SANDIA REPORT
SAND2015-7834
Unlimited Release
Printed September 2015

Reproduction of the Yucca Mountain Project TSPA-LA Model Runs using TSPA Computing Systems

Teklu Hadgu, Gordon Appel, Alexey Malashev, and Clay Payne

Prepared by
Sandia National Laboratories
Albuquerque, New Mexico 87185 and Livermore, California 94550

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

Sandia National Laboratories

Issued by Sandia National Laboratories, operated for the United States Department of Energy by Sandia Corporation.

Printed in the United States of America. This report has been reproduced directly from the best available copy.

Available to DOE and DOE contractors from
U.S. Department of Energy
Office of Scientific and Technical Information
P.O. Box 62
Oak Ridge, TN 37831

Telephone: (865) 576-8401
Facsimile: (865) 576-5728
E-Mail: reports@adonis.osti.gov
Online ordering: http://www.osti.gov/bridge

Available to the public from
U.S. Department of Commerce
National Technical Information Service
5285 Port Royal Rd.
Springfield, VA 22161

Telephone: (800) 553-6847
Facsimile: (703) 605-6900
E-Mail: orders@ntis.fedworld.gov
Online order: http://www.ntis.gov/help/ordermethods.asp?loc=7-4-0#online

SAND2015-7834
Unlimited Release
Printed September 2015

Reproduction of the Yucca Mountain Project TSPA-LA Models Runs using TSPA Computing Systems

Teklu Hadgu, Gordon Appel, Alexey Malashev and Clay Payne
Nuclear Waste Disposal research and Analysis

Sandia National Laboratories
P.O. Box 5800
Albuquerque, New Mexico 87185

Abstract

Sandia National Laboratories (SNL) conducted an evaluation of total system performance assessment (TSPA) related 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). The current work examined main components of the computing system identified in the previous work (Lee and Hadgu, 2014) to ensure the operational readiness of the TSPA-LA model capability on the server cluster. The TSPA computing hardware and storage system were replaced in late 2014 to maintain core capability and improve computation efficiency. One floating license of GoldSim Version 9.60.300 was installed on the upgraded cluster head node, and its distributed processing capability was mapped on the cluster processors. Other supporting software was tested and installed to support the TSPA-type analysis on the server cluster. All the TSPA-LA modeling cases were tested and verified for the model reproducibility on the upgraded 2014 server cluster (CL2014). All test runs were executed on multiple processors on the server cluster utilizing the GoldSim distributed processing capability, and all runs completed successfully. The model reproducibility verification was evaluated by two approaches: numerical value comparison and graphical comparison. The analysis demonstrated an excellent reproducibility of the TSPA-LA model runs on the upgraded server cluster. The 2014 server cluster and supporting software systems are fully operational to support TSPA-LA type analysis.

ACKNOWLEDGMENTS

The authors would like to acknowledge technical support by Bob D'Spain (9329). The authors would also like to express the gratitude for technical interest and programmatic support by Tito Bonano (6220) and Kevin McMahon (6222). We also would like to thank Robert Rechard for his constructive review of the report.

CONTENTS

FIGURES

TABLES

NOMENCLATURE

DLL	Dynamically Linked Libraries
DOE	Department of Energy
DTN	Data Tracking Number
GB	Gigabyte
HLW	High-Level Radioactive Waste
HPC	High Performance Computing
LA	License Application
NRC	Nuclear Regulatory Commission
NWPA	Nuclear Waste Policy Act
OCRWM	Office of Civilian Radioactive Management
RAM	Random Access Memory
SNF	Spent Nuclear Fuel
SNL	Sandia National Laboratories
SP	Service Pack
TB	Terabyte
TSPA	Total System Performance Assessment
YMP	Yucca Mountain Project

1. INTRODUCTION

The Yucca Mountain Project (YMP) was to develop a deep geological repository for the nation's high-level radioactive waste including commercial spent nuclear fuel (SNF) and United States Department Energy (DOE) managed high-level radioactive waste (HLW) and SNF. The License Application (LA) for the repository construction authorization was submitted to the United States Nuclear Regulatory Commission (NRC) in June 2008 (DOE, 2008). Sandia National Laboratories (SNL) principally served as the Lead Laboratory for the postclosure aspects of the LA. However, the YMP was terminated in 2010. Pursuant to the United States Court of Appeals for the District of Columbia Circuit ruling that the NRC complete the review of the LA; see Order, *In re: Aiken County, et al.*, No. 11-1271 (D.C. Circuit, August 13, 2013), NRC completed and published the final volumes of its safety evaluation report in January 2015.

As part of the YMP shutdown, the computer hardware, suite of software, and databases used to conduct the TSPA analyses for the LA (SNL 2008; DOE 2008), were relocated to SNL in Albuquerque, NM. In 2010 the relocated computer hardware (TSPA cluster) was replaced to update the computing system. The updated (2010) computer system was used to reproduce the total system performance assessment (TSPA) results supporting the License Application (LA). That work is documented in the report by Lee and Hadgu (2014). In late 2014 the computer hardware was again replaced with an efficient and updated TSPA cluster and storage system to allow expedited reproduction of the TSPA-LA results.

SNL conducted this 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 report by Lee and Hadgu (2014) documented the work performed prior to 2015 to achieve and maintain the readiness of the computing infrastructure (computer hardware and software) and knowledge capability to perform TSPA-type analyses. This report documents work performed since then to evaluate the upgraded TSPA cluster (CL2014) and the overall computing system. This report provides 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.

As was done in previous work (Lee and Hadgu, 2014) the goal 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. As was also done previously, the following main topics were identified for the investigation to evaluate the status of the TSPA-LA model capability on the TSPA CL2014 cluster.

- TSPA server cluster hardware

- GoldSim and other supporting software
- TSPA-LA model file retrieval
- TSPA-LA model execution on the TSPA server cluster
- TSPA-LA model reproducibility verification
- Post-processing of the output of TSPA-LA model run on CL2014

The above topics are discussed in more detail in Section 2.

2. APPROACH

Below are details of the topics listed in Section 1, identified as necessary steps to achieve the goal.

- Evaluation and maintenance of the current TSPA cluster (CL2014) for stable operations to support reliable executions of the TSPA-LA models and associated analysis and calculations.
- Retrieval of the required input files and other associated files of the TSPA-LA scenarios and/or scenario modeling cases. These files are cataloged in an archive facility by means of their Data Tracking Numbers (DTN). The archive files associated with each DTN are stored on the access-controlled read-only "Collab5" folder that resides on a Sandia network drive (named as \\FS02SNLNTY), located in Building 880 Annex inside Tech Area (TA) 1 of SNL/Albuquerque.
- Execution of the TSPA-LA model on the TSPA cluster (CL2014), ensuring reliable run executions utilizing the GoldSim (Ver. 9.6.300) distributed processing module (GoldSim, 2007) and reproducible stochastic sampling schemes (GoldSim, 2007). The model reproducibility was evaluated and verified by comparing the output of the model run using CL2014 to those retrieved from the TSPA-LA model output DTNs. The reproducibility verification was performed with the Excel spreadsheet.
- Post-processing of TSPA model test run output results from CL2014 to generate the final model output in the format that is consistent with those presented in the TSPA-LA model report (SNL 2008). The EXDOC analysis (DOE 2007) was the primary post-processing of the model output for the current work. Because of a large amount of information of the post-processed model output results, selected subsets of the post-processed model output results were compared to those from the model output DTNs to verify the post-processing reproducibility.
- Generation of the plots of the post-processed results of the model output using CL2014 in a format that is consistent with those published in the TSPA-LA model report (SNL 2008). The model reproducibility and post-processing reproducibility verification was performed graphically by comparing the plots of the model output using CL2014 with the respective plots published in the TSPA-LA model report.

The sections that follow discuss the results of the evaluations of the above selected topics, including identification of the issues or concerns and the measures taken to correct and/or improve them, which are needed to make the system operational and maintain the TSPA model capability.

3. THE TSPA-LA COMPUTING SYSTEM

The TSPA-LA computing system which constitutes the hardware and software is discussed in this section.

3.1. TSPA Server Cluster Hardware (CL2014)

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). The distributed processing 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.

Previously storage capacity was identified as an area for improvement (Lee and Hadgu, 2014). Storage limitations for TSPA model output have now been addressed with the 2014 TSPA computing system. Adequate storage space has now been allocated for the 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.

3.2. GoldSim Software

GoldSim software (GoldSim 2007) was used to develop the TSPA-LA model and GoldSim is a stochastic sampling program that integrates data with the model components and submodels of the TSPA-LA model, which allows simulation of repository performance for each realization of uncertain parameters. GoldSim manages the flow of information between and among the external process models, the model components and submodels, and the abstractions provided to the TSPA-LA model. Multiple realizations of the TSPA-LA Model yield a probability distribution of dose rate in the biosphere that shows uncertainty in dose rate based on uncertainty in all of the submodels. The latest TSPA-LA models (SNL 2008) were developed with GoldSim Version 9.60.300 or 9.60 Service Pack 3 (SP3), however, some models were developed with 9.60.100 (SP1), a version earlier than SP3 (GoldSim 2007).

Currently one GoldSim software floating license is installed on the TSPA server cluster head node. The cluster processors have been mapped for the distributed processing capability of GoldSim Version 9.60.300 (SP3) (GoldSim 2007). As discussed in more detail in Section 3.6, the TSPA-LA models were retrieved from the model output DTNs and were opened and saved successfully on the server cluster storage folder with GoldSim Version 9.60.300 (SP3) for the current study.

As pointed out in Section 4 below GoldSim 9.60.300 compute processes are limited to 10 processes per compute node.

3.3. EXDOC Software

The results generated from the GoldSim TSPA-LA Model undergo further processing to calculate the distribution of expected annual doses for each scenario class, where the term "expected annual dose" refers to the expectation of annual dose over aleatory and epistemic uncertainty (DOE 2008; Helton et al. 2014).

Aleatory uncertainty, which is also referred to as inherent or irreducible uncertainty, is the uncertainty related to the inherent randomness of the problem (such as random external events that affect safety, e.g., seismicity). *Epistemic* uncertainty, which is also referred to as reducible uncertainty, is the uncertainty related to lack of precise data (such as the uncertain composition of the current inventory of commercial spent nuclear fuel). Epistemic uncertainties can be reduced by data-gathering methods, including additional site characterization, design studies, fabrication and other demonstration tests, and other experiments both in the laboratory and in underground test facilities.

The GoldSim TSPA-LA Model results are further processed with EXDOC_LA V2.0 (DOE 2007) to determine the expected dose for each modeling case and a total expected dose combining all of the modeling cases. The overall purpose of the EXDOC post-processing is to separate aleatory and epistemic uncertainty. The solution is integrated over the aleatory uncertainty, for fixed values of the epistemic parameters, to calculate an expected value, conditional on one epistemic element. This operation is repeated for each sample element, to obtain a group of expected results. Statistics (i.e., mean and percentiles) are calculated for these results. Therefore, GoldSim and EXDOC_LA V2.0 are both required to generate the expected dose from the TSPA-LA model output. EXDOC instructions did not always include the complete steps to conduct an EXDOC run. Appendix C includes additional instruction material to provide missing information.

EXDOC_LA V2.0 software and associated input files were downloaded from the access-controlled read-only folder that resides on the \\FS02SNLNTY network drive (\\FS02SNLNTY\PAcronusL\TSPA-LA\Controlled_Files_03\EXDOC_Software), and the associated input files were downloaded from the EXDOC input file folder, \\FS02SNLNTY\PAcronusL\TSPA-LA\Controlled_Files_03\EXDOC_Input_Files.

3.4. Supporting Software

3.4.1. SigmaPlot Software

Plots for the TSPA-LA model output results (SNL 2008) were created with SigmaPlot Version 8.0. SigmaPlot Version 8 or later versions is required to open and view the plots and data of the plot files contained in the TSPA-LA model output DTN. Also, the software is required to create plots for some output results (e.g., "horsetail plots" of 300 time-history data sets) of TSPA-LA model runs of the current study. For instance the popular and easily accessible Excel graphing software is not adequate for horsetail plots (typically 300 data sets) of TSPA-LA model output as the maximum number of data sets allowed for a plot is 250.

Currently a standalone SigmaPlot Version 13.0 has been installed on the CL2014 TSPA cluster. A standalone SigmaPlot Version 12.5 has also been installed on a PC. Post processing of the model output was done on both software versions.

3.4.2. Other Supporting Software

As reported in Lee and Hadgu (2014) previous versions of the WinZip software were not adequate to fully unzip many TSPA-LA model output DTN files, and because the DTN files have many layers of the file folder structure, hence very long character strings for the file folder locations within the DTN file. Thus, the PKZIP software was used to unzip the TSPA-LA model

output DTN files. In addition, WinZip 12.0 has now increased capabilities than previous versions and is able to open TSPA-LA zipped files.
MVIEW V4.0 (DOE 2005) software is a stand-alone executable program that transforms text output describing numeric model geometry and numeric model output into two-dimensional and three-dimensional visual representations. The software was used to interpret the results of the TSPA-LA model using two-dimensional and three-dimensional visual representations and also used to statistically analyze the TSPA-LA model output. This software was not used for the current study, but will be required for a full statistical analysis of the TSPA-LA model output results. Confirmation of the statistical and sensitivity analysis will be part of future work.

Although not required for the current study, other software that may be needed for future TSPA-LA model exercise and model production runs includes a FORTRAN compiler and MathCad.

3.5. TSPA Cluster Hardware Setup and Configuration

Cluster CL2014 was setup and configured for the TSPA analyses. Symantec Endpoint Protection (SEP) that was installed on the servers has been uninstalled to ensure performance. The new 32 machines were assigned the names CL2014-1 to CL2014-32 for accounting purposes. The machine CL2014-1 was then assigned as the head node from where all GoldSim runs are to be initiated and where results are temporarily stored. CL2014-2 through CL2014-32 have been assigned as compute nodes, with a total of 620 possible compute processors. The GoldSim compute process is launched automatically by GoldSim compute manager.

GoldSim Version 9.60.300 has been installed on Cluster CL2014. All CL2014 cluster Basic Input Output System (BIOS) settings have been set to “default”, with the exception of power management profile, which has been changed to “performance”. This setting disables some power saving features of the system so that the CPUs are always ready. Tests showed this setting to be beneficial for GoldSim simulations.

Launching GoldSim in the distributed mode requires listing the compute processors that are to be used for the specific run. Scripts have been written that allow use of several combinations of processors. Run _setup.bat is a script that sets up the job with number of nodes and number of processors per node. Running Run_setup.bat prompts the user to specify the number of nodes and processors per node (CPUs). A text file is created that contains the chosen number of nodes and processors per node. The newly created text file name will then identify the set up. The user copies the content of that file into a blank text file and saves it with a .slv extension (renaming the generated file is not an option. Formatting does not allow that file to be imported into GoldSim). The user imports the newly created .slv file into GoldSim during “run on the network” set up. This script has been tested on GoldSim Version 9.60.300 and GoldSim Version 10.5.1. Further discussion can be found in Appendix A.

Testing various combinations of processors using GoldSim 9.60.300 showed that for each compute node a maximum of 10 processors can be used. Thus, even though each node has a maximum of 20 processors, only ten of them can be used for GoldSim 9.60.300 runs. This has been confirmed with GoldSim staff. These limitations have been removed in later versions of GoldSim. This limits the total number of processors available to execute a TSPA model run to a maximum of 310 when GoldSim 9.60.300 is used..

After the GoldSim runs are completed compute processes may not close properly. It is therefore strongly advised that the user reboot the cluster prior to each new GoldSim run. This will avoid having hung processes, and will ensure performance by stopping any scans or update installs from interfering. Cluster_reboot.bat is a batch file that will reboot all systems except CL2014-1. The bat file can be used to reboot the compute nodes. This is further discussed in Appendix A.

3.6. TSPA-LA Model File Retrieval

Reliable retrieval of the GoldSim TSPA-LA model files and associated files from the model output Data Tracking Number (DTN) was an important phase of the current study. To evaluate this, the following model output DTNs in a zipped file format were downloaded from the Collab5 folder of the FS02SNLNTY network server (\\FS02SNLNTY\Collab5\DTN2) (Table 1).

Table 1. Output Data Tracking Numbers (DTNs) Used

DTN MO0710ADTSPAWO.000: GW Modeling cases (v5.005) without Final Documentation
DTN MO0710PLOTSFIG.000_R1: Plots and Figures for TSPA-LA Addendum (v5.005)
DTN MO0801TSPAWPDS.000_R0: TSPA-LA Addendum, Waste Package and Drip Shield Degradation Analysis
DTN MO0801TSPAWPDS.000_R1: TSPA-LA Addendum, Waste Package and Drip Shield Degradation Analysis
DTN MO0806TSPADCOR.000_R0: TSPA DTN Corrections
DTN MO0709TSPAPLOT.000: Plots and Figures that originate from Groundwater cases (v5.000) and Igneous Eruptive cases (vE1.004)
DTN MO0709TSPAREGS.000: TSPA-LA Model (GW & E) Used for Regulatory Compliance

A suggestion was made for application of the PKZIP software to unzip the DTN files as the software was used to prepare the TSPA-LA model output DTN files. Because Sandia does not have a site license, a free trial version of the PKZIP software was downloaded from the company Web site (PKWARE, Inc.) for test purpose. The software unzipped successfully all DTN files with no errors or warnings. For instance, after complete unzipping, DTN MO0801TSPAWPDS.000_R1 contains a total of 202 files in 28 folders with the total combined size of about 11 gigabytes excluding the original zipped files; DTN MO0710ADTSPAWO.000 contains a total of 5,571 files in 109 folders with the total combined size of ~84 GB excluding the original zipped files.

The use of the PKZIP software resolved the issues associated with the unzipping of the TSPA-LA model output DTNs and retrieval of the TSPA-LA model files. A single license of the software was purchased and is installed on the cluster head node.

4. EXECUTION OF TSPA-LA MODELS ON THE SERVER CLUSTER

The TSPA-LA models that were retrieved from DTN MO0710ADTSPAWO.000 ("GW Modeling cases (v5.005) without Final Documentation") (SNL 2008) were executed on the TSPA server cluster to evaluate performance of the cluster and its operating system for TSPA-LA model runs and to verify reproducibility of the TSPA-LA model output. Required dynamic link library (DLL) files and input files were obtained following the directions in the document called "ReadMe_Rev01.doc" contained in the DTN. The readme document also provides necessary steps and preparations for TSPA-LA model runs. The following modeling cases were run on the server cluster for the current study:

- Nominal Modeling Case (300 realizations)
- Human Intrusion Scenario (9,000 realizations)
- Drip Shield Early Failure Modeling Case (3,000 realizations)
- Waste Package Early Failure Modeling Case (6,000 realizations)
- Seismic Ground Motion Modeling Case (9,000 realizations)
- Seismic Fault Displacement Modeling Case (10,800 realizations)
- Igneous Intrusion Modeling Case (3,000 realizations)
- Volcanic Eruption Modeling Case (12,000 realizations)
- Total Dose

All runs were executed on multiple processors on the cluster servers utilizing the GoldSim distributed processing modules (GoldSim 2007) (typically running each modeling case on 100 processors simultaneously). All runs were completed successfully. For each GoldSim simulation of the TSPA-LA model for the above modeling cases, the following steps are to be taken carefully to ensure successful execution and stable model output.

- Run the batch file Run_setup.bat to create a text file that contains the chosen number of nodes and processors per node.
- Copy the content of the new text file into a blank text file and save it with .slv extension.
- Open the GoldSim model and select Run on Network. Import the newly created .slv file during "Run on Network" set up. This prepares the selected processors of the compute nodes to connect to and accept the run execution directions from the master program of the GoldSim distributed processing module that is executed on the head node.
- Select "Update Status" to launch the selected processors.
- Execute the TSPA model.

Monitor the run status frequently and the progression of the model run on the compute nodes. If there are issues, the run can be terminated to save time. Once the problems have been addressed the run would then be restarted. Further discussion of the steps followed in the execution of the TSPA runs is given in Appendix A.

5. VERIFICATION OF TSPA-LA MODEL RUN RESULTS

This section discusses the verification of the TSPA-LA model reproducibility on the TSPA server cluster. Outputs of the runs using CL2014 of the TSPA-LA models of the modeling cases discussed in Section 4 were evaluated for the verification analysis. The model reproducibility verification was conducted by comparing the output from the model runs using CL2014 with the output retrieved from the DTN MO0710ADTSPAWO.000 (GW Modeling cases (v5.005) without Final Documentation) (SNL 2008). Two approaches were used for the verification effort: 1) numerical value comparison, and 2) graphical comparison.

5.1. Model Reproducibility Verification by Numerical Value Comparison

The model reproducibility verification by numerical value comparison was conducted for all the TSPA-LA modeling cases. The model output parameter Dose_Total was chosen for the reproducibility verification. The numerical value comparisons for the parameter were conducted for the values of the model output after post-processing. For each modeling case the post processed average of the mean expected annual dose from the new model run was compared with its respective value from the TSPA-LA model output retrieved from DTN MO0710ADTSPAWO.000. Excel spreadsheet calculations were performed to calculate the relative percentage difference of the new model output values as follows.

$$Difference\ (\%) = \frac{Abs\left(Dose_{LA} - Dose_{new\ run}\right)}{Dose_{LA}} \times 100$$

$Dose_{LA}$ is the dose value of the TSPA-LA model output, and $Dose_{new\ run}$ is the dose value of the output of new model run for the current study. Table 2 shows results of the comparison. The average relative percentage difference values of the selected output parameter are very small for all the modeling cases, demonstrating an excellent reproducibility. Comparison of the actual total dose values shows that the differences in output are even smaller.

Table 2. **Average relative difference for all modeling cases (using Equation 1)**

Modeling Case	Average Relative Difference %
Total Dose 10^6 Years	0.049
Total Dose 10^4 Years	0.004
Nominal Case 10^6 Years	0.031
Human Intrusion 10^6 Years	0.046
Drip Shield Early Failure 10^6 Y	0.037
Drip Shield Early Failure 10^4 Y	0.011
Waste Package Early Failure 10^6 Years	0.068
Waste Package Early Failure 10^4 Years	0.013
Seismic EF 10^6 Years	0.107
Seismic EF 10^4 Years	0.001
Seismic GM 10^6 Years	0.064
Seismic GM 10^4 Years	0.004
Igneous Intrusion 10^6 Years	0.020
Igneous Intrusion 10^4 Years	0.010
Volcanic Eruption 10^6 Years	0.002
Volcanic Eruption 10^4 Years	0.0

5.2. Model Reproducibility Verification by Graphical Comparison (Part I)

This section discusses the verification of the TSPA-LA model reproducibility on the server cluster by comparing the plots of output of new model runs using CL2014 with those reported in the TSPA-LA report (SNL 2008). Generation of comparable plots for the new model run output requires post-processing of the model output with EXDOC (DOE 2007). Outputs of EXDOC were used for the comparison.

Plots of "expected annual dose" of the modeling cases were chosen for the model reproducibility verification by graphical comparison. The plots are for the EXDOC post-processed result of output parameter "Dose_Total" of the TSPA-LA model output for each of the modeling cases. The plots also show probabilistic projections of expected annual dose.

5.2.1. Calculation of Total Expected Annual Doses

The TSPA-LA report (SNL 2008, Section 8.1.1[a]) documents projections of postclosure performance for comparison with the Postclosure Individual Protection Standard, one of the three radiation protection standards adopted by the NRC (10 CFR Part 63). The expected annual dose histories for the reasonably maximally exposed individual (RMEI) from each of the modeling cases are plotted for each realization for the 10,000 years and 1 million years modeling periods. The total mean annual dose of the combined (i.e. the sum of the modeling cases) expected dose histories is the performance measure for comparison with the Postclosure Individual Protection Standard. In this section we show comparisons of simulation results from the TSPA-LA with test runs of this study for distributions of total expected annual dose (i.e., summed over all modeling cases) for the 1,000,000 years modeling period. The output results were obtained using a GoldSim file that combines the dose histories of the individual models. Figure 1 shows comparisons of plots of distributions of total expected annual dose for the 1,000,000 years modeling period, as well as the total mean (red) dose curve and total median (blue) dose curve (Helton et al. 2014). As shown in the figure the results are almost identical. Figure 2 shows comparisons of plots of total expected annual dose for the 10,000 years modeling period. As in Figure 1, the results are almost identical. This demonstrates an excellent reproducibility of the Total Expected Annual Dose for 1, 000,000 years and 10,000 years modeling periods.

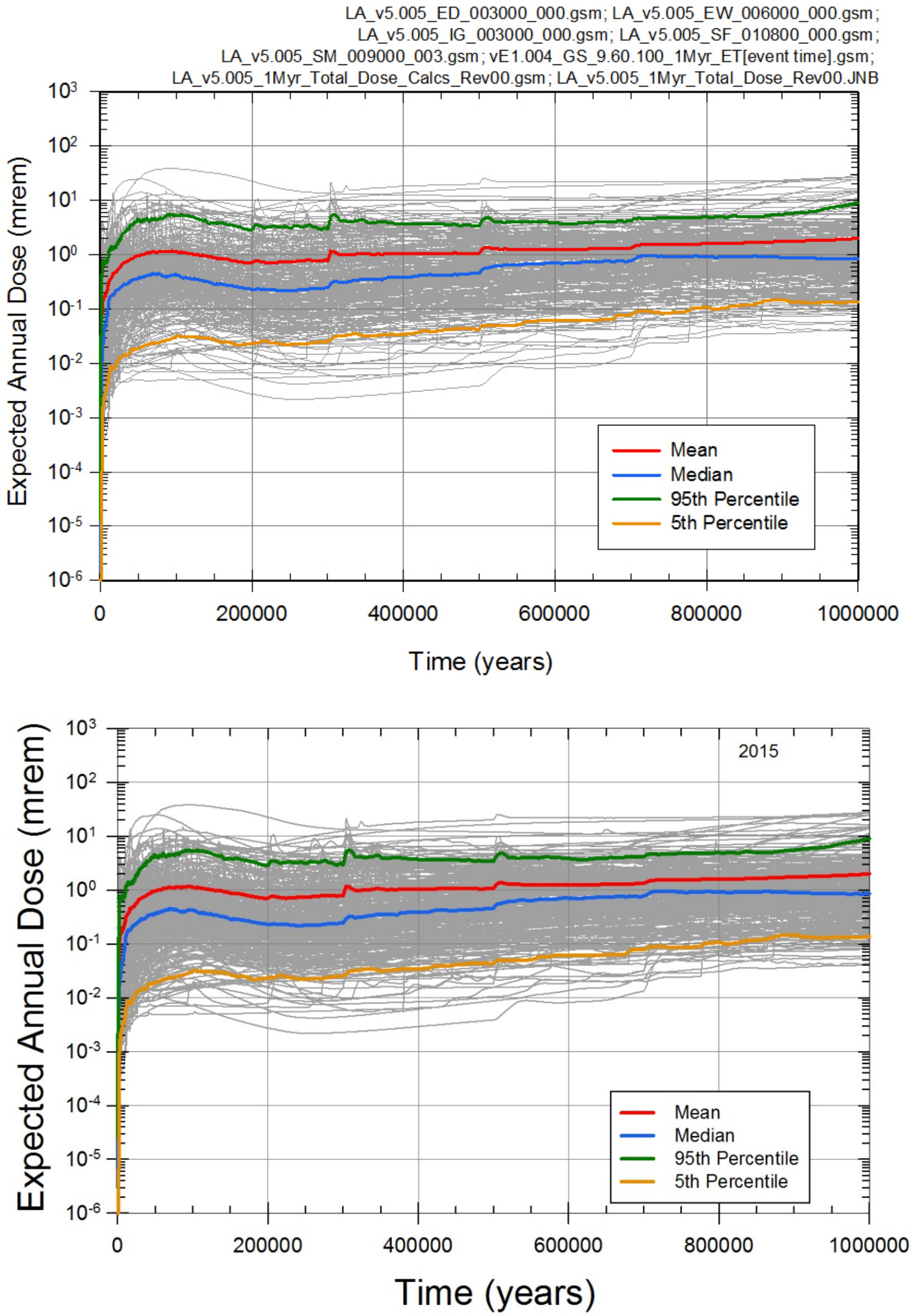


Figure 1. Comparison of Model Result for Distributions of Total Expected Annual Dose for 1,000,000 Years after Repository Closure: (top) TSPA-LA model (SNL 2008, Figure 8.1-2[a]), and (bottom) TSPA model test run of this study.

