SANDIA REPORT
SAND2016-9957
Unlimited Release
Printed October 2016

Reproduction of the Yucca Mountain Project TSPA-LA Uncertainty and Sensitivity Analyses and Preliminary Upgrade of Models

Teklu Hadgu and Gordon Appel

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

Sandia National Laboratories is a multi-mission 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.

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

SAND2016-9957
Unlimited Release
Printed September 2016

Reproduction of the Yucca Mountain Project TSPA-LA Uncertainty and Sensitivity Analyses and Preliminary Upgrade of Models

Teklu Hadgu and Gordon Appel
Nuclear Waste Disposal research and Analysis
Sandia National Laboratories
MS 0747
P.O. Box 5800
Albuquerque, New Mexico 87185

Abstract

Sandia National Laboratories (SNL) continued evaluation of total system performance assessment (TSPA) computing systems for the previously considered Yucca Mountain Project (YMP). This was done to maintain the operational readiness of the computing infrastructure (computer hardware and software) and knowledge capability for total system performance assessment (TSPA) type analysis, as directed by the National Nuclear Security Administration (NNSA), DOE 2010. This work is a continuation of the ongoing readiness evaluation reported in Lee and Hadgu (2014) and Hadgu et al. (2015). The TSPA computing hardware (CL2014) and storage system described in Hadgu et al. (2015) were used for the current analysis. One floating license of GoldSim with Versions 9.60.300, 10.5 and 11.1.6 was installed on the cluster head node, and its distributed processing capability was mapped on the cluster processors. Other supporting software were tested and installed to support the TSPA-type analysis on the server cluster. The current tasks included verification of the TSPA-LA uncertainty and sensitivity analyses, and preliminary upgrade of the TSPA-LA from Version 9.60.300 to the latest version 11.1. All the TSPA-LA uncertainty and sensitivity analyses modeling cases were successfully tested and verified for the model reproducibility on the upgraded 2014 server cluster (CL2014). The uncertainty and sensitivity analyses used TSPA-LA modeling cases output generated in FY15 based on GoldSim Version 9.60.300 documented in Hadgu et al. (2015). The model upgrade task successfully converted the Nominal Modeling case to GoldSim Version 11.1. Upgrade of the remaining of the modeling cases and distributed processing tasks will continue. 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 Jason Garland (9341), Bob D'Spain (9329), John Reynolds (9341), Jesse Saunders (6222) and GoldSim Technology Group. 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 (6222) for his constructive review of the report.

CONTENTS

FIGURES

TABLES

NOMENCLATURE

DLL	Dynamically Linked Libraries
DOE	Department of Energy
DOSTOT	Total Dose to the Reasonably Maximally Exposed Individual
DP	Distributed Processing
DTN	Data Tracking Number
EXPDOSE	Expected Dose to the Reasonably Maximally Exposed Individual
GB	Gigabyte
GTG	GoldSim Technology Group
LA	License Application
LHS	Latin Hypercube Sample
PRCC	Partial Rank Correlation Coefficients
RAM	Random Access Memory
RMEI	Reasonably Maximally Exposed Individual
SNL	Sandia National Laboratories
SP	Service Pack
TSPA	Total System Performance Assessment
YMP	Yucca Mountain Project

1. INTRODUCTION

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

As was done in previous work (Lee and Hadgu, 2014, Hadgu et al., 2015) one of the goals of this work is to demonstrate the readiness of the 2014 hardware and software systems. This is to insure that the computing system can support reliable execution of the TSPA-LA models and post-processing of the model output. This includes completing tasks started in FY15. The other goal of this work is to start upgrading the TSPA-LA from the original GoldSim version 9.60.300 to the latest version (11.1). The following main topics were identified for the current investigation to evaluate the status of the TSPA-LA model capability.

- Verification of the TSPA-LA uncertainty and sensitivity analyses results on the new TSPA cluster (CL2014) and using TSPA-LA model runs generated in FY15 using GoldSim 9.60.300.
- To begin upgrading of the TSPA-LA models with conversion from GoldSim 9.60.300 to GoldSim version 11.1

Page is intentionally blank

2. THE TSPA COMPUTING SYSTEM

2.1. The TSPA Server Cluster Hardware (CL2014)

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

The 2014 servers reside on the Sandia DMZ domain and are running under the Windows Server 2012 r2, 64-bit operating system. The system was optimized for installation and execution of the GoldSim software required to run the GoldSim distributed processing module utility (GoldSim 2010). The distributed processing module utility is a program extension to GoldSim which allows use of multiple computers connected over a network to share the computational burden of a Monte Carlo simulation. The module is the essential feature to efficiently manage and execute multiple realizations of the TSPA-LA model run on the cluster processors.

In the 2014 configuration of the total of 32 blade servers, one blade server is used as the head node, and 31 servers are used as the compute nodes dedicated to run GoldSim-based TSPA models.

2.2. 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).

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.

2.3. 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).

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 maintain the separation of aleatory and epistemic uncertainty to enhance understanding. The solution is first 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. EXDOC also performs the final integration over the epistemic uncertainty to produce the final expected dose. 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.

2.4. Supporting Software

2.4.1. 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, 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 standalone PC. Post processing of the model output was done on both software versions.

2.4.2. 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. This is because the DTN files have many layers of file folder structure, requiring 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. However, 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 used for the current study to conduct statistical analysis of the TSPA-LA model output results for verification of the TSPA-LA uncertainty and sensitivity analyses.

2.5. TSPA Cluster Hardware Setup and Configuration

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.

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. 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. This limitation has been removed in later versions (e.g., Version 10.5.1) of GoldSim.

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.

2.6. 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 archives as explained in Hadgu et al. (2015).

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

Page is intentionally blank

3. VERIFICATION OF TSPA-LA UNCERTAINTY AND SENSITIVITY ANALYSES RESULTS

Appendix K[a] of the TSPA report (SNL, 2008) presents uncertainty and sensitivity analyses for each modeling case in support of the TSPA-LA. The uncertainty analyses determine the contribution to the uncertainty in results that derives from individual uncertain inputs. Sensitivity analyses determine the contribution to the uncertainty in analysis results that derives from individual analysis inputs.

The TSPA-LA employs uncertainty and sensitivity analysis procedures based on a mapping between analysis inputs and analysis results generated with use of Latin hypercube sampling (LHS). The TSPA-LA analysis uses an LHS sample of 300. The primary sensitivity analysis procedures in use involve the determination and presentation of partial rank correlation coefficients (PRCCs), stepwise rank regression analyses, and scatterplots.

In this study, selected outputs of the TSPA-LA uncertainty and sensitivity analysis results were evaluated for the verification analysis. The model output reproducibility verification was conducted by comparing selected output of uncertainty and sensitivity analysis results using the new model runs on cluster CL2014 with the output for all the modeling cases retrieved from the DTN MO0710PLOTSFIG.000 (SNL 2008). The verification analysis used numerical value comparison as well as graphical comparison. The outputs include total dose for first 50 sample elements, partial rank correlation coefficients (PRCCs), regressions (which are numerical values) as well as scatterplots. Note that verification of outputs of total dose for the entire 300 sample elements have been conducted and are documented in Hadgu et al. (2015).

For this study the uncertainty and sensitivity analyses results were reproduced following the procedure outlined in SNL (2007). The report provides a walk-through of the steps that are to be followed to obtain the uncertainty and sensitivity analyses output.

The uncertainty and sensitivity analyses were based on TSPA-LA results of most interest to repository performance. Two of the TSPA-LA results are dose to the Reasonably Maximally Exposed Individual (RMEI) for nominal scenarios (DOSTOT) as a function of time and, for various scenarios incremental expected dose to the RMEI (EXPDOS) as a function of time. The Uncertainty and sensitivity calculations were done for the two time periods: 20,000 years and 1,000,000 years. For this study only the 1,000,000 years' results were reproduced. The analyses used independent variables that are of importance to the repository system. In the 2008 TSPA-LA the uncertainty and sensitivity analyses were conducted for all scenario classes. In this study we looked at results from all scenario classes. However, only a subset of the analyses conducted have been reproduced for verification. The uncertainty and sensitivity results are presented for the Modeling cases shown below:

- Nominal Modeling Case
- Drip Shield Early Failure Modeling Case
- Waste Package Early Failure Modeling Case
- Seismic Ground Motion Modeling Case
- Seismic Fault Displacement Modeling Case
- Igneous Intrusion Modeling case

- Total Dose to RMEI
- Human Intrusion

In the process of the uncertainty and sensitivity analysis results verification conducted for this study updates were made in two areas as described below:

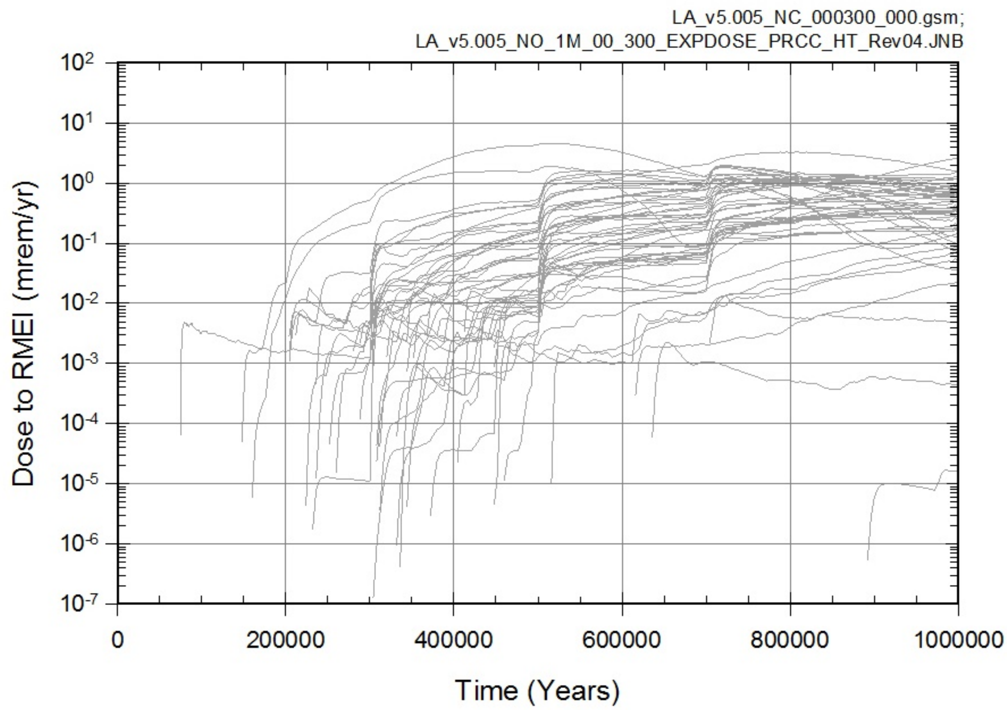
- In the TSPA-LA report (SNL 2008) for seismic ground motion 1,000,000 years the superseded GoldSim model LA_v5.005_SM_009000_000.gsm was used. The model was run on Cluster CL20014 so that results could be reproduced for the verification analysis. In addition, uncertainty and sensitivity analysis results were obtained for the final GoldSim model LA_v5.005_SM_009000_003.gsm.
- Inaccuracies were found in the TSPA-LA report (SNL 2008, Figure K7.8.2-2[a]) scatterplots for expected dose to RMEI over 1,000,000 years for all radioactive species resulting from seismic fault displacement. The correct results were used for the verification analysis.

3.1. Nominal Modeling Case

The TSPA-LA model for the Nominal Modeling Case has no associated aleatory uncertain parameters, and thus the model simulation comprises 300 realizations (i.e., 300 sets of sampled epistemic uncertain parameters).

The nominal scenario class consists of the future in which no disruptions of any kind occur. Analyses results are shown in Figures 1 to 7. The figures compare results of the original TSPA-LA model (SNL 2008, Figures K4.5-1[a] to K4.5-2[a]) and results of this study, for 1,000,000 year simulation period. Figure 1 shows comparison of GoldSim results for the dose to RMEI (DOSTOT, mrem/yr) for first 50 sample elements. Figure 2 and 3 compare PRCCs for DOSTOT for the period 0 to 1,000,000 years, and 200,000 to 1,000,000 years, respectively. Figure 4 shows comparison of results for stepwise rank regression analyses for DOSTOT at 400,000, 600,000 and 800,000 years. Figures 5 to 7 show comparison of scatterplots for DOSTOT at 600,000 years vs selected parameters.

As shown in Figures 1 to 7, 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 CL2014.



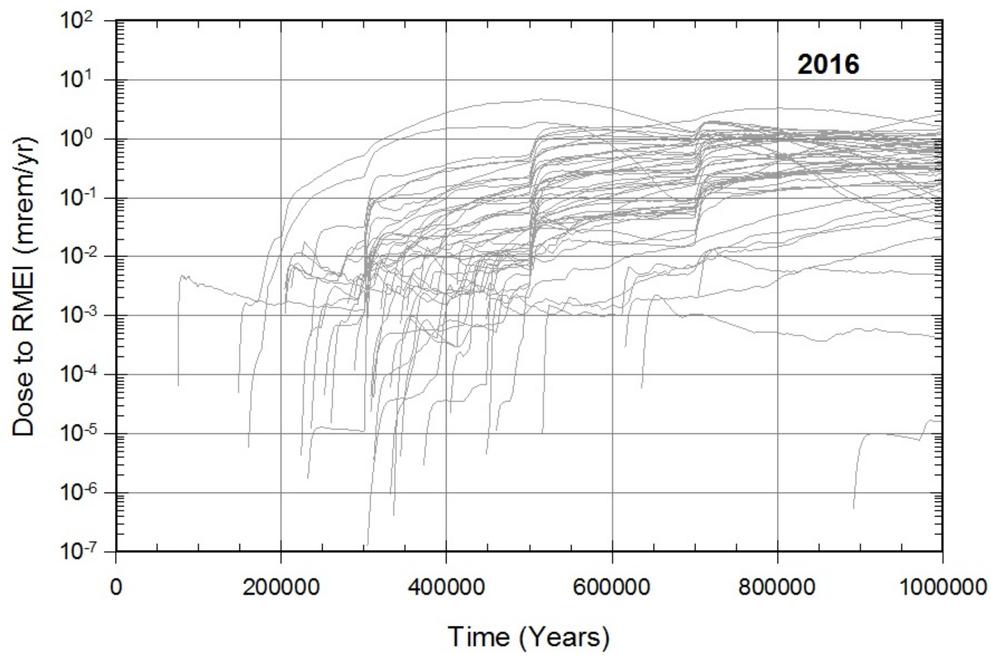


Figure 1. Comparison of model results for dose to RMEI (DOSTOT, mrem/yr) for all radioactive species under nominal conditions obtained with version 5.005 of the TSPA-LA model, DOSTOT for first 50 sample elements: (top) YMP TSPA-LA model (SNL 2008, Figure K4.5-1[a](b) and (bottom) TSPA-LA model test run of this study.

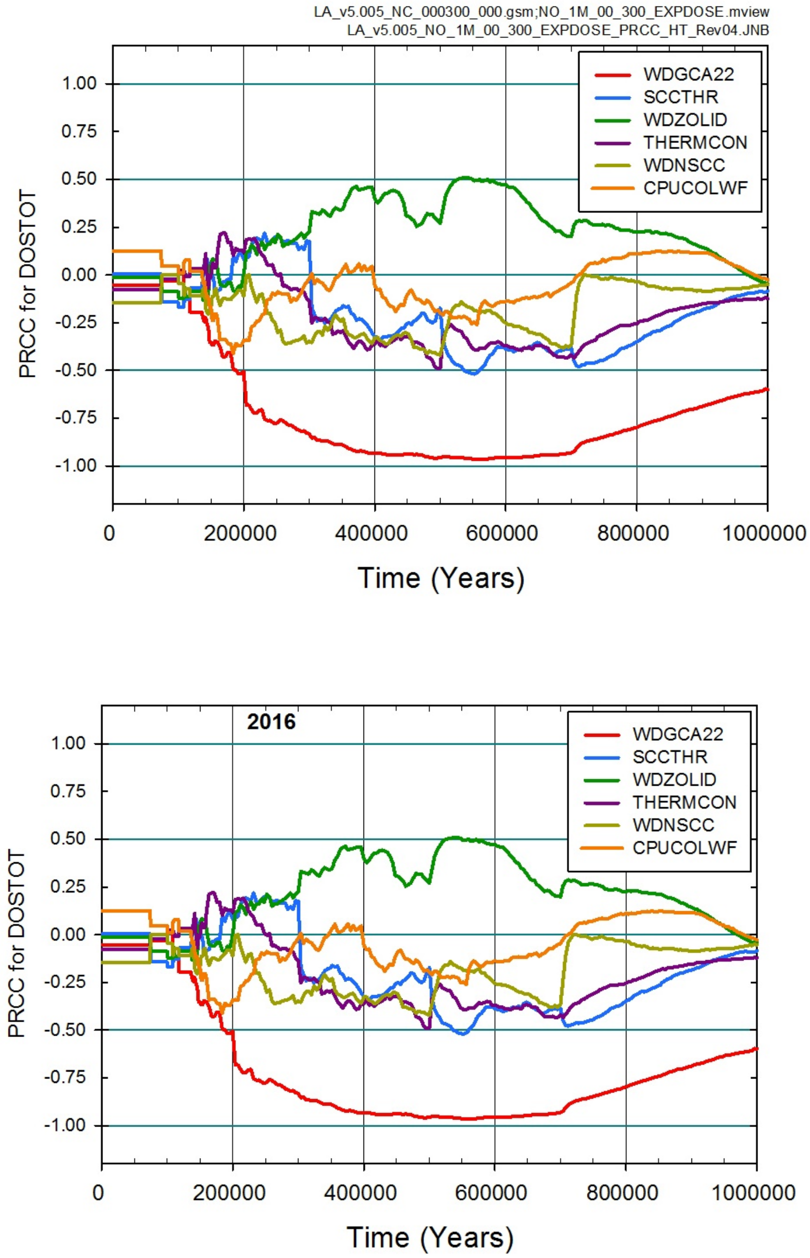
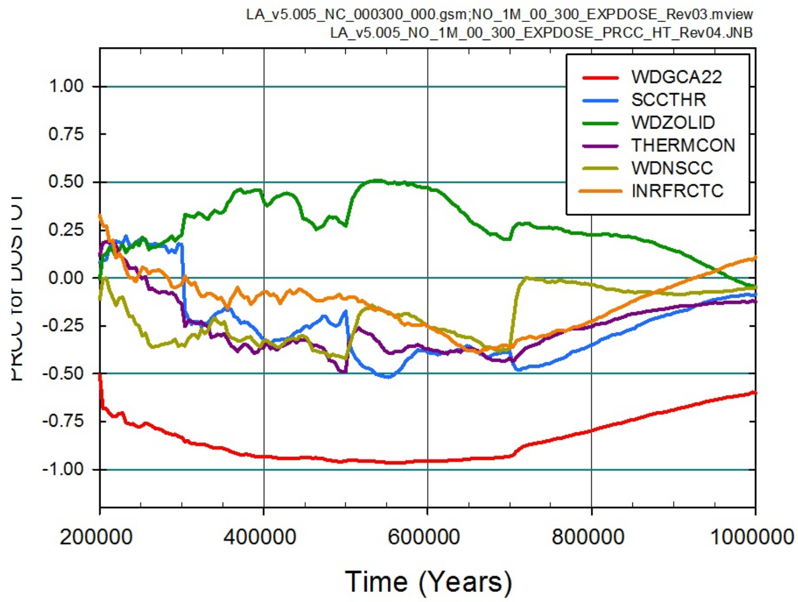


Figure 2. Comparison of model results for dose to RMEI (*DOSTOT*, mrem/yr) for all radioactive species under nominal conditions obtained with version 5.005 of the TSPA-LA model, PRCCs for *DOSTOT* for [0; 1,000,000 yr: (top) YMP TSPA-LA model (SNL 2008, Figure K4.5-1[a](c) and (bottom) TSPA-LA model test run of this study.



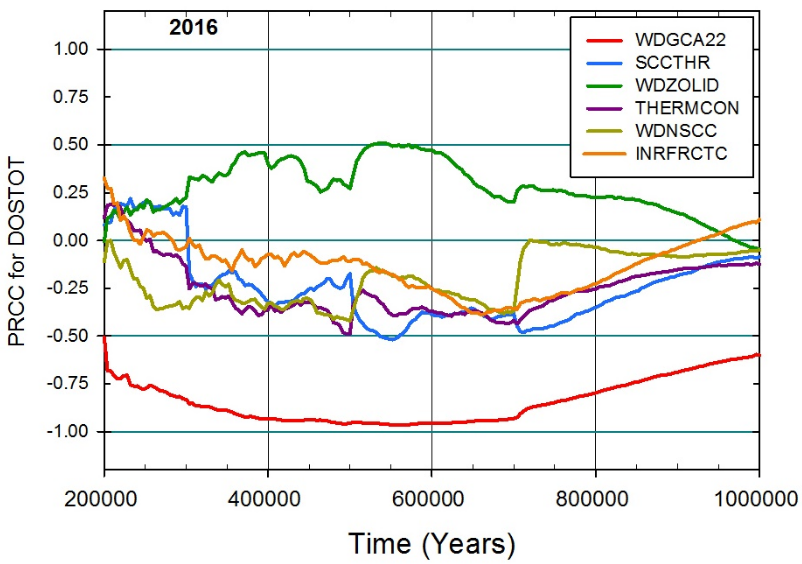
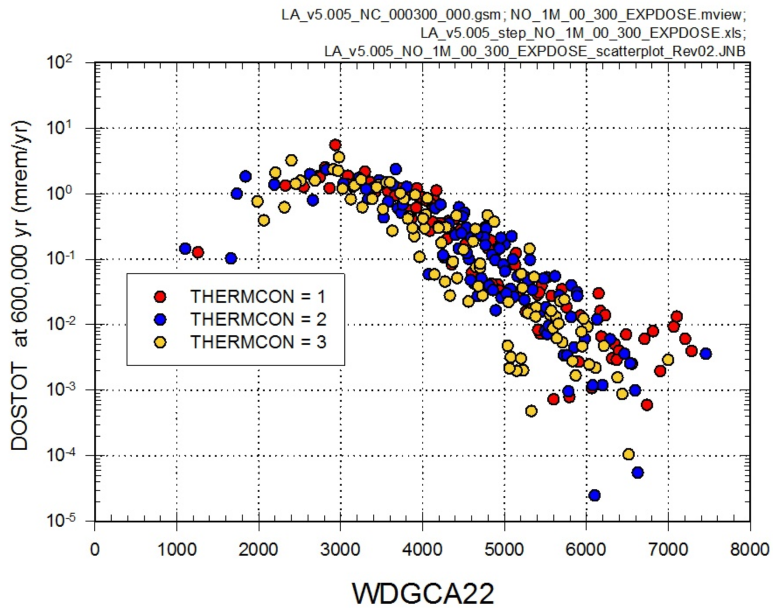


Figure 3. Comparison of model results for dose to RMEI (*DOSTOT*, mrem/yr) for all radioactive species under nominal conditions obtained with version 5.005 of the TSPA-LA model, PRCCs for *DOSTOT* for [200,000; 1,000,000 yr]: (top) YMP TSPA-LA model (SNL 2008, Figure K4.5-1[a](d) and (bottom) TSPA-LA model test run of this study.

	DOSTOT: 400,000 year			DOSTOT: 600,000 year			DOSTOT: 800,000 year		
Step	**Variable**	**R^2**	**SRRC**	**Variable**	**R^2**	**SRRC**	**Variable**	**R^2**	**SRRC**
1	WDGCA22	0.78	-0.90	WDGCA22	0.85	-0.94	WDGCA22	0.63	-0.80
2	WDZOLID	0.81	0.16	WDZOLID	0.87	0.14	WDZOLID	0.65	0.16
3	WDNSCC	0.82	-0.12	THERMCON	0.88	-0.10	MICI129	0.67	0.13
4	THERMCON	0.83	-0.13	INFIL	0.89	-0.10	SCCTHR	0.68	-0.10
5	INFIL	0.84	-0.10	SCCTHR	0.90	-0.09			
6	SCCTHR	0.85	-0.09	WDNSCC	0.91	-0.08			
7	WDGCUA22	0.85	0.07	CORRATSS	0.91	-0.07			
8	WDLCRATE	0.86	0.06	WDGCUA22	0.92	0.08			
9				MICTC99	0.92	0.07			
10				DTDRHUNC	0.92	0.04			
11				CSNFMASS	0.92	0.04			
12									
13									
14									
15									
16									

	DOSTOT: 400,000 year			DOSTOT: 600,000 year			DOSTOT: 800,000 year		
Step	**Variable**	**R^2**	**SRRC**	**Variable**	**R^2**	**SRRC**	**Variable**	**R^2**	**SRRC**
1	WDGCA22	0.78	-0.90	WDGCA22	0.85	-0.94	WDGCA22	0.63	-0.80
2	WDZOLID	0.81	0.16	WDZOLID	0.87	0.14	WDZOLID	0.65	0.16
3	WDNSCC	0.82	-0.12	THERMCON	0.88	-0.10	MICI129	0.67	0.13
4	THERMCON	0.83	-0.13	INFIL	0.89	-0.11	SCCTHR	0.68	-0.10
5	INFIL	0.84	-0.10	SCCTHR	0.90	-0.09			
6	SCCTHR	0.85	-0.09	WDNSCC	0.91	-0.08			
7	WDGCUA22	0.85	0.07	CORRATSS	0.91	-0.07			
8	WDLCRATE	0.86	0.06	WDGCUA22	0.92	0.08			
9				MICTC99	0.92	0.07			
10				DTDRHUNC	0.92	0.04			
11				CSNFMASS	0.93	0.04			
12									
13									
14									
15									
16									

Figure 4. Comparison of model results for stepwise rank regression analyses for dose to RMEI (*DOSTOT*, mrem/yr) for all radioactive species under nominal conditions obtained with version 5.005 of the TSPA-LA model, regressions for *DOSTOT* at 400,000, 600,000, and 800,000 years: (top) YMP TSPA-LA model (SNL 2008, Figure K4.5-2[a](a) and (bottom) TSPA-LA model test run of this study.



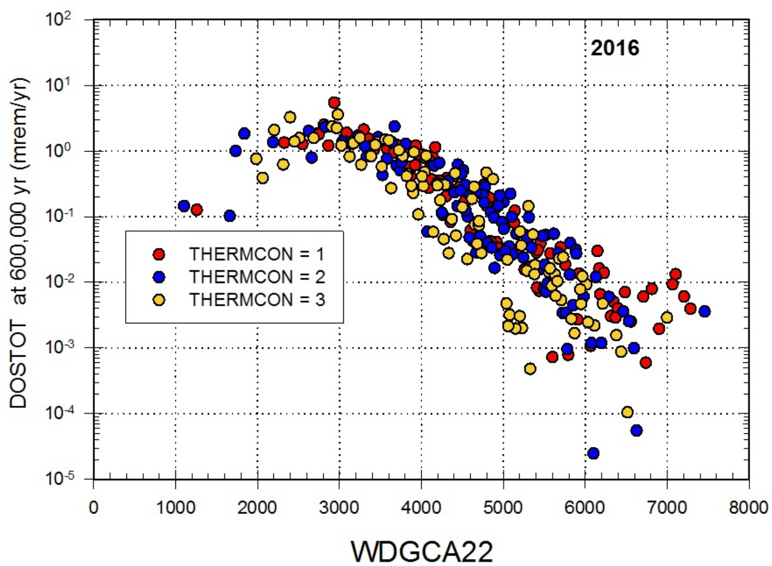
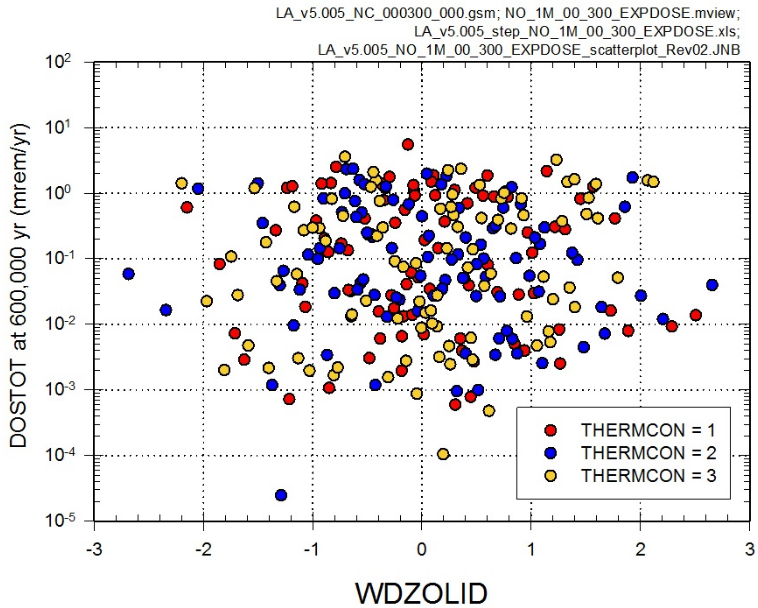


Figure 5. Comparison of model results for selected scatterplots for dose to RMEI (*DOSTOT*, mrem/yr) for all radioactive species under nominal conditions obtained with version 5.005 of the TSPA-LA model, scatterplots for *DOSTOT* at 600,000 years: (top) YMP TSPA-LA model (SNL 2008, Figure K4.5-2[a](b) and (bottom) TSPA-LA model test run of this study.



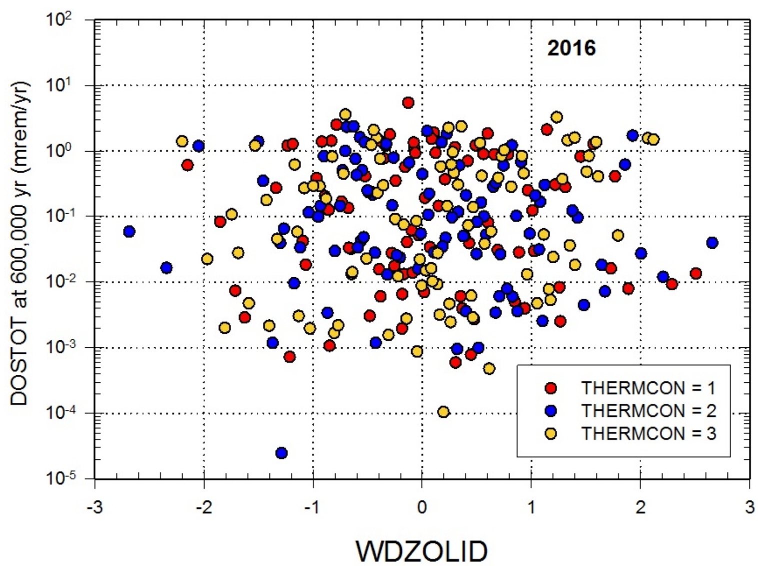
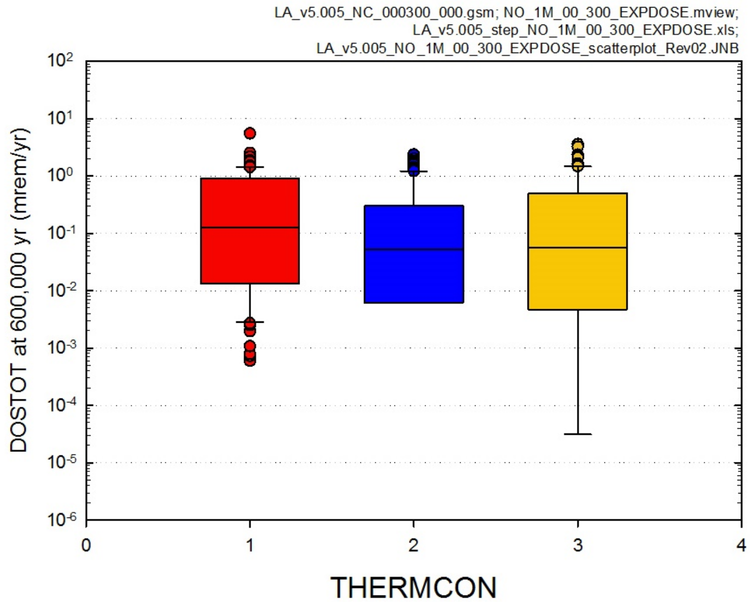


Figure 6. Comparison of model results for selected scatterplots for dose to RMEI (*DOSTOT*, mrem/yr) for all radioactive species under nominal conditions obtained with version 5.005 of the TSPA-LA model, scatterplots for *DOSTOT* at 600,000 years: (top) YMP TSPA-LA model (SNL 2008, Figure K4.5-2[a](c) and (bottom) TSPA-LA model test run of this study.



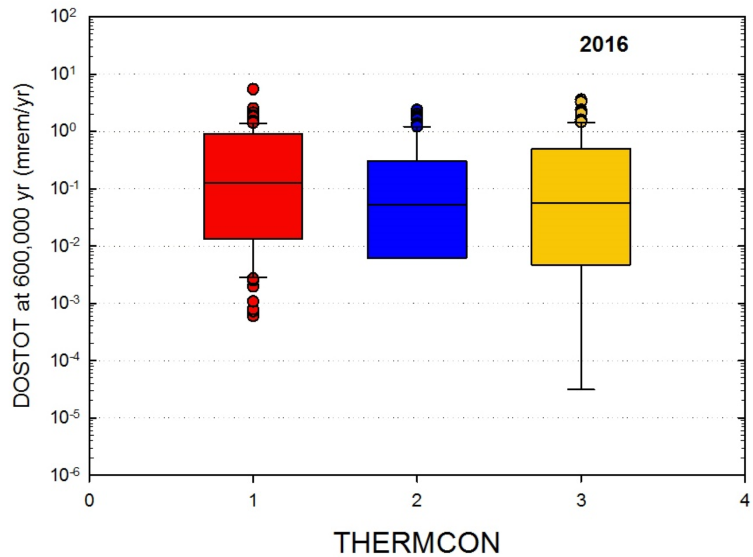


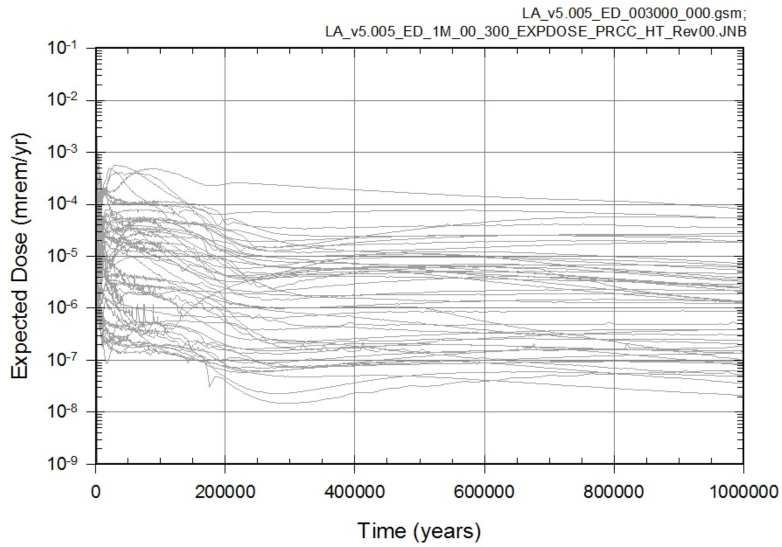
Figure 7. Comparison of model results for selected scatterplots for dose to RMEI (*DOSTOT*, mrem/yr) for all radioactive species under nominal conditions obtained with version 5.005 of the TSPA-LA model, scatterplots for *DOSTOT* at 600,000 years: (top) YMP TSPA-LA model (SNL 2008, Figure K4.5-2[a](d) and (bottom) TSPA-LA model test run of this study.

3.2. 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).

The Drip Shield Early Failure scenario class is defined based on futures that involve one or more early failure events. Results for uncertainty and sensitivity analysis are shown in Figures 8 to 13. The figures compare results of the original TSPA-LA model (SNL 2008, Figures K5.7.1[a]) and results of this study, for the 1,000,000 year simulation period. Figure 8 shows comparison of GoldSim results for dose to RMEI (EXPDOSE, mrem/yr) for the first 50 sample elements. Figure 9 compares PRCCs for EXPDOSE for the period from 0 to 1,000,000 years. Figure 10 shows comparison of results for stepwise rank regression analyses for EXPDOSE at 50,000, 200,000 and 500,000 years. Figures 11 to 13 show comparisons of scatterplots for EXPDOSE at 500,000 years vs selected parameters.

As shown in Figures 8 to 13, 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 CL2014.



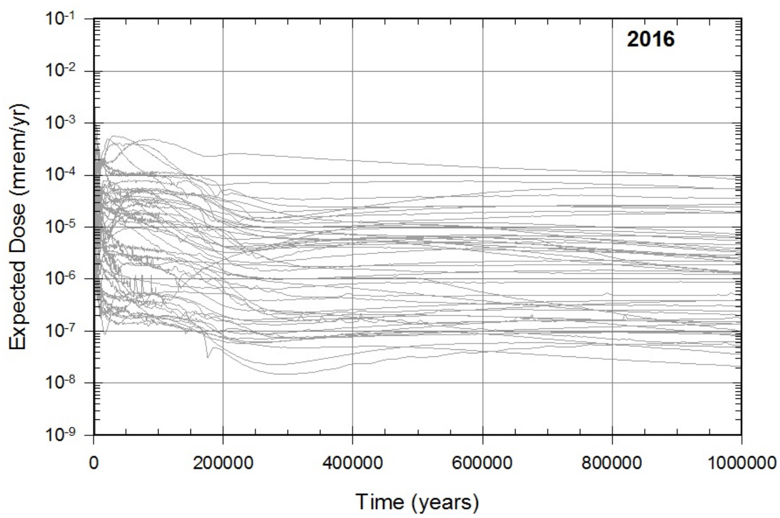
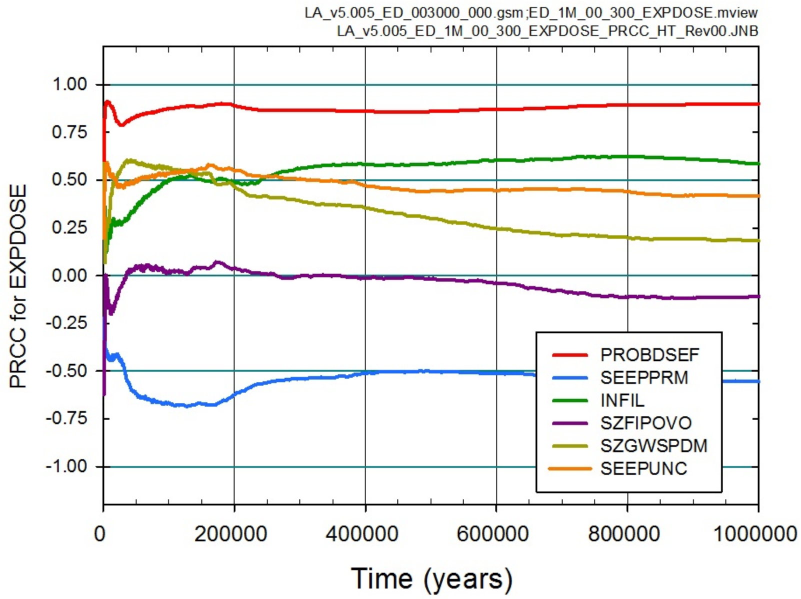


Figure 8. Comparison of model results for expected dose to RMEI (*EXPDOSE*, mrem/yr) over [0, 1,000,000 yr] for all radioactive species resulting from early Drip Shield failure obtained with version 5.005 of the TSPA-LA model, *EXPDOSE* for first 50 sample elements: (top) YMP TSPA-LA model (SNL 2008, Figure K5.7.1-3[a](b) and (bottom) TSPA-LA model test run of this study.



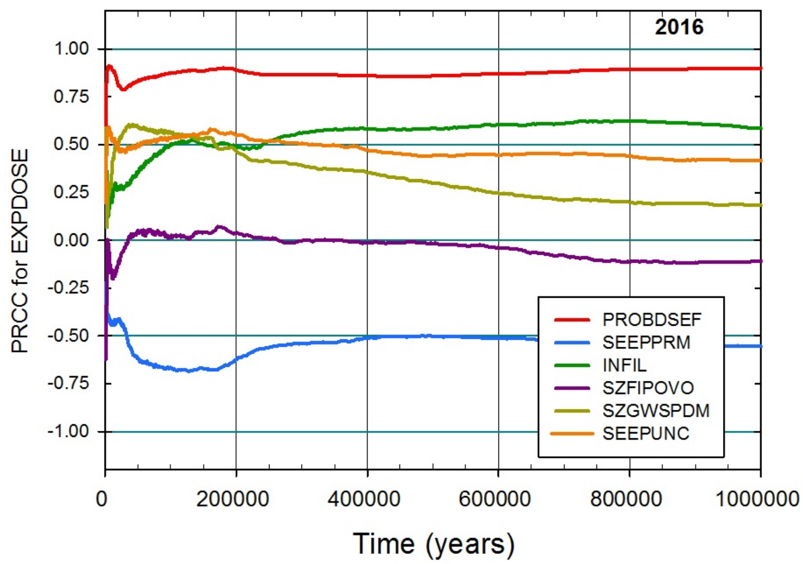
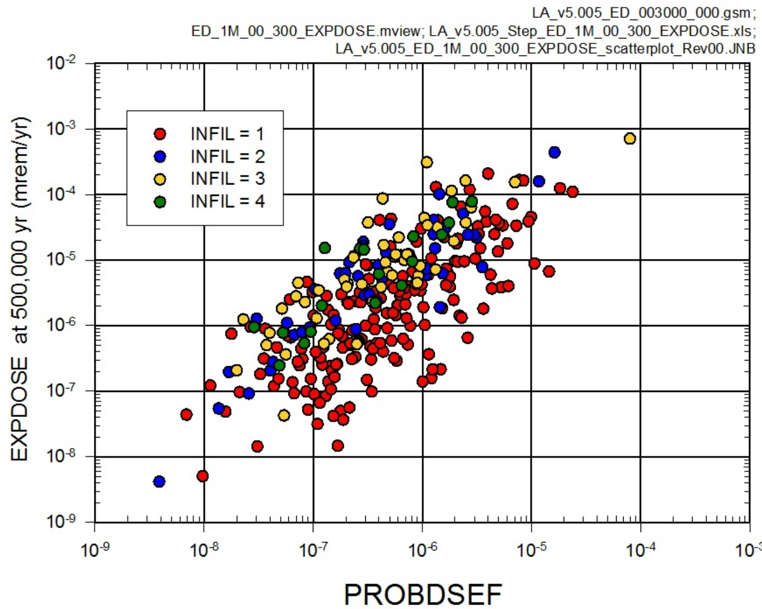


Figure 9. Comparison of model results for expected dose to RMEI (*EXPDOSE*, mrem/yr) over [0, 1,000,000 yr] for all radioactive species resulting from early Drip Shield failure obtained with version 5.005 of the TSPA-LA model, PRCCs for *EXPDOSE*: (top) YMP TSPA-LA model (SNL 2008, Figure K5.7.1-3[a](c) and (bottom) TSPA-LA model test run of this study.

