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FY 18 Status Report on the Computing Systems for the Yucca

Mountain Project TSPA-LA Models and Inventory of Software used for Process Models

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ABSTRACT

Sandia National Laboratories (SNL) continued evaluation of total system performance assessment (TSPA) computing systems for the previously considered Yucca Mountain Project (YMP). This was done to maintain the operational readiness of the computing infrastructure (computer hardware and software) and knowledge capability for total system performance assessment (TSPA) type analysis, as directed by the National Nuclear Security Administration (NNSA), DOE 2010. This work is a continuation of the ongoing readiness evaluation reported in Lee and Hadgu (2014), Hadgu et al. (2015) and Hadgu and Appel (2016), and Hadgu et al. (2017). The TSPA computing hardware (2014 server cluster -CL2014) and storage system described in Hadgu et al. (2015) were used for the current analysis. One floating license of GoldSim with Versions 9.60.300, 10.5, 11.1 and 12.0 was installed on the cluster head node, and its distributed processing capability was mapped on the cluster processors. Other supporting software were tested and installed to support the TSPA-type analysis on the server cluster. The FY18 task included developing an inventory of software used for the Yucca Mountain Project process models and preliminary assessment of status of the software; enhancing security of the cluster and setting a backup system. The 2014 server cluster and supporting software systems are fully operational to support TSPA-LA type analysis.

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The TSPA computing hardware (2014 server cluster - CL2014) and storage system described in Hadgu et al. (2015) were used for the current analysis. One floating license of GoldSim with Versions 9.60.300, 10.5, 11.1 and 12.0 was installed on the cluster head node, and its distributed processing capability was mapped on the cluster processors. Other supporting software were tested and installed to support the TSPA-type analysis on the server cluster. The FY18 task included developing an inventory of software used for the Yucca Mountain Project process models and preliminary assessment of status of the software; enhancing security of the cluster and setting a backup system. The 2014 server cluster and supporting software systems are fully operational to support TSPA-LA type analysis.

ACRONYMS AND DEFINITIONS

Abbreviation	Definition
API	Applications Programming Interface. A set of interfaces on an OS or other system, usually exposed as documented functions, that can be called by programs to perform commonly required tasks. APIs can expose parts of the system that can't be controlled in other ways.
Backwards Compatibility	The property of an evolving system, OS or API especially, to remain compatible with earlier versions of itself, so that software that runs under or uses the system, can continue to work on later versions without modification.
CL2014	2014 TSPA server cluster (Computing Hardware)
Code	Short for Engineering Code, the word "code" refers to a computer program.
COM, the Component Object Model	A binary standard for software components introduced by Microsoft in 1993. It is the basis for several other Microsoft technologies including Visual Basic, OLE, ActiveX, COM+ and DCOM.
Console Program or Application	Text-based software that runs in the console. Input is received at the command line, by an input deck (usually a structured text file) or by querying the user via output and input commands at the console.
COTS	Commercial off-the-shelf software. General-use software purchased from a software vendor. This software may have been customized for use on the YMP LA by analysts or computer programmers.
DLL	Dynamically Linked Libraries
DOE	Department of Energy
DP	Distributed Processing
DTN	Data Tracking Number
Fortran Intrinsic	Commands that are directly callable by programmers in Fortran source code.
Fortran Intrinsic, Vendor-Specific	Fortran intrinsic that is available in some Fortran compilers and not others. Vendor-specific intrinsics are nonportable and tie the source code to a specific compiler vendor.
GB	Gigabyte
GOTS, Government Off-the-Shelf	Software developed at Sandia or a U.S. Government agency for a general or non-YMP LA purpose, which may have been modified at Sandia usually by creation of an input deck. Sometimes source is received with GOTS software, sometimes not.
GTG	GoldSim Technology Group

GUI, Graphical User Interface	Software with dialogs and user interface elements, to make it more user-friendly. Such software is usually less portable but easier to use.
HAL	A Hardware Abstraction Layer is a logical division of code that serves as an abstraction layer between a computer's physical hardware and its software. It provides a device driver interface that allows a program to communicate with the hardware. In virtual machines, it also presents a raw hardware interface to the virtual client, making it look like the client software owns the hardware it's running on.
LA	License Application
NL	National Laboratory
OS	Operating system. Windows, Linux, Unix, OpenVMS, etc.
PC	Personal Computer
Preprocessor Directive	Meta code inserted into source code to cause it to compile (or not compile) different fragments depending on which system is being targeted. The presence of preprocessor directives can indicate that a programmer at least considered the possibility that the code would run on/under more than one type of hardware and/or OS.
RAM	Random Access Memory
SCM	Software Configuration Management
SNL	Sandia National Laboratories
Source Code	Series of instructions, usually in text, that when compiled produce a binary or interpreted program that can be executed.
TSPA	Total System Performance Assessment
USACE	US Army Corps of Engineers
USGS	US Geological Survey
YMP	Yucca Mountain Project

1. INTRODUCTION

Sandia National Laboratories (SNL) continued evaluation of the total system performance assessment (TSPA) computing systems for the previously considered Yucca Mountain Project (YMP). This was done to maintain the operational readiness of the computing infrastructure (computer hardware and software) and knowledge capability for total system performance assessment (TSPA) type analysis, as directed by the National Nuclear Security Administration (NNSA), DOE 2010. This work is a continuation of the ongoing readiness evaluation reported in Lee and Hadgu (2014), Hadgu et al. (2015), Hadgu and Appel (2016) and Hadgu et al. (2017). The TSPA computing hardware (2014 server cluster - CL2014) and storage system described in Hadgu et al. (2015) were used for the current analysis. One floating license of GoldSim with Versions 9.60.300, 10.5, 11.1 and 12.0 was installed on the cluster head node, and its distributed processing (DP) capability was mapped on the cluster processors. Other supporting software were tested and installed to support TSPA-type analysis on the server cluster. The current tasks included maintenance of the TSPA-LA system (hardware and software), and developing an inventory of software used as process models. CL2014 is currently running smoothly. Versions 9.60.300, 10.5, 11.1 and 12.0 are currently operational on the cluster. The 2014 server cluster and supporting software systems are now fully operational to support TSPA-LA type analysis with the GoldSim version used for the license application (GoldSim, 2007).

In FY15, through FY18 SNL conducted evaluation of the TSPA computing system to verify the readiness of the capability to perform TSPA-type analysis of the Yucca Mountain repository following the 2014 server replacement. The reports by Hadgu et al. (2015), Hadgu and Appel (2016), and Hadgu et al. (2017) documented the work performed to achieve and maintain the readiness of the computing infrastructure (computer hardware and software) and knowledge capability to perform TSPA-type analyses. The reports provided details of specifications of the 2014 computer hardware, the evaluation of the required components of the hardware and software systems, as well as the instructions to setup and conduct the TSPA-LA type simulations and post-processing of the model output. This report is a continuation of the work performed since 2015.

As was done in previous work (Lee and Hadgu, 2014, Hadgu et al., 2015, Hadgu and Appel, 2016, and Hadgu et al., 2017) one of the goals of this work is to demonstrate the readiness of the 2014 hardware and software systems. This is to insure that the computing system can support reliable execution of the TSPA-LA models and post-processing of the model output. The other goal of this work is to develop an inventory of software used in Yucca Mountain process models and to begin assessment of the current status of the software. The following main topics were identified for the current investigation to evaluate the status of the TSPA-LA model capability.

- Maintaining readiness of the TSPA-LA.
- Inventory of and assessment of software used for the YMP License Application process models.

2. THE TSPA COMPUTING SYSTEM

2.1. The TSPA Server Cluster Hardware (CL2014)

The TSPA computing system, (the hardware and software), is discussed in great detail in Hadgu et al. (2015). The new TSPA cluster (CL2014) consists of a total of 32 Dell PowerEdge R620 servers, each with 3.0 GHz Intel® Xeon® E5-2690 dual quad-core processors (20 processors per server) and 128 GB RAM. Thus, the TSPA server cluster has a total of 640 processors.

The 2014 servers reside on the Sandia DMZ domain and are running under the Windows Server 2012 r2, 64-bit operating system. The system was optimized for installation and execution of the GoldSim software required to run the GoldSim distributed processing module utility (GoldSim 2010, 2017). The distributed processing module utility is a program extension to GoldSim which allows use of multiple computers connected over a network to share the computational burden of a Monte Carlo simulation. The module is the essential feature to efficiently manage and execute multiple realizations of the TSPA-LA model run on the cluster processors. In the 2014 configuration of the total of 32 blade servers, one blade server is used as the head node, and 31 servers are used as the compute nodes dedicated to run GoldSim-based TSPA models.

2.2 The TSPA Data Storage

As stated in Hadgu and Appel (2015), adequate storage space has been allocated for current work on the network drive on which the YMP data is stored (FS02SNLNTY/collab6). The storage space is subject to 30 days daily backup.

A limited disk storage space is available on the head node of the TSPA cluster. That is intended mainly for installation of application software, storage of small files by individual users using the cluster, as well as storage of model output files while a run is carried out. The space is not enough for storing all TSPA model output files. The total size of the files contained in a TSPA LA model output DTN ranges from a few gigabytes to tens of gigabytes, and some DTNs are close to 100 gigabytes. The DTN package includes GoldSim model files, model output data files, post-processed data files, plot files, etc. The total size of the GoldSim model and model output files from a routine TSPA-LA model run typically ranges from about one gigabyte to 10 gigabytes depending on the modeling cases. To clear space on the head node, TSPA model output files need be transferred to the storage system described above.

2.3 The TSPA Server Cluster Hardware (CL2014)

The CL2014 cluster has data backup and recovery system. The backup and recovery service follows SNL corporate standards for the following:

- **Backup and Restoration of Data**: Corporate Databases follow standards and procedures defined by the Enterprise Database Administration group (Archean, CL2014 head node, and CL2014-2 compute node is backed up by Enterprise).
  - https://sharepoint.sandia.gov/sites/backup/default.asp
  - Backup and Data restoration from corporate is only for CL2014-1 (head node) and CL2014-2 (compute node). Data from the rest of the compute nodes are not restored as

all data are transferred from the compute nodes to the head node after each GoldSim run.
    - If any of the compute nodes fails, RAID array 1 is used to restore the compute node by replacing hard drives of dead servers. The backup from corporate is a just in case disaster recovery layer.
    - CL 2014 cluster data is being backed up by the SAN and disaster recovery.
    - All questions and issues are to be reported to the Corporate Enterprise team via Corporate Computing Help Desk.

- **Full File Server Backups:** Performed monthly. Incremental server backups are performed nightly.
    - Back up for the File Server is done by corporate.
        - Request for retrieving data from the backup for the CL2014 cluster is to be submitted via ticket through Corporate Computing Help Desk.
- **File Restoration:** Within 1 business day (requested via the Corporate Computing Help Desk). Customer must provide file name and location to facilitate restoration.

2.4 TSPA Server Cluster (CL2014) Hardware Status

CL2014 is functioning properly. During the year the system security was upgraded with installation of a two-factor authentication method. In addition, system back up has been implemented. The master or head node, CL2014-1 is now backed up incrementally daily and completely once a month.

3 INVENTORY AND ASSESSMENT OF SOFTWARE USED FOR THE YMP LICENSE APPLICATION PROCESS MODELS

This section provides an inventory of software used in the YMP process models. The section also provides a primary assessment of the status of the software. The TSPA-LA Model components and submodels are described in detail in the TSPA-LA report (SNL, 2008). Section 6 of the report summarizes the process models associated with the TSPA-LA models and submodels for the Nominal Scenario Class. The section also describes the event scenarios represented by Early Failure, Igneous, and Seismic Scenario Classes and the Human Intrusion Scenario. Detailed descriptions of each process and process model are described in individual analysis and model reports. The current work used the individual reports to compile a list of software utilized for the Yucca Mountain license application.

The software inventory is presented below in sections representing the TSPA-LA Model components and submodels. The following are the major sections representing the model components and processes. Each major section is further subdivided to describe the submodels.

- Unsaturated Zone (UZ) Flow
- Engineered Barrier System (EBS) Environment
- Waste Package (WP) and Drip Shield (DS) Degradation
- Waste Form (WF) Degradation and Mobilization
- EBS Flow and Transport
- UZ Transport
- Saturated Zone (SZ) Flow and Transport
- Biosphere.
- Events (Scenario classes)

For each section the process model and the individual reports where the process is described are reported. The section also includes a list of software that supported the model development. The software list details information about the software and a brief description on how it was used. The availability of each software in software configuration management (SCM) is also indicated. The software inventory is also provided in Excel Spreadsheet form in Appendix A, and in a separate Excel file. The Excel file allows a quick search of each software and the related analysis model report. Note that details may not be available in the original documents when commercial software (COTS) such as Microsoft Excel are used. A preliminary list of project developed (YMP) and COTS software is given in Appendix B.

3.2 Unsaturated Zone Flow

3.2.1 Climate Analysis

Climate analysis is documented in the report: 170002 BSC (Bechtel SAIC Company) 2004. Future Climate Analysis. ANL-NBS-GS-000008 REV 01. Las Vegas, Nevada: Bechtel SAIC Company. ACC: DOC.20040908.0005.

Software used: Microsoft Excel 2000 was used to develop graphic representations. The software is not available in SCM. No other software or models were used.

3.2.2 Infiltration Analysis

Infiltration analysis is documented in the report: 182145 SNL (Sandia National Laboratories) 2007. *Simulation of Net Infiltration for Present-Day and Potential Future Climates.* MDL-NBS-HS-000023 REV 01 AD 01, Las Vegas, Nevada: Sandia National Laboratories.

Table 1 - Simulation of Net Infiltration for Present-Day and Potential Future Climates List of Software Used

Software Name	Version	Software Tracking Number (STN)	Platform/ Operating System	Brief Description of Use	Availability
Mathcad	13.1	611161-13.1-00	PC, Windows XP	The net infiltration model (MASSIF) was developed and implemented using standard functions included with Mathcad.	Not available in SCM
LHS	2.51	10205-2.51-01	DEC Alpha Server ES45 Model 2/ Open VMS 8.2	Performs Latin hypercube sampling; generates the distribution for each parameter to be sampled; generates a correlation matrix; and detects invalid input data sets.	Available in SCM
ArcGIS	9.1	11205-9.1-00	PC, Windows XP	Integrates a collection of software files for developing a complete Geographic Information System (GIS) for the infiltration model.	Available in SCM
ENVI+IDL	4.2	11204-4.2-00	PC/Windows XP	Conducts Radiometric Corrections to the Region of Interest (ROI) data; conducts land cover characterization calculations based on ROI data; conducts geometric corrections to the ROI data.	Available in SCM
MVIEW	4.0	10072-4.0-00	PC/Windows 2000	Used for stepwise regression analysis and the calculation of partial correlation coefficients and standardized regression coefficients.	Available in SCM

The primary software used for infiltration analysis is Mathcad 13.1. The software is not available in SCM. This version is no longer supported by the software developer but it can be either located or later versions used.

Supporting software for infiltration analysis:

MVIEW is a project developed software. The version of the software that was used for YMP license application has been recently tested for the maintenance of the TSPA uncertainty and sensitivity analysis (Hadgu and Appel, 2016). Thus, this software is functional in a new operating environment.

LHS is also project developed. There is a need to test the software on updated operating environment.
ENVI and IDL are COTS that allow data extraction from geospatial and other sources. The company is Harris Geospatial Solutions. ENVI and IDL are separate codes and both are Available in SCM. There is a need to test for accuracy of data, if use of newer versions is required. Since these are pre-and post-processing software, they may be replaced with other codes in case of problems.

Another report supporting infiltration analysis is:

177081 SNL (Sandia National Laboratories) 2006. Data Analysis for Infiltration Modeling: Extracted Weather Station Data Used to Represent Present-Day and Potential Future Climate Conditions in the Vicinity of Yucca Mountain. ANL-MGR-MD-000015 REV 00. Las Vegas, Nevada: Sandia National Laboratories. ACC: DOC.20070109.0002.

Table 2 - Data Analysis for Infiltration Modeling List of Software Used

Software Name	Version	Software Tracking Number (STN)	Platform/ Operating System	Brief Description of Use	Availability
Mathcad	13.1	611161-13.1-00	PC, Windows XP	The net infiltration model (MASSIF) was developed and implemented using standard functions included with Mathcad.	Not available in SCM
CORPSCON	5.11.08	10547-5.11-08-00	PC/Windows NT 4.0	Used to convert coordinate data to the Universal Transverse Mercator (UTM) coordinate system; convert meteorological station coordinates from geographical or UTM NAD 83 coordinates to UTM NAD 27 coordinates.	Available in SCM
EARTHVISION	5.1	10174-5.1-00	IRIX 6.5	Used to extract a projected elevation given geographic coordinates as inputs.	Available in SCM

CORPSCON is a free coordinate conversion software from the US Army Corps of Engineers (UACE). There is a need to test the old version in a new computing environment.

EARTHVISION is a visualization graphics commercial software from Dynamic Graphics, Inc. The latest version of the software is 9.0. It is not clear if it is backwards compatible. IRIX 6.5 (UNIX based OS) operating system has been discontinued. There is a need to install EARTHVISION 5.1 on a current UNIX platform for testing.

3.2.3 Site Scale Unsaturated Zone Flow

Site scale unsaturated zone flow is documented in the report: 184614 SNL (Sandia National Laboratories) 2007. *UZ Flow Models and Submodels.*MDL-NBS-HS-000006 REV 03 AD 01. Las Vegas, Nevada: Sandia National Laboratories. ACC: DOC.20080108.0003.

Table 3 - UZ Flow Models and Submodels Flow List of Software Used

Software Name	Version	Software Tracking Number (STN)	Platform/Operating System	Brief Description of Use	Availability
T2R3D	1.4	10006-1.4-00	Dec Alpha/UNIX	Used for tracer transport simulations, tracer transport travel-time estimates, and modeling pore-water chemistry.	Available in SCM
TOUGHREACT	3.0	10396-3.0-00	Dec Alpha/OSF1 V5.1	Used for conducting calcite studies.	Available in SCM
TOUGH2	1.6	10007-1.6-01	Dec Alpha/OSF1 V5.1, PC-DOS Windows 98	Used to generate flow fields and to conduct model calibrations.	Available in SCM
infil2grid	1.7	10077-1.7-00	Dec Alpha/OSF1 V4.0	Used to apply infiltration maps onto the grids used for simulating flow and transport. It was also used to map infiltration maps into GENER files of TOUGH2 input data.	Available in SCM
2kgrid8.for	1.0	10503-1.0-00	Dec Alpha/OSF1 V4.0, PC-DOS Windows 95	Used to generate dual-permeability grids.	Available in SCM
bot_sum.f	1.0	10349-1.0-00	UNIX/OSF1 V4.0	Used for calculation of water mass flux at the water table boundary conditions.	Available in SCM
WINGRIDDER	2.0	10024-2.0-00	PC/Windows NT 4.0	Used to generate a three-dimensional thermal model grid.	Available in SCM
TOPTEMP_V0.f	1.0	10224-1.0-00	Dec Alpha/OSF1 V4.0	Used for estimating initial and boundary temperature conditions.	Available in SCM
GET_TEMP_V0.f	1.0	10222-1.0-00	Dec Alpha/OSF1 V4.0	Used for estimating initial and boundary temperature conditions.	Available in SCM
Tbgas3D	2.0	10882-2.0-00	SUN/SUN O. S. 5.5.1	Used for generating surface gas pressure boundary conditions.	Available in SCM

T2FEHM	4.0	10997-4.0-00	Dec Alpha/OSF1 V5.1	Converts TOUGH2 output files with the format of *flow9.dat* into files readable by FEHM.	Available in SCM
WTRISE	2.0	10537-2.0-00	Dec Alpha/OSF1 V5.1	Used to adjust the FEHM-readable files for a higher future water table.	Available in SCM
Bkread.f	1.0	10894-1.0-00	SUN/SUN O. S. 5.5.1	Used to obtain breakthrough curves.	Available in SCM
Smesh.f	1.0	10896-1.0-00	SUN/SUN O. S. 5.5.1	Used to generate grid.	Available in SCM
iTOUGH2	4.0	10003-4.0-00	SUN/SUN O. S. 5.5.1/ OS V4.0	Inverse modeling code to perform model calibration.	Available in SCM

There is a need for testing of the above codes on updated operating environment.

The following report also supports site scale unsaturated zone flow: 179545 SNL (Sandia National Laboratories) 2007. *Calibrated Unsaturated Zone Properties.* ANL-NBS-HS-000058 REV 00. Las Vegas, Nevada: Sandia National Laboratories. ACC: DOC.20070530.0013.

Table 4 - Site Scale Calibrated Unsaturated Zone Properties List of Software Used

Software Name	Version	Software Tracking Number (STN)	Platform/ Operating System	Brief Description of Use	Availability
iTOUGH2	5.0	10003-5.0-00	Linux, Red Hat V7.3	Used for property calibration against field data based on inverse modeling methodology.	Available in SCM
e9-3in	1.0	10126-1.0-00	Sun/UNIX	Used to convert coordinate data to the Universal Transverse Mercator (UTM) coordinate system. Specifically, used for converting EOS9 format of initial conditions to the corresponding EOS3 format, and converting coordinate systems for the infiltration maps.	Available in SCM
2kgrid8.for	1.0	10503-1.0-00	PC/DOSV4.00. 1111	Used to convert an ECM (Effective Continuum Model) grid to the corresponding DKM (dual-permeability model) grid.	Available in SCM
Infil2grid	1.7	10077-1.7-00	PC/DOSV4.00. 1111	Used to map infiltration data into the top boundary of a numerical grid.	Available in SCM
TBgas3D	2.0	10882-2.0-00	SUN/O.S.5.51	Used for mapping the infiltration rate data into top elements of a numerical grid, determining the top gas-flow boundary conditions for calibration simulations using pneumatic data.	Available in SCM

CORPSCON	5.11.08	10547-5.11-08-00	PC/WINDOWS NT 4.0	Used to convert coordinate data to the Universal Transverse Mercator (UTM) coordinate system. Specifically, used for converting EOS9 format of initial conditions to the corresponding EOS3 format, and converting coordinate systems for the infiltration maps.	Available in SCM

There is a need for testing the above codes on updated operating environment.

The following report also supports site scale unsaturated zone flow: 174101 BSC (Bechtel SAIC Company) 2005. *Mountain-Scale Coupled Processes (TH/THC/THM) Models.* MDL-NBS-HS-000007 REV 03. Las Vegas, Nevada: Bechtel SAIC Company. ACC: DOC.20050825.0007.

Table 5 - Mountain-Scale Coupled Processes Flow List of Software Used

Software Name	Version	STN	Platform / Operating System	Brief Description of Use	Availability
TOUGH2	1.6	10007-1.6-01	Alpha system OSF1 V4.0	Selected for its capability to model effects of heat on flow in fractured media	Available in SCM
TOUGHREACT	3.0	10396-3.0-00	Alpha System OSF1 V5.1	TOUGHREACT applies to porous media in a temperature range limited by its thermodynamic database (currently 0 to 300°C).	Available in SCM
FLAC3D	2.0	10502-2.0-00	PC/Windows 98	Used for mechanical analysis and for linked TOUGH2 and FLAC3D coupled THM analysis.	Not available in SCM
EXT	1.1	10005-1.1-00	SUN Ultra Sparc SunOS 5.5.1	The EXT code extracts data from TOUGH2 output files for plotting. The input and output formats must be standard TOUGH2 input and output formats, with eight-character element names TOUGH2 mesh.	Available in SCM
EXT	1.0	10047-1.0-00	SUN Ultra-Sparc SunOS 5.5.1	The EXT code extracts data from TOUGH2 output files for plotting. The input and output formats must be standard TOUGH2 input and output formats, five-character element names TOUGH2 mesh.	Available in SCM
Infil2grid	1.7	10077-1.7-00	PC MS-DOS V4.00.1111 under Windows 95	This software is used to extract surface infiltration rates to the top of TOUGH2 model grids. This routine is limited to eight-character element names TOUGH2 mesh.	Available in SCM

WINGRIDDER	2.0	10024-2.0-00	PC/Windows NT 4.0	A grid generator program used to produce 1-D, 2-D, or 3-D grids for numerical modeling of flow and transport problems based on the integral difference method. Output grid files are in the format compatible with TOUGH2. Inputs are distance, area, and volume that must be non- negative.	Available in SCM
GridReader	1.0	10994-1.0-00	PC/Windows NT 4.0	Gridreader is a package of utility tools used to 1) read a grid developed by WinGridder and write a mesh input file for TOUGH2 with high precision x-, y-, z-coordinates; 2) convert a TOUGH2 mesh file with 8-character cell names into a TOUGH2 mesh file with 5-character cell names. This software is to be used only with the TOUGH2 family of codes.	Available in SCM
Gpzones.dat	1.0	10509-1.0-00	PC/Windows 98	The software is used to find out which zones are connected to each grid point and how much zone volumes are connected to each grid point, and to calculate the interpolation of temperatures from TOUGH2 nodes to FLAC3D nodes. This routine is a FISH routine that can only be used for FLAC3D V2.0 or higher.	Available in SCM
Tin	1.1	10889-1.1-00	PC/Windows 98	This software takes temperature output from TOUGH2 and interpolates it into FLAC3D for coupled THM simulations. Used to transfer temperatures from TOUGH2 Version 1.6 to FLAC3D V. 2.0 during linked TOUGH2 and FLAC3D coupled THM analysis.	Available in SCM
Delb.dat	1.0	10507-1.0-00	PC/Windows 98	The code is used to calculate changes in fracture aperture for linked TOUGH2 and FLAC3D Coupled THM analyses. This software is tested for normal stress ranging from +10 MPa to -100 MPa.	Available in SCM
2KGRIDV1.F	1.0	10244-1.0-00	SUN Ultra-Sparc SunOS 5.5.1	This software is used to process data for TOUGH2 modelling for Yucca Mountain.	Available in SCM

2kgridv1a.for	1.0	10382-1.0-00	PC/Dos Emulation	Generates dual-permeability grids for the TOUGH2 family of codes	Available in SCM
Gen_incon-v0.f	1.0	10220-1.0-00	DEC Alpha OSF1 4.0	This software is used to calculate top and bottom boundary temperatures and the initial block "INCON" for starting a TOUGH2 simulation. This software only processes valid "ELEME" block input format for the TOUGH2 family of codes.	Available in SCM
Get_a_layer_v0.f	1.0	10221-1.0-00	DEC Alpha OSF1 4.0	This software is used to extract data of a given list of elements from TOUGH2 outputs for plotting. This software only processes valid "ELEME" block input format for the TOUGH2 family of codes and valid EOS3 TOUGH2 V1.4 output file formats.	Available in SCM
Get_temp_v0.f	1.0	10222-1.0-00	DEC Alpha OSF1 4.0	This software is used to search for the nearest tabulated value of temperature to assign bottom boundary conditions. The coordinates x,y and temperature (T) are within real range.	Available in SCM
Toptemp_v0.f	1.0	10224-1.0-00	DEC Alpha OSF1 4.0	This software is used to generate top temperature boundary conditions. All valid "ELEME" range of TOUGH2 input, real range of elevation, and average temperature on the Yucca Mountain surface.	Available in SCM
Hsource_v0.f	1.0	10225-1.0-00	DEC Alpha OSF1 4.0	This software is used to generate thermal GENER terms for TOUGH2 input files.	Available in SCM
2kgid8.for	1.0	10503-1.0-00	PC MS-DOS V4.00.1111 under Windows 95	This software is used to generate dual permeability meshes for the TOUGH2 family of codes. This software is limited to eight-character element names for the TOUGH2 family of codes.	Available in SCM

The above codes, with the exception of FLAC3D, are project developed. (see Appendix B). FLAC3D is COTS. It is possible that a new license will be required. There is a need to test the software on updated operating environment.

3.2.4 Drift Seepage

Drift seepage analysis is documented in the report: 177404 SNL (Sandia National Laboratories) 2007. *Drift-Scale THC Seepage Model.* MDL-NBS-HS-000001 REV 05. Las Vegas, Nevada: Sandia National Laboratories. ACC: DOC.20071010.0004.

