D is a computer code developed at Los Alamos National Laboratory to model three-dimensional fluid flow and mass transport in a porous medium. The code is being considered for use in performance assessment modeling of a potential repository for high-level radioactive wastes at Yucca Mountain in Nye County, Nevada.* This report describes modifications made during the installation and implementation of the code at Sandia National Laboratories and the results of some test problems. The operating system commands necessary to direct TRACR3D on the CRAY-1 computer at Sandia are included, and a flow chart outlining the code structure is presented.

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*The Nevada Nuclear Waste Storage Investigations (NNWSI) Project, managed by the Nevada Operations Office of the U.S. Department of Energy, is examining the feasibility of siting a repository for high-level nuclear wastes at Yucca Mountain on and adjacent to the Nevada Test Site. This work, intended to extend our understanding of potential radionuclide transport in the unsaturated geohydrologic units below Yucca Mountain, was funded by the NNWSI project. The ultimate use of this information will be to build reasonable assurance in the probabilistic predictions of postclosure waste isolation.

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Acknowledgments

Bryan Travis and Steve Hodson completed a series of comparative runs at Los Alamos National Laboratory and provided the authors invaluable help with debugging efforts. Jack Gauthier and Wynona Sexson also provided considerable help at Sandia National Laboratories in installing and debugging the TRACR3D code.

1. Introduction

Purpose

TRACR3D is a large (5500 FORTRAN lines) finite-difference code developed at Los Alamos National Laboratory (LANL) by Dr. Bryan J. Travis (Travis, 1984). The code, originally developed for applications in the oil-shale industry, models isothermal, transient fluid and gas flow and chemical transport in three dimensions in a deformable, heterogeneous, reactive porous medium. Since its original development, special-purpose subroutines have been added to the code to model fluid flow and transport of radioactive chemical species in porous materials containing discrete fractures. The general characteristics of the TRACR3D code are listed in Table 1.

The features that have been added to the original code render the TRACR3D code useful for modeling simultaneous air and water flow and accompanying radionuclide transport in three-dimensional fractured, porous media. In particular, TRACR3D has been used at LANL for analyses of isothermal radionuclide transport in both aqueous and vapor phases through variably saturated, fractured tuffs such as those that make up the prospective site for the disposal of high-level radioactive waste at Yucca Mountain in Nye County, Nevada. The purpose of these analyses was to investigate the phenomena that affect isothermal radionuclide transport on relatively small scales (on the order of 1 to 10 meters) by doing sensitivity studies, experimental analysis, data interpretation, and development of "macroscopic" models of bulk behavior. The capability to do similar analyses in three dimensions can be useful to the performance assessment group at Sandia National Laboratories (SNL) for their studies for the Nevada Nuclear Waste Storage Investigations (NNWSI) Project. Thus, a version of TRACR3D was provided to SNL for installation on the SNL CRAY-1 computer. This version, which corresponds to the version described in the TRACR3D user's manual, has been stored as T3D784 at SNL.

Table 1

Characteristics of TRACR3D

DIMENSION

1-, 2-, or 3-D

NUMERICAL TECHNIQUE

Finite difference combined with method of characteristics, orthogonal elements

GOVERNING EQUATIONS

Hydrologic: Air- and water-mass conservation, Forcheimer's equation for momenta conservation of two fluids, reducing to Richards' equation at low Reynolds numbers

Solute transport: Solute conservation considering advection, dispersion, diffusion, radioactive decay chains, equilibrium adsorption, and nonequilibrium sorption

SOLUTION TECHNIQUE

Implicit, iterative, successive overrelaxation techniques for hydrologic solution, explicit or Runge-Kutta for solute concentration solutions

BOUNDARY CONDITIONS

Specified pressure, fluid saturation or fluid flux, free flow, ponding, specified concentration or solute flux, leaching, band release; can include radioactive decay

SPECIAL-PURPOSE OPTIONAL FEATURES

Discrete Fracture Model: Discrete fractures automatically generated along user-specified grid boundaries, user-defined properties used within the fractures

Sharp-Wave Fronts: User-defined values used within weighting functions applied to calculations of concentration gradients at wave fronts

The purpose of this report is to provide the necessary documentation, supplemental to that in the user's manual (Travis, 1984), for using the SNL implementation of TRACR3D for performance assessment calculations for the NNWSI project. The information contained in this report provides many details of the code structure not found in the user's manual. This is to partially satisfy requirements for quality assurance that are applicable to all analyses and computer codes that are used for licensing a high-level nuclear waste repository. These quality assurance requirements are described in NUREG-0856 (NRC, 1983) and many DOE quality assurance documents, such as NVO-196-17 (DOE-NVO, 1986) and NNWSI procedure SOP-03-02 (currently under revision). While an even newer version of TRACR3D now exists, testing and documentation of the type described in this report and others (Travis, 1984; Hayden, 1985) have not been completed for it; the T3D784 version is the most useful at this date for performance-assessment calculations.

Background

TRACR3D was developed at LANL on a CRAY X-MP driven by the Cray Time Sharing System (CTSS). An early version of TRACR3D was implemented at SNL while development of the code was still proceeding at Los Alamos. This version was modified by the author of the code, Bryan Travis, to compensate for known differences between LANL and SNL Cray operating system functions (such as routines to check the time remaining for the job). It was compiled successfully at SNL on the CRAY-1 computer, which is run by the CRAY-1 Operating System (COS) in a batch (noninteractive) environment, using the CFT 1.10 compiler.

The first task attempted at SNL was to run the sample problem, ESTE, described in the user's manual. This three-dimensional problem tracks a nonradioactive tracer through a fracture in partially saturated, tuff-like rock. The SNL results for the ESTE problem did not compare with those obtained at LANL; in fact, the problem could not even be run to a normal completion at SNL. Differences between the two operating systems were the cause of this and several other problems with the

initial implementation of TRACR3D at SNL. Some of these problems were related to the control of the program and data files; others proved to be more subtle.

Further corrections were made at LANL to the control procedures in the code, ostensibly to compensate for any differences in operating systems. (These operating systems are described in documentation by Cray Research, Inc., and in supplements developed at LANL and SNL. (See, for example, Cray Research publication SR-0011, Los Alamos publication LA-5525-M Vol 7, and the SANDIA CRAY-1 supplement.) In May 1984, the TRACR3D documentation was published, and a new version of the code, complete with operating system corrections, was installed at SNL in June. The operating system corrections included in this published version of the code were intended to ensure that the code would run on a CRAY computer independent of the operating system used.

Six problems were eventually run on both the SNL and LANL computing systems to check out the installation of the new version of TRACR3D at SNL. Comparable results for these six problems were obtained, but minor modifications to the code were necessary at SNL. In Section 2 of this report, we describe the difficulty that was encountered and the program modifications that were implemented to correct for this difficulty.

The six test problems and the results of the comparisons are discussed in Section 3. The basic steps and operating-system commands the authors developed to run the TRACR3D code on the CRAY-1 at SNL are given in Section 4. In the installation process the authors examined the structure of the TRACR3D code in detail. This report provides future users with the fruits of those examinations by means of a flowchart of the code, lists of input parameters not described in the user's manual, and a list of the STOP statements in the code and where they occur. This information, presented in Section 5, can be useful for maximizing the efficiency of individual runs, adding subroutines, and debugging.

2. Installation of TRACR3D at SNL

The installation and initial implementation of TRACR3D at SNL made extensive use of six problems described in the user's manual. One of these problems, ESTE, is provided in the user's manual as a sample problem, giving the exact input and output from runs by Travis at LANL. Therefore, the ESTE problem was used for checking out the installation of the new version of TRACR3D (corresponding to the published user's manual) at SNL and debugging.

The published version of TRACR3D still did not produce the same results at SNL for the ESTE problem as were produced at LANL. The runs at SNL used successively smaller time steps than did the runs at LANL and showed no signs of converging to a solution. The difficulty was traced to the fact that the compilers on the two CRAY systems (both of which are CFT 1.10 compilers) used different defaults for the accuracy of floating-point numbers. The compiler at LANL provided for more than the standard 14-digit accuracy that is the default on the CFT 1.10 compiler at SNL. At SNL, floating point numbers are rounded off; values of 5 or less in the 14th digit are rounded down to zero and values of 6 or more are rounded up to 1 in the 13th digit. This caused differences in the way that effective air and gas permeabilities, which are calculated using differences between adjacent cell permeabilities, were being formulated in the TRACR3D subroutines PERME and EFPERM.

Some of the significant relative gas and liquid permeabilities for the ESTE problem become very small numbers (as low as 10^{-16}). These relative-permeability values are highly dependent on the saturation and pressure. For each iteration within a time step, the internal variables XG and XL in the subroutine PERME, and SLE1 and SLE2 in the subroutine EFPERM temporarily store the relative permeabilities, which are normalized to the saturated values of the gas and liquid permeability of the cell material, respectively. The variables XG and XL are used to calculate relative permeabilities within individual cells in the

subroutine PERME. The variables SLE1 and SLE2 are used to calculate effective permeabilities across cell interfaces in the subroutine EFPERM.

One of several averaging functions is chosen in EFPERM to calculate the effective permeability across each cell interface. The choice of the averaging function depends on the absolute values of SLE1 and SLE2, which are functions of the difference between the values of XG and XL in the adjacent cells. In some of the quasi-steady-state regions with either very low water saturation or very low air content, the significant differences between the relative permeabilities in adjacent cells were occurring only beyond the 14th digit--in the 16th digit and beyond. Therefore, there were some cells for which SLE1 and SLE2 were being evaluated as zero on the CRAY-1 at SNL, while for the same time step and node, these variables were being calculated to be very small nonzero numbers on the CRAY X-MP at LANL.

Because of the aforementioned difference in the default accuracies being used, the code was branching to different functions within the subroutine EFPERM to calculate the effective cell permeabilities across these cell interfaces. Not only were different functions being used to calculate effective permeabilities for these cells, but the function input variables SLE1 and SLE2 were different, being zero on the SNL CRAY-1 and small but nonzero on the LANL CRAY X-MP. The result was that for a few cell interfaces, TRACR3D was evaluating the effective permeability as zero on the SNL CRAY, which caused the code to take successively more and more iterations to converge within a time step, until it seemingly ran into nonconvergence problems.

This discrepancy might have been corrected by using some double precision variables on the SNL CRAY-1. However, this would have resulted a necessity for two versions of the code. Moreover, differences in the 14th digit in the relative permeabilities are not necessarily accurate. What is required is not more accuracy but the <u>same</u> accuracy.

To that end, program constraints were introduced in the subroutines PERME and EFPERM that limit the minimum value of the variables XG, XL, SLE1, and SLE2 to 1.0×10^{-13}. This in effect eliminated the

possibility for round-off error of these variables. The constraints did not noticeably affect the accuracy of the calculation, as was borne out by like results at LANL before and after adding the constraints. Further, these constraints resulted in an exact comparison between the subsequent runs of ESTE at SNL and LANL.

The constraints were introduced in TRACR3D by adding two statements to the PERME subroutine and modifying four existing statements in the EFPERM subroutine. The statements added in PERME were

```
    XG(IJK)=AMAX1(1.E-13,XG(IJK))
    XL(IJK)=AMAX1(1.E-13,XL(IJK))
```

These statements were added just prior to the continue statement labeled 10, in the do-loop for calculating cell relative permeabilities. (See program listing in Appendix A.)

The four statements that were modified in EFPERM now appear as

```
20  SLE1=AMAX1(1.E-13,(1.-F(IDONR)-SWI(MDONR))/(1.-SWI(MDONR)))
    SLE2=AMAX1(1.E-13,(1.-F(IACPT)-SWI(MACPT))/(1.-SWI(MACPT)))
```

and

```
60  SLE1=AMAX1(1.E-13,(1.-F(IDONR)-SWI(MDONR))/(1.SWI(MDONR)))
    SLE2=AMAX2(1.E-13,(1.-F(IACPT)-SWI(MACPT))/(1.SWI(MACPT)))
```

(The modifications to the original statements are underlined.)

In addition to the constraints for the minimum value of the relative permeabilities, the published version of TRACR3D was also changed to better implement the PARAMETER statements. (This program modification was made at LANL by Steve Hodson while helping the authors debug the SNL installation of TRACR3D). The PARAMETER statements are used as described in Section 4 of this report to minimize the storage allocated for small runs. An additional parameter was added to the PARAMETER list in the code. The additional parameter is NXX, which was added to store the

maximum of three other parameters, NMX, NQX, and NNX. Thus, the following statement modifications were made in the main program (statement modifications are underlined):

```
PARAMETER (NMX=13,NQX=13,NNX=43,NXX=43,NTRC=1,MQNP=9999)
```

and

```
.ATM,PTITLE(8),RHOL,ITRACF,AVR(NXX),AVY(NXX),AVZ(NXX),PRTLEV(10,3).
```

The new parameter NXX was then inserted into the following dimension statement in the subroutine BONDRY (modifications to the published version are underlined):

```
DIMENSION AVXYZ(NXX,3),IJKS(3),BB(10),ITDBDY(1)
```

The constraints on the relative permeabilities and the modifications to the PARAMETER list and DIMENSION statements were installed in the TRACR3D code at LANL, and a new version was supplied to SNL. The ESTE problem was then run to a normal completion at SNL, and the output compared exactly with that produced at LANL. The five other test problems were then run and the results compared. These comparisons are discussed in the next section and provide further installation testing of the code. The test problems GEN1, GEN2, and PIG3 provide checks on the numerical accuracy of the code because analytic solutions are available. The test problems ESTE, VARP, and LS6 provide sensitivity comparisons for the code by comparing the solutions produced on two different computer systems.

3. Summary of Test Problems

Problem Descriptions

The six problems that were run to test the installation of TRACR3D at SNL and to do initial benchmarking for numerical accuracy are described in the user's manual (Travis, 1984) and its supporting references (see REFERENCES). The first problem attempted at SNL was ESTE, which is the sample problem presented in Appendix C of the published TRACR3D user's manual. The five other problems described in the user's manual are analyses done by Travis for verification and validation of TRACR3D. The input and output to these problems were generously provided to the authors by Travis to test further the SNL implementation of TRACR3D and to do some benchmarking comparisons. Table 2 gives a brief description of each of these problems. Collectively, these test problems call on the subroutines that might be used for calculating isothermal water flow and radionuclide transport in unsaturated or saturated, fractured, porous media.

Comparison of Results

The results generated with TRACR3D at SNL and LANL have been compared in several ways. The code calculates not only saturation, pressure, and concentration fields, but also controls features such as the time steps, the number of iterations per time step, and residual errors. Variable property values are calculated. These calculated variables should compare exactly within the same time steps and cells if the code is running exactly the same on different systems. As we have already noted, however, differences in the compilers can cause minor differences in the results. These differences can be expected to be insignificant, in most cases. The experiences with running the sample problem ESTE, however, suggested that it would be prudent to investigate whether there were any further significant differences in the way the TRACR3D code was running on the SNL and LANL computer systems. Thus, the number of time steps,

Table 2

Descriptions of Test Problems

1. ESTE
   Three-dimensional, transient water flow and transport of a nonreactive solute in a low-permeability, partially saturated, porous medium with a single vertical, planar fracture. This sample problem is fully described in Appendix C of the TRACR3D user's manual (Travis, 1984).

2. GEN1
   One-dimensional transport of nonreactive solute by steady-state water flow and molecular diffusion in a saturated, homogeneous, porous medium (Van Genuchten, 1976).

3. GEN2
   One-dimensional transport of a radioactive solute by steady-state water flow and molecular diffusion in a saturated, homogeneous, porous medium; equilibrium sorption assumed. This problem was analytically solved by Genuchten (Van Genuchten, 1981).

4. VARP
   One-dimensional, transient water flow in a homogeneous, saturated porous medium using pressure-dependent permeability (Horning, 1977).

5. PIG3
   One-dimensional transport of a three-member chain of radioactive solutes by steady-state water flow in a saturated, homogeneous, porous medium; equilibrium sorption assumed (Pigford, 1980).

6. LS6
   Three-dimensional, transient water drainage through layers of crushed tuff, sand, and gravel using tables for moisture contents as functions of pressure and the Brooks-Corey model for pressure-dependent permeabilities. This problem is an analysis of a field experiment at LANL (Perkins and Travis, 1985).

time-step sizes, and number of iterations per time step were compared for each run. If these compared favorably, the results for the saturation, pressure, and concentration solutions were compared, depending on the problem. Finally, mass balances were compared. Selected output from these problems is given in the tables in Appendix C; a general discussion of the results and conclusions based on these results follows in this section.

For the first four test problems, the variables that control time-step sizes and numbers of iterations were identical out to four decimal places, as were calculated water-saturation values. Tabulated values in both space and time (where appropriate) for pressures and mass concentrations were the same out to three significant digits. In particular, water saturations and tracer concentrations as functions of time and three-dimensional space were the same to three significant digits for the ESTE problem. (Complete tables of these results are published in the TRACR3D user's manual.) For both the GEN1 and GEN2 problems, the one-dimensional, steady-state results for the tracer concentrations as functions of space were also the same to three significant digits. The transient, three-dimensional solution for pressures compared similarly well in the VARP problem.

In the fifth problem, PIG3, all but the initial value of the third member of the decay chain compared exactly to three significant digits. The initial value for the concentration of the third member of the decay chain was computed to be -8.54×10^{-17} at LANL and 2.2×10^{-17} at SNL. This discrepancy in the initial value was traced to the subroutine BOUNDRY, where the Bateman equations for radioactive decay reduce to several terms that should theoretically cancel to zero. However, because of the numerical solution scheme, differences were occurring in the 14th significant digit and beyond, resulting in the nonzero results. If necessary, a simple correction for this error could be implemented in TRACR3D by putting a practical lower limit on the variable SUM, below which SUM is set to zero. However, because of the otherwise excellent comparison of the PIG3 results, we did not think it necessary to rerun the calculation at SNL using such a correction.

The comparisons for the sixth test problem, LS6, were more difficult to interpret than the others . Results show an excellent match except for values at or near material interfaces. In LS6, a field experiment is modeled where water flows through a vertical caisson 600 cm deep. The caisson is filled with crushed tuff except at the bottom of the caisson, where a 9-in. layer of sand overlies a 9-in. layer of gravel. Between the three distinct materials--tuff, sand, and gravel--there are two interfaces where material properties change significantly. These properties, water and gas permeabilities and capillary pressure, are functions of saturation, as shown in Tables 3 through 5 and in Figures 1 through 3.

In the LS6 problem, a pulse of water was introduced at the top of the caisson and monitored as it infiltrated downward. In modeling the movement and distribution of the water pulse in the caisson, the LANL CRAY and the SNL CRAY used different numbers of iterations within time steps to converge to a pressure solution. Since TRACR3D automatically cuts down the time step after a certain number of iterations have been performed, different time-step patterns were established, making comparisons between tabulated outputs difficult. The results for water pressures and air saturations were therefore plotted as functions of time at four locations--two points in the tuff, the material interface between the sand and tuff, and the gravel at the boundary node (which is typically one of the most sensitive nodes in a calculation). These are illustrated in Figures 4 through 11.

