Modification and Application of TOUGH2 as a Variable-Density, Saturated-Flow Code and Comparison to SWIFT II Results

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1.0   Introduction

Human intrusion scenarios at the Waste Isolation Pilot Plant (WIPP) involve penetration of the repository and an underlying brine reservoir by a future borehole. Brine and gas from the brine reservoir and the repository may flow up the borehole and into the overlying Culebra formation, which is saturated with water containing different amounts of dissolved solids resulting in a spatially varying density. Current modeling approaches involve perturbing a steady-state Culebra flow field by inflow of gas and/or brine from a breach borehole that has passed through the repository. Previous studies simulating steady-state flow in the Culebra have been done. One specific study by LaVenue et al. (1990) used the SWIFT II code (Reeves et al., 1986), a single-phase flow and transport code, to develop the steady-state flow field. Because gas may also be present in the fluids from the intrusion borehole, a two-phase code such as TOUGH2 can be used to determine the effect that emitted fluids may have on the steady-state Culebra flow field. Thus a comparison between TOUGH2 and SWIFT II was prompted.

In order to compare the two codes and to evaluate the influence of gas on flow in the Culebra, modifications were made to TOUGH2. Modifications were performed by the authors to allow for element-specific values of permeability, porosity, and elevation. The analysis also used a new equation of state module for a water-brine-air mixture, EOS7 (Pruess, 1991), which was developed to simulate variable water densities by assuming a miscibile mixture of water and brine phases and allows for element-specific brine concentration in the INCON file.

2.0   Code Modifications

Comparison between SWIFT II and TOUGH2 numerical models of the Culebra Dolomite prompted changes to be made in TOUGH2. SWIFT II allows the analyst to enter element-specific formation properties; TOUGH2 did not. Thus changes were required in TOUGH2 to be able to enter element-specific formation properties such as permeability, porosity, and elevation. These properties needed to be varied at each grid-cell center. Additional changes were made in the TOUGH2 code so that portions of a SWIFT II input deck could be read and the information utilized by TOUGH2. An outline of the general changes made to the code is shown in Figure 1.

Three new subroutines were added to TOUGH2: HETERO, HINCON and EL2BETA. Three input files that hold the general information, the initial conditions and the boundary conditions are read to provide the heterogeneous formation parameters. All the heterogeneous parameters are output to the file INCON and subsequently read in RFILE. Changes to the format of INCON include addition of the permeability vectors and elevation on the same line as the "elem" and porosity values. Changes were made to the SAVE file format to mimic INCON.

HETERO is called by the main program. It reads the heterogeneous formation parameters from three input files and stores the information in specified matrices. The three input files are HETERO.INP, HETIC.INP and HETBC.INP. HETERO also converts hydraulic conductivity values to permeability if so requested.

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┌──────────────┐
│   T2CG1      │          ╭─────────────────────────────╮
│(main program)│          │  Added Common Blocks:       │
└──────────────┘          │     e7/perm(3,nel)          │
       │                  │     e8/elev(nel)            │
       │                  │     het/idhet,iiperm,ielev  │
┌──────────────┐          │     ihn/iincon              │
│      IO      │          ╰─────────────────────────────╯
└──────────────┘
       │                  ╭─────────────────────────────────╮
       │                  │  if INCON exists iincon=1       │
┌──────────────┐          │                                 │
│   SECOND     │          │  if hetero.inp exists set idhet=1│
└──────────────┘          │  if het.ic exists set    idhet=2│
       │                  │  if het.bc exists set    idhet=3│
┌──────────────┐          ╰─────────────────────────────────╯
│  HETERO      │
│(if idhet≠0)  │──┐ set iperm=1,2 or 3, ielev=1
└──────────────┘  │ Read for each indicated cell:
       │          │      Elevations
       │          │      Hydraulic cond./perm. in xyz dir.
       │          │      Xbrine
       │          │      Pressure
       │          │      Porosity
       │          │ Read viscosity and density tables if requested
┌──────────────┐  │ Change hydraulic cond to permeability if req.