	EXPDOSE: 50,000 years			EXPDOSE: 200,000 years			EXPDOSE: 500,000 years		
Step	Variable	R^2	SRRC	Variable	R^2	SRRC	Variable	R^2	SRRC
1	PROBDSEF	0.47	0.71	PROBDSEF	0.55	0.76	PROBDSEF	0.52	0.73
2	SZGWSPDM	0.55	0.29	INFIL	0.63	0.26	INFIL	0.63	0.31
3	INFIL	0.64	0.28	SEEPPRM	0.68	-0.23	SEEPPRM	0.68	-0.21
4	SEEPPRM	0.69	-0.26	SZGWSPDM	0.72	0.21	EP1LOWPU	0.71	0.18
5	EP1LOWPU	0.73	0.20	SEEPUNC	0.77	0.23	SEEPUNC	0.75	0.20
6	SEEPUNC	0.77	0.20	EP1LOWPU	0.79	0.15	SZGWSPDM	0.78	0.15
7	MICPU239	0.78	0.10	MICPU239	0.80	0.13	GOESITED	0.79	-0.12
8	SEEPPRMN	0.78	-0.08	GOESITED	0.82	-0.11	MICPU239	0.81	0.11
9	SZCOLRAL	0.79	-0.10	SEEPPRMN	0.82	-0.07	PHCSS	0.82	0.11
10	PHCSS	0.80	-0.08	HFOSA	0.83	-0.09	SEEPPRMN	0.82	-0.08
11	SZDIFCVO	0.81	-0.10	SZFISPVO	0.84	0.10	EP1LOWNU	0.83	0.11
12	SZFISPVO	0.81	0.10	SZDIFCVO	0.84	-0.09	ALPHAL	0.84	-0.10
13	ALPHAL	0.82	-0.07	ALPHAL	0.85	-0.09	UZFAG4	0.85	-0.07
14				EP1LOWNU	0.85	0.08	SZFISPVO	0.85	0.10
15				SZCONCOL	0.86	0.07	SZDIFCVO	0.86	-0.09
16				SZCOLRVO	0.86	0.06	HFOSA	0.87	-0.08

	EXPDOSE: 50,000 years			EXPDOSE: 200,000 years			EXPDOSE: 500,000 years		
Step	Variable	R^2	SRRC	Variable	R^2	SRRC	Variable	R^2	SRRC
1	PROBDSEF	0.47	0.71	PROBDSEF	0.55	0.76	PROBDSEF	0.52	0.73
2	SZGWSPDM	0.55	0.29	INFIL	0.63	0.26	INFIL	0.63	0.31
3	INFIL	0.64	0.28	SEEPPRM	0.68	-0.23	SEEPPRM	0.68	-0.21
4	SEEPPRM	0.69	-0.26	SZGWSPDM	0.72	0.21	EP1LOWPU	0.71	0.18
5	EP1LOWPU	0.73	0.20	SEEPUNC	0.77	0.23	SEEPUNC	0.75	0.20
6	SEEPUNC	0.77	0.20	EP1LOWPU	0.79	0.15	SZGWSPDM	0.78	0.15
7	MICPU239	0.78	0.10	MICPU239	0.80	0.13	GOESITED	0.79	-0.12
8	SEEPPRMN	0.78	-0.08	GOESITED	0.82	-0.11	MICPU239	0.81	0.11
9	SZCOLRAL	0.79	-0.10	SEEPPRMN	0.82	-0.07	PHCSS	0.82	0.11
10	PHCSS	0.80	-0.08	HFOSA	0.83	-0.09	SEEPPRMN	0.82	-0.08
11	SZDIFCVO	0.81	-0.10	SZCONCOL	0.84	0.07	EP1LOWNU	0.83	0.11
12	SZFISPVO	0.81	0.10	ALPHAL	0.84	-0.09	ALPHAL	0.84	-0.10
13	ALPHAL	0.82	-0.07	SZFISPVO	0.85	0.09	UZFAG4	0.85	-0.07
14				SZDIFCVO	0.85	-0.09	SZFISPVO	0.85	0.10
15				EP1LOWNU	0.86	0.08	SZDIFCVO	0.86	-0.09
16				SZCOLRVO	0.86	0.06	HFOSA	0.87	-0.08

Figure 10. Comparison of model results for stepwise rank regression analyses for expected dose to RMEI (*EXPDOSE*, mrem/yr) over [0, 1,000,000 yr] for all radioactive species resulting from early Drip Shield failure obtained with version 5.005 of the TSPA-LA model, regressions for *EXPDOSE* at 50,000, 200,000, and 500,000 years: (top) YMP TSPA-LA model (SNL 2008, Figure K5.7.1-3[a](a) and (bottom) TSPA-LA model test run of this study.



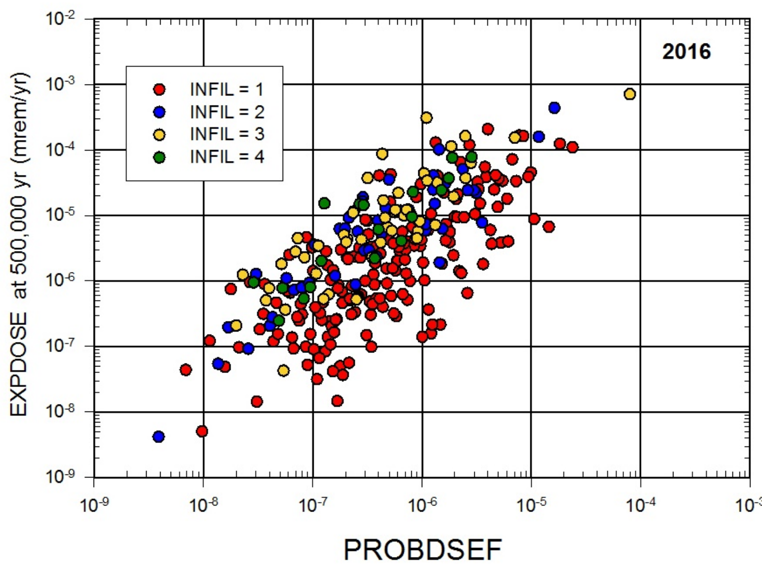
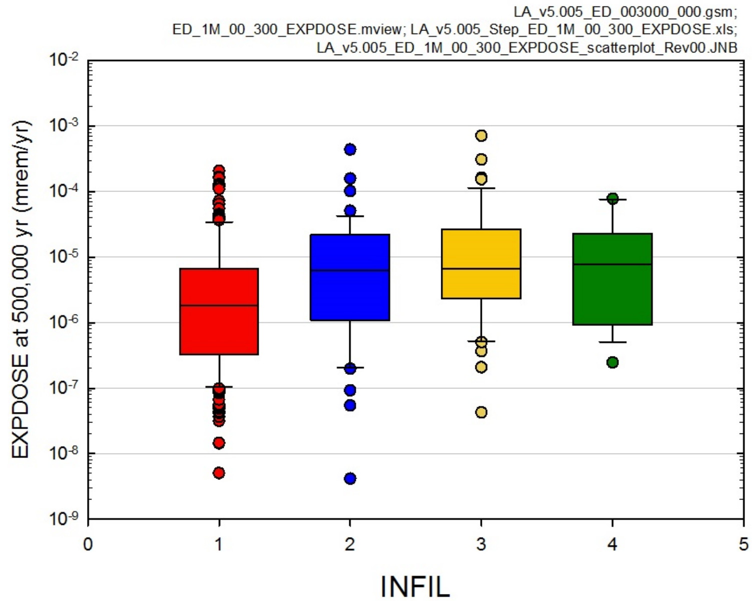


Figure 11. Comparison of model results for selected scatterplots for expected dose to RMEI (*EXPDOSE*, mrem/yr) over [0, 1,000,000 yr] for all radioactive species resulting from early Drip Shield failure obtained with version 5.005 of the TSPA-LA model, scatterplots for *EXPDOSE* at 500,000 years: (top) YMP TSPA-LA model (SNL 2008, Figure K5.7.1-3[a](b) and (bottom) TSPA-LA model test run of this study.



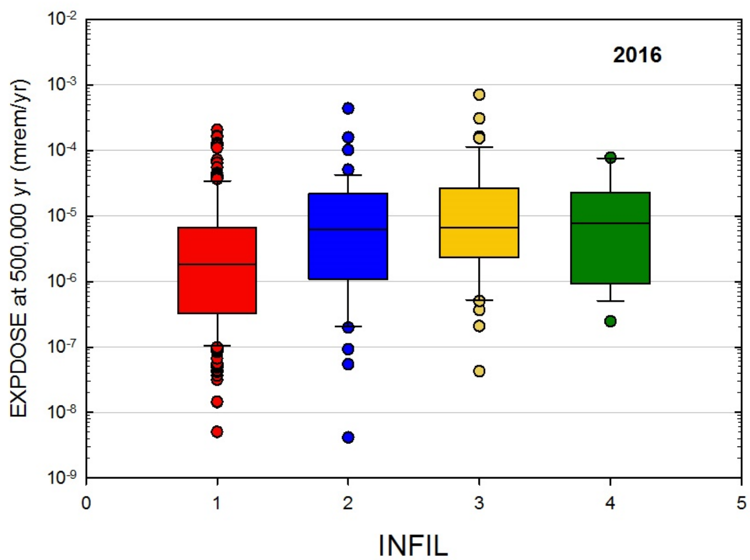
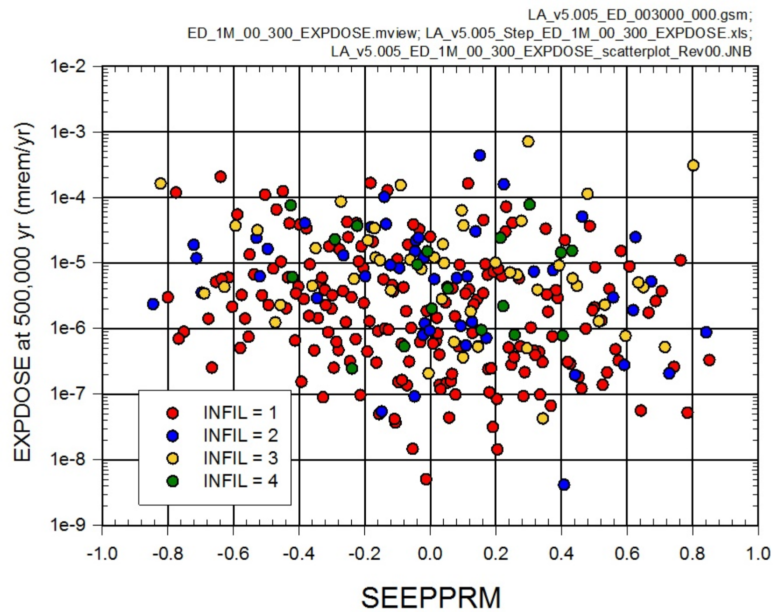


Figure 12. Comparison of model results for selected scatterplots for expected dose to RMEI (*EXPDOSE*, mrem/yr) over [0, 1,000,000 yr] for all radioactive species resulting from early Drip Shield failure obtained with version 5.005 of the TSPA-LA model, scatterplots for *EXPDOSE* at 500,000 years: (top) YMP TSPA-LA model (SNL 2008, Figure K5.7.1-3[a](c) and (bottom) TSPA-LA model test run of this study.



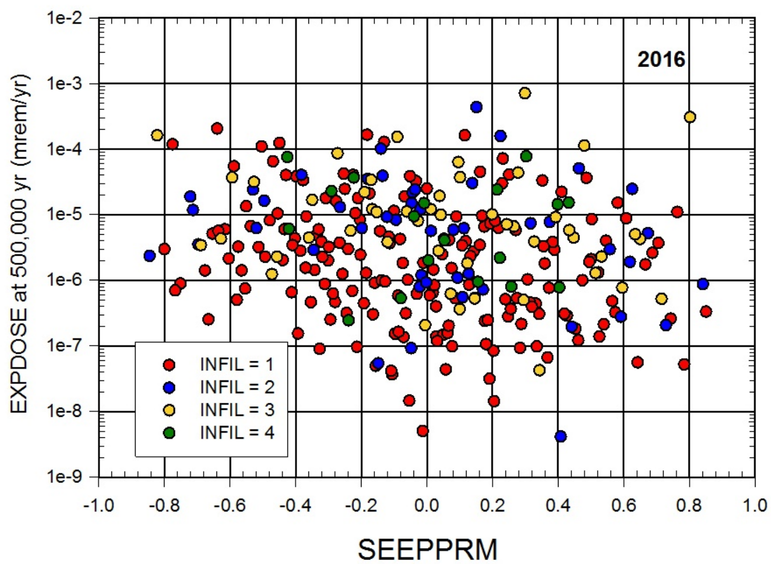


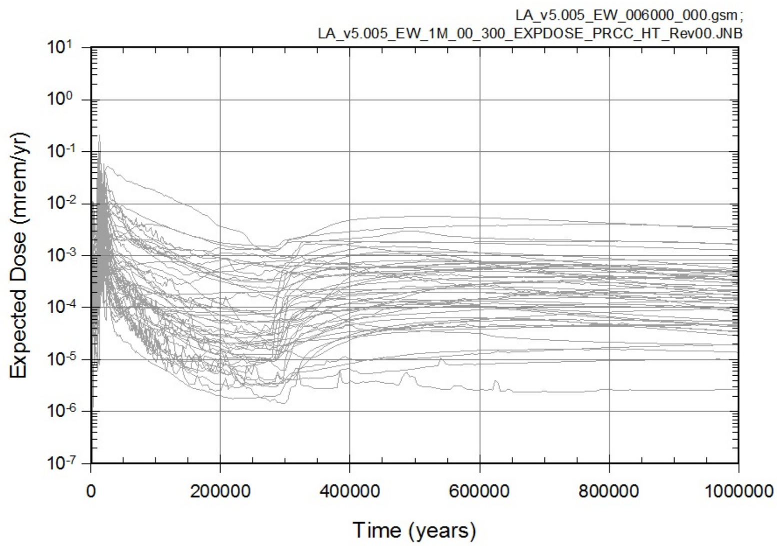
Figure 13. Comparison of model results for selected scatterplots for expected dose to RMEI (*EXPDOSE*, mrem/yr) over [0, 1,000,000 yr] for all radioactive species resulting from early Drip Shield failure obtained with version 5.005 of the TSPA-LA model, scatterplots for *EXPDOSE* at 500,000 years: (top) YMP TSPA-LA model (SNL 2008, Figure K5.7.1-3[a](d) and (bottom) TSPA-LA model test run of this study.

3.3. 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).

The Waste Package Early Failure scenario class is defined based on futures that involve one or more early failure events. Results for uncertainty and sensitivity analysis are shown in Figures 14 to 19. The figures compare results of the original TSPA-LA model (SNL 2008, Figures K5.7.1[a]) and results of this study, for the 1,000,000 year simulation period. Figure 14 shows comparisons of GoldSim results for dose to RMEI (EXPDOSE, mrem/yr) for the first 50 sample elements. Figure 15 compares PRCCs for EXPDOSE for the period from 0 to 1,000,000 years. Figure 16 shows comparisons of results for the stepwise rank regression analyses for EXPDOSE at 50,000, 200,000 and 500,000 years. Figures 17 to 19 show comparisons of scatterplots for EXPDOSE at 500,000 years vs selected parameters.

As shown in Figures 14 to 19, 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 CL2014.



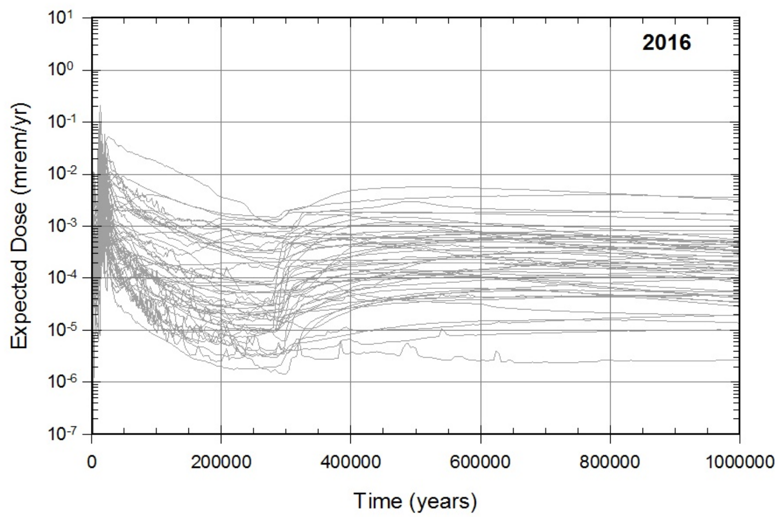
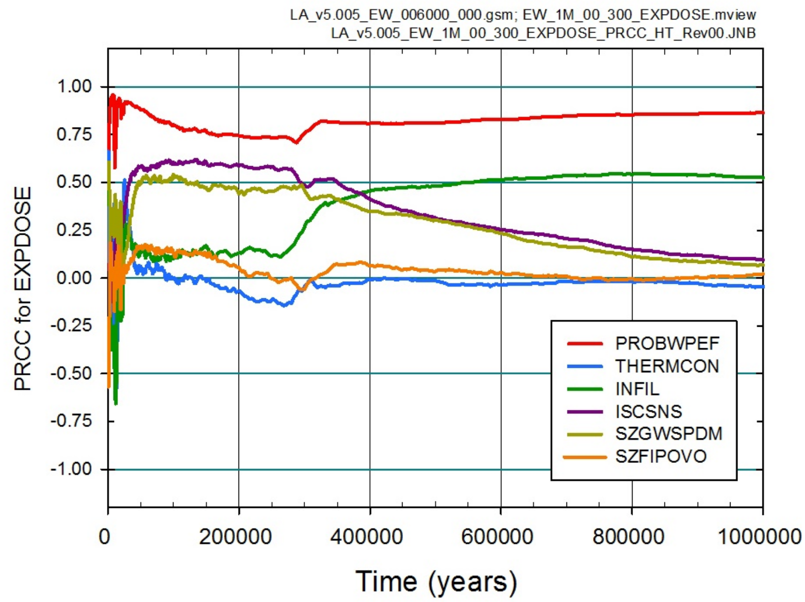


Figure 14. Comparison of model results for expected dose to RMEI (*EXPDOSE*, mrem/yr) over [0, 1,000,000 yr] for all radioactive species resulting from early waste wackage failure obtained with version 5.005 of the TSPA-LA model, *EXPDOSE* for first 50 sample elements: (top) YMP TSPA-LA model (SNL 2008, Figure K5.7.2-3[a](b) and (bottom) TSPA-LA model test run of this study.



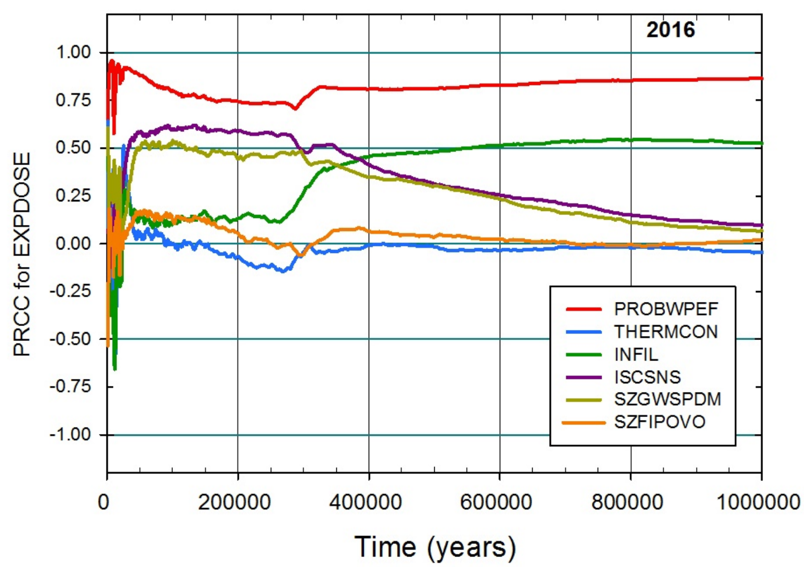


Figure 15. Comparison of model results for expected dose to RMEI (*EXPDOSE*, mrem/yr) over [0, 1,000,000 yr] for all radioactive species resulting from early waste wackage failure obtained with version 5.005 of the TSPA-LA model, PRCCs for *EXPDOSE*: (top) YMP TSPA-LA model (SNL 2008, Figure K5.7.2-3[a](c) and (bottom) TSPA-LA model test run of this study.

	EXPDOSE: 50,000 years			EXPDOSE: 200,000 years			EXPDOSE: 500,000 years		
Step	Variable	R^2	SRRC	Variable	R^2	SRRC	Variable	R^2	SRRC
1	PROBWPEF	0.60	0.79	PROBWPEF	0.37	0.62	PROBWPEF	0.39	0.70
2	ISCSNS	0.66	0.25	ISCSNS	0.50	0.38	INFIL	0.51	0.31
3	SZGWSPDM	0.72	0.22	SZGWSPDM	0.56	0.24	EP1LOWPU	0.55	0.20
4	EP1LOWPU	0.74	0.14	EP1LOWPU	0.58	0.15	SEEPPRM	0.59	-0.22
5	MICNP237	0.75	0.10	SZFISPVO	0.60	0.17	SZGWSPDM	0.62	0.17
6	SZFISPVO	0.75	0.08	SZDIFCVO	0.61	-0.14	SEEPUNC	0.65	0.19
7	SZKDSRAL	0.76	0.09	IGRATE	0.63	0.10	EP1LOWNU	0.67	0.17
8	COLU	0.77	0.08	SEEPPRM	0.64	-0.11	ALPHAL	0.69	-0.14
9				SEEPUNC	0.65	0.10	SZFISPVO	0.71	0.15
10				RHMU20	0.66	0.10	GOESITED	0.73	-0.14
11							HFOSA	0.74	-0.12
12							MICPU239	0.75	0.11
13							SZDIFCVO	0.76	-0.10
14							SEEPPRMN	0.77	-0.09
15							ISCSNS	0.77	0.09
16							HFOSITED	0.78	-0.08

	EXPDOSE: 50,000 years			EXPDOSE: 200,000 years			EXPDOSE: 500,000 years		
Step	Variable	R^2	SRRC	Variable	R^2	SRRC	Variable	R^2	SRRC
1	PROBWPEF	0.60	0.78	PROBWPEF	0.37	0.62	PROBWPEF	0.39	0.70
2	ISCSNS	0.66	0.25	ISCSNS	0.50	0.38	INFIL	0.51	0.31
3	SZGWSPDM	0.72	0.21	SZGWSPDM	0.56	0.24	EP1LOWPU	0.55	0.20
4	EP1LOWPU	0.74	0.14	EP1LOWPU	0.58	0.15	SEEPPRM	0.59	-0.22
5	MICTC99	0.75	0.08	SZFISPVO	0.60	0.17	SZGWSPDM	0.62	0.17
6	SZKDSRAL	0.75	0.08	SZDIFCVO	0.61	-0.14	SEEPUNC	0.65	0.19
7	SZFISPVO	0.76	0.09	IGRATE	0.63	0.10	EP1LOWNU	0.67	0.18
8	COLU	0.77	0.09	SEEPPRM	0.64	-0.11	ALPHAL	0.69	-0.14
9	MICPU239	0.77	0.08	SEEPUNC	0.65	0.10	SZFISPVO	0.71	0.15
10				RHMU20	0.66	0.10	GOESITED	0.73	-0.14
11							HFOSA	0.74	-0.12
12							MICPU239	0.75	0.11
13							SZDIFCVO	0.76	-0.10
14							SEEPPRMN	0.77	-0.09
15							ISCSNS	0.77	0.09
16							HFOSITED	0.78	-0.08

Figure 16. Comparison of model results for stepwise rank regression analyses for expected dose to RMEI (*EXPDOSE*, mrem/yr) over [0, 1,000,000 yr] for all radioactive species resulting from early waste wackage failure obtained with version 5.005 of the TSPA-LA model, regressions for *EXPDOSE* at 50,000, 200,000, and 500,000 years: (top) YMP TSPA-LA model (SNL 2008, Figure K5.7.2-4[a](a) and (bottom) TSPA-LA model test run of this study.

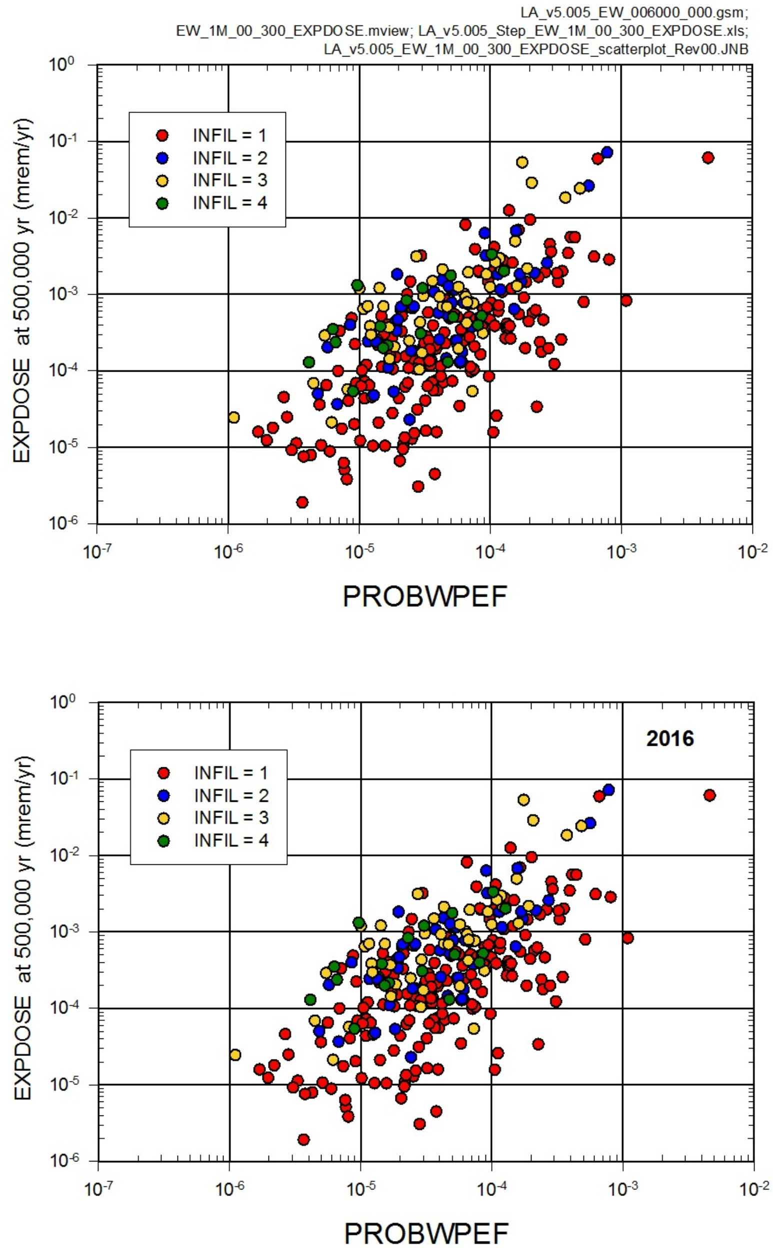
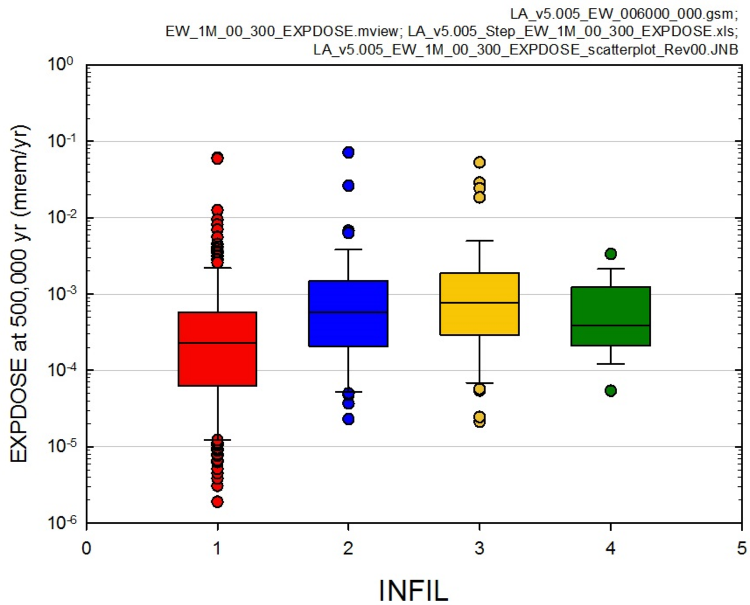


Figure 17. Comparison of model results for selected scatterplots for expected dose to RMEI (*EXPDOSE*, mrem/yr) over [0, 1,000,000 yr] for all radioactive species resulting from early waste wackage failure obtained with version 5.005 of the TSPA-LA model, scatterplots for *EXPDOSE* at 500,000 years: (top) YMP TSPA-LA model (SNL 2008, Figure K5.7.2-4[a](b) and (bottom) TSPA-LA model test run of this study.



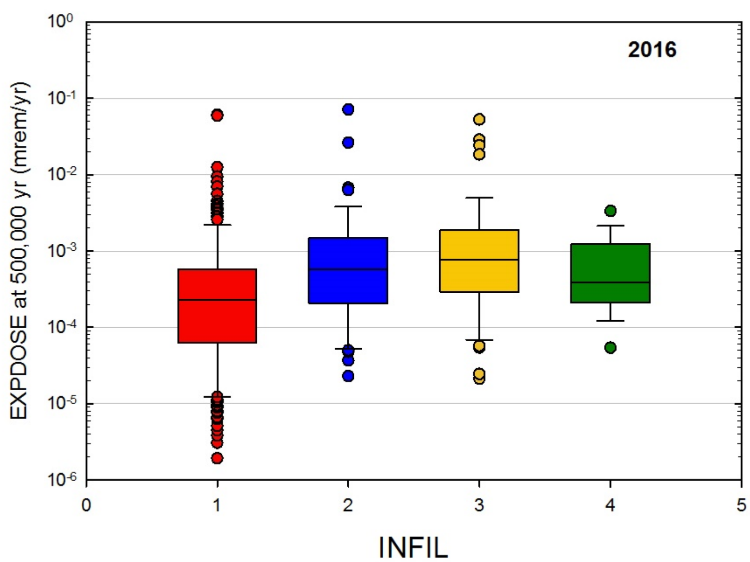
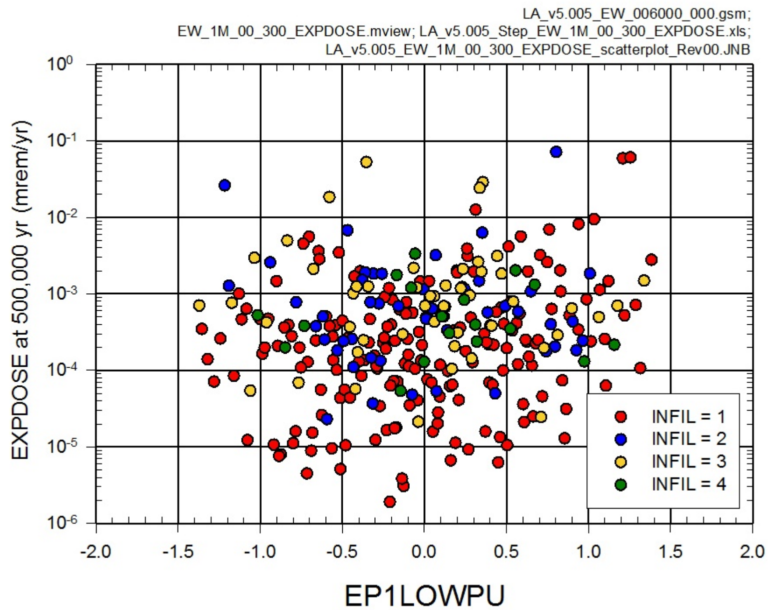


Figure 18. Comparison of model results for selected scatterplots for expected dose to RMEI (*EXPDOSE*, mrem/yr) over [0, 1,000,000 yr] for all radioactive species resulting from early waste wackage failure obtained with version 5.005 of the TSPA-LA model, scatterplots for *EXPDOSE* at 500,000 years: (top) YMP TSPA-LA model (SNL 2008, Figure K5.7.2-4[a](c) and (bottom) TSPA-LA model test run of this study.



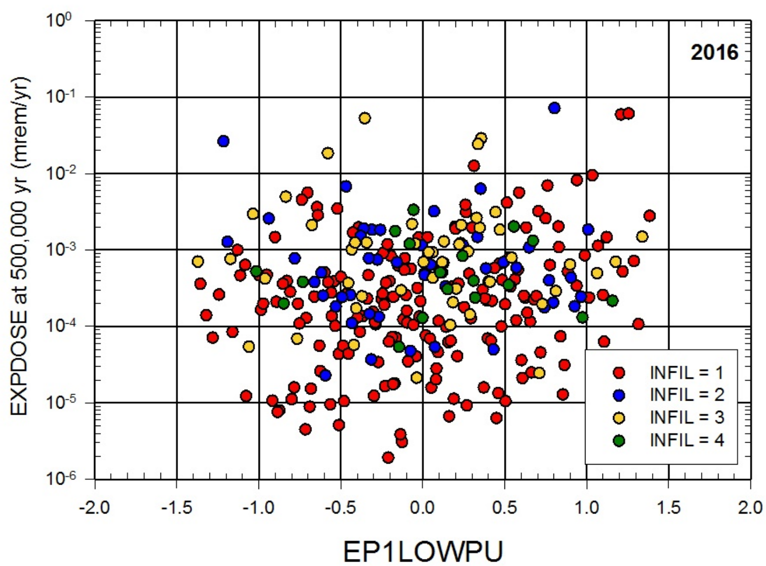


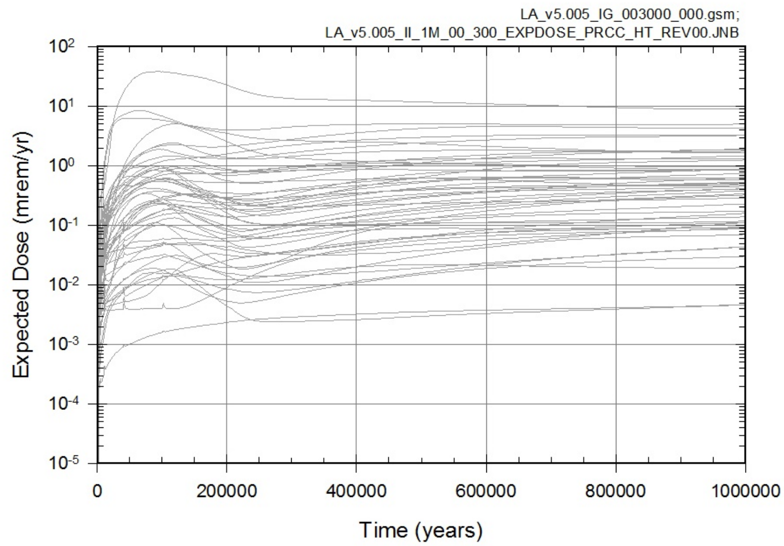
Figure 19. Comparison of model results for selected scatterplots for expected dose to RMEI (*EXPDOSE*, mrem/yr) over [0, 1,000,000 yr] for all radioactive species resulting from early waste wackage failure obtained with version 5.005 of the TSPA-LA model, scatterplots for *EXPDOSE* at 500,000 years: (top) YMP TSPA-LA model (SNL 2008, Figure K5.7.2-4[a](d) and (bottom) TSPA-LA model test run of this study.

3.4. 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).

The Igneous Intrusion scenario class is defined based on futures that involve one or more igneous events. Results for uncertainty and sensitivity analysis are shown in Figures 20 to 25. The figures compare results of the original TSPA-LA model (SNL 2008, Figures K6.7.2[a]) and results of this study, for the 1,000,000 years simulation period. Figure 20 shows comparison of GoldSim results for dose to RMEI (EXPDOSE, mrem/yr) for the first 50 sample elements. Figure 21 compares PRCCs for EXPDOSE for the period from 0 to 1,000,000 years. Figure 22 shows comparison of results for the stepwise rank regression analyses for EXPDOSE at 50,000, 200,000 and 500,000 years. Figures 23 to 25 show comparisons of scatterplots for EXPDOSE at 500,000 years vs selected parameters.

As shown in Figures 20 to 25, 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 CL2014.



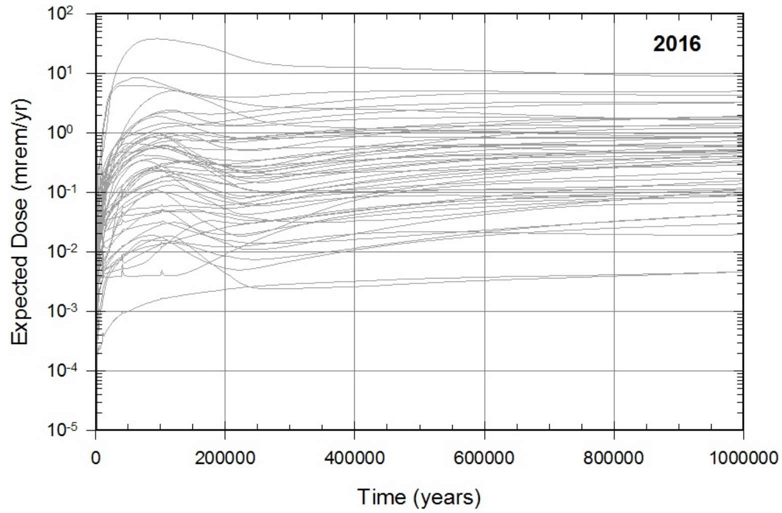
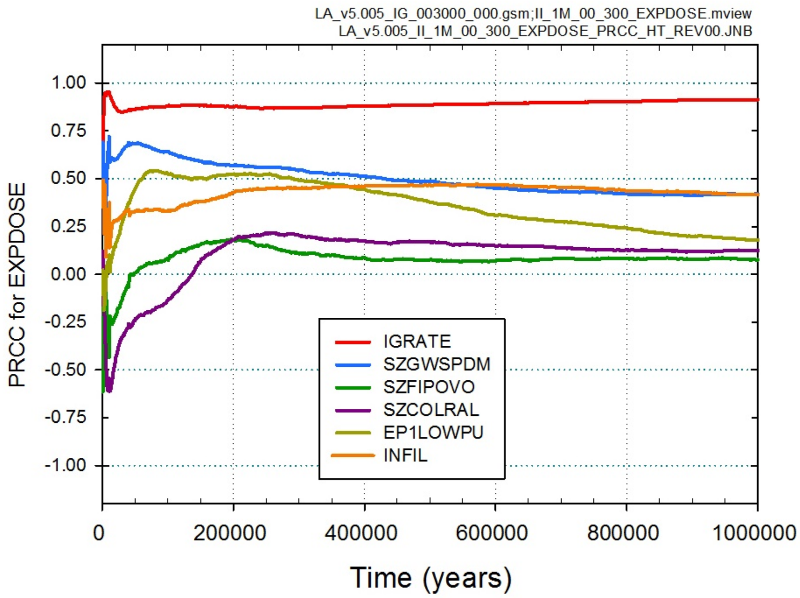


Figure 20. Comparison of model results for expected dose to RMEI (*EXPDOSE*, mrem/yr) over [0, 1,000,000 yr] for all radioactive species resulting from igneous intrusion obtained with version 5.005 of the TSPA-LA model, *EXPDOSE* for first 50 sample elements: (top) YMP TSPA-LA model (SNL 2008, Figure K6.7.2-1[a](b) and (bottom) TSPA-LA model test run of this study.



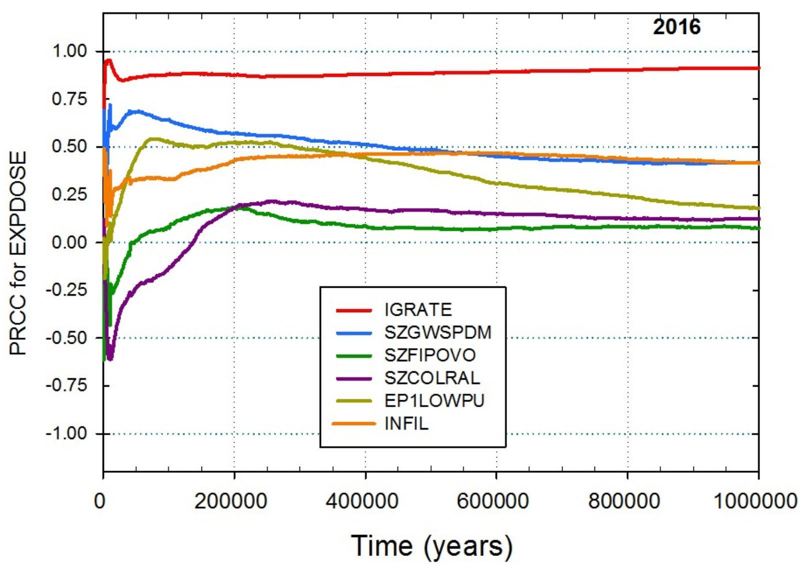
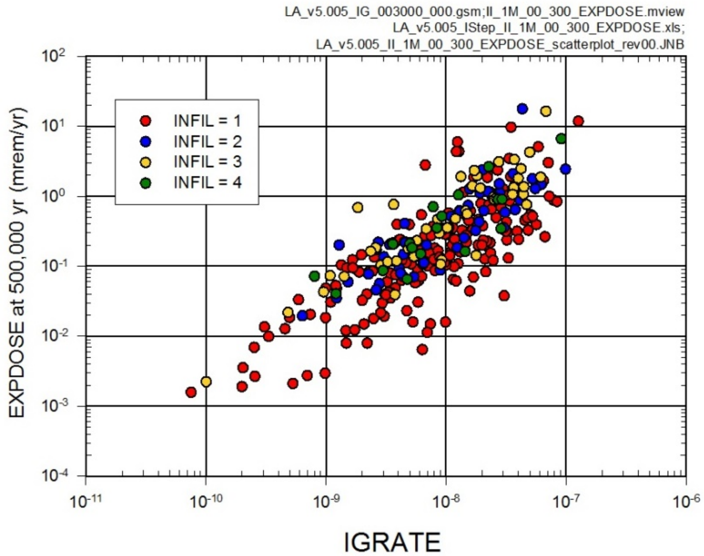


Figure 21. Comparison of model results for expected dose to RMEI (*EXPDOSE*, mrem/yr) over [0, 1,000,000 yr] for all radioactive species resulting igneous intrusion obtained with version 5.005 of the TSPA-LA model, PRCCs for *EXPDOSE*: (top) YMP TSPA-LA model (SNL 2008,Figure K6.7.2-1[a](c) and (bottom) TSPA-LA model test run of this study.

	EXPDOSE: 50,000 years			EXPDOSE: 200,000 years			EXPDOSE: 500,000 years		
Step	**Variable**	**R^2**	**SRRC**	**Variable**	**R^2**	**SRRC**	**Variable**	**R^2**	**SRRC**
1	IGRATE	0.53	0.72	IGRATE	0.57	0.75	IGRATE	0.62	0.79
2	SZGWSPDM	0.69	0.39	SZGWSPDM	0.67	0.30	SZGWSPDM	0.68	0.25
3	EP1LOWPU	0.74	0.20	EP1LOWPU	0.72	0.20	INFIL	0.73	0.19
4	INFIL	0.77	0.16	INFIL	0.75	0.19	EP1LOWPU	0.75	0.16
5	EP1NPO2	0.78	0.11	SZFISPVO	0.77	0.16	GOESITED	0.78	-0.15
6	MICNP237	0.79	0.11	GOESITED	0.79	-0.12	EP1LOWNU	0.79	0.14
7	CPUCOLWF	0.80	0.13	EP1NPO2	0.81	0.11	SZFISPVO	0.80	0.13
8	SZFISPVO	0.81	0.11	CORRATSS	0.82	-0.06	MICPU239	0.82	0.13
9	SZCOLRAL	0.82	-0.10	HFOSA	0.83	-0.09	SZCONCOL	0.83	0.10
10	KDRASMEC	0.83	0.08	EP1LOWNU	0.83	0.09	HFOSA	0.84	-0.08
11				SZDIFCVO	0.84	-0.09	UZFAG4	0.84	-0.08
12				SZCONCOL	0.85	0.08	SZDIFCVO	0.85	-0.07
13				PHCSS	0.85	-0.07	CSWFA0AK	0.85	-0.07
14				SZKDAMCO	0.85	0.06	SZKDAMCO	0.85	0.07
15				SCHOBOLT	0.86	0.07	SZSREG1X	0.86	0.07
16				MICNP237	0.86	0.11			

	EXPDOSE: 50,000 years			EXPDOSE: 200,000 years			EXPDOSE: 500,000 years		
Step	**Variable**	**R^2**	**SRRC**	**Variable**	**R^2**	**SRRC**	**Variable**	**R^2**	**SRRC**
1	IGRATE	0.53	0.72	IGRATE	0.57	0.75	IGRATE	0.62	0.79
2	SZGWSPDM	0.69	0.39	SZGWSPDM	0.67	0.30	SZGWSPDM	0.68	0.25
3	EP1LOWPU	0.74	0.20	EP1LOWPU	0.72	0.20	INFIL	0.73	0.19
4	INFIL	0.77	0.16	INFIL	0.75	0.19	EP1LOWPU	0.75	0.16
5	EP1NPO2	0.78	0.11	SZFISPVO	0.77	0.16	GOESITED	0.78	-0.15
6	MICNP237	0.79	0.11	GOESITED	0.79	-0.12	EP1LOWNU	0.79	0.14
7	CPUCOLWF	0.80	0.13	EP1NPO2	0.81	0.11	SZFISPVO	0.80	0.13
8	SZFISPVO	0.81	0.11	CORRATSS	0.82	-0.06	MICPU239	0.82	0.13
9	SZCOLRAL	0.82	-0.10	HFOSA	0.83	-0.09	SZCONCOL	0.83	0.10
10	KDRASMEC	0.83	0.08	EP1LOWNU	0.83	0.09	HFOSA	0.84	-0.08
11				SZDIFCVO	0.84	-0.09	UZFAG4	0.84	-0.08
12				SZCONCOL	0.85	0.08	SZDIFCVO	0.85	-0.07
13				PHCSS	0.85	-0.07	CSWFA0AK	0.85	-0.07
14				SZKDAMCO	0.85	0.06	SZKDAMCO	0.85	0.07
15				SCHOBOLT	0.86	0.07	SZSREG1X	0.86	0.07
16				MICNP237	0.86	0.11			

Figure 22. Comparison of model results for stepwise rank regression analyses for expected dose to RMEI (*EXPDOSE*, mrem/yr) over [0, 1,000,000 yr] for all radioactive species resulting from igneous intrusion obtained with version 5.005 of the TSPA-LA model, regressions for *EXPDOSE* at 50,000, 200,000, and 500,000 years: (top) YMP TSPA-LA model (SNL 2008, Figure K6.7.2-2[a](a) and (bottom) TSPA-LA model test run of this study.