Values obtained for water pressure and air saturation for two locations in the tuff were almost identical at times near each other (Figures 4, 5, 8, 9). For the location in the 9-in. layer of sand (at the interface with tuff), the results also matched well (Figures 6, 10). However, at first glance, there appeared to be considerable discrepancy in the results in the gravel at the boundary node (Figures 7, 11). These discrepancies have been ascribed to sensitivity in the calculation of permeabilities at this interface. The permeabilities in this region are extremely nonlinear, changing by more than 14 orders of magnitude over the water saturation range from 0.0 to 0.1 (see Figure 1). Considering

Table 3

Material Properties for Tuff in Test Problem LS6

Saturation	K_l (darcy)	K_g (darcy)	P_c (cm)
0.00005	0.00000E+00	0.00000E+00	0.60E+07
0.00050	0.00000E+00	0.00000E+00	
0.00500	0.00000E+00	0.00000E+00	
0.01000	0.00000E+00	0.00000E+00	
0.05000	0.00000E+00	0.00000E+00	
0.10000	0.00000E+00	0.25000E+00	0.05E+07
0.11500	0.70537E-14	0.24174E+00	
0.12500	0.34587E-12	0.23630E+00	
0.15000	0.68039E-10	0.22299E+00	
0.20000	0.13385E-07	0.19753E+00	0.40E+07
0.25000	0.29405E-06	0.17360E+00	0.13E+07
0.30000	0.26330E-05	0.15120E+00	0.70E+06
0.35000	0.14418E-04	0.13030E+00	0.46E+06
0.40000	0.57846E-04	0.11088E+00	0.38E+06
0.45000	0.18724E-03	0.92902E+01	0.30E+06
0.50000	0.51797E-03	0.76351E+01	0.22E+06
0.55000	0.12708E-02	0.61229E+01	0.17E+06
0.60000	0.28634E-02	0.47567E+01	0.14E+06
0.65000	0.58637E-02	0.35434E+01	0.13E+06
0.70000	0.11380E-01	0.24933E+01	0.90E+05
0.75000	0.20942E-01	0.16192E+01	0.70E+05
0.80000	0.36835E-01	0.93387E+02	0.55E+05
0.85000	0.62313E-01	0.44519E+02	0.45E+05
0.90000	0.10190E-00	0.14943E+02	0.40E+05
0.95000	0.16173E-00	0.21199E+03	
1.00000	0.25000E-00	0.00000E+00	0.00E+05

Saturation = volumetric moisture content/porosity

Table 4

Material Properties for Sand
in Test Problem LS6

Saturation	K_l (darcy)	K_g (darcy)	P_c (cm)
0.00005	0.15625E-20	0.49995E+01	0.30000E+09
0.00050	0.15625E-15	0.49950E+01	0.30000E+08
0.00500	0.15625E-10	0.49501E+01	0.30000E+07
0.01000	0.50000E-09	0.49005E+01	0.15000E+07
0.05000	0.15625E-05	0.45119E+01	0.30000E+06
0.10000	0.50000E-04	0.40459E+01	0.15000E+06
0.11500	0.10057E-03	0.39102E+01	0.13043E+06
0.12500	0.15259E-03	0.38206E+01	0.12000E+06
0.15000	0.37969E-03	0.36003E+01	0.10000E+06
0.20000	0.16000E-02	0.31744E+01	0.75000E+05
0.25000	0.48828E-02	0.27686E+01	0.60000E+05
0.30000	0.12150E-01	0.23838E+01	0.50000E+05
0.35000	0.26261E-01	0.20219E+01	0.42857E+05
0.40000	0.51200E-01	0.16848E+01	0.37500E+05
0.45000	0.92264E-01	0.13747E+01	0.33333E+05
0.50000	0.15625E-00	0.10937E+01	0.30000E+05
0.55000	0.25164E-00	0.84404E+00	0.27273E+05
0.60000	0.38880E-00	0.62720E+00	0.25000E+05
0.65000	0.58015E-00	0.44429E+00	0.23077E+05
0.70000	0.84035E-00	0.29565E+00	0.21429E+05
0.75000	0.11865E-01	0.18066E+00	0.20000E+05
0.80000	0.16384E-01	0.97600E+01	0.18750E+05
0.85000	0.22185E-01	0.43411E+01	0.17647E+05
0.90000	0.29525E-01	0.13550E+01	0.16667E+05
0.95000	0.38689E-01	0.17828E+02	0.15789E+05
1.00000	0.50000E-01	0.00000E+00	0.15000E+05

Saturation = volumetric moisture content/porosity

Table 5

Material Properties for Gravel
in Test Problem LS6

Saturation	K_l (darcy)	K_g (darcy)	P_c (cm)
0.00005	0.51740E-12	0.29997E+02	0.26922E+05
0.00050	0.82002E-09	0.29967E+02	0.21385E+05
0.00500	0.12996E-05	0.29649E+02	0.16986E+05
0.01000	0.11943E-04	0.29286E+02	0.15849E+05
0.05000	0.20598E-02	0.26331E+02	0.13493E+05
0.10000	0.18929E-01	0.22767E+02	0.12589E+05
0.11500	0.29604E-01	0.21743E+02	0.12415E+05
0.12500	0.38657E-01	0.21075E+02	0.12311E+05
0.15000	0.69281E-01	0.19450E+02	0.12089E+05
0.20000	0.17395E+00	0.16417E+02	0.11746E+05
0.25000	0.35525E+00	0.13678E+02	0.11487E+05
0.30000	0.63666E+00	0.11234E+02	0.11279E+05
0.35000	0.10427E+01	0.90789E+01	0.11107E+05
0.40000	0.15985E+01	0.72034E+01	0.10960E+05
0.45000	0.23302E+01	0.55940E+01	0.10831E+05
0.50000	0.32646E+01	0.42354E+01	0.10718E+05
0.55000	0.44288E+01	0.31103E+01	0.10616E+05
0.60000	0.58507E+01	0.21997E+01	0.10524E+05
0.65000	0.75586E+01	0.14834E+01	0.10440E+05
0.70000	0.95815E+01	0.94013E+00	0.10363E+05
0.75000	0.11949E+02	0.54738E+00	0.10292E+05
0.80000	0.14690E+02	0.28190E+00	0.10226E+05
0.85000	0.17835E+02	0.11960E+00	0.10164E+05
0.90000	0.21414E+02	0.35630E-01	0.10106E+05
0.95000	0.25459E+02	0.44771E-02	0.10051E+05
1.00000	0.30000E+02	0.00000E+00	0.10000E+05