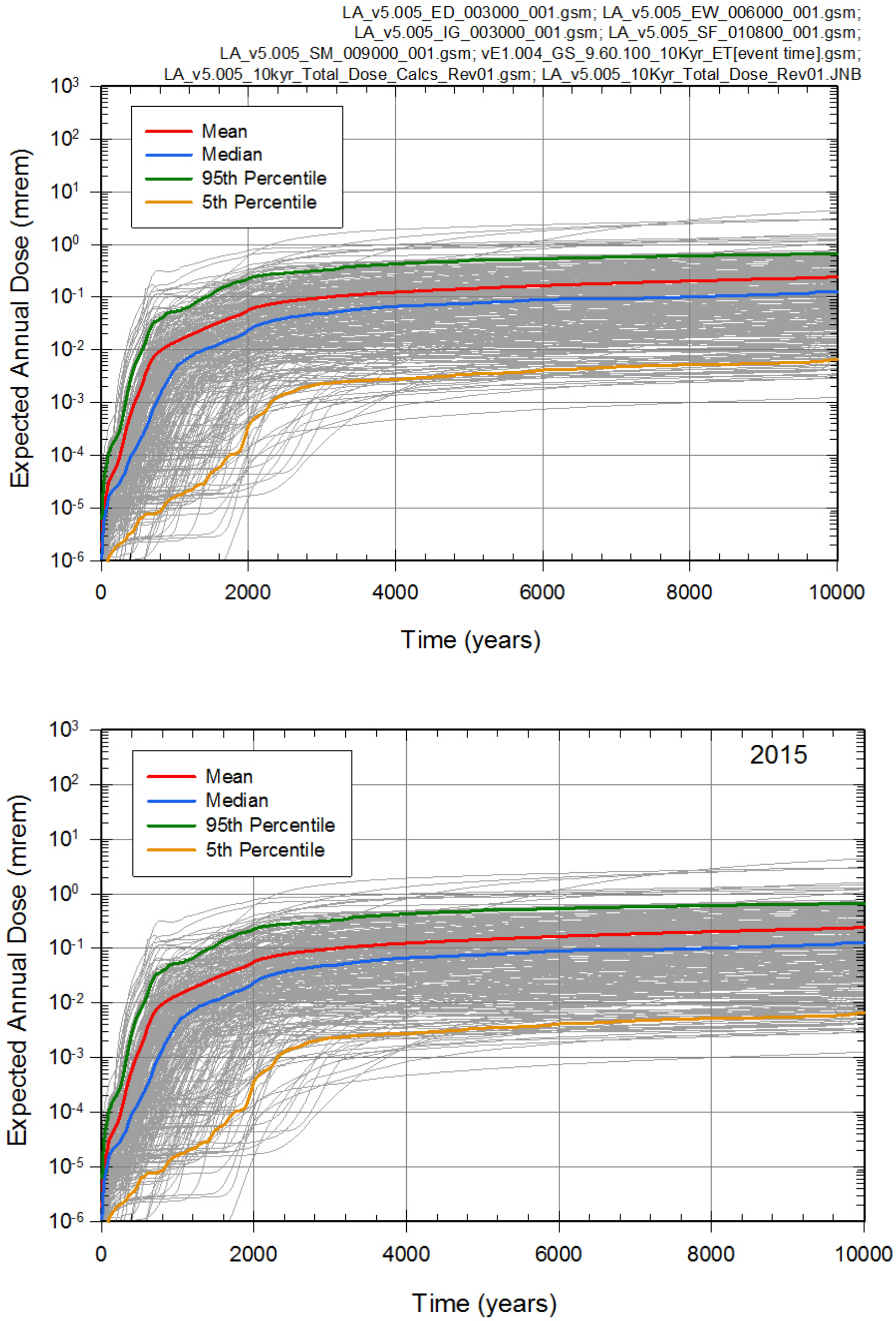


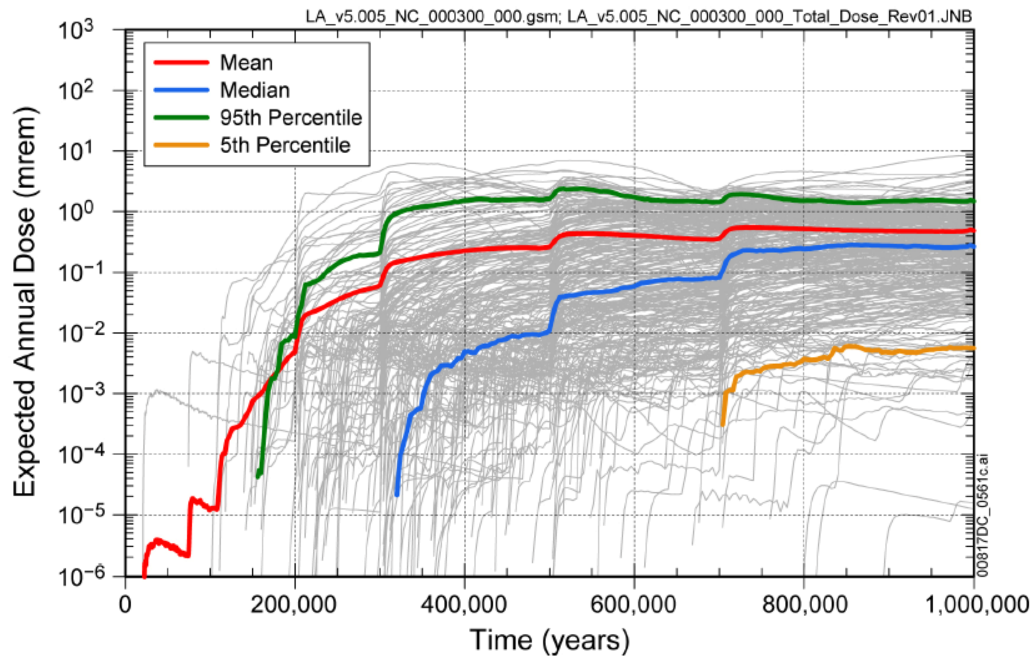
Figure 2. Comparison of Model Result for Distributions of Total Expected Annual Dose for 10,000 Years after Repository Closure: (top) TSPA-LA model (SNL 2008, Figure 8.1-1[a]), and (bottom) TSPA model test run of this study.

5.2.3. Nominal Modeling Case

EXDOC post-processing is not required for the Nominal Modeling Case because no aleatory uncertain parameter is associated with the modeling case. Figure 3 shows the model results of the distributions of expected annual dose for the Nominal Modeling Case for 1,000,000 years after repository closure for the original TSPA-LA model (top figure; SNL 2008, Figure 8.2-1[a]), and TSPA model test run of this study (bottom figure). Each figure shows horsetail plots for 300 expected annual doses, capturing effect of 300 sets of sampled epistemic uncertain parameters. The plots show probabilistic projections of expected annual dose, and the curves for the mean, median, and 5th and 95th percentiles of the distribution of expected annual doses for the simulation period.

The mean, median, and 5th and 95th percentile curves show uncertainty in the value of the expected annual dose, taking into account epistemic uncertainty associated with the modeling case. The mean expected annual dose history, which is plotted as the red curve, was computed by taking the arithmetic average of the 300 expected annual dose values, for individual time planes along the curves. Similarly, the median expected annual dose history, plotted as the blue curve, was constructed from points obtained by sorting the 300 expected values from lowest to highest, and then averaging the two middle values. Curves for the 5th and 95th percentiles are also plotted to illustrate the spread in the expected annual dose histories; 90 percent (or 270 of the 300 epistemic realizations) of the projected dose histories fall between these two percentile curves.

As shown in Figure 3, the plots of the two figures (top for the original TSPA-LA model result, and bottom for the model test run result of this study) are almost identical, and this was expected from the very small relative differences of all individual numerical values of the model output parameter discussed in Section 5.1. This demonstrates an excellent reproducibility of the Nominal modeling case for the 1,000,000 years modeling period.



Source: Output DTNs: MO0710ADTSPAWO.000 [DIRS 183752]; and MO0710PLOTSFIG.000 [DIRS 185207].

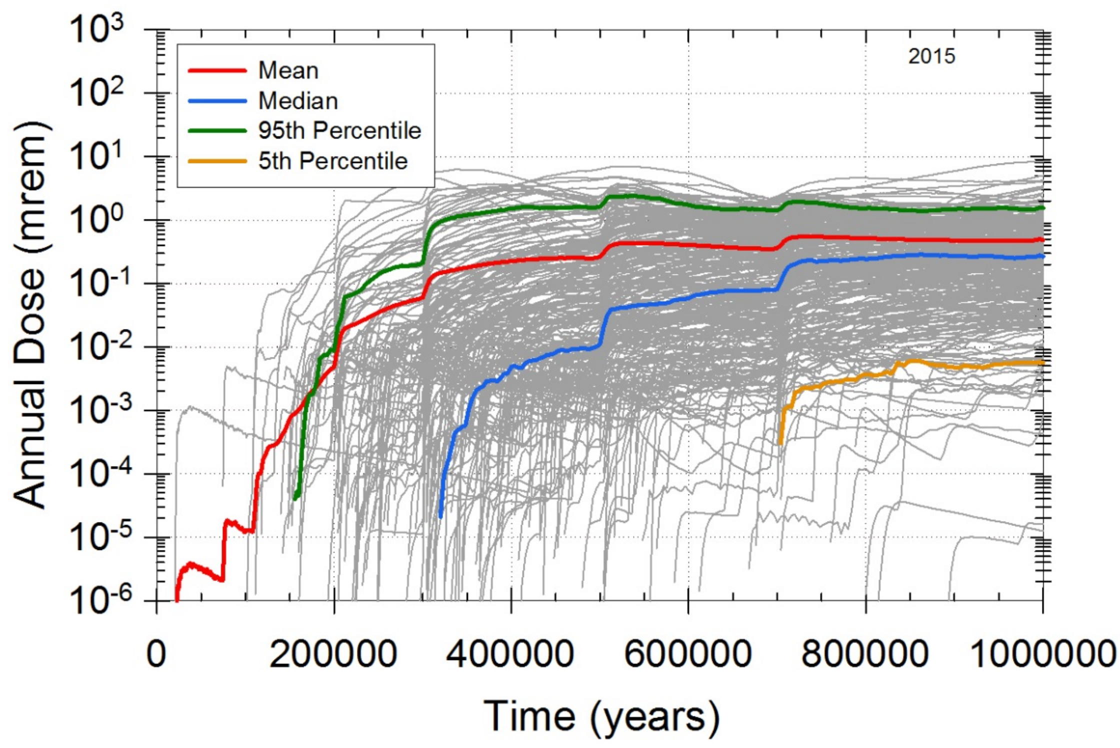


Figure 3. Comparison of Model Result for Distributions of Expected Annual Dose for the Nominal Modeling Case for 1,000,000 Years after Repository Closure: (top) TSPA-LA model (SNL 2008, Figure 8.2-1[a]), and (bottom) TSPA model test run of this study.

5.2.2. Human Intrusion Scenario

The TSPA-LA report (SNL 2008, Section 8.1.3.2[a]) also documents modeling simulations done to address the requirements of the Human Intrusion Standard. Results of TSPA probabilistic simulations were used to make projections of the annual dose following a human intrusion. The calculations of expected annual dose account for only the radionuclides released into groundwater as a consequence of the intrusion. The earliest time after disposal for the drilling intrusion was taken to be 200,000 years. The scenario considers aleatory uncertainty in the type of WP assumed to be penetrated and the location of the penetration, both within the repository footprint and in the underlying SZ.

The TSPA-LA model for the Human Intrusion Scenario has 30 associated aleatory uncertain parameters, and the model simulation comprises of 9,000 realizations (i.e., 300 sets of sampled epistemic uncertain parameters × 30 aleatory uncertain parameters per epistemic uncertain parameter set). EXDOC post-processing was used for Human Intrusion Modeling Scenario case. In the post-processing steps there is no option specified for the Human Intrusion Case. Thus, the Seismic Ground Motion (1 million years) option is selected, as it has the same number of aleatory uncertain parameters.

Table 3 lists the input parameter values for EXDOC analysis of TSPA-LA model test run output parameter "Dose_Total" for the Human Intrusion Scenario for 1,000,000 years after repository closure. Figure 4 shows the post-processed model result of the distributions of expected annual dose for the modeling scenario for 1,000,000 years after repository closure: top figure for the "original" TSPA-LA model (SNL 2008, Figure 8.2-16[a]) and bottom figure for the TSPA model test run of this study. As shown in Figure 4, the plots of the two figures are almost identical, and this demonstrates an excellent reproducibility of the original TSPA-LA model result by the model test run on the CL2014 TSPA cluster.

Table 3. Input Parameters for EXDOC Analysis of TSPA-LA Model Test Run Output "Dose_Total" for the Human Intrusion Modeling Scenario for 1,000,000 Years after Repository Closure

Input Parameters Recorded in EXDOC File "info_mc.dat"
Dose_Total !prefix quantiles.txt ! quantile filename 300 ! sample size 499 ! number of timesteps in input 1 ! number of aleatory files 30 ! aleatory sample size 3 ! number of quantiles considered 1 ! LHS element saved 1 ! analysis done (1:expected value; 2 or 4 CCDF; 3 or 5: both 0 ! option on log file
Input Parameters Recorded in EXDOC File "expc_mc.dat"
1 ! regulatory value over aleatory(1:expc; 2:quant; 3:min(quant,expc)) 1 ! regulatory value over epistemic (1:expc; 2:quant; 3:min(quant,expc))
Input Parameters Recorded in EXDOC File "ccdf_mc.dat"
1000000 ! time saved for CCDF 100 ! nber of doses considered for the statistics on the CCDF 1 ! type of discretization for statistics (0=linear ; 1=log)

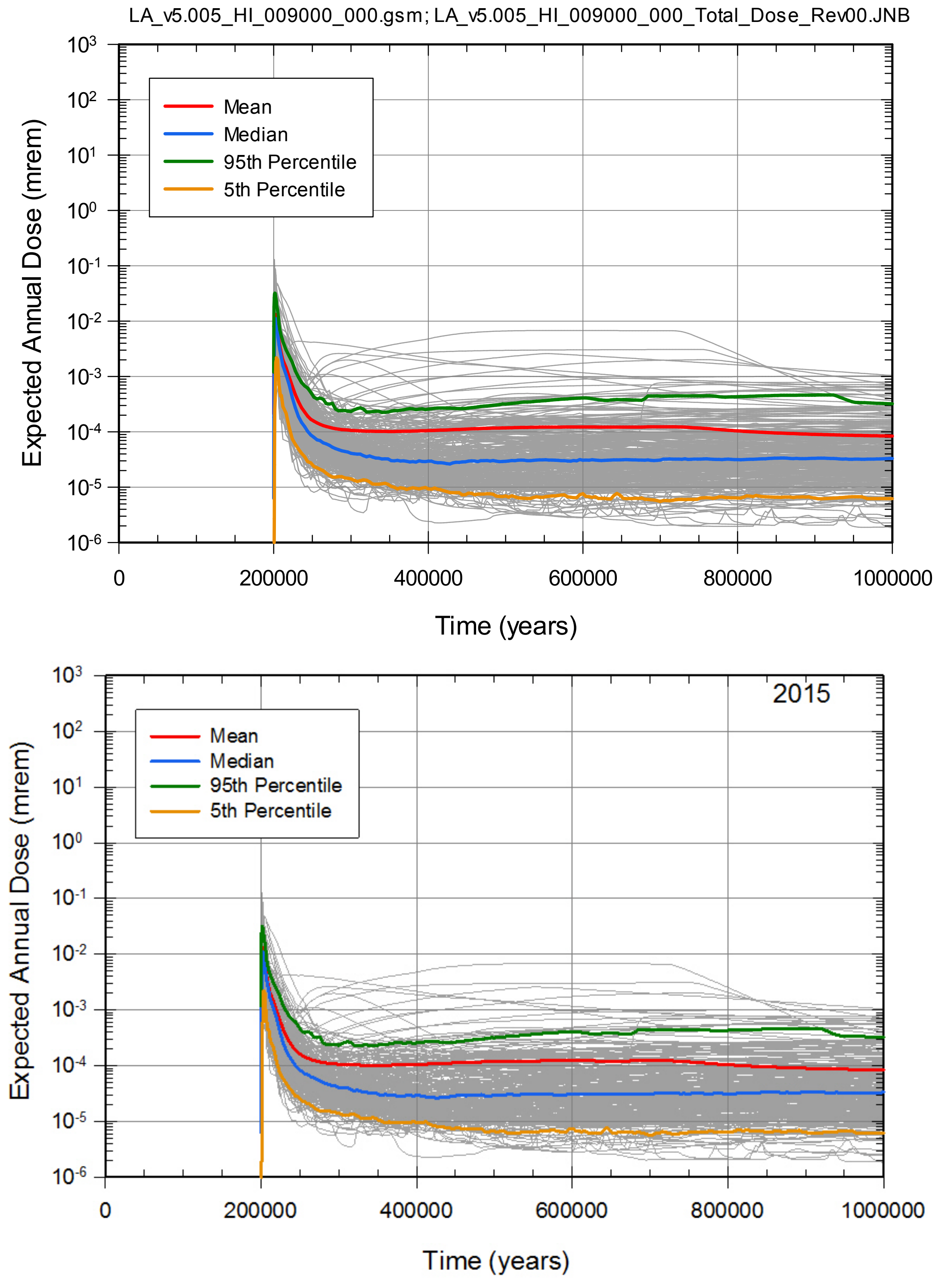


Figure 4. Comparison of Model Result for Distributions of Expected Annual Dose for the Human Intrusion Scenario for 1,000,000 Years after Repository Closure: (top) TSPA-LA model (SNL 2008, Figure 8.1-16[a]), and (bottom) TSPA model test run of this study.

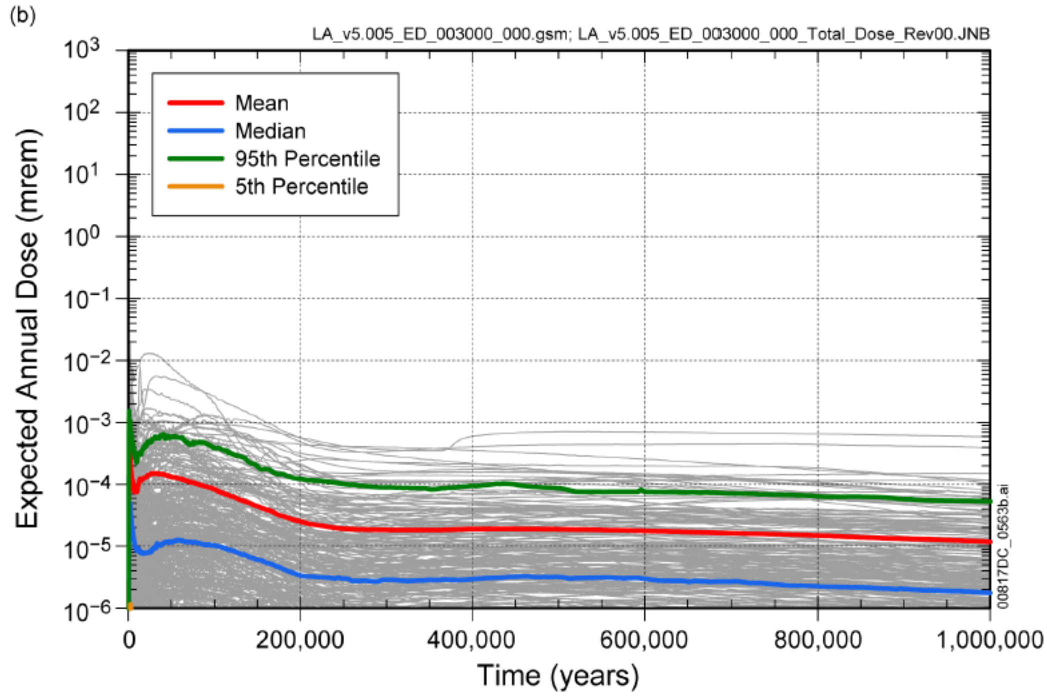
5.2.4. Drip Shield Early Failure Modeling Case

The TSPA-LA model for the Drip Shield Early Failure Modeling Case has 10 associated aleatory uncertain parameters, and the model simulation comprises 3,000 realizations (i.e., 300 sets of sampled epistemic uncertain parameters × 10 aleatory uncertain parameters per epistemic uncertain parameter set).

Tables 4 and 5 list the input parameter values for EXDOC analysis of TSPA-LA model test run output parameter "Dose_Total" for the Drip Shield Early Failure Modeling Case for 1,000,000 years and 10,000 years after repository closure, respectively. Figure 5 shows the post-processed model result of the distributions of expected annual dose for the modeling case for 1,000,000 years after repository closure: top figure for the "original" TSPA-LA model (SNL 2008, Figure 8.2-3[a]) and bottom figure for the TSPA model test run of this study. Figure 6 shows the corresponding plots for the 10,000 years simulation period after repository closure. As shown in Figures 5 and 6, the plots of the TSPA-LA and new model test run figures are almost identical, and this demonstrates an excellent reproducibility of the original TSPA-LA model result by the model test run on the cluster.

Table 4. Input Parameters for EXDOC Analysis of TSPA-LA Model Test Run Output "Dose_Total" for the Drip Shield Early Failure Modeling Case for 1,000,000 Years after Repository Closure

Input Parameters Recorded in EXDOC File "info_tr.dat"
Dose_Total ! prefix 300 ! sample size 471 ! number of timesteps 10 ! aleatory sample size 3 ! nb of aleatory parameters 3 2 1 ! order of alea. parameters 1 2 5 ! size of alea. parameters 1 ! position for alea parameter 0 1 2 ! position for alea parameter 1 1 2 3 4 5 ! position for alea parameter 2 6 ! log file indicator
Input Parameters Recorded in EXDOC File "info_cv.dat"
Dose_Total !prefix ED_lambda.txt ! lambda filename PS_frac.txt ! bins fractions filename Seep_frac_1M.txt ! Drip fractions filename wp_frac.txt ! WP fractions filename quantiles.txt ! quantile filename 300 ! sample size 471 ! number of timesteps in input 5 ! number of bins considered 2 ! number of WPs considered 3 ! number of quantiles considered 1 ! analysis done (1:expected value; 2 or 4 CCDF; 3 or 5: both 6 ! option on log file
Input Parameters Recorded in EXDOC File "expc_cv.dat"
1 ! sum over WP (0=no, 1=yes) 1 ! sum over bin (0=no, 1=yes) 1 ! sum over drip. cond. (0=no, 1=yes) 1 ! regulatory value over epistemic (1:expc; 2:quant; 3:min(quant,expc))
Input Parameters Recorded in EXDOC File "ccdf_cv.dat"
1000000.00 ! time saved for CCDF 1000 ! sample size 500 ! nber of doses considered for the statistics on the CCDF 2 ! type of discretization for statistics (0=linear ; 1=log)



Source: Output DTNs: MO0710ADTSPAWO.000 [DIRS 183752]; and MO0710PLOTSFIG.000 [DIRS 185207].

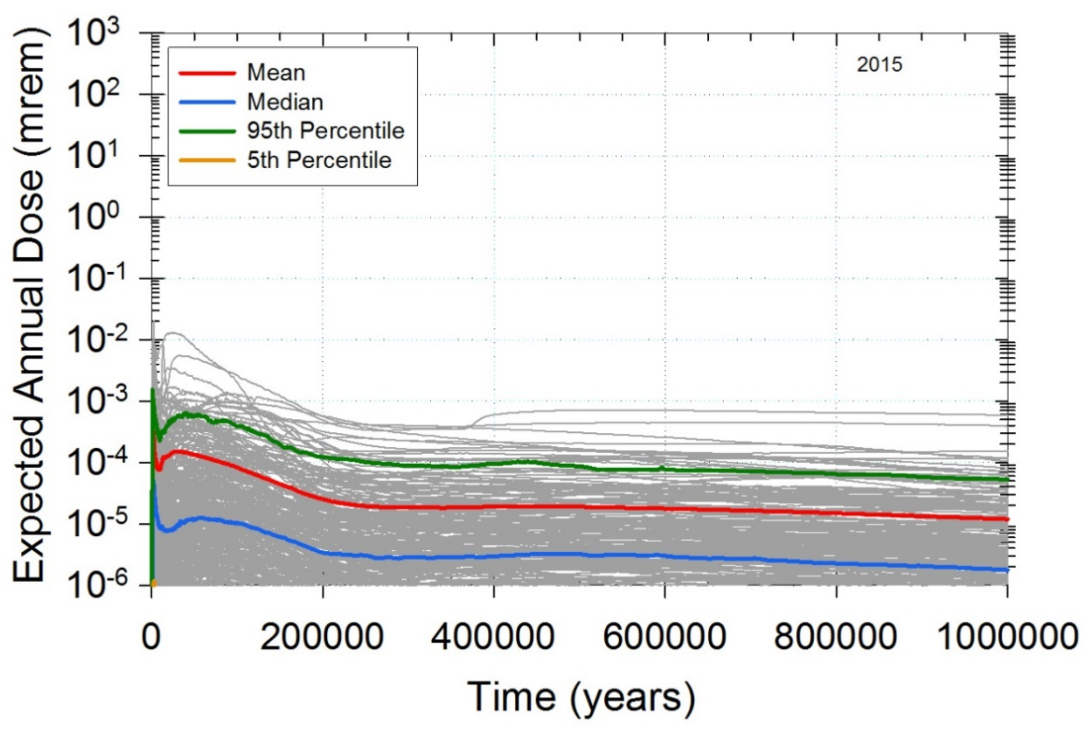


Figure 5. Comparison of Model Result for Distributions of Expected Annual Dose for the Drip Shield Early Failure Modeling Case for 1,000,000 Years after Repository Closure: (top) YMP TSPA-LA model (SNL 2008, Figure 8.2-3[a]), and (bottom) TSPA-LA model test run of this study.