Table 6 - Drift-Scale THC Seepage Model List of Software Used

Software Name	Version	Software Tracking Number	Platform/ Operating System	Brief Description of Use	Availability
TOUGHREACT	3.1.1	10396-3.1.1-00	Alpha System/ OSF1 V5.1	Used to calculate coupled thermal-hydrologic and chemical processes for kinetic and/or equilibrium mineral–water reactions and equilibrium gas–water reactions.	Available in SCM
			Linux Custer/ CAOS Linux	Used to calculate coupled thermal-hydrologic and chemical processes for kinetic and/or equilibrium mineral–water reactions and equilibrium gas–water reactions.	Available in SCM
SUPCRT92	1.0	10058-1.0-00	PC/Windows	Used to calculate the standard molal thermodynamic properties of minerals, gases, aqueous species, and reactions from 1 to 5,000 bars and 0°C to 1,000°C	Available in SCM
AMESH	1.0	10045-1.0-00	Sun UltraSparc/ SUNOS 5.5.1	Generates discrete 1-D, 2-D, or 3-D grids for numerical modeling of flow and transport problems in which the formulation is based on the integral finite difference method	Available in SCM
KREG	1.1	10318-1.1-00	PC/ DOS Emulation	Used to calculate regression coefficients of log(K) data as a function of temperature for the thermodynamic database of TOUGHREACT V3.1.1	Available in SCM
KSWITCH	1.1	10319-1.1-00	PC/ DOS Emulation	Used to switch component species in the thermodynamic database of TOUGHREACT V3.1.1 and above	Available in SCM
THERMOCHK	1.1	10895-1.1-00	PC/ DOS Emulation	Used to check the consistency (mass balance and charge balance) of reactions in the thermodynamic database of the reactive transport code TOUGHREACT V3.1.1 and above.	Available in SCM
DBCONV	1.0	10893-1.0-00	PC/ DOS Emulation	Used to convert the YMP EQ3/6 thermodynamic database to a format suitable for input into the reactive transport model TOUGHREACT V3.1.1	Available in SCM
CUTCHEM	2.0	10898-2.0-0.0	PC/ DOS Emulation	Used to extract automatically data from large output data files created by the reactive transport model TOUGHREACT V3.1.1	Available in SCM

exclude.f	1.0	10316-1.0-00	Sun UltraSparc/ SUNOS 5.5.1	Used to exclude points outside a specified radius so that points will not overlap when output is merged using merggrid.f V1.0 for 2-D THC seepage model.	Available in SCM
assign.f	1.0	10315-1.0-00	Sun UltraSparc/ SUNOS 5.5.1	Used to assign a geologic name to all TOUGH2 elements according to their location in the Z-direction for 2-D THC seepage model.	Available in SCM
merggrid2.f	1.0	10314-1.0-00	Sun UltraSparc/ SUNOS 5.5.1	Used to merge input files into one file for input into AMESH V1.0 for 2-D THC seepage model.	Available in SCM
mk_circ2	1.0	10312-1.0-00	Sun UltraSparc/ SUNOS 5.5.1	Used to create a radial grid for 2-D THC seepage model.	Available in SCM
mk_rect2	1.0	10313-1.0-00	Sun UltraSparc/ SUNOS 5.5.1	Used to create orthogonal grid for 2-D THC seepage model.	Available in SCM
2kgridv1a.for	1.0	10382-1.0-00	PC/ DOS Emulation	Generates dual-permeability grids for the TOUGH2 family of codes.	Available in SCM
mk_grav2.f	1.0	10379-1.0-00	Sun UltraSparc/ SUNOS 5.5.1	Reads AMESH V1.0 output files and creates TOUGH2 V1.4 mesh input file data, namely the gravity vector data and gridblock labeling data.	Available in SCM
sav1d_dst2d.f	1.0	10381-1.0-00	Sun UltraSparc/ SUNOS 5.5.1	Creates an INCON file for TOUGH2 input for a 2-D mesh from existing INCON and MESH data for a 1-D column.	Available in SCM

There is a need to test the software on updated operating environment.

Another report for drift seepage analysis is: 181244 SNL (Sandia National Laboratories) 2007. *Abstraction of Drift Seepage*. MDL-NBS- HS-000019 REV 01 ADD 01. Las Vegas, Nevada: Sandia National Laboratories. ACC: DOC.20070807.0001.

The software used was: Mathcad 11 for calculations, and Tecplot V9.0 for graphical display.

These two codes COTS, and thus, the versions of these software have changed. However, it is expected that any calculations and visualizations could be reproduced using later versions or other similar codes.

Drift seepage analysis is also documented in: 167652 BSC (Bechtel SAIC Company) 2004. *Seepage Model for PA Including Drift Collapse*. MDL-NBS-HS-000002 REV 03. Las Vegas, Nevada: Bechtel SAIC Company. ACC: DOC.20040922.0008; DOC.20051205.0001.

Table 7 - Model for PA Including Drift Collapse List of Software Used

Software Name	Version	Software Tracking Number (STN)	Platform/ Operating System	Brief Description of Use	Availability
iTOUGH2	5.0	10003-5.0-00	Sun UltraSparc/ SunOS 5.5.1	Performs extensive parameter sensitivity analyses based on the TOUGH2 simulator. Used for predicting seepage rates and for flow focusing study.	Available in SCM
GSLIB	V1.0SISIMV 1.204	10397-1.0SISIMV1.204-00	Sun UltraSparc/ SunOS 5.5.1	Generates three-dimensional, spatially correlated random fields by means of sequential indicator simulations. It is used to generate spatially correlated fields of log-permeability modifiers.	Available in SCM
MoveMesh	1.0	10358-1.0-00	Sun UltraSparc/ SunOS 5.5.1	Utility program that adds a constant to the coordinates of a mesh file translating the coordinate system. This allows the relabeling of a subdomain of the mesh file to be used for detailed calculations.	Available in SCM
AddBound	1.0	10357-1.0-00	Sun UltraSparc/ SunOS 5.5.1	Utility program that adds boundary elements to a mesh file.	Available in SCM
Perm2Mesh	1.0	10359-1.0-00	Sun UltraSparc/ SunOS 5.5.1	Utility program that maps a field of log-permeability modifiers onto a mesh file.	Available in SCM
CutDrift	1.0	10375-1.0-00	Sun UltraSparc/ SunOS 5.5.1	Utility program that cuts a drift portion with a diameter of 5.5 m from the mesh domain.	Available in SCM
TOUGH2	1.4	10007-1.4-01	Sun UltraSparc/ SunOS 5.5.1	Used to evaluate the effect of permeability changes due to coupled THM processes near a drift.	Available in SCM
TOUGH2	1.6	10007-1.6-01	PC/ Windows 98	Used to evaluate the effect of permeability changes due to coupled THM processes near a drift.	Available in SCM
EXT	1.0	10047-1.0-00	Sun UltraSparc/ SunOS 5.5.1	Utility program that generates three-dimensional Tecplot formatted data from iTOUGH2 output files.	Available in SCM
CutNiche	1.3	10402-1.3-00	Sun UltraSparc/ SunOS 5.5.1	Utility program that cuts a rock-fall volume above the drift in the mesh domain.	Available in SCM

The above codes, except for GSLIB, are project developed (see Appendix B). There is a need to test them on updated operating environment.

3.2.5 Drift Wall Condensation

Drift wall condensation is reported in: 181648 SNL (Sandia National Laboratories) 2007. *In-Drift Natural Convection and Condensation.* MDL-EBS-MD-000001 REV 00 AD 01. Las Vegas, Nevada: Sandia National Laboratories. ACC: DOC.20050330.0001; DOC.20051122.0005; DOC.20070907.0004.

Table 8 - In-Drift Natural Convection and Condensation List of Software Used

Software Name	Version	Software Tracking Number	Platform/ Operating System	Brief Description of Use	Availability
FLUENT	6.0.12	10550-6.0.12-01	PC, Linux v 7.3	Computational Fluid Dynamics (CFD) Calculations Convection Model	Available in SCM
GAMBIT	2.0.4	N/A	PC/Windows 2000	Visual Display of Data and Mesh	Not available in SCM
Ensight	7.4	N/A	PC/Windows 2000	Visualization of CFD Results	Not available in SCM
MS Excel	2000 SP3	N/A	PC/Windows 2000	Graphical Representation and Arithmetic Manipulation	Not available in SCM
Mathcad Professional	11.2a	N/A	PC/Windows 2000	Graphical Representation and Arithmetic Manipulation	Not available in SCM

The codes FLUENT and GAMBIT have undergone major upgrades and ownership changes. Also, software license was used on these codes and thus the license may no longer be Available in SCM. Because FLUENT is a complex modeling software, there is a strong need for testing models developed with the software on the updated platforms. Ensight is graphics software. Mathcad and Excel were used for graphical representation.

3.3 Engineered Barrier System Environment

3.3.1 Engineered Barrier System Thermal Hydrologic Environment

The Engineered Barrier System thermal hydrologic environment analysis is documented in:
181383 SNL (Sandia National Laboratories) 2007. *Multiscale Thermohydrologic Model.* ANL-EBS-MD-000049 REV 03 ADD 01. Las Vegas, Nevada: Sandia National Laboratories. ACC: DOC.20070831.0003.

Table 9 - Multiscale Thermohydrologic Model List of Software Used

Software Name	Version	Software Tracking Number	Platform/ Operating System	Brief Description of Use	Availability
NUFT	3.0s	10088-3.0s-02	Sun OS 5.8	A general-purpose code for simulating mass and heat transport in fractured porous media. Used for the MSTHM simulations.	Available in SCM
NUFT	3.0.1s	10130-3.0.1s-01	Sun OS 5.8	Used to conduct nested-mesh model calculations in the model validation exercises for the MSTHM.	Available in SCM
RADPRO	4.0	10204-4.0-00	Sun OS 5.8	Calculates the radiative heat transfer coefficients in the emplacement drift.	Available in SCM
XTOOL	10.1	10208-10.1-00	SunOS 5.6.1	Used to generate graphical representations of the results given in the NUFT and MSTHAC time-history files.	Available in SCM
MSTHAC	7.0	10419-7.0-00	Sun OS 5.8	Integrates the results of NUFT submodel calculations to predict the multiscale thermal-hydrologic conditions in the emplacement drifts and adjoining host rock throughout the repository area.	Available in SCM
readsUnits	1.0	10602-1.0-00	SunOS 5.5.1	Used to read YMESH-generated data describing a stratigraphic column and generates comment lines for NUFT input files that summarize the thicknesses of each of the hydrostratigraphic units in that column.	Available in SCM
YMESH	1.54	10172-1.54-00	Sun OS 5.8	YMESH is used to generate the thicknesses of the hydrostratigraphic units in the various MSTHM submodels based upon the grids from *Development of Numerical Grids for UZ Flow and Transport Modeling* (BSC 2004 [DIRS 169855]).	Available in SCM
boundary_conditions	1.0	11042-1.0-00	Sun OS 5.8	Used to generate upper and lower boundary conditions for the LDTH, SMT, and SDT submodels of the MSTHM, as well as for other models such as the three-dimensional thermal-hydrologic model for the Drift Scale Test (DST).	Available in SCM

heatgen_ventTable_emplace	1.0	11039-1.0-00	Sun OS 5.8	Modifies a heat-generation-rate-versus-time table: it can “age” the heat-generation table by adding a specified number of years to the time entries; it can account for the heat-removal efficiency of ventilation by multiplying the heat-generation-rate values by a specified fraction during the specified ventilation period.	Available in SCM
rme6 v1.2	1.2	10617-1.2-00	Sun OS 5.8	Converts the grid from *Development of Numerical Grids for UZ Flow and Transport Modeling* (BSC 2004 [DIRS 169855]) to a format that is readable by YMESH.	Available in SCM
xw	1.0	11035-1.0-00	Sun OS 5.8	Extends the grid from the three-dimensional unsaturated zone (UZ) flow model in the horizontal direction for the purpose of building mountain-scale submodels that extend laterally beyond the grid of the three-dimensional UZ flow model.	Available in SCM
colCen	1.0	11043-1.0-00	Sun OS 5.8	Used to determine the gridblock column in the three-dimensional UZ flow model in which a given gridblock column in a MSTHM submodel resides.	Available in SCM
repository_percolation_calculator	1.0	11041-1.0-00	Sun OS 5.8	Used to determine the value of percolation flux for each of the LDTH submodels based on the percolation flux map from the three-dimensional UZ flow model.	Available in SCM
extractBlocks_EXT	1.0	11040-1.0-00	Sun OS 5.8	Used to determine the effective thermal conductivity for the gridblocks in the drift cavity of an LDTH submodel based on a correlation accounting for the influence of natural convection.	Available in SCM
Chimney_interpolate		11038-1.0-00	Sun OS 5.8	The purpose of Chimney_interpolate is to create a set of virtual SDT and LDTH “chimney” submodels from the 108 “real” chimney submodels. The virtual chimney submodels are an input to the MSTHAC v7.0 micro-abstraction process.	Available in SCM

reformat_EXT_to_TSPA	1.0	11061-1.0-00	Sun OS 5.8	Used to post-process the micro-abstraction data produced by MSTHAC. The processing includes finding the typical waste package and location from a set of locations forming a bin and writing an output file in a format specified by TSPA-LA.	Available in SCM
MATLAB	6.1.0450			Used to prepare plots for different uses.	Not available in SCM
Mathcad	11.2a			Used to perform the calculations for developing the hydrologic properties of the invert; for comparing percolation fluxes, and for prediction of RH in the invert, respectively.	Not available in SCM

The above codes, except for MATLAB, are project developed (see Appendix B). There is a need to test them on updated operating environment. MATLAB was used for graphics and as a utility software. Other pre- and post-processing codes were also used.

3.3.2 Engineered Barrier System Chemical Environment

The Engineered Barrier System chemical environment analysis is documented in: 177412 SNL (Sandia National Laboratories) 2007. *Engineered Barrier System: Physical and Chemical Environment.* ANL-EBS-MD-000033 REV 06. Las Vegas, Nevada: Sandia National Laboratories. ACC: DOC.20070907.0003.

Table 10 - Engineered Barrier System: Physical and Chemical Environment List of Software Used

Software	Version	Software Tracking Number	Platform / Operating System	Brief Description of Use	Availability
EQ3/6	8.0	10813-8.0-00	PC/ WIN2000	a FORTRAN speciation-solubility and data processing code.	Available in SCM
GetEQData	1.0.1	10809-1.0.1-00	PC/ WIN2000	A Microsoft Excel macro used to postprocess EQ3/6 output information.	Available in SCM
ppptrk	1.0	11030-1.0-00	PC/ WIN2000	For use with particle tracking simulations only.	Available in SCM
EARTHVISION	5.0	10393-5.0-00	SGI/ IRIX 6.2 operating system has	Used to produce three-dimensional images and for data extraction.	Available in SCM

EQ3/6 and supporting codes are regularly used. There is a need to test models developed using the above codes on updated operating environment. EARTHVISION, Mathcad V. 13 and 14 as well as other COTS was also used.

The Engineered Barrier System chemical environment analysis is also documented in: 177411 SNL (Sandia National Laboratories) 2007. *In-Drift Precipitates/Salts Model.* ANL-EBS-MD-000045 REV 03. Las Vegas, Nevada: Sandia National Laboratories. ACC: DOC.20070306.0037.

Table 11 - In-Drift Precipitates/Salts Model List of Software Used

Software	Version	Software Tracking Number	Platform / OS	Brief Description of Use	Availability
EQ3/6	8.0	10813-8.0-00	PC/WINDOWS 2000	a FORTRAN speciation-solubility and data processing code.	Available in SCM
GetEQData	1.0.1	10809-1.0.1-00	PC/WINDOWS 2000	A Microsoft Excel macro used to postprocess EQ3/6 output information.	Available in SCM
SUPCRT92	1.0	10809-1.0.1-00	PC/WINDOWS NT	Used to calculate the standard molal thermodynamic properties of minerals, gases, aqueous species, and reactions from 1 to 5,000 bars and 0°C to 1,000°C.	Available in SCM

There is a need to test models developed using the above codes on updated operating environment.

3.4 Waste Package and Drip Shield Degradation

3.4.1 WAPDEG (Drip Shield General Corrosion, Waste package General Corrosion, Waste package Stress Corrosion Cracking)

The analysis is documented in the report: 181953 SNL (Sandia National Laboratories) 2007. *Stress Corrosion Cracking of Waste Package Outer Barrier and Drip Shield Materials.* ANL-EBS-MD-000005 REV 04. Las Vegas, Nevada: Sandia National Laboratories. ACC: DOC.20070913.0001.

Software used: MathCad 2001i was used on a PC/Windows environment. This software is not available in SCM and it is a version not currently supported by the software developer. There is a need locate this version of the software and test the model. It may also be necessary to test the model using an updated version of the software.

3.4.2 Localized Corrosion of Waste Package Outer Surface

The analysis is documented in the report: 178519 SNL (Sandia National Laboratories) 2007. General Corrosion and Localized Corrosion of Waste Package Outer Barrier. ANL-EBS-MD-000003 REV 03. Las Vegas, Nevada: Sandia National Laboratories. ACC: DOC.20070730.0003; DOC.20070807.0007.

List of software used: S-PLUS 2000 Professional Release 2 is not available in SCM. This a commercial Windows based software. The latest release of the software is Version 8.2. It is not clear if the software is backwards compatible. There is a need to locate and test the original version of the software on updated operating environment.

The analysis is also documented in the report: 180778 SNL (Sandia National Laboratories) 2007. *General Corrosion and Localized Corrosion of the Drip Shield.* ANL-EBS-MD-000004 REV 02 ADD 01. Las Vegas, Nevada: Sandia National Laboratories. ACC: DOC.20060427.0002; DOC.20070807.0004; DOC.20071003.0019.

List of software used: Mathcad 2001i – this Windows based software is not available in SCM. There is a need to locate and test the version of the software on updated operating environment. Excel 97 SR-2– this Windows based software is not available in SCM. It is expected that later versions of Excel could be used.

Localized corrosion resulting from salt deliquescence in dust particles was also analized. Analysis of dust deliquescence is documented in: 181267 SNL (Sandia National Laboratories) 2007. *Analysis of Dust Deliquescence for FEP Screening.* ANL-EBS-MD-000074 REV 01 AD 01. Las Vegas, Nevada: Sandia National Laboratories. ACC: DOC.20070911.0004; DOC.20070824.0001.

Table 12 - Analysis of Dust Deliquescence for FEP Screening List of Software Used

Software Name	Version	Software Tracking Number (STN)	Platform/ Operating System	Brief Description of Use	Availability
EQ3/6	8	10813-8.0-00	PC/Windows 2000 Professional	a FORTRAN speciation-solubility and data processing code.	Available in SCM
GetEQData	1.0.1	10809-1.0.1-00	PC/Windows 2000 Professional	A Microsoft Excel macro. It is used to postprocess EQ3/6 output information.	Available in SCM
XTOOL	10.1	10208-10.1-00	SUN O.S. 5.6.1	Used to generate graphical representations of the results given in the NUFT and MSTHAC time-history files.	Available in SCM

There is a need to test the software on updated operating environment.

3.5 Waste Form Degradation and Mobilization

3.5.1 Radionuclide Inventory

Radionuclide inventory is documented in the report: 180472 SNL (Sandia National Laboratories) 2007. *Initial Radionuclide Inventories.* ANL-WIS-MD-000020 REV 01 ADD 01. Las Vegas, Nevada: Sandia National Laboratories. ACC: DOC.20050927.0005; DOC.20070801.0001.

Microsoft Excel 97 was used to perform simple mathematical expressions that are standard operations in the software. No software routines or macros were developed. The software is not available in in SCM.

Another supporting document is: 177424 SNL 2007. *Radionuclide Screening.* ANL-WIS-MD-000006 REV 02. Las Vegas, Nevada: Sandia National Laboratories. ACC: DOC.20070326.0003.

Software used: GoldSim Version 8.02.500, STN: 10344-8.02-05, run under Windows 2000 PC, to do radionuclide inventory decay calculations for selected times up to a million years. The software is available in SCM. Note that GoldSim Technology Group (GTG) no longer supports versions earlier than 9.6.000. There is a need to test the software on updated operating environment.

RadNuScreen V1.0, STN: 10732-1.0-00), installed on a Dell Optiplex GX 260 PC. The software was used in radionuclide screening analyses. Software is Available in SCM. There is a need to test the software on updated operating environment.

Microsoft Excel 2003 (11.8033.8036) SP2 was used to process radionuclide inventory data and GoldSim and RadNuScreen inputs and results. Excel is appropriate for these uses because the calculations require simple mathematical expressions and operations that are available as standard functions in Excel. The software is not available in SCM.

3.5.2 In-Package Chemistry

Abstraction of in-package chemistry is documented in: 180506 SNL (Sandia National Laboratories) 2007. *In-Package Chemistry Abstraction.* ANL-EBS-MD-000037 REV 04 ADD 01. Las Vegas, Nevada: Sandia National Laboratories. ACC: DOC.20070816.0004.

Table 13 - In-Package Chemistry Abstraction List of Software Used

Software Name	Version	Software Tracking Number (STN)	Platform/ Operating System	Brief Description of Use and Components Used	Availability
EQ3/6	7.2b	UCRL-MA-110662 (LSCR198)	PC/WINDOWS 95 and HP-UX 10.20 B	EQ3NR: a FORTRAN speciation-solubility code	Available in SCM
			PC/WINDOWS 95 and HP-UX 10.20 B	EQPT: a data file preprocessor in FORTRAN	
EQ6	7.2bLV	10075-7.2bLV-02	PC/Windows 2000 and NT 4.0	EQ6: a reaction path code that models water–rock interaction or fluid mixing in either a pure reaction progress mode or a time mode	Available in SCM
GetEQData	1.0.1	10809-1.0.1-00	PC/Windows 2000, NT 4.0, 98, and 95	A Microsoft Excel macro used to postprocess EQ3/6 output information	Available in SCM
transl	2.0	10251-2.0-00	PC/Windows 2000, NT 4.0, 98, and 95	A code for translating a nonPitzer EQ3/6 database into PHREEQC format	Available in SCM
PHREEQC	2.3	10068-2.3-01	PC/Windows 2000, NT 4.0, 98, and 95	A code for geochemical speciation, reaction path modeling, reactive transport, and surface-complexation.	Available in SCM
Mathcad	11		PC/Windows 2000, NT 4.0, 98, and 95	Used for calculations	Not available in SCM

There is a need to test the codes on updated operating environment. Mathcad 11 is not available in SCM. In addition, the version is no longer supported by the software developer. There is a need to locate the software or test using later versions of the code.

3.5.3 Cladding Degradation

Cladding degradation analysis is reported in: 180616 SNL (Sandia National Laboratories) 2007. *Cladding Degradation Summary for LA.* ANL-WIS-MD-000021 REV 03 ADD 01. Las Vegas, Nevada: Sandia National Laboratories. ACC: DOC.20050815.0002; DOC.20070614.0002.

No controlled or baselined software was used.

Another supported document is: 177422 SNL (Sandia National Laboratories) 2007. *MOX Spent Nuclear Fuel and LaBS Glass for TSPA-LA.* ANL-WIS-MD-000022 REV 01. Las Vegas, Nevada: Sandia National Laboratories. ACC: DOC.20070220.0007.

No controlled or baselined software was used.

3.5.4 CSNF, DSNF, HLW Degradation

Section 3.4.4 is on Commercial Spent Fuel (CSNF), DOE-owned Spent Nuclear Fuel (DSNF) and High Level Waste (HLW) degradation analyses.

Abstraction of CSNF waste form degradation is documented in:169987 BSC (Bechtel SAIC Company) 2004. *CSNF Waste Form Degradation: Summary Abstraction.* ANL-EBS-MD-000015 REV 02. Las Vegas, Nevada: Bechtel SAIC Company. ACC: DOC.20040908.0001; DOC.20050620.0004.

Table 14 - CSNF Waste Form Degradation List of Software Used

Software Name	Version	Software Tracking Number (STN)	Platform/Operating System	Brief Description of Use	Availability
Excel	2002		PC/Windows 2000 Professional	Used to perform calculations using user-defined formulas and the application's standard	Not available in SCM
SigmaPlot	8		PC/Windows 2002	Used for the linear and nonlinear regression analyses.	Not available in SCM
Mathcad	2001i		SUN/O.S. 5.6.1	Used for the regression analysis.	Not available in SCM

It is expected that later versions of Excel can be used. The Mathcad version is not currently supported by the software developer. There is a need to either locate this software or use later versions of the software to test the model.

Abstraction of DSNF waste form degradation is documented in: 172453 BSC (Bechtel SAIC Company) 2004. *DSNF and Other Waste Form Degradation Abstraction.* ANL-WIS-MD-000004 REV 04. Las Vegas, Nevada: Bechtel SAIC Company. ACC: DOC.20041201.0007.

No computer software was used in the development of the abstracted upper-limit DSNF model described in this report.

Analysis of defense high level waste glass degradation is reported in: 169988 BSC (Bechtel SAIC Company) 2004. *Defense HLW Glass Degradation Model.* ANL-EBS-MD-000016 REV 02. Las Vegas, Nevada: Bechtel SAIC Company. ACC: DOC.20041020.0015; DOC.20050922.0002.

List of software used: Microsoft Excel 2001 was used to compile test data and perform simple arithmetic calculations, such as calculating the mean and standard deviation values that are used in this report. Excel 2001 is not available in SCM. Microsoft KaleidaGraph Version 3.0.5 was used to plot the data within this report. The software is not available in SCM. It is expected that work developed using each software can be reproduced using later versions of the software. It is also possible that the software KaleidaGraph can be replaced with another graphics software.

3.5.5 Dissolved Radionuclide Concentration Limits

Analysis of dissolved radionuclide concentration limits is reported in: 177418 SNL (Sandia National Laboratories) 2007. *Dissolved Concentration Limits of Elements with Radioactive Isotopes.* ANL-WIS-MD-000010 REV 06. Las Vegas, Nevada: Sandia National Laboratory. ACC: DOC.20070918.0010.

Table 15 - Dissolved Concentration Limits of Elements with Radioactive Isotopes List of Software Used

Software Name	Version	Software Tracking Number (STN)	Platform/Operating System	Brief Description of Use and Components Used	Availability
EQ3/6	7.2b	UCRL-MA-110662 (LSCR198)	PC/Windows 95 and HP-UX 10.20 B)	EQ3NR: a FORTRAN speciation-solubility code	Available in SCM
			Windows 95 and HP-UX 10.20 B)	EQPT: a data file preprocessor in FORTRAN	
EQ6	7.2bLV	10075-7.2bLV-02	PC/Windows 2000 and NT 4.0	EQ6: a reaction-path code that models water–rock interaction or fluid mixing in either a pure reaction progress mode or a time mode	Available in SCM
EQ3/6	8.1	10813-8.1-00	PC/Windows 2000	See above for Versions 7.2b and 7.2bLV	Available in SCM
GetEQData	1.0.1	10809-1.0.1-00	PC/Windows 2000	A Microsoft Excel macro. It is used to postprocess EQ3/6 output information.	
BUILDEQ3.BAS	1.00	10365-1.00-00	PC/DOS Emulation	A QBASIC code used to generate EQ3NR input files.	Available in SCM
PHREEQC	2.11	10068-2.11-00	PC/Windows 2000	A code for geochemical speciation, reaction path modeling, reactive transport, and surface-complexation modeling.	Available in SCM

transl	2.0	10251-2.0-00	PC/Windows 98	A code for translating a non-Pitzer EQ3/6 database into PHREEQC format.	Available in SCM

There is a need to test the software on updated operating environment.

3.5.6 WF and EBS Colloids

Analysis of waste form and engineered barrier system colloids is reported in:177423 SNL (Sandia National Laboratories) 2007. *Waste Form and In-Drift Colloids- Associated Radionuclide Concentrations: Abstraction and Summary.* MDL-EBS-PA-000004 REV 03. Las Vegas, Nevada: Sandia National Laboratories. ACC: DOC.20071018.0019.

The calculations performed in this analysis used Excel 2003 (11.8117.8107, SP-2) on a personal computer running Windows XP Service Pack 2. Excel 2003 is not available in SCM.

3.6 Engineered Barrier System Flow and Transport

3.6.1 EBS Flow

The Engineered Barrier System Flow Submodel implemented in the TSPA-LA Model is described in the report: *EBS Radionuclide Transport Abstraction* (SNL 2007 [DIRS 177407]). Software list used in both EBS Flow and EBS Transport is shown below in Section 3.5.2.

3.6.2 EBS Transport

Engineered Barrier System flow and transport abstraction is documented in: 177407 SNL (Sandia National Laboratories) 2007. *EBS Radionuclide Transport Abstraction.* ANL-WIS-PA-000001 REV 03. Las Vegas, Nevada: Sandia National Laboratories. ACC: DOC.20071004.0001.