│   INPUT      │──┘ From files hetero.inp,hetic.inp,hetbc.inp
└──────────────┘
       │                        ╭──────────────────────────────────╮
   ┌─────────┐                  │  Added:                          │
   │ MESHM   │                  │  •MATER block read of material   │
   └─────────┘                  │   type, vol and conn changes     │
    ┌────┐ ┌──────┐ ┌──────┐    │  •List elev as Z in elem block if het data used│
    │RZ2D│ │ GXYZ │ │ MINC │    │  •Beta determined by el2beta if elev│
    └────┘ └──────┘ └──────┘    │   data present                   │
              ┌──────────┐      ╰──────────────────────────────────╯
              │ EL2BETA  │
              └──────────┘  ╭────────────────────────────╮
   ┌──────────────┐         │Takes elevations and distances│
   │  HINCON      │         │between cells and generates "beta"│
   │(if iincon≠1) │         ╰────────────────────────────╯
   └──────────────┘
              ╭───────────────────────────────────────╮
              │ Generates INCON file from bc,ic het data│
┌──────┐      │ Added pemxyz and elev to INCON file    │
│ FLOP │      │ Prints out het.out a summary of nodal het info│
└──────┘      │ (unit=24)                              │
┌──────┐      ╰───────────────────────────────────────╯
│RFILE │
└──────┘        ╭────────────────────────────────────╮
┌──────────────┐│  Added:                            │
│  INDATA      ││     phi(nel) and perm(3,nel) initialization│
│(if MOP7 > 0) ││     perm(3,nel) read from INCON    │
└──────────────┘╰────────────────────────────────────╯
┌──────────┐   ╭────────────────────────────────────╮
│ SECOND   │   │  Added:                            │