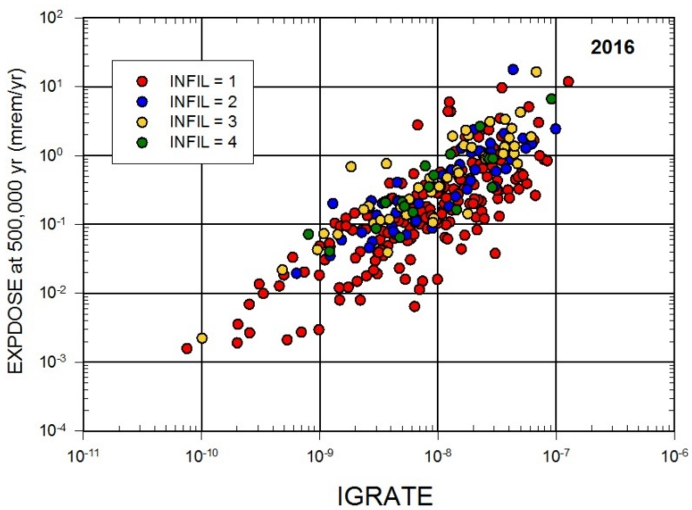
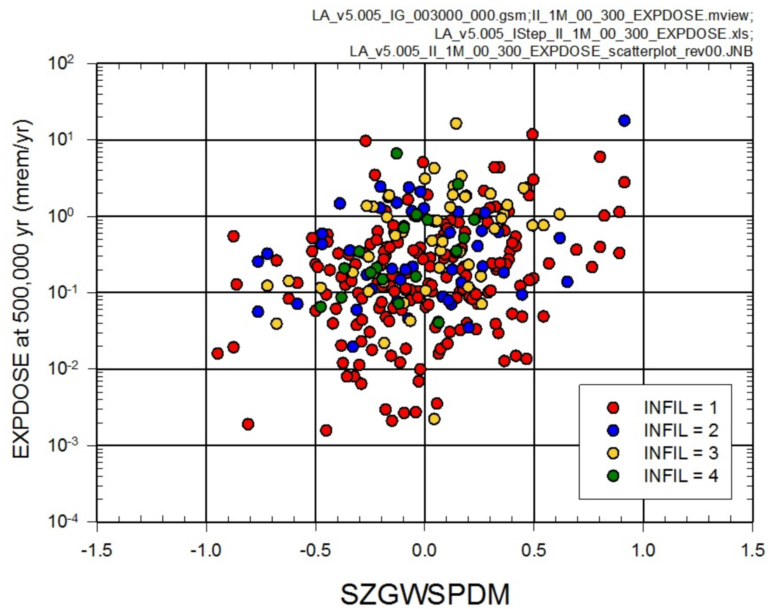


Figure 23. Comparison of model results for selected scatterplots for expected dose to RMEI (*EXPDOSE*, mrem/yr) over [0, 1,000,000 yr] for all radioactive species resulting from igneous intrusion obtained with version 5.005 of the TSPA-LA model, scatterplots for *EXPDOSE* at 500,000 years: (top) YMP TSPA-LA model (SNL 2008, Figure K6.7.2-2[a](b) and (bottom) TSPA-LA model test run of this study.



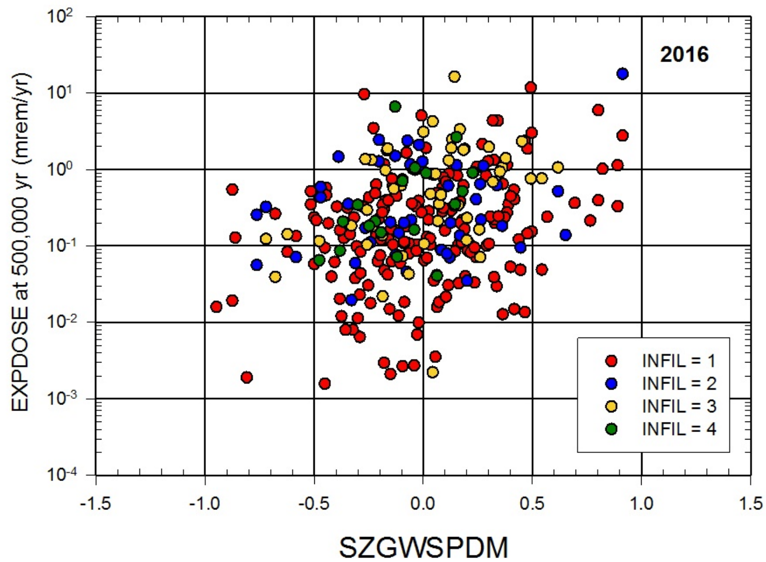
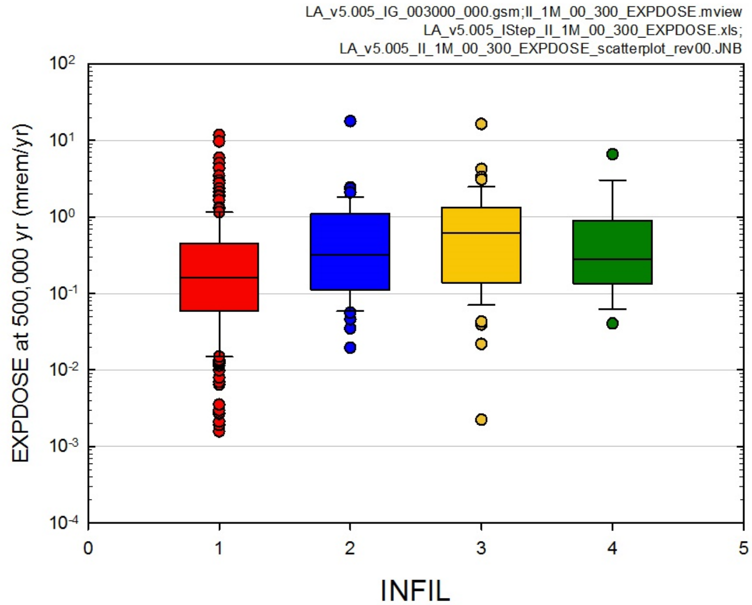


Figure 24. Comparison of model results for selected scatterplots for expected dose to RMEI (*EXPDOSE*, mrem/yr) over [0, 1,000,000 yr] for all radioactive species resulting from igneous intrusion obtained with version 5.005 of the TSPA-LA model, scatterplots for *EXPDOSE* at 500,000 years: (top) YMP TSPA-LA model (SNL 2008, Figure K6.7.2-2 [a](c) and (bottom) TSPA-LA model test run of this study.



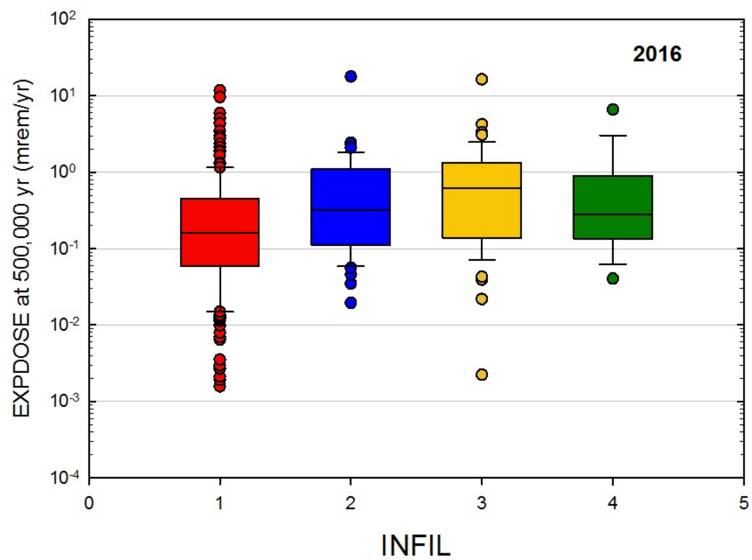


Figure 25. Comparison of model results for selected scatterplots for expected dose to RMEI (*EXPDOSE*, mrem/yr) over [0, 1,000,000 yr] for all radioactive species resulting from igneous intrusion obtained with version 5.005 of the TSPA-LA model, scatterplots for *EXPDOSE* at 500,000 years: (top) YMP TSPA-LA model (SNL 2008, Figure K6.7.2-2 [a](d) and (bottom) TSPA-LA model test run of this study.

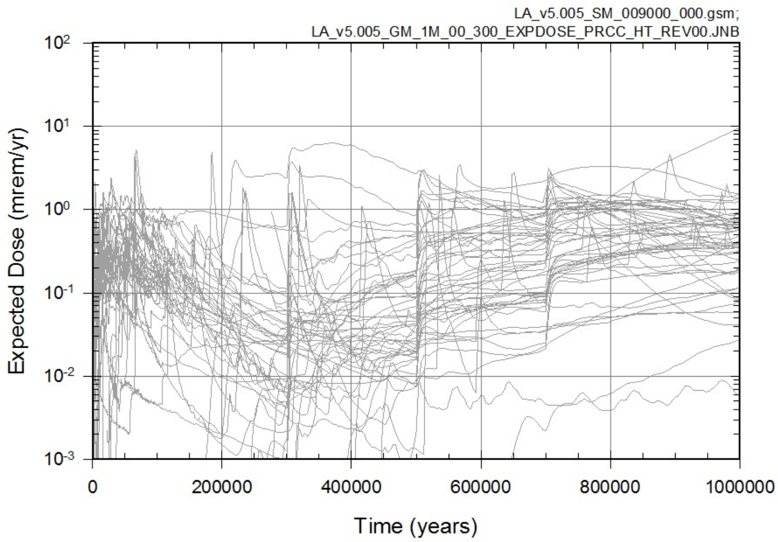
3.5. Seismic Ground Motion Modeling Case

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).

The Seismic Ground Motion scenario class is defined based on futures that involve one or more seismic events. Note that the uncertainty and sensitivity analyses documented in the TSPA-LA (SNL, 2008) appear to be based on GoldSim output results using model version LA_v5.005_SM-009000_000. However, elsewhere in the TSPA-LA report (SNL, 2008) calculations of expected dose to the RMEI were based on a newer model version LA_v5.005_SM-009000_003. The newer model was used for the verification of TSPA-LA model run results completed in 2015 (Hadgu et al., 2015). Further details of the inaccuracy can be found in Appendix A. Because of this inaccuracy model LA_v5.005_SM-009000_000 was re-run to obtain output for use in the uncertainty and sensitivity analyses. The verification of uncertainty and sensitivity analysis described below was based on dose output of model LA_v5.005_SM-009000_000. Uncertainty and sensitivity analysis using output of new model version LA_v5.005_SM-009000_003 are also reported for completeness (Figures 33 to 39).

Comparison of uncertainty and sensitivity analysis based on GoldSim output of model version LA_v5.005_SM-009000_000 are shown in Figures 26 to 32. The figures compare results of the original TSPA-LA model (SNL 2008, Figures K7.7.2) and results of this study, for the 1,000,000 year simulation period. Figure 26 shows comparisons of GoldSim results for dose to RMEI (EXPDOSE, mrem/yr) for the first 50 sample elements. Figure 27 compares PRCCs for EXPDOSE for the period from 0 to 1,000,000 years. Figure 28 shows comparisons of results for the stepwise rank regression analyses for EXPDOSE at 50,000, 200,000 and 500,000 years. Figures 29 to 32 show comparisons of scatterplots for EXPDOSE at 500,000 years vs selected parameters. As shown in Figures 26 to 32, 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.

Uncertainty and sensitivity analysis based on GoldSim output of the new model version LA_v5.005_SM-009000_003 are shown in Figures 33 to 39. The results are slightly different from those in Figures 26 to 32 but no significant difference was observed. Doses were similar (though not shown here) and the most important parameters identified were the same. The slight differences in output are the result of minor parameter changes documented in SNL (2008).



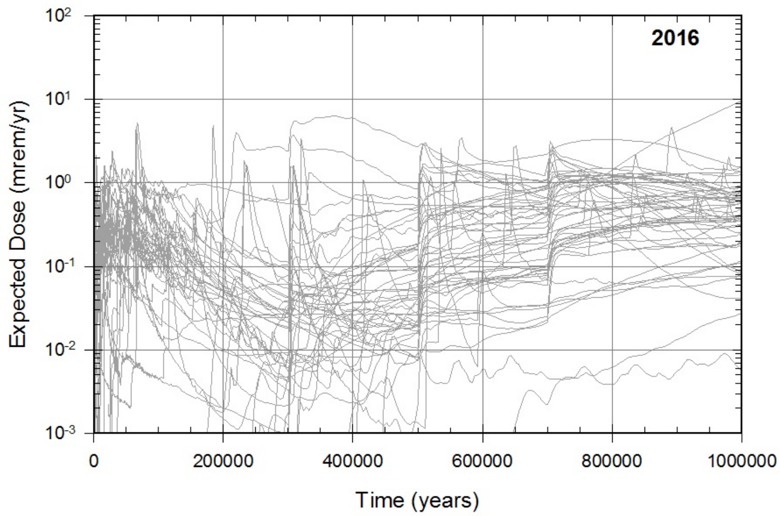
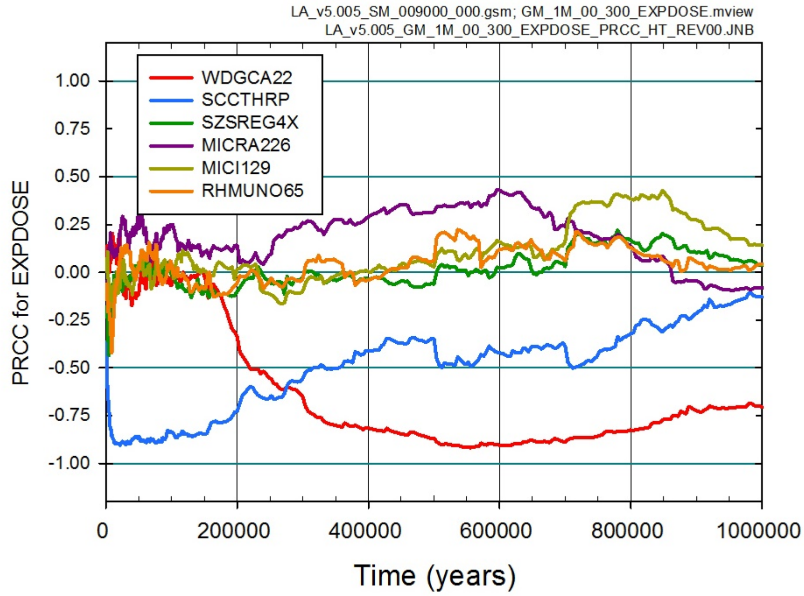


Figure 26. Comparison of model results for expected dose to RMEI (*EXPDOSE*, mrem/yr) over [0, 1,000,000 yr] for all radioactive species resulting from seismic ground motion obtained with version 5.005 of the TSPA-LA model, *EXPDOSE* for first 50 sample elements: (top) YMP TSPA-LA model (SNL 2008, Figure K7.7.2-1[a](b) and (bottom) TSPA-LA model test run of this study.



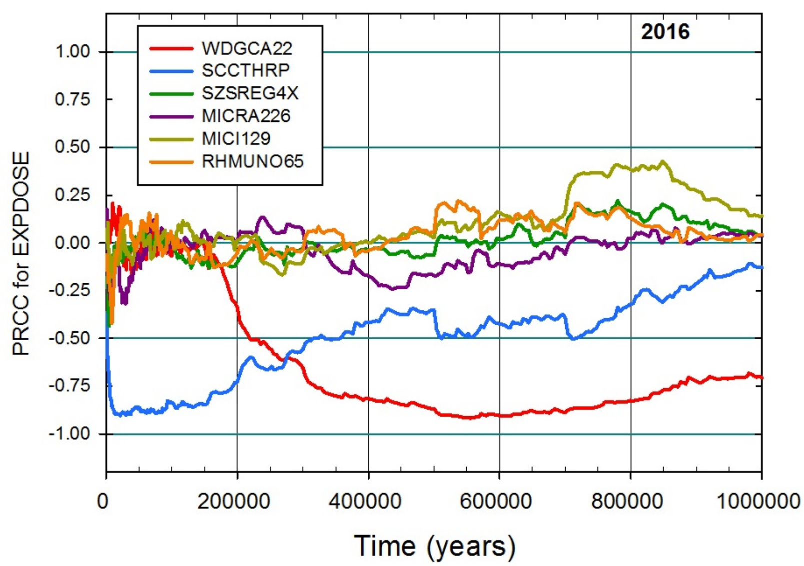
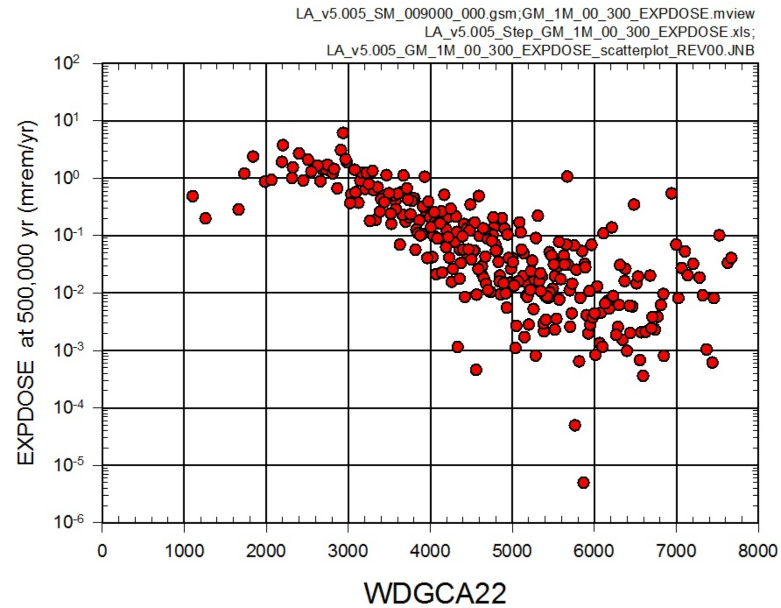


Figure 27. Comparison of model results for expected dose to RMEI (*EXPDOSE*, mrem/yr) over [0, 1,000,000 yr] for all radioactive species resulting seismic ground motion obtained with version 5.005 of the TSPA-LA model, PRCCs for *EXPDOSE*: (top) YMP TSPA-LA model (SNL 2008, Figure K7.7.2-1[a](c) and (bottom) TSPA-LA model test run of this study.

	50,000 years			200,000 years			500,000 years		
Step	**Variable**	**R^2**	**SRRC**	**Variable**	**R^2**	**SRRC**	**Variable**	**R^2**	**SRRC**
1	SCCTHRP	0.71	-0.85	SCCTHRP	0.54	-0.72	WDGCA22	0.62	-0.77
2	MICTC99	0.72	0.09	WDDSGC29	0.58	-0.18	SCCTHRP	0.71	-0.28
3	HLWDRACD	0.73	0.10	WDGCA22	0.60	-0.14	WDNSCC	0.72	-0.12
4	DSNFMASS	0.74	0.11	DSNFMASS	0.61	0.11	SZPORSAL	0.73	0.08
5	SZLODISP	0.75	-0.10	CSNFMASS	0.62	0.10	SZGWSPDM	0.73	0.11
6	SZKDSEVO	0.76	-0.09				SZCONCOL	0.74	0.09
7	CPUPERCS	0.77	0.09				EP1LOWNU	0.75	0.10
8							UZFAG4	0.76	-0.08
9									
10									
11									
12									
13									
14									
15									
16									

	50,000 years			200,000 years			500,000 years		
Step	**Variable**	**R^2**	**SRRC**	**Variable**	**R^2**	**SRRC**	**Variable**	**R^2**	**SRRC**
1	SCCTHRP	0.71	-0.85	SCCTHRP	0.54	-0.72	WDGCA22	0.62	-0.77
2	MICTC99	0.72	0.09	WDDSGC29	0.58	-0.18	SCCTHRP	0.71	-0.28
3	HLWDRACD	0.73	0.10	WDGCA22	0.60	-0.14	WDNSCC	0.72	-0.12
4	DSNFMASS	0.74	0.11	DSNFMASS	0.61	0.11	SZPORSAL	0.73	0.08
5	SZLODISP	0.75	-0.10	CSNFMASS	0.62	0.10	SZGWSPDM	0.74	0.11
6	SZKDSEVO	0.76	-0.09				SZCONCOL	0.74	0.09
7	CPUPERCS	0.77	0.09				EP1LOWNU	0.75	0.10
8							UZFAG4	0.76	-0.08
9									
10									
11									
12									
13									
14									
15									
16									

Figure 28. Comparison of model results for stepwise rank regression analyses for expected dose to RMEI (*EXPDOSE*, mrem/yr) over [0, 1,000,000 yr] for all radioactive species resulting from seismic ground motion obtained with version 5.005 of the TSPA-LA model, regressions for *EXPDOSE* at 50,000, 200,000, and 500,000 years: (top) YMP TSPA-LA model (SNL 2008, Figure K7.7.2-2[a](a) and (bottom) TSPA-LA model test run of this study.



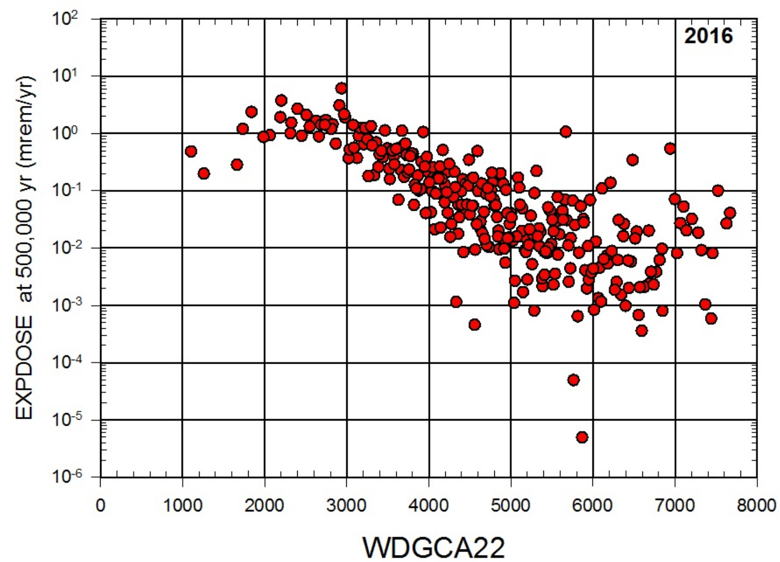
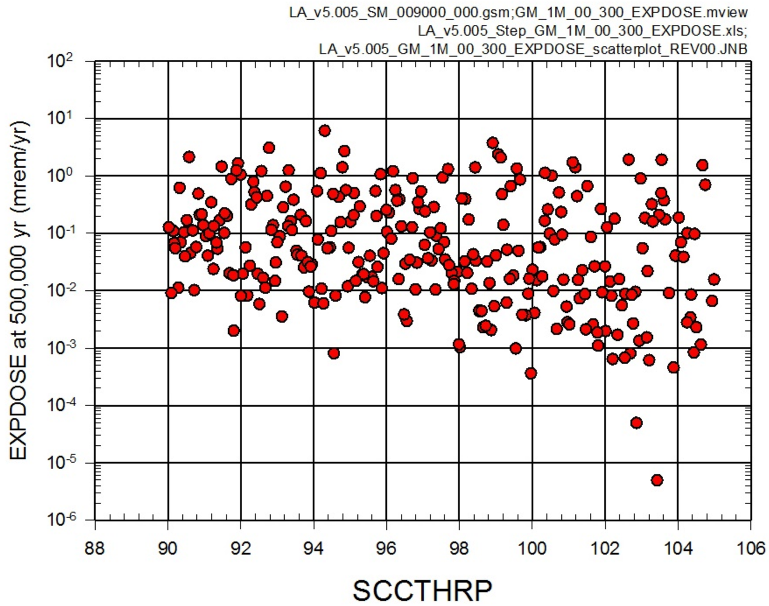


Figure 29. Comparison of model results for selected scatterplots for expected dose to RMEI (*EXPDOSE*, mrem/yr) over [0, 1,000,000 yr] for all radioactive species resulting from seismic ground motion obtained with version 5.005 of the TSPA-LA model, scatterplots for *EXPDOSE* at 500,000 years: (top) YMP TSPA-LA model (SNL 2008, Figure K7.7.2-2 [a](b) and (bottom) TSPA-LA model test run of this study.



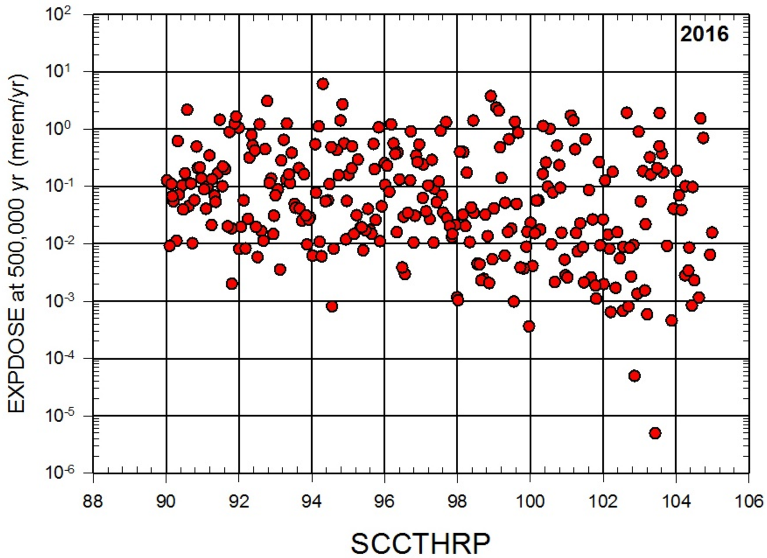
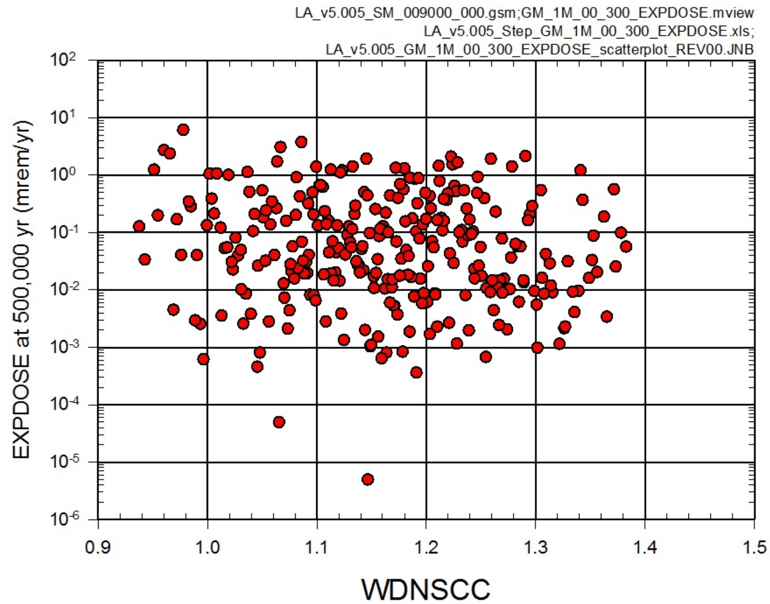


Figure 30. Comparison of model results for selected scatterplots for expected dose to RMEI (*EXPDOSE*, mrem/yr) over [0, 1,000,000 yr] for all radioactive species resulting from seismic ground motion obtained with version 5.005 of the TSPA-LA model, scatterplots for *EXPDOSE* at 500,000 years: (top) YMP TSPA-LA model (SNL 2008, Figure K7.7.2-2 [a](c) and (bottom) TSPA-LA model test run of this study.



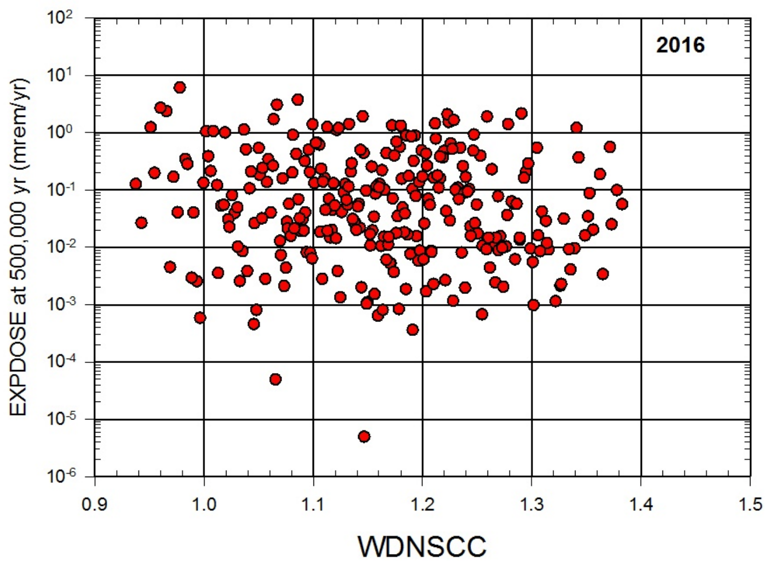
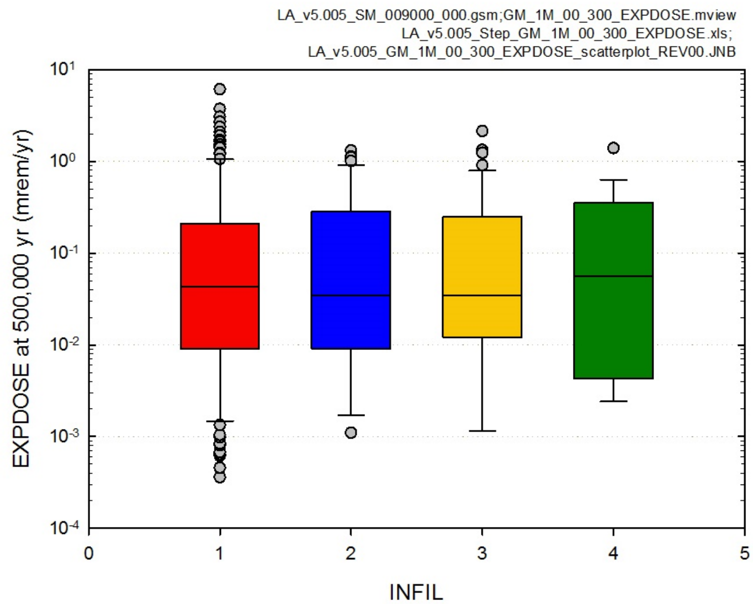


Figure 31. Comparison of model results for selected scatterplots for expected dose to RMEI (*EXPDOSE*, mrem/yr) over [0, 1,000,000 yr] for all radioactive species resulting from seismic ground motion obtained with version 5.005 of the TSPA-LA model, scatterplots for *EXPDOSE* at 500,000 years: (top) YMP TSPA-LA model (SNL 2008, Figure K7.7.2-2 [a](d) and (bottom) TSPA-LA model test run of this study.



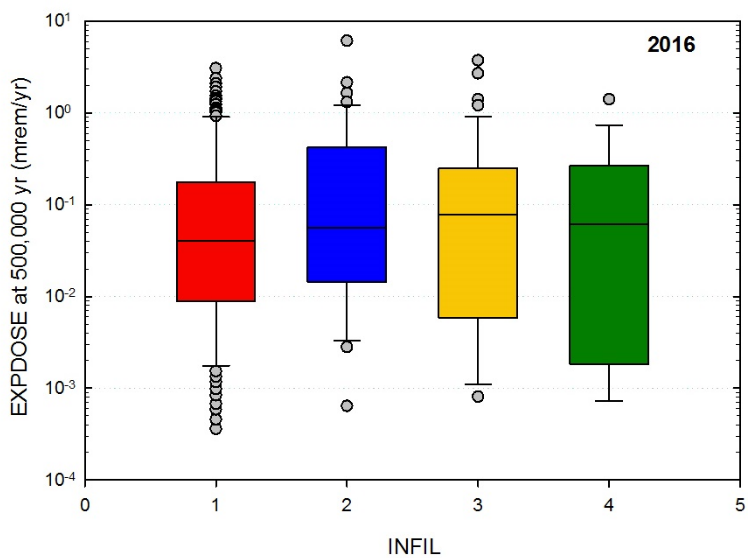


Figure 32. Comparison of model results for selected scatterplots for expected dose to RMEI (*EXPDOSE*, mrem/yr) over [0, 1,000,000 yr] for all radioactive species resulting from seismic ground motion obtained with version 5.005 of the TSPA-LA model, scatterplots for *EXPDOSE* at 500,000 years: (top) YMP TSPA-LA model (SNL 2008, Figure K7.7.2-2 [a](e) and (bottom) TSPA-LA model test run of this study.

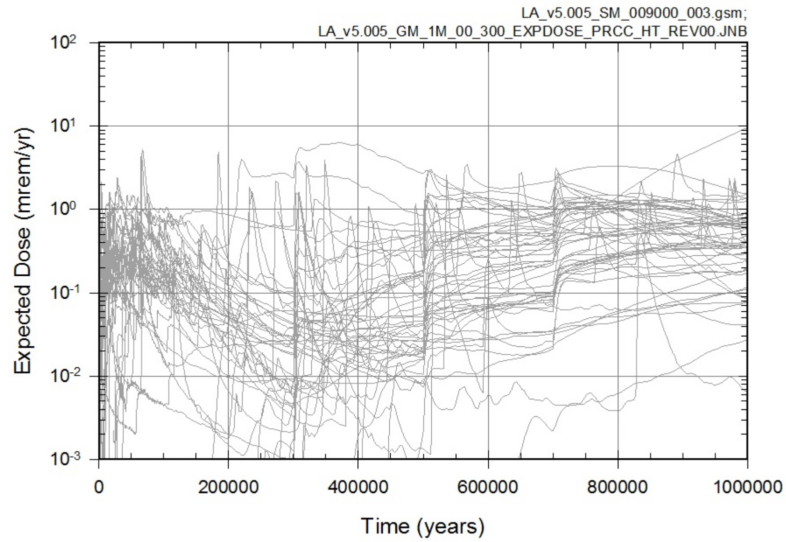


Figure 33. Expected dose to RMEI (*EXPDOSE*, mrem/yr) over [0, 1,000,000 yr] for all radioactive species resulting from seismic ground motion obtained with version 5.005 of the TSPA-LA model, *EXPDOSE* for first 50 sample elements: TSPA-LA model test run of this study using GoldSim file LA_v5.005_SM_00900_003.gsm.

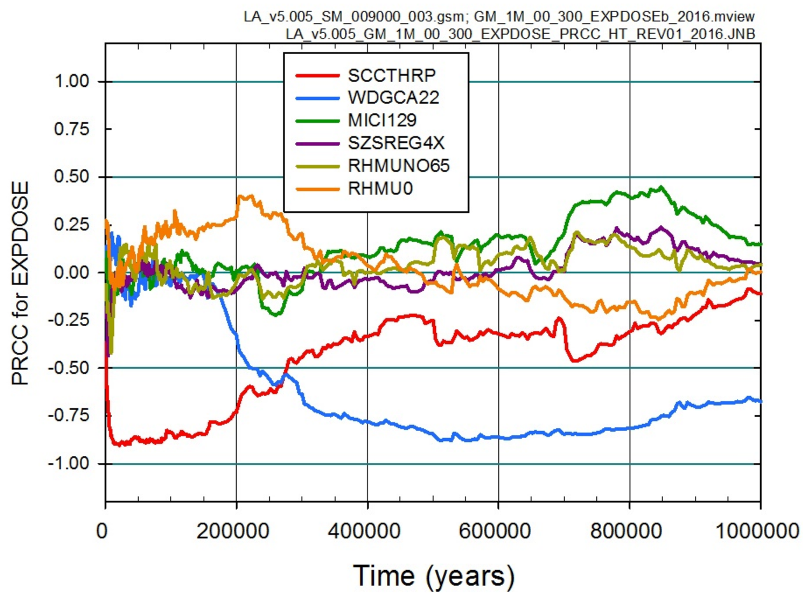


Figure 34. Expected dose to RMEI (*EXPDOSE*, mrem/yr) over [0, 1,000,000 yr] for all radioactive species resulting seismic ground motion obtained with version 5.005 of the TSPA-LA model, PRCCs for *EXPDOSE*: TSPA-LA model test run of this study using GoldSim file LA_v5.005_SM_00900_003.gsm.

	50,000 years			200,000 years			500,000 years		
Step	**Variable**	**R^2**	**SRRC**	**Variable**	**R^2**	**SRRC**	**Variable**	**R^2**	**SRRC**
1	SCCTHRP	0.71	-0.85	SCCTHRP	0.55	-0.72	WDGCA22	0.57	-0.74
2	MICTC99	0.72	0.09	WDDSGC29	0.58	-0.18	SCCTHRP	0.64	-0.25
3	HLWDRACD	0.73	0.10	WDGCA22	0.60	-0.14	WDNSCC	0.66	-0.14
4	DSNFMASS	0.74	0.11	CSNFMASS	0.61	0.11	SZPORSAL	0.67	0.10
5	SZLODISP	0.75	-0.10	DSNFMASS	0.62	0.10	SZCONCOL	0.68	0.11
6	SZKDSEVO	0.76	-0.09				SZGWSPDM	0.69	0.10
7	CPUPERCS	0.77	0.09						
8									
9									
10									
11									
12									
13									
14									
15									
16									

Figure 35. Model results for stepwise rank regression analyses for expected dose to RMEI (*EXPDOSE*, mrem/yr) over [0, 1,000,000 yr] for all radioactive species resulting from seismic ground motion obtained with version 5.005 of the TSPA-LA model, regressions for *EXPDOSE* at 50,000, 200,000, and 500,000 years: TSPA-LA model test run of this study using GoldSim file LA_v5.005_SM_00900_003.gsm.

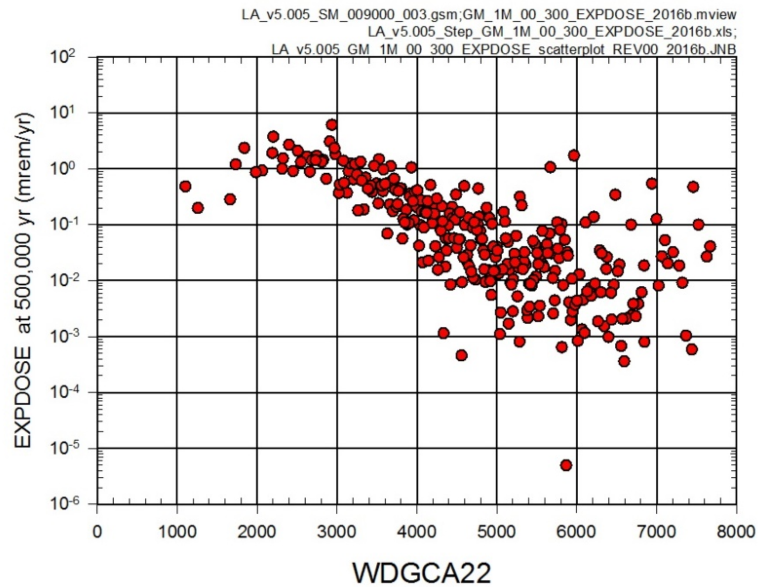


Figure 36. Model results for selected scatterplots for expected dose to RMEI (*EXPDOSE*, mrem/yr) over [0, 1,000,000 yr] for all radioactive species resulting from seismic ground motion obtained with version 5.005 of the TSPA-LA model, scatterplots for *EXPDOSE* at 500,000 years (a): model test run of this study using GoldSim file LA_v5.005_SM_00900_003.gsm

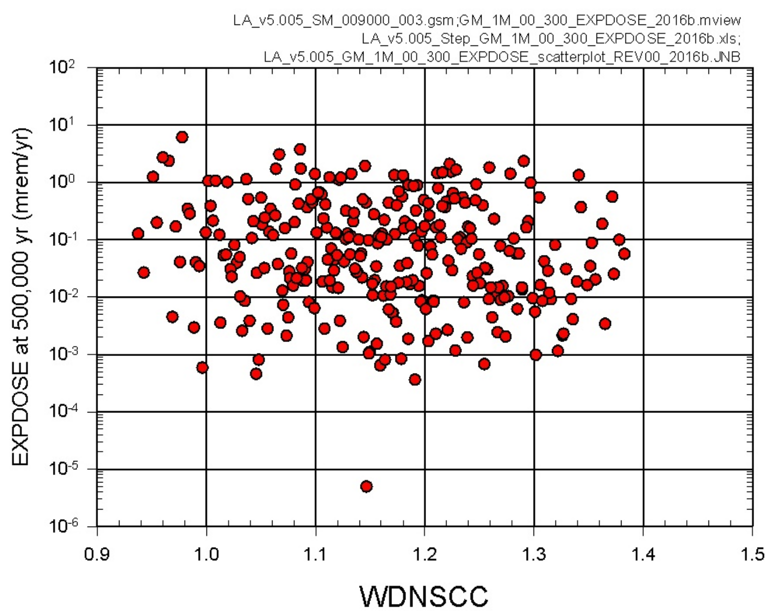


Figure 37. Model results for selected scatterplots for expected dose to RMEI (*EXPDOSE*, mrem/yr) over [0, 1,000,000 yr] for all radioactive species resulting from seismic ground motion obtained with version 5.005 of the TSPA-LA model, scatterplots for *EXPDOSE* at 500,000 years (b): model test run of this study using GoldSim file LA_v5.005_SM_00900_003.gsm

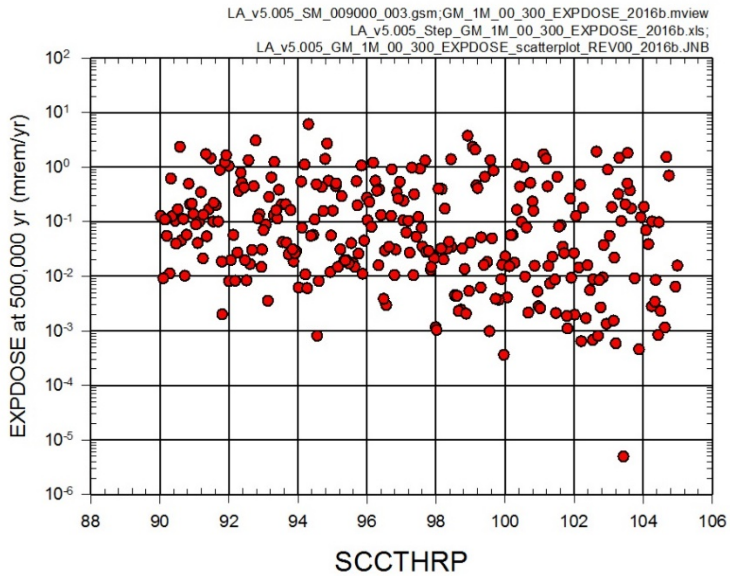


Figure 38. Model results for selected scatterplots for expected dose to RMEI (*EXPDOSE*, mrem/yr) over [0, 1,000,000 yr] for all radioactive species resulting from seismic ground motion obtained with version 5.005 of the TSPA-LA model, scatterplots for *EXPDOSE* at 500,000 years (c): model test run of this study using GoldSim file LA_v5.005_SM_00900_003.gsm

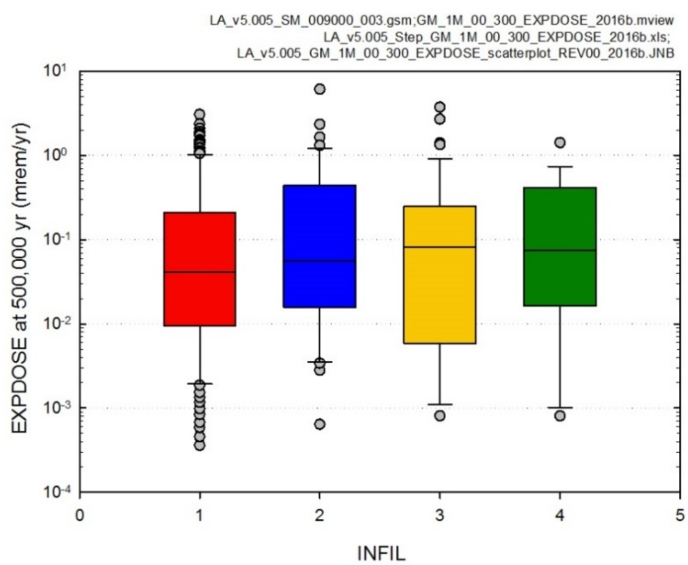


Figure 39. Model results for selected scatterplots for expected dose to RMEI (*EXPDOSE*, mrem/yr) over [0, 1,000,000 yr] for all radioactive species resulting from seismic ground motion obtained with version 5.005 of the TSPA-LA model, scatterplots for *EXPDOSE* at 500,000 years (d): model test run of this study using GoldSim file LA_v5.005_SM_00900_003.gsm

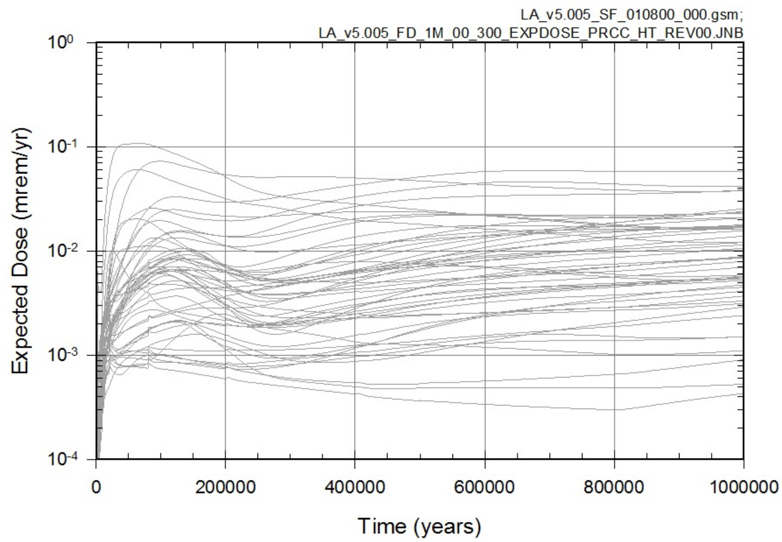
3.6. Seismic Fault Displacement Modeling Case

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).