Table 16 - EBS Radionuclide Transport Abstraction List of Software Used

Software Name	Version	Software Tracking Number (STN)	Platform/ Operating System	Brief Description of Use and Components Used	Availability
GoldSim	8.02.500	10344-8.02-05	PC/WINDOWS 2000.	Developed to perform dynamic, probabilistic simulations.	Available in SCM
GoldSim	9.60.100	10344-9.60-01	PC/WINDOWS 2000.	Developed to perform dynamic, probabilistic simulations.	Available in SCM
PHREEQC	2.11	10068-2.11-00	PC/WINDOWS 2000.	A code for geochemical speciation, reaction path modeling, reactive transport, and surface-complexation.	Available in SCM

Grab It!™				Digitizing Software is Excel-based commercial off-the-shelf software from Datatrend. Software that enables bitmap images of plots that have been captured from journal articles to be converted into (*x*, *y*) data in an Excel file for further processing.	Not available in SCM.
S-PLUS	6.0			Commercial off-the-shelf support software used in conjunction with standard desktop software such as Excel.	Not available in SCM.
JMP	5.1			Commercial off-the-shelf support statistical and data analysis software. The standard sorting and table-joining functions in JMP V. 5.1 were used to extract and sort data from UZ flow field calculations for use in the EBS-UZ interface model, described in Section 6.5.2.6 (output DTN: SN0703PAEBSRTA.001, file *Repository Values for Saturation and Flux.doc*).	Not available in SCM.

There is a need to locate unavailable software and test all the codes on updated operating environment.

3.7 Unsaturated Zone Transport

3.7.1 Unsaturated Zone Transport

Unsaturated zone transport analysis is documented in: 177396 SNL (Sandia National Laboratories) 2007. *Radionuclide Transport Models Under Ambient Conditions*. MDL-NBS-HS-000008 REV 02 ADD 01. Las Vegas, Nevada: Sandia National Laboratories. ACC: DOC.20050823.0003; DOC.20070718.0003.

Table 17 - Radionuclide Transport Models Under Ambient Conditions List of Software Used

Software Name	Version	Software Tracking Number	Platform / Operating System	Brief Description of Use	Availability
iTOUGH2	4.0	10003-4.0-00	Dec Alpha / OSF1 V4.0	Used for model calibration and prediction of Alcove 8/Niche 3 tests.	Available in SCM
TOUGH2	1.11MEOS9nTV1.0	10065-1.11MEOS9nTV1.0-00	Dec Alpha / OSF1 V4.0	Simulates flow and the decoupled transport of multiple radioactive solutes and/or colloids (parents and daughters)	Available in SCM

TOUGH2	1.4	10007-1.4-01	Dec Alpha / OSF1 V4.0	Solves the Richards equation to simulate flow in complex subsurface systems (involving porous and/or fractured	Available in SCM
TOUGH2	1.6	10007-1.6-01	Dec Alpha / OSF1 V5.1	Solves the Richards equation to simulate flow in complex subsurface systems (involving porous and/or fractured	Available in SCM
TOUGH2	1.6	10007-1.6-00	Dec Alpha / OSF1 V4.0	Solves the Richards equation to simulate flow in complex subsurface systems (involving porous and/or fractured	Available in SCM
T2R3D	1.4	10006-1.4-00	Dec Alpha / OSF1 V4.0	Simulates flow and the coupled transport of a single radioactive solute tracer in complex subsurface systems involving	Available in SCM
DCPT	2.0	10078-2.3-00	PC / Windows NT V4.0	involves the particle-tracking method to simulate transport of a single radioactive solute tracer in complex subsurface	Available in SCM
PHREEQC	2.3	10068-2.0-00	PC / Windows 98	For elements that sorb primarily through surface complexation reactions, the experimental data are augmented with	Available in SCM
Bkread.f	1.0	10894-1.0-00	Sun Sparc / SunOS 5.5.1	Used for model calibration and prediction of Alcove 8/Niche 3 tests.	Available in SCM
XtractG.f90	1.0	10930-1.0-00	Dec Alpha / OSF1 V5.1	Used to ready the mesh files for the EOS9nT simulations, for the preparation of the corresponding initial conditions	Available in SCM
Smesh.f	1.0	10896-1.0-00	Sun Sparc / SunOS 5.5.1	Developed for the test site to compare the simulation results with the relevant field observations.	Available in SCM

There is a need to test the software on updated operating environment.

Another report supporting unsaturated zone transport analysis is: 184748 SNL (Sandia National Laboratories) 2008. *Particle Tracking Model and Abstraction of Transport Processes.* MDL-NBS-HS-000020 REV 02 AD 02. Las Vegas, Nevada: Sandia National Laboratories.

Table 18 - Particle Tracking Model and Abstraction of Transport Processes List of Software Used

Software	Version	Software Tracking Number (STN)	Platform/ Operating System	Brief Description of Use	Availability
FEHM	2.20	10086-2.20-00	PC/Windows 2000 and SUN/OS 5.7 and 5.8	Used in extracting repository coordinate locations for nodes for use in the GoldSim system model.	Available in SCM
FEHM	2.21	10086-2.21-00	PC/Windows 2000, and SUN/OS 5.8	Generation of transfer function curve information using a discrete fracture model. Simulation of particle tracking validation runs. Abstraction model	Available in SCM

				simulations.	
FEHM	2.23	10086-2.23-01	SUN/OS 5.9	Simulation of particle tracking base case runs. Abstraction model simulations.	Available in SCM
GoldSim	7.50.100	10344-7.50.100-00	PC/Windows 2000	Abstraction model simulations.	Available in SCM
ppptrk	1.0	11030-1.0-00	SUN/OS 5.8 and 5.9	Post-processing of particle breakthrough curve information.	Available in SCM
discrete_tf	1.1	11033-1.1-00	PC/Windows 2000	Post-processing of discrete fracture model results to convert results to transfer functions.	Available in SCM
fehm2post	1.0	11031-1.0-00	PC/Windows 2000 and SUN/OS 5.8 and 5.9	Executes multiple FEHM simulations along with pre- and post-processing runs. Used to execute the individual simulations and generation of transfer function curves used in the TSPA-LA UZ transport abstraction model.	Available in SCM
Fortner Plot		N/A	SUN Workstation	The commercial software, Fortner Plot, was used for plotting the results of breakthrough curve simulations.	Not available in SCM
Tecplot	10	N/A	IBM PC, Window 2000 Operating System	The commercial software, Tecplot 10, was used for plotting the results of breakthrough curve simulations.	Not available in SCM

GoldSim V7.5 is an older version and is not supported by the developers (GTG). There is a need to check the unavailable software. There is also a need to test the software on updated operating environment.

3.8 Saturated Zone Flow and Transport

3.8.1 1-D Saturated Zone Flow and Transport

The 1-D SZ Flow and Transport Abstraction is implemented directly in the TSPA-LA Model in GOLDSIM to calculate the radioactive decay, ingrowth, and transport for four decay chains. Thus, there is no separate software used.

3.8.2 3-D Saturated Zone Flow and Transport

Abstraction of the saturated zone flow and transport is documented in: 183750 SNL (Sandia National Laboratories) 2008. *Saturated Zone Flow and Transport Model Abstraction.* MDL-NBS-HS-000021 REV 03 AD 02. Las Vegas, Nevada: Sandia National Laboratories. ACC: DOC.20080107.0006.

Table 19 - Saturated Zone Flow and Transport Model Abstraction List of Software Used

Software Name	Version	Software Tracking Number (STN)	Computer Type, Platform, and Location	Brief Description of Use	Availability
FEHM	2.20	10086-2.20-00	Sun /UltraSPARC - SunOS 5.7 SNL	This code is a finite-element heat- and mass-transport code that simulates nonisothermal, multiphase, multicomponent flow, and solute transport in porous media.	Available in SCM
GoldSim	7.50.100	10344-7.50.100-00	Dell OptiPlex GX260 Window 2000 Professional 5.0.2195 SNL	This code is the modeling software used in the TSPA-LA. Probabilistic simulations are represented graphically in GoldSim.	Available in SCM
GoldSim	8.01 SP4	10344-8.01SP 4-00	Computer: Master 06 Windows 2000 Advanced Server YMP Offices, Las Vegas	GoldSim (GS) is a Windows-2000–based program that provides the following general capabilities: Quantitatively address the inherent variability. Superimposes the occurrence and consequences of discrete events onto continuously varying systems. Builds top-down models, dynamically links external programs or spreadsheets directly to the GS model. Directly exchanges data between any ODBC-compliant database to the GS model.	Available in SCM
CORPSCON	5.11.08	10547-5.11.08-00	IBM Thinkpad 770Z-WINDOWS NT 4.0 SNL	This software is used to convert coordinate data to the Universal Transverse Mercator (UTM) coordinate system	Available in SCM
SZ_Pre	2.0	10914-2.0-00	Sun UltraSPARC - SunOS 5.7 SNL	This software is an automated method for preparing the FEHM input files for the SZ site-scale flow and transport model [a] for use in TSPA-LA analyses.	Available in SCM

SZ_Post	3.0	10915-3.0-00	Sun UltraSPARC - SunOS 5.7, Solaris 2.7 SNL	This software is used to translate the output files from the SZ site-scale model into the format used by the SZ_Convolute software code. SZ_Post reads the output files from the FEHM software code and writes the breakthrough curve data for radionuclide transport in the SZ.	Available in SCM
SZ_Convolute	2.2	10207-2.2-00	Dell OptiPlex GX260 Windows 2000 Professional 5.0.2195 SNL	This software is used to calculate SZ response curves based on unsaturated zone (UZ) radionuclide source terms, generic SZ responses, and climate scenarios for the YMP.	Available in SCM

The codes include project developed as well as GoldSim (see Appendix B). There is a need to test the software on updated operating environment.

The saturated flow model is documented in: 177391 SNL (Sandia National Laboratories) 2007. *Saturated Zone Site-Scale Flow Model.* MDL-NBS-HS-000011 REV 03. Las Vegas, Nevada: Sandia National Laboratories. ACC: DOC.20070626.0004; DOC.20071001.0013.

Table 20 Saturated Zone Site-Scale Flow Model List of Software Used

Software Name	Version	Software Tracking Number (STN)	Platform/Operating System	Brief Description of Use	Availability
CORPSCON	5.11.08	10547-5.11.08-00	WINDOWS NT 4.0	This software is used to convert coordinate data to the Universal Transverse Mercator (UTM) coordinate system	Available in SCM
FEHM	2.24 [a]	10086-2.24-02	PC or Sun Ultra Sparc with Sun Solaris 5.7 or 5.8 operating system	Solution to SZ flow.	Available in SCM
LaGriT	1.1 [a]	10212-1.0-00	Sun Ultra Sparc with Sun OS 2.7 operating system at LANL	Software package for grid generation, analysis, and visualization	Available in SCM
PEST	5.5 [a]	10289-5.5-00	Sun Ultra Sparc with Sun Solaris 5.7 or 5.8 operating system at LANL	Preconditioning and parameter optimization for FEHM runs	Available in SCM
EARTHVISION	5.1	10174-5.1-00	Silicon Graphics Octane workstation running IRX 6.5.	Commercial software for 3D model building and visualization used in contouring, plotting, and visualization of the data and for evaluation of results.	Available in SCM

Extract	1.0 [a]	10955-1.0-00	Sun UltraSPARC/ SunOS 5.7 operating system at SNL	Pre/postprocessor used to extract lateral flow data from the USGS regional flow model	Available in SCM
Extract	1.1 [a]	10955-1.1-00	Sun UltraSPARC – SunOS 5.7 operating system at SNL	Pre/postprocessor used to extract lateral flow data from the USGS 2001 regional flow model	Available in SCM
EXT_RECH	1.0 [a]	10958-1.0-00	Sun UltraSPARC/ SunOS 5.7 operating system at SNL	Pre/postprocessor used to extract recharge data from the USGS regional flow model	Available in SCM
Mult_Rech	1.0 [a]	10959-1.0-00	Sun UltraSPARC/ SunOS 5.7, Solaris 2.7 operating system at SNL	Pre/postprocessor that scales recharge data from the USGS regional flow model and maps the data to a new grid	Available in SCM
Xread_Distr_Rech	1.0 [a]	10960-1.0-00	Sun UltraSPARC/ SunOS 5.7 operating system at SNL	Pre/postprocessor used to extract recharge data from the USGS 1999 regional flow model	Available in SCM
Xread_Distr_Rech UZ	1.0[a]	10961-1.0-00	Sun UltraSPARC/ SunOS 5.7 operating system at SNL	Pre/postprocessor that maps recharge data onto a new grid excluding the UZ flow model region	Available in SCM
Xread_Reaches	1.0[a]	10962-1.0-00	Sun UltraSPARC/ SunOS 5.7 operating system at SNL	Pre/postprocessor that maps local recharge from four stream channels onto a new grid	Available in SCM
Xwrite_Flow_New	1.0-125[a]	10963-1.0-125-00	Sun UltraSPARC/ SunOS 5.7 operating system at SNL	Used both to map the combined UZ and SZ site-scale fluxes onto a 125-m grid and to create a flux file that is compatible with FEHM flow macros	Available in SCM
Zones	1.0 [a]	10957-1.0-00	Sun UltraSPARC/ SunOS 5.7 operating system at SNL	Used to extract zonal designation data from the USGS 2001 regional flow model	Available in SCM

[a] Project developed

There is a need to test the software on updated operating environment.

The site-scale saturated zone transport model is documented in: 177392 SNL (Sandia National Laboratories) 2007. *Site-Scale Saturated Zone Transport.* MDL-NBS-HS-000010 REV 03. Las Vegas, Nevada: Sandia National Laboratories. ACC: DOC.20070822.0003, DOC.20080117.0002.

Table 21 - Site-Scale Saturated Zone Transport List of Software Used

Software	Version	Software Tracking Number	Platform/ Operating System	Brief Description of Use	Availability
FEHM	2.24-01-00	10086-2.24-01	Sun, PC Sun OS 5.9, Windows 2000, 2003 and XP, Red Hat Linux 2.4.21, Location: LANL	Used for calculations throughout this model report. The FEHM V 2.24-01 application is based on a finite-volume/ finite-element heat- and mass-transfer code that simulates nonisothermal, multiphase, multicomponent flow and solute transport in porous media.	Available in SCM
FEHM	2.20	10086-2.20-00	Sun, PC Sun OS 5.7 & 5.8, Windows 2000, RedHat, Linux 7.1 Location: LANL	Used for calculations in Appendix C of this model report. The FEHM V 2.20 application is based on a finite-volume/finite-element heat- and mass-transfer code that simulates nonisothermal, multiphase, multicomponent flow and solute transport in porous media.	Available in SCM
cr8sptr.c	2.0	10927-2.0-00	Sun, Sun OS 5.7, Location: LANL	Used to create an input file for sptr macro in FEHM.	Available in SCM
calc_cdf.c	1.0	10924-1.0-00	Sun, Sun OS 5.7, Location: LANL	Used to calculate the cumulative distribution function of the stochastic distributions of K_d.	Available in SCM
GS2FEHM.C	1.0	10923-1.0-00	Sun, Sun OS 5.7, Location: LANL	Used to create an input file for the perm macro in FEHM.	Available in SCM
GSLIB	1.0GAMV3V 1.201	10398-1.0GAM V3V1.201-00	Sun, Sun OS 5.5.1, Location: LANL	Used to calculate a three-dimensional variogram of input data.	Available in SCM
GSLIB	2.0MSISIMV 2.0	10098-2.0MSI SIMV2.0-00	Sun, UNIX, Location: LANL	Used to generate a stochastic distribution of parameters, such as K_d and permeability.	Available in SCM
PHREEQC	2.3	10068-2.3-01	PC Windows 2000 Location: LANL	Calculates surface complexation reactions for radionuclides.	Available in SCM
RELAP	2.0	10551-2.0-00	PC, Windows 2000/NT Location: LANL	Generate BTCs	Available in SCM
FRACT_p	1.0	11009-1.0-00	PC, LINUX 2.4.18, Location: LANL	Calculates data that correlate concentrations with time for transport in the fractured media.	Available in SCM
fehm2post	1.0	11031-1.0-00	WINDOWS 2000, SUN O.S 5.8&5.7, Redhat Linux 2.4.18	Software is a set of perl scripts used to automate the repetitive series of steps required to make multiple runs of FEHM and post-process the output data.	Available in SCM?
fehm2post	1.0	11031-1.0-01	SUN O.S 5.9	Software is a set of perl scripts used to automate the repetitive series of steps required to make multiple runs of FEHM and	Available in SCM?

				post-process the output data.	
EARTHVISION	5.1	10174-5.1-00	Silicon Graphics Octane workstation running IRIX 6.5.	This software was used for plotting and visualization of data	Available in SCM
Tecplot	360		PC, Microsoft Windows 2000/NT, Sun with UNIX OS, FORTRAN	Used for plotting and visualization of analysis results in figures shown in this report. No data analysis was done with this software. Only built-in standard functions in this software were used. No software routines or macros were used with this software to prepare this report. The output was visually checked for correctness.	Not available in SCM
BestFit	V4.5		PC, Microsoft Windows 2000/NT	A statistic program that finds the distribution that best fits given data. Output of this program was used only as a guide for the selection of the distribution functions. V. 4.5 (a subset of @RISK V 4.5 STN 600806-4.5-00), Serial # 11874954, March 2000, Palisade Corporation, 798 Cascadilla Street, Ithaca, NY 14850	Not available in SCM

There is a need to test the software on updated operating environment.

Another supporting document is: 177394 SNL (Sandia National Laboratories) 2007. *Saturated Zone In-Situ Testing*. ANLNBS- HS-000039 REV 02. Las Vegas, Nevada: Sandia National Laboratories. ACC: DOC.20070608.0004.

Table 22 - Saturated Zone In-Situ Testing Transport List of Software Used

Software Name	Version	Software Tracking Number (STN)/DIRS Number	Platform/ Operating System	Brief Description of Use	Availability
2WELLS_2D	1.0	10665-1.0-00	LANL, PC, Windows 2000/NT 4.0*/98	This software is used in the analysis of longitudinal dispersivity in the Prow Pass Tuff C-wells field tracer test. It is used to obtain predicted tracer responses in homogeneous, isotropic, confined (two-dimensional) aquifers under partial recirculation conditions. It has been used both to correct dispersion-coefficient estimates for dispersion caused by a dipole-flow pattern and for pretest predictions of ATC cross-hole tracer tests.	Available in SCM
2WELLS_3D	1.0	10667-1.0-00	LANL, PC, Windows 2000/NT 4.0*/98	This software is used to obtain predicted tracer responses in homogeneous, isotropic, confined three-dimensional aquifers under partial recirculation conditions. It has been used both to correct dispersion-coefficient estimates for dispersion caused by a dipole-flow pattern and for pretest predictions of ATC cross-hole tracer tests.	Available in SCM
DIFFCELL	2.0	10557-2.0-00	LANL, PC, Windows 2000/NT 4.0*	This software is used in the analysis of laboratory diffusion cell experiments. It provides a numerical solution to an equation describing one- dimensional diffusive transport through a rock wafer with time-dependent concentration boundary conditions.	Available in SCM
EQUILFIT	1.0	10668-1.0-00	LANL, PC, Windows 2000/NT 4.0*/98	This software is used to obtain cation-exchange coefficients, given experimental data on cation sorption (both for sorbing and displaced cations) and given independent cation-exchange-capacity measurements.	Available in SCM
Filter.vi	1	10970-1-00	USGS, PC, Windows 2000/NT 4.0*/98	This software uses the standard Butterworth filter with standard coefficients. It is for filtering higher-frequency diurnal pressure changes due to barometric pressure changes and tidal effects.	Available in SCM

Injection_ Pumpback.vi	1	10675-1-00	USGS, PC, Windows 2000/NT 4.0*/98	This software is used for tracer test analysis for single-well testing. Analysis considers tracer injection, drift, and pumpback.	Available in SCM
rcv2amos.exe and MOENCH.vi, Function(1)	1.0	10583-1.0-00	USGS, PC, Windows 2000*/NT 4.0/98	The software routine rcv2amos.exe is used to analyze cross-hole tracer tests. In conjunction with the use of rcv2amos.exe, the routine MOENCH.vi was developed to serve as a user interface and to display the results.	Available in SCM
MOENCH.vi Function(2)	1.0	10582-1.0-00	USGS, PC, Windows 2000*/NT 4.0/98	This software is used for the analysis of cross-hole tracer tests.	Available in SCM
MULTRAN	1.0	10666-1.0-00	LANL, PC, Windows 2000/NT 4.0*	This is a two-dimensional numerical model that uses an implicit-in-time, alternating-direction, finite-difference method to solve the equations describing multicomponent transport of sorbing and nonsorbing solutes in a dual-porosity medium. This software is used for analysis of laboratory crushed-rock and alluvium column experiments. It is also used for the analysis of the first peak in the Bullfrog Tuff C-wells field tracer test and for prediction and analysis of ATC tracer experiments.	Available in SCM
Neuman.vi	1.0	10972-1.0-00	USGS, PC, Windows 2000/NT 4.0*/98	This software displays the standard and accepted type curve for unconfined aquifers and allows the fitting of the input data curves over the type curve. The .vi extension displays the appropriate resulting hydrologic parameters associated with the data curve matching (transmissivity and storativity).	Available in SCM
PEST	5.5	10289-5.5-00	USGS, PC, Windows 2000*	This software assists in data interpretation, model calibration, and predictive analysis. PEST adjusts model parameters and/or excitations until the fit between model output and field or laboratory observations is optimized in the weighted least-squares sense.	Available in SCM

RECIRC.vi	1.0	10673-1.0-00	USGS, PC, Windows 98/NT 4.0*/2000	This program is used for recirculating and partial-recirculation cross-hole tracer test analysis.	Available in SCM
RELAP	2.0	10551-2.0-00	LANL, PC, Windows 2000/NT*	This software models tracer transport by convoluting a Laplace-domain transfer function for transport through dual-porosity media with transfer functions that describe tracer injection, mixing in the injection and production wellbores (or flow manifolds in laboratory experiments), and recirculation of the product fluid (in field experiments only). It also performs curve fits to field or laboratory tracer test data to obtain the best-fitting transport parameter values.	Available in SCM
RETRAN	2.0	10552-2.0-00	LANL, PC, Windows 2000/NT 4.0*	This software models reactive transport in dual- porosity media with a general, nonlinear sorption isotherm and with time-varying flow rates.	Available in SCM
Streltsova-Adams.vi	1	10971-1-00	USGS, PC, Windows 2000/98/NT 4.0*	This software displays the standard and accepted Streltsova-Adams type curve for fractured aquifers and allows the fitting of the input data curves over this type curve. The .vi extension displays the appropriate resulting hydrologic parameters associated with the data curve matching (transmissivity and storativity).	Available in SCM
Theis.vi	1.0	10974-1.0-00	USGS, PC, Windows 2000/NT 4.0*/98	This software displays the standard and accepted Theis type curve and allows the fitting of the input data curves over this type curve. The .vi extension displays the appropriate resulting hydrologic parameters associated with the data curve matching (transmissivity and storativity).	Available in SCM

There is a need to test the software on updated operating environment. The COTS will need to be checked for licensing and other requirements.

Another supporting document is: 170006 BSC 2004. *Saturated Zone Colloid Transport.* ANL-NBS-HS-000031 REV 02. Las Vegas, Nevada: Bechtel SAIC Company. ACC: DOC.20041008.0007; DOC.20051215.0005.

Table 23 - Saturated Zone Colloid Transport List of Software Used

Software Name	Version	Software Tracking Number (STN)	Platform/Operating System	Brief Description of Use	Availability
RELAP	2.0	10551-2.0-00	PC, Windows 2000/NT	This software models tracer transport by convoluting a Laplace-domain transfer function for transport through dual-porosity media with transfer functions that describe tracer injection, mixing in the injection and production wellbores (or flow manifolds in laboratory experiments), and recirculation of the product fluid (in field experiments only). It also performs curve fits to field or laboratory tracer test data to obtain the best-fitting transport parameter values.	Available in SCM
Excel	2000		PC, Windows 2000/NT	Software used for statistical analysis of data and plotting of graphs.	Not available in SCM

The software RELAP is project developed. There is a need to test the software on updated operating environment. It is expected that later versions of Excel can be used on an updated operating system.

3.9 Biosphere

The Biosphere Process Model documented in Biosphere Model report [DIRS 177399] is used to develop the capabilities for calculating annual radiation dose to the RMEI using the TSPA-LA Model. The analyses and abstractions of the two exposure cases in the Biosphere Process Model and reported in *Biosphere Model Report* (SNL 2007 [DIRS 177399]) resulted in two data sets biosphere dose conversion factors (BDCFs) for the groundwater and volcanic exposure cases. The software used in the process model is listed below.

The biosphere model analysis is reported in: 177399 SNL (Sandia National Laboratories) 2007. *Biosphere Model Report.* MDL-MGR- MD-000001 REV 02. Las Vegas, Nevada: Sandia National Laboratories. ACC: DOC.20070830.0007.

Table 24 - Biosphere Model Report List of Software Used

Software	Version	Software Tracking Number (STN)	Computer Type and Platform	Brief Description of Use	Availability
GoldSim	8.02.500	10344-8.02-05	PC, Windows 2000	This version of GoldSim was used to execute the biosphere model to produce the BDCFs.	Available in SCM

GoldSim	9.60	10344-9.60-00	PC, Windows XP	Used in conjunction with ASHPLUME_DLL_LA V.2.1, this software was used for probabilistic simulations.	Available in SCM
ASHPLUME_DLL_LA	2.1	11117-2.1-00	PC, Windows XP	This software was used for calculation of initial ash/fuel areal concentrations at the location of the RMEI.	Available in SCM

GoldSim 8.02.500 is not supported by GoldSim Technology Group (GTG). There is a need to test the software on updated operating environment.

Another supporting document is: 172827 BSC (Bechtel SAIC Company) 2005. *Characteristics of the Receptor for the Biosphere Model.* ANL-MGR-MD-000005 REV 04. Las Vegas, Nevada: Bechtel SAIC Company. ACC: DOC.20050405.0005.

The only software used during this analysis was Microsoft Excel (Version 97 SR-2 and Version 2000 SR-1). The Excel versions are not available in SCM.

3.10 Events

3.10.1 Early Failure (Early Failure Scenario Class)

3.10.1.1 Drip Shield Early Failure

Drip shield early failure analysis is documented in: 178765 SNL (Sandia National Laboratories) 2007. *Analysis of Mechanisms for Early Waste Package/Drip Shield Failure.* ANL-EBS-MD-000076 REV 00. Las Vegas, Nevada: Sandia National Laboratories. ACC: DOC.20070629.0002; DOC.20071003.0015.

Table 25 - Drip Shield Early Failure List of Software Used

Software Name	Version	Software Tracking Number	Platform/ Operating System	Brief Description of Use	Availability
SAPHIRE	7.26	10325-7.26-00	PC/Windows 2000	Used to develop and quantify event trees for the analysis.	Available in SCM
Mathcad	13.0		PC/Windows XP	Used to conduct numerical manipulations and graphics.	Available in SCM

Both are COTS. There is a need to test the software on updated operating environment. licensing of the software also would need to be checked.

3.10.1.2 Waste Package Early Failure

Waste package early failure is documented in the same document as drip Shield early failure (Section 9.1.1)

3.10.2 Igneous Activity (Igneous Scenario Class)

3.10.2.1 Igneous Intrusion

Igneous activity analysis is documented in: 169989 BSC (Bechtel SAIC Company) 2004. *Characterize Framework for Igneous Activity at Yucca Mountain, Nevada.* ANL-MGR-GS-000001 REV 02. Las Vegas, Nevada: Bechtel SAIC Company. ACC: DOC.20041015.0002; DOC.20050718.0007.