└──────────┘   │     perm(1,nel) printout to output file│
┌──────────┐   ╰────────────────────────────────────╮
│ CYCIT    │       ╭────────────────────────────────────────────╮
└──────────┘       │  Added:                                    │
     ┌───────┐     │  •Change hyd.cond. values to perm if iperm=3│
     │ MULTI │     │  •Use perm(3,nel) instead of per(3,nmat) when het data pres.│
     └───────┘     │  •Use phi(nel) instead of por(nmat) when het data pres.│
     ┌───────┐     ╰────────────────────────────────────────────╯
     │ WRIFI │
     └───────┘
┌──────────┐   ╭────────────────────────────────────────────╮
│ SECOND   │   │  Added SAVE file write with perm(3,nel) and elev(nel)│
└──────────┘   ╰────────────────────────────────────────────╯
END
```
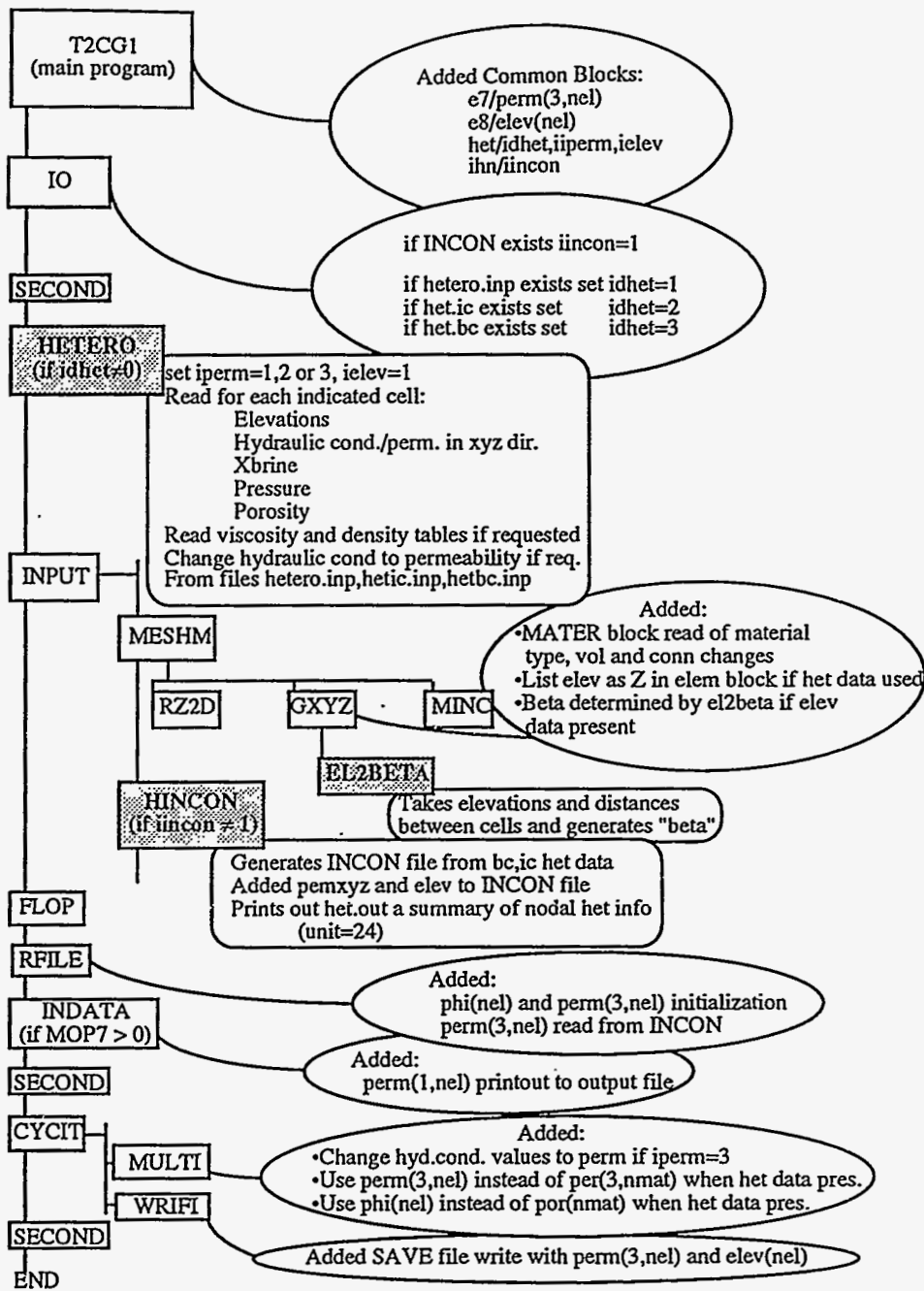
Figure 1. Flow diagram of general heterogeneous material properties changes made to TOUGH2.

HINCON is called by the subroutine INPUT. HINCON writes out the file *INCON* with the appropriate information. Additions to the *INCON* file include the values of the permeability vectors and elevation data for each node on the same line that the "elem" and porosity data are stored. HINCON also prints out *HET.OUT* a summary of the values that were processed by HETERO.

EL2BETA is called by subroutine GXYZ in MESHM. EL2BETA uses elevation data to determine the "betax" parameter (between two elements) of the CONNE.1 card. Betax is the cosine of the angle between the gravitational acceleration vector and the line between the center of the two elements (the
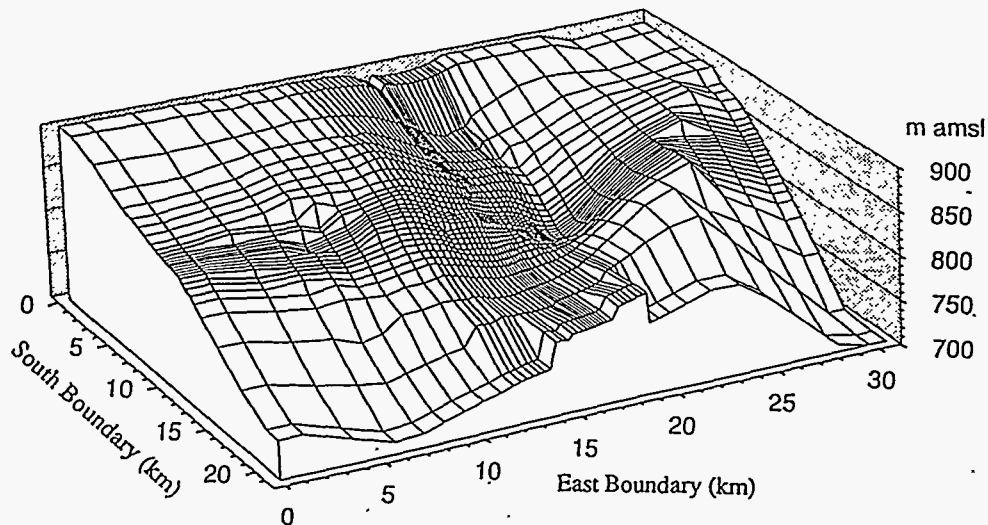
Figure 2. Surface plot of the Culebra model region mesh mid-point elevations.