Saturation = volumetric moisture content/porosity

Figure 1. Liquid Permeabilities As Functions of Saturation for Test Problem LS6

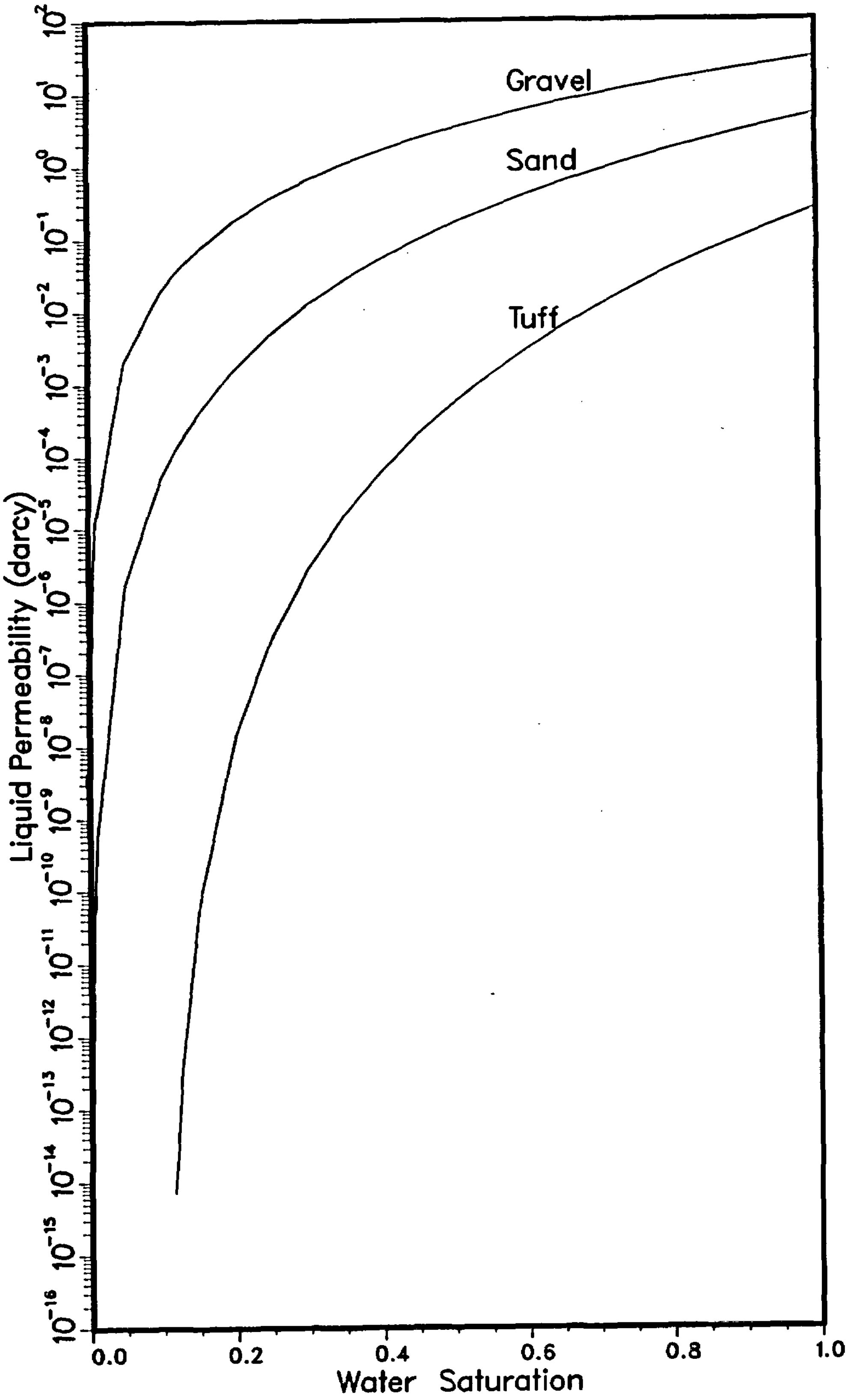


Figure 2. Gas Permeabilities As Functions of Saturation for Test Problem LS6

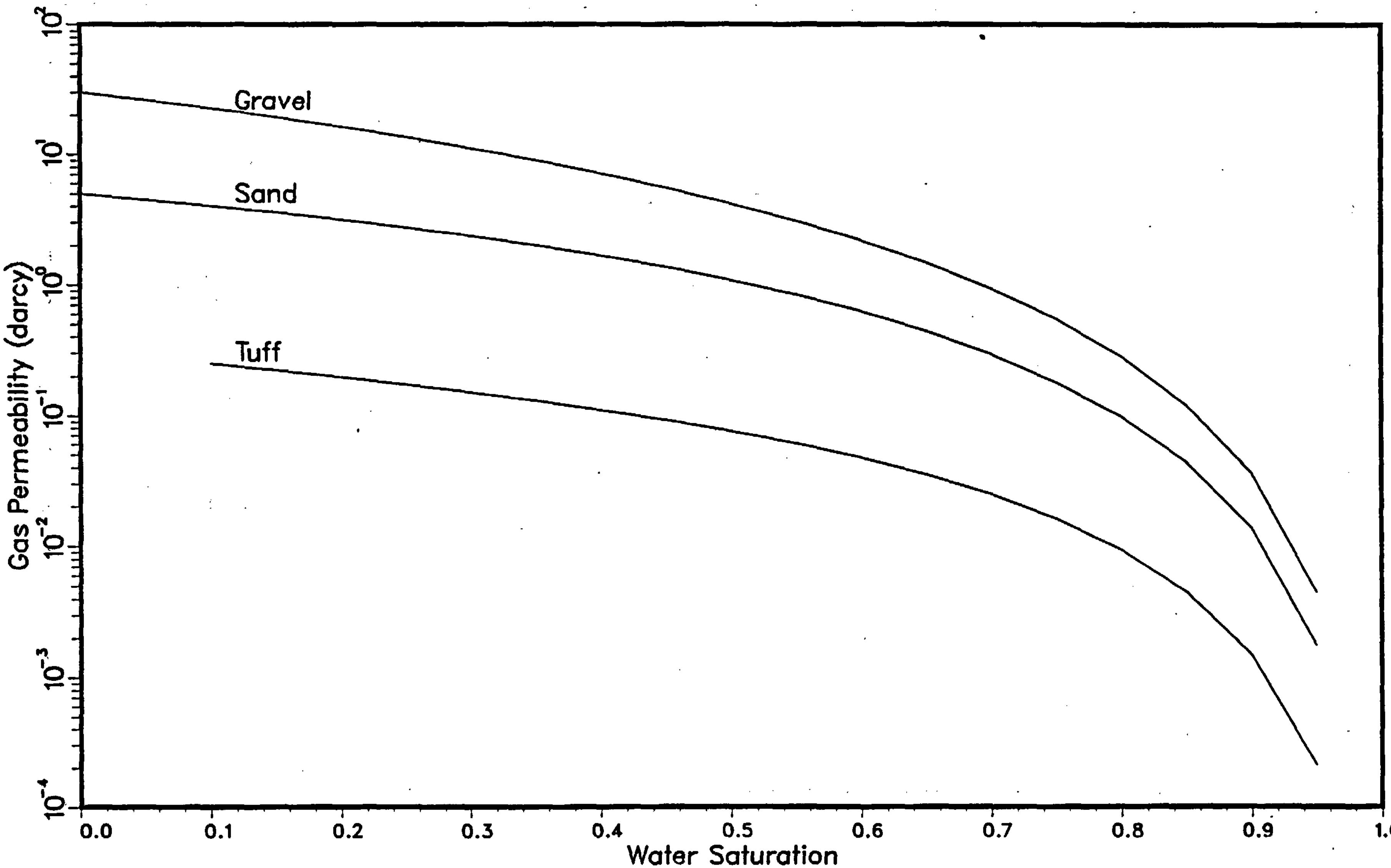


Figure 3. Capillary Pressures As Functions of Saturation
for Test Problem LS6

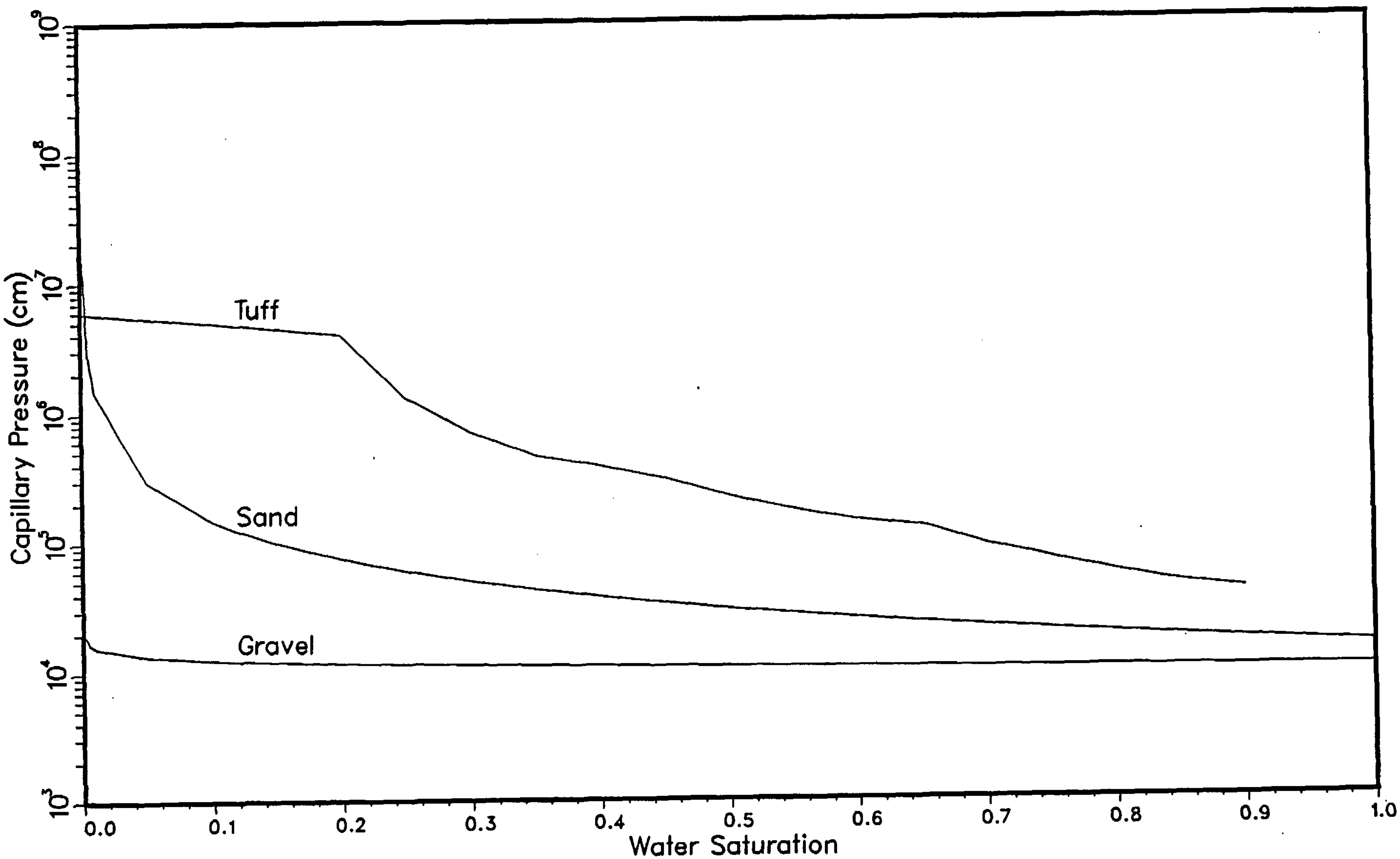


Figure 4. LS6 Comparison

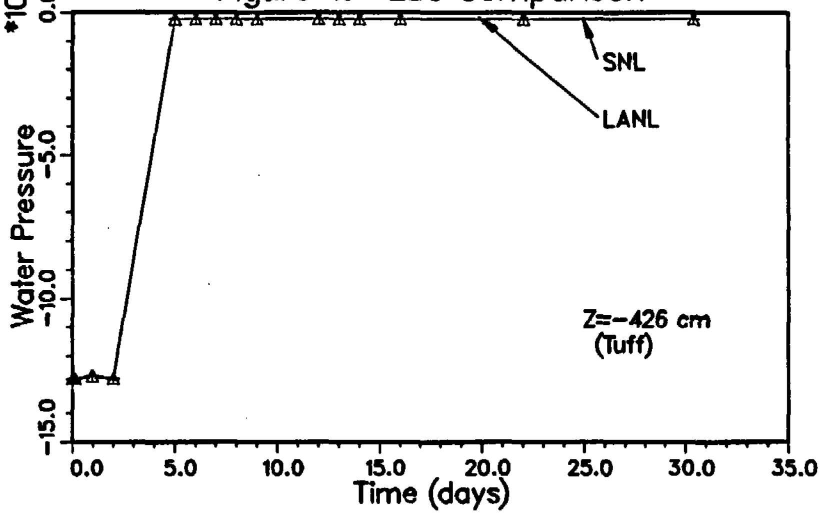


Figure 5. LS6 Comparison

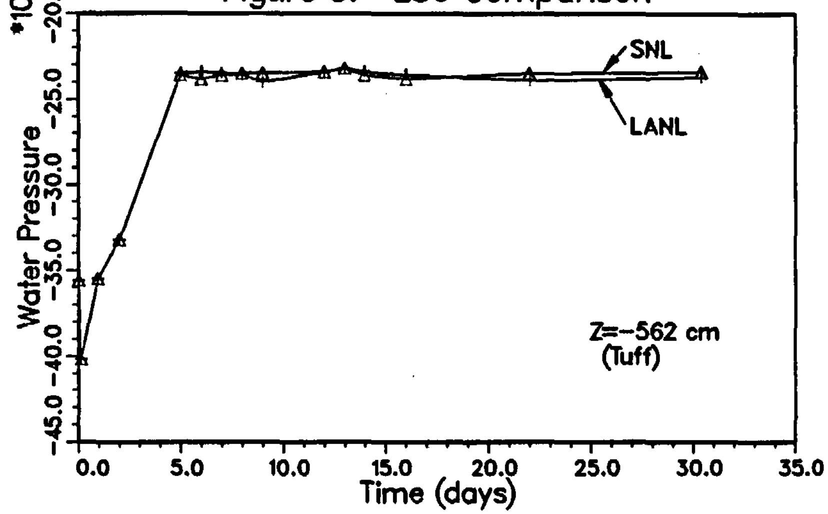


Figure 6. LS6 Comparison

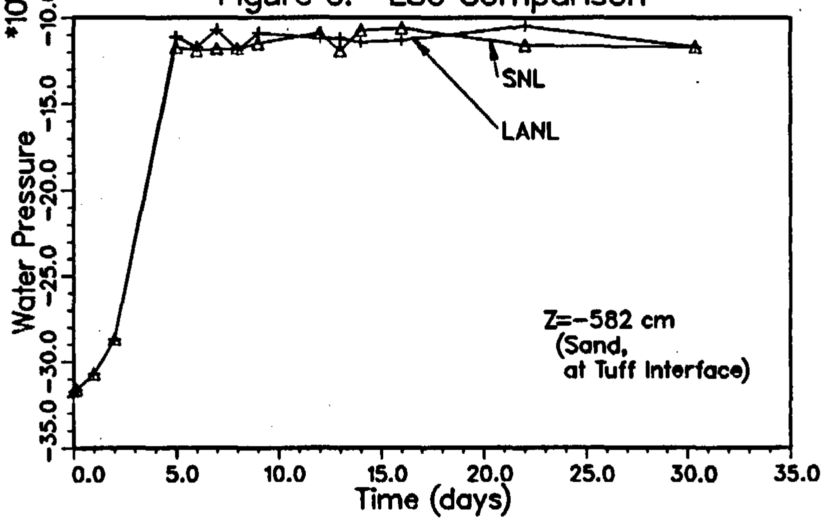


Figure 7. LS6 Comparison

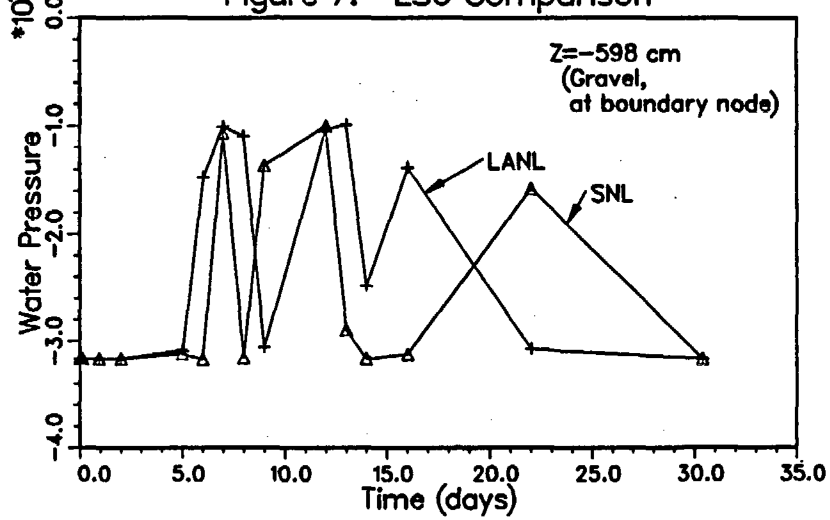


Figure 8. LS6 Comparison

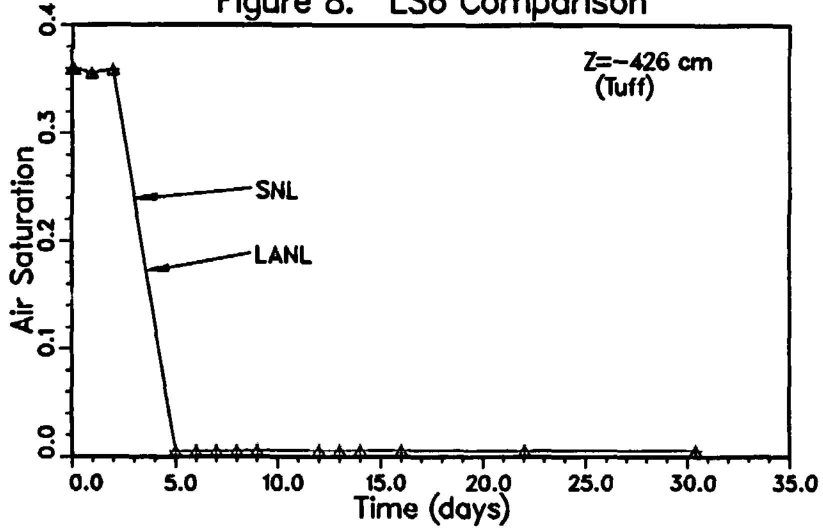


Figure 9. LS6 Comparison

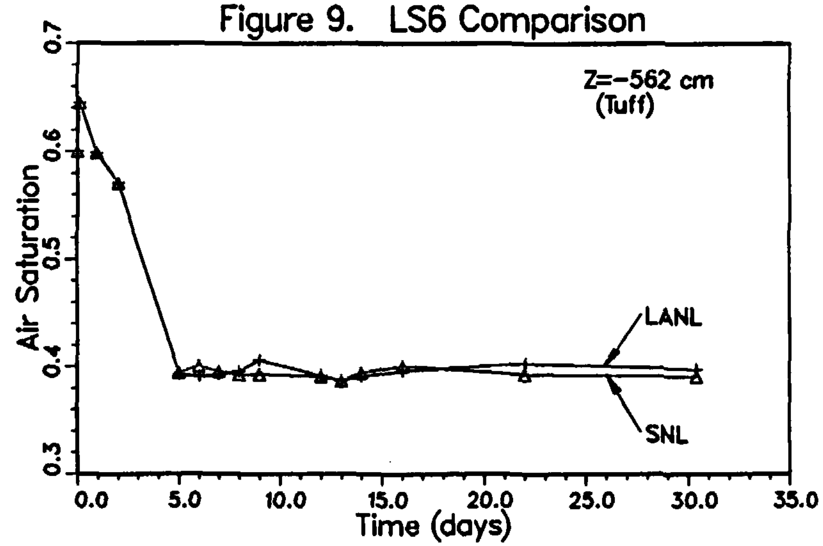


Figure 10. LS6 Comparison

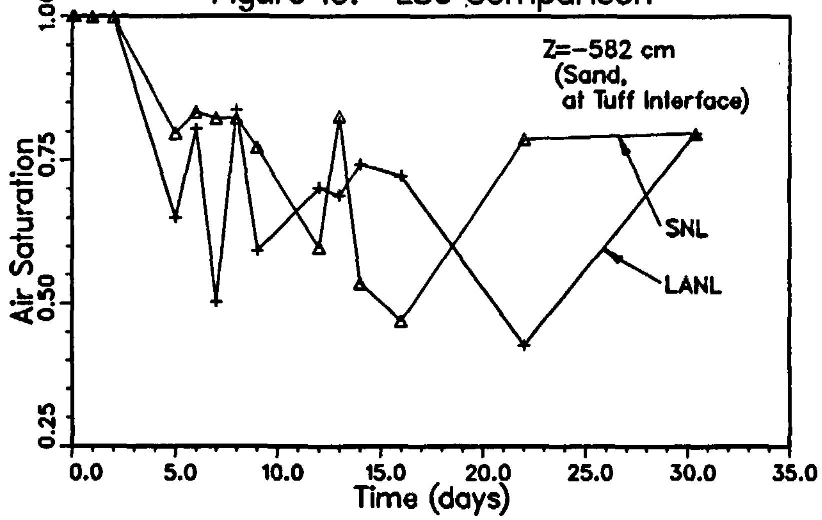
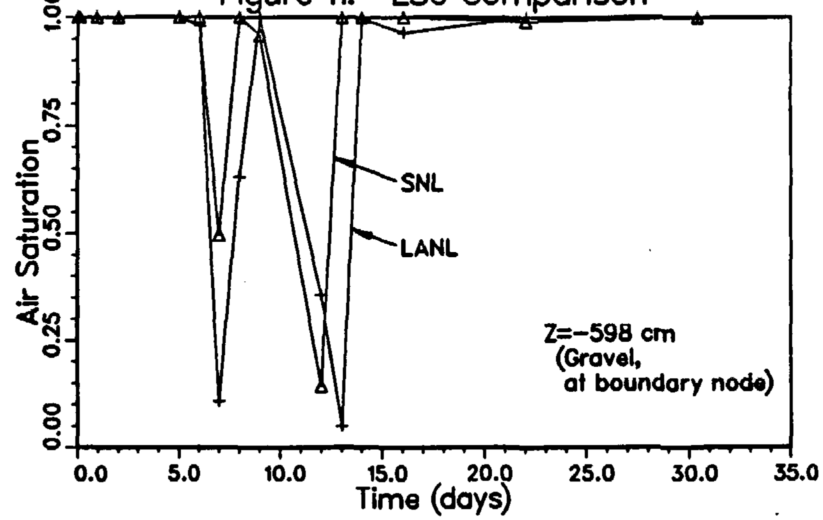


Figure 11. LS6 Comparison



this very large nonlinearity over such a relatively small range, the comparisons in Figures 7 and 11 are considered reasonable. Better comparisons could probably be attained by increasing the number of grid points, decreasing the time-step size, and making the convergence criteria more strict. Such efforts were not considered warranted, however, because of the high computer costs that would be involved.

Test problem LS6 was the only problem for which plots were generated to compare results. All other results were compared on the basis of tabulated output. To enable future users to make similar comparisons, the complete results for each problem will be stored in the NNWSI Records Center. Some representative output for each problem is reproduced in Appendix C.

Input Descriptions

The input decks for these six problems can be used as samples for preparing input files to run in TRACR3D and as test cases for future users of TRACR3D. The input file structure and input variables are described in detail in the user's manual (Travis, 1984). However, Travis provides only one sample input file, and some input descriptions can benefit from further clarification. The input files used for the six test problems are reproduced in Appendix B, and some input variables are briefly discussed below to augment the material in the user's manual.

As described by Travis in the user's manual, a TRACR3D input file consists of two data lines that control restarts and plotting. These first two lines are followed by a NAMELIST group. The values of all input variables are assigned in free format through the NAMELIST statement. This procedure results in very simple input decks, as shown in Appendix B.

TRACR3D allows the user to control the amount of computer storage allocated for each run through the use of variable array sizes. These array sizes are assigned in PARAMETER statements. The variables that control the array sizes and that are set in the PARAMETER statements are

NMX -- NO. OF X ZONES + 3 (COLUMNS, SEE INPUT PARAMETER RCM)
NQX -- NO. OF Y ZONES + 3 (ROWS, SEE INPUT PARAMETER YCM)
NNX -- NO. OF Z ZONES + 3 (LAYERS, SEE INPUT PARAMETER ZCM)
NXX -- MAXIMUM OF NMX, NQX, NNX
NTRC -- NO. OF TRACERS
MQNP -- DIMENSION OF ARRAY P . . . MUST BE MAX (MQNX, 7400)
NPTBL -- NO. OF POINTS IN INTERNAL PC AND PERMEABILITY TABLES

The default values of these parameters in the version of TRACR3D that resides on the CRAY-1 at SNL are set in the following PARAMETER statements:

```
PARAMETER (NMX=13,NQX=13,NNX=43,NXX=43,NTRC=1,MQNP=9999)
PARAMETER (NPTBL=101,NTBL=6)
PARAMETER (MQNX=NMX*NQX*NNX,MQNX3=NTRC*MQNX+1,MQNX9=MQNX*9)
PARAMETER (LENA1=8*MQNX,LENA3=5*MQNX,LENA6=12*MQNX,LENA12=2*MQNX3)
PARAMETER (LENA15=6*NPTBL*NTBL+2+MQNX*4+NTBL,LENCELL=MQNX+14)
```

The above parameter statements are read by TRACR3D prior to program execution. (For more information on using PARAMETER statements, see, for example, Cray Research publication SR-0009.) It is readily apparent that in these PARAMETER statements, the exact sizes of several large arrays are determined by the number of zones in each dimension of the grid used for the problem and by the number of data entries for material property tables.

The PARAMETER statements should be adjusted only when a particular run can be made more efficient by minimizing the amount of storage or if the default values above are not sufficient. Therefore, the variables in these PARAMETER statements do not always need to be reset. However, careful attention must be maintained to ensure that NMX, NQX, NNX, NSS, MTRC, MQNP, NPTBL, and NTBL are always large enough to accommodate the grid size of the run, the material property tables, or the number of tracers. Should a user need to change a value of one of these parameters, he must do so by changing the appropriate PARAMETER statement. The simplest way to do this is through an UPDATE directive, although this requires recompiling the object code.

4. Steps in Running TRACR3D at SNL

Basic Steps

The authors ran TRACR3D on the CRAY-1 at SNL using the COS commands. (Subsequent work will test TRACR3D using CTSS that is now available at SNL). The COS can be reached by submitting a job through the remote job entry (RJE) utility on most of the VAX computers at SNL. (For a user's guide for this utility, see Samuelson and Brown, 1982). The three files necessary to run a TRACR3D job in this way can be generated on the VAX computer. The three files are

1. Input Data File - contains the input required by TRACR3D, as described in the user's manual (Travis, 1984). The user should note that for a normal run of TRACR3D, the first line of this file should contain two zeros; this line is frequently invisible on both hard copies and CRT screens since a blank line is often used, being read in as two zeros.

2. UPDATE Directives File - a file of FORTRAN lines and UPDATE directives to modify the TRACR3D code. UPDATE is a system program that provides editing capability (for more on the UPDATE program, see the UPDATE Reference Manual). The TRACR3D code is stored as a permanent data set (file) called T3D784 on the CRAY-1 system in the proper format for UPDATE. The UPDATE modifications can be extensive, resulting in a custom version of TRACR3D, but most often should amount to no more than changing the values of variables in the FORTRAN PARAMETER statement. These variables can be used to make program compilations and execution more efficient for small problems as described in the previous section. A sample UPDATE directives file in which only one PARAMETER statement was modified is shown below for one of the test problems (PIG3, with 3 tracers and 200 cells in the z-direction). If the user is not going to modify any part of TRACR3D other than the PARAMETER statements, then an UPDATE file similar to the following should be sufficient:

UPDATE FILE FOR PIG3

```
*IDENT PIGFORD
*D PARAM.23
    PARAMETER (NMX=4, NQX=4,NNX=203,NXX=203,NTRC=3,MQNP=7400)
```

If more extensive modifications are to be made, the user will need a complete source listing of T3D784 to identify line numbers for the UPDATE directives. This can be obtained by printing the T3D784 file from UPDATE or CFT (the CRAY-1 FORTRAN compiler).

If no modifications are to be made at all, i.e., no PARAMETER statement needs to be included, the UPDATE file is not necessary.

3. COS Command File - contains commands to the RJE utility and to Secure NOS (which serves as a front end to the CRAY-1), as well as the COS statements. A sample of such a file is shown below for one of the TRACR3D test problems.

```
ESTE,T120,STSCZ.
USER,NKPRIND, {Enter NOS Password}
SEND,NKPRINDLE,BOX 419.
AUDIT.
ACCESS,DN=FT01,PDN=RESTART,UQ,NA.
ACCESS,DN=T3D784,NA.
UPDATE,P=T3D784,IN,F.
CFT,I=$CPL,L=O.
LDR.
SAVE,DN=FT01,PDN=RESTART,NA.
DISPOSE,DN=$OUT,SDN=TEMP,DC=ST,DEFER,TEXT=^
    'CTASK.  REWIND,TEMP. COPY,TEMP,OTHER.'^
    'COMQ,TEMP,DATA.  ROUTE,OTHER,DC=PR,TID=VO.'
DISPOSE,DN=FT59,DC=ST,TEXT='CTASK.  ROUTE,FT59,DC=PR,TID=VO.',^
DEFER.
AUDIT.
EXIT.
```

The first three lines in this file are described in the RJE manual (Samuelson and Brown, 1982) and in the document SANDIA CRAY-1 SUPPLEMENTS prepared in April 1984 by Division 2614 at SNL. The remaining commands are COS commands. The two DISPOSE commands include embedded text strings that are NOS commands. These are returned to the NOS front end system to direct its disposition of the job.

The AUDIT card is used to write a directory of permanent datasets to the logfile. The first ACCESS card does nothing if no restart file exists but is necessary when a restart run is done. The second ACCESS card retrieves the version of TRACR3D that the authors have stored as a permanent file on the CRAY-1. The UPDATE, CFT, and LDR commands are all described in the COS documentation. The SAVE card is required only if the problem will be restarted; the default retention time of 21 days is used here. The DISPOSE command following the SAVE command directs a microfiche to be made of the logfile. When a microfiche is requested through this DISPOSE command, the RJE utility will not send a MAIL message at the end of the job, and the user must examine the RJE unsolicited output queue to determine when his job is complete. Note that alternate forms of the DISPOSE command can be used to obtain microfiche, but the dayfile (system job summary) will not be included on the microfiche if the DEFER is eliminated.

The second DISPOSE command shown directs that an optional time-step log for the job be sent to the RJE unsolicited output queue. Not all of the commands shown are necessary to run TRACR3D; the simplest TRACR3D run requires only the ACCESS, UPDATE, CFT, LDR, and EXIT commands.

The commands for submitting the above three files to the CRAY-1 by way of the RJE utility at SNL are described in Samuelson and Brown (1982). Typically, the user will enter the RJE utility through the VAX and execute a SENDJOB command. If the user exits RJE after executing the SENDJOB command, RJE will send MAIL (VAX MAIL utility) to the user twice; once when the files for the job have been transmitted from the VAX to the NOS front end system and again after the job has been completed and the output returned to the VAX.