Table 5. Input Parameters for EXDOC Analysis of TSPA-LA Model Test Run Output "Dose_Total" for the Drip Shield Early Failure Modeling Case for 10,000 Years after Repository Closure

Input Parameters Recorded in EXDOC File "info_tr.dat"
Dose_Total ! prefix 300 ! sample size 385 ! number of timesteps 10 ! aleatory sample size 3 ! nb of aleatory parameters 3 2 1 ! order of alea. parameters 1 2 5 ! size of alea. parameters 1 ! position for alea parameter 0 1 2 ! position for alea parameter 1 1 2 3 4 5 ! position for alea parameter 2 6 ! log file indicator
Input Parameters Recorded in EXDOC File "info_cv.dat"
Dose_Total !prefix ED_lambda.txt ! lambda filename ps_frac.txt ! bins fractions filename seep_frac_10k.txt ! Drip fractions filename wp_frac.txt ! WP fractions filename quantiles.txt ! quantile filename 300 ! sample size 385 ! number of timesteps in input 5 ! number of bins considered 2 ! number of WPs considered 3 ! number of quantiles considered 1 ! analysis done (1:expected value; 2 or 4 CCDF; 3 or 5: both 6 ! option on log file
Input Parameters Recorded in EXDOC File "expc_cv.dat"
1 ! sum over WP (0=no, 1=yes) 1 ! sum over bin (0=no, 1=yes) 1 ! sum over drip. cond. (0=no, 1=yes) 1 ! regulatory value over epistemic (1:expc; 2:quant; 3:min(quant,expc))
Input Parameters Recorded in EXDOC File "ccdf_cv.dat"
20000.00 ! time saved for CCDF 1000 ! sample size 500 ! nber of doses considered for the statistics on the CCDF 2 ! type of discretization for statistics (0=linear ; 1=log)

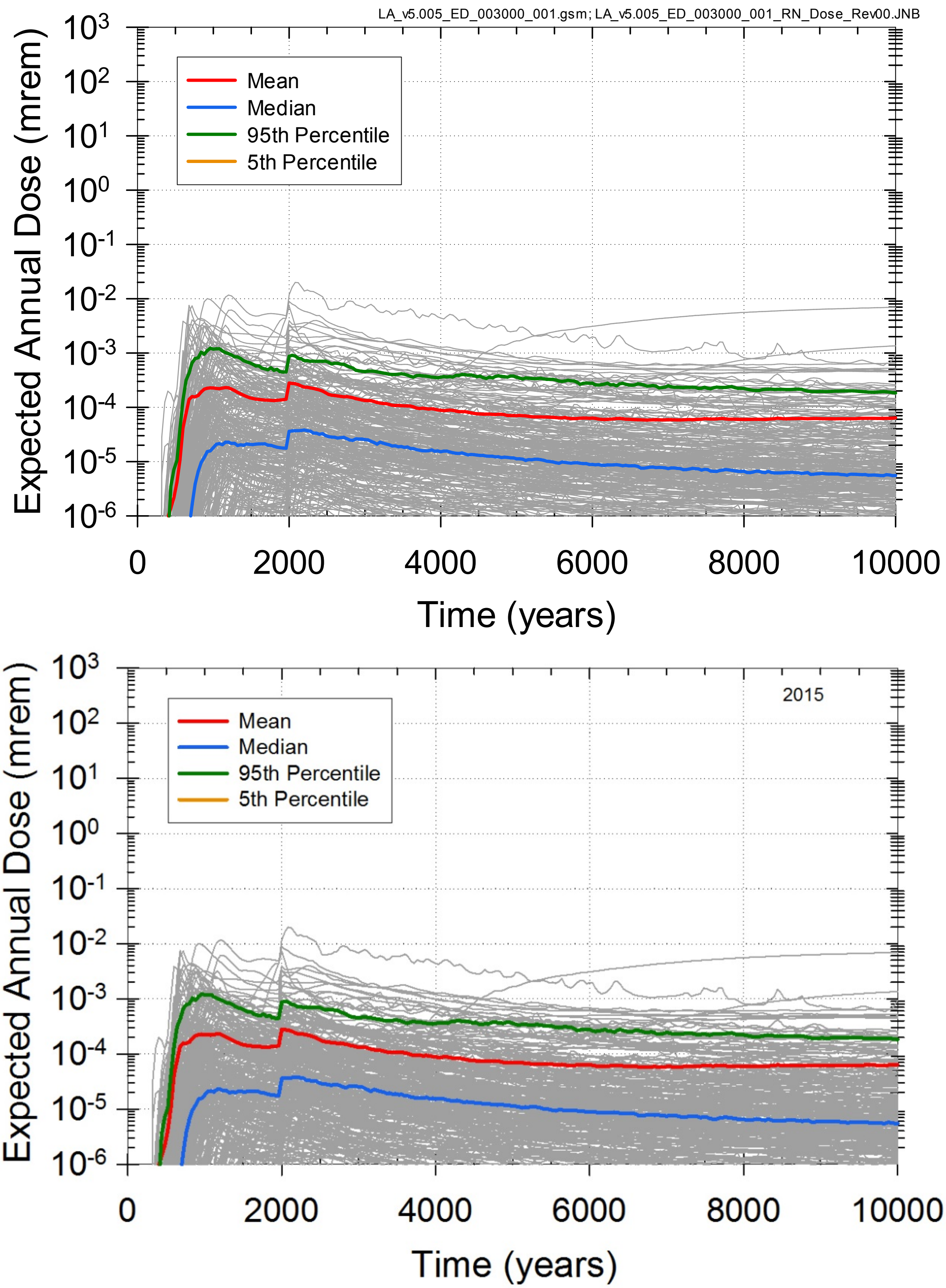


Figure 6. Comparison of Model Result for Distributions of Expected Annual Dose for the Drip Shield Early Failure Modeling Case for 10,000 Years after Repository Closure: (top) YMP TSPA-LA model (SNL 2008, Figure 8.2-3[a]), and (bottom) TSPA-LA model test run of this study.

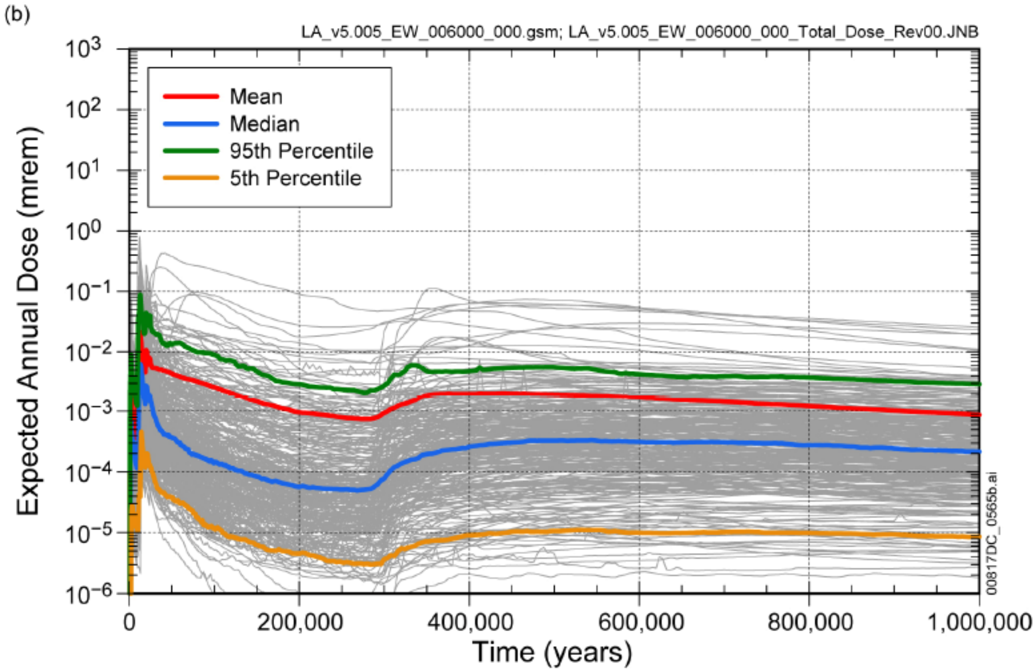
5.2.5. Waste Package Early Failure Modeling Case

The TSPA-LA model for the Waste Package Early Failure Modeling Case has 20 associated aleatory uncertain parameters, and the model simulation comprises 6,000 realizations (i.e., 300 sets of sampled epistemic uncertain parameters × 20 aleatory uncertain parameters per epistemic uncertain parameter set).

Tables 6 and 7 list the input parameter values for EXDOC post-processing analysis of TSPA-LA model test run output parameter "Dose_Total" for the Waste Package Early Failure Modeling Case for 1,000,000 years and 10,000 years after repository closure, respectively. Figure 7 shows the post-processed model result of the distributions of expected annual dose for the modeling case for 1,000,000 years after repository closure: top figure for the "original" TSPA-LA model (SNL 2008, Figure 8.2-5[a]) and bottom figure for the TSPA model test run of this study. Figure 8 shows the corresponding plots for the 10,000 years simulation period after repository closure. As shown in Figures 7 and 8, the plots of the TSPA-LA and new model test run figures are almost identical, and this demonstrates an excellent reproducibility of the original TSPA-LA model result by the model test run on the CL2014 cluster.

Table 6. Input Parameters for EXDOC Analysis of TSPA-LA Model Test Run Output "Dose_Total" for the Waste Package Early Failure Modeling Case for 1,000,000 Years after Repository Closure

Input Parameters Recorded in EXDOC File "info_tr.dat"
Dose_Total ! prefix 300 ! sample size 471 ! number of timesteps 20 ! aleatory sample size 3 ! nb of aleatory parameters 2 3 1 ! order of alea. parameters 2 2 5 ! size of alea. parameters 1 2 ! position for alea parameter 0 2 1 ! position for alea parameter 1 1 2 3 4 5 ! position for alea parameter 2 6 ! log file indicator
Input Parameters Recorded in EXDOC File "info_cv.dat"
Dose_Total !prefix EW_lambda.txt ! lambda filename ps_frac.txt ! bins fractions filename Seep_frac_1M.txt ! Drip fractions filename wp_frac.txt ! WP fractions filename quantiles.txt ! quantile filename 300 ! sample size 471 ! number of timesteps in input 5 ! number of bins considered 2 ! number of WPs considered 3 ! number of quantiles considered 1 ! analysis done (1:expected value; 2 or 4 CCDF; 3 or 5: both 6 ! option on log file
Input Parameters Recorded in EXDOC File "expc_cv.dat"
1 ! sum over WP (0=no, 1=yes) 1 ! sum over bin (0=no, 1=yes) 1 ! sum over drip. cond. (0=no, 1=yes) 1 ! regulatory value over epistemic (1:expc; 2:quant; 3:min(quant,expc))
Input Parameters Recorded in EXDOC File "ccdf_cv.dat"
1000000.00 ! time saved for CCDF 1000 ! sample size 500 ! nber of doses considered for the statistics on the CCDF 2 ! type of discretization for statistics (0=linear ; 1=log)



Source: Output DTNs: MO0710ADTSPAWO.000 [DIRS 183752]; and MO0710PLOTSFIG.000 [DIRS 185207].

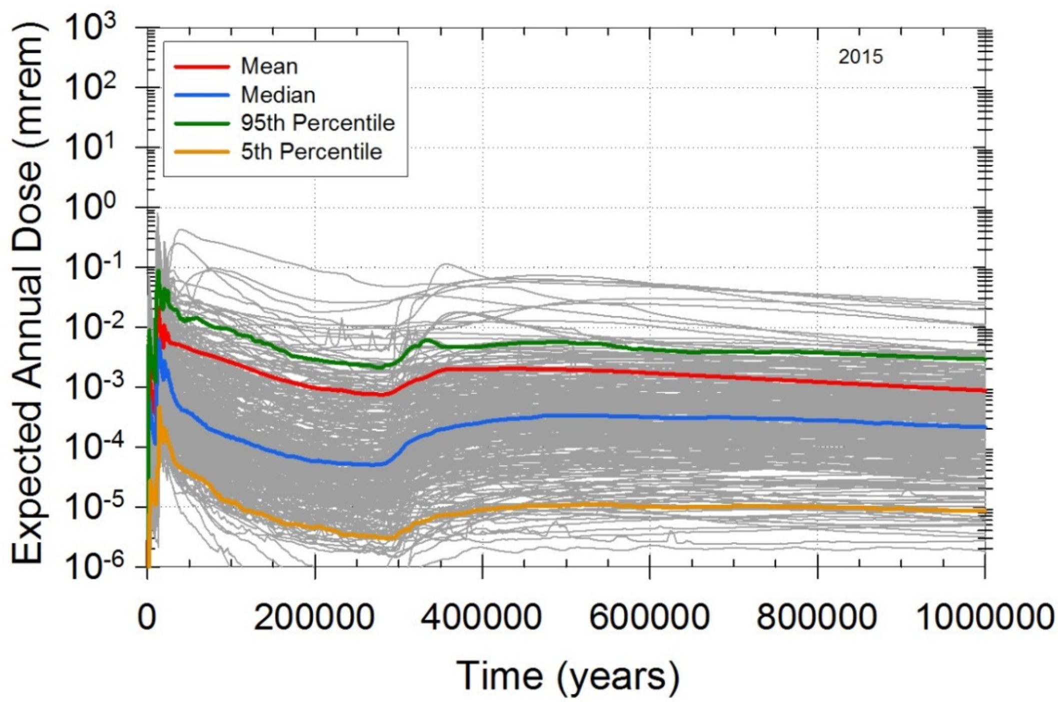


Figure 7. Comparison of Model Result for Distributions of Expected Annual Dose for the Waste Package Early Failure Modeling Case for 1,000,000 Years after Repository Closure: (top) YMP TSPA-LA model (SNL 2008, Figure 8.2-5[a]), and (bottom) TSPA-LA model test run of this study.

Table 7. Input Parameters for EXDOC Analysis of TSPA-LA Model Test Run Output "Dose_Total" for the Waste Package Early Failure Modeling Case for 10,000 Years after Repository Closure

Input Parameters Recorded in EXDOC File "info_tr.dat"
Dose_Total ! prefix 300 ! sample size 385 ! number of timesteps 20 ! aleatory sample size 3 ! nb of aleatory parameters 2 3 1 ! order of alea. parameters 2 2 5 ! size of alea. parameters 1 2 ! position for alea parameter 0 2 1 ! position for alea parameter 1 1 2 3 4 5 ! position for alea parameter 2 6 ! log file indicator
Input Parameters Recorded in EXDOC File "info_cv.dat"
Dose_Total !prefix EW_lambda.txt ! lambda filename ps_frac.txt ! bins fractions filename seep_frac_10k.txt ! Drip fractions filename wp_frac.txt ! WP fractions filename quantiles.txt ! quantile filename 300 ! sample size 385 ! number of timesteps in input 5 ! number of bins considered 2 ! number of WPs considered 3 ! number of quantiles considered 1 ! analysis done (1:expected value; 2 or 4 CCDF; 3 or 5: both 6 ! option on log file
Input Parameters Recorded in EXDOC File "expc_cv.dat"
1 ! sum over WP (0=no, 1=yes) 1 ! sum over bin (0=no, 1=yes) 1 ! sum over drip. cond. (0=no, 1=yes) 1 ! regulatory value over epistemic (1:expc; 2:quant; 3:min(quant,expc))
Input Parameters Recorded in EXDOC File "ccdf_cv.dat"
20000.00 ! time saved for CCDF 1000 ! sample size 500 ! nber of doses considered for the statistics on the CCDF 2 ! type of discretization for statistics (0=linear ; 1=log)

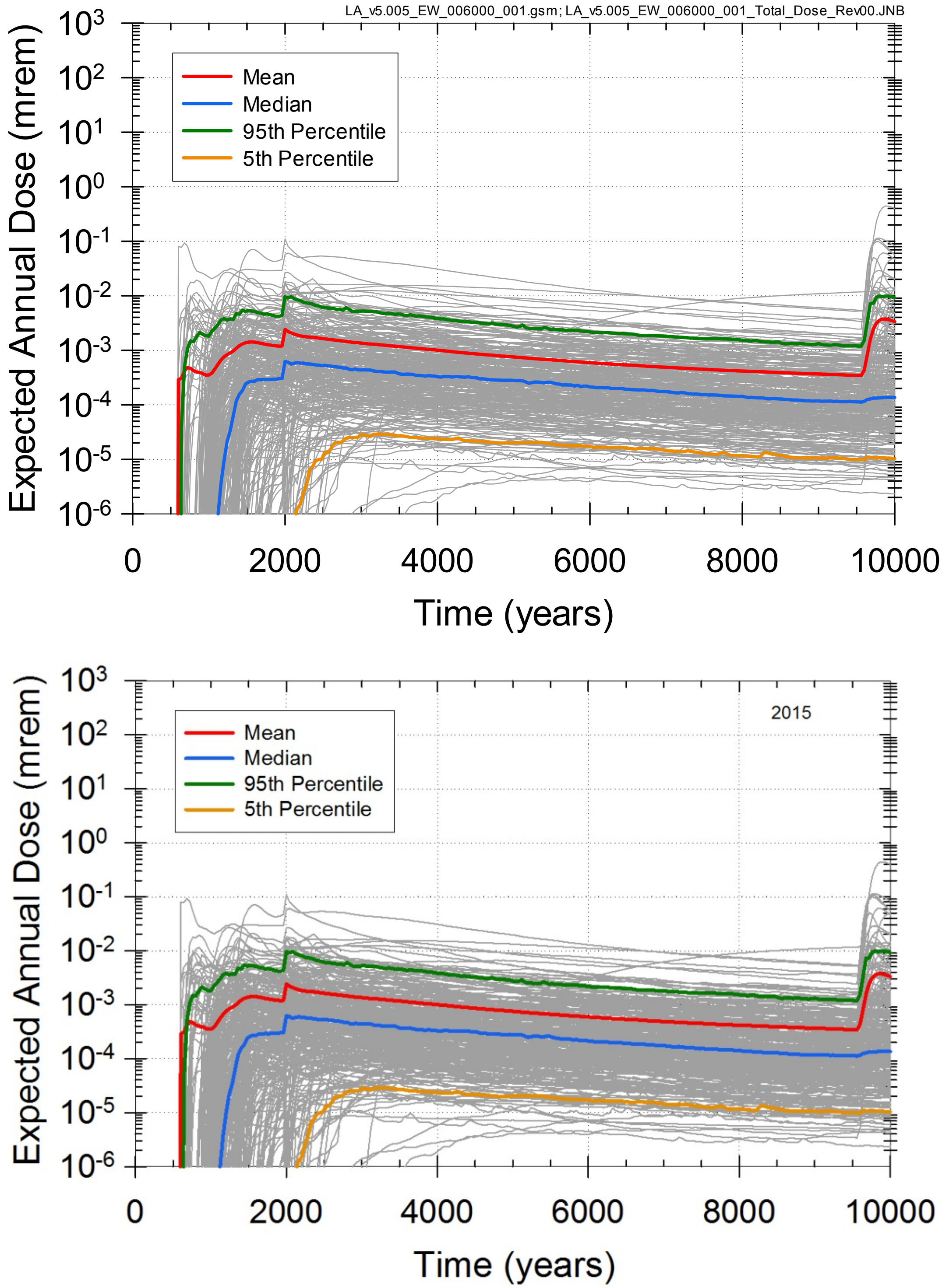


Figure 8. Comparison of Model Result for Distributions of Expected Annual Dose for the Waste Package Early Failure Modeling Case for 10,000 Years after Repository Closure: (top) YMP TSPA-LA model (SNL 2008, Figure 8.2-5[a]), and (bottom) TSPA-LA model test run of this study.

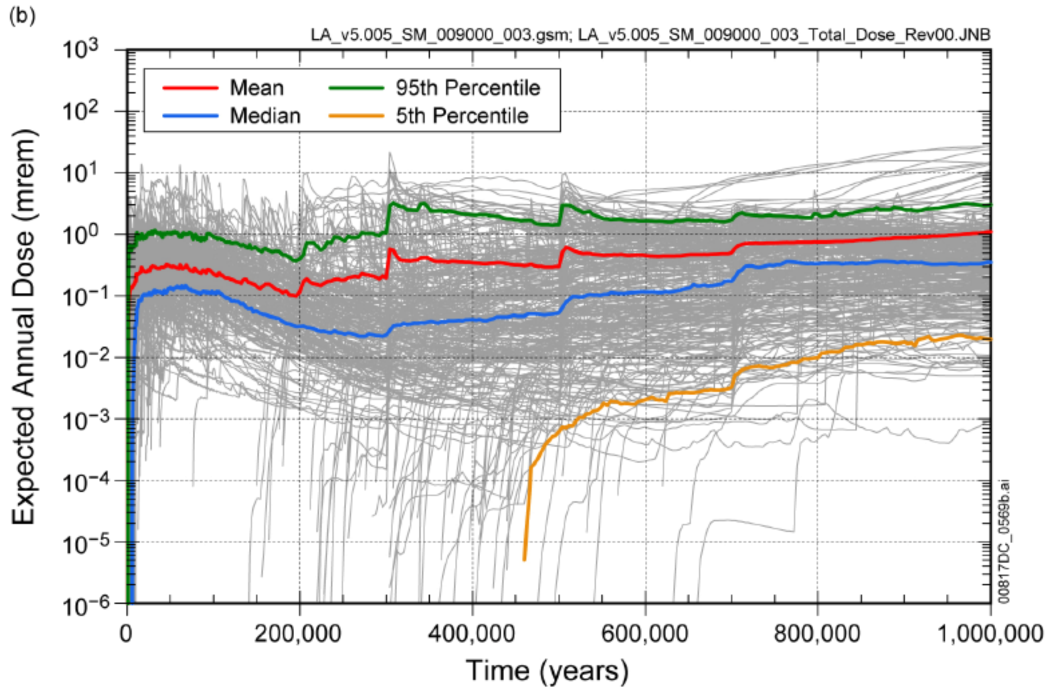
5.2.6. Seismic Ground Motion Modeling Case

The TSPA-LA model for the Seismic Ground Motion Modeling Case has 30 associated aleatory uncertain parameters, and the model simulation comprises 9,000 realizations (i.e., 300 sets of sampled epistemic uncertain parameters × 30 aleatory uncertain parameters per epistemic uncertain parameter set).

Tables 8 and 9 list the input parameter values for the EXDOC post-processing analysis of TSPA-LA model test run output parameter "Dose_Total" for the Seismic Ground Motion Modeling Case for 1,000,000 years and 10,000 years after repository closure, respectively. Prior to the EXDOC analysis, the output parameter file name should be changed from "Dose_Total.txt" to "Dose_Total_001.txt" for the post-processing analysis. Figure 9 shows the post-processed model result of the distributions of expected annual dose for the modeling case for 1,000,000 years after repository closure: top figure for the "original" TSPA-LA model (SNL 2008, Figure 8.2-11[a]) and bottom figure for the TSPA model test run of this study. Figure 10 shows the corresponding plots for the 10,000 years simulation period after repository closure. As shown in Figures 9 and 10, the plots of the TSPA-LA and new model test run figures are almost identical, and this demonstrates an excellent reproducibility of the original TSPA-LA model result by the model test run on the cluster.

Table 8. Input Parameters for EXDOC Analysis of TSPA-LA Model Test Run Output "Dose_Total" for the Seismic Ground Motion Modeling Case for 1,000,000 Years after Repository Closure

Input Parameters Recorded in EXDOC File "info_mc.dat"	
Dose_Total	!prefix
quantiles.txt	! quantile filename
300	! sample size
471	! number of timesteps in input
1	! number of aleatory files
30	! aleatory sample size
3	! number of quantiles considered
1	! LHS element saved
1	! analysis done (1:expected value; 2 or 4 CCDF; 3 or 5: both
0	! option on log file
Input Parameters Recorded in EXDOC File "expc_mc.dat"	
1	! regulatory value over aleatory(1:expc; 2:quant; 3:min(quant,expc))
1	! regulatory value over epistemic (1:expc; 2:quant; 3:min(quant,expc))
Input Parameters Recorded in EXDOC File "ccdf_mc.dat"	
1000000	! time saved for CCDF
100	! nber of doses considered for the statistics on the CCDF
1	! type of discretization for statistics (0=linear ; 1=log)



Source: Output DTNs: MO0710ADTSPAWO.000 [DIRS 183752]; and MO0710PLOTSFIG.000 [DIRS 185207].

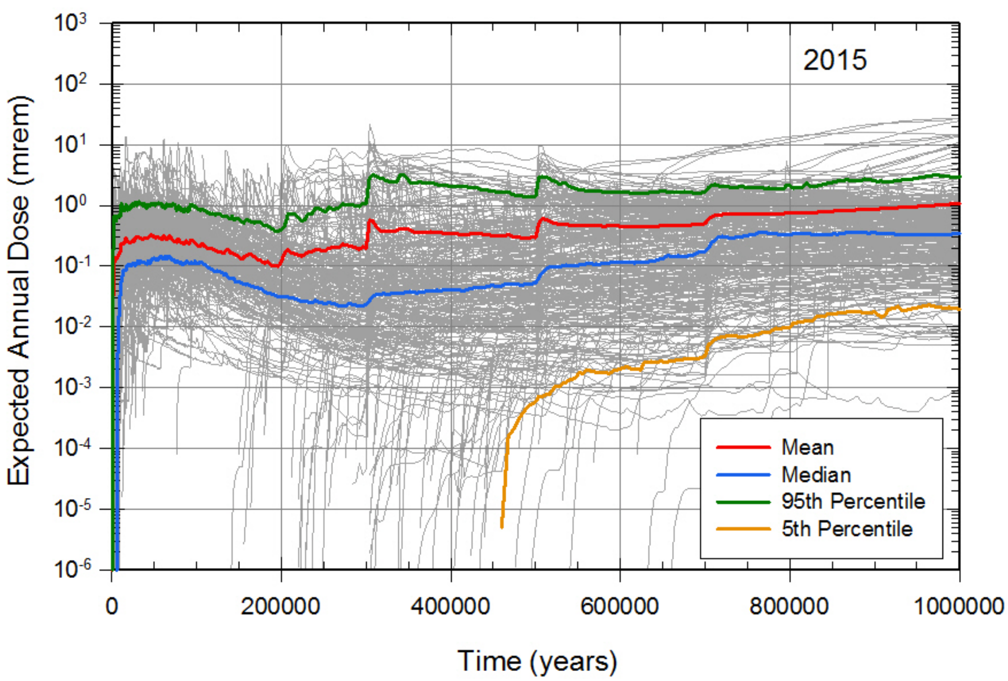
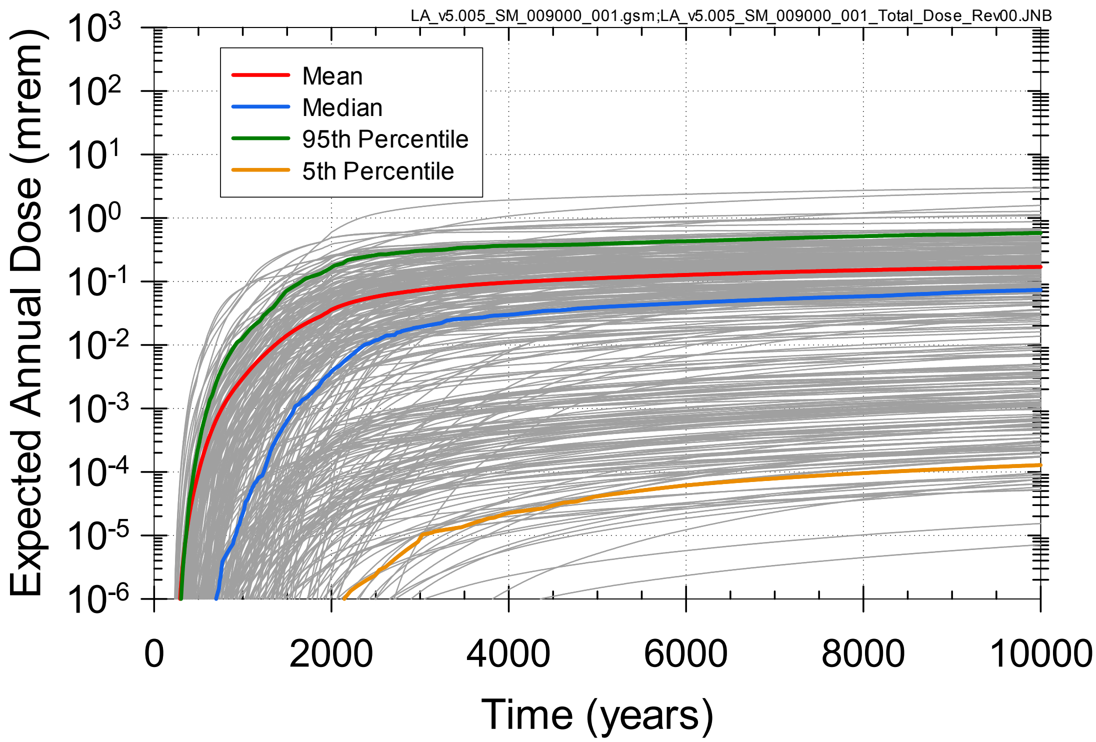


Figure 9. Comparison of Model Result for Distributions of Expected Annual Dose for the Seismic Ground Motion Modeling Case for 1,000,000 Years after Repository Closure: (top) YMP TSPA-LA model (SNL 2008, Figure 8.2-11[a]), and (bottom) TSPA-LA model test run of this study.