Table 26 – Characterize Framework for Igneous Activity List of Software Used

Software Name	Version	Software Tracking Number (STN)	Platform/ Operating System	Brief Description of Use	Availability
FITCD	1.0	10262-1.0-00	PC/Pentium 486 FORTRAN77	Computes discrete cumulative probability distributions for dike length from cumulative probabilities specified at selected values of length.	Available in SCM
SFCD	1.0	10275-1.0-00	PC/Pentium 486 FORTRAN77	Computes discrete cumulative probability distributions for dike length using user• specified distribution forms.	Available in SCM
DCPELD	1.0	10258-1.0-00	PC/Pentium 486 FORTRAN77	Computes discrete probability distribution for dike length from expert-specified distributions (output of FITCD).	Available in SCM
CPDI	1.0	10257-1.0-00	PC/Pentium 486 FORTRAN77	Computes conditional probability of intersection from volcanic events on an x,y grid using output of DCPELD and expert-specified azimuth distributions.	Available in SCM
UZVH	1.0	10277-1.0-00	PC/Pentium 486 FORTRAN77	Computes frequency of intersection from volcanic source zones using output of CPDI.	Available in SCM
UZVHLH	1.0	10278-1.0-00	PC/Pentium 486 FORTRAN77	Computes simulations of contributions to frequency of intersection on an x,y grid from volcanic source zones using Latin Hypercube sampling and output from CPDI.	Available in SCM
FKVH	1.0	10265-1.0-00	PC/Pentium 486 FORTRAN77	Computes frequency of intersection using kernel density estimation with specified h and output of CPDI.	Available in SCM
FKVHLH	1.0	10266-1.0-00	PC/Pentium 486 FORTRAN77	Computes simulations of contributions to frequency of intersection on an x,y grid using kernel density estimation with specified h, Latin Hypercube sampling, and output from CPDI.	Available in SCM
UZVPVH	1.0	10279-1.0-00	PC/Pentium 486 FORTRAN77	Computes frequency of intersection from volcanic source zones using volume predictable volcanic event rate model and output of CPDI.	Available in SCM
UZVPVHLH	1.0	10280-1.0-00	PC/Pentium 486 FORTRAN77	Computes simulations of contributions to frequency of intersection on an x,y grid from volcanic source zones using volume predictable volcanic event rate model, Latin Hypercube sampling, and	Available in SCM

Software Name	Version	Software Tracking Number (STN)	Platform/ Operating System	Brief Description of Use	Availability
				output from CPDI.	

FKVPVH	1.0	10267-1.0-00	PC/Pentium 486 FORTRAN77	Computes frequency of intersection using kernel density estimation using volume predictable volcanic event rate model and output of CPDI.	Available in SCM
FKVPVHLH	1.0	10268-1.0-00	PC/Pentium 486 FORTRAN77	Computes simulations of contributions to frequency of intersection on an x,y grid with kernel density estimation using volume predictable volcanic event rate model, Latin Hypercube sampling, and output from CPDI.	Available in SCM
ZBCKVH	1.0	10283-1.0-00	PC/Pentium 486 FORTRAN77	Computes frequency of intersection using kernel density estimation with h constrained by a source zone boundary and output of CPDI.	Available in SCM
ZBCKVHLH	1.0	10284-1.0-00	PC/Pentium 486 FORTRAN77	Computes simulations of contributions to frequency of intersection on an x,y grid using kernel density estimation with h constrained by a source zone boundary, Latin Hypercube sampling, and output from CPDI.	Available in SCM
FITFIELD	1.0	10263-1.0-00	PC/Pentium 486 FORTRAN77	Computes parameters of a bivariate Gaussian distribution that approximates boundaries of a defined polygon.	Available in SCM
FIT2CNTR	1.0	10261-1.0-00	PC/Pentium 486 FORTRAN77	Computes parameters of a bivariate Gaussian distribution from locations of volcanic events.	Available in SCM
PFGVH	1.0	10273-1.0-00	PC/Pentium 486 FORTRAN77	Computes frequency of intersection using a bivariate Gaussian distribution with specified field parameters and output of CPDI. Bivariate Gaussian distribution parameters obtained from programs FIT2CNTR or FITFIELD.	Available in SCM
PFGVHLH	1.0	10274-1.0-00		Computes simulations of contributions to frequency of intersection on an x,y grid using a 2D-Gaussian distribution with specified parameters, Latin Hypercube sampling, and output from CPDI. Gaussian distribution parameters obtained from programs FIT2CNTR or FITFIELD.	
FPFGVH	1.0	10269-1.0-00	PC/Pentium 486 FORTRAN77	Computes frequency of intersection using a bivariate Gaussian distribution with parameters fit to volcanic event locations and output of CPDI.	Available in SCM
FPFGVHLH	1.0	10270-1.0-00	PC/Pentium 486 FORTRAN77	Computes simulations of contributions to frequency of intersection on an x,y grid using a 2D-Gaussian distribution with parameters fit to volcanic event locations, Latin Hypercube sampling, and output from CPDI.	Available in SCM

VHTREE	1.0	10282-1.0-00	PC/Pentium 486 FORTRAN77	Computes mean and fractiles of frequency of intersection over an individual expert's volcanic hazard logic tree and aggregate over all experts using outputs of UZVH, UZVHB, FKVH, UZVPVH, FKVPVH, ZBCLVH, PFGVH, and FPFGVH.	Available in SCM
VHTIELHS	1.0	10281-1.0-00	PC/Pentium 486 FORTRAN77	Computes mean and fractiles of simulations of contributions to frequency of intersection on an x,y grid over an individual expert's volcanic hazard logic tree using Latin Hypercube sampling and output from UZVHLH, FKVHLH, UZVPVHLH, FKVPVHLH, ZBCLVHLH, PFGVHLH, and FPFGVHLH.	Available in SCM
NECPDS	1.1	10272-1.1-00	PC/Pentium 486 FORTRAN77	Computes distributions for number of eruptive centers per volcanic event and average spacing between eruptive centers.	Available in SCM
FITIDSR	1.0	10264-1.0-00	PC/Pentium 486 FORTRAN77	Computes discrete incremental probability distributions for dike length using input to FITCD.	Available in SCM
SFIDSR	1.0	10276-1.0-00	PC/Pentium 486 FORTRAN77	Computes discrete incremental probability distributions for dike length using input to SFCD.	Available in SCM
DLECD	1.0	10260-1.0-00	PC/Pentium 486 FORTRAN77	Computes joint discrete probability distributions for dike length and number of eruptive centers per volcanic event using output from FITIDSR.	Available in SCM
DILECDLH	1.0	10259-1.1-00	PC/Pentium 486 FORTRAN77	Computes joint conditional distribution of dike intersection length, dike azimuth, and number of eruptive centers within the repository footprint from outputs of program VHTIELHS using Latin hypercube sampling of dike length and volcanic event location distributions from DIECDIST.	Available in SCM
CFRAC	1.0	10254-1.0-00	PC/Pentium 486 FORTRAN77	Locates individual expert's simulation results that represent specified percentiles of the composite distribution for frequency of intersection from outputs of VHTIELHS.	Available in SCM
COMBSM	1.1	10256-1.1-00	PC/Pentium 486 FORTRAN77	Computes composite joint distribution of dike intersection length, dike azimuth, and number of eruptive centers within	Available in SCM

				the repository footprint across experts from outputs of DILECDLH and VHTIELHS for mean hazard.	
COMBSM	1.1	10255-1.1-00	PC/Pentium 486 FORTRAN77	Computes composite joint distribution of dike intersection length, dike azimuth, and number of eruptive centers within the repository footprint across experts from outputs of DILECDLH for selected percentiles of the hazard.	Available in SCM
MARGIN	1.1	10271-1.1-00	PC/Pentium 486 FORTRAN77	Computes marginal distributions for dike intersection length, dike azimuth, and number of eruptive centers within the repository footprint from output of COMBSM and COMBSF.	Available in SCM

There is a need to test the software on updated operating environment.

Volcanic Eruption

The analysis is documented in: 177431 SNL (Sandia National Laboratories) 2007. *Atmospheric Dispersal and Deposition of Tephra from a Potential Volcanic Eruption at Yucca Mountain, Nevada.* MDL-MGR-GS-000002 REV 03. Las Vegas, Nevada: Sandia National Laboratories. ACC: DOC.20071010.0003.

Table 27 - Volcanic Eruption List of Software Used

Software Name	Version	Software Tracking Number (STN)	Platform/ Operating System	Brief Description of Use	Availability
ArcGIS	9.1	11205-9.1-00	PC, Windows XP	Qualified geographical data visualization and basic spatial analysis; used for	Not available in SCM
ASHPLUME_DLL_LA	2.1	11117-2.1-01	PC, Windows Server 2003	This version is used by TSPA	Available in SCM
ASHPLUME_DLL_LA	2.1	11117-2.1-00	PC, Windows 2000, XP	Parameterization developed in this model report directly feeds this version of the	Available in SCM?
ASHPLUME	2.0	10022-2.0-00	PC, Windows NT 4.0	This version is used in validation studies.	Available in SCM
ASHPLUME_DLL_LA	2.0	11117-2.0-00	PC, Windows 2000	This version is used for model validation studies.	Available in SCM
ASHPLUME	1.4LV	10022-1.4LV-dll-00	PC, Windows 2000	This version is used corroboratively with V 2.0 for comparison of calculated and	Available in SCM

FAR	1.2	11190-1.2-00	PC, Windows 2000 & 2003	This software was used in the Ashplume model validation activity.	Available in SCM
GoldSim	9.60.000	10344-9.60-00	PC, Windows 2000, 2003, & XP	This software was used to run the ASHPLUME_DLL_LA V2.1 and FAR	Available in SCM
Microsoft Excel	97 SR-2 and 2000	N/A	PC, Windows 2000/NT/XP	The commercial software was used for plotting graphs and statistical calculations.	Not available in SCM
Microsoft Access	2000	N/A	PC, Windows 2000, XP	The commercial software was used for unit conversions and data segregation	Not available in SCM
OriginPro	7.5	N/A	PC, Windows 2000, XP	The commercial software was used for data visualization and generation of basic statistics using built-in functions.	Not available in SCM
Microsoft PowerPoint	97 SR-2	N/A	PC, Windows NT	The commercial software was used for visualizing model validation results.	Not available in SCM
Golden Software's Surfer	6.01	N/A	PC, Windows NT	The commercial software was used for visualizing model validation results.	Not available in SCM
Matlab	11	N/A	PC, Windows XP	The commercial software was used for generation of synthetic ash plume data sets based on simple equations.	Not available in SCM
Tecplot	360	N/A	PC, Windows XP	The commercial software was used for visualization and grid processing,	Not available in SCM

There is a need to test the software on updated operating environment. ArcGIS and GoldSim are COTS. The rest of the codes are project developed. It is possible that a new license is needed to run ArcGIS.

Another report supporting the analysis is: 179347 SNL (Sandia National Laboratories) 2007. *Redistribution of Tephra and Waste by Geomorphic Processes Following a Potential Volcanic Eruption at Yucca Mountain, Nevada.* MDL-MGR-GS-000006 REV 00. Las Vegas, Nevada: Sandia National Laboratories. ACC: DOC.20071220.0004.

Table 28 - Redistribution of Tephra and Waste by Geomorphic Processes Following a Potential Volcanic Eruption List of Software Used

Software Name	Version	Software Tracking Number (STN)	Platform/Operating System	Brief Description of Use	Availability
ASHPLUME_DLL_LA	2.1	11117-2.1-00	PC, Windows 2000/2003 server	Used to generate the initial tephra deposit required to run FAR.	Available in SCM

ArcGIS	9.2	11205-9.2-00	PC, Windows XP	Used to develop and analyze spatial data sets such as the digital	Available in SCM
FAR	1.2	11190-1.2-00	PC, Windows 2000/2003 server	Tephra redistribution model, implemented as a dynamic link library (DLL)	Available in SCM
GoldSim	9.60.100	10344-9.60-01	PC, Windows 2000, 2003, XP	commercial graphical, object-oriented, probabilistic computer	Available in SCM
MVIEW	4.0	10072-4.0-00	PC/Windows 2000	MVIEW was used to perform the stepwise linear regression analysis as part	Available in SCM
Mathcad	13.1	611161-13.1-00	PC, Windows XP	Used for standard post-processing calculations and plotting.	Not available in SCM

There is a need to test the software on updated operating environment.

Another report supporting the analysis is: 174260 SNL (Sandia National Laboratories) 2007. *Characterize Eruptive Processes at Yucca Mountain, Nevada.* ANL-MGR-GS-000002 REV 03. Las Vegas, Nevada: Sandia National Laboratories. ACC: DOC.20070301.0001.

List of software used:
Excel versions were used for this work. It is expected that use of updated platforms and operating systems will not affect the results.

Conflow, version 1.0.0, is an open-source conduit flow code developed by Mastin and Ghiorso (2000 [DIRS 170144]) and further discussed by Mastin (2002 [DIRS 178163]). This software is not available in SCM. *Conflow* was run on a Windows-based desktop PC running Windows XP and was used within its range of validation. Use of this unqualified code is limited to providing context for characterizing the conduit flow conditions and final configuration of conduit profiles during the eruptions at the study areas.

Another report supporting the analysis is: 177430 SNL (Sandia National Laboratories) 2007. *Dike/Drift Interactions.* MDL-MGRGS- 000005 REV 02. Las Vegas, Nevada: Sandia National Laboratories. ACC: DOC.20071009.0015.

Table 29 - Drift/Dike Interactions List of Software Used

Software	Version	Software Tracking Number	Computer Type Platform	Brief Description of Use	Availability
NPHF2D	1.0	10904-1.0-00	PC/Windows 2000/NT4.0	Dike Propagation Model; performs numerical modeling supporting analysis of magmatic dike propagation and analysis of the dike/drift interaction where magma enters a drift, modified and requalified for this task. This code was developed specifically for fracture propagation to the surface; no other code can evaluate the number of physical phenomena required.	Available in SCM

FLAC	4.0	10167-4.0-00	PC/Windows 2000/NT 4.0	This is commercially Available in SCM software that is used for a very broad range of geomechanical problems including hydraulic, mechanical, and thermal coupling.	Available in SCM
FLAC	4.04	10167-4.04-00	PC/Windows 2000/NT 4.0	This is commercially Available in SCM software that is used for a very broad range of geomechanical problems including hydraulic, mechanical, and thermal coupling. It is the same software as V. 4.0 but is also validated for fluid flow and coupled hydro-mechanical analyses.	Available in SCM
FLAC3D	2.1	10502-2.1-00	PC/Windows 2000/NT 4.0	This is commercially Available in SCM software that is used for a very broad range of geomechanical problems including hydraulic, mechanical, and thermal coupling. It is the preferred code for analyzing regional stresses, accounting for topography; and opening preexisting fractures by magma.	Available in SCM
FLAC3D	2.14	10502-2.14-00	PC/Windows 2000	This is commercially Available in SCM software that is used for a very broad range of geomechanical problems including hydraulic, mechanical, and thermal coupling. It is the same software as V. 2.1 but is also validated for fluid flow and coupled hydro-mechanical analyses.	Available in SCM
UDEC	3.1	10173-3.1-00	PC/Windows 2000/NT 4.0	Analyzes opening of preexisting fractures by magma. This was the only code Available in SCM for hydromechanic behavior of fracture media.	Available in SCM
UDEC	3.14	10173-3.14-00	PC/Windows 2000	Analyzes opening of preexisting fractures by magma. Same software as V. 3.1, but also validated for fluid flow and coupled hydro-mechanical analyses.	Available in SCM

Most of the above codes are commercial and used for numerical modeling (see Appendix B). Licensing requirements needs to be checked. There is a need to test the software on updated operating environment.

Another report supporting the analysis is: 177432 SNL (Sandia National Laboratories) 2007. *Number of Waste Packages Hit by Igneous Events.* ANL-MGR-GS-000003 REV 03. Las Vegas, Nevada: Sandia National Laboratories. ACC: DOC.20071002.0001.

Table 30 - Number of Waste Packages Hit by Igneous Events List of Software Used

Software	Version	Software Tracking Number (STN)	Platform/Operating System	Brief Description of Use	Availability
QUALIFIED SOFTWARE					
LHS	2.51	10205-2.51-00	DEC Alpha, with Open VMS AXP V. 7.3-1 operating system	Stochastic parameter sampling	Available in SCM
DIRECT	4.0	11121-4.0-00	PC running Windows XP operating system	Geometric intersection calculations	Available in SCM
FLAC	4.0	10167-4.0-00	PC running Windows 2000 operating system	Dike/drift proximity calculations	Available in SCM
CORPSCON	5.11.08	10547-5.11.08-00	PC running Windows 2000 operating system	Conversion of UTM to NSP coordinate	Available in SCM
EXEMPT SOFTWARE					
VULCAN	6.0	NA	PC running Windows XP operating system	Standard CAD applications	Not available in SCM
Rhinocerous (Rhino 3D)	3.0	NA	PC running Windows XP operating system	Standard CAD applications	Not available in SCM
Milkshape	1.8.1b	NA	PC running Windows XP operating system	Standard CAD applications	Not available in SCM

Codes DIRECT, FLAC and CORPSCON are commercial software. There is a need to locate unavailable software and to check for licensing requirements. There is a need to test the software on updated operating environment.

3.10.3 Seismic Activity (Seismic Scenario Class)

The list of software used for both Ground Motion and Fault Displacement Seismic Scenario cases are listed below.

Abstraction of seismic consequence is documented in: 176828 SNL (Sandia National Laboratories) 2007. *Seismic Consequence Abstraction.* MDL-WIS-PA-000003 REV 03. Las Vegas, Nevada: Sandia National Laboratories. ACC: DOC.20070928.0011.

Software used:
PFC2D V. 2.0, Software Tracking Number: 10828-2.0-00, Operating Environment: PC/Windows 2000. The software is available in SCM.

PFC2D was used to characterize the behavior of a rubblized rock mass in the lithophysal units of the repository. PFC2D was selected for its capability of modeling the nonlinear response of a rubblized rock mass by combining the behaviors of individual grain particles to simulate the overall deformation of a rubblized rock mass with voids.

The software was used to abstract output of other software. There is a need to test the software on updated operating environment.

Another supporting document is: 178851 SNL (Sandia National Laboratories) 2007. *Mechanical Assessment of Degraded Waste Packages and Drip Shields Subject to Vibratory Ground Motion.* MDLWIS- AC-000001 REV 00. Las Vegas, Nevada: Sandia National Laboratories. ACC: DOC.20070917.0006.

Table 31 - Mechanical Assessment of Degraded Waste Packages and Drip Shields Subject to Vibratory Ground Motion List of Software Used

Software	Version	Software Tracking Number	Platform/ Operating System	Brief Description of Use (Range of Use/Selection/Limitations)	Availability
UDEC	3.1	10173-3.1-00	PC/Windows 2000	UDEC was used to analyze the drip shield failure (Section 6.4) and the waste package surrounded by rubble (Section 6.5). UDEC was selected for its capability to model solid body interactions with a computationally efficient algorithm.	Available in SCM
FLAC	4.0	10167-4.0-00	PC/Windows 2000	FLAC was used to simulate the invert material during seismic shaking (Sections 6.4 through 6.5). FLAC was selected for its capability to model dynamic loading for the continuum with a computationally efficient algorithm.	Available in SCM
FLAC3D	2.1	10502-2.1-00	PC/Windows 2000	FLAC3D V. 2.1 was used to simulate the drip shield and invert during quasi-static loading (Section 6.4.6). FLAC3D V. 2.1 was selected for its capability to model dynamic loading for the continuum with a computationally efficient algorithm. FLAC3D V. 2.1 simulates the behavior of three-dimensional structures built of soil, rock, or other materials that are subject to various loading conditions.	Available in SCM

FLAC3D	2.14	10502-2.14-00	PC/Windows 2000	FLAC3D V. 2.14 was used to simulate the drip shield during quasi-static and dynamic loading (Sections 6.4.3 and 6.4.7), and to simulate the waste package loaded by the drip shield (Section 6.5.2). FLAC3D V. 2.14 was selected for its capability to model dynamic loading for the continuum with a computationally efficient algorithm. Note that FLAC3D V. 2.14 and FLAC3D V. 2.1 are identical codes.	Available in SCM
LS-DYNA SMP D	970.3858	10300-970.3858-02	DEC ALPHA/OSF1 V. 5.1	The software was used to analyze the kinematic impacts between the waste packages and between waste packages and pallets (Section 6.3). LS-DYNA was selected for its capability to model solid mechanics in dynamic loading conditions	Not available in SCM
LS-DYNA	971.7600.398	10300-971.7600.398-00	Intel Itanium/Redhat Linux Chaos 3.0	LS-DYNA V. 971.7600.398-00 Intel Itanium/Redhat Linux Chaos 3.0 was used to analyze the kinematic impacts between the waste packages and between waste packages and pallets (Section 6.3). LS-DYNA was selected for its capability to model solid mechanics in dynamic loading conditions.	Not available in SCM
LS-DYNA	971.7600.398	10300-971.7600.398-00	Intel Itanium/Redhat Linux Chaos 3.0	LS-DYNA V. 971.7600.398-00 Intel Itanium /Redhat Linux Chaos 3.0 was used to analyze the kinematic impacts between the waste packages and between waste packages and pallets (Section 6.3). LS-DYNA was selected for its capability to model solid mechanics in dynamic loading conditions.	Not available in SCM
km_impacts_pp	1.0	11235-1.0-00	Intel Itanium2 Redhat Linux 4	km_impacts_pp was used on an Intel Itanium2 Redhat Linux 4 system to postprocess output from LS-DYNA. km_impacts_pp is used to produce estimates of damaged areas for the waste packages along with estimates of the number of ruptured waste packages. km_impacts_pp was selected for its capability to process the output of	Available in SCM

				LS-DYNA and directly produce data for the seismic abstraction.	
GoldSim	8.02.500	10344-8.02-05	PC/Windows 2000	GoldSim was used to sample the rock block pattern, rock strength, and ground motion number. GoldSim is widely used for probabilistic and decision analyses and provides capability for Latin Hypercube analysis used to sample the parameters listed above.	Available in SCM
LS-PREPOST	1.0 and 2.0		AMD Opteron Redhat Linux 4, Intel Itanium2 Redhat Linux 4, and DEC ALPHA/OSF1 V. 5.1 systems.	Post processing software to visualize output.	Not available in SCM
TrueGrid	2.2.0, 2.2.6, and 2.3.0			were used to preprocess data and generate model geometry for input to LS-DYNA.	Not available in SCM
Mathcad	7.0			postprocess data from UDEC and to solve non-linear equations for stress profiles.	Available in SCM

Most of the above software are COTS (see Appendix B). There is a need to locate unavailable software and check for licensing requirements. There is a need to test the software on updated operating environment.

3.10.4 Human Intrusion (Human Intrusion Scenario Class)

The human intrusion scenario case implemented in the TSPA-LA Model is developed within the TSPA-LA report (SNL, 2018, MDL-WIS-PA-000005 REV 00 ADD 01). However, the drift degradation analysis provides input data to this scenario class and others. Thus, the list of software used for the drift degradation analysis is documented here.

Drift degradation analysis is reported in: 166107 BSC (Bechtel SAIC Company) 2004. *Drift Degradation Analysis.* ANL-EBS-MD- 000027 REV 03. Las Vegas, Nevada: Bechtel SAIC Company. ACC: DOC.20040915.0010; DOC.20050419.0001; DOC.20051130.0002; DOC.20060731.0005.

Table 32 – Drift Degradation Analysis List of Software Used

Software Name	Version	Software Tracking Number	Operating Environment (Platform/Operating System)	Brief Description of Use (Range of Use/Selection/Limitations)	Availability
UDEC	3.1	10173-3.1-00	PC/Windows 2000	UDEC was used to analyze the seismic and thermal effects on block movement in the lithophysal rock units (Section 6.4). UDEC was selected for its capability of modeling block slip and block separation in plane strain condition. Also, it is capable of thermal and dynamic simulation. There are no known limitations on outputs	Not available in SCM
3DEC	2.01	10025-2.01-00	PC/Windows 2000	3DEC was used to analyze the seismic and thermal effects on block movement in the nonlithophysal rock units (Section 6.3). 3DEC was selected for its capability of modeling of wedge type of rockfall with consideration of block slip and block separation in three- dimensional space. Also, it is capable of thermal and dynamic simulation.	Available in SCM
FLAC	4.0	10167-4.0-00	PC/Windows 2000	FLAC was used in the thermal-mechanical calculation to define the distribution of stresses around the drifts due to the progressive heating of the repository area (Section 6.2). FLAC was selected as an efficient code to run thermal-mechanical analysis. There are no known limitations on outputs.	Available in SCM
FLAC3D	2.1	10502-2.1-00	PC/Windows 2000	FLAC3D was used in the thermal-mechanical calculation to define the distribution of stresses around the drifts due to the progressive heating of the repository area (Appendix C). FLAC3D was selected as an efficient code to run thermal-mechanical analysis for the regional scale and drift scale. There are no known limitations on	Available in SCM

PFC2D	2.0	10828-2.0-00	PC/Windows 2000	PFC2D was used to characterize rock mass behavior, including the analysis of long-term strength degradation (Section 7 and Appendix S). PFC2D was selected for its capability of modeling behaviors of a rock material by combining behaviors of individual grain particles to simulate complicated non- linear deformation of a rock material including long-term mechanical strength degradation and rock mass deformation with voids.	Available in SCM
PFC2D	2.0	10828-2.0-01	PC/Windows 2000	This version of PFC2D was used to run impact analyses to confirm the initial PFC2D results (using software tracking number 10828-2.0-00), as documented in Appendix Q. The initial PFC2D software qualification did not specifically identify the library of support functions (known as Fish functions) that are used within the code. This new version (software tracking number 10828-2.0-01) specifically qualifies FishTank 041b, which is the library of Fish functions included within the code. The impact assessments in Appendix Q confirm that the results are identical using either the initial or new version of PFC2D.	Available in SCM

PFC3D	2.0	10830-2.0-00	PC/Windows 2000	PFC3D was used to characterize rock mass behavior, including the analysis of long-term strength degradation (Section 7 and Appendix S). PFC3D was selected for its capability of modeling behaviors of a rock material by combining behaviors of individual grain particles to simulate complicated non- linear deformation of a rock material including long-term mechanical strength degradation and rock mass deformation with voids.	Available in SCM
PFC3D	2.0	10830-2.0-01	PC/Windows 2000	This version of PFC3D was used to run impact analyses to confirm the initial PFC3D results (using software tracking number 10830-2.0-00), as documented in Appendix Q. The initial PFC3D software qualification did not specifically identify the library of support functions (known as Fish functions) that are used within the code. This new version (software tracking number 10830-2.0-01) specifically qualifies FishTank 041b, which is the library of Fish functions included within the code. The impact assessments in Appendix Q confirm that the results are identical using either the initial or new version of PFC3D.	Available in SCM
DRKBA	3.31	10071-3.31-00	PC/Windows 2000	DRKBA was used to analyze block development and failure in the nonlithophysal rock units (Appendix D). DRKBA was selected to assess the impact of small-scale fractures on rockfall because it has an efficient key-block simulation algorithm. DRKBA was also selected as an alternative numerical code to verify the results from 3DEC. DRKBA does not directly apply seismic and thermal loads, and therefore was not selected as the primary code for rockfall analyses.	Available in SCM

FracMan	2.512	10114-2.511-00	PC/Windows NT	FracMan was used to replicate the fracture geometry observed in the ESF to develop a representative volume of jointed rock mass (Section 6.1.6). FracMan was selected for its capability of discrete fracture data analysis, geologic fracture network construction, spatial analysis, and visualization.	Available in SCM
NUFT	3.0s	10088-3.0s-01	SUN/SUN O.S. 5.7	NUFT was used to simulate heat transfer around the emplacement drift (Section 6.2). NUFT was selected for its capability of modeling thermal-hydrology of an unsaturated zone including subsurface heat and fluid flow. There are no known limitations on outputs from NUFT.	Available in SCM
EARTHVISION	5.1	10174-5.1-00	SGI/IRIX 6.5	EarthVision was used to extract stratigraphic unit thickness and cross-sections from the Geological Framework Model (GFM2000) (Appendix M). EarthVision was selected for its capability of extracting specific data from GFM2000 and presenting the data in a common graphical format. EarthVision was not used to perform data manipulation in this report.	Available in SCM
UNWEDGE	2.3	30053 V2.3	PC/DOS Emulation	UNWEDGE was used as a reference-only example of a deterministic method for key-block analysis (Appendix D). UNWEDGE was selected for its common usage on static block analysis for the geotechnical and mining industries.	Available in SCM
Clustran	1.1	11162-1.1-00	PC/Windows 2000	Clustran was used to analyze fracture data Clustran was selected for its common usage on fracture orientation analysis for the geotechnical and mining industries.	Available in SCM

Read DXF	1.0	11159-1.0-00	PC/Windows 2000	Read DXF was used to read fracture data files in DXF format and extract polyline data with associated strike/dip tags for input into FracMan (Section 6.1.6). Read DXF was specifically developed to extract fracture data from full periphery geologic maps to facilitate the comparison of field fracture data to synthetic FracMan fracture data.	Available in SCM

Most of the codes are COTS (see Appendix B). Licensing requirements need to be checked. There is a need to test the software on updated operating environment. EARTHVISION is a visualization graphics commercial software from Dynamic Graphics, Inc. The latest version of the software is 9.0. It is not clear if it is backwards compatible. IRIX 6.5 (UNIX based OS) operating system has been discontinued. There is a need to install EARTHVISION 5.1 on a current UNIX platform for testing.