The Seismic Fault Displacement scenario class is defined based on futures that involve one or more seismic events. Note that Figures K7.8.2-2[a], Plots (b), (c), and (d) in the TSPA-LA report (SNL, 2008) are not the correct figures. Results for the 20,000 years modeling case (Figure K7.8.1-2[a], Plots (b), (c), and (d) were inadvertently repeated. The error was corrected in ERD 02 of the report. Further details are given in Appendix A of this report. For this study the correct plots were obtained from Output DTNs MO0710ADTSPAWO.000 [DIRS 183752] and MO0710PLOTSFIG.000 [DIRS 185207].

Results for uncertainty and sensitivity analysis are shown in Figures 40 to 45. The figures compare results of the original TSPA-LA model (SNL 2008, Figures K7.8.2[a] and the above DTNs) and results of this study, for the 1,000,000 year simulation period. Figure 40 shows comparison of GoldSim results for dose to RMEI (EXPDOSE, mrem/yr) for the first 50 sample elements. Figure 41 compares PRCCs for EXPDOSE for the period from 0 to 1,000,000 years. Figure 42 shows comparisons of results for the stepwise rank regression analyses for EXPDOSE at 50,000, 200,000 and 500,000 years. Figures 43 to 45 show comparisons of scatterplots for EXPDOSE at 500,000 years vs selected parameters.

As shown in Figures 40 to 45, 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 CL2014.



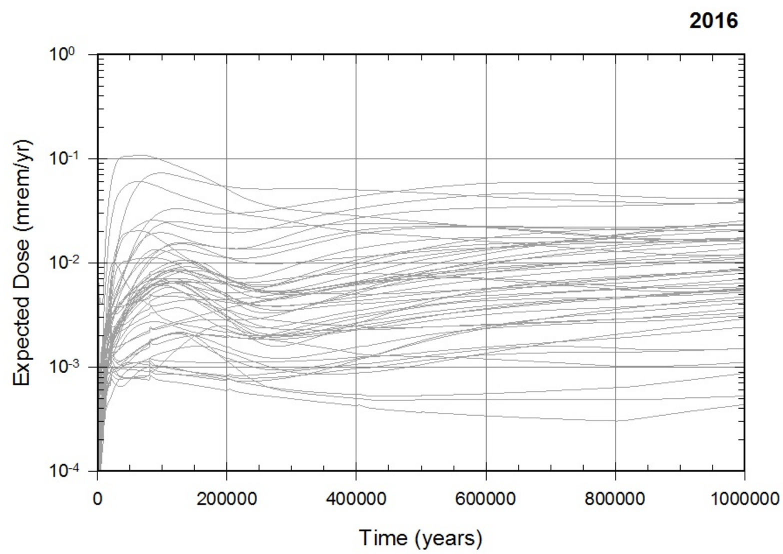
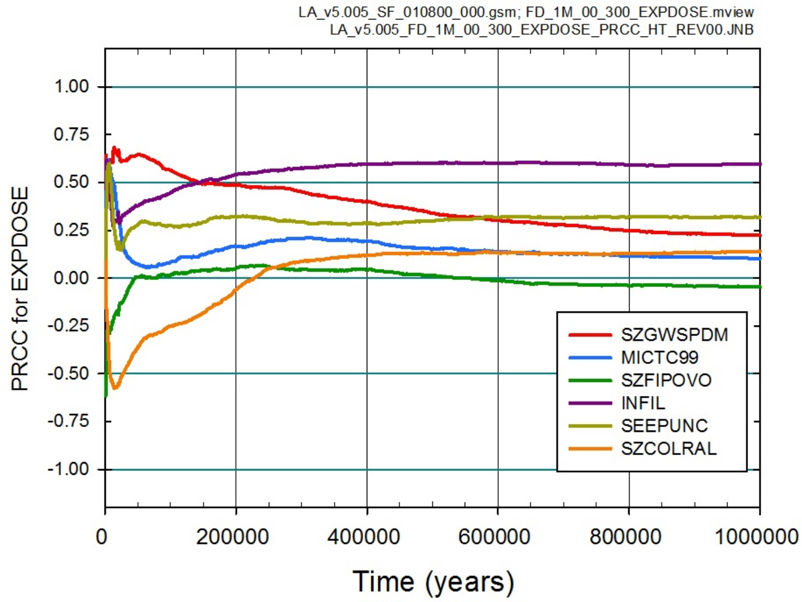


Figure 40. Comparison of model results for expected dose to RMEI (*EXPDOSE*, mrem/yr) over [0, 1,000,000 yr] for all radioactive species resulting from seismic fault displacement obtained with version 5.005 of the TSPA-LA model, *EXPDOSE* for first 50 sample elements: (top) YMP TSPA-LA model (SNL 2008, Figure K7.8.2-1[a](b) and (bottom) TSPA-LA model test run of this study.



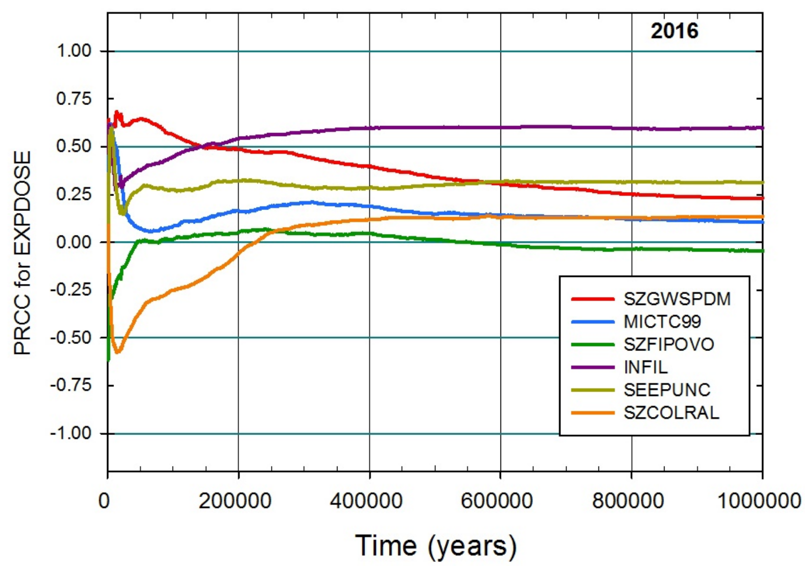
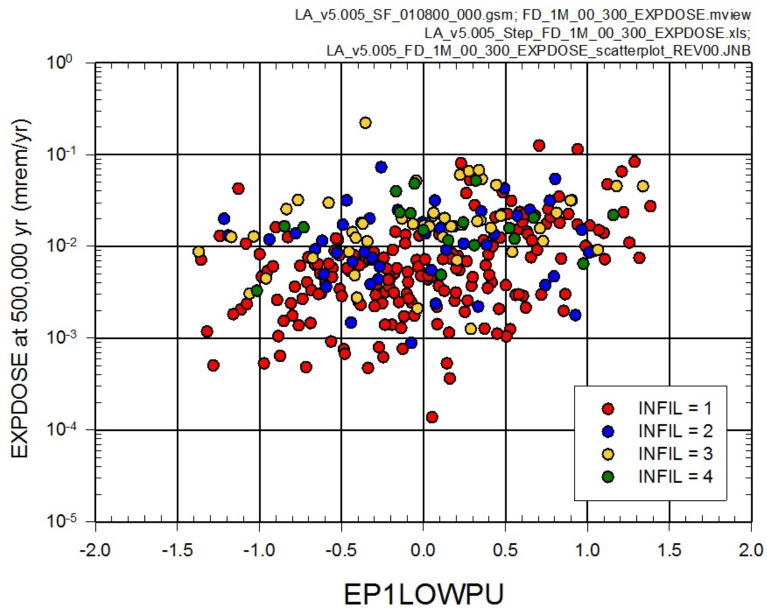


Figure 41. Comparison of model results for expected dose to RMEI (*EXPDOSE*, mrem/yr) over [0, 1,000,000 yr] for all radioactive species resulting seismic fault displacement obtained with version 5.005 of the TSPA-LA model, PRCCs for *EXPDOSE*: (top) YMP TSPA-LA model (SNL 2008, Figure K7.8.2-1[a](c) and (bottom) TSPA-LA model test run of this study.

	50,000 years			200,000 years			500,000 years		
Step	Variable	R^2	SRRC	Variable	R^2	SRRC	Variable	R^2	SRRC
1	SZGWSPDM	0.25	0.51	INFIL	0.15	0.37	INFIL	0.18	0.40
2	INFIL	0.37	0.31	SZGWSPDM	0.29	0.40	EP1LOWPU	0.29	0.33
3	WPFLUX	0.43	0.22	WPFLUX	0.37	0.28	SZGWSPDM	0.38	0.36
4	EP1LOWPU	0.48	0.21	EP1LOWPU	0.44	0.28	WPFLUX	0.43	0.25
5	SEEPPRM	0.52	-0.19	SEEPPRM	0.48	-0.22	GOESITED	0.48	-0.18
6	MICNP237	0.55	0.18	SZFISPVO	0.55	0.19	SEEPPRM	0.52	-0.20
7	CPUCOLWF	0.57	0.17	SEEPUNC	0.57	0.17	MICPU239	0.54	0.19
8	SZCOLRAL	0.60	-0.15	CORRATSS	0.59	-0.10	SEEPUNC	0.57	0.17
9	SZFISPVO	0.62	0.16	EP1NPO2	0.60	0.11	SZFISPVO	0.60	0.17
10	SEEPUNC	0.63	0.12	SZCONCOL	0.62	0.11	SZCONCOL	0.62	0.14
11	PHCSS	0.65	-0.12	EP1LOWNU	0.63	0.12	EP1LOWNU	0.64	0.18
12	HFOSA	0.66	-0.11	SZDIFCVO	0.64	-0.11	UZFAG4	0.67	-0.15
13	RUBMAXL	0.67	-0.10	SZKDAMCO	0.65	0.10	HFOSA	0.68	-0.11
14	PH2MCONS	0.67	-0.09	GOESITED	0.66	-0.11	SZDIFCVO	0.69	-0.12
15				MICPU239	0.67	0.19	KDPUSMEC	0.70	0.10
16				UZFAG4	0.68	-0.11	SZWBNDAL	0.71	-0.10

	50,000 years			200,000 years			500,000 years		
Step	Variable	R^2	SRRC	Variable	R^2	SRRC	Variable	R^2	SRRC
1	SZGWSPDM	0.25	0.51	INFIL	0.15	0.38	INFIL	0.18	0.41
2	INFIL	0.37	0.31	SZGWSPDM	0.29	0.40	EP1LOWPU	0.29	0.33
3	WPFLUX	0.43	0.22	WPFLUX	0.37	0.28	SZGWSPDM	0.38	0.35
4	EP1LOWPU	0.48	0.21	EP1LOWPU	0.44	0.28	WPFLUX	0.44	0.25
5	SEEPPRM	0.52	-0.20	SEEPPRM	0.48	-0.22	GOESITED	0.48	-0.18
6	MICNP237	0.55	0.18	SZFISPVO	0.54	0.18	SEEPPRM	0.52	-0.20
7	CPUCOLWF	0.57	0.19	SEEPUNC	0.57	0.18	MICPU239	0.54	0.18
8	SZCOLRAL	0.60	-0.14	CORRATSS	0.59	-0.09	SEEPUNC	0.57	0.18
9	SZFISPVO	0.62	0.16	EP1NPO2	0.60	0.10	SZFISPVO	0.60	0.16
10	SEEPUNC	0.63	0.12	SZCONCOL	0.62	0.12	SZCONCOL	0.62	0.14
11	PHCSS	0.65	-0.12	EP1LOWNU	0.63	0.11	EP1LOWNU	0.64	0.17
12	HFOSA	0.66	-0.11	SZDIFCVO	0.64	-0.12	UZFAG4	0.67	-0.14
13	RUBMAXL	0.67	-0.10	SZKDAMCO	0.65	0.10	HFOSA	0.68	-0.10
14	PH2MCONS	0.67	-0.09	GOESITED	0.66	-0.12	SZDIFCVO	0.69	-0.12
15				MICPU239	0.67	0.20	KDPUSMEC	0.70	0.10
16				UZFAG4	0.68	-0.11	SZWBNDAL	0.71	-0.10

Figure 42. Comparison of model results for stepwise rank regression analyses for expected dose to RMEI (*EXPDOSE*, mrem/yr) over [0, 1,000,000 yr] for all radioactive species resulting from seismic fault displacement obtained with version 5.005 of the TSPA-LA model, regressions for *EXPDOSE* at 50,000, 200,000, and 500,000 years: (top) YMP TSPA-LA model (SNL 2008, Figure K7.8.2-2[a](a) and (bottom) TSPA-LA model test run of this study.



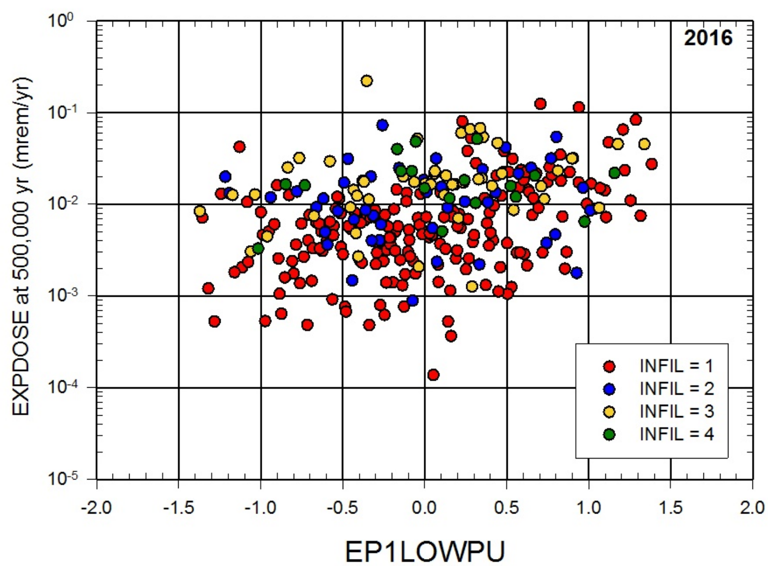
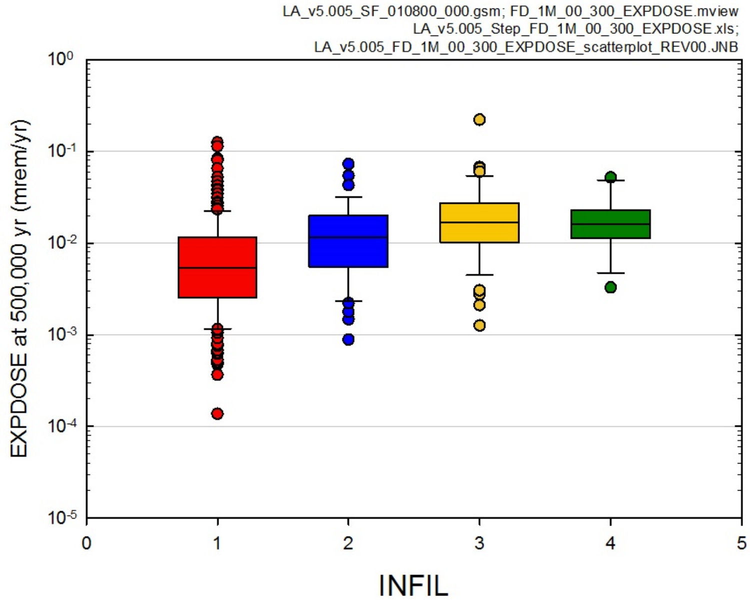


Figure 43. Comparison of model results for selected scatterplots for expected dose to RMEI (*EXPDOSE*, mrem/yr) over [0, 1,000,000 yr] for all radioactive species resulting from seismic fault displacement obtained with version 5.005 of the TSPA-LA model, scatterplots for *EXPDOSE* at 500,000 years: (top) YMP TSPA-LA model (SNL 2008 (b)) and (bottom) TSPA-LA model test run of this study.



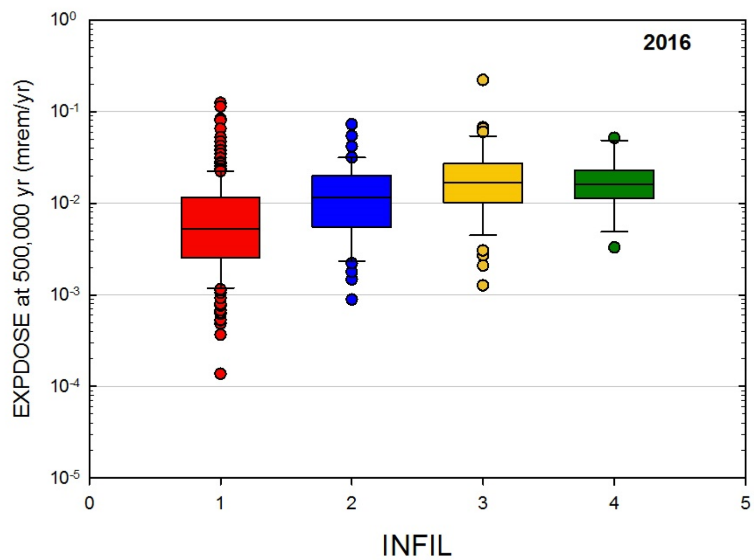
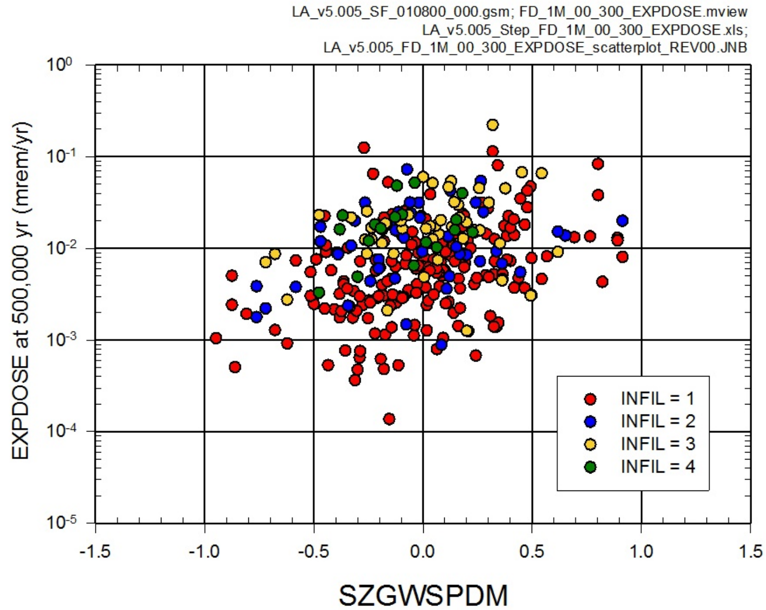


Figure 44. Comparison of model results for selected scatterplots for expected dose to RMEI (*EXPDOSE*, mrem/yr) over [0, 1,000,000 yr] for all radioactive species resulting from seismic fault displacement obtained with version 5.005 of the TSPA-LA model, scatterplots for *EXPDOSE* at 500,000 years: (top) YMP TSPA-LA model (SNL 2008 (c)) and (bottom) TSPA-LA model test run of this study.



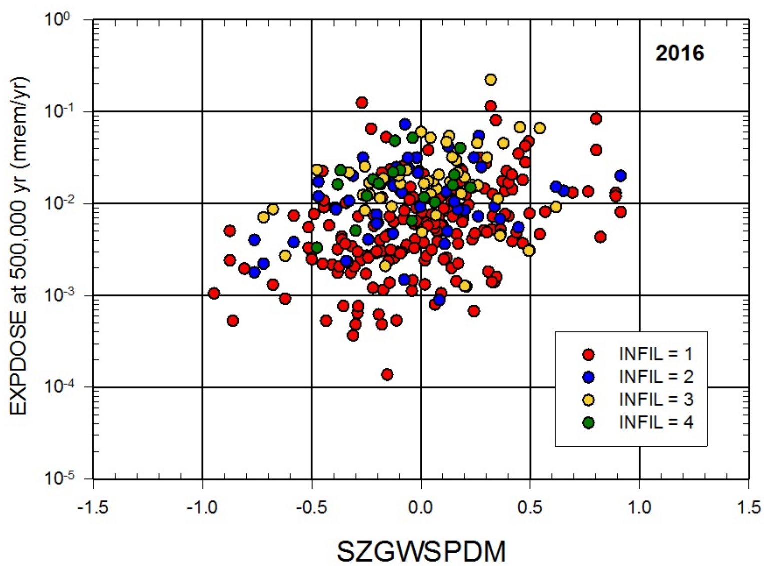


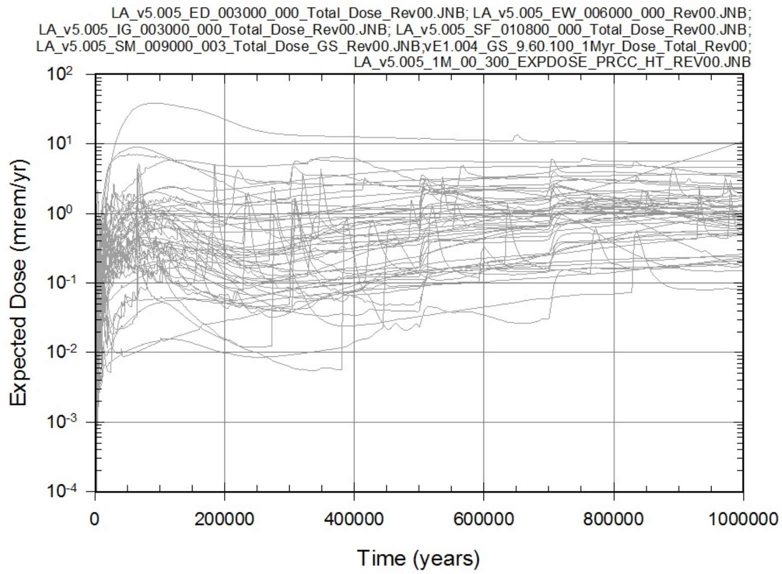
Figure 45. Comparison of model results for selected scatterplots for expected dose to RMEI (*EXPDOSE*, mrem/yr) over [0, 1,000,000 yr] for all radioactive species resulting from seismic fault displacement obtained with version 5.005 of the TSPA-LA model, scatterplots for *EXPDOSE* at 500,000 years: (top) YMP TSPA-LA model (SNL 2008 (d)) and (bottom) TSPA-LA model test run of this study.

3.7. Total Dose to the REMEI

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.

This section looks at uncertainty and sensitivity analyses verification for the total expected annual dose to the RMEI resulting from all scenario classes. Analyses results are shown in Figures 46 to 52. The figures compare results of the original TSPA-LA model (SNL 2008, Figures K8.2-1[a] to K8.2-2[a]) and results of this study, for the 1,000,000 year simulation period. Figure 46 shows comparisons of GoldSim results for expected dose to RMEI (EXPDOSE, mrem/yr) for the first 50 sample elements. Figure 47 compares PRCCs for EXPDOSE for the period from 0 to 1,000,000 years. Figure 48 shows comparisons of results for the stepwise rank regression analyses for EXPDOSE at 50,000, 200,000 and 500,000 years. Figures 49 to 52 show comparisons of scatterplots for EXPDOSE at 500,000 years vs selected parameters.

As shown in Figures 46 to 52, 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 CL2014.



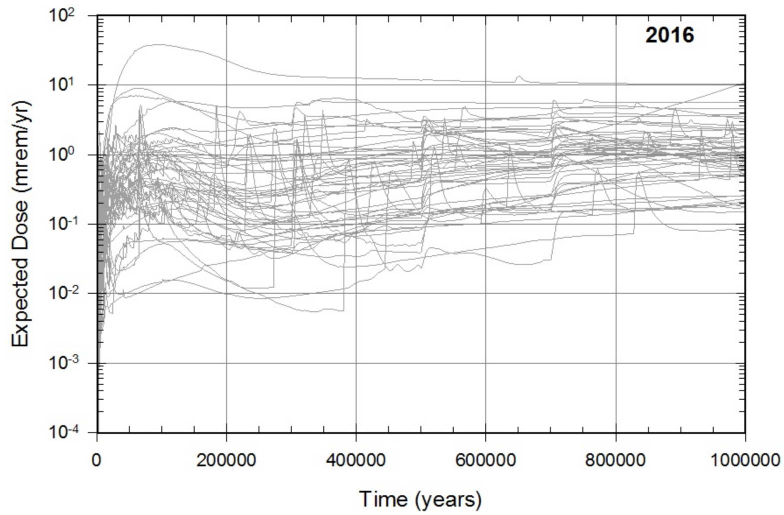
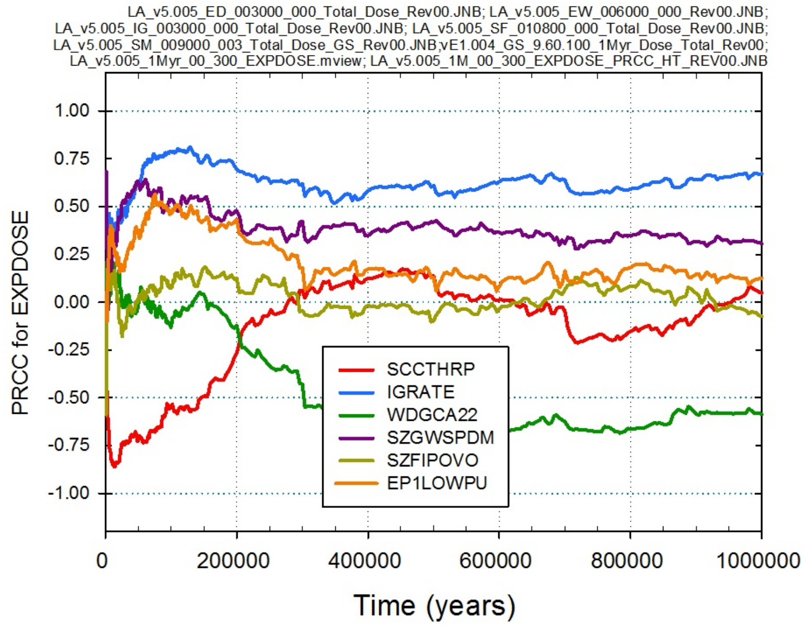


Figure 46. Comparison of model results for expected dose to RMEI (*EXPDOSE*, mrem/yr) over [0, 1,000,000 yr] for all scenario classes obtained with version 5.005 of the TSPA-LA model, *EXPDOSE* for first 50 sample elements: (top) YMP TSPA-LA model (SNL 2008, Figure K8.2-1[a](b) and (bottom) TSPA-LA model test run of this study.



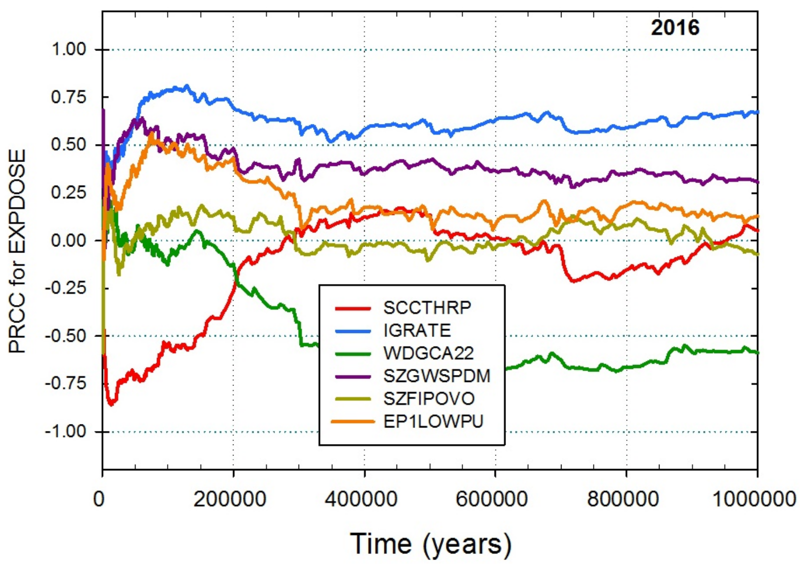
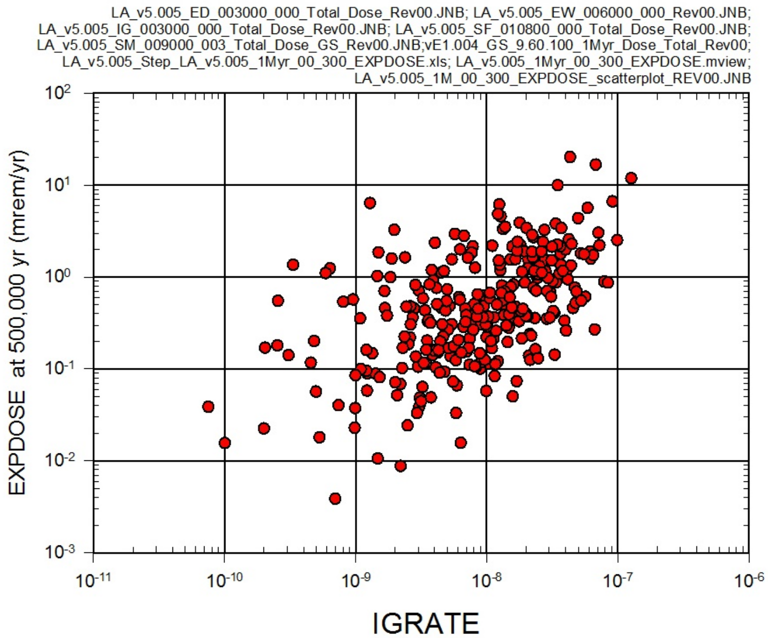


Figure 47. Comparison of model results for expected dose to RMEI (*EXPDOSE*, mrem/yr) over [0, 1,000,000 yr] for all for all scenario classes obtained with version 5.005 of the TSPA-LA model, PRCCs for *EXPDOSE*: (top) YMP TSPA-LA model (SNL 2008, Figure K8.2-1[a](c) and (bottom) TSPA-LA model test run of this study.

	EXPDOSE: 50,000 years			EXPDOSE: 200,000 years			EXPDOSE: 500,000 years		
Step	**Variable**	**R^2**	**SRRC**	**Variable**	**R^2**	**SRRC**	**Variable**	**R^2**	**SRRC**
1	SCCTHRP	0.27	-0.48	IGRATE	0.38	0.61	IGRATE	0.29	0.54
2	IGRATE	0.43	0.41	SZGWSPDM	0.48	0.28	WDGCA22	0.46	-0.38
3	SZGWSPDM	0.55	0.33	EP1LOWPU	0.53	0.23	SZGWSPDM	0.53	0.24
4	EP1LOWPU	0.60	0.20	SCCTHRP	0.57	-0.21	EP1LOWNU	0.56	0.19
5	MICNP237	0.62	0.11	SZFISPVO	0.60	0.15	MICNP237	0.59	0.16
6	INFIL	0.63	0.13	INFIL	0.62	0.16	EP1LOWPU	0.61	0.17
7	EP1NPO2	0.65	0.13	EP1NPO2	0.64	0.14	SZCONCOL	0.64	0.15
8	MICTC99	0.66	0.11	GOESITED	0.66	-0.14	SZFISPVO	0.66	0.15
9	ALPHAL	0.67	0.10	MICSE79	0.68	0.09	INFIL	0.67	0.11
10				MICNP237	0.69	0.14	GOESITED	0.68	-0.10
11				EP1LOWNU	0.70	0.11	SZKDCSVO	0.69	-0.10
12				SZCONCOL	0.71	0.11	HFOSITED	0.69	-0.09
13				PHCSS	0.72	-0.11	SZDIFCVO	0.70	-0.09
14				HFOSA	0.73	-0.09			
15				SZDIFCVO	0.73	-0.09			
16				SEEPCOND	0.74	-0.09			

	EXPDOSE: 50,000 years			EXPDOSE: 200,000 years			EXPDOSE: 500,000 years		
Step	**Variable**	**R^2**	**SRRC**	**Variable**	**R^2**	**SRRC**	**Variable**	**R^2**	**SRRC**
1	SCCTHRP	0.27	-0.48	IGRATE	0.38	0.61	IGRATE	0.29	0.54
2	IGRATE	0.43	0.41	SZGWSPDM	0.48	0.27	WDGCA22	0.46	-0.38
3	SZGWSPDM	0.55	0.33	EP1LOWPU	0.53	0.23	SZGWSPDM	0.53	0.24
4	EP1LOWPU	0.60	0.20	SCCTHRP	0.57	-0.21	EP1LOWNU	0.56	0.19
5	MICNP237	0.62	0.11	SZFISPVO	0.60	0.15	MICNP237	0.59	0.16
6	INFIL	0.63	0.13	INFIL	0.62	0.15	EP1LOWPU	0.61	0.17
7	EP1NPO2	0.65	0.13	EP1NPO2	0.64	0.14	SZCONCOL	0.64	0.15
8	MICTC99	0.66	0.11	GOESITED	0.66	-0.14	SZFISPVO	0.66	0.15
9	ALPHAL	0.67	0.10	MICSE79	0.68	0.09	INFIL	0.67	0.11
10				MICNP237	0.69	0.14	GOESITED	0.68	-0.10
11				EP1LOWNU	0.70	0.12	SZKDCSVO	0.69	-0.10
12				SZCONCOL	0.71	0.10	HFOSITED	0.69	-0.09
13				PHCSS	0.72	-0.11	SZDIFCVO	0.70	-0.09
14				HFOSA	0.73	-0.09			
15				SZDIFCVO	0.73	-0.10			

Figure 48. Comparison of model results for stepwise rank regression analyses for expected dose to RMEI (*EXPDOSE*, mrem/yr) over [0, 1,000,000 yr] for all scenario classes obtained with version 5.005 of the TSPA-LA model, regressions for *EXPDOSE* at 50,000, 200,000, and 500,000 years: (top) YMP TSPA-LA model (SNL 2008, Figure K8.2-2[a](a) and (bottom) TSPA-LA model test run of this study.



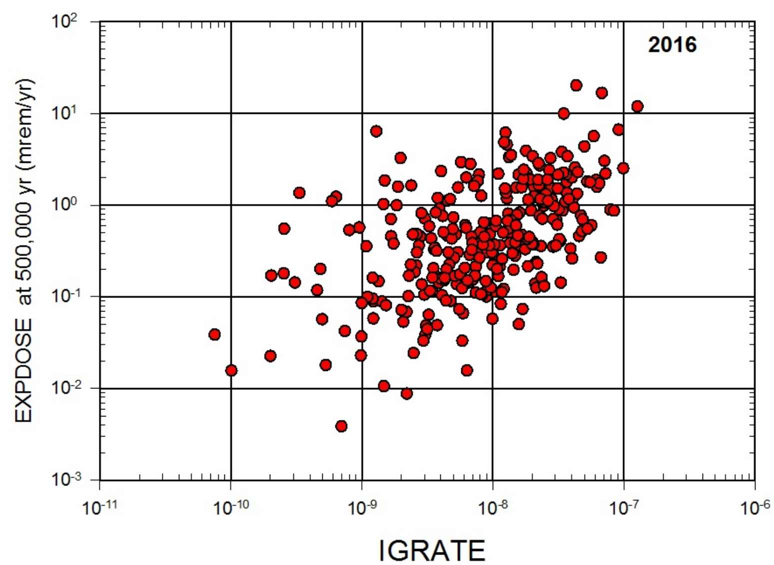
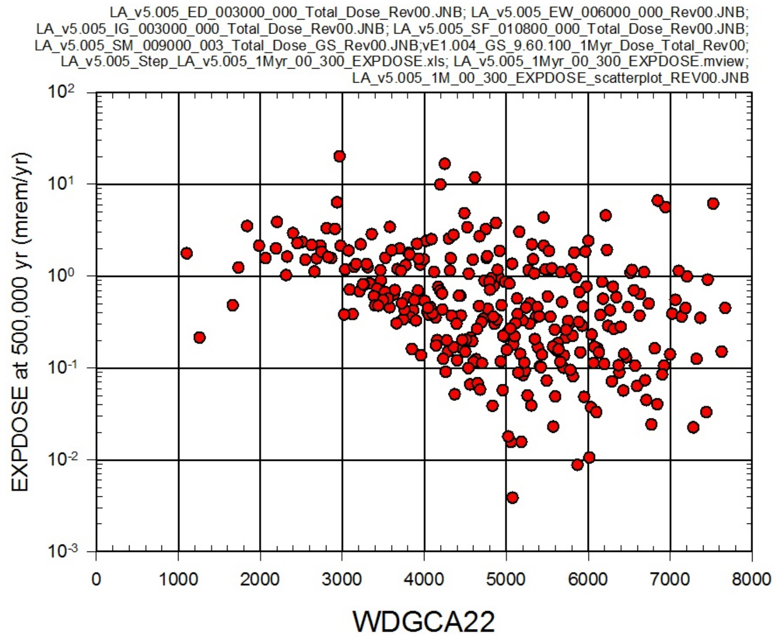


Figure 49. Comparison of model results for selected scatterplots for expected dose to RMEI (*EXPDOSE*, mrem/yr) over [0, 1,000,000 yr] for all scenario classes obtained with version 5.005 of the TSPA-LA model, scatterplots for *EXPDOSE* at 500,000 years: (top) YMP TSPA-LA model (SNL 2008, Figure K8.2-2 [a](b) and (bottom) TSPA-LA model test run of this study.



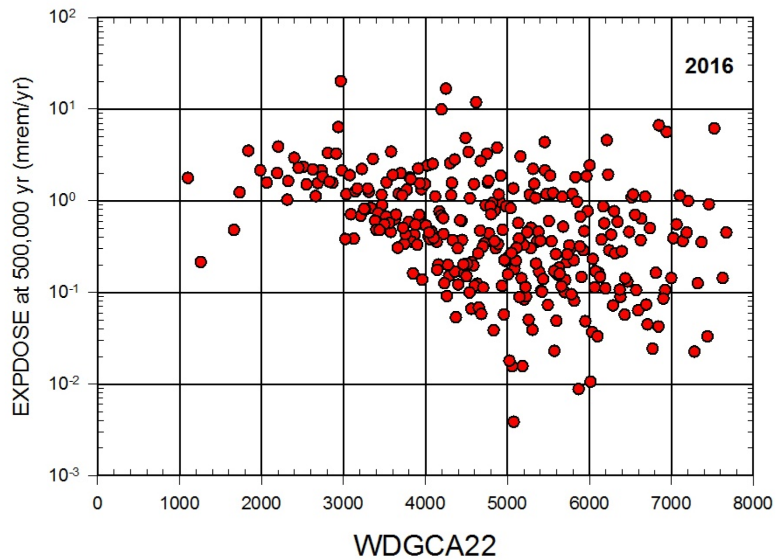
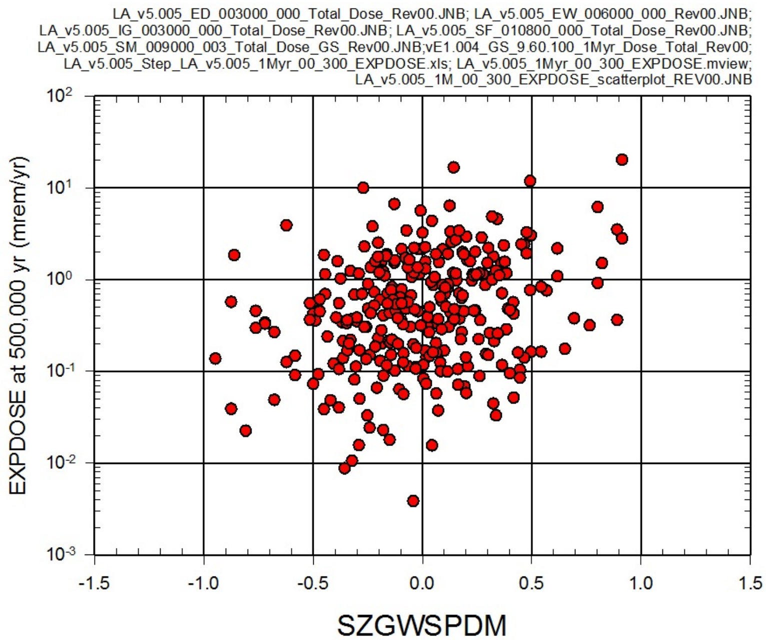


Figure 50. Comparison of model results for selected scatterplots for expected dose to RMEI (*EXPDOSE*, mrem/yr) over [0, 1,000,000 yr] for all scenario classes obtained with version 5.005 of the TSPA-LA model, scatterplots for *EXPDOSE* at 500,000 years: (top) YMP TSPA-LA model (SNL 2008, Figure K8.2-2 [a](c) and (bottom) TSPA-LA model test run of this study.



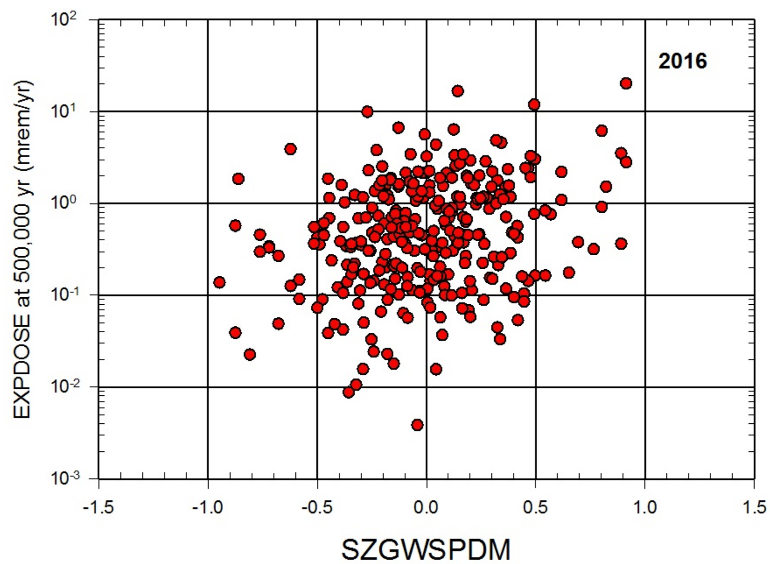
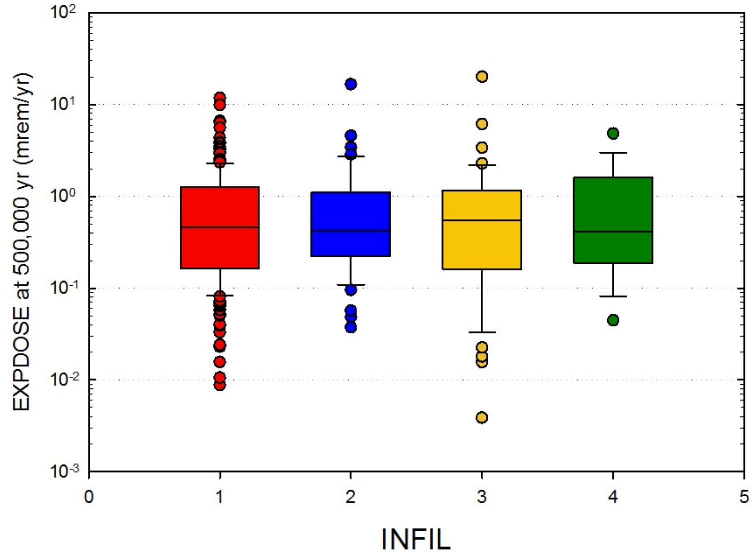


Figure 51. Comparison of model results for selected scatterplots for expected dose to RMEI (*EXPDOSE*, mrem/yr) over [0, 1,000,000 yr] for all scenario classes obtained with version 5.005 of the TSPA-LA model, scatterplots for *EXPDOSE* at 500,000 years: (top) YMP TSPA-LA model (SNL 2008, Figure K8.2-2 [a](d) and (bottom) TSPA-LA model test run of this study.