Table 9. Input Parameters for EXDOC Analysis of TSPA-LA Model Test Run Output "Dose_Total" for the Seismic Ground Motion Modeling Case for 10,000 Years after Repository Closure

Input Parameters Recorded in EXDOC File "info_tr.dat"
Dose_Total ! prefix 300 ! sample size 385 ! number of timesteps 30 ! aleatory sample size 2 ! nb of aleatory parameters 1 2 ! order of alea. parameters 6 5 ! size of alea. parameters 1 2 3 4 5 6 ! position for alea parameter 0 1 2 3 4 5 ! position for alea parameter 1 5 ! log file indicator
Input Parameters Recorded in EXDOC File "info_se.dat"
Dose_Total !prefix A1_lambda ! lambda filename A1_Event.txt ! time of event filename A1_Ampli.txt ! amplitude filename quantiles.txt ! quantile filename A1_Distrib ! amplitude distribution filename 300 ! sample size 385 ! number of timesteps in input 6 ! number of time of events 5 ! number of amplitudes 100.00 ! minimum time of event considered 20000.00 ! maximum time of event considered 0 ! minimum amplitude considered 0.005 ! maximum amplitude considered 105 ! number of point defining amplitude distribution 105 ! sample size for ampli distrib. for subs. events 3 ! number of quantiles considered 1 ! LHS element saved 1 ! analysis done (1:expected value; 2 or 4 CCDF; 3 or 5: both 5 ! option on log file
Input Parameters Recorded in EXDOC File "expc_se.dat"
0.00 ! minimum time considered 20000.00 ! maximum time considered 2001 ! number of timesteps 2001 ! number of times of event 100 ! number of amplitudes 1 ! regulatory value over epistemic (1:expc; 2:quant; 3:min(quant,expc))
Input Parameters Recorded in EXDOC File "ccdf_se.dat"
10000.00 ! time saved for CCDF 1000 ! sample size 100 ! nber of doses considered for the statistics on the CCDF 1 ! type of discretization for statistics (0=linear ; 1=log)



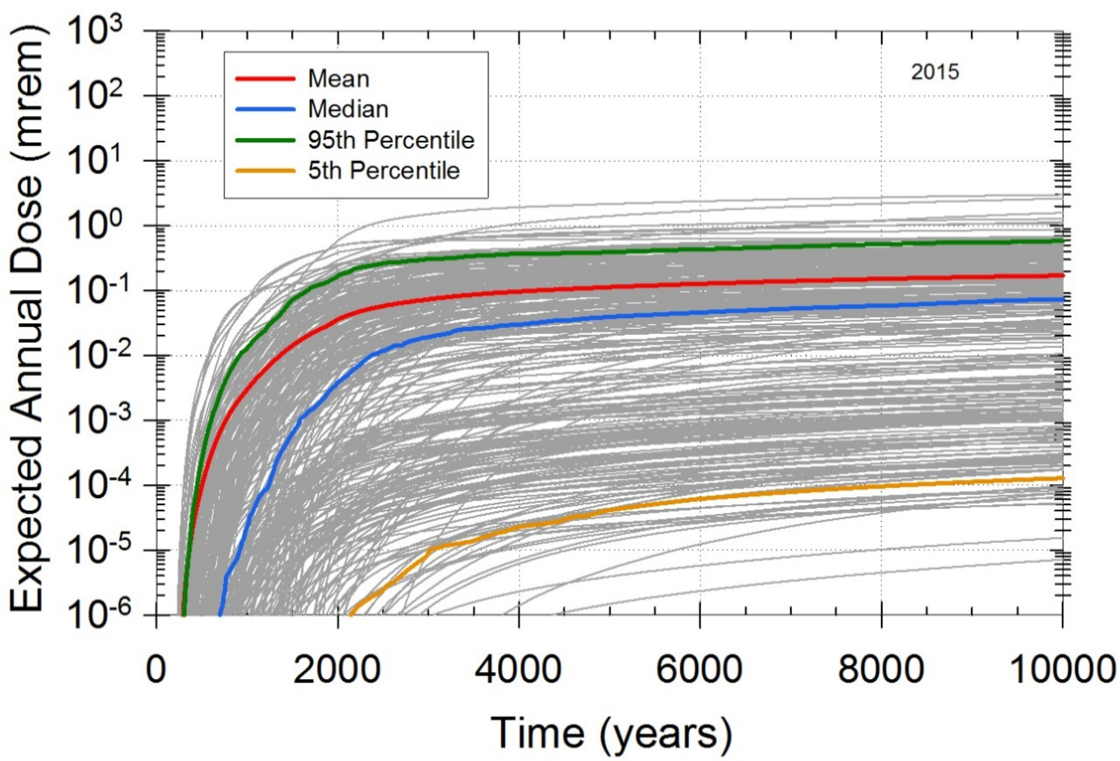


Figure 10. Comparison of Model Result for Distributions of Expected Annual Dose for the Seismic Ground Motion Modeling Case for 10,000 Years after Repository Closure: (top) YMP TSPA-LA model (SNL 2008, Figure 8.2-11[a]), and (bottom) TSPA-LA model test run of this study.

5.2.7. *Seismic Fault Displacement Modeling Case*

The TSPA-LA model for the Seismic Fault Displacement Modeling Case has 36 associated aleatory uncertain parameters, and the model simulation comprises 10,800 realizations (i.e., 300 sets of sampled epistemic uncertain parameters × 36 aleatory uncertain parameters per epistemic uncertain parameter set).

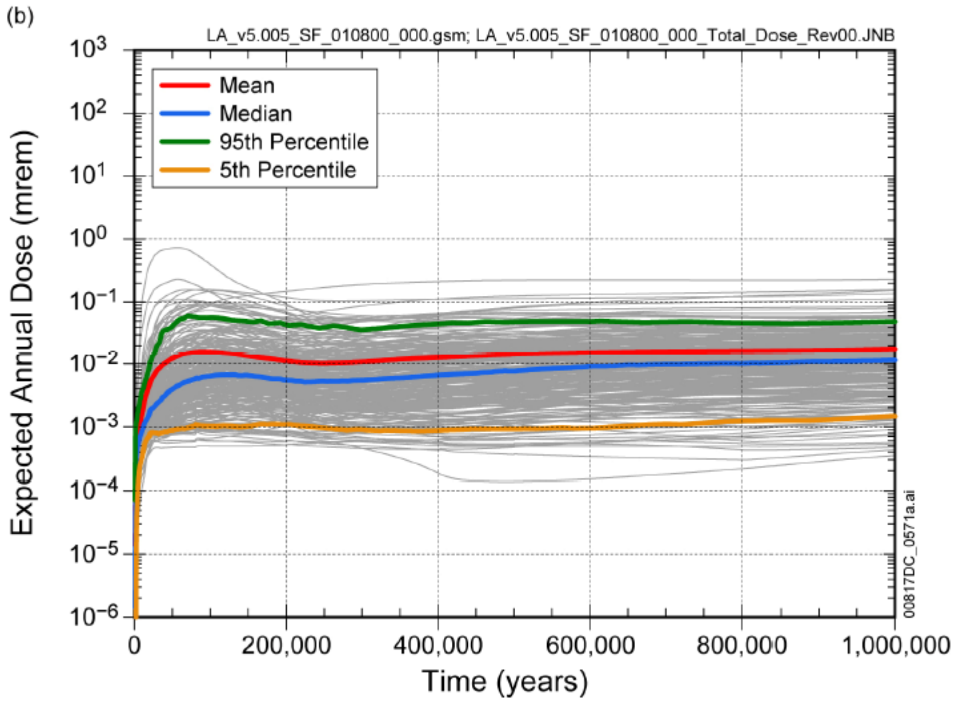
Care should be exercised in using the documentation for EXDOC post processing steps for this modeling case. In the "EXDOC Split Menu Screen Capture" for both the 10,000 years and 1 million years modeling cases the entry for "index for each parameter value" does not show the last line which consists of "1 2 3". This line has to be entered for proper splitting of the dose file.

Tables 10 and 11 list the input parameter values for the EXDOC post-processing analysis of TSPA-LA model test run output parameter "Dose_Total" for the Seismic Fault Displacement Modeling Case for 1,000,000 years after repository closure. Figure 11 shows the post-processed model result of the distributions of expected annual dose for the modeling case for 1,000,000 years after repository closure: top figure for the "original" TSPA-LA model (SNL 2008, Figure 8.2-13[a]) and bottom figure for the TSPA model test run of this study. Figure 12 shows the corresponding plots for the 10,000 years simulation period after repository closure. As shown in Figures 11 and 12, the plots of the TSPA-LA and new model test run figures are almost identical, and this demonstrates an excellent reproducibility of the original TSPA-LA model result by the model test run on the cluster.

Table 10. Input Parameters for EXDOC Analysis of TSPA-LA Model Test Run Output "Dose_Total" for the Seismic Fault Displacement Modeling Case for 1,000,000 Years after Repository Closure

Input Parameters Recorded in EXDOC File "info_tr.dat"
Dose_Total ! prefix 300 ! sample size 471 ! number of timesteps 36 ! aleatory sample size 5 ! nb of aleatory parameters 3 5 1 4 2 ! order of alea. parameters 1 1 6 2 3 ! size of alea. parameters 1 ! position for alea parameter 0 1 ! position for alea parameter 1 1 2 3 4 5 6 ! position for alea parameter 2 1 2 ! position for alea parameter 3 1 2 3 ! position for alea parameter 4 0 ! log file indicator
Input Parameters Recorded in EXDOC File "info_fd.dat"
Dose_Total !prefix A2_1M_event.txt ! time of event filename A2_Ampli ! amplitude filename A2_PS_Frac.txt ! bins fractions filename A2_Seep_Frac.txt ! Drip fractions filename A2FD_wp_Frac.txt ! WP fractions filename quantiles.txt ! quantile filename A2_FD_FSAD ! prefix for amplitude distribution filenames 300 ! sample size 471 ! number of timesteps in input 1 ! number of bins considered 2 ! number of WPs considered 6 ! number of time of events 3 ! number of amplitudes 1000.0 ! minimum time of event considered 1000000.0 ! maximum time of event considered 0 ! minimum amplitude considered 0.101 ! maximum amplitude considered 12 ! number of point defining amplitude distribution 5 ! number of point defining distribution of nWPD 3 ! number of quantiles considered 1 ! analysis done (1:expected value; 2 or 4 CCDF; 3 or 5: both 0 ! inclusion of DS failure (0=no, 1=yes) 0 ! option on log file
Input Parameters Recorded in EXDOC File "expc_fd.dat"
0.00 ! minimum time considered 1000000.0 ! maximum time considered 2001 ! number of timesteps 2001 ! number of times of event 100 ! number of amplitudes 1 ! sum over WP (0=no, 1=yes)

1	! sum over bin (0=no, 1=yes)
1	! sum over drip. cond. (0=no, 1=yes)
1	! regulatory value over epistemic (1:expc; 2:quant; 3:min(quant,expc))
Input Parameters Recorded in EXDOC File "ccdf_fd.dat"	
1000000.00	! time saved for CCDF
1000	! sample size
100	! nber of doses considered for the statistics on the CCDF
1	! type of discretization for statistics (0=linear ; 1=log)



Source: Output DTNs: MO0710ADTSPAWO.000 [DIRS 183752]; and MO0710PLOTSFIG.000 [DIRS 185207].

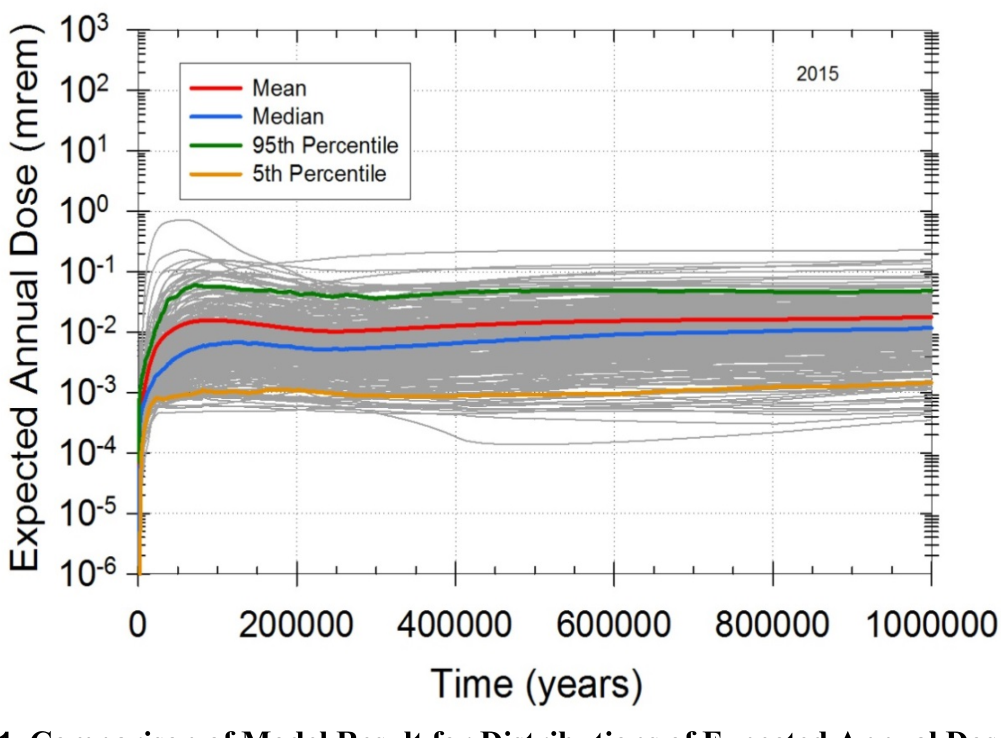


Figure 11. Comparison of Model Result for Distributions of Expected Annual Dose for the Seismic Fault Displacement Modeling Case for 1,000,000 Years after Repository Closure: (top) YMP TSPA-LA model (SNL 2008, Figure 8.2-13[a]), and (bottom) TSPA-LA model test run of this study.

Table 11. Input Parameters for EXDOC Analysis of TSPA-LA Model Test Run Output "Dose_Total" for the Seismic Fault Displacement Modeling Case for 10,000 Years after Repository Closure

Input Parameters Recorded in EXDOC File "info_tr.dat"
Dose_Total ! prefix 300 ! sample size 385 ! number of timesteps 36 ! aleatory sample size 5 ! nb of aleatory parameters 3 5 1 4 2 ! order of alea. parameters 1 1 6 2 3 ! size of alea. parameters 1 ! position for alea parameter 0 1 ! position for alea parameter 1 1 2 3 4 5 6 ! position for alea parameter 2 1 2 ! position for alea parameter 3 1 2 3 ! position for alea parameter 4 0 ! log file indicator
Input Parameters Recorded in EXDOC File "info_fd.dat"
Dose_Total !prefix A2_10k_Event.txt ! time of event filename A2_Ampli ! amplitude filename A2_PS_frac.txt ! bins fractions filename A2_Seep_Frac.txt ! Drip fractions filename A2FD_WP_Frac.txt ! WP fractions filename quantiles.txt ! quantile filename A2_FD_FSAD ! prefix for amplitude distribution filenames 300 ! sample size 385 ! number of timesteps in input 1 ! number of bins considered 2 ! number of WPs considered 6 ! number of time of events 3 ! number of amplitudes 200.00 ! minimum time of event considered 20000.00 ! maximum time of event considered 0 ! minimum amplitude considered 0.101 ! maximum amplitude considered 12 ! number of point defining amplitude distribution 5 ! number of point defining distribution of nWPD 3 ! number of quantiles considered 1 ! analysis done (1:expected value; 2 or 4 CCDF; 3 or 5: both 0 ! inclusion of DS failure (0=no, 1=yes) 5 ! option on log file
Input Parameters Recorded in EXDOC File "expc_fd.dat"
0.00 ! minimum time considered 20000.00 ! maximum time considered 2001 ! number of timesteps 2001 ! number of times of event 100 ! number of amplitudes 1 ! sum over WP (0=no, 1=yes) 1 ! sum over bin (0=no, 1=yes)

1	! sum over drip. cond. (0=no, 1=yes)
1	! regulatory value over epistemic (1:expc; 2:quant; 3:min(quant,expc))
Input Parameters Recorded in EXDOC File "ccdf_fd.dat"	
20000.00	! time saved for CCDF
1000	! sample size
100	! nber of doses considered for the statistics on the CCDF
1	! type of discretization for statistics (0=linear ; 1=log)

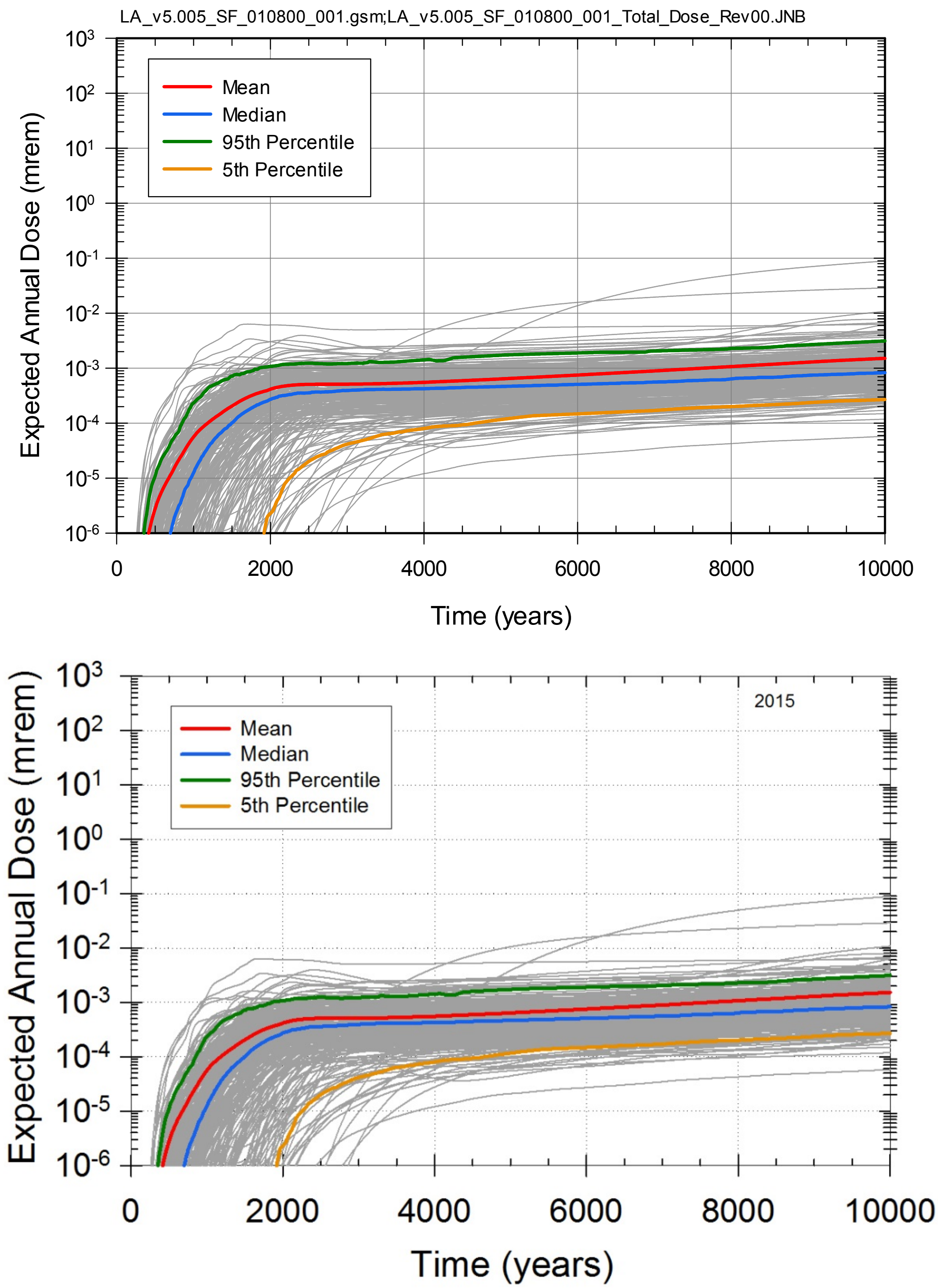


Figure 12. Comparison of Model Result for Distributions of Expected Annual Dose for the Seismic Fault Displacement Modeling Case for 10,000 Years after Repository Closure: (top) YMP TSPA-LA model (SNL 2008, Figure 8.2-13[a]), and (bottom) TSPA-LA model test run of this study.

5.2.8. Igneous Intrusion Modeling Case

The TSPA-LA model for the Igneous Intrusion Modeling Case has 10 associated aleatory uncertain parameters, and the model simulation comprises 3000 realizations (i.e., 300 sets of sampled epistemic uncertain parameters × 10 aleatory uncertain parameters per epistemic uncertain parameter set).

Tables 12 and 13 list the input parameter values for the EXDOC post-processing analysis of TSPA-LA model test run output parameter "Dose_Total" for the Igneous Intrusion Modeling Case for 1,000,000 years and 10,000 years after repository closure, respectively. Figure 13 shows the post-processed model result of the distributions of expected annual dose for the modeling case for 1,000,000 years after repository closure: top figure for the "original" TSPA-LA model (SNL 2008, Figure 8.2-13[a]) and bottom figure for the TSPA model test run of this study. Figure 14 shows the corresponding plots for the 10,000 years simulation period after repository closure. As shown in Figures 13 and 14, the plots of the TSPA-LA and new model test run using CL2014 figures are almost identical, and this demonstrates an excellent reproducibility of the original TSPA-LA model result by the model test run on the cluster.

Table 12. Input Parameters for EXDOC Analysis of TSPA-LA Model Test Run Output "Dose_Total" for the Igneous Intrusion Modeling Case for 1,000,000 Years after Repository Closure

Input Parameters Recorded in EXDOC File "info_tr.dat"
Dose_Total ! prefix 300 ! sample size 471 ! number of timesteps 10 ! aleatory sample size 2 ! nb of aleatory parameters 2 1 ! order of alea. parameters 1 10 ! size of alea. parameters 1 ! position for alea parameter 0 1 2 3 4 5 6 7 8 9 10 ! position for alea parameter 1 6 ! log file indicator
Input Parameters Recorded in EXDOC File "info.dat"
Dose_Total !prefix IG_Lambda.txt ! lambda filename IG_1M_Event.txt ! time of event filename IG_Amplitude.txt ! amplitude filename Quantiles.txt ! quantile filename IG_Law_Ampli.txt ! amplitude distribution filename 0 ! scenario considered 300 ! sample size 471 ! number of timesteps in input 10 ! number of time of events 1 ! number of amplitudes 10.00 ! minimum time of event considered 1000000.0 ! maximum time of event considered 11629.0 ! minimum amplitude considered 11629.0 ! maximum amplitude considered 11 ! number of point defining amplitude distribution 3 ! number of quantiles considered 2 ! LHS element saved 1 ! analysis done (1:expected value; 2 or 4 CCDF; 3 or 5: both 4 ! option on log file
Input Parameters Recorded in EXDOC File "expc.dat"
11629.00 ! expected value of amplitude 0.00 ! minimum time considered 1000000.0 ! maximum time considered 2001 ! number of timesteps 2001 ! number of times of event 100 ! number of amplitudes 20 ! number of time of event saved 1 ! regulatory value over epistemic (1:expc; 2:quant; 3:min(quant,expc))
Input Parameters Recorded in EXDOC File "ccdf_cv.dat"
1000000.0 ! time saved for CCDF 200 ! sample size 1 ! multiplicator of sample 2 ! type of discretization on amplitude (0=linear ; 1=log ; 2=quant) 100 ! nber of doses considered for the statistics on the CCDF 1 ! type of discretization for statistics (0=linear ; 1=log)

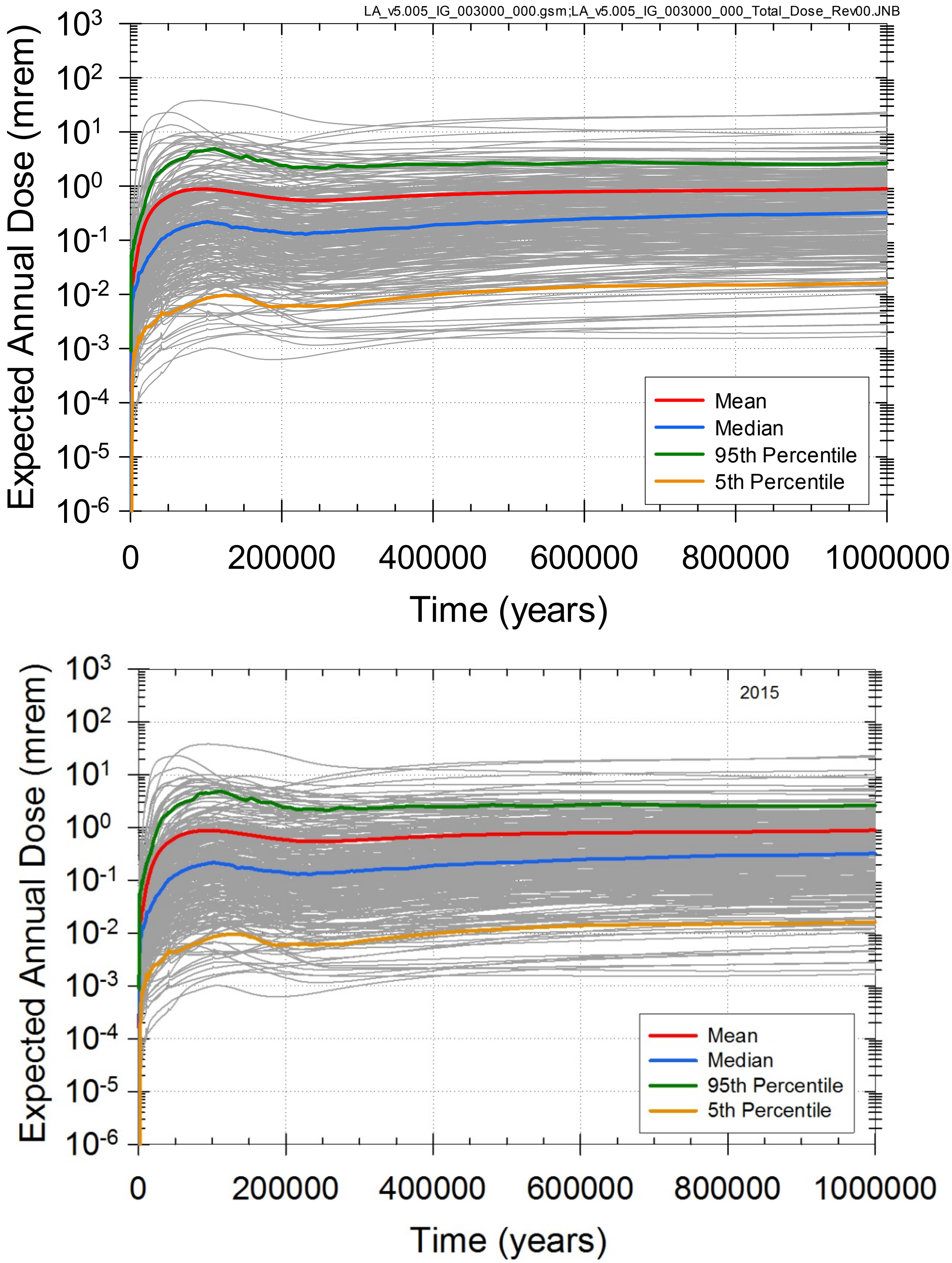
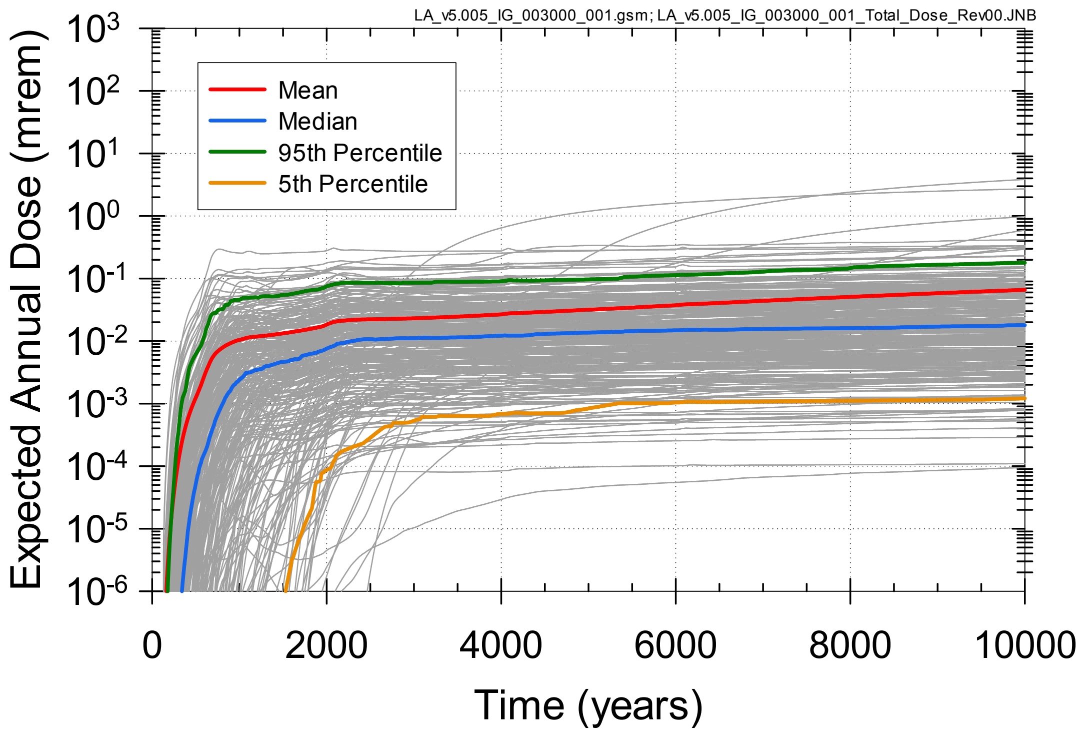


Figure 13. Comparison of Model Result for Distributions of Expected Annual Dose for the Igneous Intrusion Modeling Case for 1,000,000 Years after Repository Closure: (top) YMP TSPA-LA model (SNL 2008, Figure 8.2-7[a]), and (bottom) TSPA-LA model test run of this study.