3.11 Preliminary Assessment of Software Status

A preliminary assessment of the current condition of the software was also carried out. To facilitate the assessment, the list of software was divided into major modeling codes and supporting utility and graphics software. Each group was also subdivided into project developed (YMP) COTS. A preliminary list of software in each category is given in Appendix B. A detailed analysis on YMP LA software fitness categorization and strategy is given in Appenidx C. The analysis provides a general assessment of legacy software, and provides techniques for mitigation of possible software failures.

In general, it is expected that assessment of project developed codes will be easier than commercial codes. Some of the project developed codes are currently in use in National Laboratories and elsewhere on updated operating environment. Commercial software usually has licensing requirements. Some licenses are in-perpetuity while others are term-limited. In both cases there is a chance that the version of the software that was used for YMP license application may not be supported because of substantial upgrades to the software. This may require testing of the model with a new software version. If the commercial software was used for graphics or as a utility code, the software could be replaced in case of software issues. Further software assessment would require an in depth analysis that may include locating of unavailable software, analyzing licensing requirements of commercial software and testing of individual codes on updated operating environment. There may also be a need to run software on legacy operating systems. Running legacy operating systems on virtual machines is an option; however, the underlying hardware would not be emulated and would actually be modern hardware made accessible through a hardware abstraction layer (HAL).

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APPENDIX A. TABULATED INVENTORY OF SOFTWARE USED IN THE YMP PROCESS MODELS

Note: The discussion for a particular code in this table can be located in the body of the report by searching for the six digit code prefacing the Reference in the table

Appendix A

FY 18 Status Report on the Computing Systems for the Yucca Mountain Project TSPA-LA Models and Inventory of Software used for Process Models

Topic	Sub topic	Primary / Supporting	Software Name	Version	STN	Platform	OS	SCM?	Source	Comment	Problem / Mitigation Code(s)	Reference
UZ Flow	Climate		Excel	2000						Excel 2000 – no software issue anticipated		170002 BSC (Bechtel SAIC Company) 2004. Future Climate Analysis. ANL-NBS-GS-000008 REV 01. Las Vegas, Nevada: Bechtel SAIC Company. ACC: DOC.20040908.0005.
	Infiltration		Excel	2000	611161-13.1-00	PC, Windows XP		N				182145 SNL (Sandia National Laboratories) 2007. Simulation of Net Infiltration for Present-Day and Potential Future Climates. MDL-NBS-HS-000023 REV 01 AD 01, Las Vegas, Nevada: Sandia National Laboratories.
	Infiltration	P	Mathcad	13.1				N	COTS	Version 13.1 no longer supported by PTC		
	Infiltration	S	LHS	2.51	10205-2.51-01	DEC Alpha Server ES45 Model 2	Open VMS 8.2	Y	NL		S-CP, S-FN, S-AM	
	Infiltration		ArcGIS	9.1	11205-9.1-00	PC, Windows XP		Y	COTS	Developed by Esri	B-CT	
	Infiltration	S	ENVI+IDL	4.2	11204-4.2-00	PC	Windows XP	Y	COTS	COTS Harris Geospatial Solutions	B-CT	
	Infiltration	S	MVIEW	4	10072-4.0-00	PC	Windows 2000	Y	NL/YM		B-CT	
	Infiltration											177081 SNL (Sandia National Laboratories) 2006. Data Analysis for Infiltration Modeling: Extracted Weather Station Data Used to Represent Present-Day and Potential Future Climate Conditions in the Vicinity of Yucca Mountain. ANL-MGR- MD-000015 REV 00. Las Vegas, Nevada: Sandia National Laboratories. ACC: DOC.20070109.0002
	Infiltration		CORPSCON	5.11.08	10547-5.11-08-00	PC	Windows NT 4.0	Y	USACE	US Army Corps of Engineers	B-GT	
	Infiltration		EARTHVISION	5.1	10174-5.1-00	IRIX 6.5		Y	COTS	COTS Dynamic Graphics, Inc	B-CT	IRIS has not been actively maintained. The most current version is 6.5 and SNL can probably acquire the source code if needed.
	Site Scale UZ Flow											184614 SNL (Sandia National Laboratories) 2007. UZ Flow Models and Submodels. MDL-NBS-HS-000006 REV 03 AD 01. Las Vegas, Nevada: Sandia National Laboratories. ACC: DOC.20080108.0003.
	Site Scale UZ Flow		T2R3D	1.4	10006-1.4-00	Dec Alpha	UNIX	Y	YM			
	Site Scale UZ Flow		TOUGHREACT	3	10396-3.0-00	Dec Alpha	OSF1 V5.1	Y	YM		S-FN	
	Site Scale UZ Flow		TOUGH2	1.6	10007-1.6-01	Dec Alpha	OSF1 V5.1, PC-DOS Window98	Y	YM		S-FN	
	Site Scale UZ Flow		infil2grid	1.7	10077-1.7-00	Dec Alpha	OSF1 V4.0	Y	YM			
	Site Scale UZ Flow		2kgrid8.for	1	10503-1.0-00	Dec Alpha	OSF1 V4.0, PC-DOS Window95	Y	YM		S-FN	
	Site Scale UZ Flow		bot_sum.f	1	10349-1.0-00	UNIX	OSF1 V4.0	Y	YM		S-FN	
	Site Scale UZ Flow		WINGRIDDER	2	10024-2.0-00	PC	Windows NT 4.0	Y	YM			
	Site Scale UZ Flow		TOPTEMP_V0.f	1	10224-1.0-00	Dec Alpha	OSF1 V4.0	Y	YM		S-FN	
	Site Scale UZ Flow		GET_TEMP_V0.f	1	10222-1.0-00	Dec Alpha	OSF1 V4.0	Y	YM		S-FN	
	Site Scale UZ Flow		Tbgas3D	2	10882-2.0-00	SUN	SUN O. S. 5.5.1	Y	YM			
	Site Scale UZ Flow		T2FEHM	4	10997-4.0-00	Dec Alpha	OSF1 V5.1	Y	YM		S-FN	
	Site Scale UZ Flow		WTRISE	2	10537-2.0-00	Dec Alpha	OSF1 V5.1	Y	YM		S-FN	
	Site Scale UZ Flow		Bkread.f	1	10894-1.0-00	SUN	SUN O. S. 5.5.1	Y	YM		S-FN	
	Site Scale UZ Flow		Smesh.f	1	10896-1.0-00	SUN	SUN O. S. 5.5.1	Y	YM		S-FN	
	Site Scale UZ Flow		iTOUGH2	4	10003-4.0-00	SUN O. S. 5.5.1	OS V4.0	Y	YM		S-FN	
	Site Scale UZ Flow											179545 SNL (Sandia National Laboratories) 2007. Calibrated Unsaturated Zone Properties. ANL-NBS-HS-000058 REV 00. Las Vegas, Nevada: Sandia National Laboratories. ACC: DOC.20070530.0013
	Site Scale UZ Flow		iTOUGH2	5	10003-5.0-00	Linux	Red Hat V7.3	Y	YM		S-FN	
	Site Scale UZ Flow		e9-3in	1	10126-1.0-00	Sun	UNIX	Y	YM			
	Site Scale UZ Flow		2kgrid8.for	1	10503-1.0-00	PC	DOSV4.00.1111	Y	YM		S-FN	
	Site Scale UZ Flow		Infil2grid	1.7	10077-1.7-00	PC	DOSV4.00.1111	Y	YM			
	Site Scale UZ Flow		TBgas3D	2	10882-2.0-00	SUN	O.S.5.51	Y	YM			
	Site Scale UZ Flow		CORPSCON	5.11.08	10547-5.11-08-00	PC	WINDOWS NT 4.0	Y	USACE	US Army Corps of Engineers		

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Topic	Sub-topic	Primary / Supporting	Software Name	Version	STN	Platform	OS	SCM?	Source	Comment	Problem / Mitigation Code(s)	Reference
	Mountain Scale Coupled Processes											174101 BSC (Bechtel SAIC Company) 2005. Mountain Scale Coupled Processes (TH/THC/THM) Models. MDL-NBS-HS-000007 REV 03. Las Vegas, Nevada: Bechtel SAIC Company. ACC: DOC.20050825.0007.
	Mountain Scale Coupled Processes		TOUGH2	1.6	10007-1.6-01	Alpha system OSF1 V4.0		Y	YM	Selected for its capability to model effects of heat on flow in fractured media	S-FN	
	Mountain Scale Coupled Processes		TOUGHREACT	3	10396-3.0-00	Alpha System OSF1 V5.1		Y	YM	TOUGHREACT applies to porous media in a temperature range limited by its thermodynamic database (currently 0 to 300°C).	S-FN	
	Mountain Scale Coupled Processes		FLAC3D	2	10502-2.0-00	PC	Windows 98	N	COTS	Used for mechanical analysis and for linked TOUGH2 and FLAC3D coupled THM analysis.		
	Mountain Scale Coupled Processes		EXT	1.1	10005-1.1-00	SUN Ultra Sparc	SunOS 5.5.1	Y	YM	TOUGH2 output files for plotting. The input and output formats must be standard TOUGH2 input and output formats, with eight-character element names TOUGH2 mesh.		
	Mountain Scale Coupled Processes		EXT	1	10047-1.0-00	SUN Ultra Sparc	SunOS 5.5.1	Y	YM	The EXT code extracts data from TOUGH2 output files for plotting. The input and output formats must be standard TOUGH2 input and output formats, five-character element names TOUGH2 mesh.		
	Mountain Scale Coupled Processes		Infil2grid	1.7	10077-1.7-00	PC	MS-DOS V4.00.1111 under Windows 95	Y	YM	This software is used to extract surface infiltration rates to the top of TOUGH2 model grids. This routine is limited to eight-character element names TOUGH2 mesh.		
	Mountain Scale Coupled Processes		WINGRIDDER	2	10024-2.0-00	PC	Windows NT 4.0	Y	YM	A grid generator program used to produce 1-D, 2-D, or 3-D grids for numerical modeling of flow and transport problems based on the integral difference method. Output grid files are in the format compatible with TOUGH2. Inputs are distance, area, and volume that must be non- negative.		
	Mountain Scale Coupled Processes		GridReader	1	10994-1.0-00	PC	Windows NT 4.0	Y	YM	Gridreader is a package of utility tools used to 1) read a grid generated by WinGridder and write a mesh input file for TOUGH2 with high precision x-, y-, z-coordinates; 2) convert a TOUGH2 mesh file with 8-character cell names into a TOUGH2 mesh file with 5-character cell names. This software is to be used only with the TOUGH2 family of codes.		
	Mountain Scale Coupled Processes		Gpzones.dat	1	10509-1.0-00	PC	Windows 98	Y	YM	The software is used to find out which zones are connected to each grid point and how much zone volumes are connected to each grid point, and to calculate the interpolation of temperatures from TOUGH2 nodes to FLAC3D nodes. This routine is a FISH routine that can only be used for FLAC3D V2.0 or higher.		

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	Mountain Scale Coupled Processes		Tin	1.1	10889-1.1-00	PC	Windows 98	Y	YM	This software takes temperature output from TOUGH2 and interpolates it into FLAC3D for coupled THM simulations. Used to transfer temperatures from TOUGH2 Version 1.6 to FLAC3D V. 2.0 during linked TOUGH2 and FLAC3D coupled THM analysis.		
	Mountain Scale Coupled Processes		Delb.dat	1	10507-1.0-00	PC	Windows 98	Y	YM	The code is used to calculate changes in fracture aperture for linked TOUGH2 and FLAC3D Coupled THM analyses. This software is tested for normal stress ranging from +10 MPa to -100 MPa.		
	Mountain Scale Coupled Processes		2KGRIDV1.F	1	10244-1.0-00	SUN Ultra-Sparc	SunOS 5.5.1	Y	YM	This software is used to process data for TOUGH2 modelling for Yucca Mountain.	S-FN	
	Mountain Scale Coupled Processes		2kgridv1a.for	1	10382-1.0-00	PC	Dos Emulation	Y	YM	Generates dual-permeability grids for the TOUGH2 family of codes	S-FN	
	Mountain Scale Coupled Processes		Gen_incon-v0.f	1	10220-1.0-00	DEC Alpha	OSF1 4.0	Y	YM	This software is used to calculate top and bottom boundary temperatures and the initial block "INCON" for starting a TOUGH2 simulation. This software only processes valid "ELEME" block input format for the TOUGH2 family of codes.	S-FN	
	Mountain Scale Coupled Processes		Get_a_layer_v0.f	1	10221-1.0-00	DEC Alpha	OSF1 4.0	Y	YM	This software is used to extract data of a given list of elements from TOUGH2 outputs for plotting. This software only processes valid "ELEME" block input format for the TOUGH2 family of codes and valid EOS3 TOUGH2 V1.4 output file formats.	S-FN	
	Mountain Scale Coupled Processes		Get_temp_v0.f	1	10222-1.0-00	DEC Alpha	OSF1 4.0	Y	YM	This software is used to search for the nearest tabulated value of temperature to assign bottom boundary conditions. The coordinates x,y and temperature (T) are within real range.	S-FN	
	Mountain Scale Coupled Processes		Toptemp_v0.f	1	10224-1.0-00	DEC Alpha	OSF1 4.0	Y	YM	This software is used to generate top temperature boundary conditions. All valid "ELEME" range of TOUGH2 input, real range of elevation, and average temperature on the Yucca Mountain surface.	S-FN	
	Mountain Scale Coupled Processes		Hsource_v0.f	1	10225-1.0-00	DEC Alpha	OSF1 4.0	Y	YM	This software is used to generate thermal GENER terms for TOUGH2 input files.	S-FN	
	Mountain Scale Coupled Processes		2kgid8.for	1	10503-1.0-00	PC	MS-DOS V4.00.1111 under Windows 95	Y	YM	This software is used to generate dual permeability meshes for the TOUGH2 family of codes. This software is limited to eight-character element names for the TOUGH2 family of codes.	S-FN	
	Drift Seepage											177404 SNL (Sandia National Laboratories) 2007. Drift-Scale THC Seepage Model. MDL-NBS-HS-000001 REV 05. Las Vegas, Nevada: Sandia National Laboratories. ACC: DOC.20071010.0004

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	Drift Seepage		TOUGHREACT	3.1.1	10396-3.1.1-	Alpha System	OSF1 V5.1	Y	YM	Used to calculate coupled thermal-hydrologic and chemical processes for kinetic and/or equilibrium mineral–water reactions and equilibrium gas–water reactions.	S-FN	
	Drift Seepage		TOUGHREACT	3.1.1	10396-3.1.1-	Linux Custer	CAOS Linux	Y	YM	Used to calculate coupled thermal-hydrologic and chemical processes for kinetic and/or equilibrium mineral–water reactions and equilibrium gas–water reactions.	S-FN	
	Drift Seepage		SUPCRT92	1	10058-1.0-00	PC	PC Windows	Y	YM	Used to calculate the standard molal thermodynamic properties of minerals, gases, aqueous species, and reactions from 1 to 5,000 bars and 0°C to 1,000°C		
	Drift Seepage		AMESH	1	10045-1.0-00	Sun UltraSparc	SUNOS 5.5.1	Y	YM	D grids for numerical modeling of flow and transport problems in which the formulation is based on the integral finite difference method		
	Drift Seepage		KREG	1.1	10318-1.1-00	PC	DOS Emulation	Y	YM	Used to calculate regression coefficients of log(K) data as a function of temperature for the thermodynamic database of TOUGHREACT V3.1.1		
	Drift Seepage		KSWITCH	1.1	10319-1.1-00	PC	DOS Emulation	Y	YM	Used to switch component species in the thermodynamic database of TOUGHREACT V3.1.1 and above		
	Drift Seepage		THERMOCHK	1.1	10895-1.1-00	PC	DOS Emulation	Y	YM	Used to check the consistency (mass balance and charge balance) of reactions in the thermodynamic database of the reactive transport code TOUGHREACT V3.1.1 and above		
	Drift Seepage		DBCONV	1	10893-1.0-00	PC	DOS Emulation	Y	YM	Used to convert the YMP EQ3/6 thermodynamic database to a format suitable for input into the reactive transport model TOUGHREACT V3.1.1		
	Drift Seepage		CUTCHEM	2	10898-2.0-0.0	PC	DOS Emulation	Y	YM	Used to extract automatically data from large output data files created by the reactive transport model TOUGHREACT V3.1.1		
	Drift Seepage		exclude.f	1	10316-1.0-00	Sun UltraSparc	SUNOS 5.5.1	Y	YM	Used to exclude points outside a specified radius so that points will not overlap when output is merged using merggrid.f V1.0 for 2-D THC seepage model	S-FN	
	Drift Seepage		assign.f	1	10315-1.0-00	Sun UltraSparc	SUNOS 5.5.1	Y	YM	Used to assign a geologic name to all TOUGH2 elements according to their location in the Z-direction for 2-D THC seepage model	S-FN	
	Drift Seepage		merggrid2.f	1	10314-1.0-00	Sun UltraSparc	SUNOS 5.5.1	Y	YM	Used to merge input files into one file for input into AMESH V1.0 for 2-D THC seepage model	S-FN	
	Drift Seepage		mk_circ2	1	10312-1.0-00	Sun UltraSparc	SUNOS 5.5.1	Y	YM	Used to create a radial grid for 2-D THC seepage model		
	Drift Seepage		mk_rect2	1	10313-1.0-00	Sun UltraSparc	SUNOS 5.5.1	Y	YM	Used to create orthogonal grid for 2-D THC seepage model		

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	Drift Seepage		2kgridv1a.for	1	10382-1.0-00	PC	DOS Emulation	Y	YM	Generates dual-permeability grids for the TOUGH2 family of codes	S-FN	
	Drift Seepage		mk_grav2.f	1	10379-1.0-00	Sun UltraSparc	SUNOS 5.5.1	Y	YM	Reads AMESH V1.0 output files and creates TOUGH2 V1.4 mesh input file data, namely the gravity vector data and gridblock labeling data	S-FN	
	Drift Seepage		sav1d_dst2d.f	1	10381-1.0-00	Sun UltraSparc	SUNOS 5.5.1	Y	YM	Creates an INCON file for TOUGH2 input for a 2-D mesh from existing INCON and MESH data for a 1-D column	S-FN	
	Drift Seepage											181244 SNL (Sandia National Laboratories) 2007. Abstraction of Drift Seepage. MDL-NBS-HS-000019 REV 01 ADD 01. Las Vegas, Nevada: Sandia National Laboratories. ACC: DOC.20070807.0001
	Drift Seepage		Mathcad	11					COTS	for calculations	S-MC	
	Drift Seepage		Tecplot	9					COTS	for graphical display		
	Seepage w/ Collapse											167652 BSC (Bechtel SAIC Company) 2004. Seepage Model for PA Including Drift Collapse. MDL-NBS-HS-000002 REV 03. Las Vegas, Nevada: Bechtel SAIC Company. ACC: DOC.20040922.0008; DOC.20051205.0001
	Seepage w/ Collapse		iTOUGH2	5	10003-5.0-00	Sun UltraSparc	SunOS 5.5.1	Y	YM			
	Seepage w/ Collapse		GSLIB	V1.0SISIM	10397-1.0SISIMV1.20 4-00	Sun UltraSparc	SunOS 5.5.1	Y	COTS	Geostatistical software library		
	Seepage w/ Collapse		MoveMesh	1	10358-1.0-00	Sun UltraSparc	SunOS 5.5.1	Y	YM			
	Seepage w/ Collapse		AddBound	1	10357-1.0-00	Sun UltraSparc	SunOS 5.5.1	Y	YM			
	Seepage w/ Collapse		Perm2Mesh	1	10359-1.0-00	Sun UltraSparc	SunOS 5.5.1	Y	YM			
	Seepage w/ Collapse		CutDrift	1	10375-1.0-00	Sun UltraSparc	SunOS 5.5.1	Y	YM			
	Seepage w/ Collapse		TOUGH2	1.4	10007-1.4-01	Sun UltraSparc	SunOS 5.5.1	Y	YM		S-FN	
	Seepage w/ Collapse		TOUGH2	1.6	10007-1.6-01	PC	Windows 98	Y	YM		S-FN	
	Seepage w/ Collapse		EXT	1	10047-1.0-00	Sun UltraSparc	SunOS 5.5.1	Y	YM			
	Seepage w/ Collapse		CutNiche	1.3	10402-1.3-00	Sun UltraSparc	SunOS 5.5.1	Y	YM			
	Drift Wall Condensation											181648 SNL (Sandia National Laboratories) 2007. In-Drift Natural Convection and Condensation. MDL-EBS-MD-000001 REV 00 AD 01. Las Vegas, Nevada: Sandia National Laboratories. ACC: DOC.20050330.0001; DOC.20051122.0005; DOC.20070907.0004
	Drift Wall Condensation		FLUENT	6.0.12	10550-6.0.12-01	PC – Linux v 7.3		Y	COTS	Computational Fluid Dynamics (CFD) Calculations Convection Model	B-CT	
	Drift Wall Condensation		GAMBIT	2.0.4	N/A	PC	Windows 2000	N	COTS	Visual Display of Data and Mesh	B-CT	
	Drift Wall Condensation		Ensight	7.4	N/A	PC	Windows 2000	N	COTS	Visualization of CFD Results	B-CT	
	Drift Wall Condensation		MS Excel	2000 SP3	N/A	PC	Windows 2000	N	COTS	Graphical Representation and Arithmetic Manipulation	B-CT	
	Drift Wall Condensation		Mathcad Professional	11.2a	N/A	PC	Windows 2000	N	COTS	Graphical Representation and Arithmetic Manipulation	B-CT	
EBS Environment	Thermo-hydrologic											181383 SNL (Sandia National Laboratories) 2007. Multiscale Thermohydrologic Model. ANL-EBS-MD-000049 REV 03 ADD 01. Las Vegas, Nevada: Sandia National Laboratories. ACC: DOC.20070831.0003
	Thermo-hydrologic		NUFT	3.0s	10088-3.0s-02	Sun	OS 5.8	Y	YM			
	Thermo-hydrologic		NUFT	3.0.1s	10130-3.0.1s-01	Sun	OS 5.8	Y	YM			
	Thermo-hydrologic		RADPRO	4	10204-4.0-00	Sun	OS 5.8	Y	YM			
	Thermo-hydrologic		XTOOL	10.1	10208-10.1-00	Sun	OS 5.6.1	Y	YM			
	Thermo-hydrologic		MSTHAC	7	10419-7.0-00	Sun	OS 5.8	Y	YM			
	Thermo-hydrologic		readsUnits	1	10602-1.0-00	Sun	OS 5.5.1	Y	YM			
	Thermo-hydrologic		YMESH	1.54	10172-1.54-00	Sun	OS 5.8	Y	YM			
	Thermo-hydrologic		boundary_conditions	1	11042-1.0-00	Sun	OS 5.8	Y	YM			

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	Thermo-hydrologic		heatgen_ventTable_emplace	1	11039-1.0-00	Sun	OS 5.8	Y	YM			
	Thermo-hydrologic		rme6 v1.2	1.2	10617-1.2-00	Sun	OS 5.8	Y	YM			
	Thermo-hydrologic		xw	1	11035-1.0-00	Sun	OS 5.8	Y	YM			
	Thermo-hydrologic		colCen	1	11043-1.0-00	Sun	OS 5.8	Y	YM			
	Thermo-hydrologic		repository_percolation_calculator	1	11041-1.0-00	Sun	OS 5.8	Y	YM			
	Thermo-hydrologic		extractBlocks_EXT	1	11040-1.0-00	Sun	OS 5.8	Y	YM			
	Thermo-hydrologic		Chimney_interpolate		11038-1.0-00	Sun	OS 5.8	Y	YM			
	Thermo-hydrologic		reformat_EXT_to_TSPA	1	11061-1.0-00	Sun	OS 5.8	Y	YM			
	Thermo-hydrologic		MATLAB	6.1.0450				N	COTS		S-ML	
	Thermo-hydrologic		Mathcad	11.2a				N	COTS		S-MC	
	Chemical											177412 SNL (Sandia National Laboratories) 2007. Engineered Barrier System: Physical and Chemical Environment. ANL-EBS-MD-000033 REV 06. Las Vegas, Nevada: Sandia National Laboratories. ACC: DOC.20070907.0003.
	Chemical		EQ3/6	8	10813-8.0-00	PC	WIN2000	Y	NL/YM	Temperature, pressure, and composition range determined by the input thermodynamic database		
	Chemical		GetEQData	1.0.1	10809-1.0.1-00	PC	WIN2000	Y	NL/YM	Requires EQ3/6 V.8.0 or V.7.2b output files		
	Chemical		ppptrk	1	11030-1.0-00	PC	WIN2000	Y	YM	For use with particle tracking simulations only		
	Chemical		EARTHVISION	5	10393-5.0-00	SGI	IRIX 6.2	Y	COTS	Used to produce three-dimensional images and for data extraction. Operating system has been discontinued		
	In-Drift Precip.											177411 SNL (Sandia National Laboratories) 2007. In-Drift Precipitates/Salts Model. ANL-EBS-MD-000045 REV 03. Las Vegas, Nevada: Sandia National Laboratories. ACC: DOC.20070306.0037
	In-Drift Precip.		EQ3/6	8	10813-8.0-00	PC	WINDOWS 2000	Y	NL/YM			
	In-Drift Precip.		GetEQData	1.0.1	10809-1.0.1-00	PC	WINDOWS 2000	Y	ML/YM			
	In-Drift Precip.		SUPCRT92	1	10809-1.0.1-00	PC	WINDOWS NT	Y	YM			
WP and DS Degradation												
	WAPDEG											181953 SNL (Sandia National Laboratories) 2007. Stress Corrosion Cracking of Waste Package Outer Barrier and Drip Shield Materials. ANL-EBS-MD-000005 REV 04. Las Vegas, Nevada: Sandia National Laboratories. ACC: DOC.20070913.0001.
	WAPDEG		Mathcad	2001i		PC Windows		N	COTS	Not supported by PTC	S-MC	
	Localized Corrosion of Waste Package Outer Surface											178519 SNL (Sandia National Laboratories) 2007. General Corrosion and Localized Corrosion of Waste Package Outer Barrier. ANL-EBS-MD-000003 REV 03. Las Vegas, Nevada: Sandia National Laboratories. ACC: DOC.20070730.0003; DOC.20070807.0007
	Localized Corrosion of Waste Package Outer Surface		Mathcad	13		Windows		Y	COTS		S-MC	
	Localized Corrosion of Waste Package Outer Surface		S-PLUS 2000	Professional Release 2		Windows		N	COTS			
	General Localized Corrosion of Drip Shield											180778 SNL (Sandia National Laboratories) 2007. General Corrosion and Localized Corrosion of the Drip Shield. ANL-EBS-MD-000004 REV 02 ADD 01. Las Vegas, Nevada: Sandia National Laboratories. ACC: DOC.20060427.0002; DOC.20070807.0004; DOC.20071003.0019
	General Localized Corrosion of Drip Shield		Mathcad	2000i				N	COTS		S-MC	
	General Localized Corrosion of Drip Shield		Excel	97 SR-2				N	COTS			