hypotenuse of the triangle). EL2BETA uses the elevation data (elev1 and elev2) and the distances from the element centroids to their common interface (x1 and x2) to determine betax. MULTI uses betax in conjunction with the gravity vector value to determine density pressure changes due to height differences.

3.0 Culebra Steady-State Flow Field Results

The Culebra Dolomite is generally considered to be the principal groundwater-transport pathway for radionuclides to the accessible environment if a human-intrusion breach in the repository should occur. The Culebra is the most permeable and laterally continuous hydrostratigraphic unit above the repository. It is a fractured, finely crystalline, vuggy dolomite. The transmissivity of the Culebra varies by more than six orders of magnitude in the vicinity of the WIPP (Sandia WIPP Project, 1992). Transmissivity is controlled by the extent of fracturing and the degree to which the fractures are filled by evaporite minerals.

The region of Culebra Dolomite chosen for simulation coincides exactly with the model of LaVenue et al. (1990), who used the SWIFT II code (Reeves et al., 1986). The spatial scale of the model, which includes the WIPP-site boundary, is 21.3 km in the east-west direction by 30.6 km in the north-south direction, for a total area of 651.8 km^2. The model geometry consists of a two-dimensional model of the Culebra as is shown in Figure 2. The Culebra varies in elevation almost 200 meters, from approximately 700 to 900 meters above mean sea level (m amsl). The thickness of the Culebra is 7.7 meters, the median thickness reported for this unit. The permeability distribution for the modeled region is shown in Figure 3. The brine-water density distribution is shown in Figure 4.

Results of the saturated, steady-state pressure and flow fields calculated from the modified version of TOUGH2/EOS7 are essentially the same as those produced by SWIFT II. Figure 5 shows the comparison of the TOUGH2 pressure field to that of the comparable steady-state model of LaVenue et al. (1990). The results show that the pressures trend primarily from east to west, with the higher pressures in the east. The velocity distributions indicate that the largest flux of groundwater occurs along the western portion of the model, where permeabilities are highest. Within the WIPP site boundary the velocities range from 5.0 x 10^{-8} m/s in the northwestern corner to 1.3 x 10^{-10} m/s on the southeastern boundary.