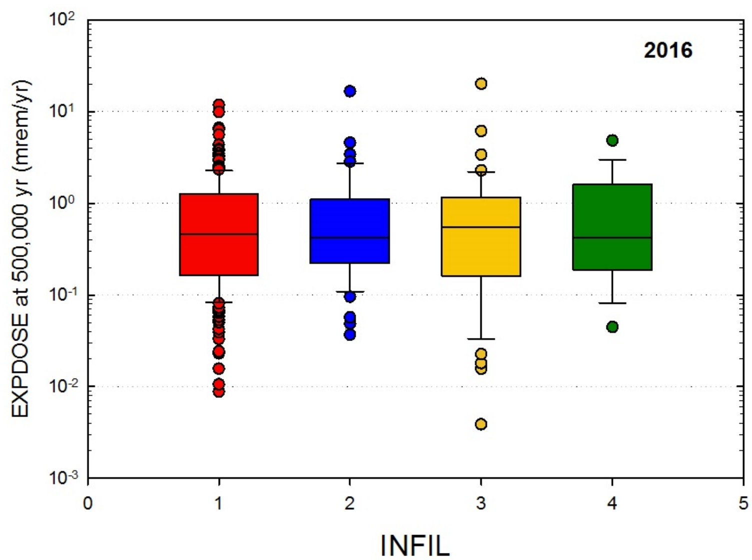


Figure 52. Comparison of model results for selected scatterplots for expected dose to RMEI (*EXPDOSE*, mrem/yr) over [0, 1,000,000 yr] for all scenario classes obtained with version 5.005 of the TSPA-LA model, scatterplots for *EXPDOSE* at 500,000 years: (top) YMP TSPA-LA model (SNL 2008, Figure K8.2-2 [a](e) and (bottom) TSPA-LA model test run of this study.

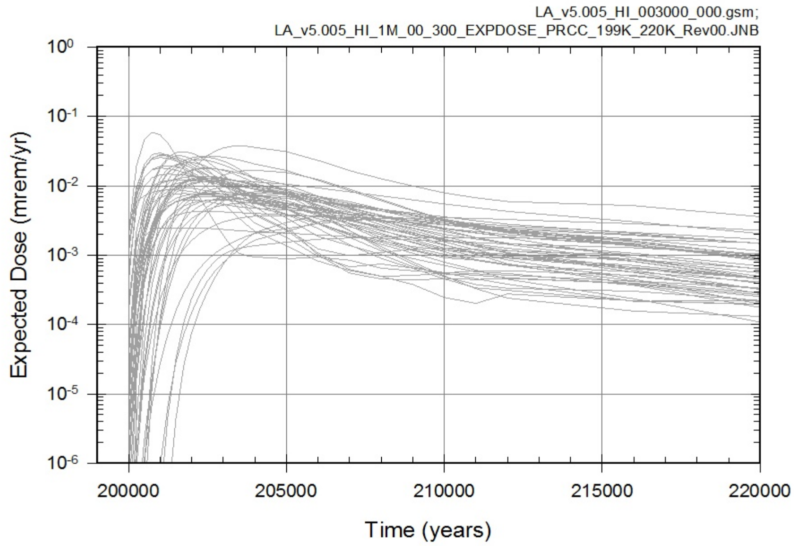
3.8. Human Intrusion Scenario

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). The human intrusion results are calculated for comparison with the human intrusion standard. The analyses for the other scenario classes are calculated for comparison with the individual protection standard.

This section looks at uncertainty and sensitivity analyses verification for human intrusion at 200, 000 years. The TSPA-LA results were presented in two sets. The first set is expected dose to the RMEI (EXPDOSE, mrem/yr) over the time period [200,00 and 220,000]. The second set is for expected dose to the RMEI (EXPDOSE, mrem/yr) over the time period [220,000 and 1,000,000]. The division was made because of the rapid changes in *EXPDOSE* that occur in the first 20,000 years after a drilling intrusion. Analyses results for the two sets are shown in Figures 53 to 68. The figures compare results of the original TSPA-LA model (SNL 2008, Figures K10-1[a] to K10-4[a]) and results of this study, for the 1,000,000 year simulation period. Results of the first set are reported in Figures 53 to 61. Figure 53 shows comparison of GoldSim results for dose to RMEI (EXPDOSE, mrem/yr) for the first 50 sample elements. Figure 54 compares PRCCs for EXPDOSE for the period 200,000 to 220,000 years resulting from human intrusion at 200,000 years. Figure 55 shows comparison of results for the stepwise rank regression analyses for EXPDOSE at 201,000, 203,000 and 205,000 years. Figures 56 to 58 show comparison of scatterplots for EXPDOSE at 201,000 years vs selected parameters. Figures 59 to 61 show comparison of scatterplots for EXPDOSE at 205,000 years vs selected parameters.

Results of the second set are reported in Figures 62 to 68. Figure 62 shows comparisons of GoldSim results for the dose to RMEI (EXPDOSE, mrem/yr) for the first 50 sample elements. Figure 63 compares PRCCs for EXPDOSE for the period 220,000 to 1,000,000 years resulting from human intrusion at 200,000 years. In this particular case the plot from this study (bottom) looks somehow different from that of the TSPA-LA (top). Two of the parameters that were considered important (SZGWSPDM and SZFISPVO) have been replaced by other parameters. This is not expected as the rest of the results conform with those of the 2008 TSPA-LA. As shown in Hadgu et al. (2015) the total dose is also about the same. This issue will be looked at more closely in FY17.

Figure 64 shows comparisons of results for the stepwise rank regression analyses for EXPDOSE at 240,000, 500,000 and 760,000 years. Figures 65 to 68 show comparisons of scatterplots for EXPDOSE at 500,000 years vs selected parameters. As shown in Figures 53 to 68 (except for Figure 63), 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.



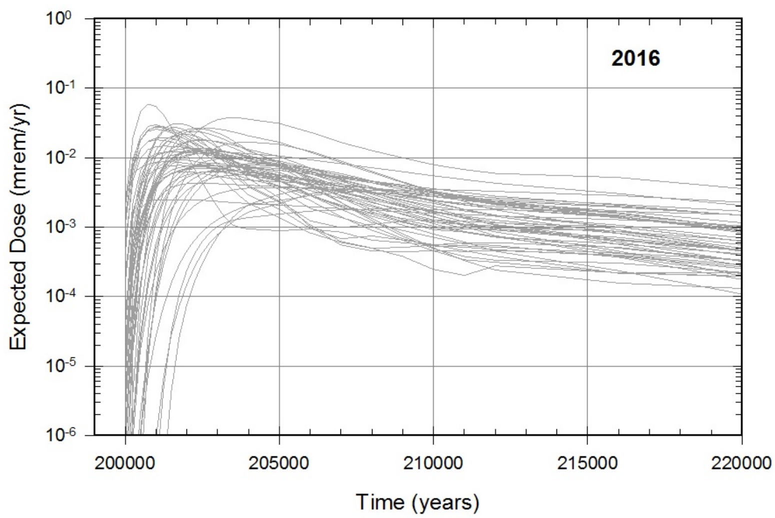
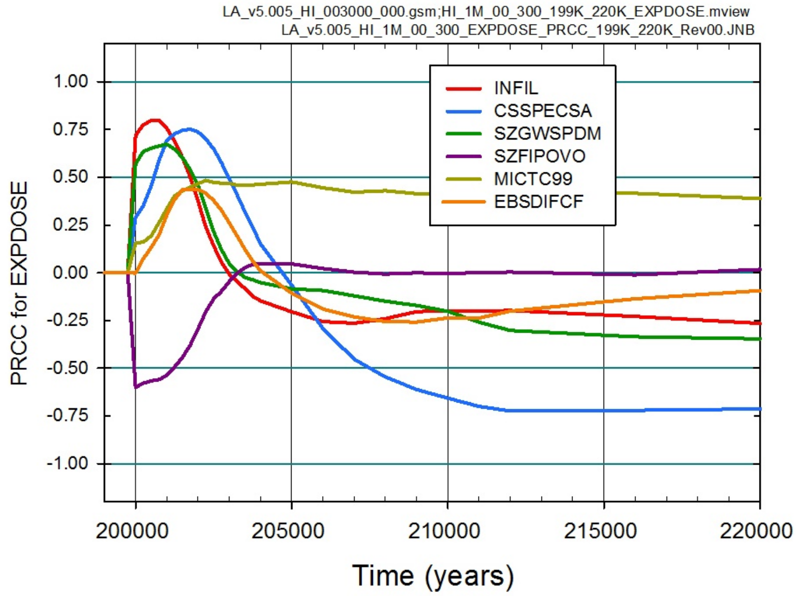


Figure 53. Comparison of model results for expected dose to RMEI (*EXPDOSE*, mrem/yr) over [200,000, 220,000 yr] resulting from human intrusion at 200,000 years obtained with version 5.005 of the TSPA-LA model, *EXPDOSE* for first 50 sample elements: (top) YMP TSPA-LA model (SNL 2008, Figure K10-1[a](b) and (bottom) TSPA-LA model test run of this study.



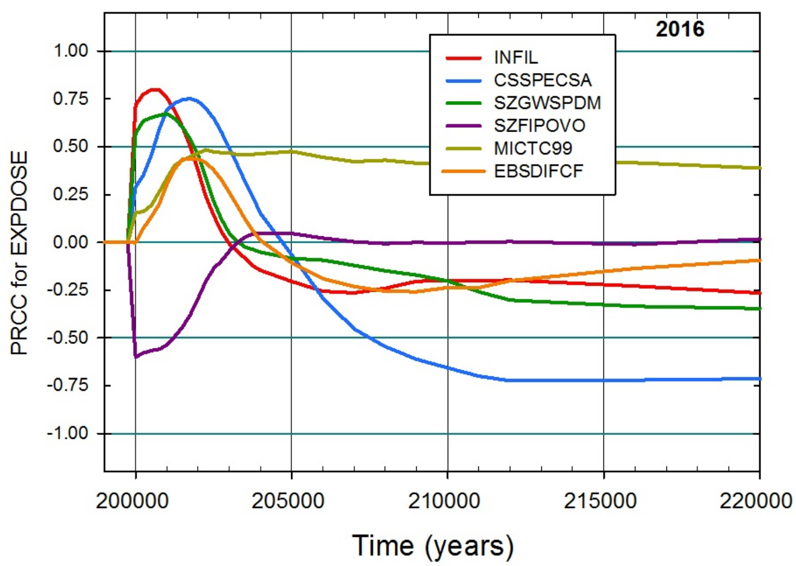
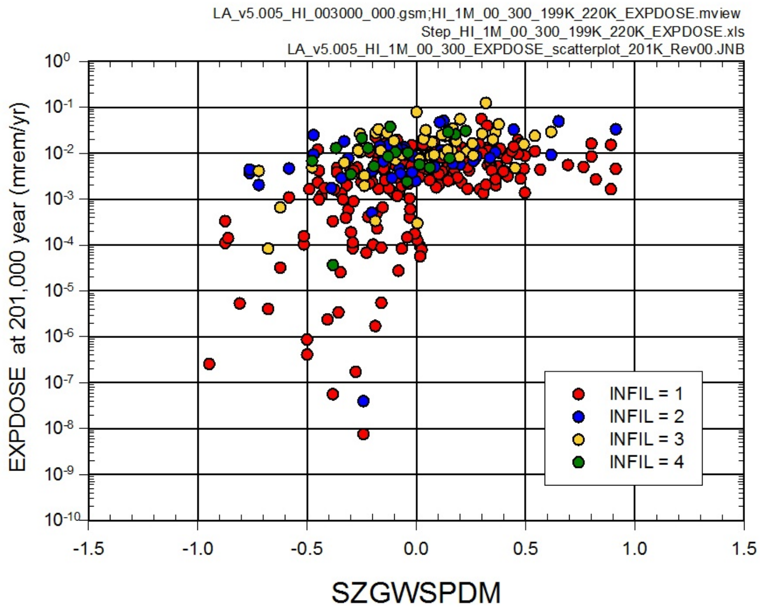


Figure 54. Comparison of model results for expected dose to RMEI (*EXPDOSE*, mrem/yr) over [200,000, 220,000 yr] resulting from human intrusion at 200,000 years obtained with version 5.005 of the TSPA-LA model, PRCCs for *EXPDOSE*: (top) YMP TSPA-LA model (SNL 2008, Figure K10-1[a](c) and (bottom) TSPA-LA model test run of this study.

	EXPDOSE: 201,000 Year			EXPDOSE: 203,000 Year			EXPDOSE: 205,000 Year		
Step	Variable	R^2	SRRC	Variable	R^2	SRRC	Variable	R^2	SRRC
1	SZGWSPDM	0.20	0.45	MICTC99	0.15	0.44	MICTC99	0.33	0.58
2	INFIL	0.40	0.48	CSSPECSA	0.33	0.44	CSNFMASS	0.38	0.22
3	CSSPECSA	0.54	0.41	SZFISPVO	0.40	0.26	INFIL	0.41	-0.18
4	SZFISPVO	0.61	0.28	SZGWSPDM	0.43	0.18			
5	SZFIPOVO	0.65	-0.20	CSNFMASS	0.47	0.19			
6	SZDIFCVO	0.68	-0.18	SZDIFCVO	0.50	-0.19			
7	MICTC99	0.70	0.14	INFIL	0.51	-0.13			
8	CSWFA4AC	0.71	0.11	CSRINDPO	0.53	-0.11			
9	PHCSS	0.72	-0.11						
10	EP1NP2O5	0.73	-0.10						
11	CSNFMASS	0.73	0.10						
12	SZPORSAL	0.74	0.09						
13	DIAMCOLL	0.75	0.08						
14									
15									
16									

	EXPDOSE: 201,000 Year			EXPDOSE: 203,000 Year			EXPDOSE: 205,000 Year		
Step	Variable	R^2	SRRC	Variable	R^2	SRRC	Variable	R^2	SRRC
1	SZGWSPDM	0.20	0.45	MICTC99	0.15	0.44	MICTC99	0.33	0.58
2	INFIL	0.40	0.48	CSSPECSA	0.33	0.44	CSNFMASS	0.38	0.22
3	CSSPECSA	0.54	0.41	SZFISPVO	0.40	0.26	INFIL	0.41	-0.18
4	SZFISPVO	0.61	0.28	SZGWSPDM	0.43	0.18			
5	SZFIPOVO	0.65	-0.20	CSNFMASS	0.47	0.19			
6	SZDIFCVO	0.68	-0.18	SZDIFCVO	0.50	-0.19			
7	MICTC99	0.70	0.14	INFIL	0.51	-0.13			
8	CSWFA4AC	0.71	0.11	CSRINDPO	0.53	-0.11			
9	PHCSS	0.72	-0.11						
10	EP1NP2O5	0.73	-0.10						
11	CSNFMASS	0.73	0.10						
12	SZPORSAL	0.74	0.09						
13	DIAMCOLL	0.75	0.08						
14									
15									
16									

Figure 55. Comparison of model results for stepwise rank regression analyses for expected dose to RMEI (*EXPDOSE*, mrem/yr) over [200,000, 220,000 yr] resulting from human intrusion at 200,00 years obtained with version 5.005 of the TSPA-LA model, regressions for *EXPDOSE* at 201,000, 203,000, and 205,000 years: (top) YMP TSPA-LA model (SNL 2008, Figure K10-2[a](a) and (bottom) TSPA-LA model test run of this study.



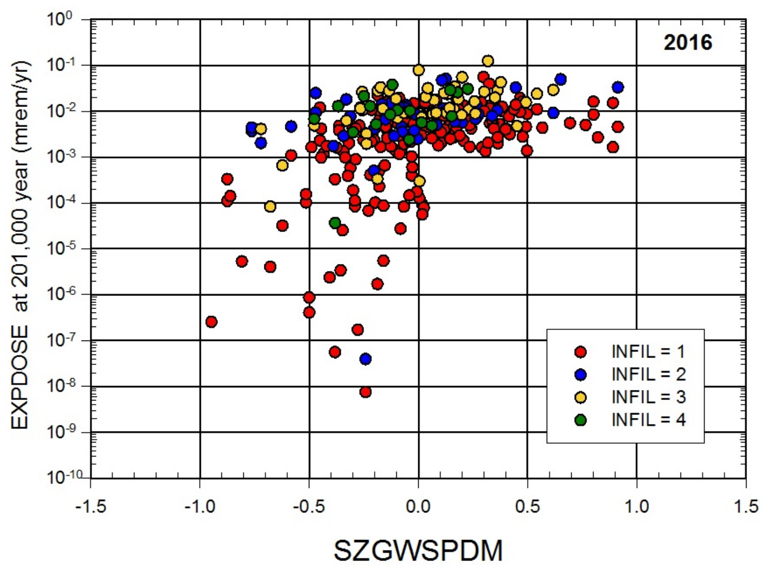
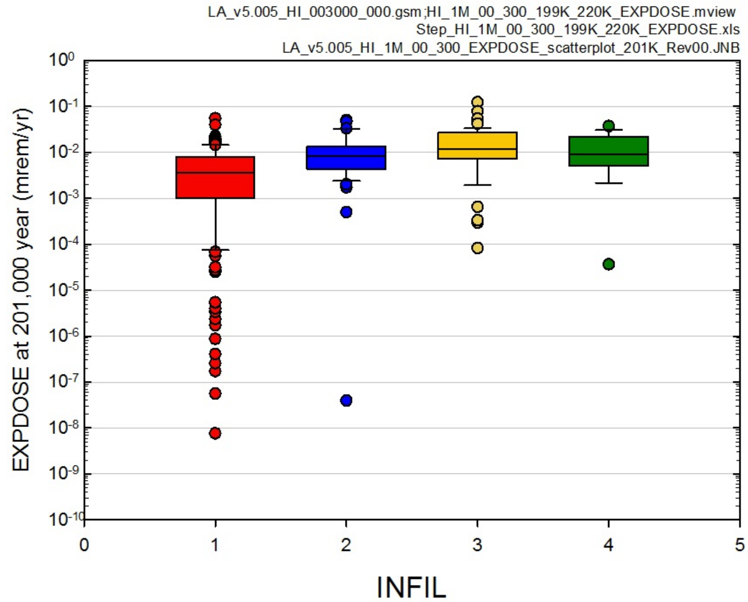


Figure 56. Comparison of model results for selected scatterplots for expected dose to RMEI (*EXPDOSE*, mrem/yr) over [200,000, 220,000 yr] resulting from human intrusion at 200,00 years obtained with version 5.005 of the TSPA-LA model, scatterplots for *EXPDOSE* at 201,000 years: (top) YMP TSPA-LA model (SNL 2008, Figure K10-2[a](b) and (bottom) TSPA-LA model test run of this study.



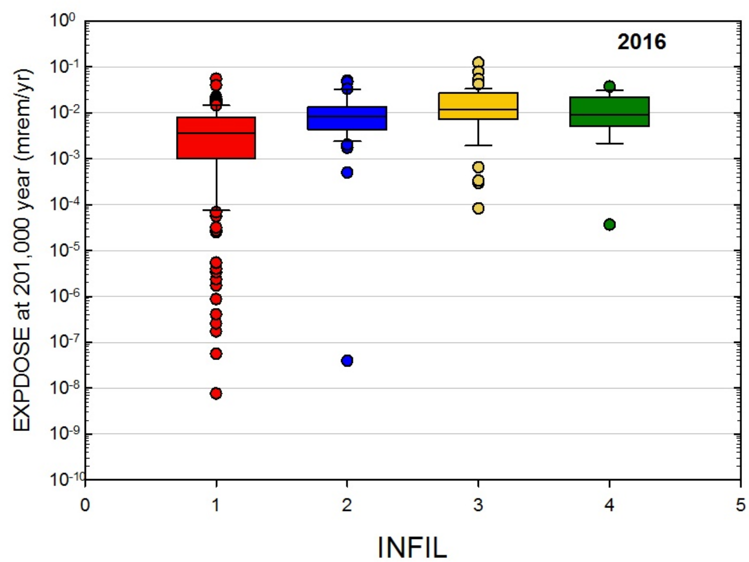


Figure 57. Comparison of model results for selected scatterplots for expected dose to RMEI (*EXPDOSE*, mrem/yr) over [200,000, 220,000 yr] resulting from human intrusion at 200,00 years obtained with version 5.005 of the TSPA-LA model, scatterplots for *EXPDOSE* at 201,000 years: (top) YMP TSPA-LA model (SNL 2008, Figure K10-2[a](c) and (bottom) TSPA-LA model test run of this study.

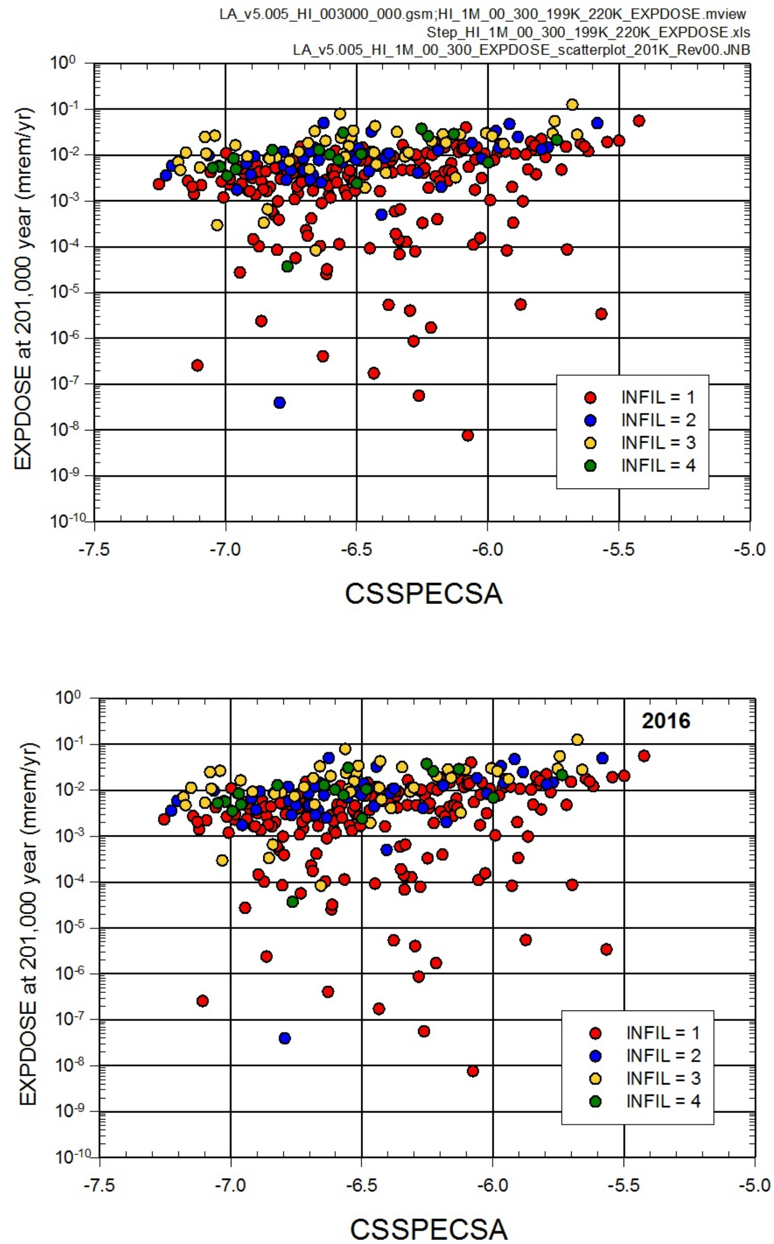
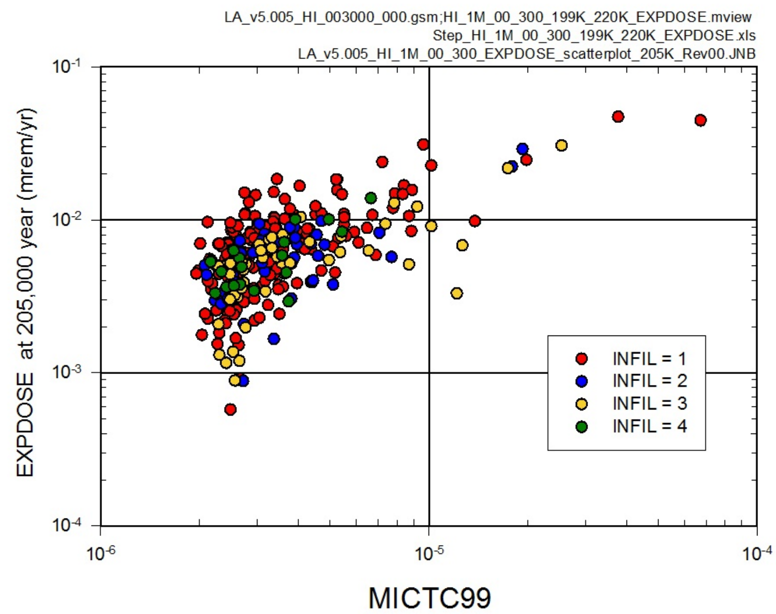


Figure 58. Comparison of model results for selected scatterplots for expected dose to RMEI (*EXPDOSE*, mrem/yr) over [200,000, 220,000 yr] resulting from human intrusion at 200,00 years obtained with version 5.005 of the TSPA-LA model, scatterplots for *EXPDOSE* at 201,000 years: (top) YMP TSPA-LA model (SNL 2008, Figure K10-2[a](d) and (bottom) TSPA-LA model test run of this study.



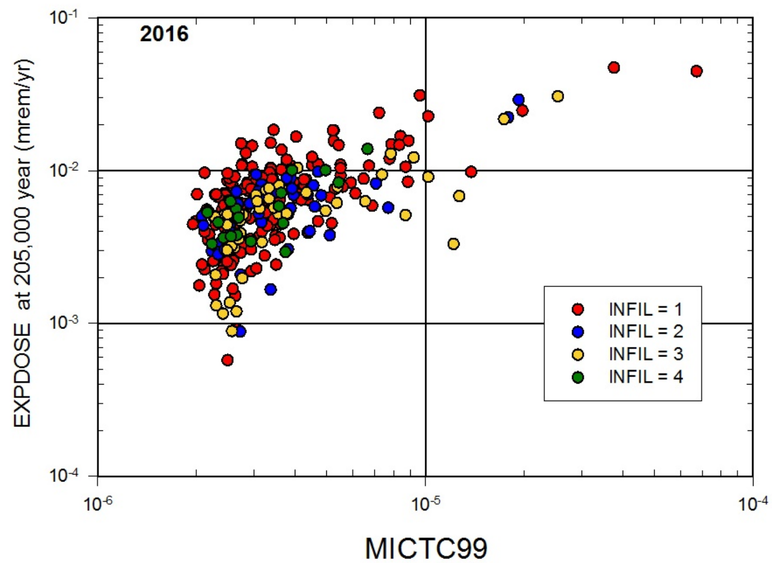
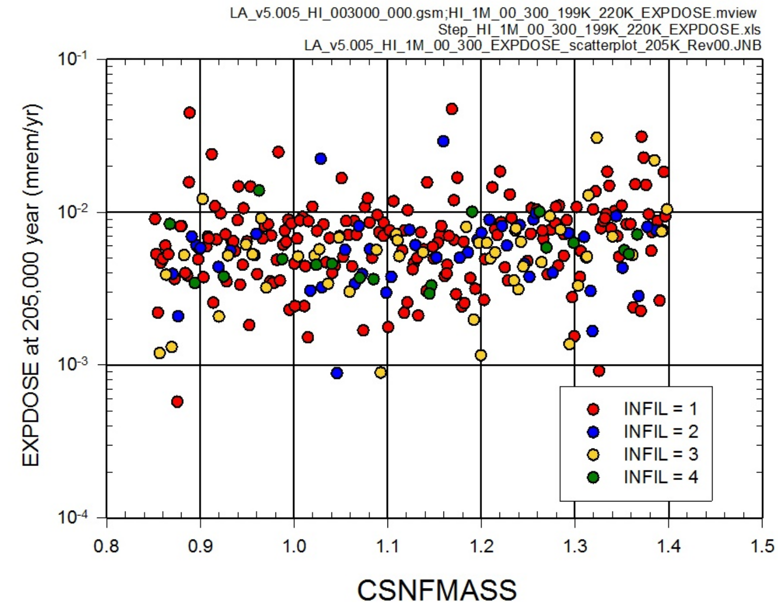


Figure 59. Comparison of model results for selected scatterplots for expected dose to RMEI (*EXPDOSE*, mrem/yr) over [200,000, 220,000 yr] resulting from human intrusion at 200,00 years obtained with version 5.005 of the TSPA-LA model, scatterplots for *EXPDOSE* at 205,000 years: (top) YMP TSPA-LA model (SNL 2008, Figure K10-2[a](e) and (bottom) TSPA-LA model test run of this study.



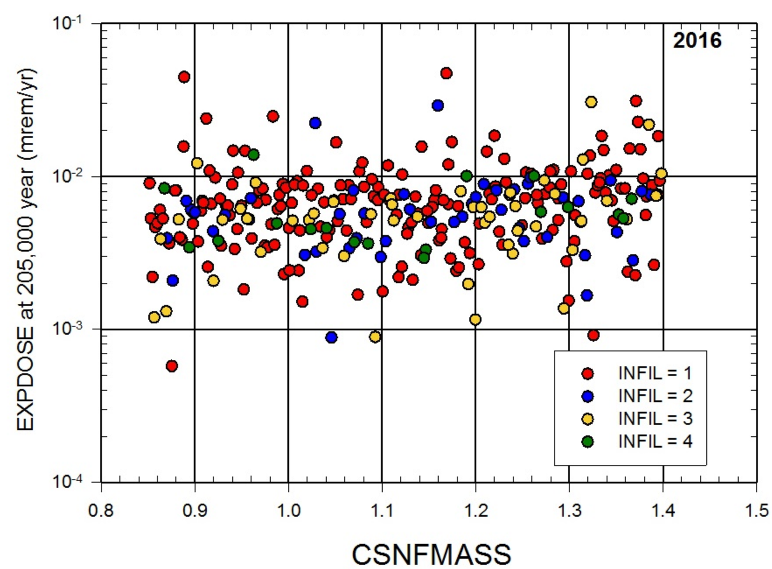
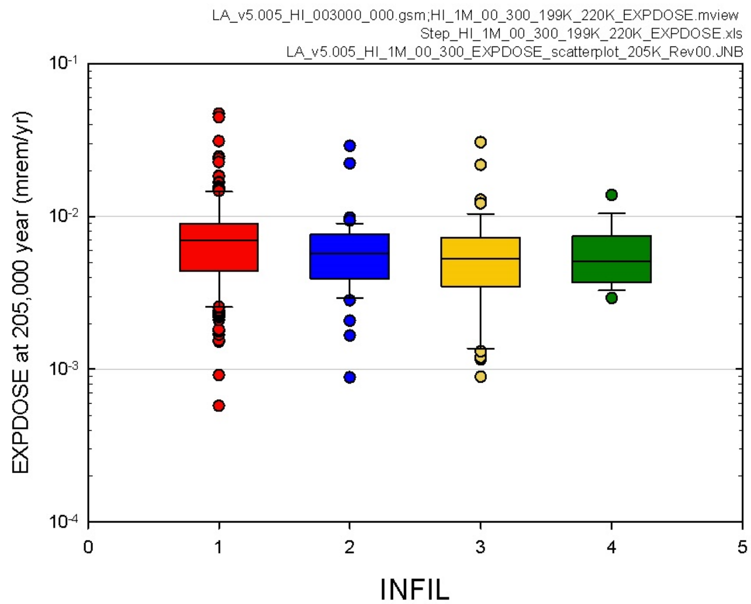


Figure 60. Comparison of model results for selected scatterplots for expected dose to RMEI (*EXPDOSE*, mrem/yr) over [200,000, 220,000 yr] resulting from human intrusion at 200,00 years obtained with version 5.005 of the TSPA-LA model, scatterplots for *EXPDOSE* at 205,000 years: (top) YMP TSPA-LA model (SNL 2008, Figure K10-2[a](f) and (bottom) TSPA-LA model test run of this study.



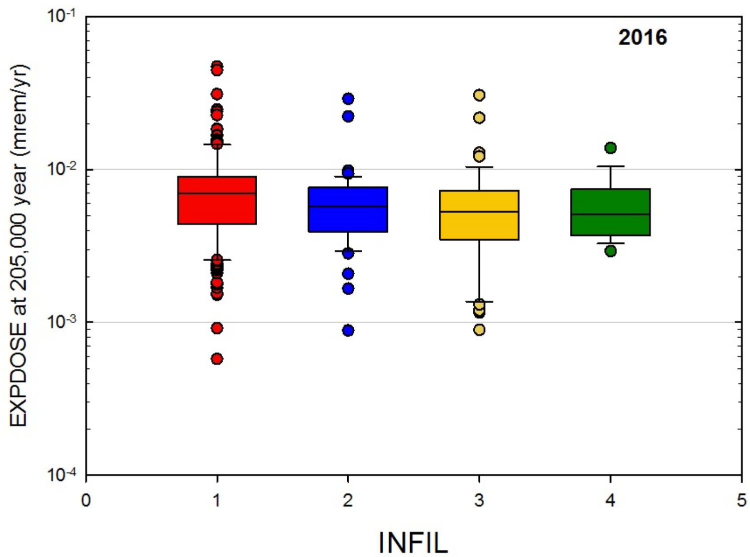
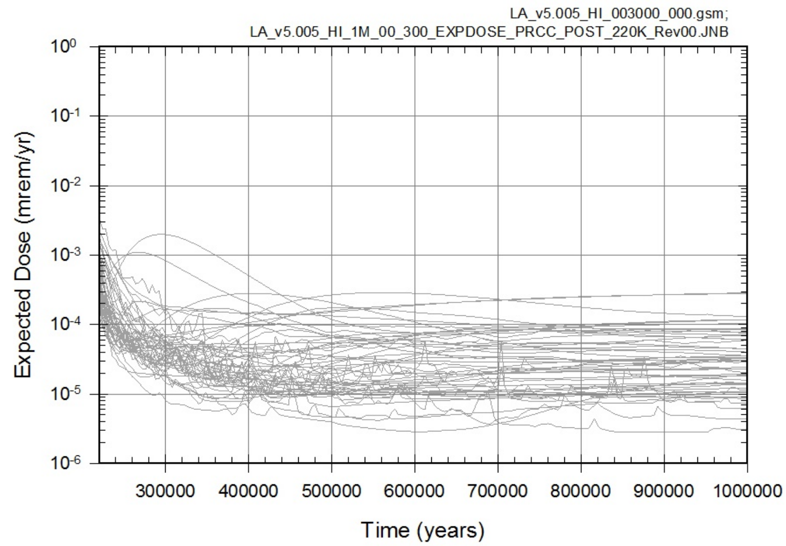


Figure 61. Comparison of model results for selected scatterplots for expected dose to RMEI (*EXPDOSE*, mrem/yr) over [200,000, 220,000 yr] resulting from human intrusion at 200,00 years obtained with version 5.005 of the TSPA-LA model, scatterplots for *EXPDOSE* at 205,000 years: (top) YMP TSPA-LA model (SNL 2008, Figure K10-2[a](g) and (bottom) TSPA-LA model test run of this study.



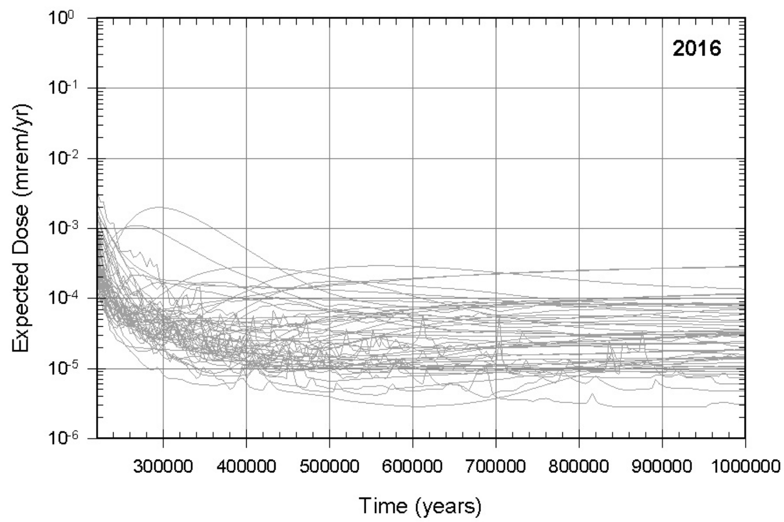
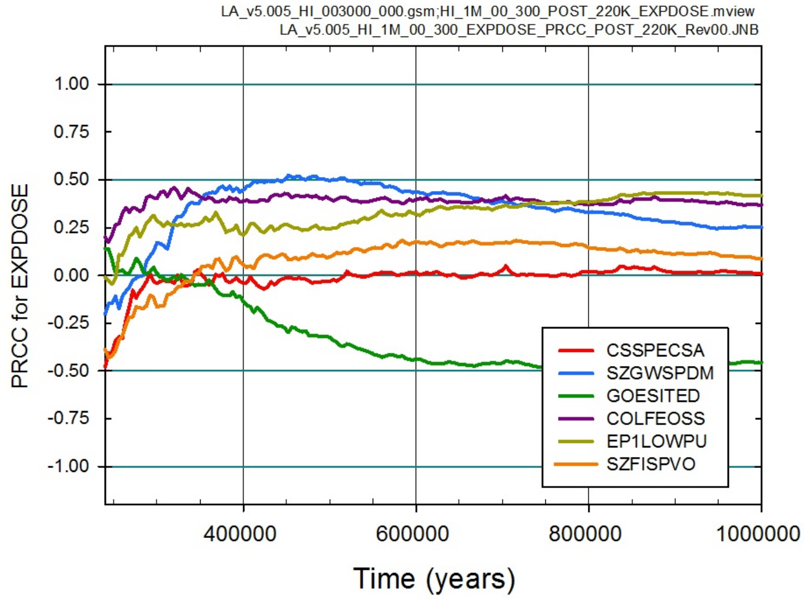


Figure 62. Comparison of model results for expected dose to RMEI (*EXPDOSE*, mrem/yr) over [220,000, 1,000,000 yr] resulting from human intrusion at 200,000 years obtained with version 5.005 of the TSPA-LA model, *EXPDOSE* for first 50 sample elements: (top) YMP TSPA-LA model (SNL 2008, Figure K10-3[a](b) and (bottom) TSPA-LA model test run of this study.



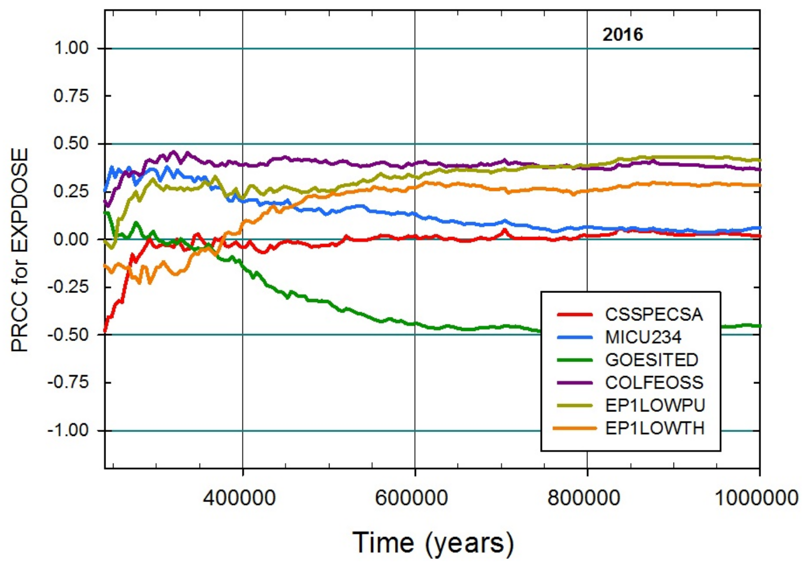
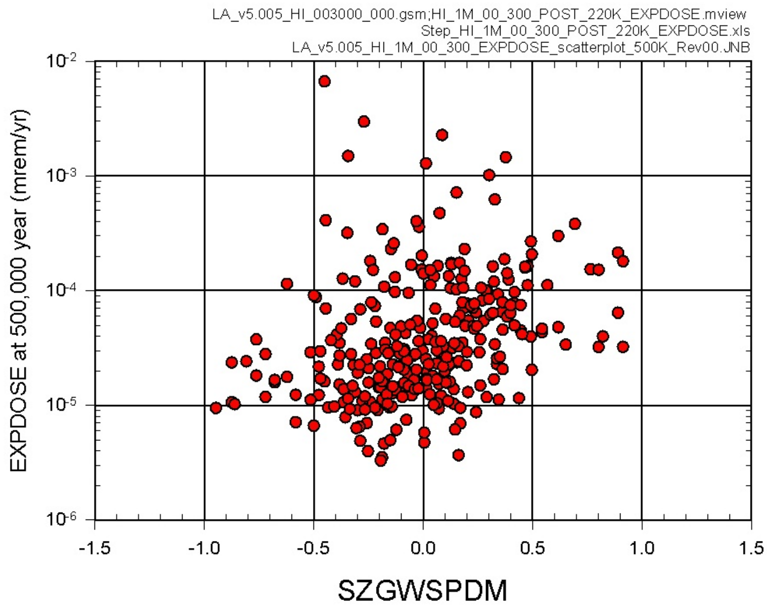


Figure 63. Comparison of model results for expected dose to RMEI (*EXPDOSE*, mrem/yr) over [220,000, 1,000,000 yr] resulting from human intrusion at 200,000 years obtained with version 5.005 of the TSPA-LA model, PRCCs for *EXPDOSE*: (top) YMP TSPA-LA model (SNL 2008, Figure K10-3[a](c) and (bottom) TSPA-LA model test run of this study.