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WF Degradation and Mobilization												
	Radionuclide Inventory		N/A									180472 SNL (Sandia National Laboratories) 2007. Initial Radionuclide Inventories. ANL-WIS-MD-000020 REV 01 ADD 01. Las Vegas, Nevada: Sandia National Laboratories. ACC: DOC.20050927.0005; DOC.20070801.0001 REV 01 Initial Radionuclide Inventories
	Radionuclide Inventory											177424 SNL (Sandia National Laboratories) 2007. Radionuclide Screening. ANLWIS-MD-000006 REV 02. Las Vegas, Nevada: Sandia National Laboratories. ACC: DOC.20070326.0003.
	Radionuclide Inventory		GoldSim	8.02.500	10344-8.02-05	Windows 2000		Y	COTS	To do radionuclide inventory decay calculations for selected times up to a million years	B-CT	
	Radionuclide Inventory		RadNuScreen	1	10732-1.0-00	Dell Optiplex GX 260 PC		Y				
	In-Package Chemistry											180506 SNL (Sandia National Laboratories) 2007. In-Package Chemistry Abstraction ANL-EBS-MD-000037 REV 04 ADD 01. Las Vegas, Nevada: Sandia National Laboratories. ACC: DOC.20070816.0004
	In-Package Chemistry		EQ3/6	7.2b	UCRL-MA-110662	Qualified on Windows 95 and HP-UX 10.20 B		Y	NL/YM			
	In-Package Chemistry		EQ6	7.2bLV	10075-7.2bLV-02	Qualified on Windows 2000 and NT 4.0		Y	NL/YM			
	In-Package Chemistry		GetEQData	1.0.1	10809-1.0.1-00	Qualified on Windows 2000, NT 4.0, 98, and 95		Y	NL/YM			
	In-Package Chemistry		transl	2	10251-2.0-00	Qualified on Windows 98		Y	YM			
	In-Package Chemistry		PHREEQ	2.3	10068-2.3-01			y	NL/YM	reaction path modeling, reactive transport, and surface-complexation		
	In-Package Chemistry		Mathcad	11				N	COTS	Older version n longer supported by PTC	B-CT	
	Cladding Degradation		N/A									180616 SNL (Sandia National Laboratories) 2007. Cladding Degradation Summary for LA. ANL-WIS-MD-000021 REV 03 ADD 01. Las Vegas, Nevada: Sandia National Laboratories. ACC: DOC.20050815.0002; DOC.20070614.0002
	Cladding Degradation		N/A									177422 SNL (Sandia National Laboratories) 2007. MOX Spent Nuclear Fuel and LaBS Glass for TSPA-LA. ANL-WIS-MD-000022 REV 01. Las Vegas, Nevada: Sandia National Laboratories. ACC: DOC.20070220.0007
	CSNF, DSNFD, HLW Degradation											
	Dust Deliquescence											181267 SNL (Sandia National Laboratories) 2007. Analysis of Dust Deliquescence for FEP Screening. ANL-EBS-MD-000074 REV 01 AD 01. Las Vegas, Nevada: Sandia National Laboratories. ACC: DOC.20070911.0004; DOC.20070824.0001
	Dust Deliquescence		EQ3/6	8	10813-8.0-00	Windows 2000 Professional			YM			
	Dust Deliquescence		GetEQData	1.0.1	10809-1.0.1-00	Windows 2000 Professional			YM			
	Dust Deliquescence		XTOOL	10.1	10208-10.1-00	SUN	O.S. 5.6.1		YM			
	Waste Form Degradation - Summary Abstraction											169987 BSC (Bechtel SAIC Company) 2004. CSNF Waste Form Degradation: Summary Abstraction. ANL-EBS-MD-000015 REV 02. Las Vegas, Nevada: Bechtel SAIC Company. ACC: DOC.20040908.0001; DOC.20050620.0004
	Waste Form Degradation - Summary Abstraction		Excel	2002		PC	Windows 2000 Professional					
	Waste Form Degradation - Summary Abstraction		SigmaPlot	8		PC	Windows 2002		COTS		B-CT	
	Waste Form Degradation - Summary Abstraction		Mathcad	2001i		SUN	O.S. 5.6.1		COTS		S-MC	
	DNSF Degradation Abstraction		N/A									172453 BSC (Bechtel SAIC Company) 2004. DSNF and Other Waste Form Degradation Abstraction. ANL-WIS-MD-000004 REV 04. Las Vegas, Nevada: Bechtel SAIC Company. ACC: DOC.20041201.0007
	HLW Glass Degradation											169988 BSC (Bechtel SAIC Company) 2004. Defense HLW Glass Degradation Model. ANL-EBS-MD-000016 REV 02. Las Vegas, Nevada: Bechtel SAIC Company. ACC: DOC.20041020.0015; DOC.20050922.00

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Topic	Sub-topic	Primary / Supporting	Software Name	Version	STN	Platform	OS	SCM?	Source	Comment	Problem / Mitigation Code(s)	Reference
	HLW Glass Degradation		Excel MAC 2001							Used to compile test data and perform simple arithmetic calculations, such as calculating the mean and standard deviation values that are used in this report		
	HLW Glass Degradation		Microsoft KaleidaGraph	3.0.5						Used to plot the data within this report		
	Dissolved Radionuclide Concentration Limits											177418 SNL (Sandia National Laboratories) 2007. *Dissolved Concentration Limits of Elements with Radioactive Isotopes.* ANL-WIS-MD-000010 REV 06. Las Vegas, Nevada: Sandia National Laboratory. ACC: DOC.20070918.0010.
	Dissolved Radionuclide Concentration Limits		EQ3/6	7.2b	UCRL-MA-110662 (LSCR198)				NL/YM	EQ3NR: a FORTRAN speciation-solubility code	S-FN	
	Dissolved Radionuclide Concentration Limits		EQ3/6	7.2b	(Qualified on Windows 95 and HP-UX 10.20 B)				NL/YM	EQPT: a data file preprocessor in FORTRAN	S-FN	
	Dissolved Radionuclide Concentration Limits		EQ6	7.2bLV	10075-7.2bLV-02 (Qualified on Windows 2000 and NT 4.0)				NL/YM	models water–rock interaction or fluid mixing in either a pure reaction progress mode or a time mode		
	Dissolved Radionuclide Concentration Limits		EQ3/6	8.1	10813-8.1-00 (Qualified on Windows 2000)				NL/YM	See above for Versions 7.2b and 7.2bLV		
	Dissolved Radionuclide Concentration Limits		GetEQData	1.0.1	10809-1.0.1-00 (Qualified on Windows 2000)					A Microsoft Excel macro. It is used to postprocess EQ3/6 output information.		
	Dissolved Radionuclide Concentration Limits		BUILDEQ3. BAS	1	10365-1.00-00 (DOS Emulation)					A QBASIC code used to generate EQ3NR input files		
	Dissolved Radionuclide Concentration Limits		PHREEQC	2.11	10068-2.11-00 (Qualified on Windows 2000)				NL/YM	A code for geochemical speciation, reaction path modeling, reactive transport, and surface-complexation modeling		
	Dissolved Radionuclide Concentration Limits		transl	2	10251-2.0-00 (Qualified on Windows 98)				NL/YM	A code for translating a non-Pitzer EQ3/6 database into PHREEQC format		
	WF and EBS Colloids		Excel 2003			PC/Windows						177423 SNL (Sandia National Laboratories) 2007. Waste Form and In-Drift Colloids-Associated Radionuclide Concentrations: Abstraction and Summary. MDL-EBS-PA-000004 REV 03. Las Vegas, Nevada: Sandia National Laboratories. ACC: DOC.20071018.0019
EBS Flow and Transport												
	EBS Flow									The EBS Flow Submodel implemented in the TSPA-LA Model is described in EBS Radionuclide Transport Abstraction (SNL 2007 [DIRS 177407]). Software list used in both EBS Flow and EBS Transport is shown below in Section 5.2		177407 SNL (Sandia National Laboratories) 2007. EBS Radionuclide Transport Abstraction. ANL-WIS-PA-000001 REV 03. Las Vegas, Nevada: Sandia National Laboratories. ACC: DOC.20071004.0001.
	EBS Transport											177407 SNL (Sandia National Laboratories) 2007. EBS Radionuclide Transport Abstraction. ANL-WIS-PA-000001 REV 03. Las Vegas, Nevada: Sandia National Laboratories. ACC: DOC.20071004.0001.
	EBS Transport		GoldSim	8.02.500	10344-8.02-05	run on Microsoft Windows 2000 on a Dell workstation with Intel Xeon processor		Y	COTS		B-CT	

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	EBS Transport		GoldSim	9.6	10344-9.60-01	run on Microsoft Windows 2000 on a Dell workstation with Intel Xeon processor		Y	COTS		B-CT	
	EBS Transport		PHREEQ	2.11	10068-2.11-00	run on Microsoft Windows 2000 on a Dell Precision 670 PC with an Intel Xeon processor		Y	NL/YM			
	EBS Transport		Grab-It!					N	COTS	Datatrend Software enables bitmap images of plots that have been captured from journal articles to be converted into (x, y) data in an Excel file for further processing		
	EBS Transport		S-Plus	6				N	COTS			
	EBS Transport		JMP	5.1				N	COTS		B-CT	
UZ Transport	UZ Transport											177396 SNL (Sandia National Laboratories) 2007. Radionuclide Transport Models Under Ambient Conditions. MDL-NBS-HS-000008 REV 02 ADD 01. Las Vegas, Nevada: Sandia National Laboratories. ACC: DOC.20050823.0003; DOC.20070718.0003.
	UZ Transport		iTOUGH2	4	10003-4.0-00	Dec Alpha	OSF1 V4.0	Y	NL		S-FN	
	UZ Transport		TOUGH2	1.11MEOS9	10065-1.11 MEOS9nT	Dec Alpha	OSF1 V4.0	Y	NL		S-FN	
	UZ Transport		TOUGH2	1.4	10007-1.4-01	Dec Alpha	OSF1 V4.0	Y	NL		S-FN	
	UZ Transport		TOUGH2	1.6	10007-1.6-01	Dec Alpha	OSF1 V5.1	Y	NL		S-FN	
	UZ Transport		TOUGH2	1.6	10007-1.6-00	Dec Alpha	OSF1 V4.0	Y	NL		S-FN	
	UZ Transport		T2R3D	1.4	10006-1.4-00	Dec Alpha	OSF1 V4.0	Y	NL		S-FN	
	UZ Transport		DCPT	2	10078-2.0-00	PC	Windows NT V4.0	Y	NL		S-FN	
	UZ Transport		PHREEQ	2.3	10068-2.11-00	PC	Windows 98	?	NL/YM		S-FN	
	UZ Transport		Bkread.f	1	10894-1.0-00	Sun Sparc	SunOS 5.5.1	Y	NL		S-FN	
	UZ Transport		XtractG.f90	1	10930-1.0-00	Dec Alpha	OSF1 V5.1	Y	NL		S-FN	
	UZ Transport		Smesh.f	1	10896-1.0-00	Sun Sparc	SunOS 5.5.1	Y	NL		S-FN	
	UZ Transport											184748 SNL (Sandia National Laboratories) 2008. Particle Tracking Model and Abstraction of Transport Processes. MDL-NBS-HS-000020 REV 02 AD 02. Las Vegas, Nevada: Sandia National Laboratories
	UZ Transport		FEHM	2.2	10086-2.20-00	PC-Windows 2000 and SUN	OS 5.7 and 5.8	Y	NL	Used in extracting repository coordinate locations for nodes for use in the GoldSim system model.	S-FN	
	UZ Transport		FEHM	2.21	10086-2.21-00	PCWindows 2000, and SUN	OS 5.8	Y	NL	Generation of transfer function curve information using a discrete fracture model. Simulation of particle tracking validation runs. Abstraction model simulations.	S-FN	
	UZ Transport		FEHM	2.23	10086-2.23-01	SUN	OS 5.9	Y	NL/YM	Simulation of particle tracking base case runs. Abstraction model simulations.	S-FN	
	UZ Transport		GoldSim	7.50.100	10344-7.50.100-00	PC	Windows 2000	Y	COTS	Abstraction model simulations.	B-CT	
	UZ Transport		ppptrk	1	11030-1.0-00	SUN	OS 5.8 and 5.9	Y	YM	Post-processing of particle breakthrough curve information.		
	UZ Transport		discrete_tf	1.1	11033-1.1-00	PC	Windows 2000	Y	YM	Post-processing of discrete fracture model results to convert results to transfer functions.	S-FN	

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Topic	Sub-topic	Primary / Supporting	Software Name	Version	STN	Platform	OS	SCM?	Source	Comment	Problem / Mitigation Code(s)	Reference
	UZ Transport		fehm2post	1	11031-1.0-00	PC-Windows 2000 and SUN	OS 5.8 and 5.9	Y	YM	Executes multiple FEHM simulations along with pre- and post-processing runs. Used to execute the individual simulations and generation of transfer function curves used in the TSPA-LA UZ transport abstraction model.	S-FN	
	UZ Transport		Fortner Plot		N/A	SUN Workstation		N	COTS	Plot, was used for plotting the results of breakthrough curve simulations. Only built-in standard functions in this software were used. No software routines or macros were used with this software to prepare this report. The output was visually checked for correctness.	B-CT	
	UZ Transport		Techplot	10	N/A	IBM PC	Window 2000 Operating System	N	COTS	The commercial software, Techplot 10, was used for plotting the results of breakthrough curve simulations. Only built-in standard functions in this software were used. No software routines or macros were used with this software to prepare this report. The output was visually checked for correctness.	B-CT	
SZ Flow and Transport												
	SZ Flow and Transport											183750 SNL (Sandia National Laboratories) 2008. Saturated Zone Flow and Transport Model Abstraction. MDL-NBS-HS-000021 REV 03 AD 02. Las Vegas, Nevada: Sandia National Laboratories. ACC: DOC.20080107.0006
	SZ Flow and Transport		FEHM	2.2	10086-2.20-00	Sun UltraSPARC	SunOS 5.7	Y	NL/YM	and mass-transport code that simulates nonisothermal, multiphase, multicomponent flow, and solute transport in porous media.	S-FN	
	SZ Flow and Transport		GoldSim	7.50.100	10344-7.50.100-00	Dell OptiPlex GX260	Window 2000 Professional 5.0.2195	Y	COTS	This code is the modeling software used in the TSPA-LA. Probabilistic simulations are represented graphically in GoldSim.	B-CT	
	SZ Flow and Transport		GoldSim	8.01 SP4	10344-8.01SP 4-00	Computer: Master 06 Windows 2000 Advanced Server		Y	COTS	GoldSim (GS) is a Windows-2000–based program that provides the following general capabilities: • Quantitatively address the inherent variability. • Superimposes the occurrence and consequences of discrete events onto continuously varying systems. • Builds top-down models, dynamically links external programs or spreadsheets directly to the GS model. • Directly exchanges data between any ODBC-compliant database to the GS model.	B-CT	
	SZ Flow and Transport		CORPSCON	5.11.08	10547-5.11.08-00	IBM Thinkpad 770Z-	WINDOWS NT 4.0 SNL	Y	USACE	US Army Corps of Engineers. This software is used to convert coordinate data to the Universal Transverse Mercator (UTM) coordinate system		

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Topic	Sub-topic	Primary / Supporting	Software Name	Version	STN	Platform	OS	SCM?	Source	Comment	Problem / Mitigation Code(s)	Reference
	SZ Flow and Transport		SZ_Pre	2	10914-2.0-00	Sun UltraSPARC	SunOS 5.7	Y	NL/YM	This software is an automated method for preparing the FEHM input files for the SZ site-scale flow and transport model a for use in TSPA-LA analyses.		
	SZ Flow and Transport		SZ_Post	3	10915-3.0-00	Sun UltraSPARC	SunOS 5.7, Solaris 2.7	Y	NL/YM	scale model b into the format used by the SZ_Convolute software code. SZ_Post reads the output files from the FEHM software code and writes the breakthrough curve data for radionuclide transport in the SZ.		
	SZ Flow and Transport		SZ_Convolute	2.2	10207-2.2-00	Dell OptiPlex GX260	Windows 2000 Professional 5.0.2195	Y	NL/YM	This software is used to calculate SZ response curves based on unsaturated zone (UZ) radionuclide source terms, generic SZ responses, and climate scenarios for the YMP.		
	SZ Flow and Transport											177391 SNL (Sandia National Laboratories) 2007. Saturated Zone Site-Scale Flow Model. MDL-NBS-HS-000011 REV 03. Las Vegas, Nevada: Sandia National Laboratories. ACC: DOC.20070626.0004; DOC.20071001.0013
	SZ Flow and Transport		CORPSCON	5.11.08	10547-5.11.08-00		WINDOWS NT 4.0	Y	USACE	US Army Corps of Engineers. This software is used to convert coordinate data to the Universal Transverse Mercator (UTM) coordinate system	S-GT	
	SZ Flow and Transport		FEHM	2.24	10086-2.24-02	PC or Sun Ultra Sparc	Sun Solaris 5.7 or 5.8 operating system	Y	NL/YM	Solution to SZ flow	S-FN	
	SZ Flow and Transport		LaGriT	1.1	10212-1.0-00	Sun Ultra Sparc	Sun OS 2.7 operating system at LANL	Y	NL/YM	Software package for grid generation, analysis, and visualization		
	SZ Flow and Transport		PEST	5.5	10289-5.5-00	Sun Ultra Sparc	Sun Solaris 5.7 or 5.8 operating system at LANL	Y		Preconditioning and parameter optimization for FEHM runs		
	SZ Flow and Transport		EARTHVISION	5.1	10174-5.1-00	Silicon Graphics Octane workstation	IRX 6.5.	Y	COTS	Commercial software for 3D model building and visualization used in contouring, plotting, and visualization of the data and for evaluation of results.	B-CT	
	SZ Flow and Transport		Extract	1	10955-1.0-00	Pre/postprocessor used to extract lateral flow data from the USGS regional flow model		Y	YM	Pre/postprocessor used to extract lateral flow data from the USGS regional flow model		
	SZ Flow and Transport		Extract	1.1	10955-1.1-00	Pre/postprocessor used to extract lateral flow data from the USGS regional flow model		Y	YM	Pre/postprocessor used to extract lateral flow data from the USGS 2001 regional flow model		
	SZ Flow and Transport		EXT_RECH	1	10958-1.0-00	Pre/postprocessor used to extract lateral flow data from the USGS regional flow model		Y	YM	Pre/postprocessor used to extract recharge data from the USGS regional flow model		

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Topic	Sub-topic	Primary / Supporting	Software Name	Version	STN	Platform	OS	SCM?	Source	Comment	Problem / Mitigation Code(s)	Reference
	SZ Flow and Transport		Mult_Rech	1.0 b	10959-1.0-00	Pre/postprocessor used to extract lateral flow data from the USGS regional flow model		Y	YM	Pre/postprocessor that scales recharge data from the USGS regional flow model and maps the data to a new grid		
	SZ Flow and Transport		Xread_Distr_Rech	1.0 b	10960-1.0-00	Pre/postprocessor used to extract lateral flow data from the USGS regional flow model		Y	YM	Pre/postprocessor used to extract recharge data from the USGS 1999 regional flow model		
	SZ Flow and Transport		Xread_Distr_Rech_UZ	1.0b	10961-1.0-00	Pre/postprocessor used to extract lateral flow data from the USGS regional flow model		Y	YM	Pre/postprocessor that maps recharge data onto a new grid excluding the UZ flow model region		
	SZ Flow and Transport		Xread_Reaches	1.0b	10962-1.0-00	Pre/postprocessor used to extract lateral flow data from the USGS regional flow model		Y	YM	Pre/postprocessor that maps local recharge from four stream channels onto a new grid		
	SZ Flow and Transport		Xwrite_Flow_New	1.0-125b	10963-1.0-125-00	map the combined UZ and SZ site-scale fluxes onto a 125-m grid and to create a flux file that is compatible with FEHM flow		Y	YM	Used both to map the combined UZ and SZ site-scale fluxes onto a 125-m grid and to create a flux file that is compatible with FEHM flow macros		
	SZ Flow and Transport		Zones	1.0 b	10957-1.0-00	Used to extract zonal designation data from the USGS 2001 regional flow model		Y	YM	Used to extract zonal designation data from the USGS 2001 regional flow model		
	SZ Flow and Transport											177392 SNL (Sandia National Laboratories) 2007. Site-Scale Saturated Zone Transport. MDL-NBS-HS-000010 REV 03. Las Vegas, Nevada: Sandia NationalLaboratories. ACC: DOC.20070822.0003, DOC.20080117.0002
	SZ Flow and Transport		FEHM	2.24-01-00	10086-2.24-01	Sun, PC	Sun OS 5.9, Microsoft Windows 2000, 2003	Y	NL/YM	Used for calculations throughout this model report. The FEHM V 2.24-01 application is based on a finite-volume/ finite-element heat- and mass-transfer code that simulates nonisothermal, multiphase, multicomponent flow and solute transport in porous media		
	SZ Flow and Transport		FEHM	2.2	10086-2.20-00	Sun, PC	Sun OS 5.7 & 5.8, Windows 2000,	Y	NL/YM	Used for calculations in Appendix C of this model report. The FEHM V 2.20 application is based on a finite-volume/ finite-element heat- and mass-transfer code that simulates nonisothermal, multiphase, multicomponent flow and solute transport in porous media.		

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	SZ Flow and Transport		cr8sptr.c	2	10927-2.0-00	Sun	Sun OS 5.7, Location: LANL	Y	NL/YM	Used to create an input file for sptr macro in FEHM.	S-CP	
	SZ Flow and Transport		calc_cdf.c	1	10924-1.0-00	Sun	Sun OS 5.7, Location: LANL	Y	NL/YM	Used to calculate the cumulative distribution function of the stochastic distributions of Kd	S-CP	
	SZ Flow and Transport		GS2FEHM.C	1	10923-1.0-00	Sun	Sun OS 5.7, Location: LANL	Y	NL/YM	Used to create an input file for the perm macro in FEHM	S-CP	
	SZ Flow and Transport		GSLIB	1.0GAMV3	10398-1.0GAM V3V1.2	Sun	Sun OS 5.5.1,	Y		dimensional variogram of input data.		
	SZ Flow and Transport		GSLIB	2.0MSISIM	10098-2.0MSI SIMV2.0	Sun	UNIX	Y		Used to generate a stochastic distribution of parameters, such as Kd and permeability		
	SZ Flow and Transport		PHREEQC	2.3	10068-2.3-01	PC	Windows 2000 Location: LANL	Y	NL/YM	Calculates surface complexation reactions for radionuclides.		
	SZ Flow and Transport		RELAP	2	10551-2.0-00	PC	Windows 2000 Location: LANL	Y	NL/YM	Generate BTCs	S-FN, S-GT	
	SZ Flow and Transport		FRACT_p	1	11009-1.0-00	PC	LINUX 2.4.18, Location: LANL	Y	YM	Calculates data that correlate concentrations with time for transport in the fractured media		
	SZ Flow and Transport		fehm2post	1	11031-1.0-00		WINDOWS 2000, SUN O.S 5.8&5.7, Redhat Linux 2.4.18	Y	NL/YM	Software is a set of perl scripts used to automate the repetitive series of steps required to make multiple runs of FEHM and post-process the output data		
	SZ Flow and Transport		fehm2post	1	11031-1.0-01		SUN O.S 5.9	Y	NL/YM	Software is a set of perl scripts used to automate the repetitive series of steps required to make multiple runs of FEHM and post-process the output data		
	SZ Flow and Transport		EARTHVISION	5.1	10174-5.1-00	Silicon Graphics Octane workstation	IRIX 6.5.			This software was used for plotting and visualization of data		
	SZ Flow and Transport		Tecplot	360		PC	Microsoft Windows 2000 NT, Sun with UNIX OS, FORTRAN	N	COTS	of analysis results in figures shown in this report. No data analysis was done with this software. Only built-in standard functions in this software were used. No software routines or macros were used with this software to prepare this report. The output was visually checked for correctness	B-CT	
	SZ Flow and Transport		BestFit	V4.5		PC	Microsoft Windows 2000 NT		COTS	distribution that best fits given data. Output of this program was used only as a guide for the selection of the distribution functions. Only built-in standard functions in this software were used. No software routines or macros were used with this software to prepare this report. The output was visually checked for correctness. V. 4.5 (a subset of @RISK V 4.5 STN 600806-4.5-00), Serial # 11874954, March 2000, Palisade Corporation, 798 Cascadilla Street, Ithaca, NY 14850	B-CT	
	Saturated Zone In-Situ Testing											177394 SNL (Sandia National Laboratories) 2007. Saturated Zone In-Situ Testing. ANL-NBS-HS-000039 REV 02. Las Vegas, Nevada: Sandia National Laboratories. ACC: DOC.20070608.0004.

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	Saturated Zone In-Situ Testing		2WELLS_2D	1	10665-1.0-00	LANL, PC	Windows 2000 NT 4.0*/98	Y	NL/YM	This software is used in the analysis of longitudinal dispersivity in the Prow Pass Tuff C-wells field tracer test. It is used to obtain predicted tracer responses in homogeneous, isotropic, confined (two-dimensional) aquifers under partial recirculation conditions. It has been used both to correct dispersion-coefficient estimates for dispersion caused by a dipole-flow pattern and for pretest predictions of ATC cross-hole tracer tests.		
	Saturated Zone In-Situ Testing		2WELLS_3D	1	10667-1.0-00	LANL, PC	Windows 2000 NT 4.0*/99	Y	NL/YM	This software is used to obtain predicted tracer responses in homogeneous, isotropic, confined three-dimensional aquifers under partial recirculation conditions. It has been used both to correct dispersion-coefficient estimates for dispersion caused by a dipole-flow pattern and for pretest predictions of ATC cross-hole tracer tests.		
	Saturated Zone In-Situ Testing		DIFFCELL	2	10557-2.0-00	LANL, PC	Windows 2000 NT 4.0*/100	Y	NL/YM	This software is used in the analysis of laboratory diffusion cell experiments. It provides a numerical solution to an equation describing one- dimensional diffusive transport through a rock wafer with time-dependent concentration boundary conditions.		
	Saturated Zone In-Situ Testing		EQUILFIT	1	10668-1.0-00	LANL, PC	Windows 2000 NT 4.0*/101	Y	NL/YM	This software is used to obtain cation-exchange coefficients, given experimental data on cation sorption (both for sorbing and displaced cations) and given independent cation-exchange-capacity measurements.		
	Saturated Zone In-Situ Testing		Filter.vi	1	10970-1-00	USGS, PC	Windows 2000 NT 4.0*/98	Y	USGS	This software uses the standard Butterworth filter with standard coefficients. It is for filtering higher- frequency diurnal pressure changes due to barometric pressure changes and tidal effects.		
	Saturated Zone In-Situ Testing		Injection_Pumpback.vi	1	10675-1-00	USGS, PC	Windows 2000 NT 4.0*/99	Y	USGS	This software is used for tracer test analysis for single-well testing. Analysis considers tracer injection, drift, and pumpback.		
	Saturated Zone In-Situ Testing		rcv2amos.exe and MOENCH.vi, Function(1)	1	10583-1.0-00	USGS, PC	Windows 2000 NT 4.0*/100	Y	USGS	The software routine rcv2amos.exe is used to analyze cross-hole tracer tests. In conjunction with the use of rcv2amos.exe, the routine MOENCH.vi was developed to serve as a user interface and to display the results.		
	Saturated Zone In-Situ Testing		MOENCH.vi Function(2)	1	10582-1.0-00	USGS, PC	Windows 2000 NT 4.0*/101	Y	USGS	This software is used for the analysis of cross-hole tracer tests.		

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Topic	Sub-topic	Primary / Supporting	Software Name	Version	STN	Platform	OS	SCM?	Source	Comment	Problem / Mitigation Code(s)	Reference
	Saturated Zone In-Situ Testing		MULTRAN	1	10666-1.0-00	LANL, PC	Windows 2000 NT 4.0*/98	Y	NL/YM	numerical model that uses an implicit-in-time, alternating-direction, finite-difference method to solve the equations describing multicomponent transport of sorbing and nonsorbing solutes in a dual-porosity medium. This software is used for analysis of laboratory crushed-rock and alluvium column experiments. It is also used for the analysis of the first peak in the Bullfrog Tuff C-wells field tracer test and for prediction and analysis of ATC tracer experiments.		
	Saturated Zone In-Situ Testing		Neuman.vi	1	10972-1.0-00	USGS, PC	Windows 2000 NT 4.0*/101	Y	USGS	This software displays the standard and accepted type curve for unconfined aquifers and allows the fitting of the input data curves over the type curve. The .vi extension displays the appropriate resulting hydrologic parameters associated with the data curve matching (transmissivity and storativity).		
	Saturated Zone In-Situ Testing		PEST	5.5	10289-5.5-00	USGS, PC	Windows 2000*	Y		interpretation, model calibration, and predictive analysis. PEST adjusts model parameters and/or excitations until the fit between model output and field or laboratory observations is optimized in the weighted least-squares sense.		
	Saturated Zone In-Situ Testing		RECIRC.vi	1	10673-1.0-00	USGS, PC	Windows 98 NT 4.0*/2000	Y	USGS	recirculating and partial-recirculation cross-hole tracer test analysis.		
	Saturated Zone In-Situ Testing		RELAP	2	10551-2.0-00	LANL, PC	Windows 2000 NT*	Y	YM	This software models tracer transport by convoluting a Laplace-domain transfer function for transport through dual-porosity media with transfer functions that describe tracer injection, mixing in the injection and production wellbores (or flow manifolds in laboratory experiments), and recirculation of the product fluid (in field experiments only). It also performs curve fits to field or laboratory tracer test data to obtain the best-fitting transport parameter values.		
	Saturated Zone In-Situ Testing		RETRAN	2	10552-2.0-00	LANL, PC	Windows 2000 NT 4.0*	Y	YM	This software models reactive transport in dual- porosity media with a general, nonlinear sorption isotherm and with time-varying flow rates.		