The procedures described above were used for running the test problems for installation and initial verification of the TRACR3D code using the COS for the CRAY-1 at SNL. The three required files are reproduced for each problem (Appendix B). It is expected that future procedures will be developed to use CTSS at SNL and the Integrated File System (IFS) with the MASS utility. These procedures may be similar to those used at LANL.

Some of the control statements described above are necessary to use features mentioned but not discussed in the user's manual. These features have been mentioned previously in this document as well; they are described more fully below.

Other Helpful Procedures

1. Time-Step Log

The optional time-step log requested through the second DISPOSE command can be very useful for analyzing output, comparing runs, and improving efficiency. The log is a table generated during every run of TRACR3D. A portion of such a time-step log is shown in Appendix C for the ESTE problem.

For every time step, the table lists the current time, the time-step size, the Courant time-step limit, the number of iterations required to converge to a pressure solution within the time step, and the CPU time used during the time step. The first three of these variables are labeled TIME, DT, and DTI in the table and are calculated according to the equations given in the user's manual for t, t_f, and t_c, respectively. The fourth variable is labeled LGL and is used in the code as a check to see whether the time step should be reduced or increased. The last variable is evaluated using the system function TREMAIN and indicates to the user where the bulk of the computer time is being used.

To get the file containing the time-step log for a run, the user must include the DISPOSE command shown above in the COS file and execute the following command on the VAX: RJE > GET jobname. This command will transfer the file containing the time-step log into the user's directory. The transferred file will have the same name as shown for the jobname in the unsolicited output queue with the VAX extension LOG appended.

2. Restart

The restart feature in TRACR3D can be helpful when simulating radionuclide transport in very slow flow fields or for long time periods (as for nuclides with long half-lives). The SNL implementation of TRACR3D uses the system routine TREMAIN to check for job time remaining and writes a restart file when the job time is running out. By reading this restart file, a job can be restarted at the point where it was interrupted, rather than resubmitting it from the beginning with a higher job time allocation. In addition to saving computer time when job times are underestimated, this allows a user to submit jobs in several pieces with higher priorities to improve turnaround. (This eliminates the need to wait overnight only to find that your job aborted after running for 10 seconds!) Before submitting a restart, the TRACR3D input data file must have a nonzero digit placed somewhere in the first 10 columns of its first line (which may otherwise appear blank) as described in the user's manual.

The restart capability is implemented at SNL using the ACCESS and SAVE statements with PDN=RESTART. These are included in the COS file shown. As described above, the TRACR3D run is not affected by either the presence or absence of a RESTART file. The RESTART file is saved by the SNL system for only 21 days (although this may be changed by systems personnel or by changing the SAVE statement). If more than one problem is being run using the restart capability, unique filenames in SAVE and PDN statements must be specified.

3. Plotting

The TRACR3D user's manual describes the variables used to save plot data for subsequent plotting. However, no plot routine is included in the TRACR3D program. The data saved in plot files is written by unformatted FORTRAN WRITE statements. Further utilization of these data must be through a user-supplied plotting program. Plotting programs have been used to analyze TRACR3D runs at LANL. These programs use the DISSPLA graphics package and the data stored by TRACR3D in the unformatted plotfiles.

5. Structure of TRACR3D

During analysis work on the SNL version of the TRACR3D code, a flowchart and lists of the subroutine calls and STOP statements were developed as aids in following the program logic. These are discussed below.

Subroutine Calls

A list of the subroutine calls in TRACR3D is given in Table 6. Each program segment that calls one or more subroutines is underlined followed by the subroutines called within each of these routines in columnar order. If the call is an alternate entry point, the entry point is followed by the name of the subroutine (in parentheses) in which the entry point occurs. Those subroutines that are library functions or system-dependent routines are indicated in the same manner.

STOP Statements

Input data errors may cause TRACR3D to stop at internal FORTRAN STOP statements. The subroutine in which each STOP occurs is given in Table 7, followed by the nearest numbered line of code (plus or minus a few lines). Since the FORTRAN statement numbers in TRACR3D are usually in numerical order, this list of TRACR3D STOP statements can be used to find the subroutine in which the STOP occurred and the line last executed.

Flowchart

A flowchart of the TRACR3D code is shown in Figure 12. This chart has been invaluable in understanding the method of iteration used in the pressure solution, the calculation of time-step sizes, and in segregating blocks of independent code during debugging and modifications. The flowchart uses three symbols. A rectangular block indicates FORTRAN statement(s) that can be considered as an entity, since they contain no

Table 6

Subroutine Calls in TRACR3D

TRACR3D	APRINT	PERME	VELOCT
APRINT	ASELCT	EFPERM	SLOPE
BONDRY			
CONPLT			
-(PLTSAV)	BONDRY	PLTSAV	ZEROIN
DSPRSN	INTERP	PMESH	FCSET
FCSET	PCSET		
INPUT			
INTERP		PMESH	
MOVIT	DSPRSN	CNVTIM	
NEWIN	DMDU	SSRCH	
-(INPUT)			
PCSET			
PERME	INPUT	PRESSR	
PLT3DV	APRINT	PCSET	
PRESSR	BONDRY	SLOPE	
RRSTRT	LOC	ZEROIN	
RZPLT	-(Sys Dep)		
-(PLTSAV)	PCSET		
SAVETH	RELPRM	RRSTRT	
-(PLTSAV		LOC	
SCOPY		-(Sys Dep)	
-(Library	MOVIT		
SSCAL	BONDRY		
-(Library	GAUSS		
TREMAIN	INTERP		
-(Sys Dep)	SCOPY		
VELOCT	-(Library)		
WRSTRT			
-(RRSTRT)			

FORTRAN Functions Used:			
	MOD	SIN	ASIN
	SQRT	ALOG	ALOGIO
	EXP	COS	

Table 7

STOP Statements in TRACR3D

STOP #	Program Segment	FORTRAN Statement #
2	TRACR3D	480 - 1
777	TRACR3D	490 - 2
600	RELPRM	20 - 2
601	RELPRM	20 + 2
602	RELPRM	30 + 3
603	RELPRM	40 + 2
442	PCSET	15 + 1
445	PCSET	25 - 1
444	INPUT	422 - 1
123	INPUT	490 - 1
3	INPUT	630 - 1
1	INPUT	850 - 1
2	INPUT	860 - 1
333	INPUT	1270 + 1
334	INPUT	1320 - 1
5	RRSTRT	10 - 1
607	BONDRY	340 + 1
610	BONDRY	380 - 1
621	BONDRY	410 + 1
622	BONDRY	450 - 1
615	BONDRY	470 + 1
623	BONDRY	510 - 1

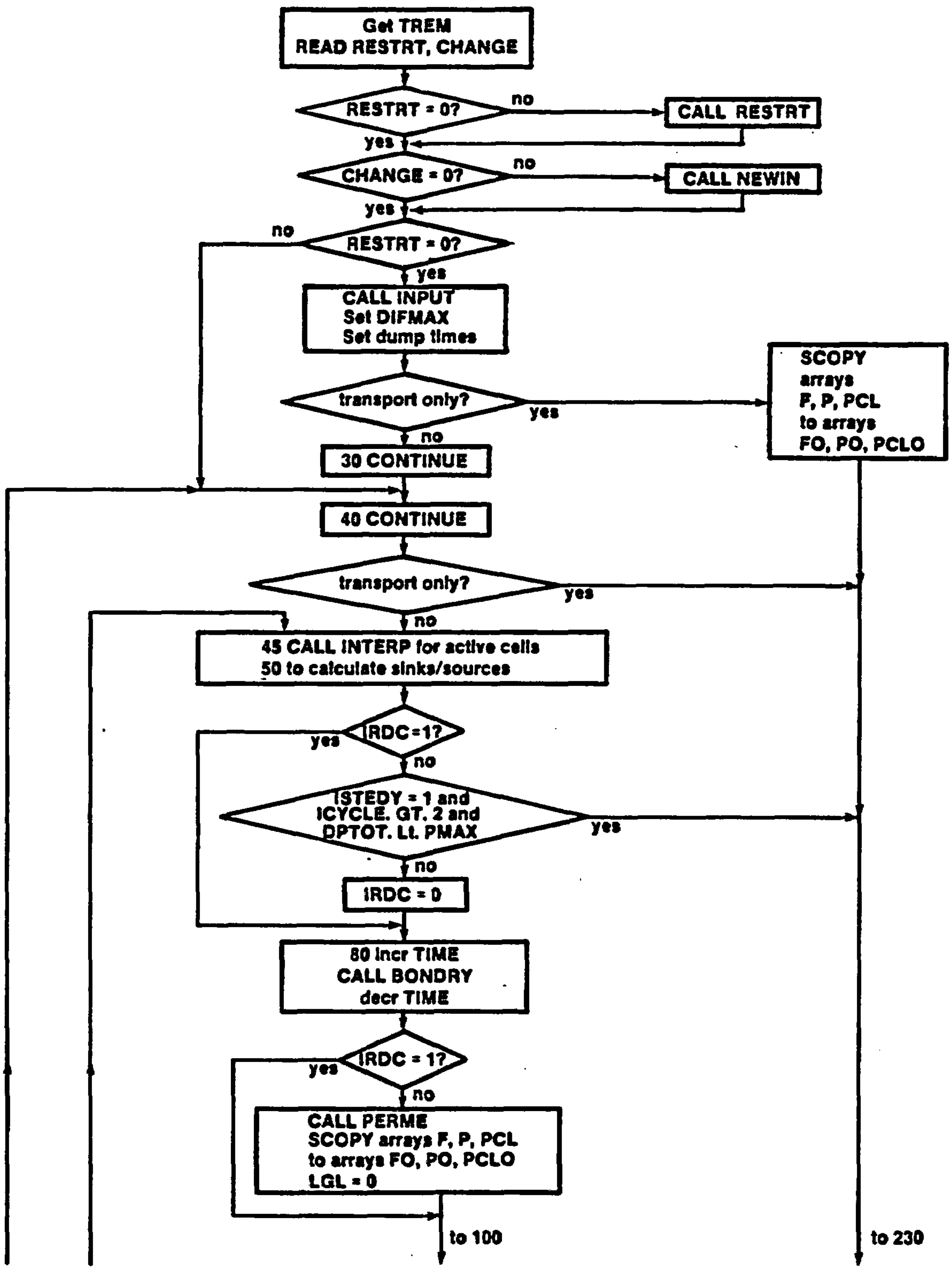


Figure 12. Flowchart of TRACR3D

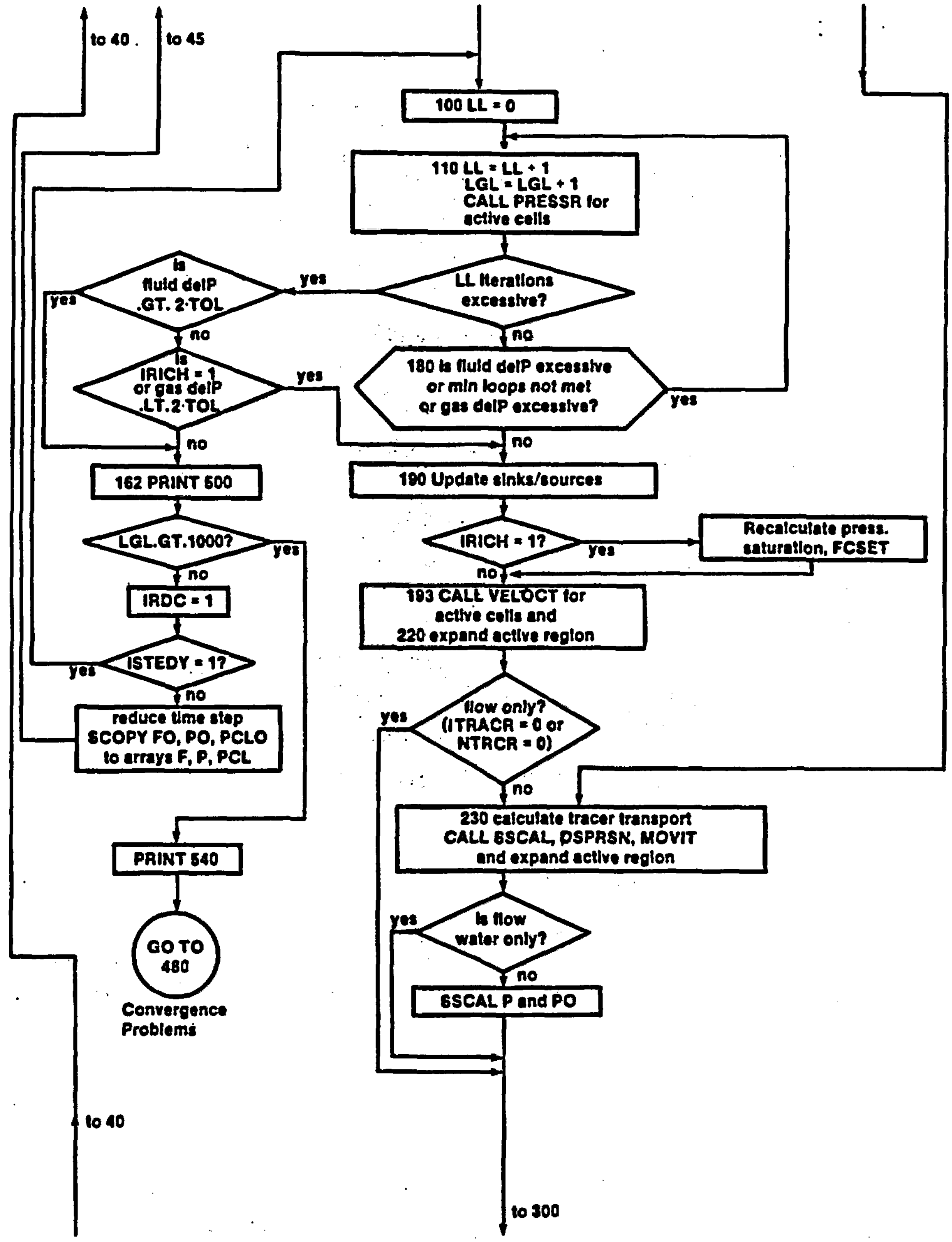


Figure 12. Flowchart of TRACR3D (cont'd)

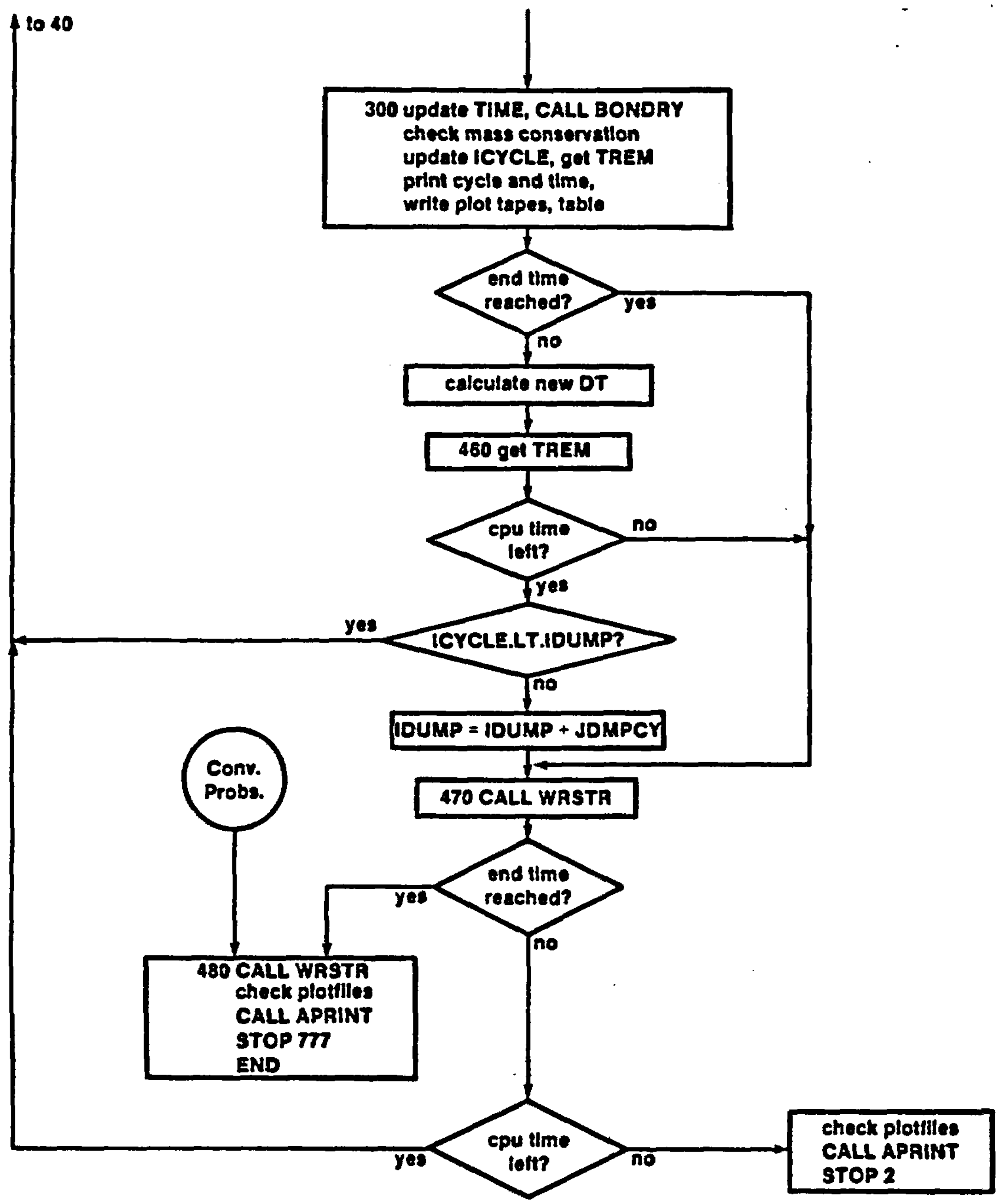


Figure 12. Flowchart of TRACR3D (cont'd)

branches to or from other parts of the code. These blocks are entered only at the top and exited only at the bottom after completion of some function or task. A diamond shape (or a truncated diamond) indicates a test and branch block of code. The circle symbol is used to show the continuation of a path of minor consequence to the iterative scheme.

The flowchart shows that TRACR3D contains one major forward branch, to statement 230, which is taken for cases of transport only. Two substantial backward branches are present to statements 40 and 45. The flowchart also shows that the branch back to statement 40 is part of the loop that steps through time, while the branch back to statement 45 is a part of the pressure iteration performed for each time step.

6. Summary of TRACR3D Status at SNL

The previous five sections describe the work done to install and implement the TRACR3D code on the CRAY-1 system at SNL. Several modifications were described that will suffice for most applications of the code. In particular, the version of the code stored on the CRAY-1 is, to the best of our knowledge, ready to be used for analyses for the NNWSI project. Further certification of the code, however, will be necessary to validate the physical models in the code to the specifications of NUREG-0856 (Silling, 1983) and NVO-196-17 (US DOE, 1986). In addition to the analyses described in the user's manual, certification of TRACR3D for use in performance assessments of Yucca Mountain has been initiated through the participation of Travis in the NNWSI Code Verification (COVE) activity (Hayden, 1985).