	EXPDOSE: 240,000 yr			EXPDOSE: 500,000 yr			EXPDOSE: 760,000 yr		
Step	**Variable**	**R^2**	**SRRC**	**Variable**	**R^2**	**SRRC**	**Variable**	**R^2**	**SRRC**
1	CSSPECSA	0.20	-0.44	SZGWSPDM	0.15	0.37	GOESITED	0.10	-0.33
2	SZGWSPDM	0.29	-0.29	GOESITED	0.23	-0.27	SZGWSPDM	0.20	0.27
3	SZFISPVO	0.36	-0.34	ISCSS	0.29	-0.26	COLFEOSS	0.27	0.29
4	MICTC99	0.42	0.22	COLFEOSS	0.34	0.22	EP1LOWPU	0.34	0.23
5	SZDIFCVO	0.45	0.19	EP1LOWPU	0.39	0.22	ISCSS	0.39	-0.23
6	MICI129	0.46	0.14	HFOSA	0.43	-0.20	EP1LOWNU	0.44	0.18
7	UZKDCSDT	0.48	-0.12	EP1LOWNU	0.46	0.17	HFOSA	0.48	-0.20
8	CSNFMASS	0.49	0.12	MICCS135	0.48	0.14	MICCS135	0.51	0.17
9	ISCSS	0.50	-0.11	SZDIFCVO	0.49	-0.16	MICPU239	0.54	0.16
10				SZFISPVO	0.51	0.17	SZDIFCVO	0.55	-0.17
11				SZCOLRAL	0.53	-0.14	SZFISPVO	0.57	0.14
12				UZRCOL	0.54	0.12	HFOSITED	0.59	-0.15
13				HFOSITED	0.55	-0.11	WDGCUA22	0.60	0.12
14							SZSREG2Y	0.61	0.13
15							SZKDSRVO	0.62	-0.11
16							SZLODISP	0.63	-0.10

	EXPDOSE: 240,000 yr			EXPDOSE: 500,000 yr			EXPDOSE: 760,000 yr		
Step	**Variable**	**R^2**	**SRRC**	**Variable**	**R^2**	**SRRC**	**Variable**	**R^2**	**SRRC**
1	CSSPECSA	0.20	-0.44	SZGWSPDM	0.15	0.37	GOESITED	0.10	-0.33
2	SZGWSPDM	0.29	-0.29	GOESITED	0.23	-0.27	SZGWSPDM	0.20	0.27
3	SZFISPVO	0.36	-0.34	ISCSS	0.28	-0.26	COLFEOSS	0.27	0.29
4	MICTC99	0.42	0.22	COLFEOSS	0.34	0.22	EP1LOWPU	0.34	0.23
5	SZDIFCVO	0.45	0.19	EP1LOWPU	0.39	0.22	ISCSS	0.39	-0.23
6	MICI129	0.46	0.14	HFOSA	0.42	-0.20	EP1LOWNU	0.44	0.18
7	UZKDCSDT	0.48	-0.12	EP1LOWNU	0.46	0.17	HFOSA	0.48	-0.20
8	CSNFMASS	0.49	0.12	MICCS135	0.47	0.14	MICCS135	0.51	0.17
9	ISCSS	0.50	-0.11	SZDIFCVO	0.49	-0.17	MICPU239	0.54	0.17
10				SZFISPVO	0.51	0.17	SZDIFCVO	0.55	-0.17
11				SZCOLRAL	0.53	-0.14	SZFISPVO	0.57	0.15
12				UZRCOL	0.54	0.11	HFOSITED	0.59	-0.15
13				HFOSITED	0.55	-0.11	WDGCUA22	0.60	0.12
14							SZSREG2Y	0.61	0.13
15							SZKDSRVO	0.62	-0.11
16							SZLODISP	0.63	-0.10

Figure 64. Comparison of model results for stepwise rank regression analyses for expected dose to RMEI (*EXPDOSE*, mrem/yr) over [220,000, 1,000,000 yr] resulting from human intrusion at 200,00 years obtained with version 5.005 of the TSPA-LA model, regressions for *EXPDOSE* at 240,000, 500,000, and 760,000 years: (top) YMP TSPA-LA model (SNL 2008, Figure K10-4[a](a) and (bottom) TSPA-LA model test run of this study.



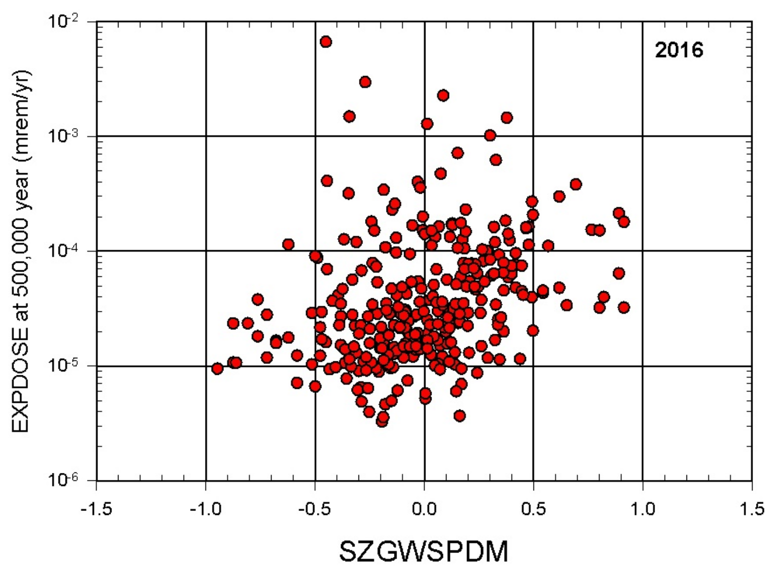
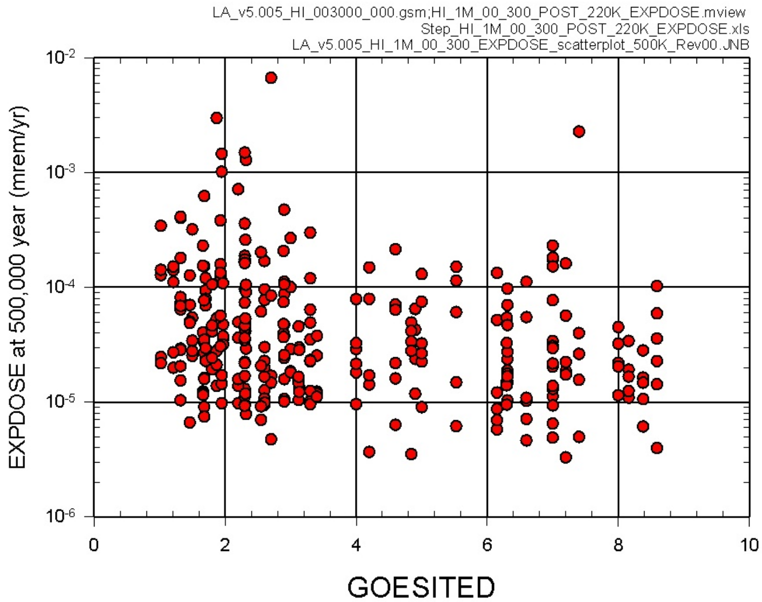


Figure 65. Comparison of model results for selected scatterplots for expected dose to RMEI (*EXPDOSE*, mrem/yr) over [220,000, 1,000,000 yr] resulting from human intrusion at 200,00 years obtained with version 5.005 of the TSPA-LA model, scatterplots for *EXPDOSE* at 500,000 years: (top) YMP TSPA-LA model (SNL 2008, Figure K10-4[a](b) and (bottom) TSPA-LA model test run of this study.



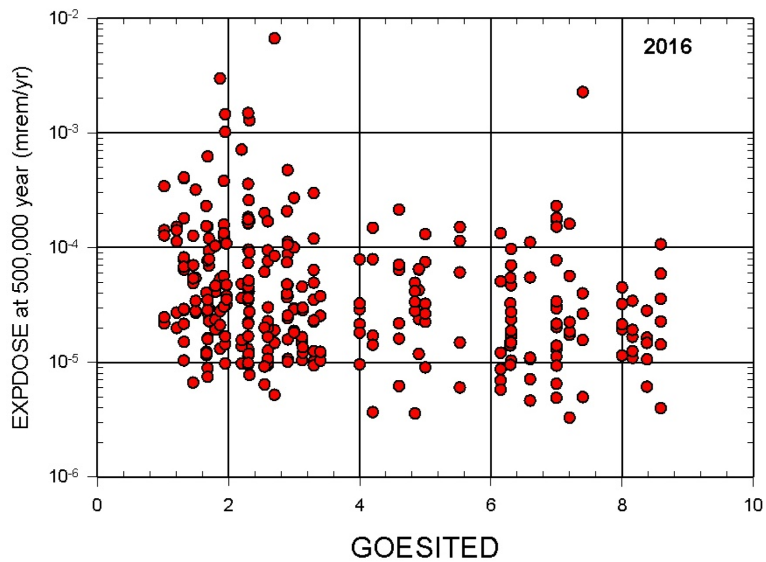
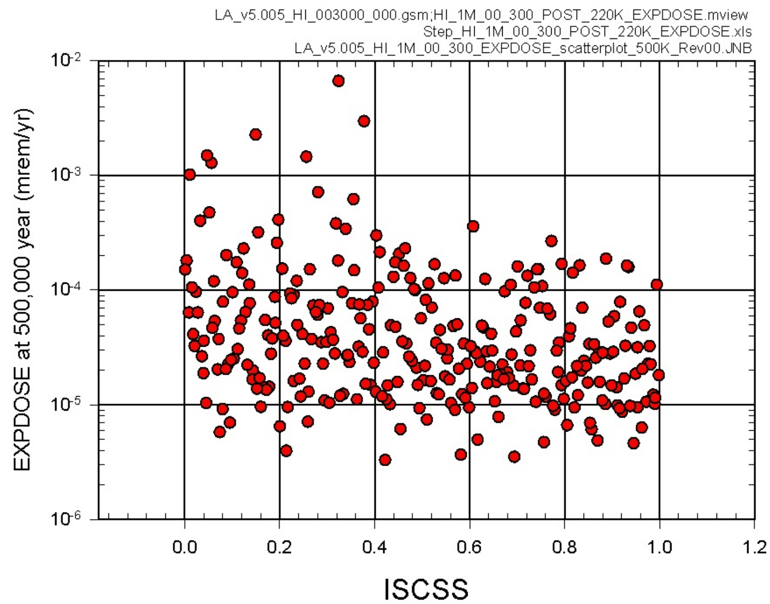


Figure 66. Comparison of model results for selected scatterplots for expected dose to RMEI (*EXPDOSE*, mrem/yr) over [220,000, 1,000,000 yr] resulting from human intrusion at 200,00 years obtained with version 5.005 of the TSPA-LA model, scatterplots for *EXPDOSE* at 500,000 years: (top) YMP TSPA-LA model (SNL 2008, Figure K10-4[a](c) and (bottom) TSPA-LA model test run of this study.



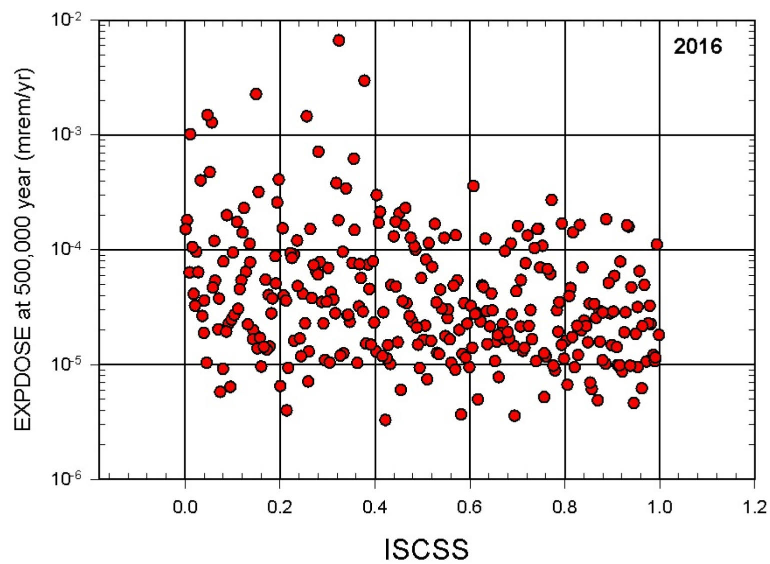


Figure 67. Comparison of model results for selected scatterplots for expected dose to RMEI (*EXPDOSE*, mrem/yr) over [220,000, 1,000,000 yr] resulting from human intrusion at 200,00 years obtained with version 5.005 of the TSPA-LA model, scatterplots for *EXPDOSE* at 500,000 years: (top) YMP TSPA-LA model (SNL 2008, Figure K10-4[a](d) and (bottom) TSPA-LA model test run of this study.

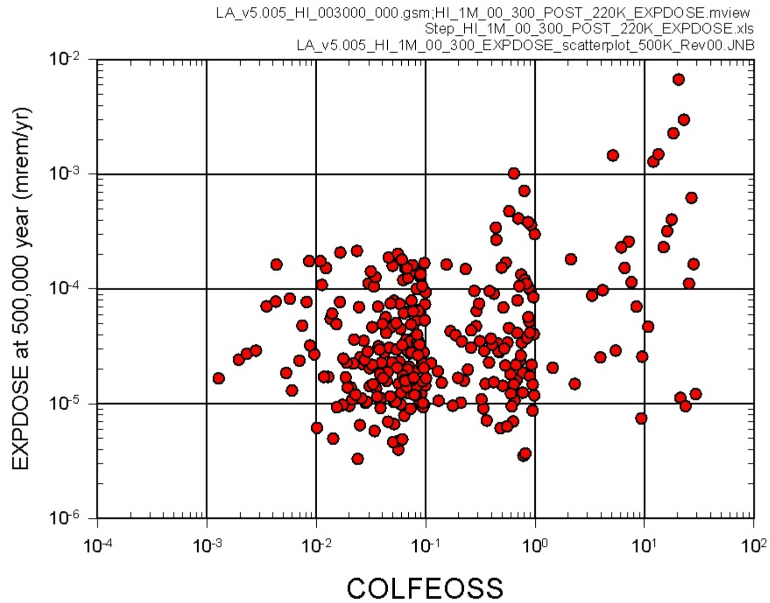


Figure 68. Comparison of model results for selected scatterplots for expected dose to RMEI (*EXPDOSE*, mrem/yr) over [220,000, 1,000,000 yr] resulting from human intrusion at 200,00 years obtained with version 5.005 of the TSPA-LA model, scatterplots for *EXPDOSE* at 500,000 years: (top) YMP TSPA-LA model (SNL 2008, Figure K10-4[a](e) and (bottom) TSPA-LA model test run of this study.

4. TSPA-LA MODEL UPGRADE

4.1. TSPA-LA model Conversion

The 2008 TSPA-LA simulations that were an integral part of the license application were based on GoldSim 9.60.300. Since then several upgrades have been made to GoldSim software to update components of the software. The latest version is GoldSim 11.1. Because of the possibility that the older version will not be supported in the near future by GoldSim as well as the WINDOWS operating system, we have started upgrading the TSPA-LA to GoldSim version 11.1.

Opening of the 2008 TSPA-LA modeling cases in GoldSim 11.1 results in a number of error messages. That indicates that changes have to be made to each of the modeling cases in order to make them operational with GoldSim 11.1. To facilitate the conversion effort, the process was started with the Nominal Modeling case. This modeling case consists of a future in which no disruptions occur and thus has no aleatory parameters. That reduces the total number of realizations for the modeling case to 300. Thus, upgrading it would be more efficient than the rest of the modeling cases which are much more complex. The model conversion effort was carried out with the support of the GoldSim Technology Group.

Because of the numerous changes in GoldSim software between Version 9.60.300 (9.60 SP3) and the version 11.1 it was decided to do the conversion in two stages. In stage 1 conversion of the Nominal Modeling case was done from Version 9.60.300 to 10.5. In stage 2 conversion was done from Version 10.5 to 11.1 Details of the conversion process have been documented by the GoldSim Technology Group and the report is included in Appendix B.

The conversion process of the Nominal Modeling case from GoldSim 9.60.300 to 11.1 required addressing the following issues:

1) <u>SubModel output interface conversions</u>: Two SubModels were flagged for conversions made to the outputs on their output interface. The conversion messages note that this version of GoldSim "*changes how simulation data are exported from SubModel elements*". The SubModels are Aleatory_Params (located in \Time_Zero) and Epistemic_Params (located in \Epistemic_Uncertainty). The conversion messages note that all outputs were converted successfully. This conversion is not expected to affect model results.

2) <u>Table log interpolation changed to linear interpolation</u>: Five Lookup Table elements were flagged because they "*used to do log interpolation on the independent variable*". As of GoldSim version 11.0, the log interpolation option is no longer available for Lookup Tables. The conversion message noted that these were converted to linear interpolation.

3) <u>Conversion of custom unit built-in SI unit</u>: One conversion message noted the "*unit cdeg is not defined*". The cdeg is a custom unit defined in the TSPA model. The conversion message presents the following question and provides 'Yes' and 'No' options: "*Did you mean the SI unit Cdeg?*" The 'Yes' option was selected.

4) Time Series Definition: The external exchange format for the Time Series data type has changed. Thus, the old DLL (TS_Proc.dll) function does not operate correctly. This DLL has now been replaced with the latest DLL (TSProc.dll).

5) Custom Resampling Logic: The resampling logic for a Stochastic element correlated to another element has been changed. In the current version these options are mutually exclusive, and thus the correlation option has been changed to "not correlated". This affected eight Stochastic elements.

6) Recording Time Series Workaround: Located in the Submodel 'EBS_Submodel' (at \Global_Inputs_and_Calcs\Global_Events\Seismic_Scenario\Model_Input_Seismic\Model_Feeds_Seismic\Aleatory_Feeds_Seismic), there is a Time Series element, 'Seismic_Event_Occurs', that generates an error when the TSPA model is run in GoldSim version 11.1.5. The error message is "No data in Time Series …". This issue was addressed by implementing a workaround described in detail in Appendix B.

7) Running with Distributive Process: Running the Nominal Modeling case on many processors results in error messages. These messages seem to be related to unavailability of certain input files when they are needed by a process.

At this time all of the error messages related to the Nominal Modeling case, except for the Distributive process case, have been addressed. Changes have been made to the modeling case to address the errors. Some of these changes have the potential to affect output results. A study of the effect of the changes on output will be needed. The following changes resulting from the conversion process could affect model results:

1) The correlation option for eight Stochastic elements was changed to 'not correlated'.
2) The log interpolation setting for five Lookup Tables was converted to linear interpolation.
3) A custom unit (cdeg) was converted to the built-in SI unit Cdeg.

The following changes from the conversion process should not affect model results:

1) A change in the external exchange format for the Time Series data type required the use of a different DLL (TSProc.dll) in place of TS_Proc.dll.
2) Outputs on the output interface of two SubModel elements were converted.

Also, the workaround implemented in the 11.1.5 version of the model is not expected to impact model results.

4.1.1. Nominal Modeling Case: Reproduction of Expected Annual Dose for 1,000,000 Years Using GoldSim 11.1

As pointed out above, the Nominal Modeling case was converted to GoldSim Version 11.1 and was run on a few processors. The output results were then used for comparison with the 2008 TSPA-LA output. EXDOC post-processing is not required for the Nominal Modeling Case because no aleatory uncertain parameters are associated with it. Figure 69 shows the model results of the distributions of expected annual dose for the Nominal Modeling Case for the 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 using GoldSim 11.1 (bottom figure). Each figure shows horsetail plots for 300 expected annual doses, capturing effect of 300 sets of sampled epistemically 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. Figure 70 shows comparison of mean expected annual dose.

The results show that there are slight differences in the horsetail plots. The difference is indicated in the mean annual dose history curves (Figures 69 and 70). Most of the differences are at early time at very low annual dose values, which is not consequential. There are also small differences at other times. Figure 69 shows that the plots for the rest of the percentiles are very close. Overall, the differences between the 2008 TSPA-LA results and the current GoldSim 11.1 results are very small. Further study will be needed to identify the causes of the differences.

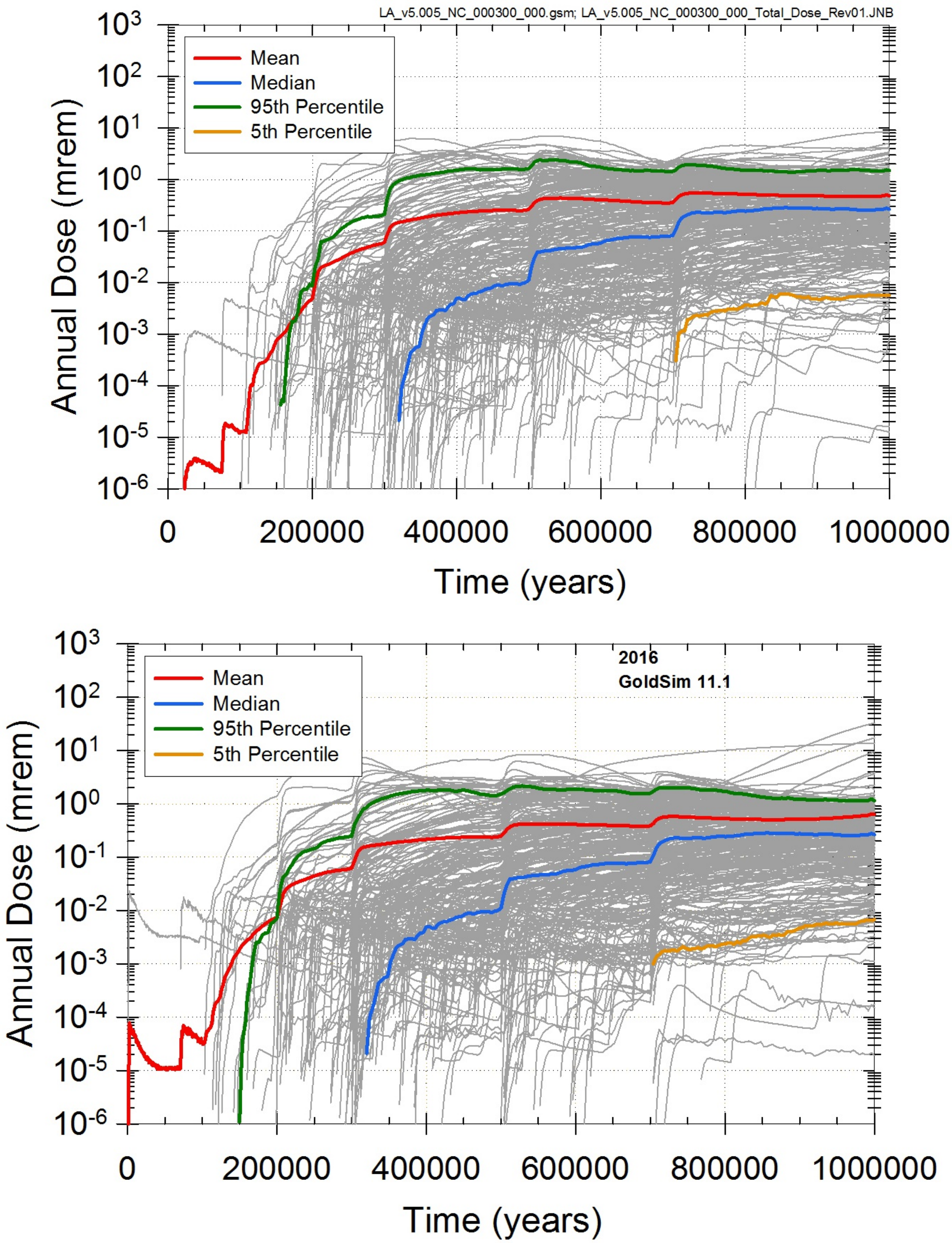


Figure 69. Comparison of Model Result for Distributions of Expected Annual Dose for the Nominal Modeling Case for 1,000,000 Years after Repository Closure: (top) TSPA-LA model (SNL 2008, Figure 8.2-1[a]), and (bottom) TSPA model test run of this study.

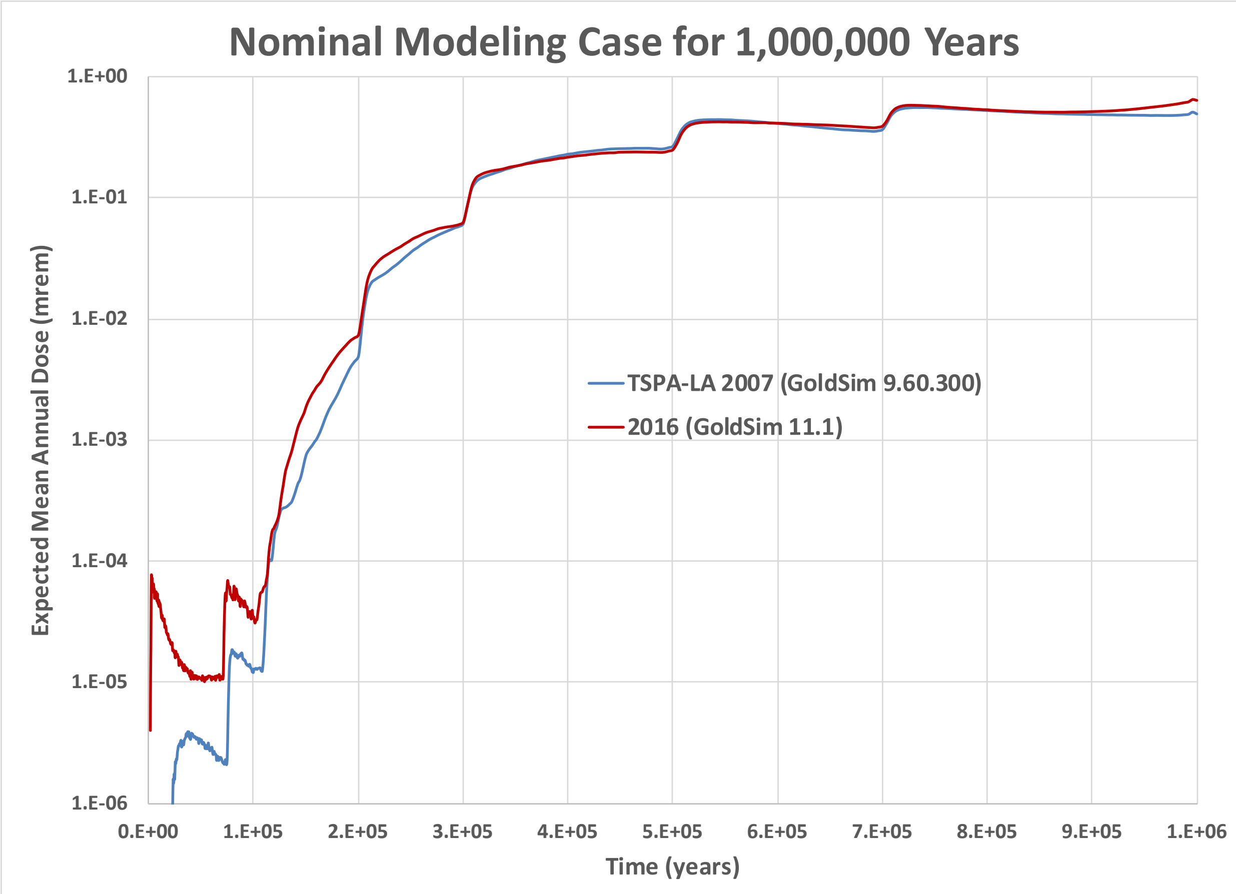


Figure 70. Comparison of Model Results for Expected Mean Annual Dose of the Nominal Modeling Case for 1,000,000 Years after Repository Closure.

4.2. Distributed Process

As described in Section 2.5 all the modeling cases are run under GoldSim distributed processing system, where simulation is done on a user specified number of processors. When running the Nominal Modeling case using GoldSim 11.1 on a few processors the 300 realization are completed without problems. However, this results in a long computation time. When the modeling case is run on a large number of processors numerous error messages are encountered. Details of the problems are documented in Appendix C. The problems seem to be related to file access issues. Solutions to these problems include making changes in an external DLL and/or changes in GoldSim. This issue will be addressed in future work.

This page is intentionally blank

5. 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 MVIEW software to reproduce the TSPA-LA uncertainty and sensitivity analyses.

The modeling analysis documented in Hadgu et al. (2015) concentrated on demonstrating the capability of the TSPA cluster to reproduce the TSPA-LA modeling cases with the use of GoldSim Version 9.60.300 and post-processing software. In thus study the TSPA-LA uncertainty and sensitivity analyses (SNL, 2008, Appendix K[a]) were reproduced based on the TSPA-LA output of GoldSim Version 9.60.300 to demonstrate system readiness. In this study conversion of the TSPA-LA model from GoldSim Version 9.60.300 to the latest version of GoldSim Version 11.1 was started. Recommendation for future work include completion of the model conversion task, verification of the TSPA-LA models using GoldSim 11.1 and associated uncertainty and sensitivity analyses.

5.1. 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.

The above steps were mainly completed in 2015 and documented in Hadgu et al. (2015). For this study an earlier version of the Seismic Ground Motion Modeling case was run as part of the verification of the uncertainty and sensitivity analyses (Section 3.5). The run was completed successfully. A GoldSim 11.1 version of the Nominal Modeling Case was also run as part of TSPA-LA upgrade (Section 4.1). This run was completed successfully on a small number of processors. Running on a larger number of processors will be conducted once issues with the distributed processing system are addressed (Section 4.2 and Appendix C).

5.2. 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. GoldSim Versions 10.5 and 11.1 were also installed on the cluster as part of TSPA-LA model upgrade to the latest version of GoldSim (Section 4).

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 maintain separation between aleatory and epistemic uncertainty in the TSPA-LA model output to enhance understanding. EXDOC also performs the final integration over both the aleatory and epistemic uncertainty to produce the final expected mean dose for comparison to the regulatory limits.

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.

5.3. 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 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 based on 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.

Page is intentionally blank

6. 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.

Hadgu, T., Appel, G., Malashev, A., and Payne, C. 2015. Reproduction of the Yucca Mountain Project TSPA-LA model Runs using TSPA Computing Systems, SAND2015-7834.

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.

Page is intentionally blank

Appendix A. Uncertainty and Sensitivity Analyses of the Seismic Fault Displacement and Seismic Ground Motion Modeling Cases

A-1. Seismic Fault Displacement Modeling Case

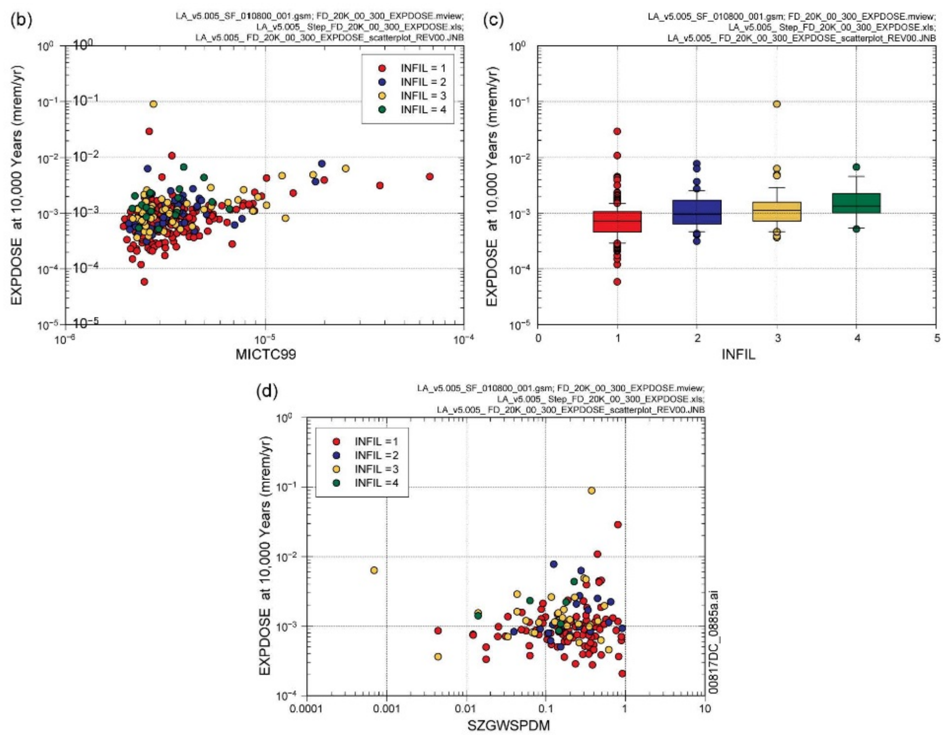
Expected Doses to RMEI for 20,000 and 1,000,000 years (Seismic Fault Displacement) MDL-WIS-PA-000005 REV 00 ADD 01 Figure K7.8.1-2[a] and Figure K7.8.2-2[a]:

Results Tables (a) on these pages appear correct. Results Plots (b), (c), and (d) for 20K yr case are repeated on 1,000,000 yr. This appears to be simply a matter of having pasted the incorrect Plots (b), (c), and (d) on 1,000,000 yr Figure K7.8.2-2[a]. The DTNs have correct figures. 2016 results match the correct figures in the DTN.

- The errors were fixed in ERD 02 - see entry for CR 11885, and associated replacement figure K7.8.2-2[a]
- SAR – Does not seem these figures are in the SAR Section 2.4.

(a)

	3,000 years			5,000 years			10,000 years		
Step[a]	Variable[b]	R^{2c}	SRRC[d]	Variable	R^2	SRRC	Variable	R^2	SRRC
1	INFIL	0.18	0.45	INFIL	0.19	0.44	MICTC99	0.15	0.36
2	MICTC99	0.31	0.32	MICTC99	0.32	0.34	INFIL	0.27	0.35
3	SZGWSPDM	0.40	0.31	SEEPPRM	0.42	-0.31	SZGWSPDM	0.37	0.33
4	SEEPPRM	0.49	-0.29	SZGWSPDM	0.49	0.29	DTDRHUNC	0.45	0.26
5	SEEPUNC	0.57	0.30	SEEPUNC	0.57	0.31	SEEPPRM	0.49	-0.16
6	CSSPECSA	0.62	0.22	CSSPECSA	0.62	0.21	SZCOLRAL	0.52	-0.19
7	SZFISPVO	0.66	0.22	SZFISPVO	0.65	0.18	SZFISPVO	0.55	0.18
8	CSNFMASS	0.68	0.15	ALPHAL	0.67	-0.16	SZFIPOVO	0.56	-0.14
9	MICC14	0.69	0.14	CSNFMASS	0.68	0.18	CSNFMASS	0.58	0.13
10	SZDIFCVO	0.71	-0.14	MICC14	0.70	0.12	SZDIFCVO	0.59	-0.13
11	ALPHAL	0.73	-0.14	SZCOLRAL	0.71	-0.14	MICAM243	0.61	0.13
12	MICSE79	0.74	0.09	SZFIPOVO	0.72	-0.12	CSSPECSA	0.62	0.13
13	SZFIPOVO	0.74	-0.10	SZCOLRVO	0.73	-0.12	CSWFA4AC	0.63	0.12
14	SZCOLRVO	0.75	-0.08	MICSN126	0.74	0.10	KDUSMEC	0.64	0.11
15	THERMCON	0.76	-0.08	SZDIFCVO	0.75	-0.10			
16				CSWFA4AC	0.76	0.09			



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

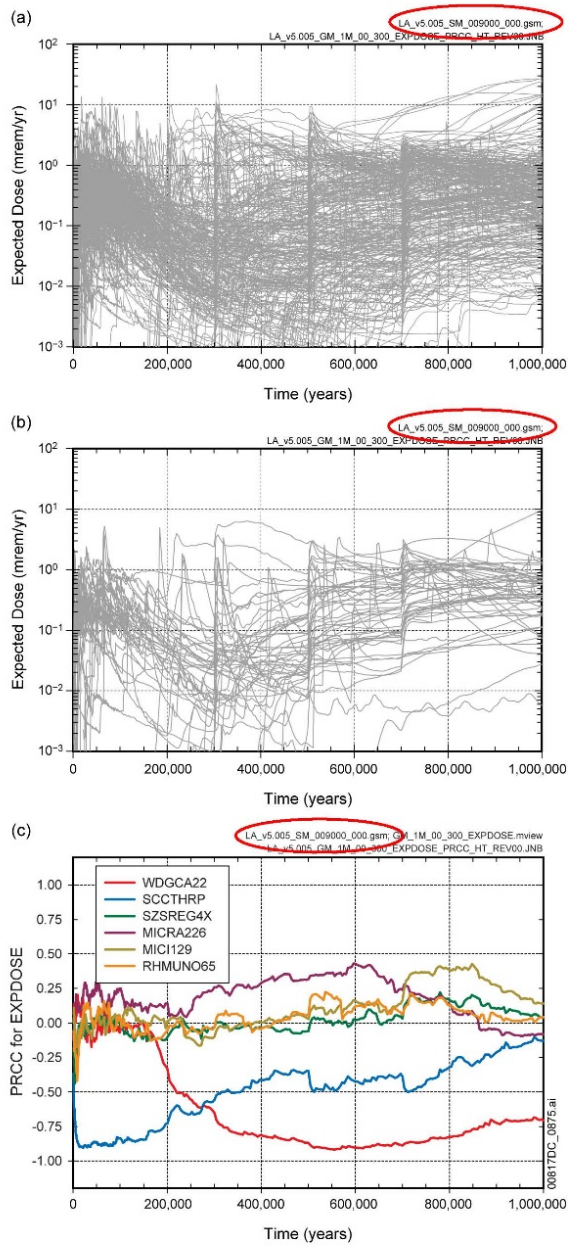
NOTE: In (c), the box extends from 0.25 to 0.75 quantile; lower and upper bar and whisker extend to 0.1 and 0.9 quantile, respectively; dots represent values outside 0.1 to 0.9 quantile range; median indicated by light horizontal line.

Figure K7.8.1-2[a]. Stepwise rank regression analyses and selected scatterplots for expected dose to RMEI (*EXPDOSE*, mrem/yr) over [0, 20,000 yr] for all radioactive species resulting from seismic fault displacement: (a) regressions for *EXPDOSE* at 3,000, 5,000, and 10,000 years, and (b,c,d) scatterplots for *EXPDOSE* at 10,000 years

A-2. Seismic Ground Motion Modeling case

MDL-WIS-PA-000005 REV 00 ADD 01 Figure K7.7.2-1[a] and Figure K7.7.2-2[a]. Results Plots on these pages appear derived from earlier Seismic Ground Motion (SGM) model version. SGM model version LA_v5.005_SM-009000_000 vs. LA_v5.005_SM-009000_003. It appears earlier version of SGM used in TSPA-LA for Sensitivity and Uncertainty Analysis. 2016 results confirm use of outdated SGM and indicate very small effect on TSPA results. TSPA Figure 8.2-11[a] graph b, presents 'Distributions of Expected Annual Dose for the Seismic Ground Motion Modeling Case (b) 1,000,000 Years after Repository Closure (the same as Figure K7.7.2-1[a]). However, it is labeled as using LA_v5.005_SM-009000_003.

- Figure K7.7.2-1[a] does not appear in ERDs. This indicates that the discrepancy was not addressed in ERDs.
- These figures are in the SAR:
    - SAR Figure 2.4-150 is TSPA Figure K7.7.2-1[a] . SAR Figure 2.4-151 is TSPA Figure K7.7.2-2[a]



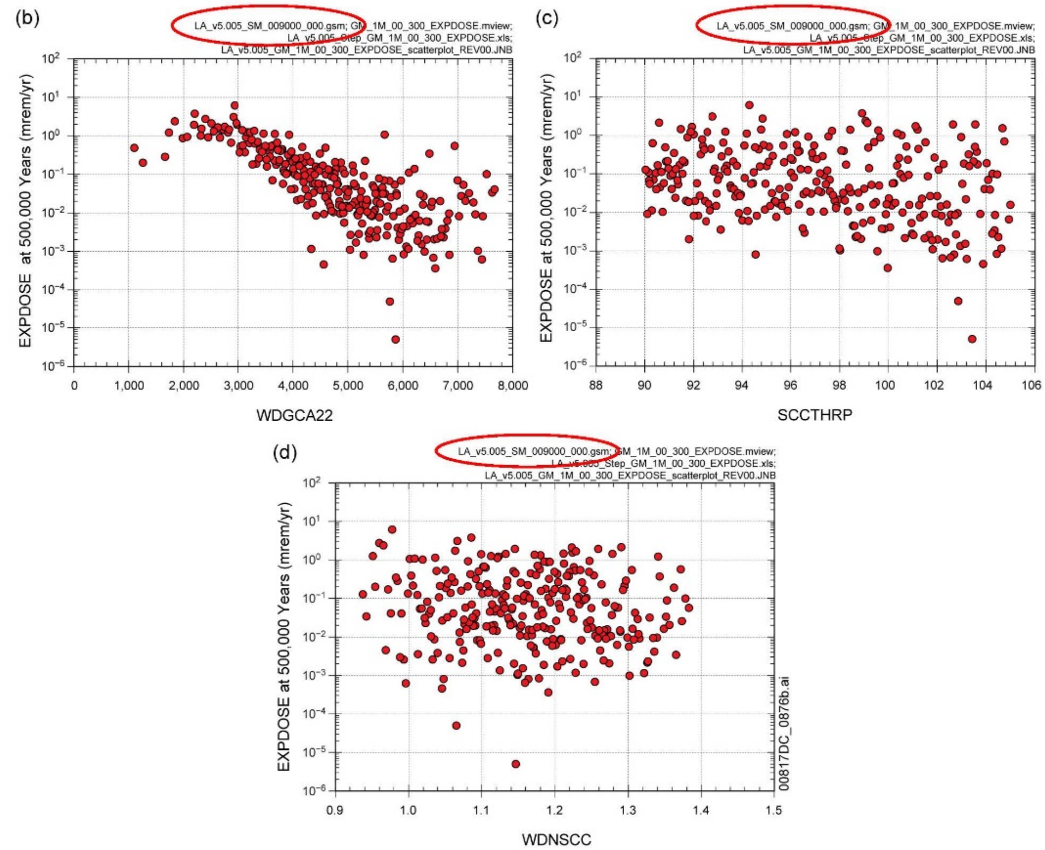
Source: Output DTNs: MO0710ADTSPAWO.000 [DIRS 183752]; and MO0710PLOTSFIG.000 [DIRS 185207].