Table 13. Input Parameters for EXDOC Analysis of TSPA-LA Model Test Run Output "Dose_Total" for the Igneous Intrusion Modeling Case for 10,000 Years after Repository Closure

Input Parameters Recorded in EXDOC File "info_tr.dat"
Dose_Total ! prefix 300 ! sample size 385 ! number of timesteps 10 ! aleatory sample size 2 ! nb of aleatory parameters 2 1 ! order of alea. parameters 1 10 ! size of alea. parameters 1 ! position for alea parameter 0 1 2 3 4 5 6 7 8 9 10 ! position for alea parameter 1 6 ! log file indicator
Input Parameters Recorded in EXDOC File "info.dat"
Dose_Total !prefix IG_lambda.txt ! lambda filename IG_10k_event.txt ! time of event filename IG_amplitude.txt ! amplitude filename quantiles.txt ! quantile filename IG_law_ampli.txt ! amplitude distribution filename 0 ! scenario considered 300 ! sample size 385 ! number of timesteps in input 10 ! number of time of events 1 ! number of amplitudes 10.00 ! minimum time of event considered 20000.00 ! maximum time of event considered 11629.0 ! minimum amplitude considered 11629.0 ! maximum amplitude considered 11 ! number of point defining amplitude distribution 3 ! number of quantiles considered 2 ! LHS element saved 1 ! analysis done (1:expected value; 2 or 4 CCDF; 3 or 5: both 4 ! option on log file
Input Parameters Recorded in EXDOC File "expc.dat"
11629.00 ! expected value of amplitude 0.00 ! minimum time considered 20000.00 ! maximum time considered 2001 ! number of timesteps 2001 ! number of times of event 100 ! number of amplitudes 20 ! number of time of event saved 1 ! regulatory value over epistemic (1:expc; 2:quant; 3:min(quant,expc))
Input Parameters Recorded in EXDOC File "ccdf_cv.dat"
20000.00 ! time saved for CCDF 200 ! sample size 1 ! multiplicator of sample 2 ! type of discretization on amplitude (0=linear ; 1=log ; 2=quant) 100 ! nber of doses considered for the statistics on the CCDF 1 ! type of discretization for statistics (0=linear ; 1=log)



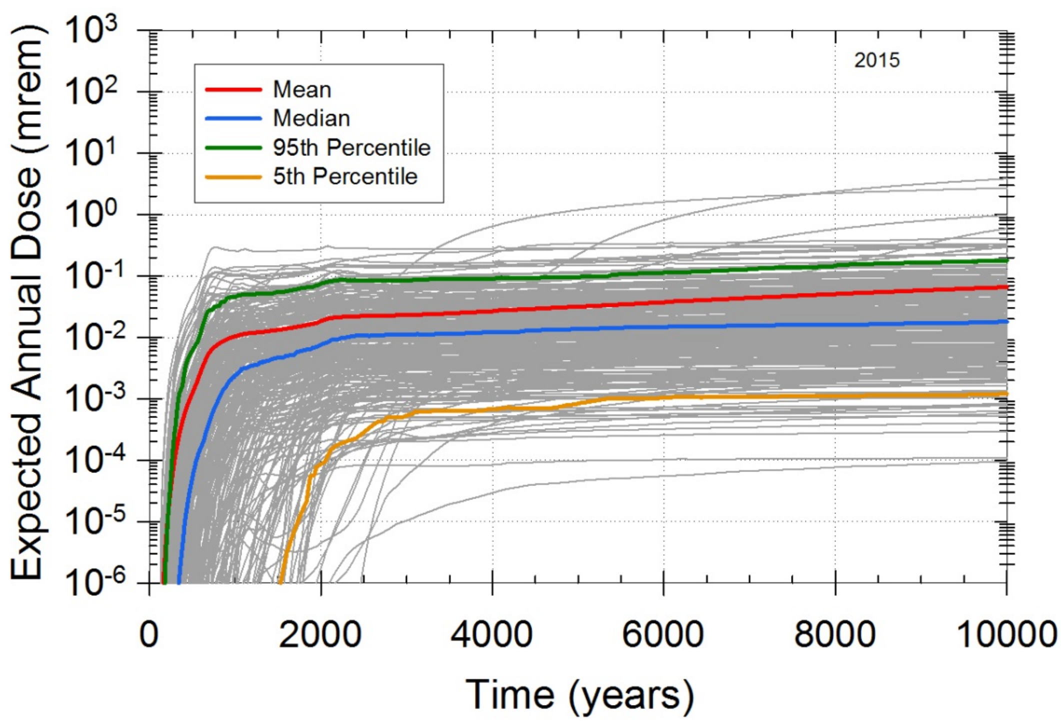


Figure 14. Comparison of Model Result for Distributions of Expected Annual Dose for the Igneous Intrusion Modeling Case for 10,000 Years after Repository Closure: (top) YMP TSPA-LA model (SNL 2008, Figure 8.2-7[a]), and (bottom) TSPA-LA model test run of this study.

5.2.9. Volcanic Eruption Modeling Case

The TSPA-LA model for the Volcanic Eruption Modeling Case has 40 associated aleatory uncertain parameters, and the model simulation comprises 12000 realizations (i.e., 300 sets of sampled epistemic uncertain parameters × 40 aleatory uncertain parameters per epistemic uncertain parameter set).

Tables 14 and 15 list the input parameter values for the EXDOC post-processing analysis of TSPA-LA model test run output parameter "Dose_Total" for the Volcanic Eruption Modeling Case for 1,000,000 years and 10,000 years after repository closure, respectively. The Volcanic Eruption modeling case for the 1,000,000 years period was run ten times for the ten eruption event times (250 years; 600 years; 1,000 years; 4,000 years; 10,000 years; 40,000 years; 100,000 years; 200,000 years; 400,000 years; 800,000 years). Figure 15 shows the post-processed model result of the distributions of expected annual dose for the modeling case for 1,000,000 years after repository closure: top figure for the "original" TSPA-LA model (SNL 2008, Figure 8.2-9) and bottom figure for the TSPA model test run of this study.

The Volcanic Eruption modeling case for the 20,000 years period was run nine times for the nine eruption event times (10 years; 100 years; 600 years; 2,000 years; 4,000 years; 6,000 years; 10,000 years; 14,000 years; 18,000 years). Figure 16 shows the post-processed model result of the distributions of expected annual dose for the modeling case for 10,000 years after repository closure: top figure for the "original" TSPA-LA model (SNL 2008, Figure 8.2-9) and bottom figure for the TSPA model test run of this study.

As shown in Figures 15 and 16, the plots of the TSPA-LA and new model test run using CL2014 figures are almost identical, and this demonstrates an excellent reproducibility of the original TSPA-LA model result by the model test run on the cluster.

Table 14. Input Parameters for EXDOC Analysis of TSPA-LA Model Test Run Output "Dose_Total" for the Volcanic Eruption Modeling Case for 1,000,000 Years after Repository Closure

Input Parameters Recorded in EXDOC File "info_tr.dat"
VE_010 ! prefix 300 ! sample size 153 ! number of timesteps 40 ! aleatory sample size 1 ! nb of aleatory parameters 1 ! order of alea. parameters 40 ! size of alea. parameters 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 ! position for alea parameter 0 6 ! log file indicator
Input Parameters Recorded in EXDOC File "info_mct.dat"
VE !prefix VE_lambda.txt ! lambda filename VE_1M_Event.txt ! time of event filename VE_Amplitude.txt ! amplitude filename quantiles.txt ! quantile filename VE_Law_Ampli.txt ! amplitude distribution filename 300 ! sample size 363 ! number of timesteps in input 10 ! number of time of events 1 ! number of amplitudes 40 ! aleatory sample size 250 ! minimum time of event considered 1000000 ! maximum time of event considered 0.1 ! minimum amplitude considered 3.5 ! maximum amplitude considered 5002 ! number of point defining amplitude distribution 3 ! number of quantiles considered 1 ! LHS element saved 1 ! analysis done (1:expected value; 2 or 4 CCDF; 3 or 5: both 6 ! option on log file
Input Parameters Recorded in EXDOC File "expc_mct.dat"
1.128 ! expected value of amplitude 250.00 ! minimum time considered 1000000 ! maximum time considered 2001 ! number of timesteps 2001 ! number of times of event 100 ! number of time of event saved 1 ! regulatory value over epistemic (1:expc; 2:quant; 3:min(quant,expc))
Input Parameters Recorded in EXDOC File "ccdf_mct.dat"
100000.00 ! time saved for CCDF 1000 ! sample size 100 ! nber of doses considered for the statistics on the CCDF 1 ! type of discretization for statistics (0=linear ; 1=log)

Table 15. Input Parameters for EXDOC Analysis of TSPA-LA Model Test Run Output "Dose_Total" for the Volcanic Eruption Modeling Case for 10,000 Years after Repository Closure

Input Parameters Recorded in EXDOC File "info_tr.dat"
VE_009 ! prefix 300 ! sample size 79 ! number of timesteps 40 ! aleatory sample size 1 ! nb of aleatory parameters 1 ! order of alea. parameters 40 ! size of alea. parameters 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 ! position for alea parameter 0 6 ! log file indicator
Input Parameters Recorded in EXDOC File "info_mct.dat"
VE !prefix VE_lambda.txt ! lambda filename VE_10k_event.txt ! time of event filename VE_amplitude.txt ! amplitude filename quantiles.txt ! quantile filename VE_law_ampli.txt ! amplitude distribution filename 300 ! sample size 171 ! number of timesteps in input 9 ! number of time of events 1 ! number of amplitudes 40 ! aleatory sample size 10.00 ! minimum time of event considered 20000.00 ! maximum time of event considered 0.1 ! minimum amplitude considered 3.5 ! maximum amplitude considered 5002 ! number of point defining amplitude distribution 3 ! number of quantiles considered 1 ! LHS element saved 1 ! analysis done (1:expected value; 2 or 4 CCDF; 3 or 5: both 6 ! option on log file
Input Parameters Recorded in EXDOC File "expc_mct.dat"
1.128 ! expected value of amplitude 10.00 ! minimum time considered 20000.00 ! maximum time considered 2001 ! number of timesteps 2001 ! number of times of event 100 ! number of time of event saved 1 ! regulatory value over epistemic (1:expc; 2:quant; 3:min(quant,expc))
Input Parameters Recorded in EXDOC File "ccdf_mct.dat"
20000.00 ! time saved for CCDF 1000 ! sample size 100 ! nber of doses considered for the statistics on the CCDF 1 ! type of discretization for statistics (0=linear ; 1=log)

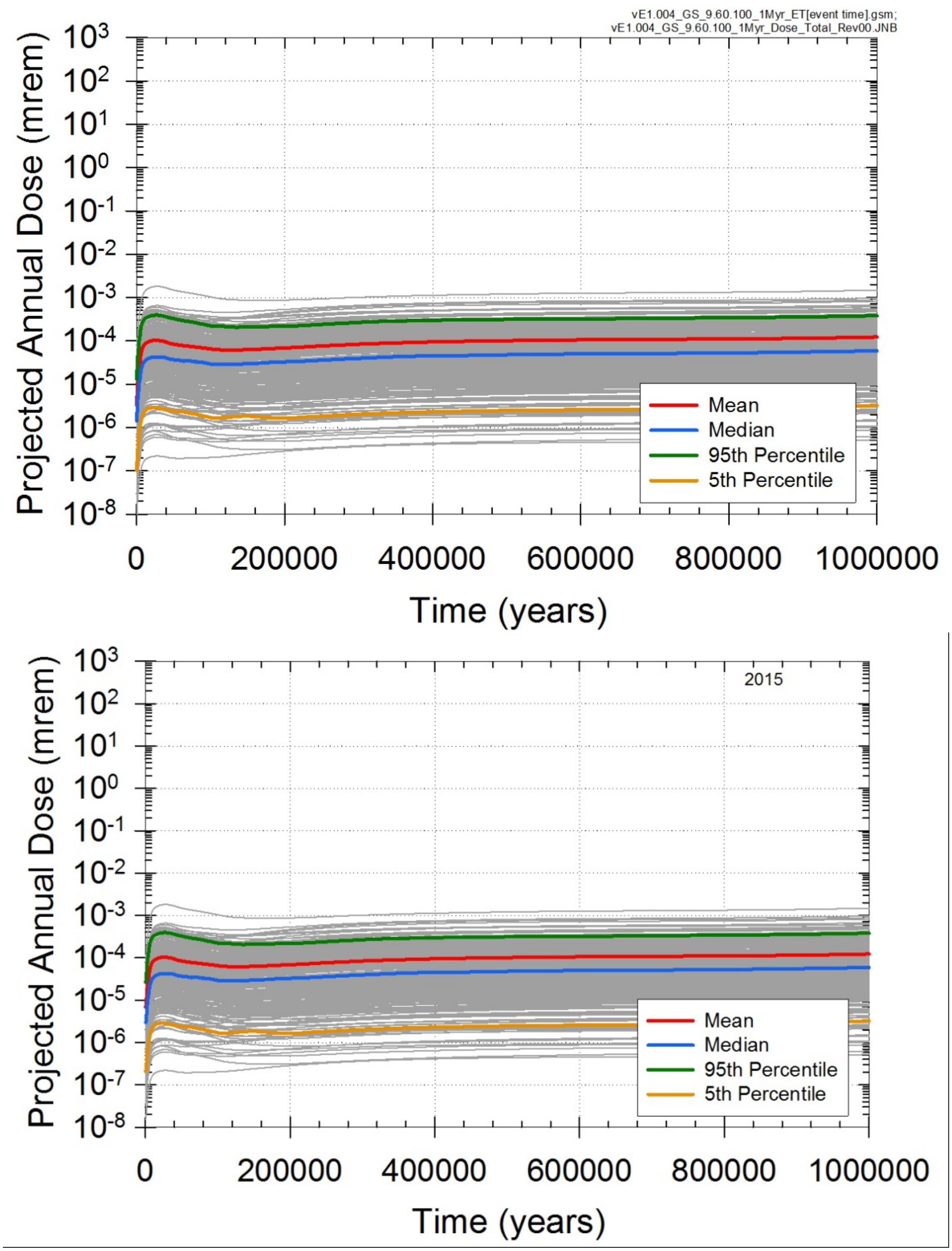
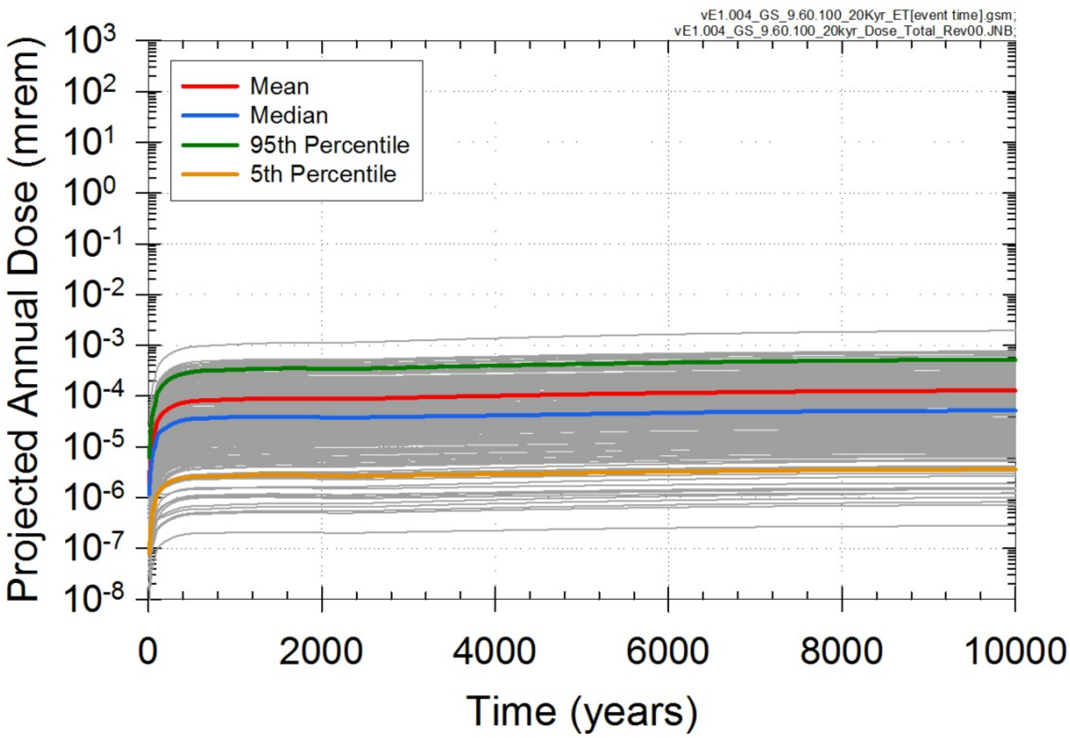


Figure 15. Comparison of Model Result for Distributions of Expected Annual Dose for the Volcanic Eruption Modeling Case for 1,000,000 Years after Repository Closure: (top) YMP TSPA-LA model (SNL 2008, Figure 8.2-9), and (bottom) TSPA-LA model test run of this study.



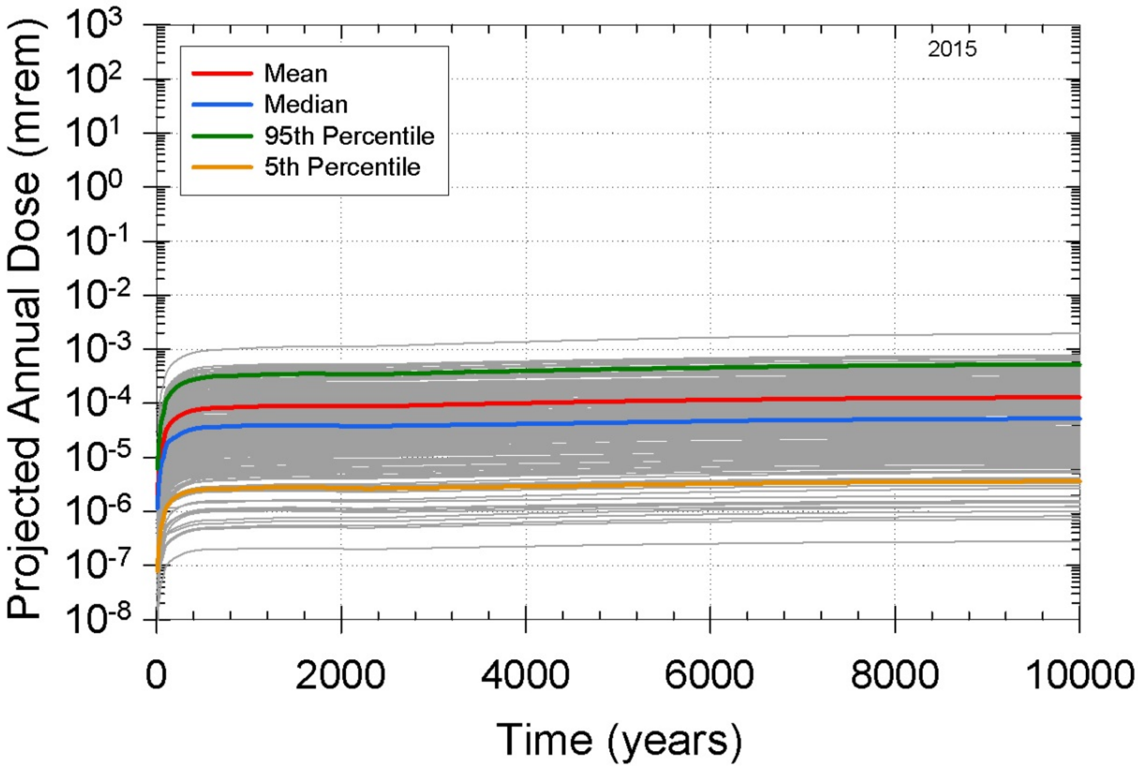


Figure 16. Comparison of Model Result for Distributions of Expected Annual Dose for the Volcanic Eruption Modeling Case for 10,000 Years after Repository Closure: (top) YMP TSPA-LA model (SNL 2008, Figure 8.2-9), and (bottom) TSPA-LA model test run of this study.

5.3. Model Reproducibility Verification by Graphical Comparison (Part II)

In this section new calculated mean annual dose results of the modeling cases using CL2014 are compared with results of the TSPA-LA. In order to get a direct graphical comparison of the TSPA-LA results and the results from the model test runs using the TSPA Cluster, plots were made of EXDOC mean expected dose output for the different modeling cases. Figures 17 to 32 show curves for the mean of the distribution of expected annual doses of all the modeling cases. The figures show results from the TSPA-LA and from test runs of this study. The solid line represents TSPA-LA results and the dots represent results of the test runs. As shown in Figures 17 to 32, the plots of the TSPA-LA and new model test run are almost identical, and this demonstrates an excellent reproducibility of the original TSPA-LA model result by the model test runs on the CL2014 cluster.

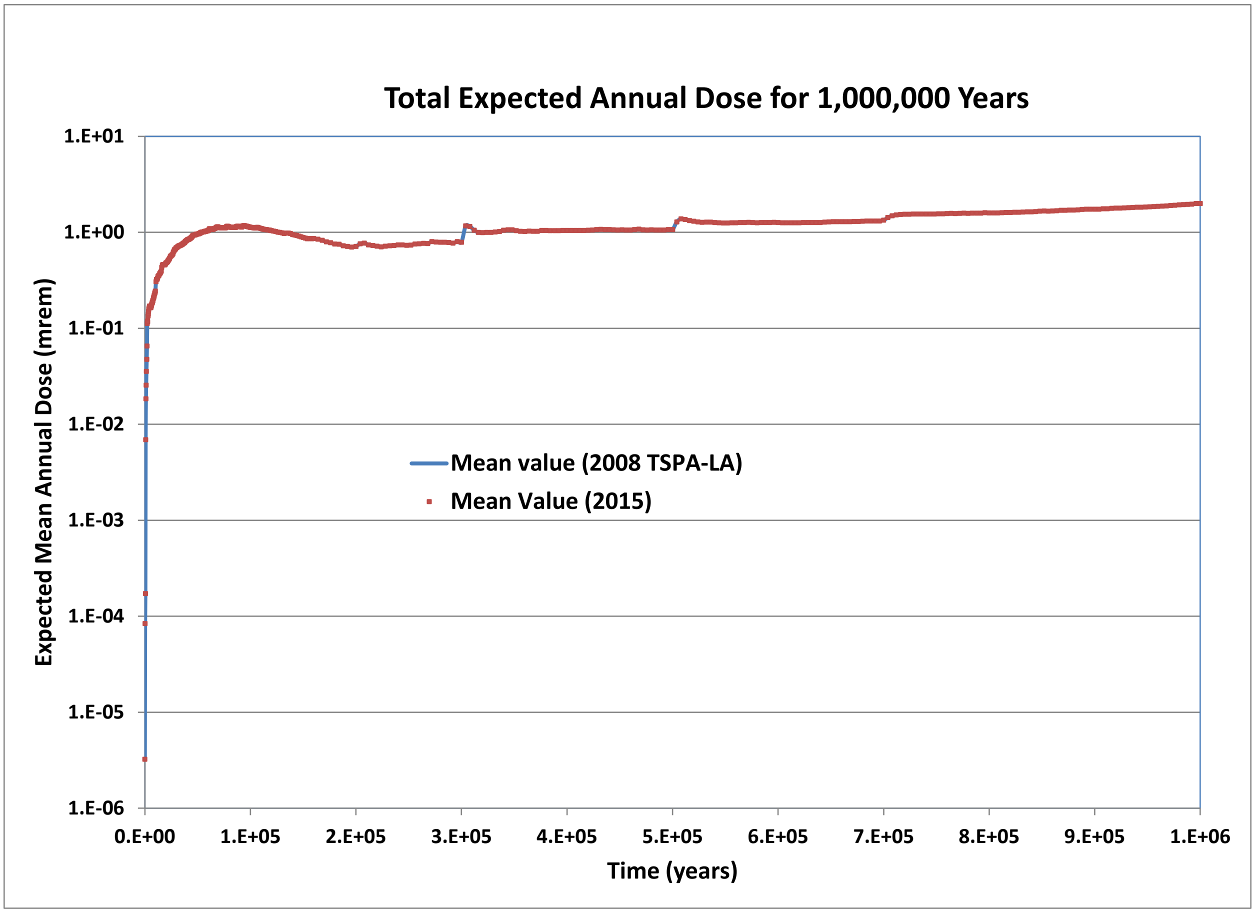


Figure 17. Comparison of Model Results for Total Expected Mean Annual Dose for 1,000,000 Years after Repository Closure.