The TRACR3D code is stored on the CRAY-1 at SNL under the filename T3D784. This file has been used to run the six problems described in this report. The successful comparisons between the runs at SNL and LANL extend the verification work done at LANL to the SNL implementation. File T3D784 can be used to solve the conservation and momentum equations for one- two- or three-dimensional, transient or steady-state distributions of water, gas, and radioactive solutes in a reacting, porous medium. The reactions of the solute with the medium may be either equilibrium or nonequilibrium.

In the process of installing and implementing the code at SNL, the authors examined the structure of TRACR3D and performed sensitivity studies of some of the control parameters. The currently stored version seems to be free of bugs and to run effectively on the CRAY-1 at SNL. The code will not be maintained by the authors, however. It is conceivable (if not probable) that in future applications of the code, heretofore undiscovered problems may be found. Therefore, some parts of the code structure (i.e., subroutine calls, program logic flow, and program STOP statements) have been reproduced in this report to

supplement the information in the user's manual. In addition, Appendix B lists the input, UPDATE, and COS control files as they were used to run the six test problems; Appendix C lists selected output from the test problems. This material can be used to provide supplemental example problems for new users of TRACR3D, to reproduce the results described in this report at other installations, and to verify any new versions of the code that may be developed at SNL.

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Appendix A

TRACR3D Code Listing As Stored at SNL

The TRACR3D code has been stored as permanent file T3D784 on the CRAY-1 under COS. This file is in UPDATE format for use as described in this report. The same file is stored on the IFS in VAX native text for backup purposes. These files correspond to the listing in this appendix. The second file is accessible by the MASS utility for use on CTSS where it can be run by the CTSS UPDATE facility or by the utility program HISTORN, as at LANL. In addition, control procedures can be developed to run TRACR3D interactively from CTSS or to submit TRACR3D to CTSS from the user's VAX system.

Since TRACR3D is itself not interactive and program runs are most often lengthy, interactive usage is not a significant advantage and may require a user-modifiable FORTRAN (non-UPDATE) file. Job submission via UPDATE allows necessary user modifications while maintaining stricter control over the code for quality assurance purposes, including audit trails of code modifications.

The complete TRACR3D code listing for this appendix is 90 pages long and has been reproduced on microfiche included at the end of this report.

Appendix B

Input Files for Test Problems

The tables in this appendix contain listings of the three files that were used to run each test problem, the COS control file, the UPDATE directives file, and the input data file.

1. ESTE
   - COS Command File
   - UPDATE File
   - Input Data File

2. GEN1
   - COS Command File
   - UPDATE File
   - Input Data File

3. GEN2
   - COS Command File
   - UPDATE File
   - Input Data File

4. VARP
   - COS Command File
   - UPDATE File
   - Input Data File

5. PIG3
   - COS Command File
   - UPDATE File
   - Input Data File

6. LS6
   - COS Command File
   - UPDATE File
   - Input Data File

Table B.1

Sample Problem ESTE

COS Control File

```
ESTEST2,T599,STSCZ.
USER, your username,{Enter NOS Password}.
SEND, your name, your box number.
CHARGE(your charge number)
ACCESS, DN=T3D784,NA.
UPDATE, P=T3D784,IN,F.
CFT,I=$CPL,L=0.
LDR.
DISPOSE,DN=$OUT,SDN=TEMP,DC=ST,DEFER,TEXT=
  'CTASK.  REWIND,TEMP.  COPY,TEMP,OTHER.'
  'COMQ,TEMP,DAT.  ROUTE,OTHER,DC=PR,TID=VO.'
DISPOSE,DN=FT59,DC=ST,TEXT='CTASK.  ROUTE,FT59,DC=PR,TID=VO.',DEFER.
EXIT.
```

UPDATE Directives File

```
*IDENT ESTEST
*D PARAM.23
      PARAMETER (NMX=13,NQX=13,NNX=43,NXX=43,NTRC=1,MQNP=9999)
```

Table B.1 (cont'd)

Input Data File

```
      0         0
 EXPLORATORY SHAFT TRACER EXPERIMENT - 1
$SETUP
 RCM=0.,10,100., YCM=0.,1,.0017,1,.2,2,1.,1,2.,4,10.,1,15.,
 ZCM=-400.,40,0.,
 MATCEL=1,10,1,10,1,40,1, 1,10,1,1,1,40,2, 1,1,1,10,30,30,3,
 TABMAT=1,1.E-6,1.E-6,1.E-6,.20,.1,0.,.50,2.,.05E6,2.5,1.,0.,
        2,1.E2,1.E2,1.E2,.95,.01,0.,.50,5.,.01E6,0.,1.,1.,
        3,1.E6,1.E6,1.E6,.20,0.,0.,0.,10.,0.,0.,1.,0.,
 TIME=0., DT=1., DTMAX=100., TEND=1800., COURNT=1., OMEGAP=1.,
 IBL=1,10,1,40,1, IBR=1,10,1,40,1, IBF=1,10,1,40,1, IBBK=1,10,1,40,1,
 IBB=1,10,1,10,2, IBT=1,10,1,10,1,   IJPT=1,1,1,10,30,30,10,
 TDBDY=10,6, 0.,1.1E6,0.,0., 900.,1.1E6,0.,0.,
      900.001,1.1E6,0.,1.E-3, 1020.,1.1E6,0.,1.E-3,
      1020.001,1.1E6,0.,0., 1.E7,1.1E6,0.,0.,
 PIN=1,10,1,10,1,40,1.E6,   CIN=1,10,1,10,1,40,0.,
 FIN=1,10,1,10,0,41,.50, 1,10,1,1,1,40,.50,
     1,1,1,10,30,30,0., 1,10,1,1,0,0,0.,
 IACT=1,2,1,10,29,31,1,1, TOLC=1.E-9, FMIN=1.E-6,
 IFLOW=2, ITRACF=2, ICHMOD=0, ICOORD=1, IDIM=3, DIFC=1.E-5,
 IFORCH=0, ISTEDY=0, ITRACR=1, HAFLIF=0., NTRCR=1, CDONOR=0.25,
 ICNVEC=1, GRAV=980., IDSPSN=0, IPRSDP=0, IRICH=0,
 TOL=10., ATM=1.E6,  TOLP=1.E3, TOLF=.01, COMPRL=0., POSTIM=3.,
 NPASST=1, IPRNT=1,1,10, JPRNT=1,1,7, KPRNT=1,14,15,5,35,
 TABTP=540.,540.,1080.,360.,1800., LGLMIN=30, LGLMAX=200,
 NXPCON=111, IVELP=3, PLOTT=0.,180.,1.E7,   ICPLAN=2,1, 3,20,
 IJTH=1,1,10, 5,1,10, 10,1,10, 1,5,10, 1,10,10,
 THDT=30., THP=1, THF=1, THC1=1,
 IPROD=1,1,30, 1,2,30, 1,3,30, 1,4,30, 1,5,30, 1,6,30, 1,7,30,
      1,8,30, 1,9,30, 1,10,30,  IPRODN=10,
          $
```

Table B.2

Sample Problem GEN1

COS Control File

```
GEN11,T599,STSCZ.
USER, your username,{Enter NOS Password}.
SEND, your name, your box number.
CHARGE(your charge number)
ACCESS, DN=T3D784,NA.
UPDATE, P=T3D784,IN,F.
CFT,I=$CPL,L=0.
LDR.
DISPOSE,DN=$OUT,SDN=TEMP,DC=ST,DEFER,TEXT=
  'CTASK.  REWIND,TEMP.  COPY,TEMP,OTHER.'
  'COMQ,TEMP,DAT.  ROUTE,OTHER,DC=PR,TID=VO.'
DISPOSE,DN=FT59,DC=ST,TEXT='CTASK.  ROUTE,FT59,DC=PR,TID=VO.',DEFER.
EXIT.
```

UPDATE Directives File

```
*IDENT GENUC1D
*D PARAM.23
      PARAMETER (NMX=4,NQX=4,NNX=53,NXX=53,NTRC=1,MQNP=7400)
```

Table B.2 (cont'd)

Input Data File

```
       0         0
  GENUCHTEN TEST, 1-D
$SETUP
  ZCM=0.,50,182.9, YCM=0.,1,1., RCM=0.,1,1.,
  MATCEL=1,1,1,1,1,50,1,
  TABMAT=1,1.,1.,1.,1.,0.,0.,0.,10.,0.,2.5,1.,0.,
  IBB=1,1,1,1,10, IBT=1,1,1,1,2,
  IBL=1,1,1,50,1, IBR=1,1,1,50,1,
  IBF=1,1,1,50,1, IBBK=1,1,1,50,1,
  IFLOW=0, ITRACR=-1, ITRACF=2, ISTEDY=1,  ICHMOD=0,
  IDIM=1, NTRCR=1, IACT=1,1,1,1,1,10,0,1, TOLC=1.0E-6,
  IJV=1,1,1,1,0,51, 0.,0.,0.,0.,0.,.01411,
  TIME=0., DT=100., DTMAX=100., TEND=10000.,
  KPRNT=10,1,50,  TABTP=3250.,3250.,13000.,
  NXPCON=0, NPASST=1, ICONS=1,   THDT=0., CDONOR=-1.,
   LINEZ=1,1, RZTIME=0.,3250.,13000., IPICK=3,19*0,
  FIN=0,2,0,2,0,51,0., CIN=0,2,0,2,0,51,0.,
  PIN=0,2,0,2,0,51,1.E6,
  DIFC=.001, POSTIM=60.,
  TDBDY=10, 2, 0.,1.E6,0.,1., 1.E5,1.E6,0.,1.,
        $
```

Table B.3

Sample Problem GEN2

COS Control File

```
GEN22,T599,STSCZ.
USER, your username,{Enter NOS Password}.
SEND, your name, your box number.
CHARGE(your charge number)
ACCESS, DN=T3D784,NA.
UPDATE, P=T3D784,IN,F.
CFT,I=$CPL,L=0.
LDR.
DISPOSE,DN=$OUT,SDN=TEMP,DC=ST,DEFER,TEXT=
  'CTASK.  REWIND,TEMP.  COPY,TEMP,OTHER.'
  'COMQ,TEMP,DAT.  ROUTE,OTHER,DC=PR,TID=VO.'
DISPOSE,DN=FT59,DC=ST,TEXT='CTASK.  ROUTE,FT59,DC=PR,TID=VO.',DEFER.
EXIT.
```

UPDATE Directives File

```
*IDENT GENUC2
*D PARAM.23
      PARAMETER (NMX=4,NQX=4,NNX=103,NXX=103,NTRC=1,MQNP=7400)
```

Input Data File

```
     0          0
 COMPARISON OF TRACR3D WITH GENUCHTENS TEST CASE, J.HYDROLOGY,VOL.49
$SETUP
  ZCM=0.,100,250., YCM=0.,1,1., RCM=0.,1,1.,
  MATCEL=1,1,1,1,1,100,1,
  TABMAT=1,1.,1.,1.,1.,0.,0.,0.,10.,0.,2.,1.,0.,
   EQUILK=1.0,
  CIN=1,1,1,1,0,101,0.,
  FIN=1,1,1,1,0,101,0.,
  PIN=1,1,1,1,0,101,1.E6,
  IBL=1,1,1,100,1, IBR=1,1,1,100,1, IBB=1,1,1,1,10, IBT=1,1,1,1,1,
  IBF=1,1,1,100,1, IBBK=1,1,1,100,1,
  GRAV=0., IFORCH=0, IPRSDP=0, VISL=.01, IFLOW=0, ISTEDY=1,
  NTRCR=1, ITRACR=-1, ITRACF=2, POSTIM=20., ICOORD=1,
  IJV=1,1,1,1,0,101, 0.,0.,0., 0.,0.,25.,
  TDBDY=10,4, 0.,1.E6,0.,1., 5.,1.E6,0.,1., 5.0000001,1.E6,0.,0.,
         1.E3,1.E6,0.,0.,
  TABTP=20.,5.,40.,  DELCY=25., KPRNT=1,9,10,10,60,20,80,
  TIME=0., TEND=15., DT=.1, DTMAX=.1, COURNT=.5,
  NXPCON=0, CDONOR=-1.0,
  IACT=1,1,1,1,1,10,0,1,
  IDIM=1, TOLC=1.E-6,
  THDT=0.,
   LINEZ=1,1, RZTIME=0.,5.,5.,2.5,15., IPICK=3,0,
  CMIN=1.E-14, DIFC=37.5, HAFLIF=8.317767, ICHMOD=1,
      $
```

Table B.4

Sample Problem VARP

COS Control File

```
VARPER,T599,STSCZ.
USER, your username,{Enter NOS Password}.
SEND, your name, your box number.
CHARGE(your charge number)
ACCESS, DN=T3D784,NA.
UPDATE, P=T3D784,IN,F.
CFT,I=$CPL,L=0.
LDR.
DISPOSE,DN=$OUT,SDN=TEMP,DC=ST,DEFER,TEXT=
  'CTASK.  REWIND,TEMP.  COPY,TEMP,OTHER.'
  'COMQ,TEMP,DAT.  ROUTE,OTHER,DC=PR,TID=VO.'
DISPOSE,DN=FT59,DC=ST,TEXT='CTASK.  ROUTE,FT59,DC=PR,TID=VO.',DEFER.
EXIT.
```

UPDATE Directives File

```
*IDENT VARPER
*D PARAM.23
      PARAMETER (NMX=4,NQX=4,NNX=13,NXX=13,NTRC=0,MQNP=7400)
```

Table B.4 (cont'd)

Input Data File

```
          0          0
  TEST OF VARIABLE PERMEABILITY
$SETUP
   RCM=0.,1,1., YCM=0.,1,1.,
   ZCM=0.,10,1.,
  MATCEL=1,1,1,1,1,10,1,
  TABMAT=1,1.,1.,1.,.3,0.,5.E-8,0.,10.,0.,1.,1.,0.,
  IBL=1,1,1,10,1, IBR=1,1,1,10,1, IBF=1,1,1,10,1, IBBK=1,1,1,10,1,
  IBB=1,1,1,1,2, IBT=1,1,1,1,2,
  TIME=0., DT=.1, DTMAX=.1, TEND=.2,
  NTRCR=0, IDIM=1, IFORCH=0, IPRSDP=1,  IFLOW=0,
  ITRACR=0, IDSPSN=0, TOL=1.E-1,
  IACT=1,1,1,1,1,10,1,0,
  FIN=1,1,1,1,0,11,0.,
  PIN=1,1,1,1,1,11,1.E6, 1,1,1,1,0,0,11.E6,
  TABTP=0.,.1,.1,
  IPRNT=1,1,1, JPRNT=1,1,1, KPRNT=1,1,10,
       $
```

Table B.5

Sample Problem PIG3

COS Control File

```
PIG3TRC,T1200,STSCZ.
USER, your username,{Enter NOS Password}.
SEND, your name, your box number.
CHARGE(your charge number)
ACCESS, DN=T3D784,NA.
UPDATE, P=T3D784,IN,F.
CFT,I=$CPL,L=0.
LDR.
DISPOSE,DN=$OUT,SDN=TEMP,DC=ST,DEFER,TEXT=
  'CTASK.  REWIND,TEMP.  COPY,TEMP,OTHER.'
  'COMQ,TEMP,DAT.  ROUTE,OTHER,DC=PR,TID=VO.'
DISPOSE,DN=FT59,DC=ST,TEXT='CTASK.  ROUTE,FT59,DC=PR,TID=VO.',DEFER.
EXIT.
```

UPDATE Directives File

```
*IDENT PIGFORD
*D PARAM.23
      PARAMETER (NMX=4,NQX=4,NNX=203,NXX=203,NTRC=3,MQNP=7400)
```

Table B.5 (cont'd)

Input Data File

```
       0          0
  THREE CHAIN DECAY AND TRANSPORT      (pigford)
$SETUP
  YCM=0.,1,1., RCM=0.,1,1.,
  ZCM=0.,200,2000.,
  MATCEL=1,1,1,1,1,200,1,
  TABMAT=1,1.,1.,1.,1.,1.,0.,0.,10.,0.,1.,1.,0.,
  IBL=1,1,1,200,1, IBR=1,1,1,200,1, IBB=1,1,1,1,4, IBT=1,1,1,1,3,
  IBF=1,1,1,200,1, IBBK=1,1,1,200,1,
  TIME=0., DT=15., DTMAX=15., TEND=5.E4,
  CDONOR=-1.0, NTRCR=3, ICHMOD=1, IFLOW=0, ISTEDY=1, ITRACF=2,
  ITRACR=-1, IDSPSN=0, IFORCH=0, IDIM=1, IPRSDP=0,
  TOLC=.005,2.E-5,2.E-6,
  IACT=1,1,1,1,1,5,0,1,1,1,
  FIN=1,1,1,1,0,201,0.,
  CIN=1,1,1,1,0,201,0.,0.,0.,
  SNIN=1,1,1,1,0,201,0.,0.,0.,
  PIN=1,1,1,1,0,201,1.E6,
  CBIN=1.,0.,0., TLEACH=3.3300001E4,
  HAFLIF=2.44E5,7.7E4,1.6E3,
  EQUILK(1,1)=27.6, EQUILK(1,2)=99., EQUILK(1,3)=0.,
  IJV=1,1,1,1,0,200, 0.,0.,0., 0.,0.,.22,
  DIFC=3.52,3.52,3.52,
  MOLC=234.,230.,226.,
  TABTP=1.E4,4.E4,1.E5, DELCY=1.E6,
  IPRNT=1,1,1, JPRNT=1,1,1, KPRNT=0,1,10,5,200,
  NXPCON=0, THDT=0.,
  IPICK=3,5,7,0, RZTIME=0.,1.E4,1.E5, LINEZ=1,1,
        $
```

Table B.6

Sample Problem LS6

COS Control File

```
LS6CAIS,T2400,STSCZ.
USER, your username,{Enter NOS Password}.
SEND, your name, your box number.
CHARGE(your charge number)
ACCESS, DN=T3D784,NA.
UPDATE, P=T3D784,IN,F.
CFT,I=$CPL,L=0.
LDR.
DISPOSE,DN=$OUT,SDN=TEMP,DC=ST,DEFER,TEXT=
  'CTASK.  REWIND,TEMP.  COPY,TEMP,OTHER.'
  'COMQ,TEMP,DAT.  ROUTE,OTHER,DC=PR,TID=VO.'
DISPOSE,DN=FT59,DC=ST,TEXT='CTASK.  ROUTE,FT59,DC=PR,TID=VO.',DEFER.
EXIT.
```

UPDATE Directives File

```
*IDENT LS6CAI
*D PARAM.23
      PARAMETER (NMX=4,NQX=4,NNX=153,NXX=153,NTRC=0,MQNP=7400)
*D PRESSR.143
*D PRESSR.144
*D PRESSR.145
```

Table B.6 (cont'd)