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Topic	Sub-topic	Primary / Supporting	Software Name	Version	STN	Platform	OS	SCM?	Source	Comment	Problem / Mitigation Code(s)	Reference
	Saturated Zone In-Situ Testing		Streltsova- Adams.vi	1	10971-1-00	USGS, PC	Windows 2000 NT 4.0®/98	Y	USGS	This software displays the standard and accepted Streltsova-Adams type curve for fractured aquifers and allows the fitting of the input data curves over this type curve. The .vi extension displays the appropriate resulting hydrologic parameters associated with the data curve matching (transmissivity and storativity).		
	Saturated Zone In-Situ Testing		Theis.vi	1	10974-1.0-00	USGS, PC	Windows 2000 NT 4.0®/99	Y	USGS	This software displays the standard and accepted Theis type curve and allows the fitting of the input data curves over this type curve. The .vi extension displays the appropriate resulting hydrologic parameters associated with the data curve matching (transmissivity and storativity).		
	Saturated Zone Colloid Transport											170006 BSC (Bechtel SAIC Company) 2004. Saturated Zone Colloid Transport. ANL-NBS-HS-000031 REV 02. Las Vegas, Nevada: Bechtel SAIC Company. ACC: DOC.20041008.0007; DOC.20051215.0005; LLR.20080527.0086; DOC.20090520.0003
			RELAP	2	10551-2.0-00	PC, Windows 200	NT			This software models tracer transport by convoluting a Laplace-domain transfer function for transport through dual-porosity media with transfer functions that describe tracer injection, mixing in the injection and production wellbores (or flow manifolds in laboratory experiments), and recirculation of the product fluid (in field experiments only). It also performs curve fits to field or laboratory tracer test data to obtain the best-fitting transport parameter values.		
			Excel	2000		PC, Windows 200	NT			analysis of data and plotting of graphs.		
Biosphere	Biosphere Model											177399 SNL (Sandia National Laboratories) 2007. Biosphere Model Report. MDL-MGR-MD-000001 REV 02. Las Vegas, Nevada: Sandia National Laboratories. ACC: DOC.20070830.0007
	Biosphere Model		GoldSim	8.02.500	10344-8.02-05	PC	Windows 2000	Y	COTS	This version of GoldSim was used to execute the biosphere model to produce the BDCFs		
	Biosphere Model		GoldSim	9.6	10344-9.60-00	PC	Windows XP	Y	COTS	Used in conjunction with ASHPLUME_DLL_LA V.2.1, this software was used for probabilistic simulations (Appendix G)		
	Biosphere Model		ASHPLUME_DLL_LA	2.1	11117-2.1-00	PC	Windows XP	Y	YM	This software was used for calculation of initial ash/fuel areal concentrations at the location of the RMEI (Appendix G)		
	Receptor Characteristics		Excel	Version 97 SR-2 and Version 2000 SR-1					COTS		B-CT	172827 BSC (Bechtel SAIC Company) 2005. Characteristics of the Receptor for the Biosphere Model. ANL-MGR-MD-000005 REV 04. Las Vegas, Nevada: Bechtel SAIC Company. ACC: DOC.20050405.0005
Events											B-CT	

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Topic	Sub-topic	Primary / Supporting	Software Name	Version	STN	Platform	OS	SCM?	Source	Comment	Problem / Mitigation Code(s)	Reference
	Waste Package Early Failure										B-CT	178765 SNL (Sandia National Laboratories) 2007. Analysis of Mechanisms for Early Waste Package/Drip Shield Failure. ANL-EBS-MD-000076 REV 00. Las Vegas, Nevada: Sandia National Laboratories. ACC: DOC.20070629.0002; DOC.20071003.0015
	Waste Package Early Failure		SAPHIRE	7.26	10325-7.26-00		Windows 2000	Y	COTS		B-CT	
	Waste Package Early Failure		Mathcad	13			Windows XP	Y	COTS		B-CT	
											B-CT	178765 SNL (Sandia National Laboratories) 2007. Analysis of Mechanisms for Early Waste Package/Drip Shield Failure. ANL-EBS-MD-000076 REV 00. Las Vegas, Nevada: Sandia National Laboratories. ACC: DOC.20070629.0002; DOC.20071003.0015
	Waste Package Early Failure		SAPHIRE	7.26	10325-7.26-00		Windows 2000	Y	COTS		B-CT	
	Waste Package Early Failure		Mathcad	13			Windows XP	Y	COTS		B-CT	
	Igneous Intrusion											169989 BSC (Bechtel SAIC Company) 2004. Characterize Framework for Igneous Activity at Yucca Mountain, Nevada. ANL-MGR-GS-000001 REV 02. Las Vegas, Nevada: Bechtel SAIC Company. ACC: DOC.20041015.0002; DOC.20050718.0007
	Igneous Intrusion		FITCD	1	10262-1.0-00	PC	Pentium 486 FORTR	Y	YM	Computes discrete cumulative probability distributions for dike length from cumulative probabilities specified at selected values of length.		
	Igneous Intrusion		SFCD	1	10275-1.0-00	PC	Pentium 486 FORTR	Y	YM	Computes discrete cumulative probability distributions for dike length using user• specified distribution forms.		
	Igneous Intrusion		DCPELD	1	10258-1.0-00	PC	Pentium 486 FORTR	Y	YM	Computes discrete probability distribution for dike length from expert-specified distributions (output of FITCD).		
	Igneous Intrusion		CPDI	1	10257-1.0-00	PC	Pentium 486 FORTR	Y	YM	Computes conditional probability of intersection from volcanic events on an x,y grid using output of DCPELD and expert-specified azimuth distributions.		
	Igneous Intrusion		UZVH	1	10277-1.0-00	PC	Pentium 486 FORTR	Y	YM	Computes frequency of intersection from volcanic source zones using output of CPDI.		
	Igneous Intrusion		UZVHLH	1	10278-1.0-00	PC	Pentium 486 FORTR	Y	YM	Computes simulations of contributions to frequency of intersection on an x,y grid from volcanic source zones using Latin Hypercube sampling and output from CPDI.		
	Igneous Intrusion		FKVH	1	10265-1.0-00	PC	Pentium 486 FORTR	Y	YM	intersection using kernel density estimation with specified hand output of CPDI.		
	Igneous Intrusion		FKVHLH	1	10266-1.0-00	PC	Pentium 486 FORTR	Y	YM	Computes simulations of contributions to frequency of intersection on an x,y grid using kernel density estimation with specified h, Latin Hypercube sampling, and output from CPDI.		
	Igneous Intrusion		UZVPVH	1	10279-1.0-00	PC	Pentium 486 FORTR	Y	YM	intersection from volcanic source zones using volume predictable volcanic event rate model and output of CPDI.		

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	Igneous Intrusion		UZVPVHLH	1	10280-1.0-00	PC	Pentium 486 FORTR	Y	YM	Computes simulations of contributions to frequency of intersection on an x,y grid from volcanic source zones using volume predictable volcanic event rate model, Latin Hypercube sampling, and output from CPDI.		
	Igneous Intrusion		FKVPVH	1	10267-1.0-00	PC	Pentium 486 FORTR	Y	YM	intersection using kernel density estimation using volume predictable volcanic event rate model and output of CPDI.		
	Igneous Intrusion		FKVPVHLH	1	10268-1.0-00	PC	Pentium 486 FORTR	Y	YM	Computes simulations of contributions to frequency of intersection on an x,y grid with kernel density estimation using volume predictable volcanic event rate model, Latin Hypercube sampling, and output from CPDI.		
	Igneous Intrusion		ZBCKVH	1	10283-1.0-00	PC	Pentium 486 FORTR	Y	YM	intersection using kernel density estimation with h constrained by a source zone boundary and output of CPDI.		
	Igneous Intrusion		ZBCKVHLH	1	10284-1.0-00	PC	Pentium 486 FORTR	Y	YM	Computes simulations of contributions to frequency of intersection on an x,y grid using kernel density estimation with h constrained by a source zone boundary, Latin Hypercube sampling, and output from CPDI.		
	Igneous Intrusion		FITFIELD	1	10263-1.0-00	PC	Pentium 486 FORTR	Y	YM	Computes parameters of a bivariate Gaussian distribution that approximates boundaries of a defined polygon.		
	Igneous Intrusion		FIT2CNTR	1	10261-1.0-00	PC	Pentium 486 FORTR	Y	YM	Computes parameters of a bivariate Gaussian distribution from locations of volcanic events.		
	Igneous Intrusion		PFGVH	1	10273-1.0-00	PC	Pentium 486 FORTR	Y	YM	intersection using a bivariate Gaussian distribution with specified field parameters and output of CPDI. Bivariate Gaussian distribution parameters obtained from programs FIT2CNTR or FITFIELD.		
	Igneous Intrusion		PFGVHLH	1	10274-1.0-00			Y	YM	contributions to frequency of intersection on an x,y grid using a 2D-Gaussian distribution with specified parameters, Latin Hypercube sampling, and output from CPDI. Gaussian distribution parameters obtained from programs FIT2CNTR or FITFIELD.		
	Igneous Intrusion		FPFGVH	1	10269-1.0-00	PC	Pentium 486 FORTR	Y	YM	Computes frequency of intersection using a bivariate Gaussian distribution with parameters fit to volcanic event locations and output of CPDI.		

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	Igneous Intrusion		FPFGVHLH	1	10270-1.0-00	PC	Pentium 486 FORTR	Y	YM	Computes simulations of contributions to frequency of intersection on an x,y grid using a 2D-Gaussian distribution with parameters fit to volcanic event locations, Latin Hypercube sampling, and output from CPDI.		
	Igneous Intrusion		VHTREE	1	10282-1.0-00	PC	Pentium 486 FORTR	Y	YM	Computes mean and fractiles of frequency of intersection over an individual expert's volcanic hazard logic tree and aggregate over all experts using outputs of UZVH, UZVHB, FKVH, UZVPVH, FKVPVH, ZBCLVH, PFGVH, and FPFGVH.		
	Igneous Intrusion		VHTIELHS	1	10281-1.0-00	PC	Pentium 486 FORTR	Y	YM	Computes mean and fractiles of simulations of contributions to frequency of intersection on an x,y grid over an individual expert's volcanic hazard logic tree using Latin Hypercube sampling and output from UZVHLH, FKVHLH, UZVPVHLH, FKVPVHLH, ZBCLVHLH, PFGVHLH, and FPFGVHLH.		
	Igneous Intrusion		NECPDS	1.1	10272-1.1-00	PC	Pentium 486 FORTR	Y	YM	Computes distributions for number of eruptive centers per volcanic event and average spacing between eruptive centers.		
	Igneous Intrusion		FITIDSR	1	10264-1.0-00	PC	Pentium 486 FORTR	Y	YM	Computes discrete incremental probability distributions for dike length using input to FITCD.		
	Igneous Intrusion		SFIDSR	1	10276-1.0-00	PC	Pentium 486 FORTR	Y	YM	Computes discrete incremental probability distributions for dike length using input to SFCD.		
	Igneous Intrusion		DLECD	1	10260-1.0-00	PC	Pentium 486 FORTR	Y	YM	Computes joint discrete probability distributions for dike length and number of eruptive centers per volcanic event using output from FITIDSR.		
	Igneous Intrusion		DILECDLH	1	10259-1.1-00	PC	Pentium 486 FORTR	Y	YM	Computes joint conditional distribution of dike intersection length, dike azimuth, and number of eruptive centers within the repository footprint from outputs of program VHTIELHS using Latin hypercube sampling of dike length and volcanic event location distributions from DIECDIST.		
	Igneous Intrusion		CFRAC	1	10254-1.0-00	PC	Pentium 486 FORTR	Y	YM	Locates individual expert's simulation results that represent specified percentiles of the composite distribution for frequency of intersection from outputs of VHTIELHS.		

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	Igneous Intrusion		COMBSM	1.1	10256-1.1-00	PC	Pentium 486 FORTR	Y	YM	Computes composite joint distribution of dike intersection length, dike azimuth, and number of eruptive centers within the repository footprint across experts from outputs of DILECDLH and VHTIELHS for mean hazard.		
	Igneous Intrusion		COMBSM	1.1	10255-1.1-00	PC	Pentium 486 FORTR	Y	YM	Computes composite joint distribution of dike intersection length, dike azimuth, and number of eruptive centers within the repository footprint across experts from outputs of DILECDLH for selected percentiles of the hazard.		
	Igneous Intrusion		MARGIN	1.1	10271-1.1-00	PC	Pentium 486 FORTR	Y	YM	Computes marginal distributions for dike intersection length, dike azimuth, and number of eruptive centers within the repository footprint from output of COMBSM and COMBSF.		
	Volcanic Eruption											177431 SNL (Sandia National Laboratories) 2007. Atmospheric Dispersal and Deposition of Tephra from a Potential Volcanic Eruption at Yucca Mountain, Nevada. MDL-MGR-GS-000002 REV 03. Las Vegas, Nevada: Sandia National Laboratories. ACC: DOC.20071010.0003
	Volcanic Eruption		ArcGIS	9.1	11205-9.1-00	PC	Windows XP	N	COTS	Qualified geographical data visualization and basic spatial analysis; used for visualization of ASHPLUME and ASHFALL model output in the code comparison model validation activity (Section 7.5)		
	Volcanic Eruption		ASHPLUME_DLL_LA	2.1	11117-2.1-01	PC	Windows Server 2003	Y	YM	This version is used by TSPA		
	Volcanic Eruption		ASHPLUME_DLL_LA	2.1	11117-2.1-00	PC	Windows 2000, XP	Y	YM	Parameterization developed in this model report directly feeds this version of the software for TSPA usage. This version is used for model validation studies described in Section 7.		
	Volcanic Eruption		ASHPLUME	2	10022-2.0-00	PC	Windows NT 4.0	Y	YM	This version is used in validation studies as described in Section 7.		
	Volcanic Eruption		ASHPLUME_DLL_LA	2	11117-2.0-00	PC	Windows 2000	Y	YM	This version is used for model validation studies described in Section 7.		
	Volcanic Eruption		ASHPLUME	1.4LV	10022-1.4LV-dll-00	PC	Windows 2000	Y	YM	corroboratively with V 2.0 for comparison of calculated and measured ash deposition thickness for 1995 Cerro Negro eruption (see Section 7.3).		
	Volcanic Eruption		FAR	1.2	11190-1.2-00	PC	Windows 2000 & 2003	Y	YM	This software was used in the Ashplume model validation activity reported in Section 7.6		
	Volcanic Eruption		GoldSim	9.60.000	10344-9.60-00	PC	Windows 2000, 2003, & XP	Y	COTS	This software was used to run the ASHPLUME_DLL_LA V2.1 and FAR V.1.2 codes in the Ashplume model validation activity reported in Section 7.6	B-CT	
	Volcanic Eruption											179347 SNL (Sandia National Laboratories) 2007. Redistribution of Tephra and Waste by Geomorphic Processes Following a Potential Volcanic Eruption at Yucca Mountain, Nevada. MDL-MGR-GS-000006 REV 00. Las Vegas, Nevada: Sandia National Laboratories. ACC: DOC.20071220.0004

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	Volcanic Eruption		ASHPLUME_DLL_LA	2.1	11117-2.1-00	PC	Windows 2000 2003 server	Y	YM			
	Volcanic Eruption		ArcGIS	9.2	11205-9.2-00	PC	Windows XP	Y	COTS		B-CT	
	Volcanic Eruption		FAR	1.2	11190-1.2-00	PC	Windows 2000 2003 server	Y	YM			
	Volcanic Eruption		GoldSim	9.60.100	10344-9.60-01	PC	Windows 2000, 2003, XP	Y	COTS		B-CT	
	Volcanic Eruption		MVIEW	4	10072-4.0-00	PC	Windows 2000	Y	YM			
	Volcanic Eruption		Mathcad	13.1	611161-13.1-00	PC	Windows XP	N	COTS		B-CT	
	Volcanic Eruption											174260 SNL (Sandia National Laboratories) 2007. Characterize Eruptive Processes at Yucca Mountain, Nevada. ANL-MGR-GS-000002 REV 03. Las Vegas, Nevada: Sandia National Laboratories. ACC: DOC.20070301.0001
	Volcanic Eruption		Excel					Y				
	Volcanic Eruption		Conflow	1.0.0			Windows XP	N	YM	Use of this unqualified code is limited to providing context for characterizing the conduit flow conditions and final configuration of conduit profiles during the eruptions at the study areas		
	Dike/Drift Interactions											177430 SNL (Sandia National Laboratories) 2007. Dike/Drift Interactions. MDL-MGR-GS-000005 REV 02. Las Vegas, Nevada: Sandia National Laboratories. ACC: DOC.20071009.0015
	Dike/Drift Interactions		NPHF2D	1	10904-1.0-00	PC	Windows 2000 NT4.(	Y	YM	Dike Propagation Model; performs numerical modeling supporting analysis of magmatic dike propagation and analysis of the dike/drift interaction where magma enters a drift, modified and requalified for this task. This code was developed specifically for fracture propagation to the surface; no other code can evaluate the number of physical phenomena required.		
	Dike/Drift Interactions		FLAC	4	10167-4.0-00	PC	Windows 2000 NT4.(	Y	COTS	This is commercially available in SCM software that is used for a very broad range of geomechanical problems including hydraulic, mechanical, and thermal coupling.	B-CT	
	Dike/Drift Interactions		FLAC	4.04	10167-4.04-00	PC	Windows 2000 NT4.(	Y	COTS	SCM software that is used for a very broad range of geomechanical problems including hydraulic, mechanical, and thermal coupling. It is the same software as V. 4.0 but is also validated for fluid flow and coupled hydro-mechanical analyses.	B-CT	
	Dike/Drift Interactions		FLAC3D	2.1	10502-2.1-00	PC	Windows 2000 NT4.(	Y	COTS	SCM software that is used for a very broad range of geomechanical problems including hydraulic, mechanical, and thermal coupling. It is the preferred code for analyzing regional stresses, accounting for topography; and opening preexisting fractures by magma.	B-CT	

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	Dike/Drift Interactions		FLAC3D	2.14	10502-2.14-00	PC	Windows 2000	Y	COTS	SCM software that is used for a very broad range of geomechanical problems including hydraulic, mechanical, and thermal coupling. It is the same software as V. 2.1 but is also validated for fluid flow and coupled hydro-mechanical analyses.	B-CT	
	Dike/Drift Interactions		UDEC	3.1	10173-3.1-00	PC	Windows 2000 NT4.(	Y	COTS	Analyzes opening of preexisting fractures by magma. This was the only code available in SCM for hydromechanic behavior of fracture media.	B-CT	
	Dike/Drift Interactions		UDEC	3.14	10173-3.14-00	PC	Windows 2000	Y	COTS	fractures by magma. Same software as V. 3.1, but also validated for fluid flow and coupled hydro-mechanical analyses.	B-CT	
	Waste Packages / Igneous Events											177432 SNL (Sandia National Laboratories) 2007. Number of Waste Packages Hit by Igneous Events. ANL-MGR-GS-000003 REV 03. Las Vegas, Nevada: Sandia National Laboratories. ACC: DOC.20071002.0001
	Waste Packages / Igneous Events		LHS	2.51	10205-2.51-00	DEC Alpha	Open VMS AXP V. 7.3-1	Y	NL/YM	Stochastic parameter sampling (Qualified Software)		
	Waste Packages / Igneous Events		DIRECT	4	11121-4.0-00	PC	Windows XP	Y	YM	Geometric intersection calculations (Qualified Software)		
	Waste Packages / Igneous Events		FLAC	4	10167-4.0-00	PC	Windows 2000	Y	COTS	Dike/drift proximity calculations (Qualified Software)	B-CT	
	Waste Packages / Igneous Events		CORPSCON	5.11.08	10547-5.11.08-00	PC	Windows 2000	Y	USAE	Conversion of UTM to NSP coordinate (Qualified Software)		
	Waste Packages / Igneous Events		VULCAN	6	NA	PC	Windows XP	N	COTS	Standard CAD applications (Exempt Software)	B-CT	
	Waste Packages / Igneous Events		Rhinocerous (Rhino 3D)	3	NA	PC	Windows XP	N	COTS	Standard CAD applications (Exempt Software)	B-CT	
	Waste Packages / Igneous Events		Milkshape	1.8.1b	NA	PC	Windows XP	N	COTS	Standard CAD applications (Exempt Software)	B-CT	
	Ground Motion											
	Fault Displacement											176828 SNL (Sandia National Laboratories) 2007. Seismic Consequence Abstraction. MDL-WIS-PA-000003 REV 03. Las Vegas, Nevada: Sandia National Laboratories. ACC: DOC.20070928.0011.
	Fault Displacement		PFC2D	V2.0	10828-2.0-00	PC	Windows 2000		COTS	Used to characterize the behavior of a rubblized rock mass in the lithophysal units of the repository	B-CT	
	Fault Displacement											178851 SNL (Sandia National Laboratories) 2007. Mechanical Assessment of Degraded Waste Packages and Drip Shields Subject to Vibratory Ground Motion. MDL-WIS-AC-000001 REV 00. Las Vegas, Nevada: Sandia National Laboratories. ACC: DOC.20070917.0006.
	Fault Displacement		UDEC	3.1	10173-3.1-00	PC	Windows 2000	Y	COTS	shield failure (Section 6.4) and the waste package surrounded by rubble (Section 6.5). UDEC was selected for its capability to model solid body interactions with a computationally efficient algorithm.	B-CT	
	Fault Displacement		FLAC	4	10167-4.0-00	PC	Windows 2000	Y	COTS	invert material during seismic shaking (Sections 6.4 through 6.5). FLAC was selected for its capability to model dynamic loading for the continuum with a computationally efficient algorithm.	B-CT	

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Topic	Sub-topic	Primary / Supporting	Software Name	Version	STN	Platform	OS	SCM?	Source	Comment	Problem / Mitigation Code(s)	Reference
	Fault Displacement		FLAC3D	2.1	10502-2.1-00	PC	Windows 2000	Y	COTS	FLAC3D V. 2.1 was used to simulate the drip shield and invert during quasi-static loading (Section 6.4.6). FLAC3D V. 2.1 was selected for its capability to model dynamic loading for the continuum with a computationally efficient algorithm. FLAC3D V. 2.1 simulates the behavior of three-dimensional structures built of soil, rock, or other materials that are subject to various loading conditions.	B-CT	
	Fault Displacement		FLAC3D	2.14	10502-2.14-00	PC	Windows 2000	Y	COTS	simulate the drip shield during quasi-static and dynamic loading (Sections 6.4.3 and 6.4.7), and to simulate the waste package loaded by the drip shield (Section 6.5.2). FLAC3D V. 2.14 was selected for its capability to model dynamic loading for the continuum with a computationally efficient algorithm. Note that FLAC3D V. 2.14 and FLAC3D V. 2.1 are identical codes.	B-CT	
	Fault Displacement		LS-DYNA SMP D	970.3858	10300-970.3858-02	DEC ALPHA	OSF1 V. 5.1	N	COTS	the kinematic impacts between the waste packages and between waste packages and pallets (Section 6.3). LS-DYNA was selected for its capability to model solid mechanics in dynamic loading conditions	B-CT	
	Fault Displacement		LS-DYNA	971.7600.3	10300-971.7600.398-0(	Intel Itanium	Redhat Linux Chaos 3.0	N	COTS	Intel Itanium/Redhat Linux Chaos 3.0 was used to analyze the kinematic impacts between the waste packages and between waste packages and pallets (Section 6.3). LS-DYNA was selected for its capability to model solid mechanics in dynamic loading conditions.	B-CT	
	Fault Displacement		LS-DYNA	971.7600.3	10300-971.7600.398-0(	Intel Itanium	Redhat Linux Chaos 3.0	N	COTS	Intel Itanium /Redhat Linux Chaos 3.0 was used to analyze the kinematic impacts between the waste packages and between waste packages and pallets (Section 6.3). LS-DYNA was selected for its capability to model solid mechanics in dynamic loading conditions.	B-CT	

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Topic	Sub-topic	Primary / Supporting	Software Name	Version	STN	Platform	OS	SCM?	Source	Comment	Problem / Mitigation Code(s)	Reference
	Fault Displacement		km_impacts_pp	1	11235-1.0-00	Intel Itanium2	Redhat Linux 4	Y	YM	Intel Itanium2 Redhat Linux 4 system to postprocess output from LS-DYNA. km_impacts_pp is used to produce estimates of damaged areas for the waste packages along with estimates of the number of ruptured waste packages. km_impacts_pp was selected for its capability to process the output of LS-DYNA and directly produce data for the seismic abstraction.		
	Fault Displacement		GoldSim	8.02.500	10344-8.02-05	PC	Windows 2000	Y	COTS	GoldSim was used to sample the rock block pattern, rock strength, and ground motion number. GoldSim is widely used for probabilistic and decision analyses and provides capability for Latin Hypercube analysis used to sample the parameters listed above.	B-CT	
	Fault Displacement		LS-PREPOST	1.0 and 2.0		AMD Opteron Redhat Linux 4, Intel Itanium2 Redhat Linux 4, and DEC ALPHA	OSF1 V. 5.1 systems.	N	YM	Post processing software to visualize output.		
	Fault Displacement		TrueGrid	2.2.0, 2.2.6, and 2.3.0				N	YM	were used to preprocess data and generate model geometry for input to LS-DYNA.		
	Fault Displacement		Mathcad	7				Y	COTS	postprocess data from UDEC and to solve non-linear equations for stress profiles.	B-CT	
	Human Intrusion (Human Intrusion Scenario Class)											166107 BSC (Bechtel SAIC Company) 2004. Drift Degradation Analysis. ANL-EBSMD-000027 REV 03. Las Vegas, Nevada: Bechtel SAIC Company. ACC: DOC.20040915.0010; DOC.20050419.0001; DOC.20051130.0002; DOC.20060731.0005.
	Human Intrusion (Human Intrusion Scenario Class)		UDEC	3.1	10173-3.1-00	PC	Windows 2000	Y	COTS	seismic and thermal effects on block movement in the lithophysal rock units (Section 6.4). UDEC was selected for its capability of modeling block slip and block separation in plane strain condition. Also, it is capable of thermal and dynamic simulation. There are no known limitations on outputs	B-CT	
	Human Intrusion (Human Intrusion Scenario Class)		3-DEC code	2.01	10025-2.01-00	PC	Windows 2000	Y	COTS	3DEC was used to analyze the seismic and thermal effects on block movement in the nonlithophysal rock units (Section 6.3). 3DEC was selected for its capability of modeling of wedge type of rockfall with consideration of block slip and block separation in three- dimensional space. Also, it is capable of thermal and dynamic simulation.	B-CT	

Topic	Sub-topic	Primary / Supporting	Software Name	Version	STN	Platform	OS	SCM?	Source	Comment	Problem / Mitigation Code(s)	Reference
	Human Intrusion (Human Intrusion Scenario Class)		FLAC	4	10167-4.0-00	PC	Windows 2000	Y	COTS	FLAC was used in the thermal-mechanical calculation to define the distribution of stresses around the drifts due to the progressive heating of the repository area (Section 6.2).FLAC was selected as an efficient code to run thermal-mechanical analysis. There are no known limitations on outputs.	B-CT	
	Human Intrusion (Human Intrusion Scenario Class)		FLAC3D	2.1	10502-2.1-00	PC	Windows 2000	Y	COTS	mechanical calculation to define the distribution of stresses around the drifts due to the progressive heating of the repository area (Appendix C).FLAC3D was selected as an efficient code to run thermal-mechanical analysis for the regional scale and drift scale. There are no known limitations on outputs.	B-CT	
	Human Intrusion (Human Intrusion Scenario Class)		PFC2D	2	10828-2.0-00	PC	Windows 2000	Y	YM	PFC2D was used to characterize rock mass behavior, including the analysis of long-term strength degradation (Section 7 and Appendix S). PFC2D was selected for its capability of modeling behaviors of a rock material by combining behaviors of individual grain particles to simulate complicated non- linear deformation of a rock material including long-term mechanical strength degradation and rock mass deformation with voids.		
	Human Intrusion (Human Intrusion Scenario Class)		PFC2D	2	10828-2.0-01	PC	Windows 2000	Y	YM	run impact analyses to confirm the initial PFC2D results (using software tracking number10828-2.0-00), as documented in Appendix Q. The initial PFC2D software qualification did not specifically identify the library of support functions (known as Fish functions) that are used within the code. This new version (software tracking number 10828-2.0-01) specifically qualifies FishTank 041b, which is the library of Fish functions included within the code. The impact assessments in Appendix Q confirm that the results are identical using either the initial or new version of PFC2D.		