Figure K7.7.2-1[a]. Expected dose to RMEI (*EXPDOSE*, mrem/yr) over [0, 1,000,000 yr] for all radioactive species resulting from seismic ground motion obtained with version 5.005 of the TSPA-LA Model: (a) *EXPDOSE* for all (i.e., 300) sample elements, (b) *EXPDOSE* for first 50 sample elements, and (c) PRCCs for *EXPDOSE*

(a)

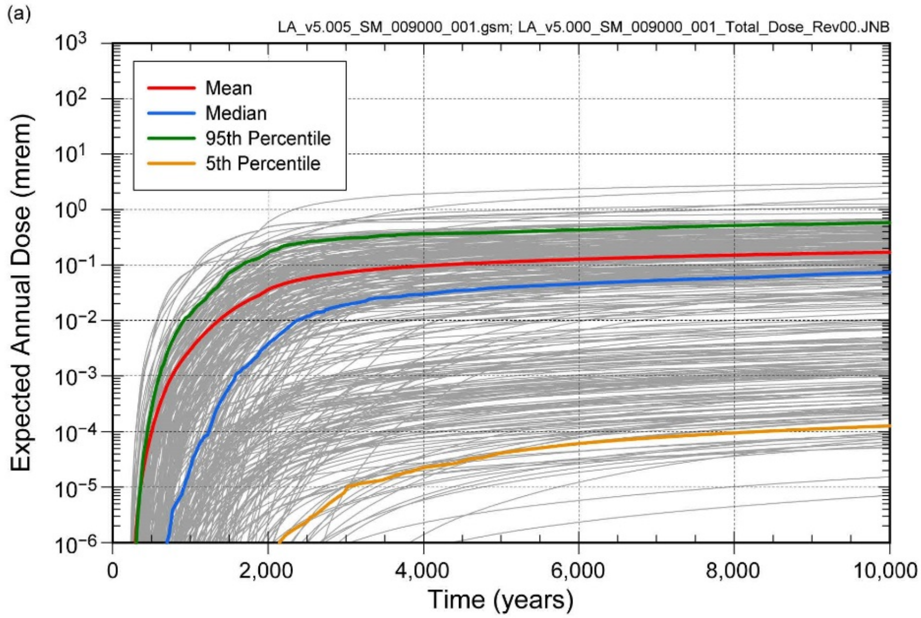
	50,000 Years			200,000 Years			500,000 Years		
Step[a]	Variable[b]	R^2 [c]	SRRC[d]	Variable	R^2	SRRC	Variable	R^2	SRRC
1	SCCTHRP	0.71	−0.85	SCCTHRP	0.54	−0.72	WDGCA22	0.62	−0.77
2	MICTC99	0.72	0.09	WDDSGC29	0.58	−0.18	SCCTHRP	0.71	−0.28
3	HLWDRACD	0.73	0.10	WDGCA22	0.60	−0.14	WDNSCC	0.72	−0.12
4	DSNFMASS	0.74	0.11	DSNFMASS	0.61	0.11	SZPORSAL	0.73	0.08
5	SZLODISP	0.75	−0.10	CSNFMASS	0.62	0.10	SZGWSPDM	0.73	0.11
6	SZKDSEVO	0.76	−0.09				SZCONCOL	0.74	0.09
7	CPUPERCS	0.77	0.09				EP1LOWNU	0.75	0.10
8							UZFAG4	0.76	−0.08

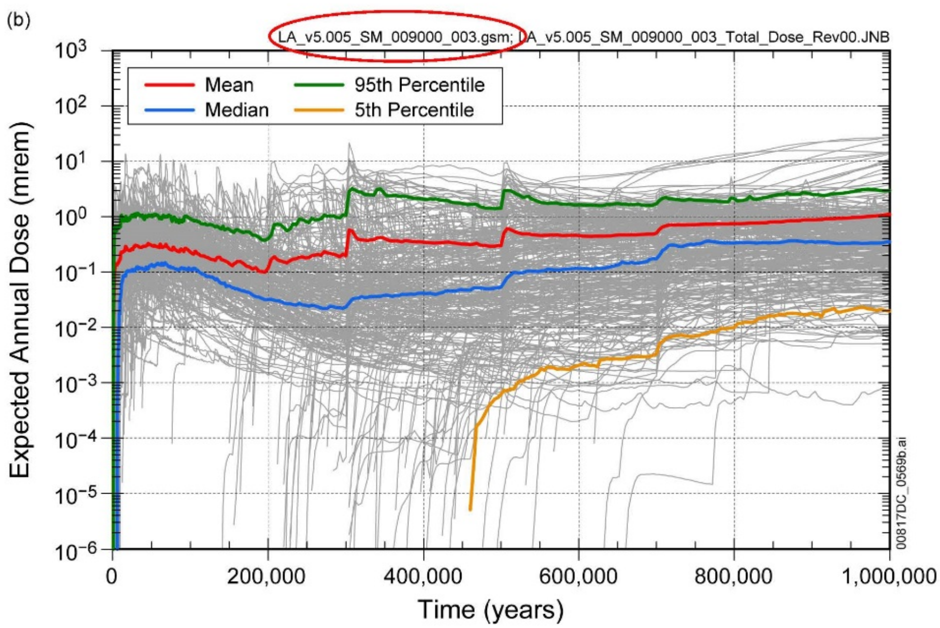
a: Steps in stepwise rank regression analysis
b: Variables listed in order of selection in stepwise regression
c: Cumulative R^2 value with entry of each variable into regression model
d: Standardized rank regression coefficients (SRRCs) in final regression model



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

Figure K7.7.2-2[a]. Stepwise rank regression analyses and selected scatterplots for expected dose to RMEI (*EXPDOSE*, mrem/yr) over [0, 1,000,000 yr] for all radioactive species resulting from seismic ground motion obtained with version 5.005 of the TSPA-LA Model: (a) regressions for *EXPDOSE* at 50,000, 200,000, and 500,000 years, and (b,c,d) scatterplots for *EXPDOSE* at 500,000 years





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

Figure 8.2-11[a]. Distributions of Expected Annual Dose for the Seismic Ground Motion Modeling Case for (a) 10,000 Years and (b) 1,000,000 Years after Repository Closure

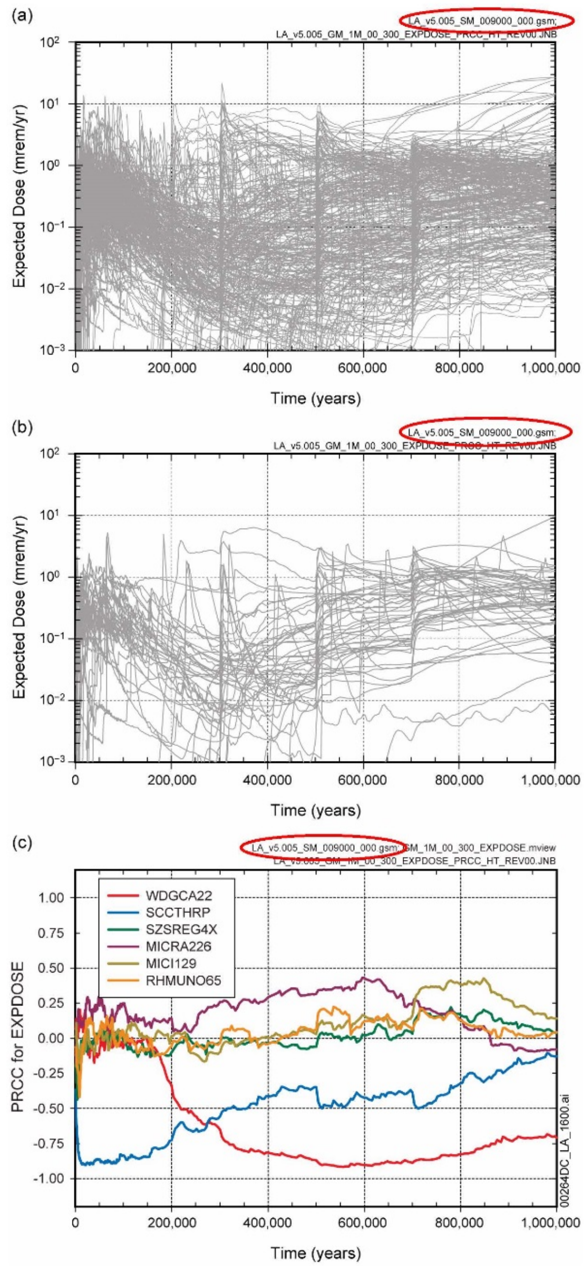


Figure 2.4-150. Expected Dose to RMEI (*EXPDOSE*, mrem/yr) over [0, 1,000,000 Year] for All Radioactive Species for the Seismic Ground Motion Modeling Case: (a) *EXPDOSE* for All (i.e., 300) Sample Elements, (b) *EXPDOSE* for First 50 Sample Elements, and (c) Partial Rank Correlation Coefficients for *EXPDOSE*

Source: SNL 2008a, Appendix K, Figure K7.7.2-1[a].

(a)

	50,000 Years			200,000 Years			500,000 Years		
Step[a]	Variable[b]	R^2 [c]	SRRC[d]	Variable	R^2	SRRC	Variable	R^2	SRRC
1	SCCTHRP	0.71	−0.85	SCCTHRP	0.54	−0.72	WDGCA22	0.62	−0.77
2	MICTC99	0.72	0.09	WDDSGC29	0.58	−0.18	SCCTHRP	0.71	−0.28
3	HLWDRACD	0.73	0.10	WDGCA22	0.60	−0.14	WDNSCC	0.72	−0.12
4	DSNFMASS	0.74	0.11	DSNFMASS	0.61	0.11	SZPORSAL	0.73	0.08
5	SZLODISP	0.75	−0.10	CSNFMASS	0.62	0.10	SZGWSPDM	0.73	0.11
6	SZKDSEVO	0.76	−0.09				SZCONCOL	0.74	0.09
7	CPUPERCS	0.77	0.09				EP1LOWNU	0.75	0.10
8							UZFAG4	0.76	−0.08

a: Steps in stepwise rank regression analysis
b: Variables listed in order of selection in stepwise regression
c: Cumulative R^2 value with entry of each variable into regression model
d: Standardized rank regression coefficients (SRRCs) in final regression model

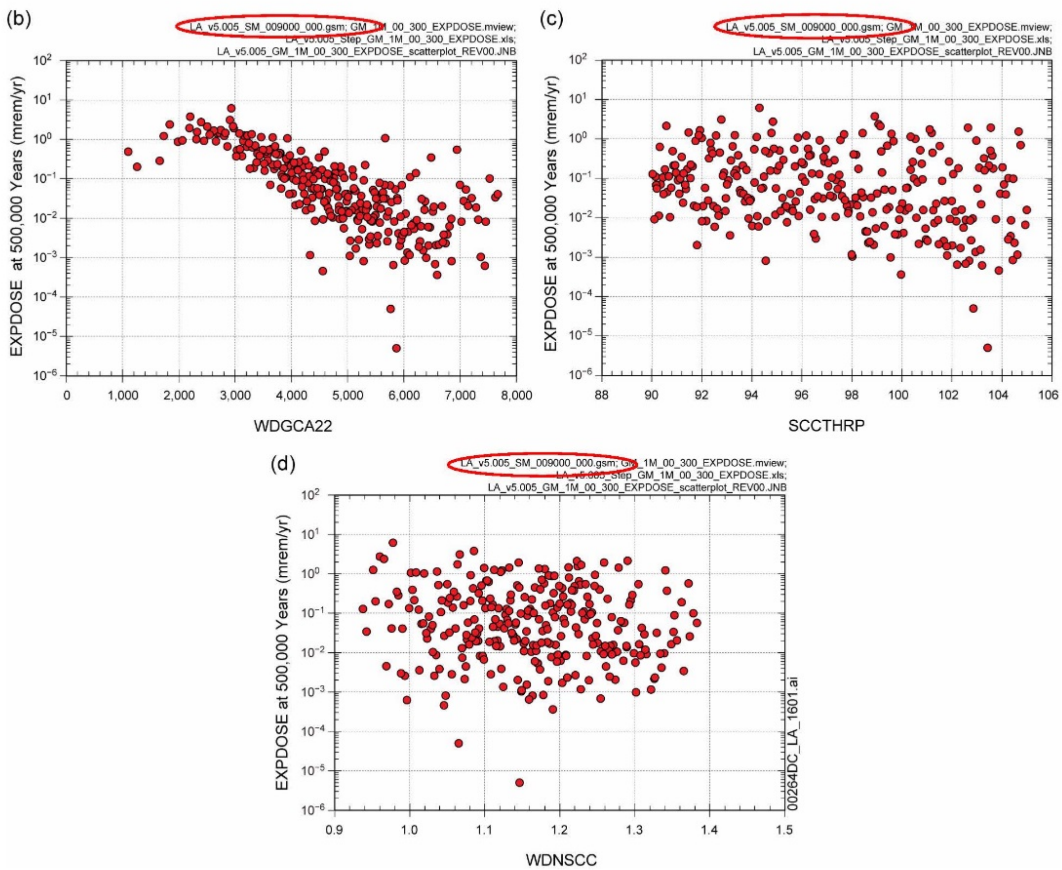


Figure 2.4-151. Stepwise Rank Regression Analyses and Selected Scatterplots for Expected Dose to RMEI (*EXPDOSE*, mrem/yr) over [0, 1,000,000 Year] for All Radioactive Species for the Seismic Ground Motion Modeling Case: (a) Regressions for *EXPDOSE* at 50,000, 200,000, and 500,000 Years, and (b,c,d) Scatterplots for *EXPDOSE* at 500,000 Years

Source: SNL 2008a, Appendix K, Figure K7.7.2-2[a].

Appendix B. Goldsim Technology Group Report on Nominal Modeling Case Conversion

TSPA Model Conversion

GoldSim Technology Group

Ryan Roper
22 September 2016

Note: document date innaccurate - Document received as a Word file attached to an email dated 7/13/2016 with automatic date field enabled.

Contents

Overview of the TSPA Model Conversion

A zip file, *Nominal_Modeling_Case.zip*, was provided by Sandia National Labs to GoldSim Technology Group which contained a GoldSim 9.60 SP3 version of the Total System Performance Assessment (TSPA) model and supporting files (including .dll, .dat, .txt, .ou and other files) needed to run the model. The original GoldSim model file name is *LA_v5.005_NC_000300_000.gsm*. This model file was converted to the latest version (at the time of this writing) of GoldSim, version 11.1.5.

The following is a summary of the conversion process:

1) It was confirmed that the original 9.60 SP3 version of the model file, with supporting files provided in the zip file (*Nominal_Modeling_Case.zip*), could run successfully. It was run for 3 realizations with distributed processing on a Windows 7 laptop machine.

2) The 9.60 SP3 version of the model was converted to GoldSim version 10.5 SP7. Screenshots of all conversion messages are included in the Appendix of this document.

3) It was confirmed that the 10.5 SP7 version of the model could run successfully. It was run for 2 realizations with distributed processing on the same Windows 7 laptop.

4) The 10.5 SP7 version of the model was converted to GoldSim version 11.1.5. Screenshots of all conversion messages are included in the Appendix of this document.

5) It was confirmed that the 11.1.5 version of the model could run successfully (after implementing a workaround for an issue described later in this document). It was run for 2 realizations with distributed processing. Again, this was done on the same machine.

Details of the TSPA Model Conversion Steps

Each of the steps in the TSPA model conversion summarized in the previous section are described in more detail in the sections that follow.

Step 1: Ran the Original 9.60 SP3 Version of the Model without Errors

The zip file provided by Sandia (*Nominal_Modeling_Case.zip*) was unzipped at the following folder location on the test machine: C:\TSPA\Nominal_Modeling_Case. Note that an initial attempt to run the model at a location with a longer folder path failed. The apparent reason for this was that the path string was truncated in one of the DLL function calls that reads/writes data from/to a file. To avoid this issue, all subsequent testing was done in the folder location mentioned.

All files in the unzipped folder were selected and the 'Read-Only' attribute was unselected for all files. This was to ensure that necessary file copy commands could be executed by external DLLs. The model file was opened in GoldSim version 9.60 SP3 and the number of realizations was set to 3. A distributed processing (DP) run was carried out and successfully completed with 1 slave.

Note that the model was originally run without DP. When run without DP, there appears to be a file access conflict at the beginning of the second realization, which results in an error. Presumably, an external DLL is still 'holding onto' a .dat file from realization 1 when the DLL MFCP_LA.dll attempts to copy data to the same file. To get around this issue, the model was run using DP.

Step 2: Converted the Model File to GoldSim Version 10.5 SP7

After confirming that the original 9.60 SP3 version of the model file could run successfully for 3 realizations, the model file was converted to GoldSim version 10.5 SP7. Screenshots of all conversion messages can be found in the Appendix of this document. Below is a summary of the conversion messages.

1) Time Series definition format: The external element TS_PROC_DLL was flagged because it "*transfers at least one Time Series Definition in or out of a Dynamic Link Library (DLL)*". The conversion message noted that, in GoldSim 10.1, the "*external exchange format for the Time Series data type has changed.*"

2) Stochastic correlation option changed: Eight Stochastic elements were flagged because they "*[define] custom resampling logic and [are] correlated to another Stochastic element*". The conversion message noted that starting in GoldSim 10 "*these options are mutually exclusive*" and "*the correlation option has been changed to 'not correlated'*." **Note that this change could affect model results**.

Step 3: Ran the 10.5 SP7 Version of the Model without Errors

After converting the original 9.60 SP3 model file to version 10.5 SP7, the converted model was run to confirm that it would run without errors. It was run for 2 realizations using DP (1 slave) to avoid the file access conflict described previously.

Note that the model was first run using the DLL *TS_Proc.dll*, provided in the original zip file. Errors were encountered, as described in the Appendix of this document. As explained in the previous section, this was due to a change in the format in which time series definitions are specified in an external DLL.

The model was then run using a different 'TS_Proc' DLL with the file name '*TSProc.dll*'. This DLL uses the new time series definition format and is distributed with the latest version of GoldSim (11.1). The DLL can be found by first unzipping '*GSExampleDLLs.zip*', located here: <*GoldSim 11.1 installation folder*>\General Examples\External. Once the file has been unzipped, *TSProc.dll* can be found here: \GSExampleDLLs\TSProc\Win32\Release.

TSProc.dll was copied to the model file location (C:\TSPA\Nominal_Modeling_Case) and the External Element TS_PROC_DLL (located at \Time_Zero\EBS_PS_Loop\EBS_PSE_Loop) was edited to reference the DLL *TSProc.dll*, rather than *TS_Proc.dll*. Then the model was run for 2 realizations using DP. The run completed successfully.

Step 4: Converted the Model File to GoldSim Version 11.1.5

After confirming that the 10.5 SP7 version of the model file could run successfully for 2 realizations, the model file was converted to GoldSim version 11.1.5. Screenshots of all conversion messages are included in the Appendix of this document. Below is a summary of conversion messages.

1) SubModel output interface conversions: Two SubModels were flagged for conversions made to the outputs on their output interface. The conversion messages note that this version of GoldSim "*changes how simulation data are exported from SubModel elements*". The SubModels are Aleatory_Params (located in \Time_Zero) and Epistemic_Params (located in \Epistemic_Uncertainty). The conversion messages note that all outputs were converted successfully. This conversion is not expected to affect model results.

2) Table log interpolation changed to linear interpolation: Five Lookup Table elements were flagged because they "*used to do log interpolation on the independent variable*". As of GoldSim version 11.0, the log interpolation option is no longer available for Lookup Tables. The conversion message noted that these were converted to linear interpolation. **Note that this change could affect model results**.

3) Conversion of custom unit to built-in SI unit: One conversion message noted the "*unit cdeg is not defined*". Presumably cdeg is a custom unit defined in the TSPA model. The conversion message presents the following question and provides 'Yes' and 'No' options: "*Did you mean the SI unit Cdeg?*" The 'Yes' option was selected. **Note that this change could affect model results**.

Step 5: Ran the 11.1.5 Version of the Model without Errors

After converting the 10.5 SP7 model file to version 11.1.5, the converted model was run to confirm that it could run without errors. Note, however, that the model was only successfully run after implementing a workaround for an issue that was encountered. The issue and workaround are described in the Appendix of this document. The model was run for 2 realizations using DP (1 slave) to avoid the file access conflict described previously.

Final Results of Model Conversion

Summary of Results

As described previously in this document, a GoldSim 9.60 SP3 version of the Total System Performance Assessment (TSPA) model was converted to the latest version (at the time of this writing) of GoldSim, version 11.1.5. Conversion from version 9.60 SP3 to 10.5 and subsequent conversion from version 10.5 to 11.1.5 was successful. The Appendix of this document contains screenshots of all conversion messages encountered during the two stages of conversion. The final model file is *LA_v5.005_NC_000300_000_11_1_5.gsm*.

All three versions (9.60 SP3, 10.5 SP7 and 11.1.5) of the model were run with 2 or 3 realizations using distributed processing (DP) on a laptop with Windows 7. In all three cases, the model ran without errors. Note that to successfully run the model in 11.1.5 required implementation of a workaround to avoid an issue that was encountered. The issue and workaround are described in the Appendix of this document.

The following changes resulting from the conversion process could affect model results:

1) The correlation option for eight Stochastics was changed to 'not correlated'.
2) The log interpolation setting for five Lookup Tables was converted to linear interpolation.
3) A custom unit (cdeg) was converted to the built-in SI unit Cdeg.

The following changes from the conversion process should not affect model results:

1) A change in the external exchange format for the Time Series data type required the use of a different DLL (TSProc.dll) in place of TS_Proc.dll.
2) Outputs on the output interface of two SubModel elements were converted.

Also, the workaround implemented in the 11.1.5 version of the model is not expected to impact model results.

Files Provided to Sandia

Relevant model files and conversion documentation have been provided to Sandia in a zip file, *TSPA_Model_Conversion.zip*. Model files provided to Sandia include the following:

- *LA_v5.005_NC_000300_000_3Rlz.gsm*: This is a 9.60 SP3 version of the model that contains results for 3 realizations. Other than changing the number of realizations, no other changes were made relative to the original model file provided to GoldSim Technology Group.

- *LA_v5.005_NC_000300_000_10_5_SP7_2Rlz.gsm*: This is a 10.5 SP7 version of the model that contains results for 2 realizations. Changes relative to the original model file include the following: (1) conversion-related changes (the correlation option was changed to 'not correlated' for eight stochastics), (2) the number of realizations was changed to two and (3) the External Element TS_PROC_DLL was changed to reference TSProc.dll instead of TS_Proc.dll.

- *LA_v5.005_NC_000300_000_11_1_5_2Rlz.gsm*: This is an 11.1.5 version of the model that contains results for 2 realizations. Changes relative to the 10.5 SP7 version of the model include conversion-related changes and implementation of the workaround described in the Appendix. Changes related to conversion include the following: conversion of outputs on SubModel output interfaces, change in the interpolation setting on Lookup Tables and conversion of the custom unit cdeg to the built-in SI unit Cdeg.

- *LA_v5.005_NC_000300_000_11_1_5.gsm*: This is an 11.1.5 version of the model that does not contain any results. The number of realizations (300) was left unchanged from the original model file and the External Element TS_PROC_DLL was edited to reference TSProc.dll instead of TS_Proc.dll. All other conversion-related changes described above apply to this version. Also, note that the workaround described in the Appendix is implemented in this version of the model.

Documentation provided to Sandia includes this TSPA Model Conversion document. This document contains (1) an overview of conversion steps, (2) important details about each of the conversion steps, (3) a summary of the results of model conversion, (4) instructions for running the converted model and

(5) an appendix that includes screenshots of all conversion messages encountered during the two stages of conversion, error messages related to TS_Proc.dll encountered when running the model in 10.5 SP7 and a detailed description of an issue originally encountered when running the 11.1.5 version of the model and a workaround implemented in the 11.1.5 version to avoid the issue.

Instructions for Running the Converted Model

To run the converted model (version 11.1.5), carry out the following steps:

1) Unzip Nominal_Modeling_Case.zip to a folder location that is not too deeply nested in subfolders (note that if the path to the supporting files is too long, the path strings could be truncated in function executions by one or more DLLs).

2) Select all files in the unzipped folder (using Ctrl+A), right-click any one of the files and select 'Properties' in the context menu. Uncheck the 'Read-only' attribute and click OK.

3) Move or copy the converted model file, *LA_v5.005_NC_000300_000_11_1_5.gsm*, to the unzipped folder.

4) Copy the file *TSProc.dll* to the unzipped folder. Note that this can be found in the GoldSim 11.1.5 installation folder. First unzip '*GSExampleDLLs.zip*', which is located here: *<GoldSim 11.1 installation folder>*\General Examples\External. Once the file has been unzipped, *TSProc.dll* can be found here: \GSExampleDLLs\TSProc\Win32\Release.

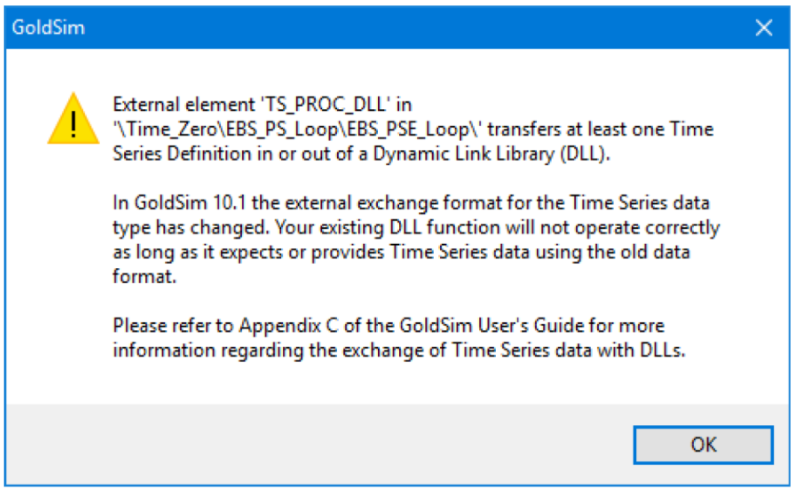
5) Open the model file in GoldSim 11.1.5 and confirm that TS_PROC_DLL (located at \Time_Zero\EBS_PS_Loop\EBS_PSE_Loop) correctly references *TSProc.dll*, rather than *TS_Proc.dll*.

6) Run the model with distributed processing (to avoid the file access conflict described previously).

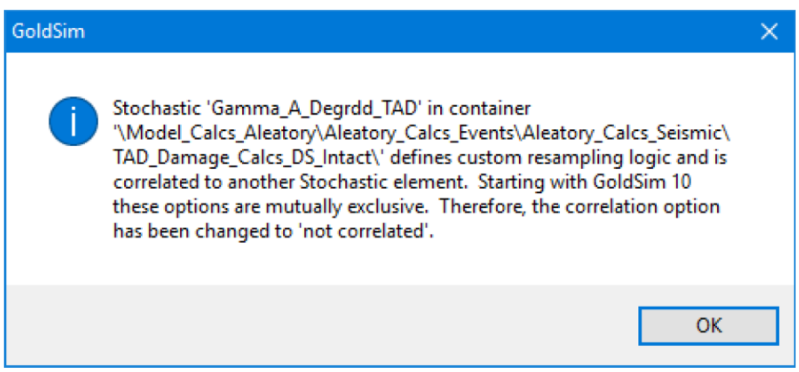
Appendix

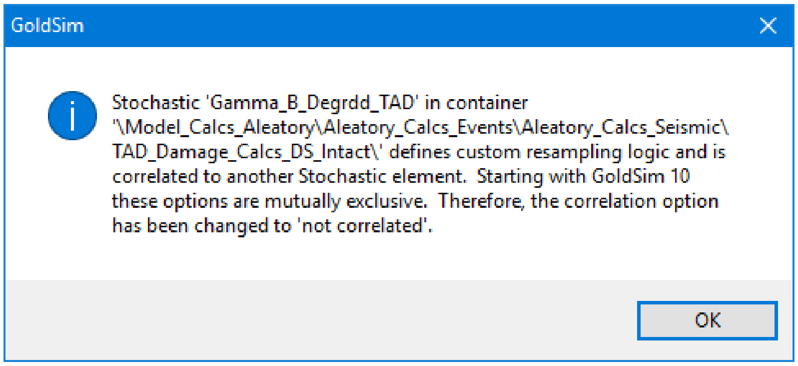
Conversion Messages (9.60 SP3 to 10.5 SP7)

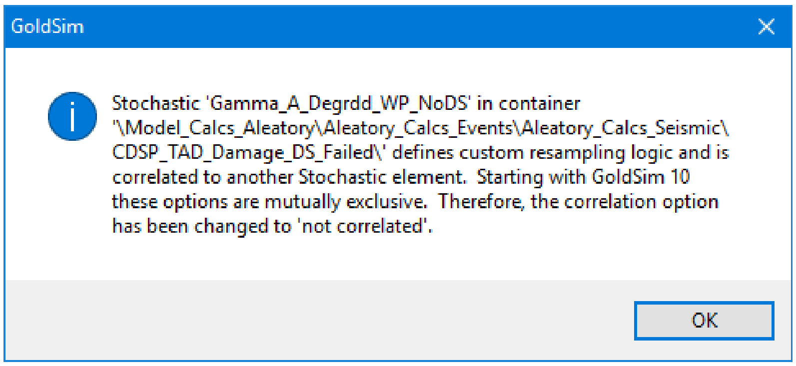
Change in Time Series Definition Import Format

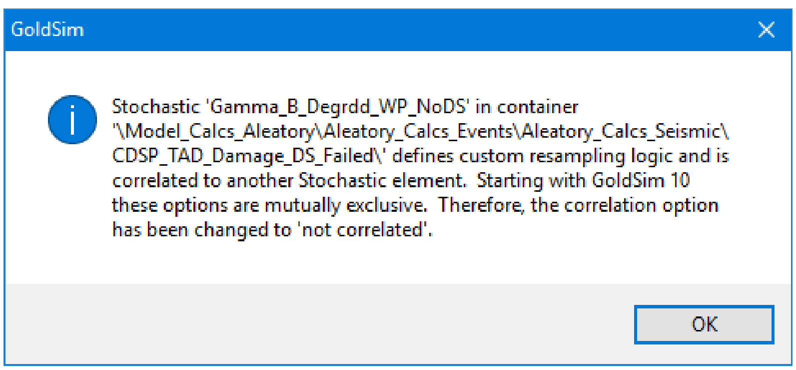


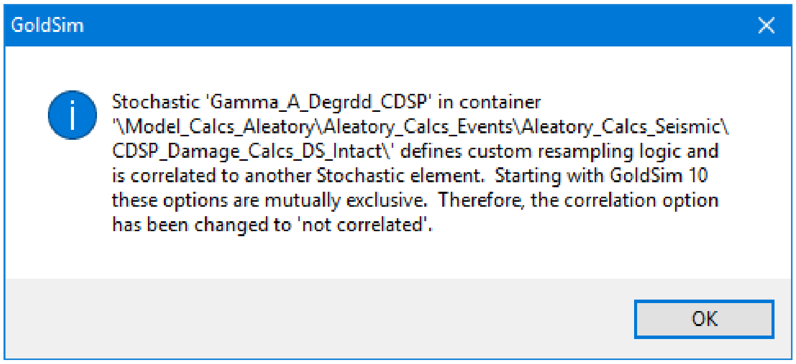
Correlation Option Changed to 'Not Correlated' (8 Stochastics)

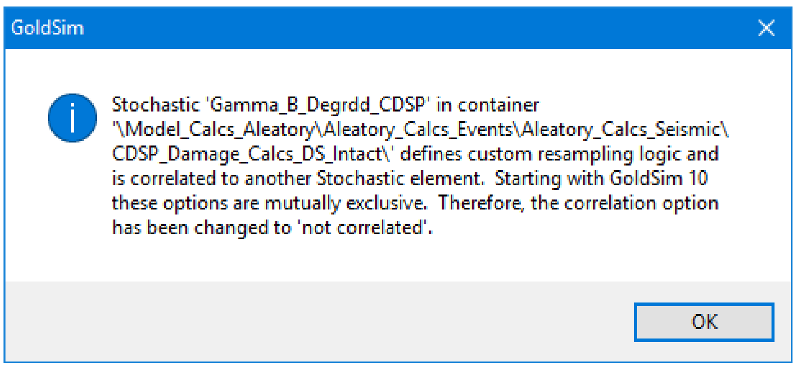


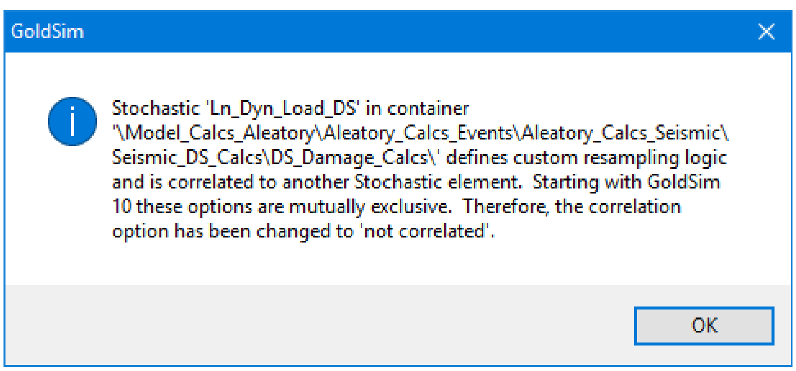

GoldSim
Stochastic 'Gamma_B_Degrdd_TAD' in container '\Model_Calcs_Aleatory\Aleatory_Calcs_Events\Aleatory_Calcs_Seismic\TAD_Damage_Calcs_DS_Intact\' defines custom resampling logic and is correlated to another Stochastic element. Starting with GoldSim 10 these options are mutually exclusive. Therefore, the correlation option has been changed to 'not correlated'.
OK

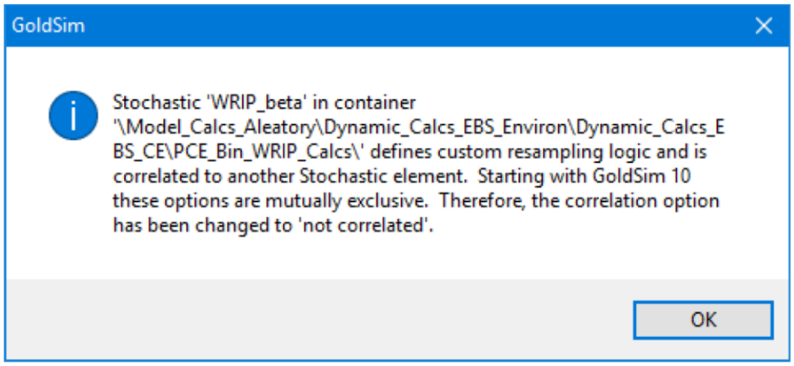

GoldSim
Stochastic 'Gamma_A_Degrdd_WP_NoDS' in container '\Model_Calcs_Aleatory\Aleatory_Calcs_Events\Aleatory_Calcs_Seismic\CDSP_TAD_Damage_DS_Failed\' defines custom resampling logic and is correlated to another Stochastic element. Starting with GoldSim 10 these options are mutually exclusive. Therefore, the correlation option has been changed to 'not correlated'.
OK


GoldSim
Stochastic 'Gamma_B_Degrdd_WP_NoDS' in container '\Model_Calcs_Aleatory\Aleatory_Calcs_Events\Aleatory_Calcs_Seismic\CDSP_TAD_Damage_DS_Failed\' defines custom resampling logic and is correlated to another Stochastic element. Starting with GoldSim 10 these options are mutually exclusive. Therefore, the correlation option has been changed to 'not correlated'.
OK


GoldSim
Stochastic 'Gamma_A_Degrdd_CDSP' in container '\Model_Calcs_Aleatory\Aleatory_Calcs_Events\Aleatory_Calcs_Seismic\CDSP_Damage_Calcs_DS_Intact\' defines custom resampling logic and is correlated to another Stochastic element. Starting with GoldSim 10 these options are mutually exclusive. Therefore, the correlation option has been changed to 'not correlated'.
OK


GoldSim
Stochastic 'Gamma_B_Degrdd_CDSP' in container '\Model_Calcs_Aleatory\Aleatory_Calcs_Events\Aleatory_Calcs_Seismic\CDSP_Damage_Calcs_DS_Intact\' defines custom resampling logic and is correlated to another Stochastic element. Starting with GoldSim 10 these options are mutually exclusive. Therefore, the correlation option has been changed to 'not correlated'.
OK

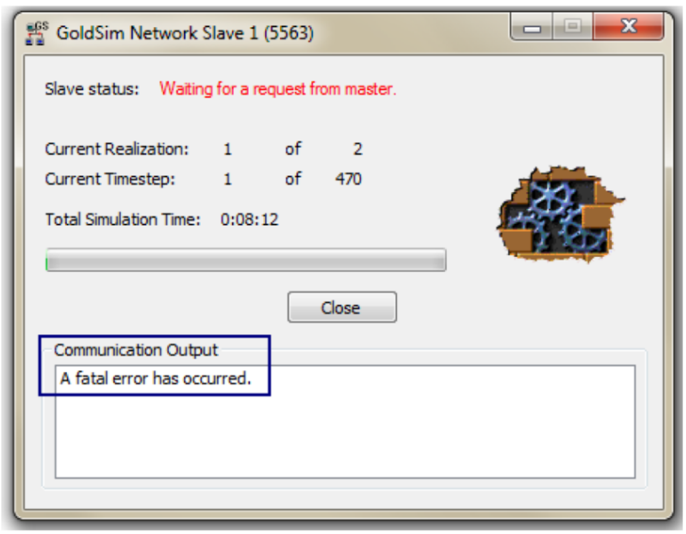

GoldSim
Stochastic 'Ln_Dyn_Load_DS' in container '\Model_Calcs_Aleatory\Aleatory_Calcs_Events\Aleatory_Calcs_Seismic\Seismic_DS_Calcs\DS_Damage_Calcs\' defines custom resampling logic and is correlated to another Stochastic element. Starting with GoldSim 10 these options are mutually exclusive. Therefore, the correlation option has been changed to 'not correlated'.
OK

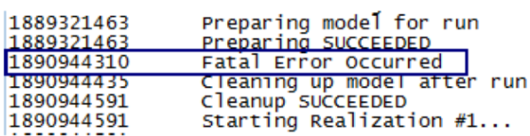


Error Messages when Running with TS_Proc.dll

Slave Log for DP Run (with TS_Proc.dll)

The slave 'Communication Output' and run log indicates a fatal error, but does not provide details.

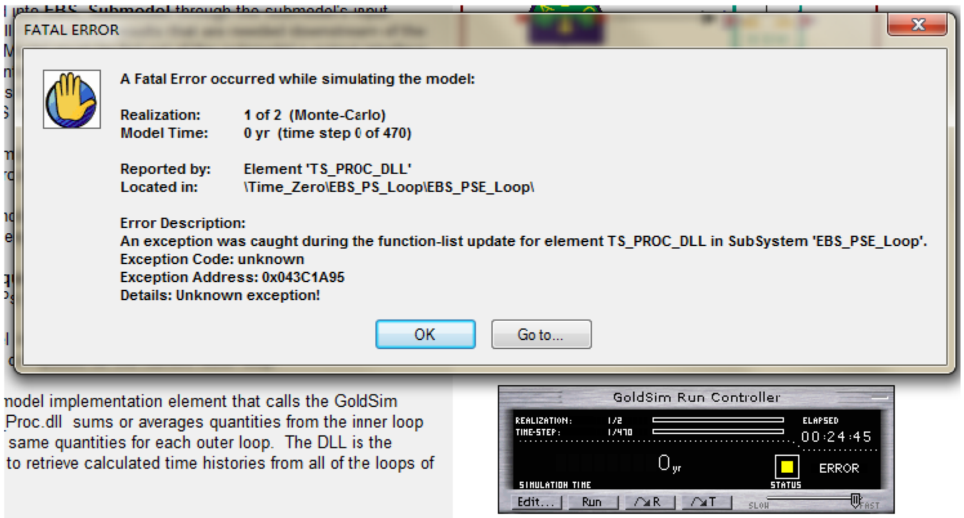


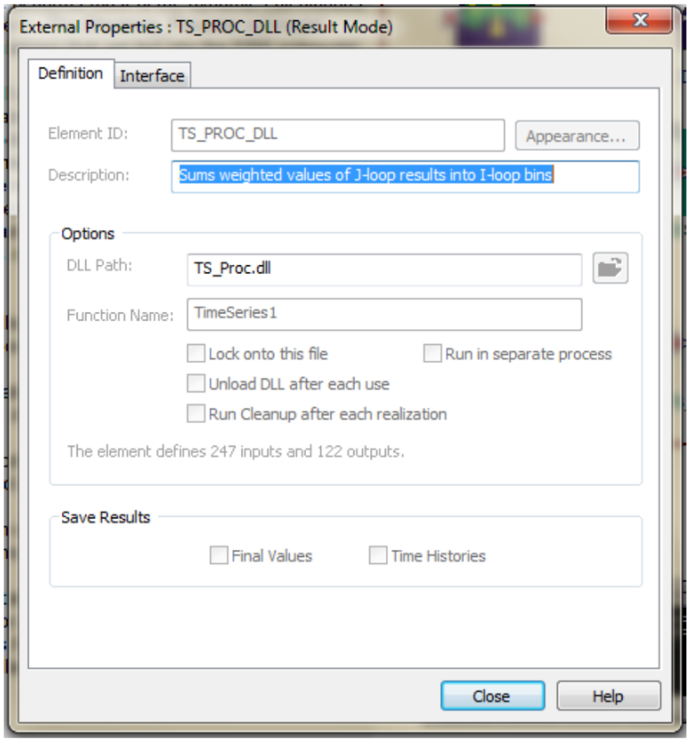


```
1889321463      Preparing model for run
1889321463      Preparing SUCCEEDED
1890944310      Fatal Error Occurred
1890944435      Cleaning up model after run
1890944591      Cleanup SUCCEEDED
1890944591      Starting Realization #1...
```

Error Message for Non-DP Run (with TS_Proc.dll)

More information was obtainable by running the model without distributed processing. In this case, a fatal error message dialog is displayed indicating that the problem is with the element TS_PROC_DLL. The error message only indicates that there was an 'unknown exception'. The error is the result of a change in the time series definition format for an external DLL. This format change occurred in GoldSim 10.1.





Conversion Messages (10.5 SP7 to 11.1.5)

SubModel Output Interface Conversions

Important Conversion Information for SubModel

This version of GoldSim changes how simulation data are exported from SubModel elements. For **deterministic simulations** the SubModel output interface provides the **final value** of the selected SubModel output using an output with a matching data type. For **Monte Carlo simulations** SubModels provide **statistics** for selected value- or condition-type outputs. For more information on SubModel conversion, please refer to the GoldSim documentation.

GoldSim made the following changes to SubModel 'Aleatory_Params' in container '\Time_Zero\'.

Success: Output interface 'BIN_Prob_FB1_a' successfully converted to final value statistic output.

Success: Output interface 'BIN_Prob_FB2_a' successfully converted to final value statistic output.

Success: Output interface 'BIN_Prob_FB3_a' successfully converted to final value statistic output.

Success: Output interface 'Num_EF_WP_Cond_a' successfully converted to final value statistic output.

Success: Output interface 'Rand_Env_FB1_a' successfully converted to final value statistic output.

Success: Output interface 'Rand_Env_FB2_a' successfully converted to final value statistic output.

Success: Output interface 'Rand_Env_FB3_a' successfully converted to final value statistic output.

Success: Output interface 'Num_EF_WP_CDSP_a' successfully converted to final value statistic output.

Success: Output interface 'HI_BIN_Prob_a' successfully converted to final value statistic output.

Success: Output interface 'HI_SZ_Region_Prob_PS1_a' successfully converted to final value statistic output.

Success: Output interface 'HI_SZ_Region_Prob_PS2_a' successfully converted to final value statistic output.

Success: Output interface 'HI_SZ_Region_Prob_PS3_a' successfully converted to final value statistic output.

Success: Output interface 'HI_SZ_Region_Prob_PS4_a' successfully converted to final value statistic output.

Success: Output interface 'HI_SZ_Region_Prob_PS5_a' successfully converted to final value statistic output.

Success: Output interface 'HI_WP_Type_Rand_a' successfully converted to final value statistic output.

Success: Output interface 'Igneous_Event_1_Time_a' successfully converted to final value statistic output.

Success: Output interface 'Igneous_Event_2_Time_a' successfully converted to final value statistic output.

Success: Output interface 'Igneous_Event_3_Time_a' successfully converted to final value statistic output.

Success: Output interface 'Igneous_Event_4_Time_a' successfully converted to final value statistic output.

Success: Output interface 'Igneous_Event_5_Time_a' successfully converted to final value statistic output.

Success: Output interface 'Igneous_Num_Event_Rand_a' successfully converted to final value statistic output.

Success: Output interface 'Num_WPs_Hit_Intrusive_1_a' successfully converted to final value statistic output.

Success: Output interface 'Num_WPs_Hit_Intrusive_2_a' successfully converted to final value statistic output.

Success: Output interface 'Num_WPs_Hit_Intrusive_3_a' successfully converted to final value statistic output.

Success: Output interface 'Num_WPs_Hit_Intrusive_4_a' successfully converted to final value statistic output.

Success: Output interface 'Num_WPs_Hit_Intrusive_5_a' successfully converted to final value statistic output.

Success: Output interface 'Exceedance_Freq_FD_a' successfully converted to final value statistic output.

Success: Output interface 'Seismic_Event_Time_FD_a' successfully converted to final value statistic output.

Success: Output interface 'Seismic_Event_Time_Max_FD' successfully converted to final value statistic output.

Success: Output interface 'Seismic_Event_Time_Min_FD' successfully converted to final value statistic output.

Success: Output interface 'Rubble_Fill_Time_NonLith' successfully converted to final value statistic output.

Success: Output interface 'Rubble_Fill_Time_Lith' successfully converted to final value statistic output.

```
Success: Output interface 'DS_Frame_Fail_Time' successfully converted to final value statistic output.
Success: Output interface 'DS_Plate_Fail_Time' successfully converted to final value statistic output.
Success: Output interface 'DS_GC_Fail_Time' successfully converted to final value statistic output.
Success: Output interface 'TAD_Failed_Area_a' successfully converted to final value statistic output.
Success: Output interface 'Num_EF_DS_Cond_a' successfully converted to final value statistic output.
Success: Output interface 'Num_EF_DS_CDSP_a' successfully converted to final value statistic output.
Success: Output interface 'Seismic_Lambda_Max_FD' successfully converted to final value statistic output.
Success: Output interface 'Seismic_Lambda_Min_FD' successfully converted to final value statistic output.
Success: Output interface 'CDSP_Failed_Area_a' successfully converted to final value statistic output.
Success: Output interface 'TimeStep_Length_by_TS_Index' successfully converted to final value statistic output.
Success: Output interface 'Rubble_Vol_Accum_Lith_max' successfully converted to final value statistic output.
Success: Output interface 'Rubble_Vol_Accum_NonLith_max' successfully converted to final value statistic output.
Success: Output interface 'WRIP_beta_rand_a' successfully converted to final value statistic output.
Success: Output interface 'Puncture_Area_a' successfully converted to final value statistic output.
Success: Output interface 'CDSP_Rupture_Area_a' successfully converted to final value statistic output.
Success: Output interface 'TAD_Rupture_Area_a' successfully converted to final value statistic output.
Success: Output interface 'Seismic_FD_Rubble_Vol_Lith' successfully converted to final value statistic output.
Success: Output interface 'Seismic_FD_Rubble_Vol_NonLith' successfully converted to final value statistic output.
Success: Output interface 'Seismic_First_Event_Time_CSNF' successfully converted to final value statistic output.
Success: Output interface 'Seismic_First_Event_Time_CDSP' successfully converted to final value statistic output.
```

Important Conversion Information for SubModel

This version of GoldSim changes how simulation data are exported from SubModel elements. For **deterministic simulations** the SubModel output interface provides the **final value** of the selected SubModel output using an output with a matching data type. For **Monte Carlo simulations** SubModels provide **statistics** for selected value- or condition-type outputs. For more information on SubModel conversion, please refer to the GoldSim documentation.

GoldSim made the following changes to SubModel 'Epistemic_Params' in container '\Epistemic_Uncertainty\'.

Success: Output interface 'Infiltration_Scenario_a' successfully converted to final value statistic output.

Success: Output interface 'Alpha_ACM_Weights_a' successfully converted to final value statistic output.

Success: Output interface 'LogK_Uncert_Lith_a' successfully converted to final value statistic output.

Success: Output interface 'LogK_Uncert_NonLith_a' successfully converted to final value statistic output.

Success: Output interface 'Seepage_Uncertainty_a' successfully converted to final value statistic output.

Success: Output interface 'Alpha_Uncert_Lith_a' successfully converted to final value statistic output.

Success: Output interface 'Alpha_Uncert_NonLith_a' successfully converted to final value statistic output.

Success: Output interface 'Random_Seed_1' successfully converted to final value statistic output.