Input Data File

```
      0         0
 LS-6 EXPERIMENT, 13 CM PULSE,  CAISSON A
$SETUP
  RCM=0.,1,270., ZCM=-600.,150,0., YCM=0.,1,270.,
  MATCEL= 0,2,0,2,0,6,2, 0,2,0,2,7,12,3, 0,2,0,2,151,151,4,
           0,2,0,2,13,150,1,
  TABMAT=1, .25,.25,.25,.346,.1,0.,.1,.4329,-1.,2.5,1.,0.,
     2, 30.,30.,30.,.45,1.,0.,0.,10.,0.01E6,2.5,1.,0.,
     3, 5.,5.,5.,.33,.1,0.,0.,1.,.015E6,2.5,1.,0.,
     4, .25,.25,.25,.346,.1,0.,.1,.4329,0.,2.5,1.,0.,
  PCTB=1,18,  0.,0., .10,.04E6, .15,.045E6, .20,.055E6, .25,.07E6,
      .30,.09E6, .35,.125E6, .40,.14E6, .45,.17E6, .50,.22E6,
      .55,.30E6, .60,.38E6, .65,.46E6,
      .70,.70E6, .75,1.3E6, .80,4.E6, .90,5.E6, 1.,6.E6,
  TIME=0., DT=100., DTMAX=1.E10, TEND=3.024E6,
   POSTIM=20., DELCY=1.E5, ICHMOD=0, NTRCR=0,
  ICOORD=1, ISTEDY=0, IFLOW=2, IPRSDP=0, IFORCH=0, ITRACR=0,
  GRAV=980., PIN=0,2,0,2,0,150, 0.00E0,
  CIN=0,2,0,2,0,150, 0.,
  FIN=0,2,0,2,0,6,1., 0,2,0,2,13,32,.243, 0,2,0,2,33,52,.36,
      0,2,0,2,53,72,.40, 0,2,0,2,73,92,.44, 0,2,0,2,93,111,.474,
      0,2,0,2,112,130,.462, 0,2,0,2,131,150,.483, 0,2,0,2,7,12,.60,
  IBL=1,1,1,150,1, IBR=1,1,1,150,1, IBB=1,1,1,1,2, IBT=1,1,1,1,20,
    IBF=1,1,1,150,1, IBBK=1,1,1,150,1,
  TDBDY=20,2, 0.0,0.,1., 0.,13.,0.,
  NXPCON=0,  LINEZ=1,1, IPICK=2,0,0,0,0,0,14*0,
  RZTIME=0.,10800.,10800.,72000.,82800.,90000.,172800.,259200.,432000.,
   86400.,777600.,259200.,1036800.,86400.,1210600.,172800.,1383400.,
   518400.,1901800.,1123200.,3025000.,432000.,3457000.,432000.,1.E7,
  IJTH=1,1,1, 1,1,5, 1,1,6, 1,1,9, 1,1,10, 1,1,25, 1,1,44, 1,1,63,
       1,1,82, 1,1,102, 1,1,121, 1,1,140, 1,1,150,
   THDT=1200., THDTPT=1, THP=1, THF=1, THSMBL=2,
  TABTP=0.,10800.,10800.,72000.,82800.,90000.,172800.,259200.,432000.,
   86400.,777600.,259200.,1036800.,86400.,1210600.,172800.,1383400.,
   518400.,1901800.,1123200.,3025000.,432000.,3457000.,432000.,1.E7,
  IPRNT=1,1,1, JPRNT=1,1,1, KPRNT=1,4,5,5,10,34,44,19,63,19,82,20,
         102,19,121,19,140,1,150,
    OMEGAP=1.00, COURNT=1., TOLC=1.E-7, ITRACF=2, IDIM=1, IRICH=1,
  IACT=1,1,1,1,1,150,1,0,  TOLP=1.E10, TOLF=1.E10,
   TOL=1., FMIN=1.E-10, DIFC=1.E-5, IDSPSN=0, MOLC=80.,
  LGLMIN=30, LGLMAX=50,
           $
```

Appendix C

Selected Output from Test Problems

The amount of output from any run of TRACR3D is controlled by the user. The output returned from runs of the six test problems presented in this report amounted to 1400 pages, with a like amount produced at LANL for comparison. A small portion of this output is included here for each problem as examples for the TRACR3D user. Complete listings of all of this output have been stored in the NNWSI Records Center.

1. Sample Time-Step Log from ESTE
2. ESTE Results
3. GEN1 Results
4. GEN2 Results
5. VARP Results
6. PIG3 Results
7. LS6 Results

Table C.1

Sample Time-Step Log from ESTE

Time Step Number		t		Δ_{tf}		Δ_{tc}		Iterations		CPU time
1	TIME=	1.0000E+00	DT=	1.0000E+00	DTI=	0.0000E+00	LGL	174	TTOT=	1.587
2	TIME=	2.0000E+00	DT=	1.0000E+00	DTI=	8.9216E+01	LGL	200	TTOT=	1.480
3	TIME=	3.0000E+00	DT=	1.0000E+00	DTI=	7.7486E+01	LGL	128	TTOT=	1.097
4	TIME=	4.0000E+00	DT=	1.0000E+00	DTI=	6.5035E+01	LGL	66	TTOT=	0.716
5	TIME=	5.0000E+00	DT=	1.0000E+00	DTI=	5.3646E+01	LGL	57	TTOT=	0.697
6	TIME=	6.0000E+00	DT=	1.0000E+00	DTI=	4.3306E+01	LGL	56	TTOT=	0.746
7	TIME=	7.0000E+00	DT=	1.0000E+00	DTI=	3.4007E+01	LGL	59	TTOT=	0.844
8	TIME=	8.0000E+00	DT=	1.0000E+00	DTI=	2.5767E+01	LGL	66	TTOT=	1.005
9	TIME=	9.0000E+00	DT=	1.0000E+00	DTI=	1.8907E+01	LGL	61	TTOT=	1.050
10	TIME=	1.0000E+01	DT=	1.0000E+00	DTI=	1.7885E+01	LGL	39	TTOT=	0.811
11	TIME=	1.1000E+01	DT=	1.0000E+00	DTI=	1.9820E+01	LGL	27	TTOT=	0.677
12	TIME=	1.2200E+01	DT=	1.2000E+00	DTI=	2.3792E+01	LGL	25	TTOT=	0.679
13	TIME=	1.3640E+01	DT=	1.4400E+00	DTI=	2.6323E+01	LGL	20	TTOT=	0.618
14	TIME=	1.5368E+01	DT=	1.7280E+00	DTI=	2.2769E+01	LGL	21	TTOT=	0.668
15	TIME=	1.7442E+01	DT=	2.0736E+00	DTI=	1.9212E+01	LGL	22	TTOT=	0.722
16	TIME=	1.9930E+01	DT=	2.4883E+00	DTI=	1.6908E+01	LGL	21	TTOT=	0.734
17	TIME=	2.2916E+01	DT=	2.9860E+00	DTI=	1.6609E+01	LGL	19	TTOT=	0.718
18	TIME=	2.6499E+01	DT=	3.5832E+00	DTI=	1.5392E+01	LGL	19	TTOT=	0.756
19	TIME=	3.0799E+01	DT=	4.2998E+00	DTI=	1.7087E+01	LGL	19	TTOT=	0.798
20	TIME=	3.5959E+01	DT=	5.1598E+00	DTI=	1.7818E+01	LGL	18	TTOT=	0.809

Note: The log file as output by TRACR3D includes only the 20 lines (often much more) for the time steps calculated during that program run. The headings were added for purposes of this report.

Table C.2

ESTE Results

Output from problem ESTE is published in its entirety in Travis (1984) (LA-9667-MS), Appendix D and is not repeated here. Appendix C of that reference includes a description of the TRACR3D output tables produced by subroutine APRINT as controlled by input variables TABTP, IPRNT, JPRNT, and KPRNT. Tables C.3c, C.4b, C.5b, C.6b, and C.7b in this appendix are examples of this type of output.

<u>NOTE:</u> The originals of these tables were of poor quality.

```
GENIK6F                                    UPDATE 1.11 83097           08/07/84      14:43:15     PAGE    1
*** INPUT LISTING ***                                                  PLDATE 07/31/84 LASTID GENUC1D

*IDENT GENUC1D
              1.          *IDENT GENUC1D
              2.          *D PARAM.23
              .                     PARAMETER (NMX=4,NQX=4,NNX=53,NXX=53,NTRC=1,MQNP=7400)

 ***       3 RECORDS      2 DIRECTIVES      1 MOD IDENTS      0 INPUT ERRORS
```

C-04

Table C.3a

Output Produced by UPDATE

This output serves to document the program changes made for this run of GEN1.

```
          PAGE 1                    UN=ELMPJRV                08/07/84-14:43:20    CFT 1.11(04/16/84)  PAGE 1
  5541       1. 1                                                                        SSRCH.46
 PRNAME $MAIN     WARNING -     STATEMENT NUMBER ON BLANK CARD IGNORED ************************************************************ P=0035433C
  5541       1. 1                                                                        SSRCH.46
 PRNAME $MAIN     WARNING -     MISSING END STATEMENT ***************************************************************************** P=0035064D
  M=   1   R INPUT FOLLOWS
     0.0      1.0      1.0
  X IN CM FOLLOWS
     0.0      0.0      1.0      1.0
  Q=   1   Y INPUT FOLLOWS
     0.0      1.0      1.0
  Y IN CM FOLLOWS
     0.0      0.0      1.0      1.0
  N=  50   ZCM INPUT FOLLOWS
     0.0     50.0    182.9
  Z IN CM FOLLOWS
     0.0      0.0      3.7      7.3     11.0     14.6     18.3     21.9     25.6     29.3     32.9     36.6     40.2     43.9     47.6
    51.2     54.9     58.5     62.2     65.8     69.5     73.2     76.8     80.5     84.1     87.8     91.4     95.1     98.8    102.4
   106.1    109.7    113.4    117.1    120.7    124.4    128.0    131.7    135.3    139.0    142.7    146.3    150.0    153.6    157.3
   161.0    164.6    168.3    171.9    175.6    179.2    182.9    182.9
 MATERIAL TABLE FOLLOWS
     1.   0.100E+01    0.100E+01    0.100E+01 1.0000 0.0000 0.0000 0.000010.0000  0.000E+00  2.500  1.000  0.000

  CELL MATERIAL DATA FOLLOWS
     1   1   1   1   1  50  1
  CHANGES TO INITIAL TRACER CONCENTRATION (GM/CC)
    0.  2.  0.  2.  0. 51. 0.00000E+00
  CHANGES TO INITIAL ADSORBED CONCENTRATION (GM/GM)

  CHANGES TO INITIAL GAS SATURATION
    0.  2.  0.  2.  0. 51. 0.00000E+00     0.
  CHANGES TO INITIAL PRESSURE (P=ATM) DISTRIBUTION
    0.  2.  0.  2.  0. 51. 0.10000E+07     0.
  TIME DEPENDENT BOUNDARY NUMBER AND LOCATION
  10      3
     LEFT BOUNDARY SET UP FOLLOWS

    1
    1
    1
    1
    1
    1
    1
    1
    1
    1
    1
    1
    1
    1
    1
```

Table C.3b

First Page of Output from TRACR3D

This page recapitulates the input data for the problem. (The two warnings from CFT are the result of two extraneous characters at the end of the FORTRAN source code and have since been deleted.)

```
     GENUCHTEN TEST, 1-D                                                                      Z LEVEL    16  Z =         56.699
TIME      55.00  MINS   CYCLE       33 DT  0.10E+03
                           MASS (GM)-GAS-     L,R,B,T,F,BK      0.0000E+00    0.0000E+00    0.0000E+00    0.0000E+00    0.0000E+00    0.0000E+00
                           MASS (GM)-LIQUID-  L,R,B,T,F,BK      0.0000E+00    0.0000E+00    0.4656E+02    0.4656E+02    0.0000E+00    0.0000E+00
                                 1
                              0.50
                                 1
   1      0.50   1  1.00E+06   1        0.50   1
                           1.00E+06
                           0.00E+00
                           2.95E-02
                           0.00E+00
                            01,0010
                            S 0,P 0    S
                                 1
                              0.50
                                 1
```

Table C.3c

Main Output from TRACR3D

Problem GEN1 produced 205 pages of such output for 41 Z-values at 5 time values.

```
14:43:14   0.0000     CSP
14:43:14   0.0000     CSP            SANDIA NATIONAL LABORATORY - ALBUQUERQUE, NEW MEXICO    08/07/84
14:43:14   0.0000     CSP
14:43:14   0.0000     CSP            CRAY-1 S/1000 (S/N 39)  COS 1.11 (BF3S)   ASSEMBLY DATE 03/28/84
14:43:14   0.0000     CSP
14:43:14   0.0000     CSP
14:43:14   0.0000     CSP     JOB,JN=   GEN1K6F,US=256JFOS,T=   600,P=2.        BOX=419
14:43:14   0.0007     CSP     ACCOUNT,AC=1561231-06312,PW=N77496.
14:43:15   0.0018     CSP     -- INVOKING PROCEDURE   SEND
14:43:15   0.0045   1 EXP     *, ************************************************************************
14:43:15   0.0045   1 EXP     *, *
14:43:15   0.0045   1 EXP     *, *              PLEASE SEND THIS LISTING TO -
14:43:15   0.0045   1 EXP     *, *
14:43:15   0.0045   1 EXP     *, *
14:43:15   0.0045   1 EXP     *, *              JFOSTER      BOX 419
14:43:15   0.0045   1 EXP     *, *
14:43:15   0.0045   1 EXP     *, ************************************************************************
14:43:15   0.0046     CSP     CHARGE(1561231)
14:43:15   0.0049     CSP     ACCESS,DN=T3D784,NA.
14:43:15   0.0049     PDM     PD000 - PDN = T3D784            ID = 256JFOS    ED =    1  US = 256JFOS
14:43:15   0.0049     PDM     PD000 - ACCESS  COMPLETE
14:43:15   0.0053     CSP     UPDATE,P=T3D784,IN,F.
14:43:15   0.0059     USER    UD001 - PL DATE 07/31/84 LEVEL: SSRCH
   43:19   0.7875     CSP     CFT,I=$CPL,L=0.
   43:21   0.7876     USER    CF000 - CFT VERSION -    04/16/84 1.11
   43:41   3.7196     USER    CF001 - COMPILE TIME =     2.9320 SECONDS
   43:41   3.7196     USER    CF002 -       5541 LINES,      4031 STATEMENTS
   43:41   3.7196     USER    CF003 -     67559 WORDS,     10512 I/O BUFFERS USED
   43:42   3.7200     CSP     LDR.
   43:49   3.8888     USER    LD000 - BEGIN EXECUTION
   43:52   5.3464     USER    FT063 -      STOP 777           IN TRACR3D
   43:52   5.3469     CSP     DISPOSE,DN=$OUT,SDN=TEMP,DC=ST,DEFER,TEXT=*
14:43:52   5.3473     CSP     *
14:43:52   5.3477     CSP     .
14:43:52   5.3485     CSP     DISPOSE,DN=FT59,DC=ST,TEXT=,DEFER.
14:43:52   5.3486     CSP     EXIT.
14:43:52   5.3487     CSP     END OF JOB
14:43:52   5.3487     CSP
14:43:52   5.3487     CSP
14:43:52   5.3489     USER        JOB NAME -                                GEN1K6F
14:43:52   5.3489     USER        USER NUMBER -                             256JFOS
14:43:52   5.3489     USER        TIME EXECUTING IN CPU -                   0000:00:05.3489
14:43:52   5.3489     USER        TIME WAITING TO EXECUTE -                 0000:00:26.2335
14:43:52   5.3489     USER        TIME WAITING FOR I/O -                    0000:00:06.5881
14:43:52   5.3490     USER        TIME WAITING IN INPUT QUEUE -             0001:59:23.2122
14:43:52   5.3490     USER        MEMORY * CPU TIME (MWDS*SEC) -                   0.45161
14:43:52   5.3490     USER        MEMORY * I/O WAIT TIME (MWDS*SEC) -              0.54705
14:43:52   5.3490     USER        MINIMUM MEMORY WORDS USED -                55296
14:43:52   5.3491     USER        MAXIMUM MEMORY WORDS USED -               120832
14:43:52   5.3491     USER        DISK SECTORS MOVED -                         790
14:43:52   5.3491     USER        USER I/O REQUESTS -                          209
14:43:52   5.3491     USER        OPEN CALLS -                                  32
14:43:52   5.3491     USER        CLOSE CALLS -                                 18
14:43:52   5.3491     USER        MEMORY RESIDENT DATASETS -                     0
14:43:52   5.3491     USER        TEMPORARY DATASET SECTORS USED -               5
14:43:52   5.3491     USER        PERMANENT DATASET SECTORS ACCESSED -          56
14:43:52   5.3491     USER        PERMANENT DATASET SECTORS SAVED -              0
14:43:52   5.3491     USER        SECTORS RECEIVED FROM FRONT END -              0
14:43:52   5.3492     USER        SECTORS QUEUED TO FRONT END -                  0
14:43:52   5.3492     USER        COST OF CPU USAGE (DOLLARS) -               1.30
```

Table C.3d

Dayfile from COS for Problem GEN1

```
      PAGE 1                    UN=ELMPJRV               08/07/84-14:44:02     CFT 1.11(04/16/84)  PAGE 1

  5541      1. 1                                                               SSRCH.46
PRNAME $MAIN    WARNING -    STATEMENT NUMBER ON BLANK CARD IGNORED ***************************************************** P=0035433C
  5541      1. 1                                                               SSRCH.46
PRNAME $MAIN    WARNING -    MISSING END STATEMENT ******************************************************************** P=0035064D
N=    1  R INPUT FOLLOWS
   0.0     1.0     1.0
X IN CM FOLLOWS
   0.0     0.0     1.0     1.0
U=    1  Y INPUT FOLLOWS
   0.0     1.0     1.0
Y IN CM FOLLOWS
   0.0     0.0     1.0     1.0
N= 100   ZCM INPUT FOLLOWS
   0.0   100.0   250.0
Z IN CM FOLLOWS
   0.0     0.0     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   102.5   105.0   107.5
 110.0   112.5   115.0   117.5   120.0   122.5   125.0   127.5   130.0   132.5   135.0   137.5   140.0   142.5   145.0
 147.5   150.0   152.5   155.0   157.5   160.0   162.5   165.0   167.5   170.0   172.5   175.0   177.5   180.0   182.5
 185.0   187.5   190.0   192.5   195.0   197.5   200.0   202.5   205.0   207.5   210.0   212.5   215.0   217.5   220.0
 222.5   225.0   227.5   230.0   232.5   235.0   237.5   240.0   242.5   245.0   247.5   250.0   250.0
MATERIAL TABLE FOLLOWS
     1  0.100E+01    0.100E+01    0.100E+01 1.0000 0.0000 0.0000 0.000010.0000  0.000E+00  2.000  1.000  0.000

       MATERIAL DATA FOLLOWS
          1    1    1    1 100   1
       ES TO INITIAL TRACER CONCENTRATION (GM/CC)
        1.  1.  1.  0.101. 0.00000E+00
       ES TO INITIAL ADSORBED CONCENTRATION (GM/GM)

 ......ES TO INITIAL GAS SATURATION
   1.  1.  1.  1.  0.101. 0.00000E+00    0.
 CHANGES TO INITIAL PRESSURE (P=ATM) DISTRIBUTION
   1.  1.  1.  1.  0.101. 0.10000E+07    0.
 TIME DEPENDENT BOUNDARY NUMBER AND LOCATION
 10    3
    LEFT BOUNDARY SET UP FOLLOWS

    1
    1
    1
    1
    1
    1
    1
    1
    1
    1
    1
    1
    1
    1
    1
```