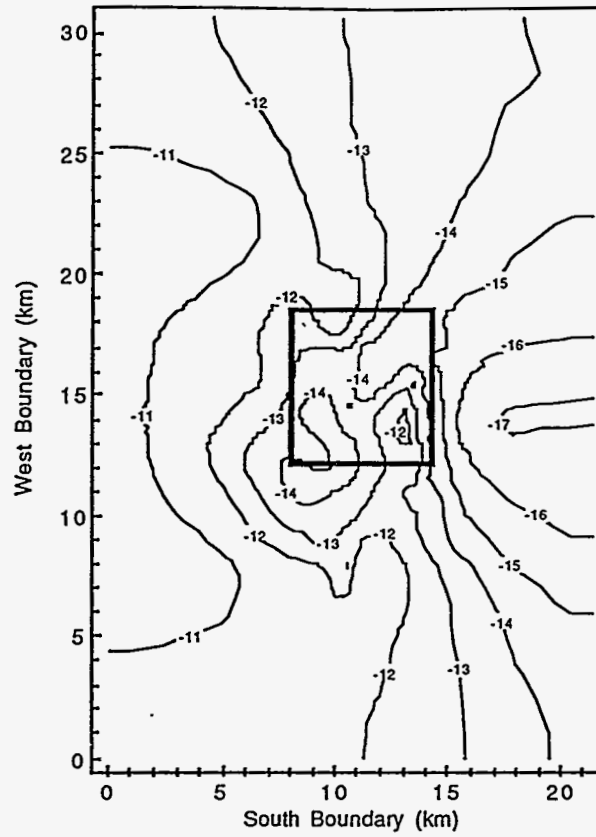
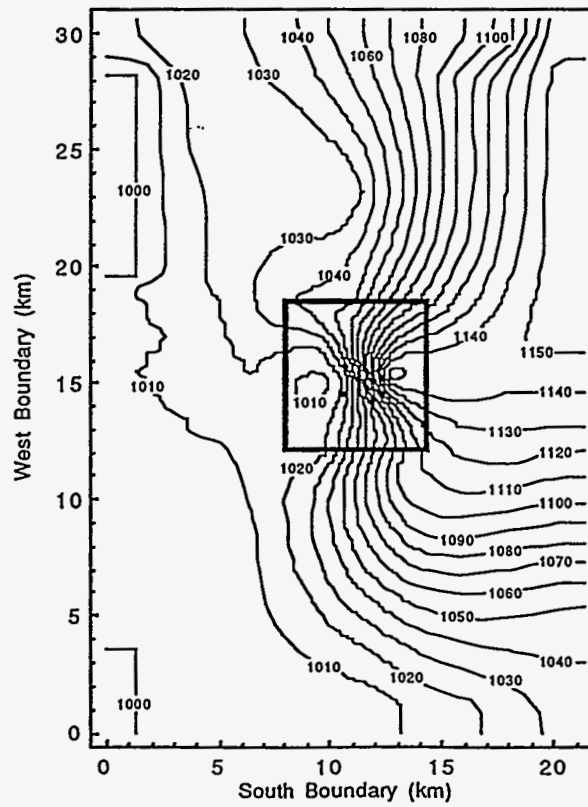Figure 3. Culebra permeability distribution (log m^2). Box in the center indicates WIPP site boundary.

Figure 4. Culebra brine-water density (kg/m^3) distribution. Box in the center indicates WIPP site boundary.
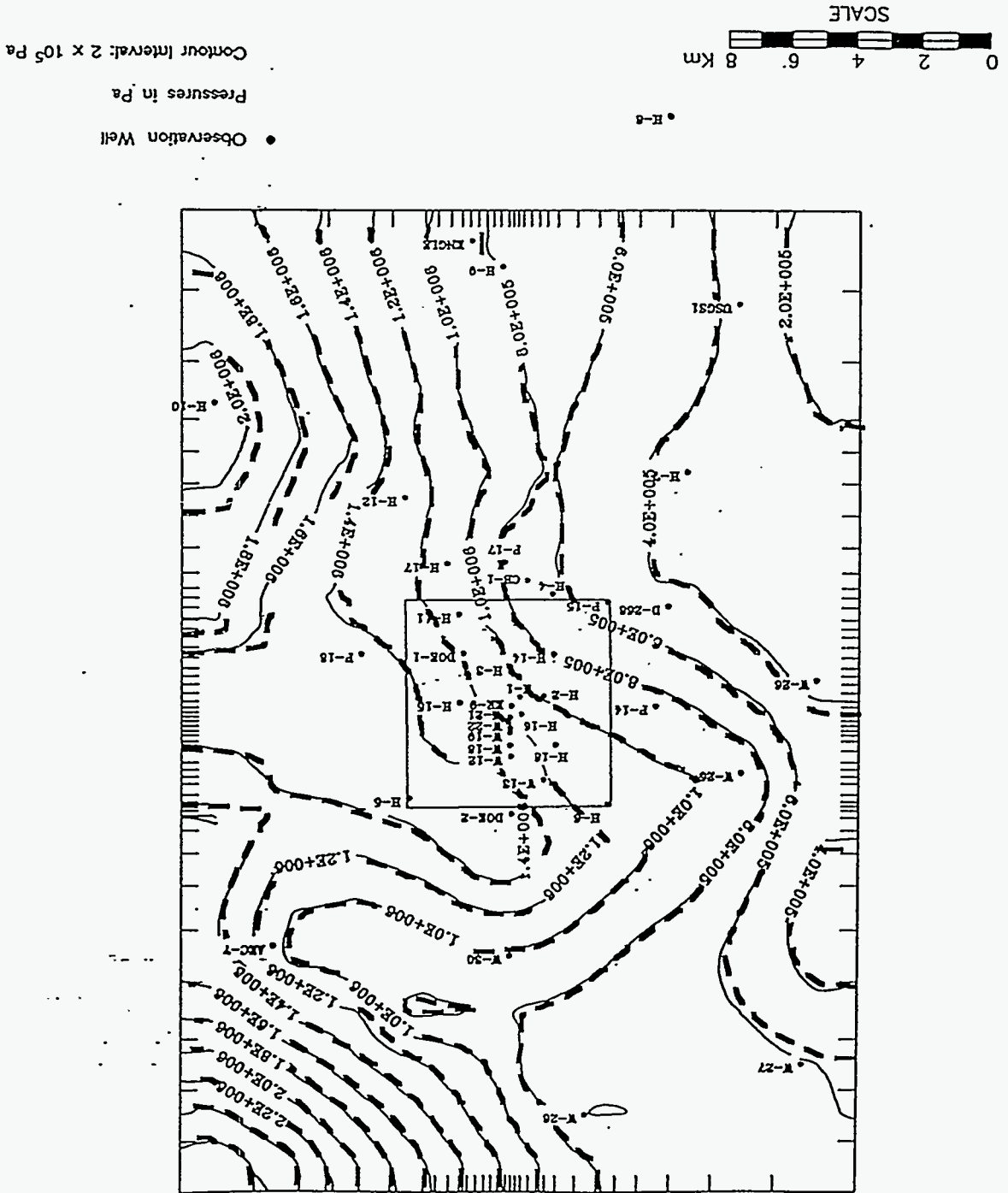
SCALE

0   2   4   6.   8 Km

● Observation Well

Pressures in Pa

Contour Interval: 2×10^5 Pa

Figure 5. Comparison of steady-state pressure fields of LaVenue et al. (1990) (solid lines) to modified TOUGH2/EOS7 (dashed lines). Box in the center indicates WIPP site boundary.

Page 5

4.0 Conclusions

Steady-state simulations of a Culebra Dolomite in the region surrounding the WIPP site were made. The resulting steady-state pressure and flow fields produced from these simulations are essentially the same as those produced by LaVenue et al. [1990]. This model comparison provides a useful benchmark of the newly developed EOS7 module for the TOUGH2 code, illustrating application of TOUGH2 to a variable-density regional groundwater flow problem.

Acknowledgments

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References

LaVenue, A. M., T. L. Cauffman, and J. F. Pickens, 1990, *Ground-Water Flow Modeling of the Culebra Dolomite Volume 1: Model Calibration,* Contractor Report SAND89-7068/1, Sandia National Laboratories, Albuquerque, NM.

Pruess, K., 1991. "EOS7, An Equation-of-State Module for the TOUGH2 Simulator for Two-Phase Flow of Saline Water and Air," *Lawrence Berkeley Laboratory LBL-31114,* August 1991.

Reeves, M., D. S. Ward, N. D. Johns, and R. M. Cranwell, 1986, *Theory and Implementation for SWIFT II, the Sandia Waste-Isolation Flow and Transport Model, Release 4.84,* SAND83-1159, Sandia National Laboratories, Albuquerque, NM.

Cauffman, T.L., A.M. LaVenue, and J.P. McCord, 1990, *Ground-Water Flow Modeling of the Culebra Dolomite Volume II: Data Base,* Contractor Report SAND89-7068/2, Sandia National Laboratories, Albuquerque, NM.

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