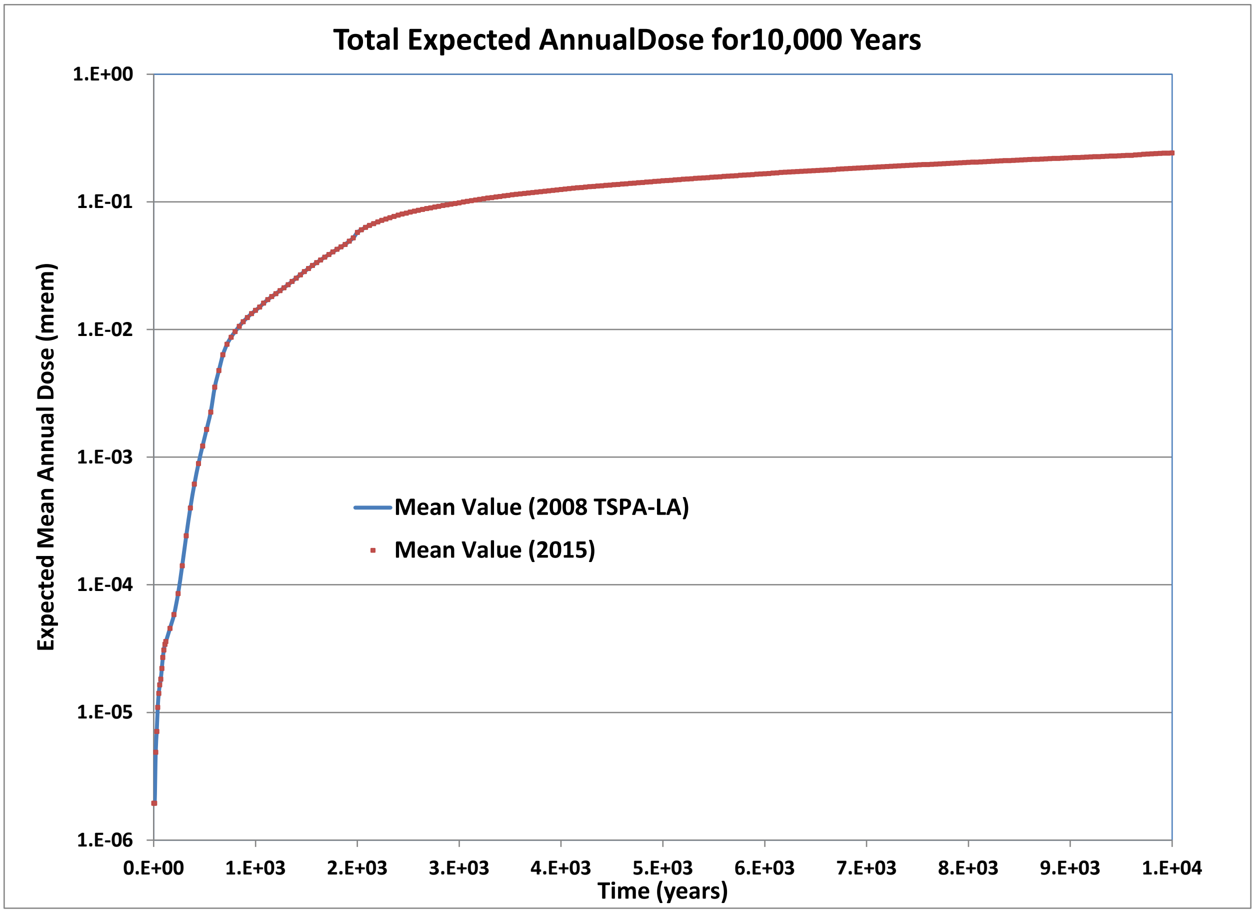


Figure 18. Comparison of Model Results for Total Expected Mean Annual Dose for 10,000 Years after Repository Closure.

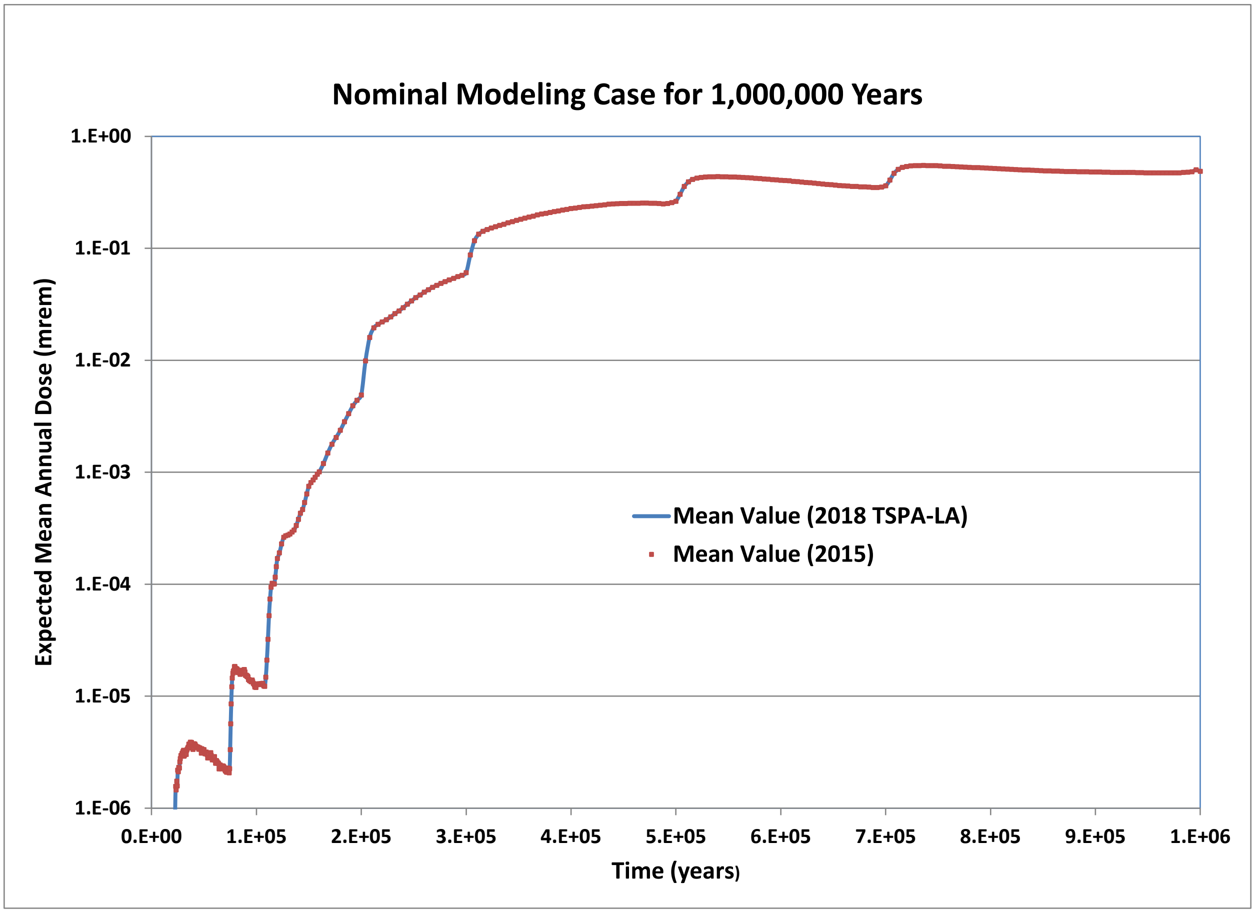


Figure 19. Comparison of Model Results for Expected Mean Annual Dose of the Nominal Modeling Case for 1,000,000 Years after Repository Closure.

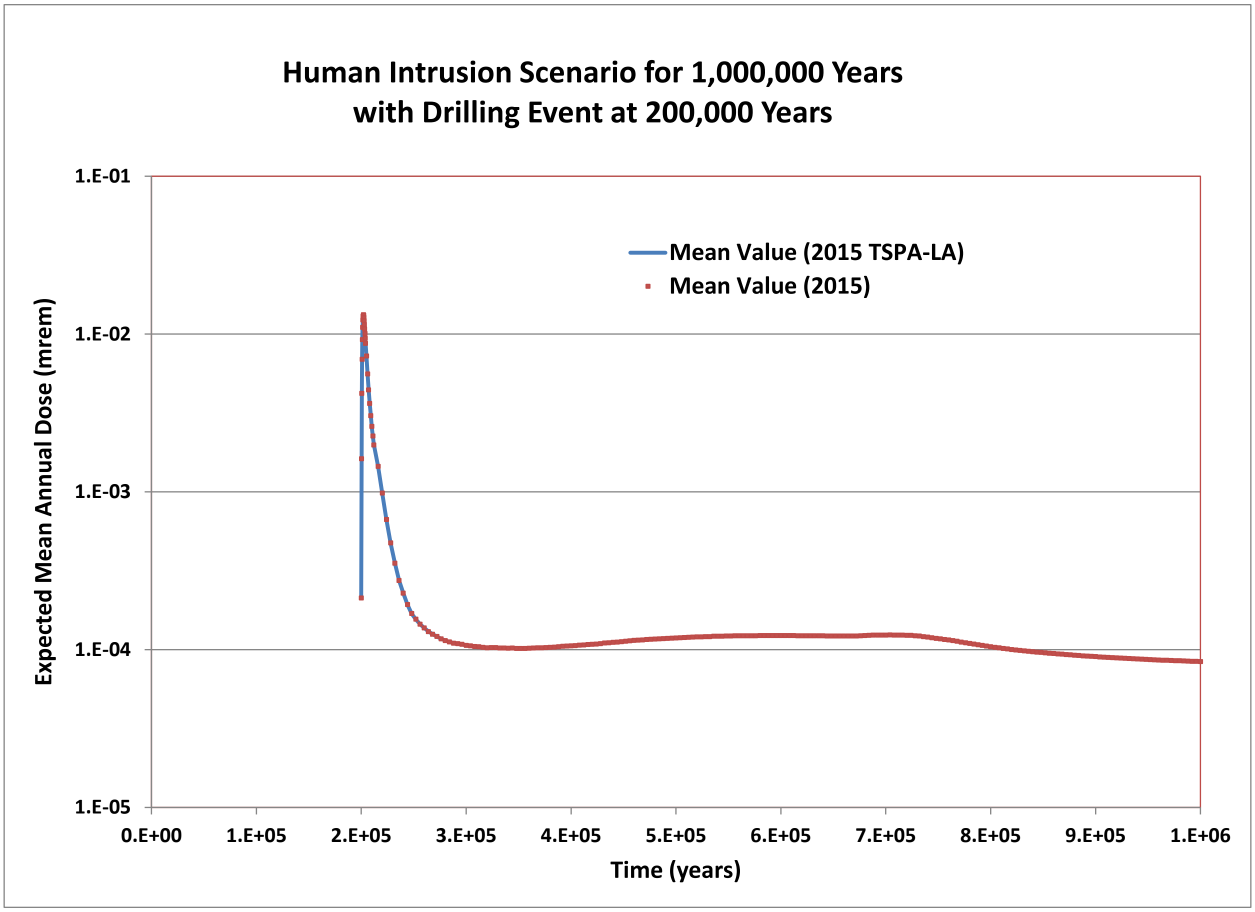


Figure 20. Comparison of Model Results for Expected Mean Annual Dose of the Human Intrusion Modeling Case for 1,000,000 Years after Repository Closure.

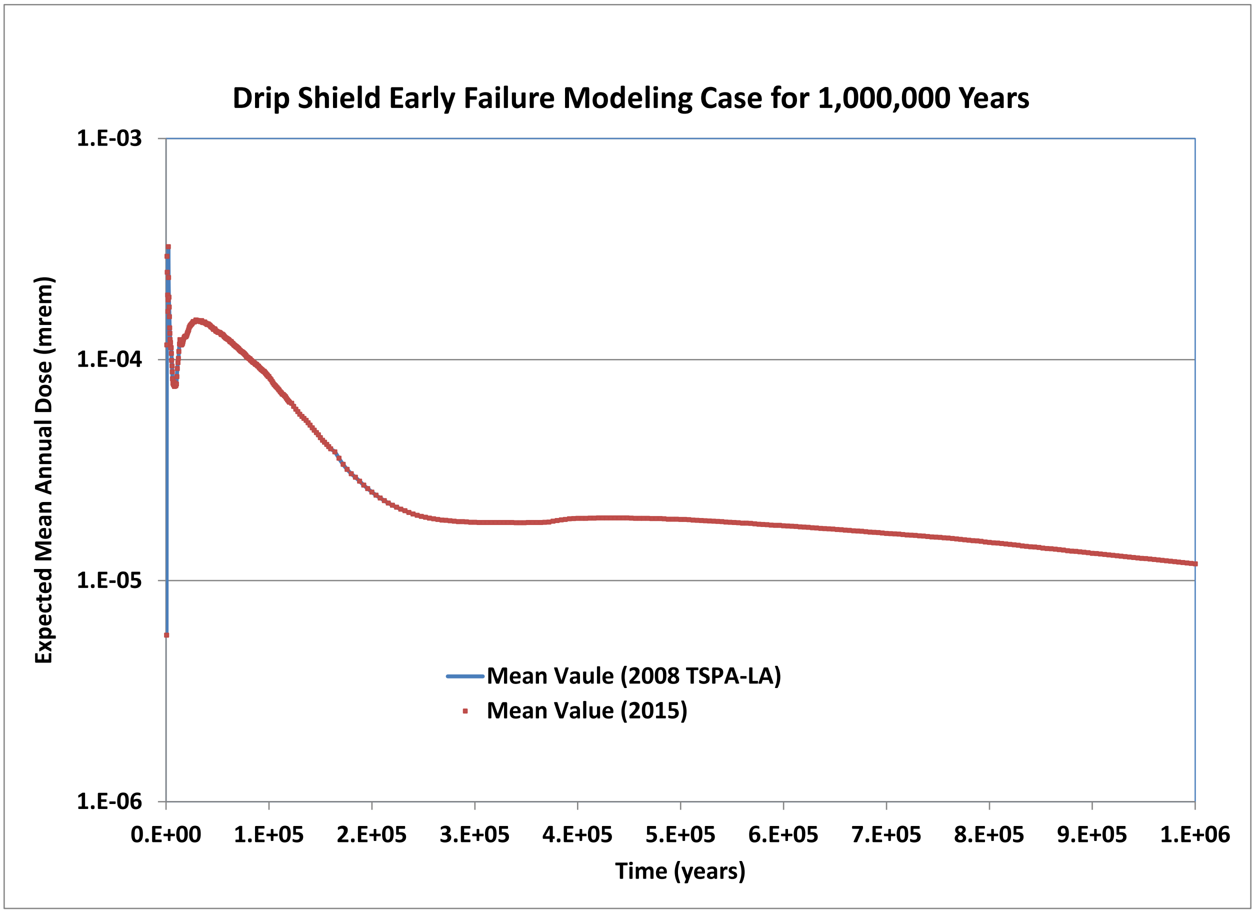


Figure 21. Comparison of Model Results for Expected Mean Annual Dose of the Drip Shield Early Failure Modeling Case for 1,000,000 Years after Repository Closure.

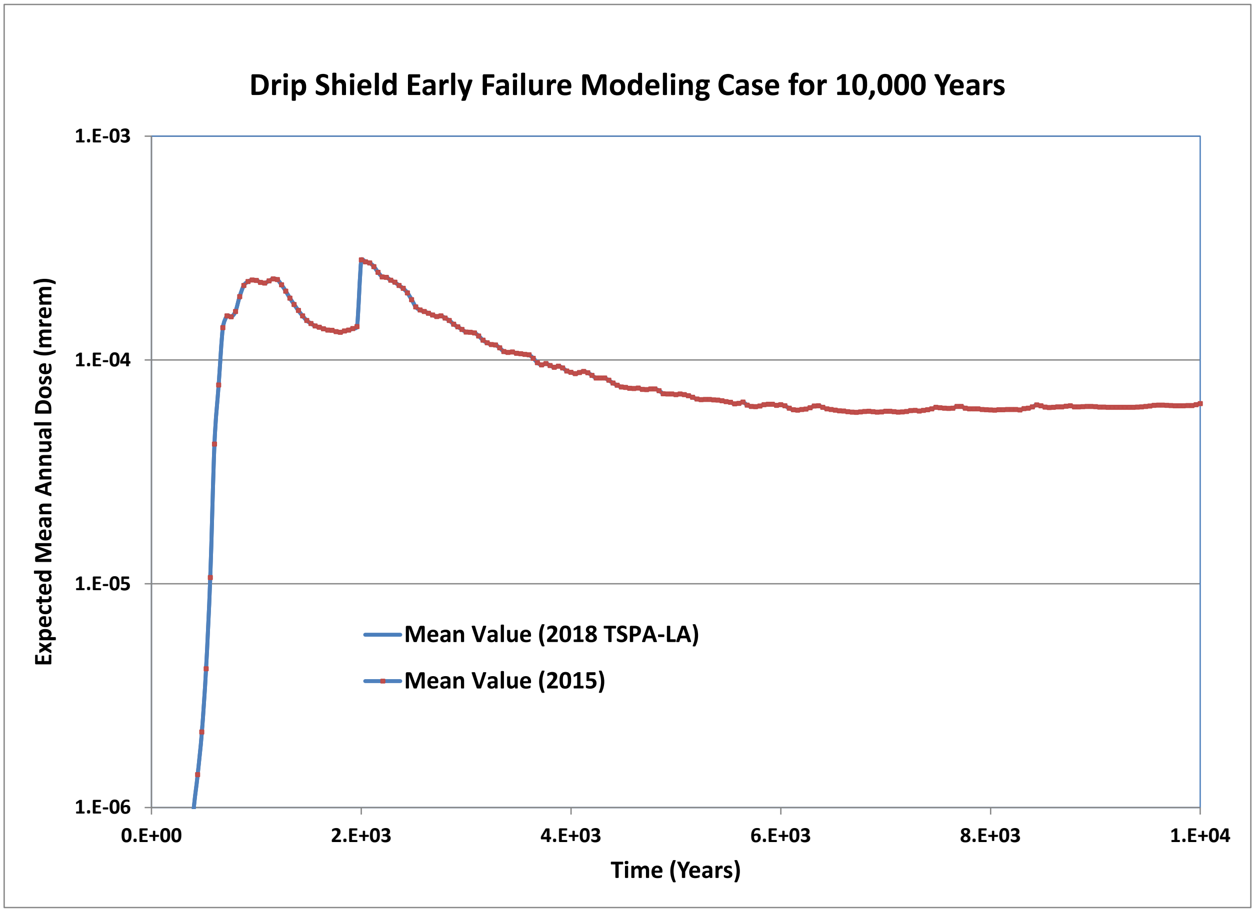


Figure 22. Comparison of Model Results for Expected Mean Annual Dose of the Drip Shield Early Failure Modeling Case for 10,000 Years after Repository Closure.

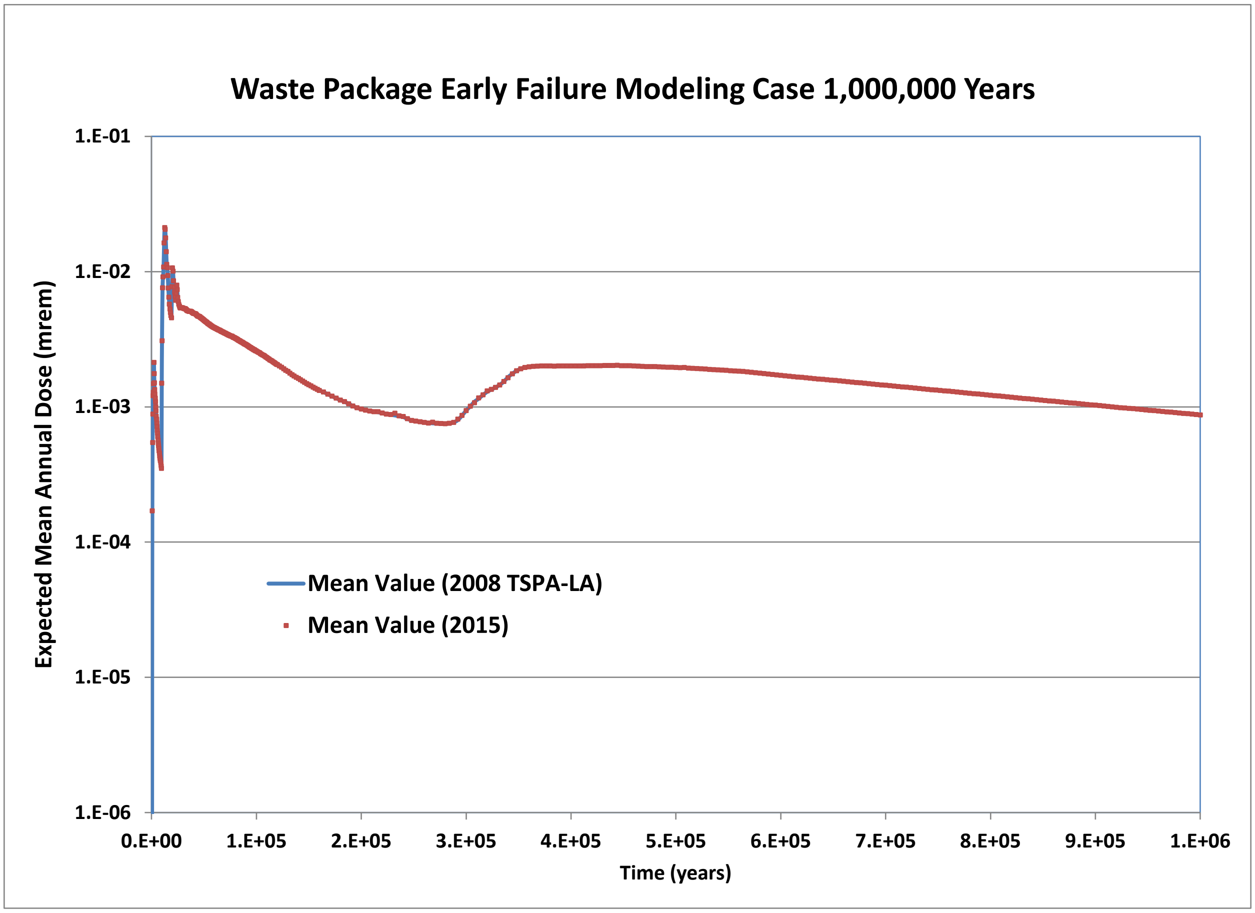


Figure 23. Comparison of Model Results for Expected Mean Annual Dose of the Waste Package Early Failure Modeling Case for 1,000,000 Years after Repository Closure.

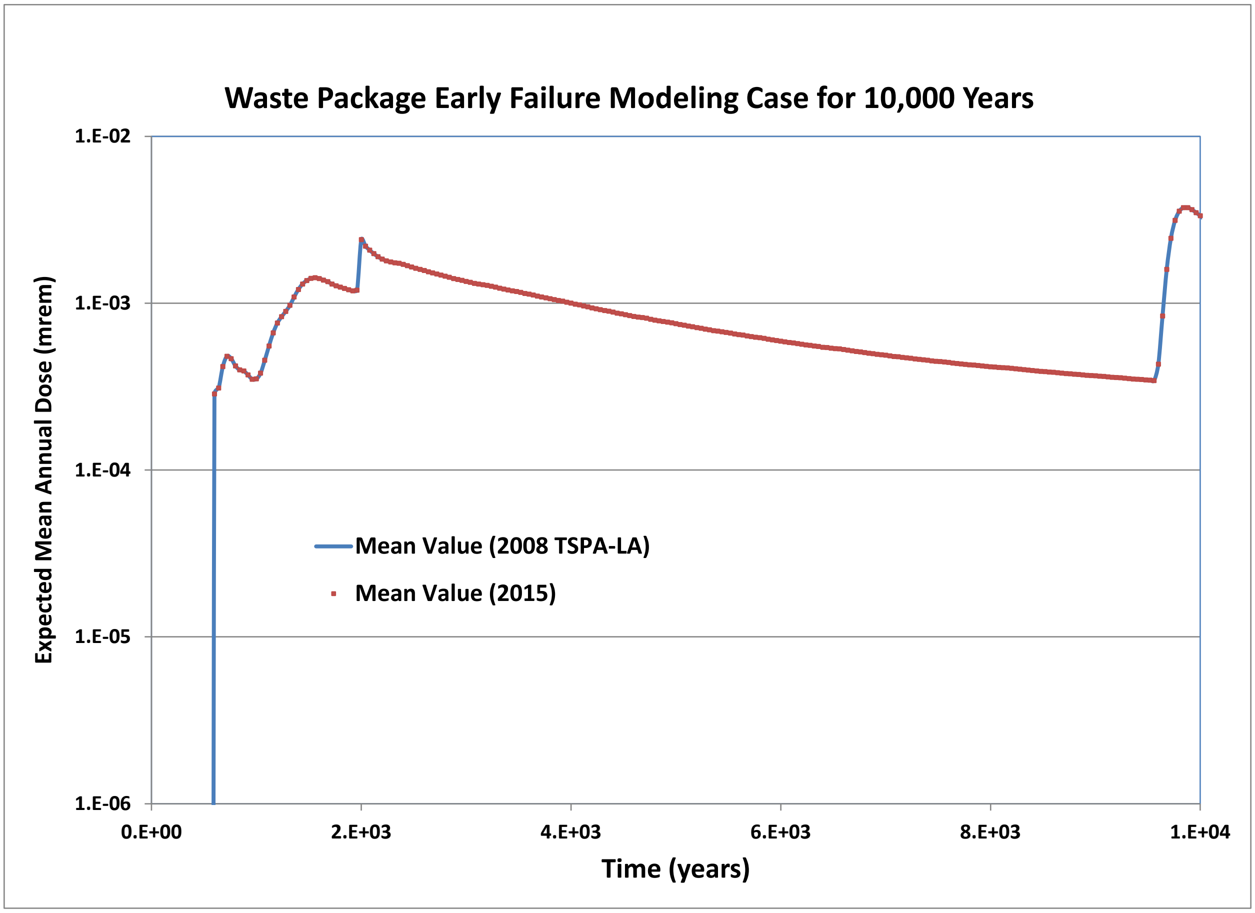


Figure 24. Comparison of Model Results for Expected Mean Annual Dose of the Waste Package Early Failure Modeling Case for 10,000 Years after Repository Closure.

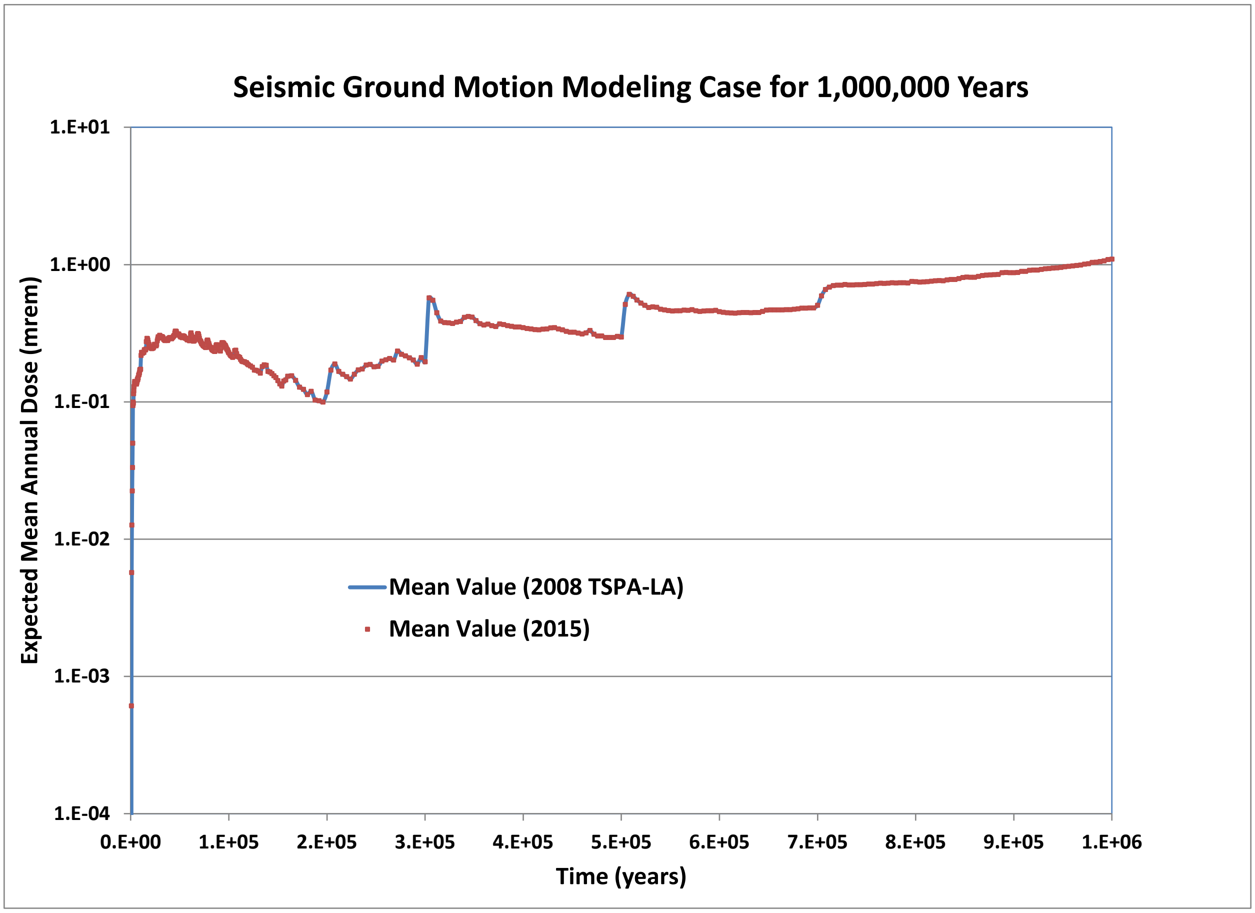


Figure 25. Comparison of Model Results for Expected Mean Annual Dose of the Seismic Ground Motion Modeling Case for 1,000,000 Years after Repository Closure.