Table C.4a

TRACR3D Input Data Recapitulation for Problem GEN2

```
   COMPARISON OF TRACR3D WITH GENUCHTENS TEST CASE, J.HYDROLOGY,V Z LEVEL    10  Z =       23.750
TIME      0.65  SECS   CYCLE      25 DT  0.23E-01
                         MASS (GM)-GAS-     L,R,B,T,F,BK    0.0000E+00   0.0000E+00   0.0000E+00   0.0000E+00   0.0000E+00   0.0000E+00
                         MASS (GM)-LIQUID-  L,R,B,T,F,BK    0.0000E+00   0.0000E+00   0.1614E+02   0.0000E+00   0.0000E+00   0.0000E+00
                              1
                              0.50
                              1
  1     0.50   1   1.00E+06  1     0.50  1
                         1.00E+06
                         0.00E+00
                         2.85E-04
                         0.00E+00
                          01,0010
                          S 0,P 0    S
                              1
                              0.50
                              1
```

C-09

Table C.4b

Main Output for Problem GEN2

Similar output was obtained for 8 Z-values at 28 time values, amounting to 224 pages.

```
           PAGE 1                     ON=ELNPQRV                           08/07/84-14:50:16      CFT 1.11(04/16/84)  PAGE 1
    5541        1. 1                                                                                   SSRCH.46
 PRNAME $MAIN    WARNING -     STATEMENT NUMBER ON BLANK CARD IGNORED ****************************************************** P=0035433C
    5541        1. 1                                                                                   SSRCH.46
 PRNAME $MAIN    WARNING -     MISSING END STATEMENT ******************************************************************** P=0035064D
   M=   1  R INPUT FOLLOWS
     0.0      1.0      1.0
   X IN CM FOLLOWS
     0.0      0.0      1.0      1.0
   Q=   1  Y INPUT FOLLOWS
     0.0      1.0      1.0
   Y IN CM FOLLOWS
     0.0      0.0      1.0      1.0
   N=  10  ZCM INPUT FOLLOWS
     0.0     10.0      1.0
   Z IN CM FOLLOWS
     0.0      0.0      0.1      0.2      0.3      0.4      0.5      0.6      0.7      0.8      0.9      1.0      1.0
 MATERIAL TABLE FOLLOWS
     1.   0.100E+01   0.100E+01   0.100E+01 0.3000 0.0000 0.0000 0.000010.0000  0.000E+00  1.000  1.000  0.000

   CELL MATERIAL DATA FOLLOWS
        1    1    1    1    1   10   1
    HANGES TO INITIAL GAS SATURATION
     1.  1.  1.  1.  0. 11. 0.00000E+00     0.
    HANGES TO INITIAL PRESSURE (P=ATM) DISTRIBUTION
     1.  1.  1.  1.  1. 11. 0.10000E+07     1.  1.  1.  1.  0.  0. 0.11000E+08     0.
      LEFT BOUNDARY SET UP FOLLOWS

    1
    1
    1
    1
    1
    1
    1
    1
    1
    1
     RIGHT BOUNDARY SET UP FOLLOWS

    1
    1
    1
    1
    1
    1
    1
    1
    1
    1
```

Table C.5a

TRACR3D Input Data Recapitulation for Problem VARP

```
      TEST OF VARIABLE PERMEABILITY                                               Z LEVEL     1  Z =          0.050
TIME      0.10  SECS   CYCLE        1 DT  0.10E+00
                         MASS (GM)-GAS-     L,R,B,T,F,BK     0.0000E+00     0.0000E+00     0.0000E+00     0.0000E+00     0.0000E+00     0.0000E+0
                         MASS (GM)-LIQUID-  L,R,B,T,F,BK     0.0000E+00     0.0000E+00     0.1038E+01     0.9622E+00     0.0000E+00     0.0000E+0
                              1
                              0.50
                              1
  1       0.50   1   1.05E+07   1       0.50  1
                         1.05E+07
                         0.00E+00
                          01,0001
                          S 0,P 0    S
                              1
                              0.50
                              1
```

Table C.5b

Main Output for Problem VARP

Fifty similar pages were produced for 10 Z-values at 5 time values.

```
  1   0.100E+00   0.156E-02   50    0  0.3742E+02  0.3742E+02
  1   0.100E+00   0.125E-02  100    1  0.1775E+02  0.1775E+02
  1   0.100E+00   0.997E-03  150    1  0.7055E+01  0.7055E+01
  1   0.100E+00   0.798E-03  200    1  0.2264E+01  0.2264E+01
  1   0.100E+00   0.638E-03  250    1  0.5704E+00  0.5704E+00
CYCLE      2 TIME  0.10051E+00 DT=  0.51062E-03 P-ITER=  300 P-TOL=   0.11 PCL-TOL=   0.11  MASS BAL.=0.999998 CT= 0.053
```


Table C.5c

Diagnostic Output from TRACR3D for Problem VARP

The first five lines are from program statement no. 162 (see flow chart) and are printed every time the number of pressure iterations is excessive, causing the time step to be reduced (except for steady-state problems). The last line is printed after each time cycle for any problems doing flow calculations.

```
          PAGE 1                     DN=ELMP3RV                     08/11/84-04:46:27      CFT 1.11(04/16/84)  PAGE 1

  5541       1. 1                                                                             SSRCH.46
PRNAME $MAIN    WARNING -     STATEMENT NUMBER ON BLANK CARD IGNORED ************************************************ P=0035433C
  5541       1. 1                                                                             SSRCH.46
PRNAME $MAIN    WARNING -     MISSING END STATEMENT ************************************************************** P=0035064D
 M=   1   R INPUT FOLLOWS
    0.0     1.0     1.0
 X IN CM FOLLOWS
    0.0     0.0     1.0     1.0
 Q=   1   Y INPUT FOLLOWS
    0.0     1.0     1.0
 Y IN CM FOLLOWS
    0.0     0.0     1.0     1.0
 N= 200   ZCM INPUT FOLLOWS
    0.0   200.0  2000.0
 Z IN CM FOLLOWS
    0.0     0.0    10.0    20.0    30.0    40.0    50.0    60.0    70.0    80.0    90.0   100.0   110.0   120.0   130.0
  140.0   150.0   160.0   170.0   180.0   190.0   200.0   210.0   220.0   230.0   240.0   250.0   260.0   270.0   280.0
  290.0   300.0   310.0   320.0   330.0   310.0   350.0   360.0   370.0   380.0   390.0   400.0   410.0   420.0   430.0
  440.0   450.0   460.0   470.0   480.0   490.0   500.0   510.0   520.0   530.0   540.0   550.0   560.0   570.0   580.0
     .0   600.0   610.0   620.0   630.0   640.0   650.0   660.0   670.0   680.0   690.0   700.0   710.0   720.0   730.0
     .0   750.0   760.0   770.0   780.0   790.0   800.0   810.0   820.0   830.0   840.0   850.0   860.0   870.0   880.0
     .0   900.0   910.0   920.0   930.0   940.0   950.0   960.0   970.0   980.0   990.0  1000.0  1010.0  1020.0  1030.0
     .0  1050.0  1060.0  1070.0  1080.0  1090.0  1100.0  1110.0  1120.0  1130.0  1140.0  1150.0  1160.0  1170.0  1180.0
     .0  1200.0  1210.0  1220.0  1230.0  1240.0  1250.0  1260.0  1270.0  1280.0  1290.0  1300.0  1310.0  1320.0  1330.0
     .0  1350.0  1360.0  1370.0  1380.0  1390.0  1400.0  1410.0  1420.0  1430.0  1440.0  1450.0  1460.0  1470.0  1480.0
     .0  1500.0  1510.0  1520.0  1530.0  1540.0  1550.0  1560.0  1570.0  1580.0  1590.0  1600.0  1610.0  1620.0  1630.0
     .0  1650.0  1660.0  1670.0  1680.0  1690.0  1700.0  1710.0  1720.0  1730.0  1740.0  1750.0  1760.0  1770.0  1780.0
 1790.0  1800.0  1810.0  1820.0  1830.0  1840.0  1850.0  1860.0  1870.0  1880.0  1890.0  1900.0  1910.0  1920.0  1930.0
 1940.0  1950.0  1960.0  1970.0  1980.0  1990.0  2000.0  2000.0
MATERIAL TABLE FOLLOWS
     1.   0.100E+01    0.100E+01    0.100E+01 1.0000 1.0000 0.0000 0.000010.0000   0.000E+00  1.000   1.000   0.000

 CELL MATERIAL DATA FOLLOWS
     1    1    1    1    1 200   1
 CHANGES TO INITIAL TRACER CONCENTRATION (GM/CC)
   1.  1.  1.  1.  0.201. 0.00000E+00    0.  0.
 CHANGES TO INITIAL ADSORBED CONCENTRATION (GM/GM)
   1.  1.  1.  1.  0.201. 0.00000E+00    0.  0.
 CHANGES TO INITIAL GAS SATURATION
   1.  1.  1.  1.  0.201. 0.00000E+00    0.
 CHANGES TO INITIAL PRESSURE (P=ATM) DISTRIBUTION
   1.  1.  1.  1.  0.201. 0.10000E+07    0.
     LEFT BOUNDARY SET UP FOLLOWS

   1
   1
   1
   1
   1
   1
   1
   1
   1
```

Table C.6a

TRACR3D Input Data Recapitulation for Problem PIG3

```
    THREE CHAIN DECAY AND TRANSPORT       (PIGFORD)                    Z LEVEL     5  Z =       45.000
TIME      2.78  HRS    CYCLE     924 DT  0.11E+02
                       MASS (GM)-GAS-    L,R,B,T,F,BK    0.0000E+00   0.0000E+00   0.0000E+00   0.0000E+00   0.0000E+00   0.0000E+00
                       MASS (GM)-LIQUID- L,R,B,T,F,BK    0.0000E+00   0.0000E+00   0.2201E+04   0.2201E+04   0.0000E+00   0.0000E+00
                            1
                            0.50
                            1
  1     0.50   1   1.00E+06   1      0.50   1
                       1.00E+06
                       0.00E+00
                       8.19E-01
                       0.00E+00
                       7.08E-03
                       0.00E+00
                       1.93E-03
                       0.00E+00
                        01,1110
                        S 0,P 0    S
                            1
                            0.50
                            1
```


Table C.6b

Main Output for Problem PIG3

Problem PIG3 returned 196 similar pages. This output included more numbers than for previous problems since PIG3 includes three tracers. See Appendix C of Travis (1984) (LA-9667-MS) for a complete description of this output.

```
          PAGE 1                  C.=LIMPURY                      08/11/84-22:30:41      CFT 1.11(04/16/84)  PAGE 1

 5536        1. 1                                                                             SSRCH.46
PRNAPE SPAIN     WARNING =      STA. MENT ORDER ON FLAG CARD IGNORED ******************************************************** P=00035433C
 5538        1. 1                                                                             SSRCH.46
PRNAPE SPAIN     WARNING =      MISSING END STATEMENT ****************************************************************** P=00035064D
 M=   1   R INPUT FOLLOWS
   0.0      1.0    270.0
 X IN CM FOLLOWS
   0.0      0.0    270.0    270.0
 U=   1   Y INPUT FOLLOWS
   0.0      1.0    270.0
 Y IN CM FOLLOWS
   0.0      0.0    270.0    270.0
 N= 150  ZCM INPUT FOLLOWS
 -600.0   150.0      0.0
 Z IN CM FOLLOWS
 -600.0  -600.0  -596.0  -592.0  -588.0  -584.0  -580.0  -576.0  -572.0  -568.0  -564.0  -560.0  -556.0  -552.0  -548.0
 -544.0  -540.0  -536.0  -532.0  -528.0  -524.0  -520.0  -516.0  -512.0  -508.0  -504.0  -500.0  -496.0  -492.0  -488.0
 -484.0  -480.0  -476.0  -472.0  -468.0  -464.0  -460.0  -456.0  -452.0  -448.0  -444.0  -440.0  -436.0  -432.0  -428.0
     .0  -420.0  -416.0  -412.0  -408.0  -404.0  -400.0  -396.0  -392.0  -388.0  -384.0  -380.0  -376.0  -372.0  -368.0
     .0  -360.0  -356.0  -352.0  -348.0  -344.0  -340.0  -336.0  -332.0  -328.0  -324.0  -320.0  -316.0  -312.0  -308.0
     .0  -300.0  -296.0  -292.0  -288.0  -284.0  -280.0  -276.0  -272.0  -268.0  -264.0  -260.0  -256.0  -252.0  -248.0
     .0  -240.0  -236.0  -232.0  -228.0  -224.0  -220.0  -216.0  -212.0  -208.0  -204.0  -200.0  -196.0  -192.0  -188.0
     .0  -180.0  -176.0  -172.0  -168.0  -164.0  -160.0  -156.0  -152.0  -148.0  -144.0  -140.0  -136.0  -132.0  -128.0
     .0  -120.0  -116.0  -112.0  -108.0  -104.0  -100.0   -96.0   -92.0   -88.0   -84.0   -80.0   -76.0   -72.0   -68.0
     .0   -60.0   -56.0   -52.0   -48.0   -44.0   -40.0   -36.0   -32.0   -28.0   -24.0   -20.0   -16.0   -12.0    -8.0
     .0     0.0     0.0
MATERIAL TABLE FOLLOWS
    1.   0.250E+00    0.250E+00    0.250E+00 0.3460 0.1000 0.0000 0.1000 0.4329 -0.100E+01   2.500   1.000  0.000
    2.   0.300E+02    0.300E+02    0.300E+02 0.4500 1.0000 0.0000 0.000010.0000  0.100E+05   2.500   1.000  0.000
    3.   0.500E+01    0.500E+01    0.500E+01 0.3300 0.1000 0.0000 0.0000 1.0000  0.150E+05   2.500   1.000  0.000
    4.   0.250E+00    0.250E+00    0.250E+00 0.3460 0.1000 0.0000 0.1000 0.4329  0.000E+00   2.500   1.000  0.000

 CELL MATERIAL DATA FOLLOWS
      0   2   0   2   0   6  2       0   2   0   2   7  12   3       0   2   0   2 151 151   4       0   2   0   2  13 150   1
 CHANGES TO INITIAL GAS SATURATION
    0.  2.  0.  2.  0.  6. 0.10000E+01     0.  2.  0.  2. 13. 32. 0.24300E+00     0.  2.  0.  2. 33. 52. 0.36000E+00

    0.  2.  0.  2. 53. 72. 0.40000E+00     0.  2.  0.  2. 73. 92. 0.44000E+00     0.  2.  0.  2. 93.111. 0.47400E+00

    0.  2.  0.  2.112.130. 0.46200E+00     0.  2.  0.  2.131.150. 0.48300E+00     0.  2.  0.  2.  7. 12. 0.60000E+00

    0.
 CHANGES TO INITIAL PRESSURE (P=P1*) DISTRIBUTION
    0.  2.  0.  2.  0.150. 0.00000E+00    0.
 TIME DEPENDENT BOUNDARY NUMBER AND LOCATION
 10       0  11       0  12       0  13       0  14       0  15       0  16       0  17       0  18       0  19       0  20       3
HAVE 13 POINTS FOR TIME HISTORY,  TMPT=    1200.0     SEC. 1.0.K FOR POINTS FOLLOWS
     1,  1,  1       1,  1,  5       1,  1,  6       1,  1,  9
     1,  1, 44       1,  1, 63       1,  1, 82       1,  1,102
     1,  1,150
     LEFT BOUNDARY SET UP FOLLOWS

    1
    1
    1
```

Table C.7a

TRACR3D Input Data Recapitulation for Problem LS6

```
      LS-6 EXPERIMENT, 13 CM PULSE,  CAISSON A                              Z LEVEL      1  Z =      =598.000
TIME      3.13  HRS     CYCLE       19 DT  0.11E+04
                                MASS (GM)-GAS-    L,P,B,T,F,PK       0.0000E+00      0.0000E+00      0.0000E+00      0.0000E+00      0.0000E+00      0.0000E+00
                                MASS (GM)-LIQUID- L,P,B,T,F,PK       0.0000E+00      0.0000E+00     -0.2115E-09     -0.4843E+06      0.0000E+00      0.0000E+00
                                   1
                                  135.00
                                   1
  1    135.00   1   0.00E+00   1    135.00   1
                               -3.17E+04
                                1.00E+00
                                 02,0001
                                 S 0,P 0    S
                                   1
                                  135.00
                                   1
```