Topic	Sub-topic	Primary / Supporting	Software Name	Version	STN	Platform	OS	SCM?	Source	Comment	Problem / Mitigation Code(s)	Reference
	Human Intrusion (Human Intrusion Scenario Class)		PFC3D	2	10830-2.0-00	PC	Windows 2000	Y	YM	PFC3D was used to characterize rock mass behavior, including the analysis of long-term strength degradation (Section 7 and Appendix S). PFC3D was selected for its capability of modeling behaviors of a rock material by combining behaviors of individual grain particles to simulate complicated non- linear deformation of a rock material including long-term mechanical strength degradation and rock mass deformation with voids.		
	Human Intrusion (Human Intrusion Scenario Class)		PFC3D	2	10830-2.0-01	PC	Windows 2000	Y	YM	run impact analyses to confirm the initial PFC3D results (using software tracking number10830-2.0-00), as documented in Appendix Q. The initial PFC3D software qualification did not specifically identify the library of support functions (known as Fish functions) that are used within the code. This new version (software tracking number 10830-2.0-01) specifically qualifies FishTank 041b, which is the library of Fish functions included within the code. The impact assessments in Appendix Q confirm that the results are identical using either the initial or new version of PFC3D.		
	Human Intrusion (Human Intrusion Scenario Class)		DRKBA	3.31	10071-3.31-00	PC	Windows 2000	Y	YM	development and failure in the nonlithophysal rock units (Appendix D). DRKBA was selected to assess the impact of small-scale fractures on rockfall because it has an efficientkey-block simulation algorithm. DRKBA was also selected as an alternative numerical code to verify the results from 3DEC. DRKBA does not directly apply seismic and thermal loads, and therefore was not selected as the primary code for rockfall analyses.		
	Human Intrusion (Human Intrusion Scenario Class)		FracMan	2.512	10114-2.511-00	PC	Windows NT	Y	COTS	fracture geometry observed in the ESF to develop a representative volume of jointed rock mass (Section 6.1.6). FracMan was selected for its capability of discrete fracture data analysis, geologic fracture network construction, spatial analysis, and visualization.	B-CT	

Appendix A

FY 18 Status Report on the Computing Systems for the Yucca Mountain Project TSPA-LA Models and Inventory of Software used for Process Models

Topic	Sub-topic	Primary / Supporting	Software Name	Version	STN	Platform	OS	SCM?	Source	Comment	Problem / Mitigation Code(s)	Reference
	Human Intrusion (Human Intrusion Scenario Class)		NUFT	3.0s	10088-3.0s-01	SUN	SUN O.S. 5.7	Y	NL/YM	NUFT was used to simulate heat transfer around the emplacement drift (Section 6.2). NUFT was selected for its capability of modeling thermal-hydrology of an unsaturated zone including subsurface heat and fluid flow. There are no known limitations on outputs from NUFT.		
	Human Intrusion (Human Intrusion Scenario Class)		EARTHVISON	5.1	10174-5.1-00	SGI	IRIX 6.5		COTS	EarthVision was used to extract stratigraphic unit thickness and cross-sections from the Geological Framework Model (GFM2000) (Appendix M). EarthVision was selected for its capability of extracting specific data from GFM2000 and presenting the data in a common graphical format. EarthVision was not used to perform data manipulation in this report.		
	Human Intrusion (Human Intrusion Scenario Class)		UNWEDGE	2.3	30053 V2.3	PC	DOS Emulation	Y	YM	reference-only example of a deterministic method forkey-block analysis (Appendix D). UNWEDGE was selected for its common usage on static block analysis for the geotechnical and mining industries.		
	Human Intrusion (Human Intrusion Scenario Class)		Clustran	1.1	11162-1.1-00	PC	Windows 2000	Y	YM	fracture data in Section 6.1.6. Clustran was selected for its common usage on fracture orientation analysis for the geotechnical and mining industries.		
	Human Intrusion (Human Intrusion Scenario Class)		Read DXF	1	11159-1.0-00	PC	Windows 2000	Y	YM	fracture data files in DXF format and extract polyline data with associated strike/dip tags for input into FracMan (Section 6.1.6). Read DXF was specifically developed to extract fracture data from full periphery geologic maps to facilitate the comparison of field fracture data to synthetic FracMan fracture data.		

APPENDIX B. CATEGORIZED SOFTWARE LISTS

The software inventory provided in Section 3 and in Appendix A is further subdivided into various categories to help in the assessment of current condition of the software. The categories are:

- Modeling codes, project developed
- Modeling codes, commercial or non-project developed
- Utility/graphics codes, project developed
- Utility/graphics codes, commercial or non-project developed

The list of software in the various categories are shown below.

B.1. List of project developed modeling codes

2WELLS_2D	PFGVH
2WELLS_3D	PFGVHLH
3-DEC	FPFGVH
ASHPLUME	FPFGVHL
ASHPLUME_DLL_LA	VHTREE
calc_cdf.c	VHTIELHS
DCPT	NECPDS
DIFFCELL	FITIDSR
Delb.dat	SFIDSR
EQ3/6	DLECD
EQ6	DILECDLH
FAR	CFRAC
FEHM	COMBSM
iTOUGH2	MARGIN
LHS	RETRAN
MVIEW	
NUFT	
PHREEQ	
PHREEQC	
SUPCRT92	
T2R3D	
TOUGHREACT	
TOUGH2	
FITCD	
SFCD	
DCPELD	
CPDI	
UZVH	
UZVHLH	
FKVH	
FKLH	
UZVPVH	
UZVPVHLH	
FKVPVH	
FKVPVHLH	
ZBCKVH	
ZBCKVHLH	
FITFIELD	
FIT2CNTR	

B.2. List of commercial or non-project developed modeling codes

3-DEC
FLUENT
FracMan
FLAC
FLAC3D
GSLIB
GoldSim
LS-DYNA SMP D
LS-DYNA
Mathcad
MATLAB
UDEC
PEST

B.3. List of utility codes and graphics software that are project developed:

2KGRIDV1.F	GS2FEHM.C,	Tbgas3D
2kgridv1a.for	Hsource_v0.f	T2FEHM
2kgid8.for	heatgen_ventTable_emplace	Theis.vi
assign.f	Injection_Pumpback.vi	Tin
AMESH	Infil2grid	Transl
AddBound	KREG	THERMOCHK
boundary_conditions	KSWITCH,km_impacts_pp	VHTREE
bot_sum.f	LaGriT,Mult_Rech	WINGRIDDER
Bkread.f	MSTHAC	WTRISE
BUILDEQ3.BAS	MoveMesh	Xread_Distr_Rech
BestFit,calc_cdf.c	merggrid2.f	Xread_Distr_Rech_UZ,Xread_Reaches
CutDrift	mk_circ2	Xwrite_Flow_New
CutNiche	mk_rect2	XtractG.f90
colCen	mk_grav2.f	Xw
Chimney_interpolate	MOENCH.vi.Function(1)	XTOOL
CUTCHEM	MOENCH.vi,Function(2)	YMESH
cr8sptr.c	MULTRAN	Zones
Delb.dat	NPHF2D	
DBCONV	Perm2Mesh	
discrete_tf	Ppptrk	
e93in	RADPRO	
EXT,exclude.f	readsUnits	
extractBlocks_EXT	repository_percolation_calculator	
Extract	rcv2amos.exe	
EXT_RECH	ReadDXF	
EQUILFIT	RadNuScreen	
fehm2post	RECIRC.vi	
FRACT_p	RELAP	
Filter.vi	rme6	
fehm2post	reformat_EXT_to_TSPA	
GridReader	Streltsova-Adams.vi	
Gpzones.dat	sav1d_dst2d.f	
Gen_inconv0.f	Smesh.f	
Get_a_layer_v0.f	SZ_Pre,SZ_Post	
Get_temp_v0.f	SZ_Convolute	

GetEQData	TOPTEMP_V0.f	

B.4. List of utility codes and graphics software that are commercial or non-project developed:

ArcGIS
BestFit
Mathcad
MATLAB
Milkshape
PFC2D
PFC3D
Rhinocerous (Rhino 3D)
SAPHIRE
S-Plus
S-PLUS 2000
SigmaPlot
Tecplot
UNWEDGE
VULCAN

APPENDIX C. YMP LA SOFTWARE FITNESS CATEGORIZATION AND STRATEGY

C.1. Overview

Being able to use legacy YMP LA tools for current and future studies depends on:

- How compatible those tools are with modern operating systems (OS) and hardware
- Whether SNL has the source code, and what language the software was written in.
- That tool's purpose
    - Problem-specific, taking input and generating simulation that can be post-processed
    - Conversion/post-processing, taking output from one code and converting that output to input for another code
    - Graphical, generating plots/graphs for user consumption

C.2. Software Categories

To aid in assessing fitness of any particular software package, the following categories were enumerated:

C.2.1. Binary Categories (B)

Binary categories apply if SNL does not have access to source code.

C.2.1.1. Windows DLLs for use in GoldSim (B-DGS)

It has been determined that all the Windows Dynamic-Link Libraries (DLLs) used on the original TSPA calculations can be recompiled. Once compiled they work as expected and generate output exactly the same, or consistent with, output from the original DLLs. It is expected that any legacy DLLs that aren't recompiled to exhibit the same successful behavior.

C.2.1.2. Written in Visual Basic (B-VB)

Microsoft stopped supporting Visual Basic, applications written in Visual Basic (VB) and Visual Basic programmers in 2008. Since then there have been multiple versions of Windows released, along with thousands of Windows updates and system policy changes. Additionally, at least one time since then, Microsoft has made decisions that broke backwards compatibility of Component Object Model (COM) DLLs distributed with Windows. This is an issue because Visual Basic is built on COM. Most Visual Basic applications use third party programming tools distributed using COM. All Visual Basic applications, regardless of complexity, use Windows COM interfaces and require them to be compatible with the COM environment existing at the time they were compiled. These factors affect whether any given Visual Basic application will run on Windows. The author estimates a 50/50 success rate based on what he has seen in the past few years. YMP LA software may do better or worse. See mitigation heading below about Wine for a compelling solution to the problem of running old Windows binaries.

C.2.2. Written in Fortran (B-FN)

During the YMP LA there were two major Fortran compiler vendors: Lahey and COMPAQ. Applications (even console applications) compiled using Lahey are especially unlikely to work on modern OS versions. Console applications compiled using the COMPAQ compiler don't fare much better. In short, there's no guarantee that compiled Fortran applications will run on modern systems without individual testing. See mitigation heading below about Wine for a compelling solution to this problem.

C.2.2.1. Written in C++ (B-CP)

It is expected that most C++ console applications will work without modification on later versions of the same OS and similar hardware. This might not be the case. See mitigation heading below about Wine for a solution to the problem of C++ binaries crashing on later OS versions and newer hardware.

C.2.3. COTS Software (B-CT)

Software was licensed from external vendors for use on the project. There are multiple issues possible with COTS software. The license may no longer be valid. The vendor might refuse to support the version in use during the original YMP LA, and may require purchase of a new, updated version of the software. An updated version of the software probably requires input changes, and likely requires changes to how its output is consumed by downstream codes.

C.2.4. GOTS Software (B-GT)

Software, without source, was licensed from other government agencies for use on the YMP LA project. Because this software was originally funded by the government, one is probably able to acquire source code from the originating agency at no cost. If the source is still available, which is likely, there may be export control issues or other licensing issues or agreements that would need to be worked out between the originating and using agency. SNL contacted a couple of agencies informally to inquire about receiving source and received no replies. However, the SNL Licensing and IP office would probably be successful in requesting source through formal channels. Insurmountable barriers are not expected in acquiring source for any Government Off-the-Shelf Software (GOTS) package used by the project. Delays on the order of months are likely, however.

C.2.5. C2.2 Source Categories

Having source code significantly reduces the risk that a specific software package might not be able to run on a newer or different OS. But different software categories carry with them different risk factors. These are enumerated below.

C.2.5.1. Project Actively Maintained (S-AM)

This category is valid for any programming language. If a software package is known to be actively maintained, its availability is assumed. Time should be scheduled towards verifying this on a code by code basis, but current versions of actively-maintained software will compile and can probably be plugged into the YMP LA calculation without modification.

C.2.6. MATLAB (S-ML)

MATLAB code used in the YMP LA is not likely to work without modification in later versions of MATLAB. For this code to work, most of it must either be compiled and run under the original version of MATLAB used then, or modified to work under current versions of MATLAB. Such modification is probably not extensive, but each code must be evaluated separately.

C.2.7. Mathcad (S-MC)

The Mathcad data format, features and instruction set are not 100% compatible with previous versions. When upgrading from one version to the next, some modification of the source code is to be expected. To upgrade to the current version of Mathcad from the version used during the YMP LA, having to make changes is almost a certainty. Running the code under an older version of Mathcad is the best solution in the short term, if possible.

C.2.8. Windows DLLs for use in GoldSim (S-DGS)

It has been determined that all of the Windows DLLs used on the original TSPA calculations can be recompiled. Once compiled they work as expected and generate output the same as, or consistent with, output from the original DLLs.

C.2.9. Written in Visual Basic (S-VB)

Chance for successful compilation is fairly good if you have the Visual Basic source. But many VB programmers used third-party libraries from companies that no longer exist. Many of these libraries require a valid product key file to exist on a developer's computer before they will enable compilation. If such a license can't be acquired (something that is very likely), an alternative to the third-party library must be devised. Alternatives include (but are not limited to) writing custom code in VB, wrapping another third-party library -- in Visual Basic.NET, C#.NET or C++ -- and calling that library from VB. If the original tool exists on CD, it's possible that it can be installed and used on a modern system. It's also quite possible that installation simply no longer works.

C.2.10. Written in Fortran (S-FN)

Software written in Fortran for which SNL has the source code, carries low risk. Depending on many factors detailed elsewhere in this appendix such as complexity, purpose, the use of preprocessor directives and the use of system-specific code and Fortran intrinsics, compiling on or porting to a new system might be time-consuming. But the risk of the code not generating identical or consistent output is low.

C.2.11. Written in C++ (S-CP)

If C++ standards were adhered to originally, minimal problems are expected recompiling C++ projects under a later version of the compiler. The same possible issues exist as in Fortran – the use of non-standard code is a possibility to contend with, as is the expectation that minor changes will be required when changing OSes due to differences between what Microsoft considers standard and put into their compilers, and what the rest of the world considers standard.

C.2.12. GOTS Software (S-GT)

Having the source code to a GOTS software package carries the same benefits as having the source to any other package. The source may be better structured than single-purpose source code created

by a single developer at SNL, but would also be more complex. Thus, porting such a package, or updating to run on a newer OS and/or different hardware would carry similar risks.

C.3. Mitigations

There are many ways to mitigate the issues discussed in this appendix. Applicability must be considered for each individual case.

C.3.1. Run Original OS on Original Hardware (M-OH)

If a code can't be made to run on a newer system with newer OS, or ported to a different system, it can always be made to run on the original hardware with original OS. But there are issues to consider when doing this:

1) The original system will probably be denied access to any corporate network due to security issues with the old OS. This would require creating a private subnet or running software offline and manually transferring results between computer systems.
2) Certainly, the original computers no longer exist.
3) Most modern OSes run on commodity computer hardware. But some of the codes in this study were run on DEC Alpha workstations and servers – hardware that halted production in the 1990s.
4) Most original hardware no longer exists at SNL and would probably have to be purchased from used computer vendors.

C.3.2. Run Original OS on Virtual Machine (M-VM)

Although a virtual machine running on a modern computer is based on the hardware of that computer, it's fairly likely that the original operating system can be made to work with the software in a compatible fashion. It should be noted that there would be no way, under a virtual machine, to emulate the original hardware, however. But trying out this option would be inexpesive and low-risk.

C.3.3. Run Original OS on Emulation of Original Hardware

Although it might be difficult to source the hardware originally used to run a calculation, it might be possible to purchase an emulator for that hardware and install the original operating system and software. Whether or not suitable emulators are available hasn't yet been explored. It's fairly likely, however, that if emulators are available for a specific set of hardware, it would be fairly expensive.

C.3.4. Linux/Unix to Windows (M-LW)

As long as the developer tried to adhere to application software programming standards and wrote code in languages available on both platforms (C++, Fortran, etc.), it is usually fairly straightforward to get code written on one OS to compile and run correctly on another, regardless of complexity. Success is likely, but the time it takes to attain success is unknown and will differ for each software package.

C.3.5. Linux/Unix to Windows – GUI (M-LW-G)

Getting a Unix Graphical User Interface (GUI) built in C++ to run on Windows is almost always easier than going the other direction. Most (not all) popular Linux GUI packages have a Windows counterpart, for example. Also, Cygwin is an option that reduces cross platform issues considerably.

C.3.6. The use of Cross-Platform Toolkits (M-LW-TK)

Qt, wxWidgets (previously wxWindows) and other GUI programmer toolkits sport native implementations on Linux and Windows. If either of these packages were used to create Unix or Linux software packages, it is likely that other portability aspects were considered by the developer as well. This knowledge can be used to help predict portability success on software source code, even when the developer is no longer around.

C.3.7. Conversion to Console (M-LW-Co)

The lowest risk route to getting GUI apps ported to another platform might just be conversion to a console-only program. For this approach to work, the developer would need to enumerate all possible GUI inputs and pass them as command-line arguments or in a separate input file. If GUI outputs (such as graphs displayed with interactive user input) are supplied, this might not be an option.

C.3.8. Target Local Linux Environment (M-LW-LL)

Cygwin and MinGW are two software packages that supply a Linux environment, including a complete build system, on Windows. Much software written to run on Linux and never intended for Windows, can be ported more easily to run as a guest under these packages than under native Windows.

C.3.9. Windows to Linux (M-WL)

Getting Windows applications to run on Linux carries many of the same issues as going from Linux to Windows.

C.3.10. Windows to Linux with GUI (M-WL-G)

On Linux an application is more likely to use a cross-platform GUI toolkit. But for Windows developers who use more integrated development environments (IDEs), a Windows-specific, nonportable GUI is far more likely. Therefore, the default expectation is that GUI code is non-portable. Below are mitigations for either case.

C.3.11. Target Local Windows Environment (M-WL-G-W)

This may be counterintuitive, but using Wine on Linux might be a better option than targeting the older Windows OS on older computer hardware. Linux features the Wine package, software designed to allow Windows applications to run on Linux by emulating services and APIs from Windows environments. Wine targeting is an option for any Windows program and is probably the first thing that should be tried if recompiling or porting are not options. With Wine, success is never guaranteed. And traditionally, running newer Windows software packages on Wine can be more problematic than running older software. However, Wine ensures good backwards compatibility with older Windows OSes all the way to Windows 3.1. In some cases, better backwards compatibility than Microsoft Windows itself!

C.3.12. Conversion to Console (M-WL-G-CC)

A route to getting GUI apps ported to another platform might just be conversion to a console-only program. For this approach to work, the developer would need to enumerate all possible GUI inputs and pass them as command-line arguments or in a separate input file. If GUI outputs (such as graphs displayed with interactive user input) are supplied, this might not be an option.

C.3.13. The use of Cross-Platform Toolkits (M-WL-G-TK)

It is unlikely that programs originally written to run on Windows use cross-platform GUI toolkits. But it is a possibility. Qt, wxWidgets (previously wxWindows) and other GUI programmer toolkits sport native implementations on Linux and Windows. If either of these tools were used to create Windows software packages, it is likely that other portability aspects were considered by the developer as well. This knowledge can be used to help predict portability success on software source code, even when the developer is no longer around.

C.3.14. Windows to Linux – Console

Any of the strategies outlined for GUI are also valid for console programs.

C.4. Notes About Source Code

When considering whether a package will compile under newer compilers, work under newer interpreter versions of run on a different computer system or later OS, many of the same issues are encountered regardless of programming language. This section attempts to talk about these issues as they relate to the programming languages used to write codes used in the YMP LA calculation.

C.4.1. C4.1 Fortran Portability

Getting older Fortran to compile under newer Fortran compilers is usually fairly straightforward. It's never a question of whether the code will compile. The only question is how long will it take to make that happen, and there are only as few variables that need to be considered when asking that question:

C.4.1.1. Standard Fortran

If efforts were made to write code in standard Fortran originally, one can have a high degree of confidence that the same code will build without problems today. However, use of intrinsics and non-standard Fortran source code are items that must be considered on a project-by-project basis, when determining how long it will take to get software running on new platforms or under a new or updated compiler.

C.4.1.2. Fortran Intrinsics

Fortran intrinsics are commands innately available to the language, such as ABS, LOG, SIG, WRITE, etc. Most of these intrinsics are enumerated in the Fortran Language Standard and are referred to as standard intrinsics. Standard intrinsics are generally portable. Though minor namespace changes might be required when different compilers are used, a successful recompile virtually guarantees identical operation at runtime.

However, Fortran standards can't address every issue encountered by programmers on every platform. So standard intrinsics don't exist for every problem encountered. In these cases, a developer can either use vendor-supplied intrinsics where provided, or write code that doesn't adhere to the standard and is therefore inherently nonportable. Sometimes a needed language feature is ignored by the standard because system solutions are too diverse to be tackled by a general document, or because the Fortran Standards Committee can't come to agreement on how to handle the differences between systems or how to implement a particular feature.
Most compiler vendors provide nonportable intrinsics to deal with system-specific resources like timers and keyboard interrupts. Some needs may be supplied by some vendors and not others. And some programmers may eschew a standard intrinsic in favor of a competing-and-better vendor-specific intrinsic or their own hand-crafted solution. In all these cases, compiling the code under a newer compiler version, different compiler vendor or newer operating system is likely to require code changes. In most of these cases, such code changes, regardless of complexity, are not likely to affect the implemented algorithms or program output.

C.4.2. Preprocessor Directives

Any reasonably complicated code base, whether Fortran or C++, is almost guaranteed to have *some* nonportable code. The program author has the choice of using preprocessor directives to provide different code for different platforms when s/he knows the code won't compile on a different platform. When preprocessor directives (like #ifdef) are used, separate working code fragments are supplied for each platform the program author expects to compile on. Searching for preprocessor directives in source code is one way to assess whether the software was developed with portability in mind.

C.4.3. MATLAB Portability

MATLAB code used in the YMP LA is not likely to work without modification in later versions of MATLAB. For this code to work, most of it must either be compiled and run under the original version of MATLAB used then, or modified to work under current versions of MATLAB. Such modification is probably not extensive, but each code must be evaluated separately.

C.4.4. Mathcad Portability

The Mathcad data format, features and instruction set are not 100% compatible with previous versions. When upgrading from one version to the next, some modification of the source code is to be expected. To upgrade to the current version of Mathcad from the version used during the YMP LA, having to make changes is almost a certainty. Running the code under an older version of Mathcad is the best solution in the short term, if possible.

C.4.5. C++ Portability

Like Fortran, C++ has a published standard. If code is written to adhere to that standard, portability between platforms and compilers is not an issue – the code will always compile. Even when the standard is adhered to, however, some dependency notations may need to change. This is not

executable code, however, and getting it to compile is normally handled by using preprocessor directives.

Without examining the code base of a specific C/C++ project, it's impossible to predict how simple it is going to be to get code to compile on a different platform. It can be assumed, however, that at a minimum, a developer is going to need to make minor changes to dependency notation. These changes will not affect program operation or output.
If a program passes all arguments on the command line and has no user interaction at runtime, no other source code changes are likely to be called for. If it receives input from the user after the program has started, minor code changes that do not affect program operation or output are likely. These changes are therefore low risk. If the program is not a console program and has a graphical user interface (GUI), however, having to make source code changes is practically guaranteed.

C.4.5.1. Visual Studio IDE (MSVS)

When discussing cross-platform C++ where one of the platforms (in either direction) is Windows, it is wise to consider the Microsoft Visual Studio IDE and C++ compiler. This is because many of the issues encountered are due to Microsoft's fuzzy approach to standards compliance. Some namespaces are defined in nonstandard places or have slightly different names. Additionally, MSVS creates and manages some code for the user, especially when a developer is maintaining Graphical User Interface (GUI) code. This code is not always standard. Thus, it can be assumed that migrating a code base from Windows to another OS is usually going to be more difficult than going from another OS to Windows. However, problems **will** exist going either direction.

C.4.6. Metrics to use to Assess Code Porting Effort and Success

Most of the YMP LA software developers have moved on or retired. Hiring enough people to individually assess over 350 software packages would be expensive. But there are metrics that can be used to predict:

1) Portability success
2) Programmer hours per software package for code porting or recompile
3) The number of changes required for successful compilation of each software package
4) Whether an existing binary will run under modern OSes as-is

Such prediction is out of scope of this document. But it attempts to lay out some metrics that can be used for prediction. If accurate records are kept by developers while migrating each package, such prediction will become more reliable over time.

C.4.6.1. Metrics

When estimating any software development endeavor including the amount of time it will take to port a software package to another OS, anything you can assign a value to and anything you can measure is a candidate you should consider using to assist in making predictions. If it's countable, then count. Otherwise, a predictive or modifying constant can be applied and adjusted as projects are successfully ported. As time goes on, keeping accurate records is important as it improves forecasting accuracy.

C.4.6.2. Number of Code Lines

Although rating programmers based on how many lines of source code are written per day would likely reward the wrong things, the line count can still provide valid and useful insights that can be used for prediction. If two software packages are similar in complexity, use of intrinsics, and whether compiler directives were used, an estimate based on careful assessment of one package can be extrapolated to other packages based on the difference in lines of code.

C.4.6.3. Number of Source Code Files

The number of source code files used can be indicative of the organization skills of a software developer. Does he break software down into manageable chunks? Is she an object-oriented programmer? Does he reuse code instead of copying and modifying snippets? Additionally, creating a make system on a new platform takes more time when there are more source files. A modifier that relates the number of code lines to the number of files can be useful in prediction.

C.4.6.4. Whether Compiler Directives are Present in the Code

If compiler directives are present in the code, then at least *some* time was spent thinking about portability. A numerical modifier can be created based on whether compiler directives are used, whether an #ifdef is followed by an #else, and whether this #else contains actual executable code, code comments, or text intended to cause a compiler error. Either of these possibilities will increase or reduce the time investment needed to get the code to compile on a new platform.

C.4.6.5. Whether System-Specific Calls are Used (Without Compiler Directives)

If system-specific calls are used and are not surrounded by compiler directives, having to modify code to enable correct behavior on other platforms is guaranteed. Such code is easy to scan for using a custom script. Function prototypes for shared objects (on Linux) and dynamic link libraries (on Windows) are unique and obvious. It is possible and even easy, to write scripts to determine whether the function prototypes exist and how many of them there are. These two pieces of information can be used to modify an expected time for completion when applied to the number of lines of source code.

C.4.6.6. Whether System-Specific Calls are Used (With Compiler Directives)

If system-specific calls are used and *are* surrounded by compiler directives, this makes it far more likely that the package being evaluated will compile and work without changes. The developer will still spend an unknown quantity of time preparing for the build and doing things like creating a make file, creating a project file for an IDE, and troubleshooting minor build and link errors. These times can vary depending on the number of files and number of lines of source code.

C.4.6.7. Source Code Commenting

There are probably a few metrics that can be teased out of source code commenting, as well. Ratio of comment lines to source code lines. Number of identical (copy-and-pasted) comments. One position might be if there are a lot of comments, the code is unnecessarily complex. Another might be that the software author wished to enhance readability.

C.5. Conclusion

This appendix was created in the hopes that it would help to guide future detailed examination of software packages used to conduct the original YMP LA calculation in determining what it would take to, not only run the calculation again using modern systems, but to migrate the entire collection of software packages to a modern system. It should be expanded to include additional mitigations, additional completion metric strategies and even actual metrics applied as the next phase of this project commences.

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