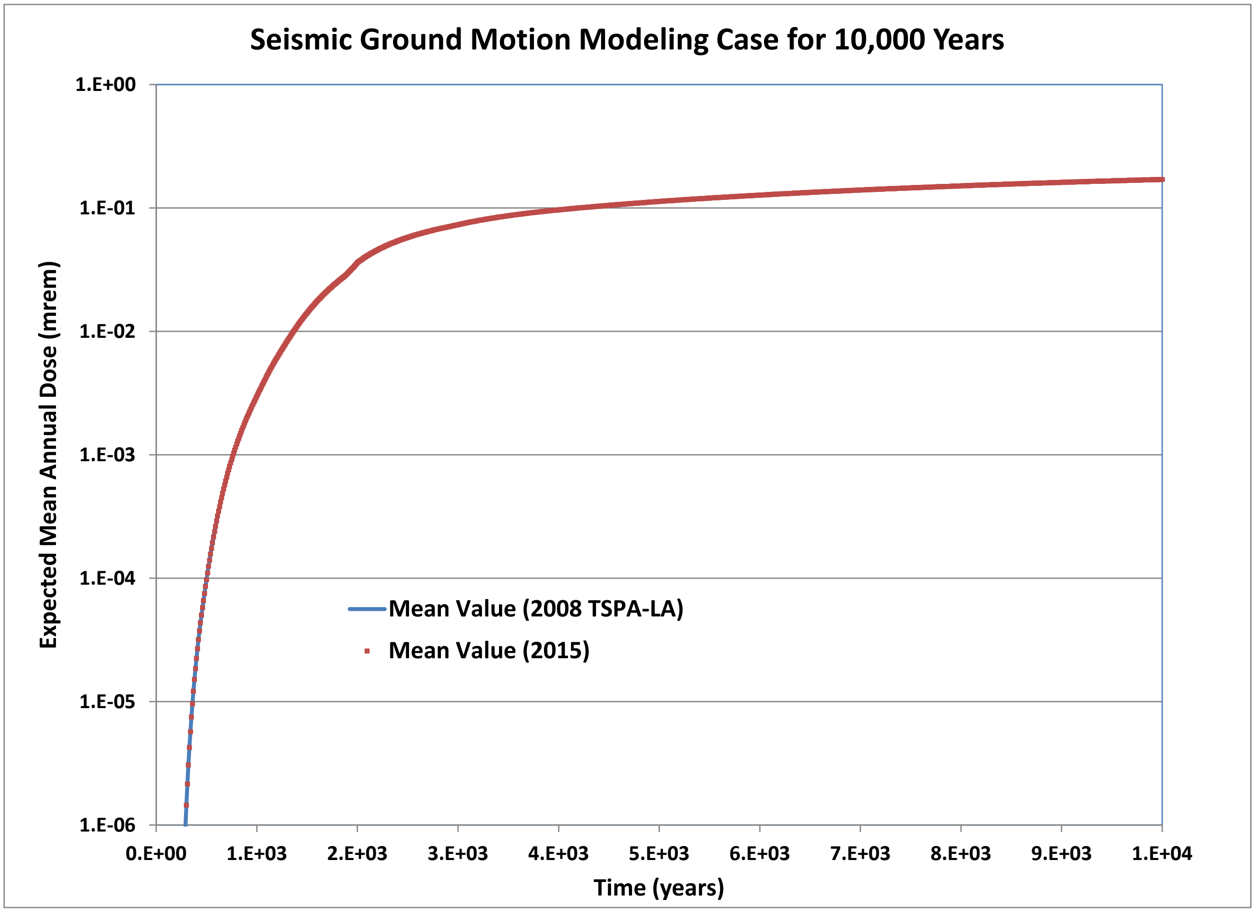


Figure 26. Comparison of Model Results for Expected Mean Annual Dose of the Seismic Ground Motion Modeling Case for 10,000 Years after Repository Closure.

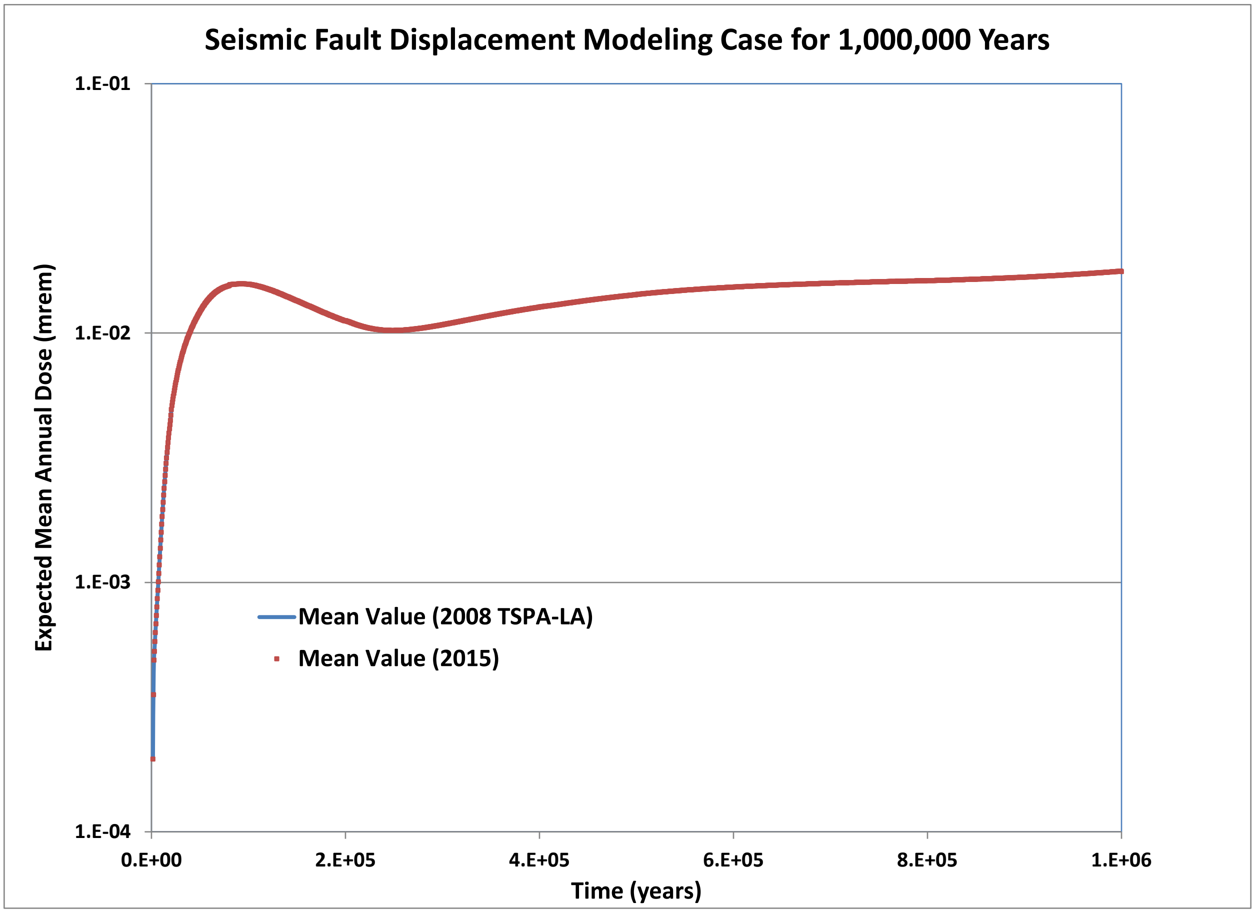


Figure 27. Comparison of Model Results for Expected Mean Annual Dose of the Seismic fault Displacement Modeling Case for 1,000,000 Years after Repository Closure.

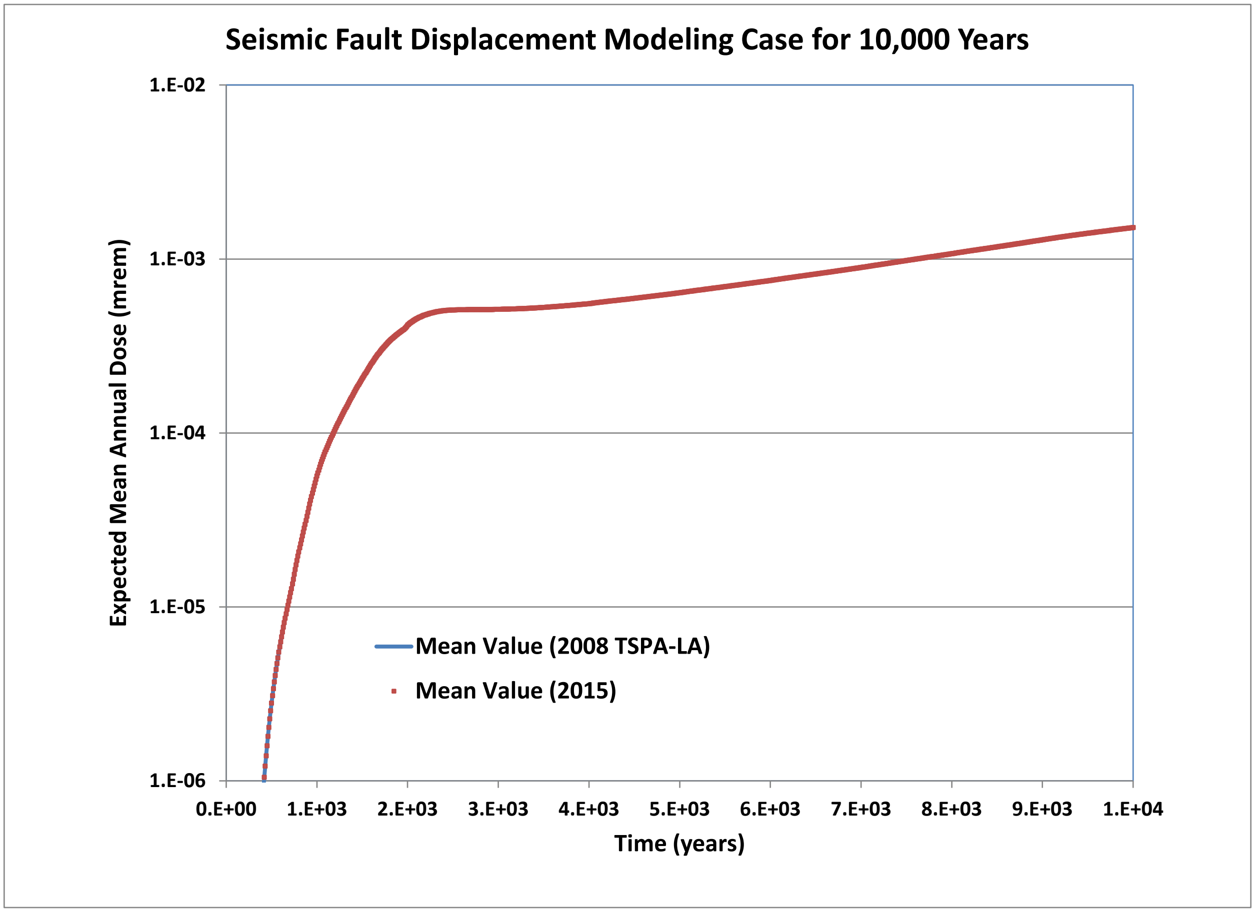


Figure 28. Comparison of Model Results for Expected Mean Annual Dose of the Seismic Fault Displacement Modeling Case for 10,000 Years after Repository Closure.

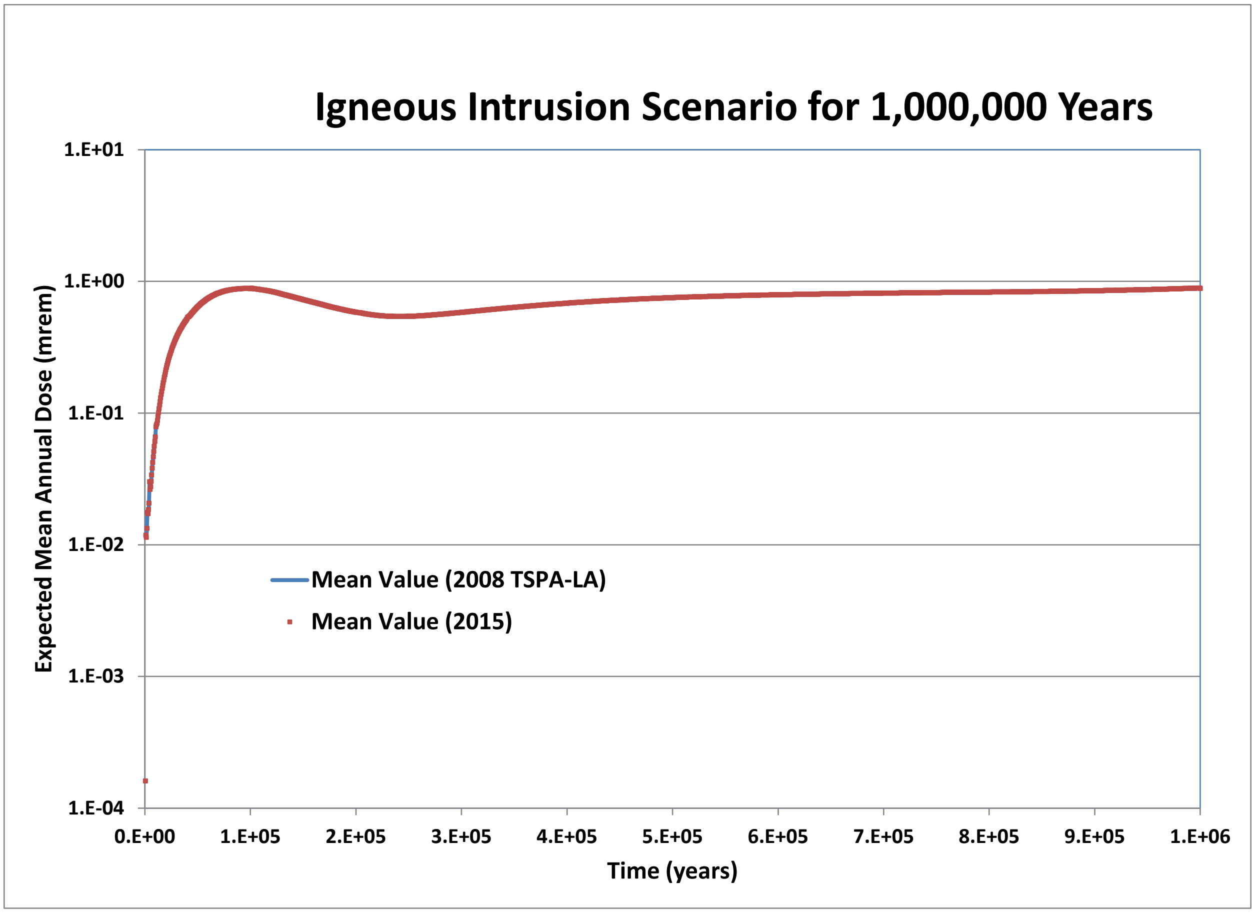


Figure 29. Comparison of Model Results for Expected Mean Annual Dose of the Igneous Intrusion Modeling Case for 1,000,000 Years after Repository Closure.

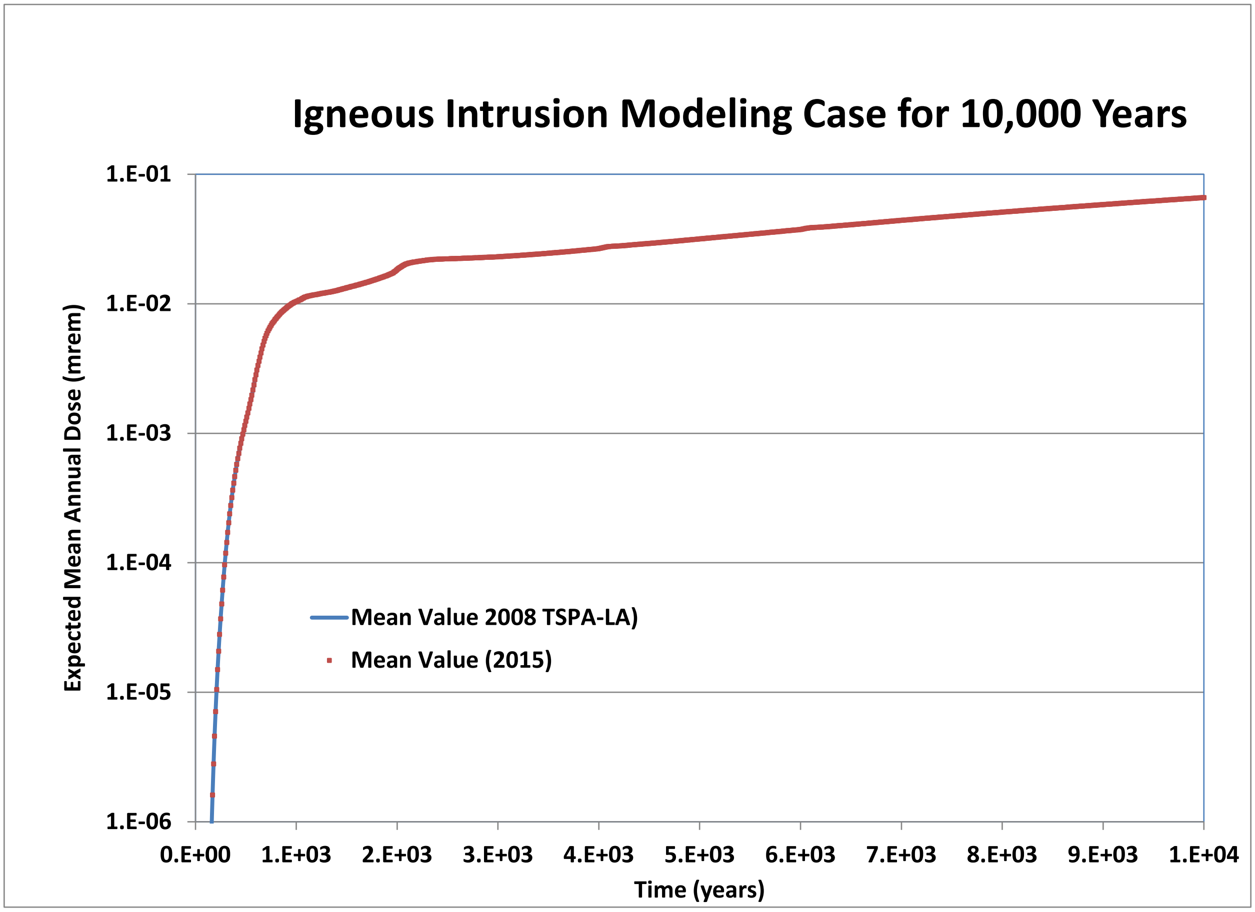


Figure 30. Comparison of Model Results for Expected Mean Annual Dose of the Igneous Intrusion Modeling Case for 10,000 Years after Repository Closure.

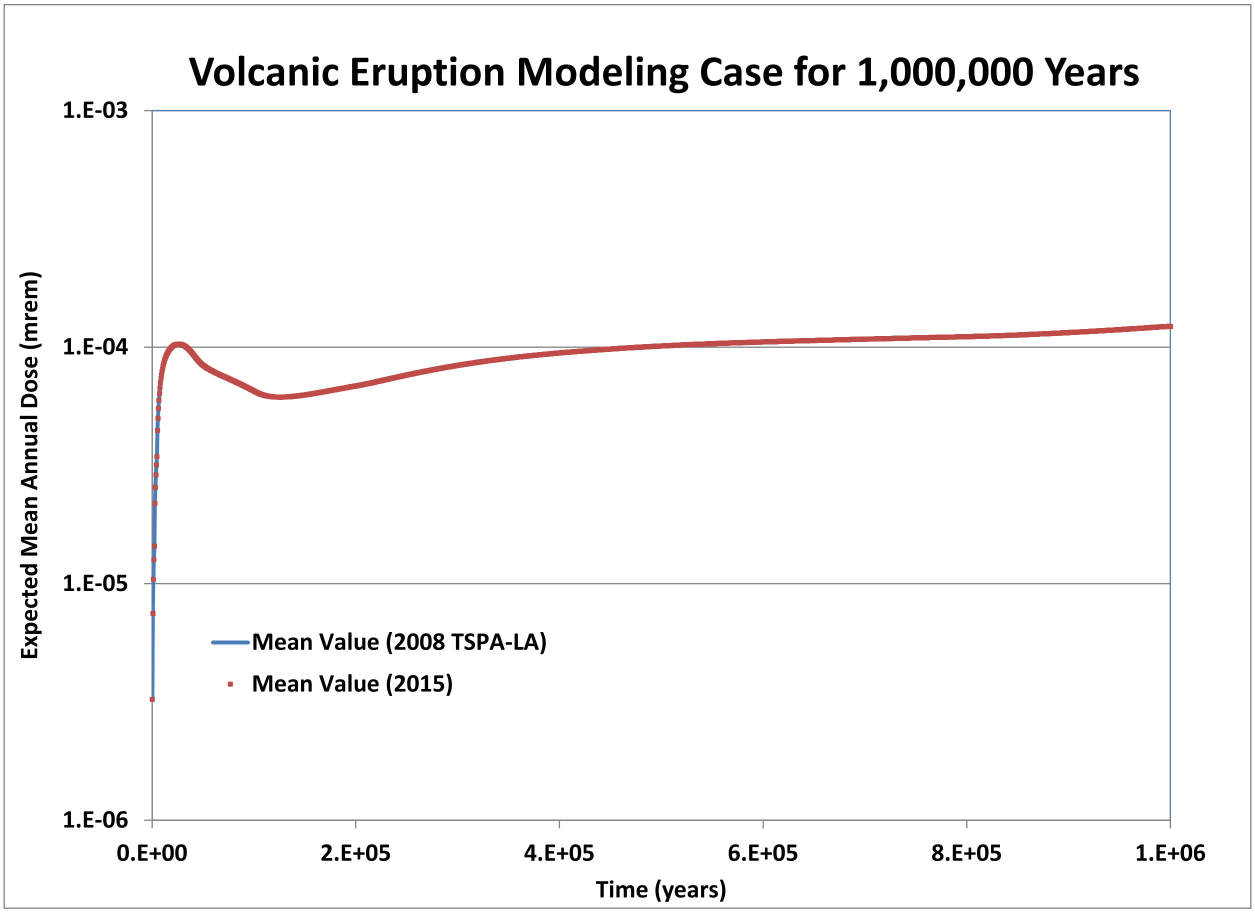


Figure 31. Comparison of Model Results for Expected Mean Annual Dose of the Volcanic Eruption Modeling Case for 1,000,000 Years after Repository Closure.

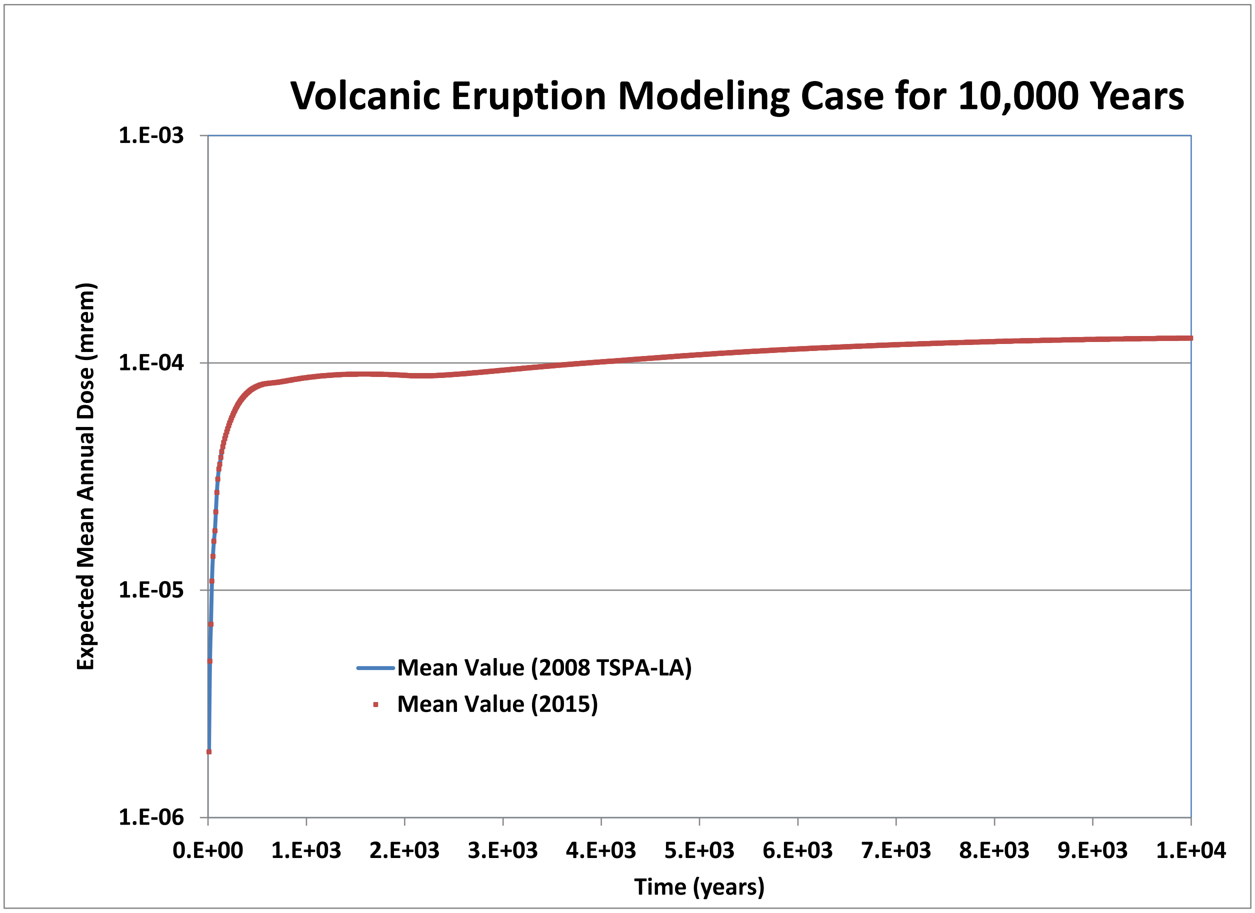


Figure 32. Comparison of Model Results for Expected Mean Annual Dose of the Volcanic Eruption Modeling Case for 10,000 Years after Repository Closure.