Table C.7b

Main Output for Problem LS6

Similar pages were obtained for 19 Z-values at 17 time values, amounting to 323 pages.

```
CYCLE   355 TIME  0.37247E+06 DT=  0.81000E+03 P-ITER=   6 P-TOL=   0.00 PCL-TOL=   0.97  MASS BAL.=1.062124 CT= 0.151
CYCLE   356 TIME  0.37344E+06 DT=  0.97700E+03 P-ITER=   7 P-TOL=   0.00 PCL-TOL=   0.97  MASS BAL.=1.061404 CT= 0.169
CYCLE   357 TIME  0.37461E+06 DT=  0.11164E+04 P-ITER=   8 P-TOL=   0.00 PCL-TOL=   0.88  MASS BAL.=1.060564 CT= 0.188
CYCLE   358 TIME  0.37601E+06 DT=  0.13957E+04 P-ITER=  14 P-TOL=   0.00 PCL-TOL=   0.84  MASS BAL.=1.059683 CT= 0.306
CYCLE   359 TIME  0.37769E+06 DT=  0.16796E+04 P-ITER=  26 P-TOL=   0.00 PCL-TOL=   0.84  MASS BAL.=1.059686 CT= 0.531
CYCLE   360 TIME  0.37966E+06 DT=  0.19964E+04 P-ITER=  22 P-TOL=   0.00 PCL-TOL=   0.88  MASS BAL.=1.058202 CT= 0.457
CYCLE   361 TIME  0.38202E+06 DT=  0.23366E+04 P-ITER=  30 P-TOL=   0.00 PCL-TOL=   0.88  MASS BAL.=1.056486 CT= 0.599
CYCLE   362 TIME  0.38436E+06 DT=  0.23367E+04 P-ITER=  38 P-TOL=   0.00 PCL-TOL=   0.97  MASS BAL.=1.054752 CT= 0.760
CYCLE   363 TIME  0.38669E+06 DT=  0.23367E+04 P-ITER=  27 P-TOL=   0.00 PCL-TOL=   0.74  MASS BAL.=1.053053 CT= 0.548
CYCLE   364 TIME  0.38903E+06 DT=  0.23367E+04 P-ITER=  42 P-TOL=   0.00 PCL-TOL=   0.92  MASS BAL.=1.070411 CT= 0.866
CYCLE   365 TIME  0.39001E+06 DT=  0.98223E+03 P-ITER=  17 P-TOL=   0.00 PCL-TOL=   0.94  MASS BAL.=1.069643 CT= 0.353
CYCLE   366 TIME  0.39119E+06 DT=  0.11767E+04 P-ITER=  20 P-TOL=   0.00 PCL-TOL=   0.95  MASS BAL.=1.068722 CT= 0.415
CYCLE   367 TIME  0.39260E+06 DT=  0.14144E+04 P-ITER=  18 P-TOL=   0.00 PCL-TOL=   0.99  MASS BAL.=1.067619 CT= 0.381
CYCLE   368 TIME  0.39430E+06 DT=  0.16973E+04 P-ITER=  22 P-TOL=   0.00 PCL-TOL=   0.58  MASS BAL.=1.070162 CT= 0.464
CYCLE   369 TIME  0.39595E+06 DT=  0.16511E+04 P-ITER=  27 P-TOL=   0.00 PCL-TOL=   0.88  MASS BAL.=1.068899 CT= 0.548
CYCLE   370 TIME  0.39793E+06 DT=  0.19813E+04 P-ITER=  24 P-TOL=   0.00 PCL-TOL=   0.97  MASS BAL.=1.067354 CT= 0.484
370    0.398E+06     0.234E+04    50      0  0.0000E+00   0.2120E+01
CYCLE   371 TIME  0.39980E+06 DT=  0.18693E+04 P-ITER= 100 P-TOL=   0.00 PCL-TOL=   1.32  MASS BAL.=1.065937 CT= 1.938
CYCLE   372 TIME  0.40136E+06 DT=  0.15578E+04 P-ITER=  35 P-TOL=   0.00 PCL-TOL=   0.68  MASS BAL.=1.064761 CT= 0.710
CYCLE   373 TIME  0.40292E+06 DT=  0.15578E+04 P-ITER=  25 P-TOL=   0.00 PCL-TOL=   0.92  MASS BAL.=1.300470 CT= 0.543
CYCLE   374 TIME  0.40308E+06 DT=  0.15838E+03 P-ITER=   4 P-TOL=   0.00 PCL-TOL=   0.32  MASS BAL.=1.300235 CT= 0.110
CYCLE   375 TIME  0.40327E+06 DT=  0.19006E+03 P-ITER=   4 P-TOL=   0.00 PCL-TOL=   0.69  MASS BAL.=1.299952 CT= 0.110
CYCLE   376 TIME  0.40350E+06 DT=  0.22807E+03 P-ITER=   5 P-TOL=   0.00 PCL-TOL=   0.43  MASS BAL.=1.299614 CT= 0.130
CYCLE   377 TIME  0.40377E+06 DT=  0.27368E+03 P-ITER=   5 P-TOL=   0.00 PCL-TOL=   0.88  MASS BAL.=1.299206 CT= 0.129
CYCLE   378 TIME  0.40410E+06 DT=  0.32842E+03 P-ITER=   6 P-TOL=   0.00 PCL-TOL=   0.87  MASS BAL.=1.298717 CT= 0.150
CYCLE   379 TIME  0.40449E+06 DT=  0.39410E+03 P-ITER=   7 P-TOL=   0.00 PCL-TOL=   0.70  MASS BAL.=1.298133 CT= 0.170
CYCLE   380 TIME  0.40496E+06 DT=  0.47292E+03 P-ITER=   7 P-TOL=   0.00 PCL-TOL=   0.85  MASS BAL.=1.297431 CT= 0.169
CYCLE   381 TIME  0.40553E+06 DT=  0.56751E+03 P-ITER=   7 P-TOL=   0.00 PCL-TOL=   0.85  MASS BAL.=1.296617 CT= 0.171
CYCLE   382 TIME  0.40621E+06 DT=  0.68101E+03 P-ITER=   6 P-TOL=   0.00 PCL-TOL=   0.78  MASS BAL.=1.297600 CT= 0.151
CYCLE   383 TIME  0.40703E+06 DT=  0.81721E+03 P-ITER=   6 P-TOL=   0.00 PCL-TOL=   0.92  MASS BAL.=1.296414 CT= 0.151
CYCLE   384 TIME  0.40801E+06 DT=  0.98066E+03 P-ITER=   8 P-TOL=   0.00 PCL-TOL=   0.94  MASS BAL.=1.295001 CT= 0.190
CYCLE   385 TIME  0.40919E+06 DT=  0.11768E+04 P-ITER=   8 P-TOL=   0.00 PCL-TOL=   0.84  MASS BAL.=1.293305 CT= 0.188
CYCLE   386 TIME  0.41060E+06 DT=  0.14121E+04 P-ITER=  14 P-TOL=   0.00 PCL-TOL=   0.91  MASS BAL.=1.291407 CT= 0.307
CYCLE   387 TIME  0.41229E+06 DT=  0.16946E+04 P-ITER=  29 P-TOL=   0.00 PCL-TOL=   0.75  MASS BAL.=1.294758 CT= 0.591
CYCLE   388 TIME  0.41402E+06 DT=  0.17250E+04 P-ITER=  21 P-TOL=   0.00 PCL-TOL=   1.00  MASS BAL.=1.292252 CT= 0.436
CYCLE   389 TIME  0.41610E+06 DT=  0.20748E+04 P-ITER=  24 P-TOL=   0.00 PCL-TOL=   0.86  MASS BAL.=1.289267 CT= 0.486
CYCLE   390 TIME  0.41843E+06 DT=  0.23367E+04 P-ITE
CYCLE   391 TIME  0.42077E+06 DT=  0.23366E+04 P-ITE
CYCLE   392 TIME  0.42311E+06 DT=  0.23367E+04 P-ITE
CYCLE   393 TIME  0.42544E+06 DT=  0.23367E+04 P-ITE
CYCLE   394 TIME  0.42587E+06 DT=  0.43004E+03 P-ITE
CYCLE   395 TIME  0.42639E+06 DT=  0.51605E+03 P-ITE
CYCLE   396 TIME  0.42701E+06 DT=  0.61925E+03 P-ITE
CYCLE   397 TIME  0.42728E+06 DT=  0.26519E+03 P-ITE
CYCLE   398 TIME  0.42759E+06 DT=  0.31823E+03 P-ITE
CYCLE   399 TIME  0.42798E+06 DT=  0.38188E+03 P-ITE
CYCLE   400 TIME  0.42843E+06 DT=  0.45825E+03 P-ITE
CYCLE   401 TIME  0.42898E+06 DT=  0.54990E+03 P-ITE
CYCLE   402 TIME  0.42964E+06 DT=  0.65988E+03 P-ITE
CYCLE   403 TIME  0.43044E+06 DT=  0.79186E+03 P-ITE
CYCLE   404 TIME  0.43139E+06 DT=  0.95023E+03 P-ITE
CYCLE   405 TIME  0.43253E+06 DT=  0.11403E+04 P-ITER=  11 P-TOL=   0.00 PCL-TOL=   0.88  MASS BAL.=1.506071 CT= 0.247
```

Table C.7c

Diagnostic Output from TRACR3D for Problem LS6

Problem LS6 went through 2804 cycles, producing 2804 lines of output like these as well as some like the interruption shown here from statement number 162. (see Table C.5c).

Appendix D

Parameters from the NNWSI Reference Information Base and the NNWSI Technical Data Base

The six test problems described in this report were used to implement the TRACR3D code at SNL and were not intended to produce any results based on the Yucca Mountain material properties or directly applicable to the planned repository. Therefore, no parameters from the NNWSI Reference Information Base or NNWSI Technical Data Base were used.

Data used in this report was identical to that used for the same test problems as run at LANL to provide comparable output.

DISTRIBUTION LIST

B. C. Rusche (RW-1)
Director
Office of Civilian Radioactive
Waste Management
U.S. Department of Energy
Forrestal Building
Washington, DC 20585

T. P. Longo (RW-25)
Program Management Division
Office of Geologic Repositories
U.S. Department of Energy
Forrestal Building
Washington, DC 20585

Ralph Stein (RW-23)
Office of Civilian Radioactive
Waste Management
U.S. Department of Energy
Forrestal Building
Washington, DC 20585

Cy Klingsberg (RW-24)
Geosciences and Technology Division
Office of Geologic Repositories
U. S. Department of Energy
Forrestal Building
Washington, DC 20585

J. J. Fiore, (RW-221)
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Forrestal Building
Washington, DC 20585

B. G. Gale (RW-223)
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Waste Management
U.S. Department of Energy
Forrestal Building
Washington, DC 20585

M. W. Frei (RW-231)
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Washington, DC 20585

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U.S. Department of Energy
Forrestal Building
Washington, D.C. 20585

C. R. Cooley (RW-24)
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U.S. Department of Energy
Forrestal Building
Washington, DC 20585

J. E. Shaheen (RW-44)
Outreach Programs
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U.S. Department of Energy
Forrestal Building
Washington, DC 20585

V. J. Cassella (RW-222)
Office of Civilian Radioactive
Waste Management
U.S. Department of Energy
Forrestal Building
Washington, DC 20585

J. O. Neff, Manager
Salt Repository Project Office
U.S. Department of Energy
505 King Avenue
Columbus, OH 43201

D. C. Newton (RW-23)
Engineering & Licensing Division
Office of Geologic Repositories
U.S. Department of Energy
Forrestal Building
Washington, DC 20585

S. A. Mann, Manager
Crystalline Rock Project Office
U.S. Department of Energy
9800 South Cass Avenue
Argonne, IL 60439

O. L. Olson, Manager
Basalt Waste Isolation Project Office
Richland Operations Office
U.S. Department of Energy
Post Office Box 550
Richland, WA 99352

K. Street, Jr.
Lawrence Livermore National
Laboratory
Post Office Box 808
Mail Stop L-209
Livermore, CA 94550

D. L. Vieth, Director (4)
Waste Management Project Office
U.S. Department of Energy
Post Office Box 14100
Las Vegas, NV 89114

L. D. Ramspott (3)
Technical Project Officer for NNWSI
Lawrence Livermore National
Laboratory
P.O. Box 808
Mail Stop L-204
Livermore, CA 94550

D. F. Miller, Director
Office of Public Affairs
U.S. Department of Energy
Post Office Box 14100
U.S. Department of Energy
Las Vegas, NV 89114

W. J. Purcell (RW-20)
Associate Director
Office of Civilian Radioactive
Waste Management
U.S. Department of Energy
Forrestal Building
Washington, DC 20585

P. M. Bodin (12)
Office of Public Affairs
U.S. Department of Energy
Post Office Box 14100
Las Vegas, NV 89114

D. T. Oakley (4)
Technical Project Officer for NNWSI
Los Alamos National Laboratory
P.O. Box 1663
Mail Stop F-619
Los Alamos, NM 87545

B. W. Church, Director
Health Physics Division
U.S. Department of Energy
Post Office Box 14100
Las Vegas, NV 89114

L. R. Hayes (3)
Technical Project Officer for NNWSI
U.S. Geological Survey
Post Office Box 25046
421 Federal Center
Denver, CO 80225

Chief, Repository Projects Branch
Division of Waste Management
U.S. Nuclear Regulatory Commission
Washington, D.C. 20555

NTS Section Leader
Repository Project Branch
Division of Waste Management
U.S. Nuclear Regulatory Commission
Washington, D.C. 20555

Document Control Center
Division of Waste Management
U.S. Nuclear Regulatory Commission
Washington, D.C. 20555

V. M. Glanzman
U.S. Geological Survey
Post Office Box 25046
913 Federal Center
Denver, CO 80225

P. T. Prestholt
NRC Site Representative
1050 East Flamingo Road
Suite 319
Las Vegas, NV 89109

J. S. Wright
Technical Project Officer for NNWSI
Westinghouse Electric Corporation
Waste Technology Services Division
Nevada Operations
Post Office Box 708
Mail Stop 703
Mercury, NV 89023

M. E. Spaeth
Technical Project Officer for NNWSI
Science Applications
International Corporation
Suite 407
101 Convention Center Drive
Las Vegas, NV 89109

ONWI Library
Battelle Columbus Laboratory
Office of Nuclear Waste Isolation
505 King Avenue
Columbus, OH 43201

SAIC-T&MSS Library (2)
Science Applications
International Corporation
Suite 407
101 Convention Center Drive
Las Vegas, NV 89109

W. M. Hewitt, Program Manager
Roy F. Weston, Inc.
955 L'Enfant Plaza, Southwest, Suite 800
Washington, DC 20024

W. S. Twenhofel, Consultant
Science Applications
International Corp.
820 Estes Street
Lakewood, CO 89215

H. D. Cunningham
General Manager
Reynolds Electrical &
Engineering Co., Inc.
Post Office Box 14400
Mail Stop 555
Las Vegas, NV 89114

A. E. Gurrola
General Manager
Energy Support Division
Holmes & Narver, Inc.
Mail Stop 580
Post Office Box 14340
Las Vegas, NV 89114

T. Hay, Executive Assistant
Office of the Governor
State of Nevada
Capitol Complex
Carson City, NV 89710

J. A. Cross, Manager
Las Vegas Branch
Fenix & Scisson, Inc.
Mail Stop 514
Post Office Box 14308
Las Vegas, NV 89114

R. R. Loux, Jr., Executive Director (3)
Nuclear Waste Project Office
State of Nevada
Evergreen Center, Suite 252
1802 North Carson Street
Carson City, NV 89701

Neal Duncan (RW-44)
Office of Policy, Integration, and
Outreach
U.S. Department of Energy
Forrestal Building
Washington, DC 20585

C. H. Johnson, Technical
Program Manager
Nuclear Waste Project Office
State of Nevada
Evergreen Center, Suite 252
1802 North Carson Street
Carson City, NV 89701

John Fordham
Desert Research Institute
Water Resources Center
Post Office Box 60220
Reno, NV 89506

Dr. Martin Mifflin
Desert Research Institute
Water Resources Center
Suite 1
2505 Chandler Avenue
Las Vegas, NV 89120

Department of Comprehensive Planning
Clark County
225 Bridger Avenue, 7th Floor
Las Vegas, NV 89155

Planning Department
Nye County
Post Office Box 153
Tonopah, NV 89049

Lincoln County Commission
Lincoln County
Post Office Box 90
Pioche, NV 89043

Economic Development Department
City of Las Vegas
400 East Stewart Avenue
Las Vegas, NV 89101

Community Planning and Development
City of North Las Vegas
Post Office Box 4086
North Las Vegas, NV 89030

Director of Community Planning
City of Boulder City
Post Office Box 367
Boulder City, NV 89005

City Manager
City of Henderson
Henderson, NV 89015

Commission of the European Communities
200 Rue de la Loi
B-1049 Brussels
BELGIUM

N. A. Norman
Project Manager
Bechtel National Inc.
P. O. Box 3965
San Francisco, CA 94119

Technical Information Center
Roy F. Weston, Inc.
955 L'Enfant Plaza, Southwest, Suite 800
Washington, DC 20024

Flo Butler
Los Alamos Technical Associates
1650 Trinity Drive
Los Alamos, New Mexico 87544

R. Harig
Parsons Brinkerhoff Quade & Douglas, Inc.
1625 Van Ness Ave.
San Francisco, CA 94109-3678

Timothy G. Barbour
Science Applications International Corporation
1626 Cole Boulevard, Suite 270
Golden, CO 80401

Dr. Madan M. Singh, President
Engineers International, Inc.
98 East Naperville Road
Westmont, IL 60559-1595

E. P. Binnall
Field Systems Group Leader
Building 50B/4235
Lawrence Berkeley Laboratory
Berkeley, CA 94720

Roger Hart
Itasca Consulting Group, Inc.
P.O. Box 14806
Minneapolis, Minnesota 55414

T. H. Isaacs (RW-22)
Office of Civilian Radioactive
Waste Management
U.S. Department of Energy
Forrestal Building
Washington, DC 20585

J. P. Knight (RW-24)
Office of Civilian Radioactive
Waste Management
U.S. Department of Energy
Forrestal Building
Washington, DC 20585

D. H. Alexander (RW-232)
Office of Civilian Radioactive
Waste Management
U.S. Department of Energy
Forrestal Building
Washington, DC 20585

Allen Jelacic (RW-233)
Office of Civilian Radioactive
Waste Management
U.S. Department of Energy
Forrestal Building
Washington, DC 20585

B. J. King, Librarian (2)
Basalt Waste Isolation Project
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J. R. Rollo
Deputy Assistant Director
for Engineering Geology
U.S. Geological Survey
106 National Center
12201 Sunrise Valley Drive
Reston, VA 22092

David K. Parrish
RE/SPEC Inc.
3815 Eubank, N.E.
Albuquerque, NM 87191

R. Lindsay Mundell
United States Bureau of Mines
P.O. Box 25086
Building 20
Denver Federal Center
Denver, Colorado 80225

D. L. Fraser, General Manager
Reynolds Electrical & Engineering
Co., Inc.
Mail Stop 555
Post Office Box 14400
Las Vegas, NV 89114-4400

Vincent Gong
Technical Project Officer for NNWSI
Reynolds Electrical & Engineering
Co., Inc.
Mail Stop 615
Post Office Box 14400
Las Vegas, NV 89114-4400

Gerald Parker (RW-241)
Office of Civilian Radioactive
Waste Management
U.S. Department of Energy
Forrestal Building
Washington, DC 20585

Christopher M. St. John
J. F. T. Agapito Associates, Inc.
27520 Hawthorne Blvd., Suite 137
Rolling Hills Estates, CA 90274

J. P. Pedalino
Technical Project Officer for NNWSI
Holmes & Narver, Inc.
Mail Stop 605
Post Office Box 14340
Las Vegas, NV 89114

S. D. Murphy
Technical Project Officer for NNWSI
Fenix & Scisson, Inc.
Mail Stop 514
Post Office Box 15408
Las Vegas, NV 89114

Eric Anderson
Mountain West Research-Southwest, Inc.
398 South Mill Avenue, Suite 300
Tempe, AZ 85281

S. H. Kale (RW-20)
Office of Civilian Radioactive
Waste Management
U. S. Department of Energy
Forrestal Building
Washington, DC 20585

Judy Foremaster (5)
City of Caliente
Post Office Box 158
Caliente, NV 89008

J. H. Anttonen, Deputy Assistant
Manager for Commercial
Basalt Waste Isolation Project
Office
U. S. Department of Energy
P.O. Box 550
Richland, WA 99352

K. Birdsell
Los Alamos National Laboratory
MS F665
Los Alamos, NM 87545

B.J. Travis
Los Alamos National Laboratory
MS F665
Los Alamos, NM 87545

1511 D. K. Gartling
1511 R. R. Eaton
6300 R. W. Lynch
6310 T. O. Hunter
6310 NNWSICF
6310 22/12144/04-1872/REP-II/QIII
6310 72-12143-0/QIII
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6311 C. Mora
6312 F. W. Bingham
6312 G. E. Barr
6312 J. Foster (6)
6312 J. Gauthier
6312 M. L. Green
6312 B. S. Langkopf
6312 W. B. Miller
6312 R. R. Peters
6312 A. C. Peterson
6312 R. W. Prindle
6312 N. K. Prindle
6312 M. S. Tierney
6312 M. Wilson
6312 J. G. Yeager
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6313 E. A. Klavetter
6314 J. R. Tillerson
6315 S. Sinnock
6315 P. C. Kaplan
6316 R. B. Pope
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6331 A. R. Lappin
6332 L. D. Tyler
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6410 N. R. Ortiz
3141 S. A. Landenberger (5)
3151 W. L. Garner (3)
8024 P. W. Dean
3154-3 C. H. Dalin (28)
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