6. SUMMARY AND CONCLUSION

The purpose of this work is to evaluate and maintain operational readiness of the computing infrastructure (computer hardware and software) and knowledge capability to perform TSPA-LA type analyses. The following tasks were identified as necessary steps to achieve the objective:

- Evaluation and maintenance of the CL2014 TSPA server cluster system to support reliable executions of the TSPA-LA models and associated analysis and calculations.
- Retrieval of the TSPA-LA model files required input files and other associated files of the TSPA-LA modeling cases.
- Execution of the TSPA-LA model on the TSPA cluster servers (CL2014), ensuring reliable run executions utilizing the GoldSim distributed processing module and reproducible stochastic sampling schemes (GoldSim 2007).
- Post-processing of TSPA model output results to generate the final model output in the format that is consistent with those presented in the TSPA-LA model report (SNL 2008).
- Generation of the plots of the post-processed model output in the format that is consistent with those published in the TSPA-LA model report (SNL 2008).

Execution of TSPA-LA Model on the CL2014 Server Cluster

The latest TSPA-LA models for individual modeling cases retrieved from DTN MO0710ADTSPAWO.000 (GW Modeling cases (v5.005) without Final Documentation) were executed on the CL2014 TSPA server cluster to evaluate performance of the cluster. The modeling cases that were run on the server cluster for the current study for both 1,000,000 and 10,000 years simulations periods include:

- Nominal Modeling Case (300 realizations)
- Drip Shield Early Failure Modeling Case (3,000 realizations)
- Waste Package Early Failure Modeling Case (6,000 realizations)
- Seismic Ground Motion Modeling Case (9,000 realizations)
- Seismic Fault Displacement Modeling Case (10,800 realizations)
- Igneous Intrusion Modeling Case (3,000 realizations)
- Human Intrusion Scenario (9,000 realizations)

All runs were executed on multiple processors on the cluster servers utilizing the GoldSim distributed processing modules (GoldSim 2007), and all runs were completed successfully.

Computing System

The 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 cluster runs under Windows Server 2012 r2, 64-bit operating system. The operating system was optimized for installation and execution of the GoldSim software required to run the GoldSim distributed processing module utility (GoldSim 2010).

The TSPA-LA models (SNL 2008) were developed with GoldSim Version 9.60.300. A floating license of Version 9.60.300 (SP3) has been installed on the cluster head node, and its distributed processing capability was mapped on the cluster processors.

The GoldSim TSPA-LA model output dose results undergo further processing with EXDOC to calculate the distribution of expected values of key model output parameters for each modeling case. The overall purpose of the EXDOC post-processing is to separate aleatory and epistemic uncertainty in the TSPA-LA model output.

Plots for the TSPA-LA model output results were created with SigmaPlot Versions 8.0, 12.5 and 13.0. SigmaPlot Version 8 or later versions is required to open and view the plots and data of the plot files contained in the TSPA-LA model output DTN.

The performance of the computing system was tested prior to full verification runs as reported in Appendix B. The testing also included safe and reliable retrieval of the GoldSim TSPA-LA model files and associated files from the model output DTN. The results confirmed that the computing system reliably reproduces components of the TSPA-LA. The confirmatory tests also showed that the CL2014 hardware is much more efficient and faster in comparison to the previous hardware.

TSPA-LA Model Reproducibility Verification

Verification of the TSPA-LA model reproducibility on the TSPA server cluster was conducted by comparing the output of the new model runs of all the TSPA-LA modeling cases with the output retrieved from the DTN MO0710ADTSPAWO.000. Two approaches were used for the verification effort: 1) numerical value comparison, and 2) graphical comparison.

For the numerical value comparison verification, relative differences of all individual values of a selected output parameter of the new model run were calculated against its respective individual value from the TSPA-LA model output retrieved from DTN MO0710ADTSPAWO.000. The relative differences were very small for all the individual dose values of the selected model output parameter, demonstrating an excellent reproducibility. In general the individual dose values were identical to the 3rd or 4th digit from the first non-zero digit, and the differences beyond the 3rd or 4th digit are due mainly to rounding errors.

The graphical comparison verification of the TSPA-LA model reproducibility on the server cluster was conducted by comparing the plots of output from the new model runs using CL2014 with those reported in the TSPA-LA report (SNL 2008). Plots of "expected annual dose" of the above individual modeling cases were chosen for the model reproducibility verification. The plots also show probabilistic projections of expected annual dose. The graphical comparison also included use of Excel plots of expected mean annual dose of the TSPA-LA and new results, for each modeling case. Both graphical comparison methods showed that the results were nearly identical. This result was expected from the very small relative differences of all individual numerical values of the model output parameter. This demonstrates an excellent reproducibility of the TSPA-LA on the CL2014 cluster.

The modeling analysis documented in this report concentrated on demonstrating the capability of the TSPA cluster to reproduce the TSPA-LA modeling cases. The TSPA-LA also included uncertainty and sensitivity analyses, which does not require use of the cluster. The next step would be to reproduce those analyses to demonstrate system readiness. Another recommendation for future work includes migrating the TSPA-LA model from GoldSim Version 9.60.300 to the latest version of GoldSim Version 11.1. This is based on suggestions by GoldSim staff who stated that Version 9.60.300 is not backwards compatible with the newer versions of GoldSim. They also stated that future Windows versions may not support GoldSim Version 9.60.300.

7. REFERENCES

DOE (U.S. Department of Energy) 2005. *User Information for: MVIEW 4.0.* Document ID: 10072-UID-4.0-00. Las Vegas, Nevada: U.S. Department of Energy, Office of Repository Development. ACC: MOL.20050712.0027. See also: MVIEW V. 4.0. 2007. WINDOWS XP. STN: 10072-4.0-01.

DOE (U.S. Department of Energy) 2007. *User Information Document for: EXDOC_LA Version 2.0.* Document ID: 11193-UID-2.0-00. Las Vegas, Nevada: U. S. Department of Energy, Office of Repository Development.

DOE (U.S. Department of Energy). 2008. *Yucca Mountain Repository License Application: Safety Analysis Report.* DOE/RW-0573, Revision 1. U.S. Department of Energy, Washington, DC. (http://www.nrc.gov/waste/hlw-disposal/yucca-lic-app/yucca-lic-app-safety-report.html#1)

DOE (U.S. Department of Energy) 2010. Direction to Withdraw Work Related to Office of Civilian Radioactive Waste Management (OCRWM) Licensing Proceedings; Contract No. DE-AC04-94AL85000; Letter from JoAnn Wright, NNSA Contracting Officer to Gary Zura, Deputy for Contracts; Dated May 12, 2010.

GoldSim (GoldSim Technology Group) 2007. *User's Guide, GoldSim Probabilistic Simulation Environment.* Version 9.60. Two volumes.; *User's Guide, GoldSim Contaminant Transport Module.* Version 4.20; *User's Guide, GoldSim Distributed Processing Module*, Version 9.60. Issaquah, Washington: GoldSim Technology Group, March 2007.

GoldSim 2010. *User's Guide, GoldSim Probabilistic Simulation Environment.* Version 10.50, Two volumes; *User's Guide, GoldSim Contaminant Transport Module.* Version 6.0; *User's Guide, GoldSim Distributed Processing Module*, Version 10.50. Issaquah, Washington: GoldSim Technology Group, December 2010.

Helton, J. C., Hansen, C. W., and Sallaberry, C. J. 2014. Conceptual Structure and Computational Organization of the 2008 Performance Assessment for the Proposed High-Level Radioactive Waste Repository at Yucca Mountain, Nevada, *Reliability Engineering and System Safety*, 122, 223-248.

Lee, J. and Hadgu, T. (2014). Evaluation of the Computing Systems for Yucca Mountain Repository TSPA-LA Model Operational Readiness, Sandia National Laboratories, Albuquerque, New Mexico. SAND2014-18178.

NWPA (Nuclear Waste Policy Act). 1983. Public Law 97-425; 96 Stat. 2201, as amended by P.L. 100- 203. December 22, 1987.

SNL (Sandia National Laboratories) 2008. *Total System Performance Assessment Model/Analysis for the License Application.* MDL-WIS-PA-000005 REV 00 ADD 01. Las Vegas, Nevada: Sandia National Laboratories.

APPENDIX A: STEPS FOR EXECUTION OF THE TSPA MODELING CASES

TSPA runs for the modeling cases were initiated from the local C: drive of the TSPA Cluster. Relevant input files from DTNs listed in Section 3.5 are copied into folders in the Local Disk (C:)/Users/. Outputs were directed to the same folders.

- In the TSPA run folder place the following:
  - The original GoldSim file that came with the DTN
  - DLL_Set_35 (this is not included in the DTN. Check readme file on instructions where to get it).
  - Input_File_Set_064_Corrected (found in DTN MO0806TSPADCOR.000)
  - TS_Proc.dll - The model location in the TSPA model for this element is: "\Time_Zero\EBS_PS_Loop\EBS_PSE_Loop\TS_PROC_DLL". In this element, the computer pathway to TS_PROC.dll must match the local installation.
  - For more information follow instructions that came with the DTN

For each test GoldSim simulation of the TSPA-LA model, the following steps are taken carefully to ensure successful execution and stable model output.

- Run the batch file Run_setup.bat to create a text file that contains the chosen number of nodes and processors per node.
- Copy the content of the newly created text file into a blank text file and save it with .slv extension.
- A shorter version of the above steps was also used to expedite making model runs:
  - Run Cluster_reboot.bat to reboot all processors (except the head node) so that any issues from a previous run do not interfere with a new run.
  - Run reboot_check.bat to check progress of rebooting the system. The batch file provides the status of all compute nodes.
- Open the GoldSim model and select Run on Network. Import the newly created .slv file during "Run on Network" set up. This prepares the selected processors of the compute nodes to connect to and accept the run execution directions from the master program of the GoldSim distributed processing module that is executed on the head node.
- Select "Update Status" to launch the selected processors.
- Execute the TSPA model.
- Monitor the run status frequently and the progression of the model run on the compute nodes. If there are issues, the run can be terminated to save time. Once the problems have been addressed the run would then be restarted.

Volcanic Eruption 1,000,000 Years Modeling Case

The Volcanic Eruption 1,000,000 years modeling case has to be run ten times representing ten eruption times. There was a problem in running the modeling case on cluster CL2014. The problem was that the external files (DLLs) located at model/simulation-settings/external files were locked and GoldSim could not get to the files. The solution was to unlock the external files before the runs were made. The same remedy was applied to the volcanic eruption 10,000 years modeling case. All the rest of the modeling cases did not have such a problem.

APPENDIX B: CONFIRMATION OF TSPA-LA MODEL RUNS ON NEW CLUSTER (CL2014) WITH GOLDSIM VERSION 9.60.300

This appendix discusses the confirmation of the TSPA-LA model reproducibility on the new TSPA server cluster (CL2014) using GoldSim Version 9.60.300. Prior to rerunning the full suite of the TSPA-LA models on Cluster CL2014, confirmatory test runs were conducted. The Nominal modeling case was selected for the confirmatory tests because it contains the lowest number of realizations (300) and is thus faster to run. Thus, the Nominal modeling case was run on the new server cluster (CL2014) for the test cases. All test runs were executed on multiple number of processors on the cluster utilizing the GoldSim distributed processing modules (GoldSim 2007).

A total of three runs were made for the confirmation tests using he nominal modeling case with 300 realizations. The three runs are listed below. Execution of the runs followed the steps described in Appendix A.

- Run1: 100 processors (10 compute nodes x 10 processors per compute node)
- Run2: 200 processors (20 compute nodes x 10 processors per compute node)
- Run3: 300 processors (30 compute nodes x 10 processors per compute node)

Outputs of the runs were evaluated for the confirmatory analysis. The model output reproducibility confirmation was conducted by comparing the output from the new model runs with the output for the TSPA-LA Nominal modeling case retrieved from the DTN MO0710ADTSPAWO.000 (GW Modeling cases (v5.005) without Final Documentation) (SNL 2008). The confirmatory analysis used numerical value comparison as well as graphical comparison.

For the model reproducibility confirmation by numerical value comparison, the model output parameter "Dose_Total" was chosen. All individual values of the selected output parameter of the new model run were compared with its respective individual value from the TSPA-LA model output retrieved from DTN MO0710ADTSPAWO.000. Excel spreadsheet calculations were performed to calculate the relative differences of the new model output values using Equation 1. The average relative difference for the three runs was 0.034% for all the individual dose values of the selected model output parameter. This demonstrates an excellent reproducibility of the TSPA-LA model output. Further testing was done with the rest of the TSPA-LA modeling cases during verification of TSPA-LA results.

Figure 33 shows a graphical comparison of the outputs of Expected Mean Annual Dose for the Nominal Modeling Case for 1,000,000 Years after repository closure. The figure includes results of TSPA-LA together with those of runs 1 to 3. As shown, the results are nearly identical.

Figure 34 shows computation times for the three runs on Cluster CL2014 for the Nominal modeling case. The figure also shows the computation time for the Nominal modeling case on an older cluster (Cl2010) with 100 processors. Comparing the computation time for the two clusters shows that Cluster CL2014 was found to be 20% faster. As would be expected, increasing the number of processors on the new cluster reduces the total computation time. That is shown with the blue line in Figure 34. The trend is also shown in Figure 35, which shows computation speed-up using computation time for Run 1 as a reference. As number of processors increases, the speed increases. However, as number of processors increases the time spent on communication between the head node and the compute nodes also increases, which takes up some CPU time. Thus, the speed-up between Run 1 (100 processors) and Run 3 (200 processors) is 2.2, less than the maximum possible of 3.

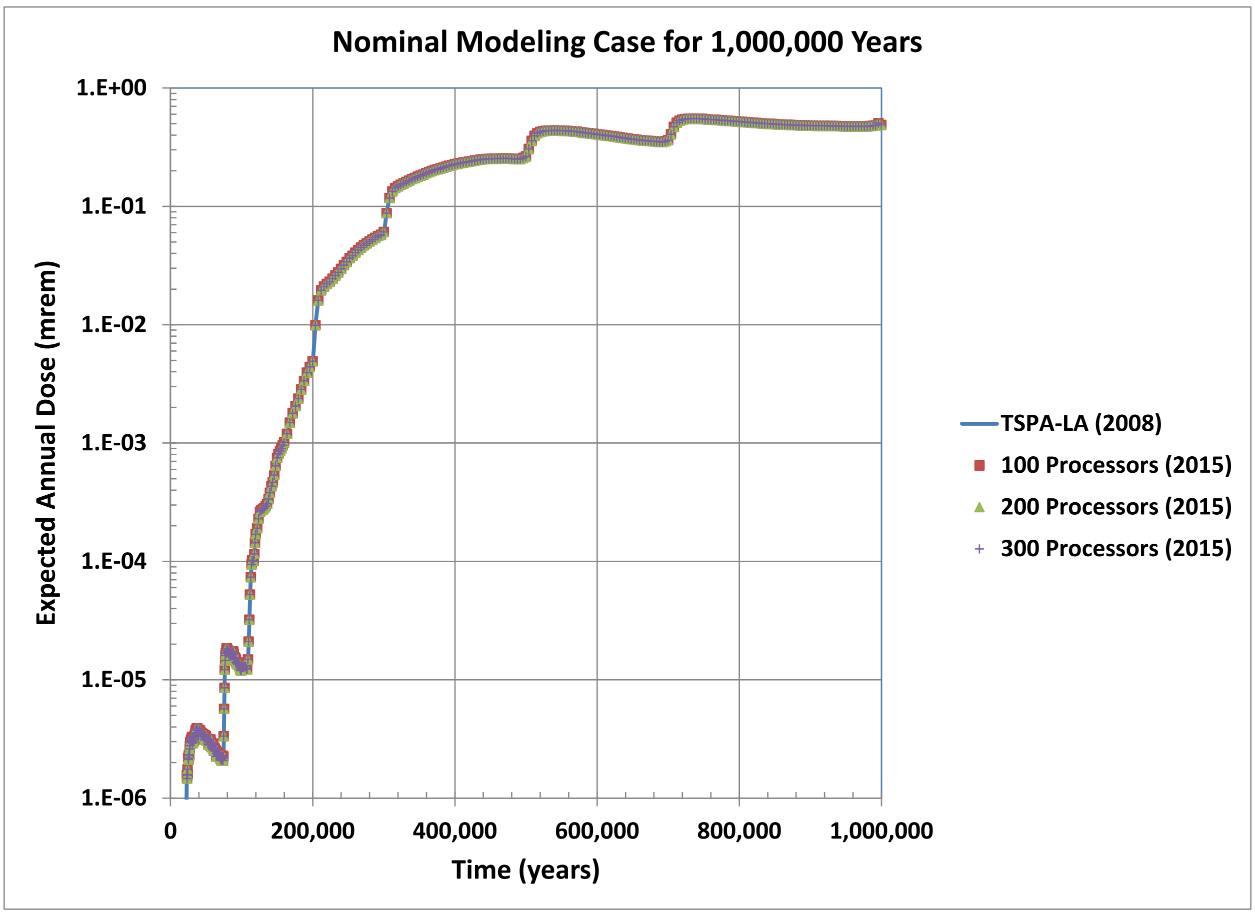


Figure 33. Comparison of Model Results of Expected Mean Annual Dose for the Nominal Modeling Case for 1,000,000 Years after repository Closure: TSPA-LA and Runs 1 to 3.

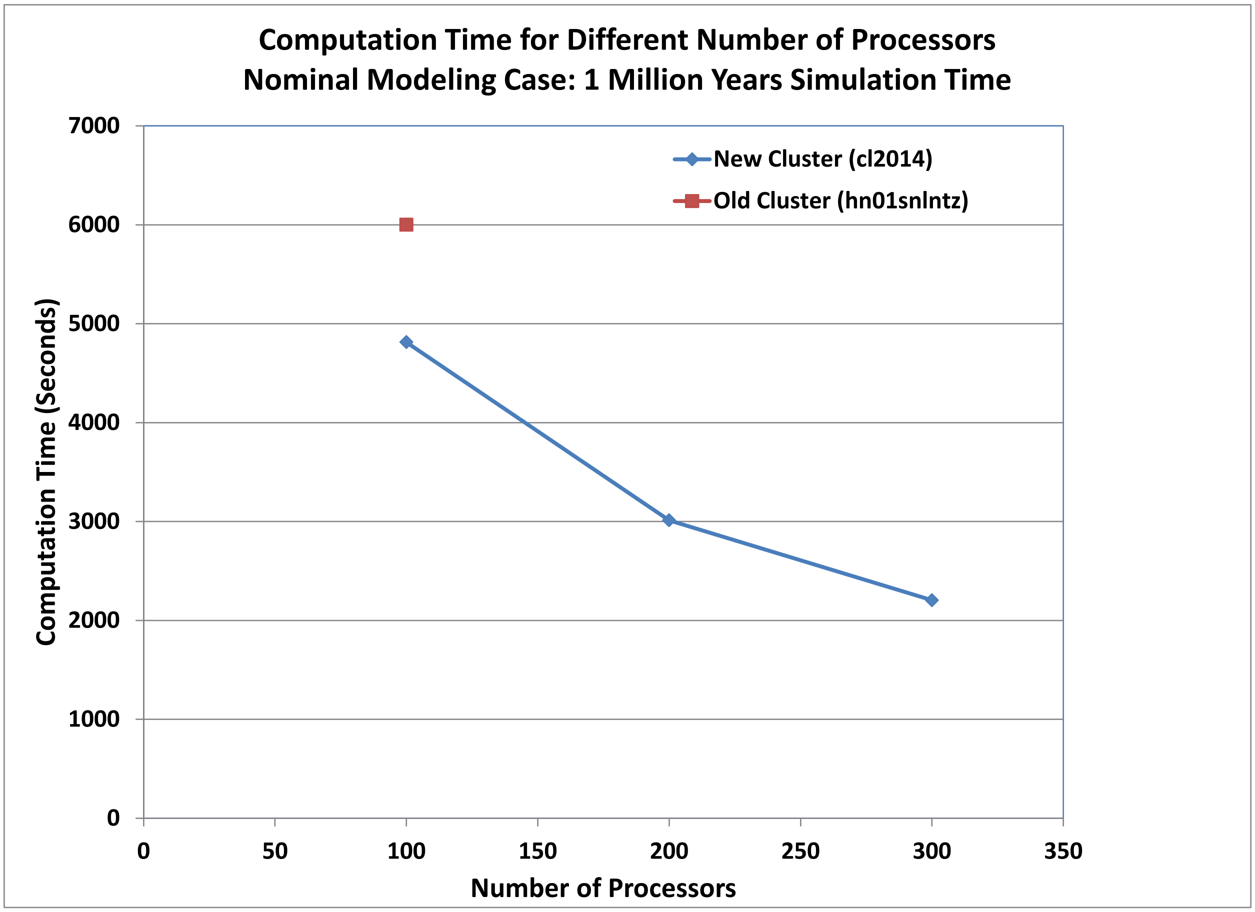


Figure 34. Comparison of Computation Times for Expected Mean Annual Dose for the Nominal Modeling Case for 1,000,000 Years after repository Closure: Cluster hn01snlntz with 100, 200 and 300 processors for Runs 1, 2 and 3, respectively on Cluster CL2014.

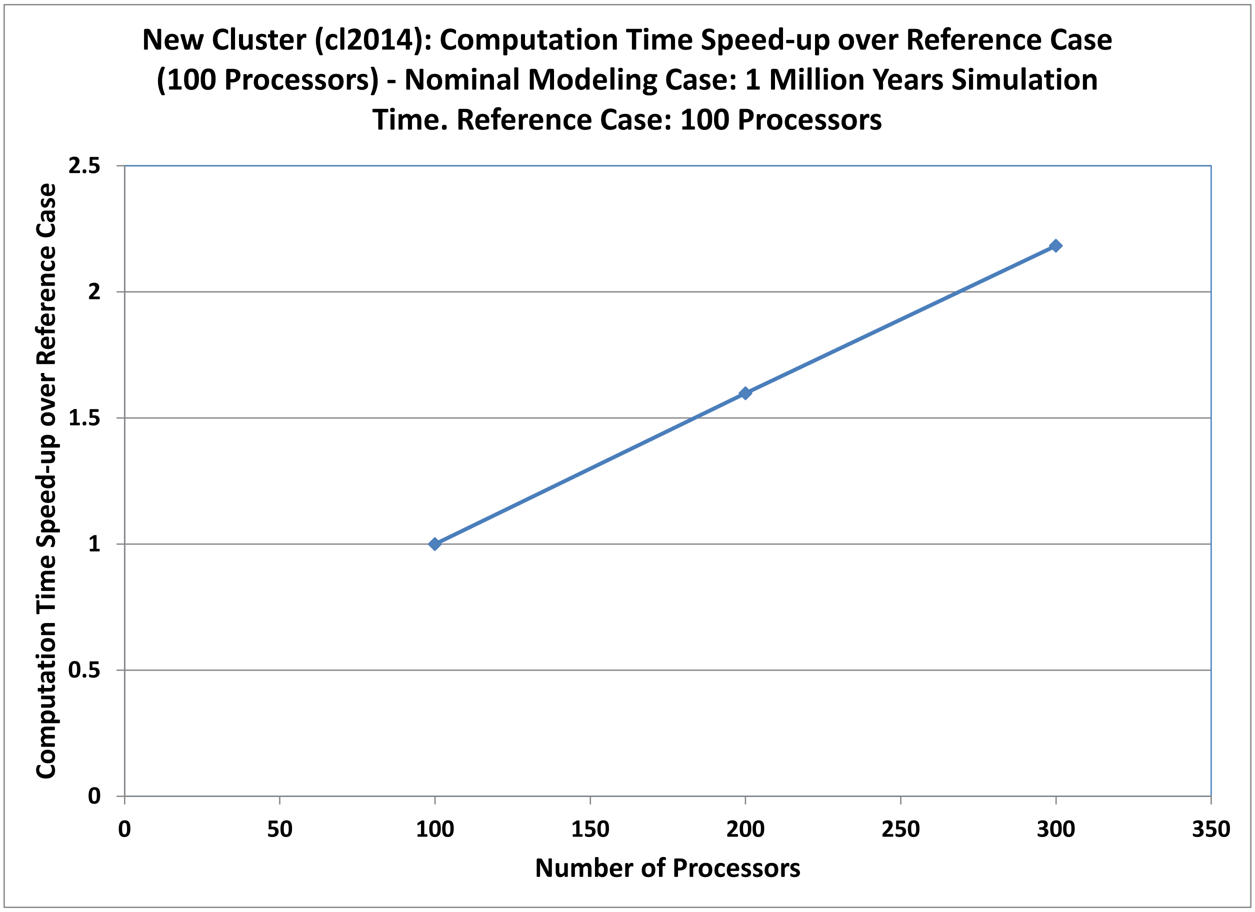


Figure 35. Comparison of Computation Time Speed-Up for Expected Mean Annual Dose for the Nominal Modeling Case for 1,000,000 Years after repository Closure: Reference Case with 100, 200 and 300 Processors for Runs 1, 2 and 3, respectively on Cluster CL2014.

APPENDIX C: POST PROCESSING WITH EXDOC

The following is a list of changes to be added to EXDOC documentation for the different TSPA-LA modeling cases for smooth execution of the software.

- Waste Package Early Failure Modeling Case, 10,000 years
  - As with Drip Shield Early Failure Modeling, 10,000 years, the split files with extension "_001.txt" have to be copied to "_002.txt". Thus files with both extensions are needed to complete the EXDOC steps.
- Waste Package Early Failure Modeling, 1,000,000 years
  - As with Drip Shield Early Failure Modeling Case, 1,000,000 years, the split files with extension "_001.txt" have to be copied to "_002.txt". Thus files with both extensions are needed to complete the EXDOC steps.
- Seismic Ground Motion Modeling Case 1,000,000 years
  - There is no EXDOC WORD document for this modeling case. It shares similar input as Human Intrusion Modeling case, 1,000,000 years. Thus, documentation for Human Intrusion Modeling case is used. There is also a document titled "EXDOC_cofirmation_Settings.doc: that has information on this.
  - There is no need for splitting files. Just rename "Dose_Total.txt" to "Dose_Total_001.txt".
- Seismic Fault Displacement, 1,000,000 years
  - Documentation on the modeling case for the Split step misses one line at the bottom. The entry for "index for each parameter value" should include "1 2 3" at the end.
  - Also, the file A2_Seep_Frac.txt should be renamed A2_1M_Seep_Frac.txt for this modeling case.
  - In Fig. 4 of the instruction file change "Dose_Th230" to "Dose_Total"
  - After the split is done, copy the 36 new files that are generated and add 36 files with the extension 002. i.e. copy and rename the files with extension 001 to extension 002.
- Seismic Fault Displacement, 10,000 years
  - The Split file misses one line at the bottom. The entry for "index for each parameter value" should include "1 2 3 " at the end.
  - After the split is done, copy the 36 new files that are generated and add 36 files with the extension 002. i.e. copy and rename the files with extension 001 to extension 002.
  - Also, A2_Seep_Frac.txt should be renamed A2_10k_Seep_Frac.txt
  - For Dose_Total analysis the Zero_Dose files and batch files are not used.
- Volcanic Eruption Modeling Case, 1,000,000 years

  - Needs number of time steps from the 10 files generated in the GoldSim runs. Open each file and record the time steps. The first two lines are not counted. The number of lines represents the total number of time steps. Use the data to run EXDOC for each file.
  - On Fig. 7 of the instruction file the maximum time given should be changed to 1000000.
- Volcanic Eruption Modeling Case, 10,000 years
  - Needs number of time steps from the 9 files generated in the GoldSim runs. Open each file and record the time steps. The first two lines are not counted. The number of lines represents the total number of time steps. Use the data to run EXDOC for each file.
  - On Fig. 7 of the instruction file the maximum time given should be changed to 20000.

DISTRIBUTION

1	MS0736	Tito Bonano	06220
1	MS0747	Kevin McMahon	06222
1	MS0747	Robert J. MacKinnon	06224
1	MS0747	Gordon Appel	06222
1	MS0747	Teklu Hadgu	06222
1	MS0899	Technical Library	9536 (electronic copy)