Success: Output interface 'Random_Seed_2' successfully converted to final value statistic output.

Success: Output interface 'DWC_Dispersivity_Cond_a' successfully converted to final value statistic output.

Success: Output interface 'DWC_Invert_Properties_Cond_a' successfully converted to final value statistic output.

Success: Output interface 'DWC_Ventilated_Cond_a' successfully converted to final value statistic output.

Success: Output interface 'Seepage_Condensation_Prob_a' successfully converted to final value statistic output.

Success: Output interface 'DWC_Std_Error_a_a' successfully converted to final value statistic output.

Success: Output interface 'DWC_Std_Error_b_a' successfully converted to final value statistic output.

Success: Output interface 'DWC_Std_Error_c_a' successfully converted to final value statistic output.

Success: Output interface 'DWC_Std_Error_d_a' successfully converted to final value statistic output.

Success: Output interface 'dt_dRh_uncertainty' successfully converted to final value statistic output.

Success: Output interface 'Thermal_Conductivity_Uncert_a' successfully converted to final value statistic output.

Success: Output interface 'Seepage_Water_Type_a' successfully converted to final value statistic output.

Success: Output interface 'C1_GenCorr_A22_a' successfully converted to final value statistic output.

Success: Output interface 'Defect_Count_a' successfully converted to final value statistic output.

Success: Output interface 'Defect_Size_a' successfully converted to final value statistic output.

Success: Output interface 'GC_ULevel_A22_a' successfully converted to final value statistic output.

Success: Output interface 'MIC_RHThresh_a' successfully converted to final value statistic output.

Success: Output interface 'n_SCC_a' successfully converted to final value statistic output.

Success: Output interface 'Stress_Thresh_SCC_a' successfully converted to final value statistic output.

Success: Output interface 'z_OL_a' successfully converted to final value statistic output.

Success: Output interface 'WDSeed_CDSP_PS1_a' successfully converted to final value statistic output.

Success: Output interface 'WDSeed_CDSP_PS2_a' successfully converted to final value statistic output.

Success: Output interface 'WDSeed_CDSP_PS3_a' successfully converted to final value statistic output.

Success: Output interface 'WDSeed_CDSP_PS4_a' successfully converted to final value statistic output.

Success: Output interface 'WDSeed_CDSP_PS5_a' successfully converted to final value statistic output.

Success: Output interface 'WDSeed_CSNF_PS1_a' successfully converted to final value statistic output.

Success: Output interface 'WDSeed_CSNF_PS2_a' successfully converted to final value statistic output.

Success: Output interface 'WDSeed_CSNF_PS3_a' successfully converted to final value statistic output.

Success: Output interface 'WDSeed_CSNF_PS4_a' successfully converted to final value statistic output.

Success: Output interface 'WDSeed_CSNF_PS5_a' successfully converted to final value statistic output.

Success: Output interface 'WDSeed_FB1_a' successfully converted to final value statistic output.

Success: Output interface 'WDSeed_FB2_a' successfully converted to final value statistic output.

Success: Output interface 'WDSeed_FB3_a' successfully converted to final value statistic output.

Success: Output interface 'WDSeed_Mktable_CDSP_PS1_a' successfully converted to final value statistic output.

Success: Output interface 'WDSeed_Mktable_CDSP_PS2_a' successfully converted to final value statistic output.

Success: Output interface 'WDSeed_Mktable_CDSP_PS3_a' successfully converted to final value statistic output.

Success: Output interface 'WDSeed_Mktable_CDSP_PS4_a' successfully converted to final value statistic output.

Success: Output interface 'WDSeed_Mktable_CDSP_PS5_a' successfully converted to final value statistic output.

Success: Output interface 'WDSeed_Mktable_CSNF_PS1_a' successfully converted to final value statistic output.

Success: Output interface 'WDSeed_Mktable_CSNF_PS2_a' successfully converted to final value statistic output.

Success: Output interface 'WDSeed_Mktable_CSNF_PS3_a' successfully converted to final value statistic output.

Success: Output interface 'WDSeed_Mktable_CSNF_PS4_a' successfully converted to final value statistic output.

Success: Output interface 'WDSeed_Mktable_CSNF_PS5_a' successfully converted to final value statistic output.

Success: Output interface 'WDSeed_Mktable_FB1_a' successfully converted to final value statistic output.

Success: Output interface 'WDSeed_Mktable_FB2_a' successfully converted to final value statistic output.

Success: Output interface 'WDSeed_Mktable_FB3_a' successfully converted to final value statistic output.

Success: Output interface 'LC_rate_a' successfully converted to final value statistic output.

Success: Output interface 'Rind_Porosity_CSNF_a' successfully converted to final value statistic output.

Success: Output interface 'Log_Specific_SA_CSNF_a' successfully converted to final value statistic output.

Success: Output interface 'CSNF_WF_Uncert_a0_Alk_a' successfully converted to final value statistic output.

Success: Output interface 'CSNF_WF_Uncert_a1_Alk_a' successfully converted to final value statistic output.

Success: Output interface 'CSNF_WF_Uncert_a2_Alk_a' successfully converted to final value statistic output.

Success: Output interface 'CSNF_WF_Uncert_a3_Alk_a' successfully converted to final value statistic output.

Success: Output interface 'CSNF_WF_Uncert_a0_Acid_a' successfully converted to final value statistic output.

Success: Output interface 'CSNF_WF_Uncert_a4_Acid_a' successfully converted to final value statistic output.

Success: Output interface 'Exposure_Factor_a' successfully converted to final value statistic output.

Success: Output interface 'HLW_Diss_kE_Acidic_a' successfully converted to final value statistic output.

Success: Output interface 'HLW_Diss_kE_Alkaline_a' successfully converted to final value statistic output.

Success: Output interface 'IPC_NDM_Vapor_Flux_a' successfully converted to final value statistic output.

Success: Output interface 'CSNF_Mass_Uncert_a' successfully converted to final value statistic output.

Success: Output interface 'DSNF_Mass_Uncert_a' successfully converted to final value statistic output.

Success: Output interface 'HLW_Mass_Uncert_a' successfully converted to final value statistic output.

Success: Output interface 'Initial_Release_Frac_Cs_a' successfully converted to final value statistic output.

Success: Output interface 'Initial_Release_Frac_I_a' successfully converted to final value statistic output.

Success: Output interface 'Initial_Release_Frac_Sr_a' successfully converted to final value statistic output.

Success: Output interface 'Initial_Release_Frac_Tc_a' successfully converted to final value statistic output.

Success: Output interface 'Kd_Am_Rev_Smectite_a' successfully converted to final value statistic output.

Success: Output interface 'Kd_Cs_Rev_Smectite_a' successfully converted to final value statistic output.

Success: Output interface 'Kd_Pa_Rev_Smectite_a' successfully converted to final value statistic output.

Success: Output interface 'Kd_Pu_Rev_Smectite_a' successfully converted to final value statistic output.

Success: Output interface 'Kd_Sn_Rev_Smectite_a' successfully converted to final value statistic output.

Success: Output interface 'Kd_Th_Rev_Smectite_a' successfully converted to final value statistic output.

Success: Output interface 'Default_Fwd_Rate_Const_a' successfully converted to final value statistic output.

Success: Output interface 'Max_Default_Fwd_Rate_Const' successfully converted to final value statistic output.

Success: Output interface 'Target_Flux_Out_Ratio_a' successfully converted to final value statistic output.

Success: Output interface 'CS_Corrosion_Rate_a' successfully converted to final value statistic output.

Success: Output interface 'Goethite_SA_a' successfully converted to final value statistic output.

Success: Output interface 'Goethite_Site_Density_a' successfully converted to final value statistic output.

Success: Output interface 'HFO_SA_a' successfully converted to final value statistic output.

Success: Output interface 'HFO_Site_Density_a' successfully converted to final value statistic output.

Success: Output interface 'Relative_Abundance_Goethite_a' successfully converted to final value statistic output.

Success: Output interface 'SS_Corrosion_Rate_a' successfully converted to final value statistic output.

Success: Output interface 'DS_Flux_Uncertainty_a' successfully converted to final value statistic output.

Success: Output interface 'WP_Flux_Uncertainty_a' successfully converted to final value statistic output.

Success: Output interface 'Invert_Diff_Coeff_Uncert_a' successfully converted to final value statistic output.

Success: Output interface 'ff_group1_antilog' successfully converted to final value statistic output.

Success: Output interface 'ff_group2_antilog' successfully converted to final value statistic output.

Success: Output interface 'ff_group3_antilog' successfully converted to final value statistic output.

Success: Output interface 'ff_group4_antilog' successfully converted to final value statistic output.

Success: Output interface 'ff_group5_antilog' successfully converted to final value statistic output.

Success: Output interface 'ff_group6_antilog' successfully converted to final value statistic output.

Success: Output interface 'ff_group7_antilog' successfully converted to final value statistic output.

Success: Output interface 'ff_group8_antilog' successfully converted to final value statistic output.

Success: Output interface 'ff_group9_antilog' successfully converted to final value statistic output.

Success: Output interface 'Interface_Area_mult_a' successfully converted to final value statistic output.

Success: Output interface 'Por_group1_a' successfully converted to final value statistic output.

Success: Output interface 'Por_group2_a' successfully converted to final value statistic output.

Success: Output interface 'Por_group3_a' successfully converted to final value statistic output.

Success: Output interface 'Por_group4_a' successfully converted to final value statistic output.

Success: Output interface 'Por_group5_a' successfully converted to final value statistic output.

Success: Output interface 'Por_group6_a' successfully converted to final value statistic output.

Success: Output interface 'Por_group7_a' successfully converted to final value statistic output.

Success: Output interface 'Por_group8_a' successfully converted to final value statistic output.

Success: Output interface 'Por_group9_a' successfully converted to final value statistic output.

Success: Output interface 'Colloidal_Concentration_uz_a' successfully converted to final value statistic output.

Success: Output interface 'Colloidal_Kd_Am_uz_a' successfully converted to final value statistic output.

Success: Output interface 'Colloidal_Kd_Cs_uz_a' successfully converted to final value statistic output.

Success: Output interface 'Colloidal_Kd_Pa_uz_a' successfully converted to final value statistic output.

Success: Output interface 'Colloidal_Kd_Pu_uz_a' successfully converted to final value statistic output.

Success: Output interface 'Colloidal_Kd_Th_uz_a' successfully converted to final value statistic output.

Success: Output interface 'Am_devit_a' successfully converted to final value statistic output.

Success: Output interface 'Cs_devit_a' successfully converted to final value statistic output.

Success: Output interface 'Cs_zeo_a' successfully converted to final value statistic output.

Success: Output interface 'Np_devit_a' successfully converted to final value statistic output.

Success: Output interface 'Pa_devit_a' successfully converted to final value statistic output.

Success: Output interface 'Pu_devit_a' successfully converted to final value statistic output.

Success: Output interface 'Ra_zeo_a' successfully converted to final value statistic output.

Success: Output interface 'Sr_devit_a' successfully converted to final value statistic output.

Success: Output interface 'Th_devit_a' successfully converted to final value statistic output.

Success: Output interface 'Colloidal_Retard_Factor_dist_a' successfully converted to final value statistic output.

Success: Output interface 'Rseed_FEHM_PT_a' successfully converted to final value statistic output.

Success: Output interface 'Rseed_FEHM_Release_a' successfully converted to final value statistic output.

Success: Output interface 'SZ_Index_a' successfully converted to final value statistic output.

Success: Output interface 'Bio_Index_a' successfully converted to final value statistic output.

Success: Output interface 'Igneous_Event_Prob_a' successfully converted to final value statistic output.

Success: Output interface 'Sn_devit_a' successfully converted to final value statistic output.

Success: Output interface 'Se_devit_a' successfully converted to final value statistic output.

Success: Output interface 'U_devit_a' successfully converted to final value statistic output.

Success: Output interface 'UZDC_STN_RG1_a' successfully converted to final value statistic output.

Success: Output interface 'UZDC_STN_RG2_a' successfully converted to final value statistic output.

Success: Output interface 'UZDC_STN_RG3_a' successfully converted to final value statistic output.

Success: Output interface 'Gamma_AFM_a' successfully converted to final value statistic output.

Success: Output interface 'WDDSGC_29_a' successfully converted to final value statistic output.

Success: Output interface 'Stress_Thresh_A22_a' successfully converted to final value statistic output.

Success: Output interface 'Inpkg_pH_2DHLW_NS_Rand_a' successfully converted to final value statistic output.

Success: Output interface 'Inpkg_pH_2DHLW_S_Rand_a' successfully converted to final value statistic output.

Success: Output interface 'Inpkg_pH_2MCO_NS_Rand_a' successfully converted to final value statistic output.

Success: Output interface 'Inpkg_pH_2MCO_S_Rand_a' successfully converted to final value statistic output.

Success: Output interface 'Inpkg_pH_CSNF_NS_Rand_a' successfully converted to final value statistic output.

Success: Output interface 'Inpkg_pH_CSNF_S_Rand_a' successfully converted to final value statistic output.

Success: Output interface 'Inpkg_IStr_2DHLW_NS_Rand_a' successfully converted to final value statistic output.

Success: Output interface 'Inpkg_IStr_2DHLW_S_Rand_a' successfully converted to final value statistic output.

Success: Output interface 'Inpkg_IStr_2MCO_NS_Rand_a' successfully converted to final value statistic output.

Success: Output interface 'Inpkg_IStr_2MCO_S_Rand_a' successfully converted to final value statistic output.

Success: Output interface 'Inpkg_IStr_CSNF_NS_Rand_a' successfully converted to final value statistic output.

Success: Output interface 'Inpkg_IStr_CSNF_S_Rand_a' successfully converted to final value statistic output.

Success: Output interface 'Am_Eps_1_high_a' successfully converted to final value statistic output.

Success: Output interface 'Am_Eps_1_low_a' successfully converted to final value statistic output.

Success: Output interface 'Am_Eps_2_CDSP_High_a' successfully converted to final value statistic output.

Success: Output interface 'Am_Eps_2_CSNF_High_a' successfully converted to final value statistic output.

Success: Output interface 'Am_Eps_2_Glass_Low_a' successfully converted to final value statistic output.

Success: Output interface 'Np2O5_Eps_1_high_a' successfully converted to final value statistic output.

Success: Output interface 'Np2O5_Eps_1_low_a' successfully converted to final value statistic output.

Success: Output interface 'Np2O5_Eps_2_CDSP_High_a' successfully converted to final value statistic output.

Success: Output interface 'Np2O5_Eps_2_CSNF_High_a' successfully converted to final value statistic output.

Success: Output interface 'Np2O5_Eps_2_Glass_Low_a' successfully converted to final value statistic output.

Success: Output interface 'NpO2_Eps_1_high_a' successfully converted to final value statistic output.

Success: Output interface 'NpO2_Eps_1_low_a' successfully converted to final value statistic output.

Success: Output interface 'NpO2_Eps_2_CDSP_High_a' successfully converted to final value statistic output.

Success: Output interface 'NpO2_Eps_2_CSNF_High_a' successfully converted to final value statistic output.

Success: Output interface 'NpO2_Eps_2_Glass_Low_a' successfully converted to final value statistic output.

Success: Output interface 'Pa_Eps_1_a' successfully converted to final value statistic output.

Success: Output interface 'Pa_Eps_2_CDSP_High_a' successfully converted to final value statistic output.

Success: Output interface 'Pa_Eps_2_CSNF_High_a' successfully converted to final value statistic output.

Success: Output interface 'Pa_Eps_2_Glass_Low_a' successfully converted to final value statistic output.

Success: Output interface 'Pu_Eps_1_high_a' successfully converted to final value statistic output.

Success: Output interface 'Pu_Eps_1_low_a' successfully converted to final value statistic output.

Success: Output interface 'Pu_Eps_2_CDSP_High_a' successfully converted to final value statistic output.

Success: Output interface 'Pu_Eps_2_CSNF_High_a' successfully converted to final value statistic output.

Success: Output interface 'Pu_Eps_2_Glass_Low_a' successfully converted to final value statistic output.

Success: Output interface 'Sn_Eps_high_a' successfully converted to final value statistic output.

Success: Output interface 'Sn_Eps_low_a' successfully converted to final value statistic output.

Success: Output interface 'Th_Eps_1_high_a' successfully converted to final value statistic output.

Success: Output interface 'Th_Eps_1_low_a' successfully converted to final value statistic output.

Success: Output interface 'Th_Eps_2_CDSP_High_a' successfully converted to final value statistic output.

Success: Output interface 'Th_Eps_2_CSNF_High_a' successfully converted to final value statistic output.

Success: Output interface 'Th_Eps_2_Glass_Low_a' successfully converted to final value statistic output.

Success: Output interface 'Schoepite_Boltwoodite_Interp_a' successfully converted to final value statistic output.

Success: Output interface 'U_Eps_1_high_Other_a' successfully converted to final value statistic output.

Success: Output interface 'U_Eps_1_low_Other_a' successfully converted to final value statistic output.

Success: Output interface 'U_Eps_2_Boltwoodite_CDSP_Hig_a' successfully converted to final value statistic output.

Success: Output interface 'U_Eps_2_Boltwoodite_CSNF_Hig_a' successfully converted to final value statistic output.

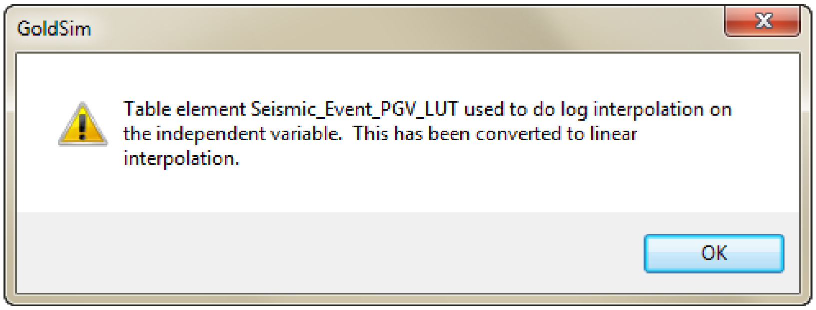
Success: Output interface 'U_Eps_2_Boltwoodite_Glass_Lo_a' successfully converted to final value statistic output.

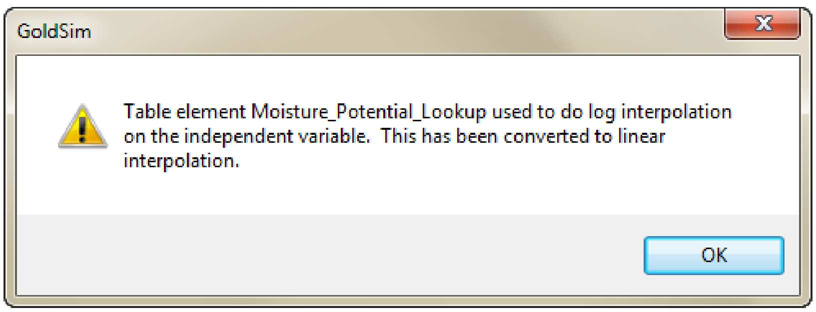
Success: Output interface 'U_Eps_2_Schoepite_CDSP_High_a' successfully converted to final value statistic output.

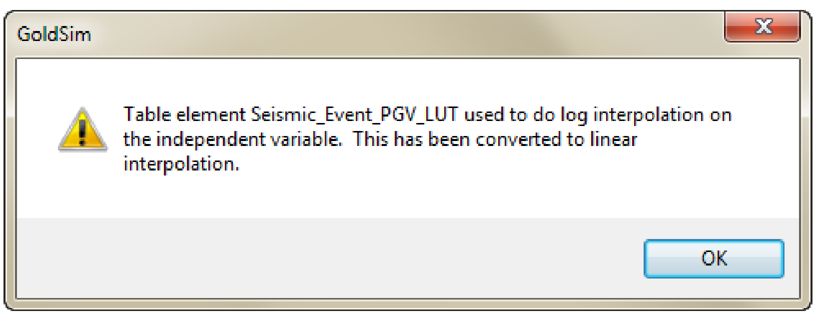
Success: Output interface 'U_Eps_2_Schoepite_CSNF_High_a' successfully converted to final value statistic output.

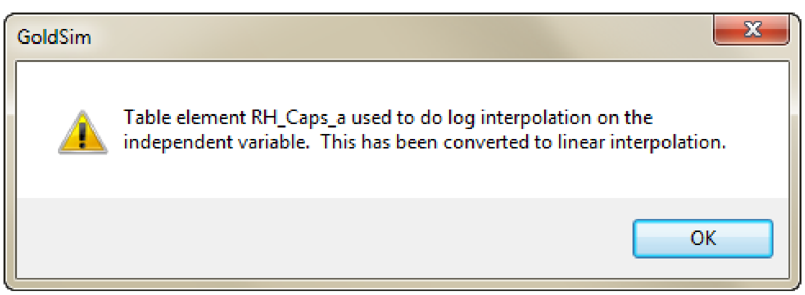
```
Success: Output interface 'U_Eps_2_Schoepite_Glass_Low_a' successfully converted to final value statistic output.
Success: Output interface 'U_Eps_1_high_Nominal_a' successfully converted to final value statistic output.
Success: Output interface 'U_Eps_1_low_Nominal_a' successfully converted to final value statistic output.
Success: Output interface 'U_Eps_2_CSNF_High_Nominal_a' successfully converted to final value statistic output.
Success: Output interface 'U_Eps_2_CSNF_Low_Nominal_a' successfully converted to final value statistic output.
Success: Output interface 'PCE_Delta_pCO2_a' successfully converted to final value statistic output.
Success: Output interface 'PCE_Cl_MU_RH_0_20_a' successfully converted to final value statistic output.
Success: Output interface 'PCE_Cl_MU_RH_20_40_a' successfully converted to final value statistic output.
Success: Output interface 'PCE_Cl_MU_RH_40_65_a' successfully converted to final value statistic output.
Success: Output interface 'PCE_Cl_MU_RH_65_85_a' successfully converted to final value statistic output.
Success: Output interface 'PCE_Cl_MU_RH_85_100_a' successfully converted to final value statistic output.
Success: Output interface 'PCE_Cl_N_MU_RH_40_65_a' successfully converted to final value statistic output.
Success: Output interface 'PCE_Cl_N_MU_RH_65_85_a' successfully converted to final value statistic output.
Success: Output interface 'PCE_Cl_N_MU_RH_85_100_a' successfully converted to final value statistic output.
Success: Output interface 'PCE_Cl_NO3_MU_RH_0_20_a' successfully converted to final value statistic output.
Success: Output interface 'PCE_Cl_NO3_MU_RH_20_65_a' successfully converted to final value statistic output.
Success: Output interface 'PCE_Cl_NO3_MU_RH_65_85_a' successfully converted to final value statistic output.
Success: Output interface 'PCE_Cl_NO3_MU_RH_85_100_a' successfully converted to final value statistic output.
Success: Output interface 'PCE_Gp1_Cl_NO3_CDF_a' successfully converted to final value statistic output.
Success: Output interface 'PCE_Gp2_Cl_NO3_CDF_a' successfully converted to final value statistic output.
Success: Output interface 'PCE_Gp3_Cl_NO3_CDF_a' successfully converted to final value statistic output.
Success: Output interface 'PCE_Gp4_Cl_NO3_CDF_a' successfully converted to final value statistic output.
Success: Output interface 'PCE_I_Uncert_RH_85_100_a' successfully converted to final value statistic output.
Success: Output interface 'PCE_pH_Uncert_RH_0_65_a' successfully converted to final value statistic output.
Success: Output interface 'PCE_pH_Uncert_RH_65_75_a' successfully converted to final value statistic output.
Success: Output interface 'PCE_pH_Uncert_RH_75_100_a' successfully converted to final value statistic output.
Success: Output interface 'Diameter_Colloid_a' successfully converted to final value statistic output.
Success: Output interface 'Conc_Col_FeOx_CS_Sampled_a' successfully converted to final value statistic output.
Success: Output interface 'Conc_Col_FeOx_SS_Sampled_a' successfully converted to final value statistic output.
Success: Output interface 'Conc_Col_Gw_Sampled_a' successfully converted to final value statistic output.
Success: Output interface 'Conc_Col_U_Sampled_a' successfully converted to final value statistic output.
Success: Output interface 'CPu_Col_CSNF_Sampled_a' successfully converted to finalvalue statistic output.
Success: Output interface 'CPu_Col_Wf_Embed_Sampled_a' successfully converted to final value statistic output.
Success: Output interface 'CPu_Per_CSNF_Embed_Col_a' successfully converted to final value statistic output.
Success: Output interface 'CPu_Per_WF_Embed_Col_a' successfully converted to final value statistic output.
Success: Output interface 'Specific_SA_Smectite_Col_a' successfully converted to final value statistic output.
Success: Output interface 'Kd_Np_Rev_Smectite_a' successfully converted to final value statistic output.
Success: Output interface 'Kd_Ra_Rev_Smectite_a' successfully converted to final value statistic output.
Success: Output interface 'Kd_U_Rev_Smectite_a' successfully converted to final value statistic output.
Success: Output interface 'Kd_Am_Rev_U_Col_a' successfully converted to final value statistic output.
Success: Output interface 'Kd_Cs_Rev_U_Col_a' successfully converted to final value statistic output.
Success: Output interface 'Kd_Np_Rev_U_Col_a' successfully converted to final value statistic output.
Success: Output interface 'Kd_Pa_Rev_U_Col_a' successfully converted to final value statistic output.
Success: Output interface 'Kd_Pu_Rev_U_Col_a' successfully converted to final value statistic output.
Success: Output interface 'Kd_Ra_Rev_U_Col_a' successfully converted to final value statistic output.
Success: Output interface 'Kd_Sn_Rev_U_Col_a' successfully converted to final value statistic output.
Success: Output interface 'Kd_Th_Rev_U_Col_a' successfully converted to final value statistic output.
Success: Output interface 'pH_Cell2_Regression_Error_a' successfully converted to final value statistic output.
Success: Output interface 'Cr2O3_SA_a' successfully converted to final value statistic output.
Success: Output interface 'NiO_SA_a' successfully converted to final value statistic output.
Success: Output interface 'Diff_Path_Length_Invert_Top_a' successfully converted to final value statistic output.
Success: Output interface 'CSNF_Rind_SA_a' successfully converted to final value statistic output.
Success: Output interface 'Density_CSNF_Rind_a' successfully converted to final value statistic output.
Success: Output interface 'FHH_Isotherm_k_CP_a' successfully converted to final value statistic output.
Success: Output interface 'FHH_Isotherm_k_CSNF_Rind_a' successfully converted to final value statistic output.
Success: Output interface 'FHH_Isotherm_s_CP_a' successfully converted to final value statistic output.
Success: Output interface 'FHH_Isotherm_s_CSNF_Rind_a' successfully converted to final value statistic output.
Success: Output interface 'HLWG_Rind_SA_a' successfully converted to final value statistic output.
Success: Output interface 'IPC_pH_CSNF_lowRH_Rand_a' successfully converted to final value statistic output.
Success: Output interface 'Colloidal_Kd_Sn_uz_a' successfully converted to final value statistic output.
Success: Output interface 'WDDSAggrGC_a' successfully converted to final value statistic output.
Success: Output interface 'WDDSBenignGC_a' successfully converted to final value statistic output.
Success: Output interface 'Vol_Rubble_Max_Lith_a' successfully converted to final value statistic output.
Success: Output interface 'Vol_Rubble_Max_NonLith_a' successfully converted to final value statistic output.
Success: Output interface 'UNC_WP_EF' successfully converted to final value statistic output.
Success: Output interface 'UNC_DS_EF' successfully converted to final value statistic output.
Success: Output interface 'DS_Crack_Area_Density_a' successfully converted to finalvalue statistic output.
Success: Output interface 'WP_Crack_Area_Density_a' successfully converted to final value statistic output.
Success: Output interface 'Background_Ra226_Ra228_a' successfully converted to final value statistic output.
Success: Output interface 'Background_Alpha_a' successfully converted to final value statistic output.
Success: Output interface 'UNC_DS_EF_conv_from_ln' successfully converted to finalvalue statistic output.
Success: Output interface 'UNC_WP_EF_conv_from_ln' successfully converted to final value statistic output.
Success: Output interface 'FHH_Isotherm_k_CP_a_5003' successfully converted to final value statistic output.
Success: Output interface 'FHH_Isotherm_s_CP_a_5003' successfully converted to final value statistic output.
```

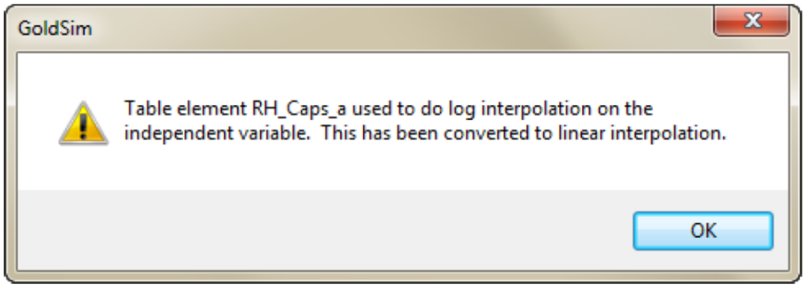
Table Log Interpolation Changed to Linear Interpolation



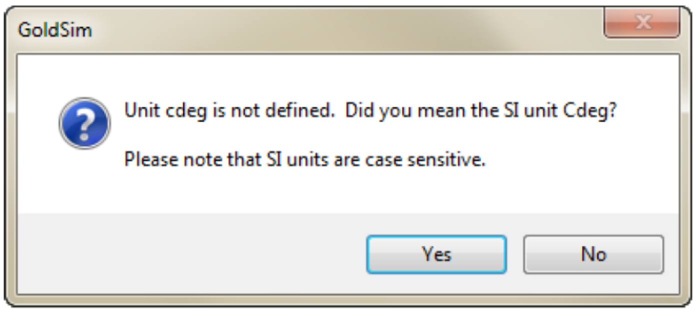








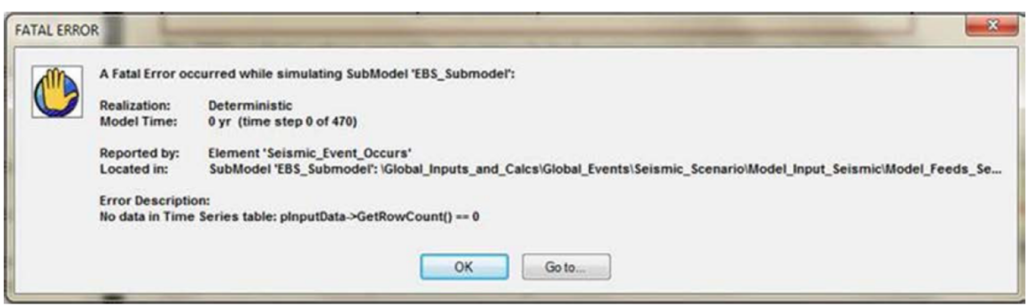
Conversion of Custom Unit ‘cdeg’ to SI Unit ‘Cdeg’



Workaround for Recording Time Series Issue

Description of the Recording Time Series Issue

Located in the Submodel ‘EBS_Submodel’ (at \Global_Inputs_and_Calcs\Global_Events\Seismic_Scenario\Model_Input_Seismic\Model_Feeds_Seismic\Aleatory_Feeds_Seismic), there is a Time Series element, ‘Seismic_Event_Occurs’, that generates an error when the TSPA model is run in GoldSim version 11.1.5. The error message is the following:



Note that in the release version of GoldSim 11.1.5, a different error message with limited and misleading information is shown. An internal test build version of GoldSim (11.1.5015) was used to provide this more detailed and accurate error message above.

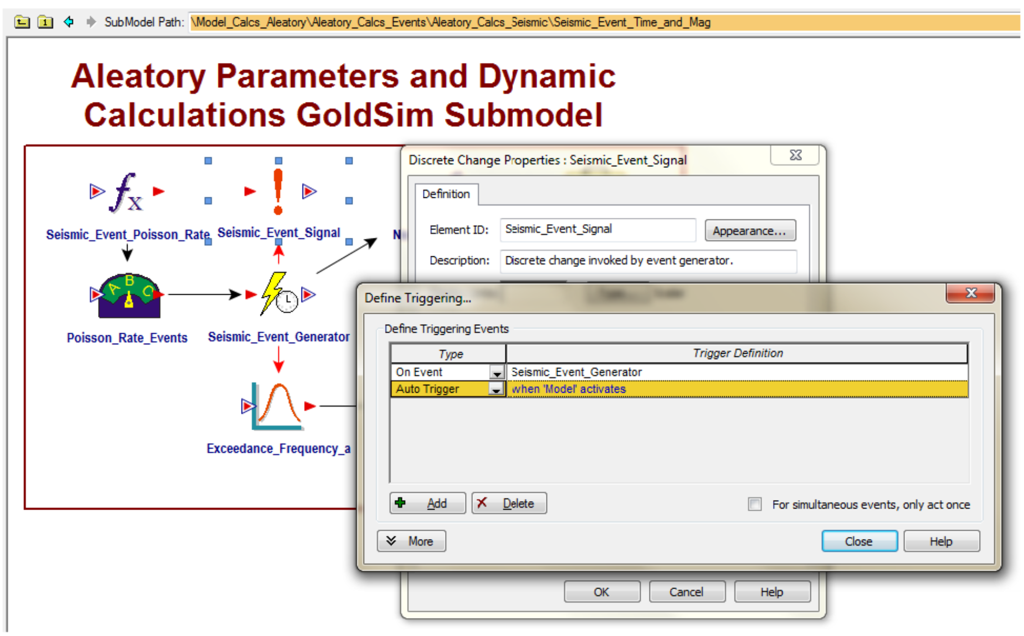
This Time Series Element is linked to a Time Series definition that is passed through the input interface of the SubModel 'EBS_Submodel'. The definition is provided by a Time Series Element in a separate SubModel, 'Aleatory_Params', which records the output of a Discrete Change Element. The recording Time Series Element is 'Seismic_Event_Occurs' and is located here (inside of the SubModel 'Aleatory_Params'): \Event_Export_TS_Recorder. The Discrete Change Element recorded by this Time Series Element is 'Seismic_Event_Signal' and is located here: \Model_Calcs_Aleatory\Aleatory_Calcs_Events\Aleatory_Calcs_Seismic\Seismic_Event_Time_and_Mag.

It seems that the issue (which generates the error message shown above) arises when the Discrete Change Element 'Seismic_Event_Signal' does not trigger at all on a given update of the SubModel 'Aleatory_Params'. In this case, the recorded Time Series definition has no data and this gives rise to an error condition that is caught in GoldSim versions 11.0 and later, but not in earlier versions of GoldSim.

Workaround Implemented in the Converted 11.1.5 Model

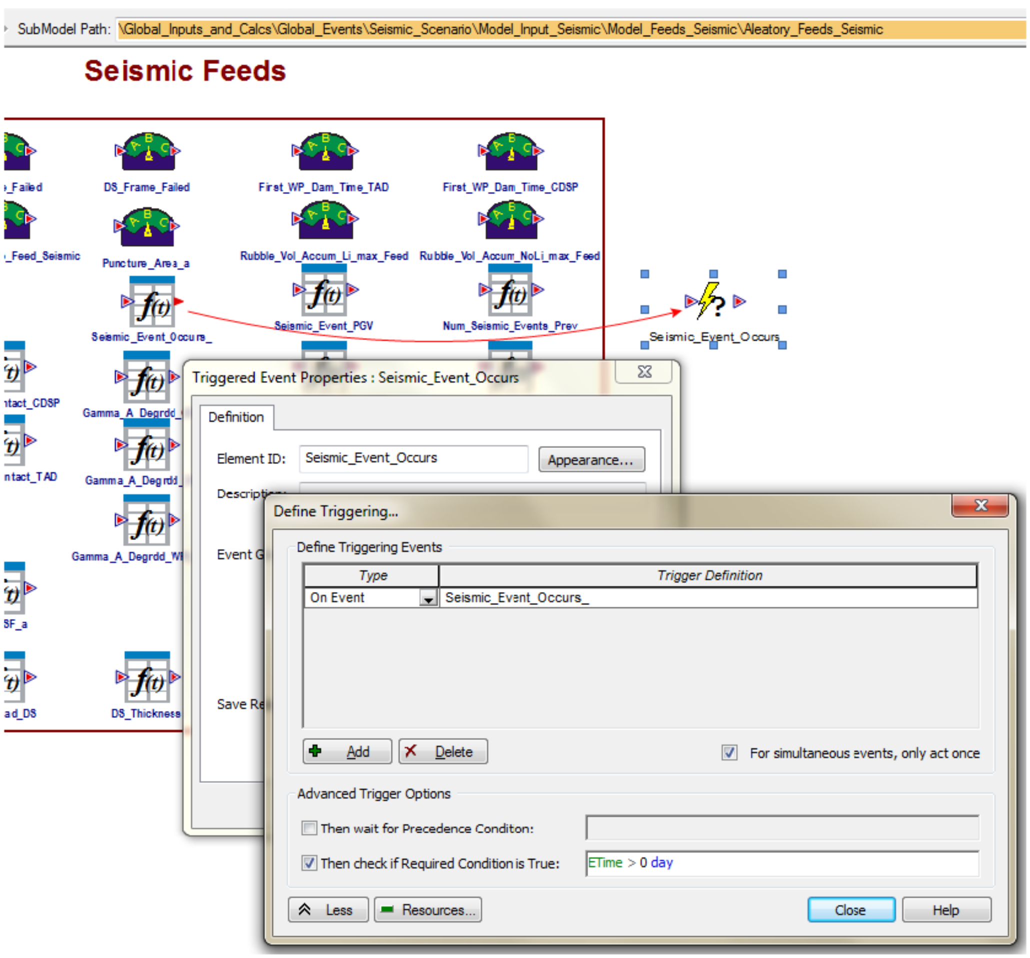
A workaround for the issue described above was implemented in the converted 11.1.5 model. This consisted of two parts, as described below:

1) To ensure that the recording Time Series Element ('Seismic_Event_Occurs'), located inside the SubModel 'Aleatory_Params', always records at least one discrete change event, an 'Auto Trigger' event was added to the Discrete Change Element 'Seismic_Event_Signal' as shown in the screenshot below:



This way, the recording Time Series Element will always record a discrete change event at least at time zero, each time the SubModel 'Aleatory_Params' is updated.

2) The receiving Time Series Element (i.e. that which receives the definition from the recording Time Series Element), located in the SubModel 'EBS_Submodel' and also named 'Seismic_Event_Occurs' (like the recording Time Series Element), was linked to a Triggered Event Element. The receiving Time Series Element was renamed to 'Seismic_Event_Occurs_' and the Triggered Event Element was named 'Seismic_Event_Occurs'. A required condition (ETime > 0 day) was specified for the Triggered Event Element so that it would never trigger at time 0. This can be seen below:



The purpose for adding the required condition was to eliminate the 'Auto Trigger' added to the Discrete Change Element 'Seismic_Event_Signal'. Thus, the Auto Trigger serves to ensure that the Time Series Element 'Seismic_Event_Occurs' (renamed 'Seismic_Event_Occurs_') always has at least one entry. Using the Triggered Event Element with the required condition (ETime > 0 day) then allows that event to be eliminated. Because the original, recorded Discrete Change Element (Seismic_Event_Signal) is triggered by a Timed Event Element, it cannot otherwise ever be triggered at time 0. So the elimination (using the required condition on the Triggered Event Element) of the added time 0 event (i.e. the Auto Trigger on the Discrete Change Element, 'Seismic_Event_Signal') should not be problematic.

Also, since none of the elements originally triggered by the Time Series Element 'Seismic_Event_Occurs' (located in the SubModel 'EBS_Submodel') actually use the value portion of the discrete change output of the Time Series Element (they only use the event), it should be appropriate to use the Triggered Event Element instead of the Time Series Element to trigger these downstream events.

Appendix C. Goldsim Technology Group Report on Problems with the Distributed Process

TSPA Model: Analysis of Distributed Processing Issue

GoldSim Technology Group

Ryan Roper

22 September 2016

Note: Document date inaccurate - Document received as Word file attached to email dated 8/15/2016 with automatic date field enabled.

Contents

Background

In early June 2016, Sandia provided GoldSim Technology Group (GTG) with a 9.60 SP3 version of the Total System Performance Assessment (TSPA) model to be converted to the latest version of GoldSim, 11.1.5. The conversion was successful and we provided, on June 28, 2016, a zip file containing the converted model file (*LA_v5.005_NC_000300_000_11_1_5.gsm*) and a conversion report ('*TSPA Model Conversion Report.docx*').

We had confirmed that the converted 11.1.5 model ran successfully for 2 realizations with distributed processing (DP) on one of our machines. On July 1, 2016, Sandia reported they had successfully run the 11.1.5 version of the model for 300 realizations with 300 slaves (30 machines with 10 slaves each). However, they noted that the run took about 23 hours, in contrast to only 34 minutes that it took when running the 9.60 version of the model with the same slave configuration.

We analyzed the run log for the 11.1.5 DP run and discovered that the majority of slaves completed only 1 or no realizations. Some slaves completed around 2-5 realizations and one completed 60 realizations. At the time, we did not know the reason for the failed or aborted realizations on some slaves. We were able to confirm, however, that successful run times for individual realizations were comparable to run times in 9.60 SP3 (about 17 to 32 minutes).

On August 1, 2016, Sandia reported they had run two more tests. In one test, four realizations were run with two processors. This completed without any errors. In the other test, 300 realizations were run on 30 different machines, each using one slave. It was reported that this run stopped after 280 realizations.

Log files for both of these runs were provided to GTG.

Overview

GoldSim Technology Group provided advanced support to Sandia to help diagnose the source of the failed DP runs with 300 realizations and to provide recommendations to successfully run the 11.1.5 model with the desired DP configuration: 300 realizations on 30 machines with 10 slaves each. This support consisted of the following:

1) Analyzing the run log, provided by Sandia, for the test case in which they attempted to run 300 realizations on 30 machines with 1 slave each.

2) Reproducing the same issue, in-house, in both a 20-realization DP run with 3 machines and 8 total slaves and also a standalone (non-DP) run.

Based on these efforts, we discovered that aborting a model run or realization during the time-zero initialization/pre-processing can leave the WD4DLL.thk file in such a state that subsequent runs will fail. Encountering this issue in a DP run with many realizations is not uncommon, because of how GoldSim manages the assignment of realizations to slaves.

The following sections describe (1) relevant details of slave/realization management in DP runs in GoldSim, (2) key results of our analysis that shed light on the issue and (3) steps that can be taken to successfully complete a DP run with the TSPA model.

GoldSim Distributed Processing

When a realization is completed in a GoldSim DP run, the master assigns to the slave a new realization that is not currently being worked on by another slave. If all remaining realizations are already assigned to a slave, the master will assign one of the incomplete realizations to one or more idle slaves. It is, therefore, possible for more than one slave to work on a given realization at a time. As soon as one of the slaves completes the realization, the master instructs the other slaves to abort the realization and then assigns new realizations to the slaves.

This behavior was implemented in support of the Yucca Mountain project, in which significant variability in slave run times (even for a given realization) were sometimes observed. One slave, hung up on a realization, could become a bottleneck and prevent the simulation from finishing. With the current design for managing slave runs, such bottlenecks are more likely to be avoided.

Observations in the TSPA Model

In an attempt to reproduce the issue encountered by Sandia, we ran the 11.1.5 version of the TSPA model for 20 realizations on 8 slaves. Two of the slaves were on the same machine as the master and the other six slaves ran on two additional machines, three slaves on each. Run times per realization were typically around 20 to 28 minutes. The time-zero initialization of a realization usually took around 10-12 minutes. We did, in fact, observe behavior in this smaller test case that was similar to what Sandia observed. Specifically, one or more realizations failed with the same error message: "*Error reading WD4DLL.thk file.*"

During the initialization, we observed that the size of the WD4DLL.thk file repeatedly increased to a certain point and then dropped back down to 1 KB. It appears that data is written to the .thk file and then, presumably once this data has been read by another process, the file is deleted and replaced by a new, empty file.

Analysis of the run log provided by Sandia (for a 300-realization run on 30 machines with 1 slave each) revealed the following:

1) The first 268 realizations successfully run to completion without being assigned to multiple slaves. Thereafter, many realizations are assigned to more than one slave (in accordance with GoldSim's designed behavior). No failed realizations are observed until after this point in the simulation.

2) A failed realization never occurs on a given slave until at least one realization has been aborted on that slave (due to completion of the realization on a different slave). Once a failure does occur on a slave, all realizations on the same slave either fail or are aborted.

The table below shows all realizations assigned to (but not necessarily completed on) slave #16. In green font color, realization #258, is the last realization that finished successfully on slave #16. In blue font color are realizations that ran for some time on slave #16 until aborted by the master because the realization either finished or failed on a different slave. In red font color are realizations that failed on slave #16.

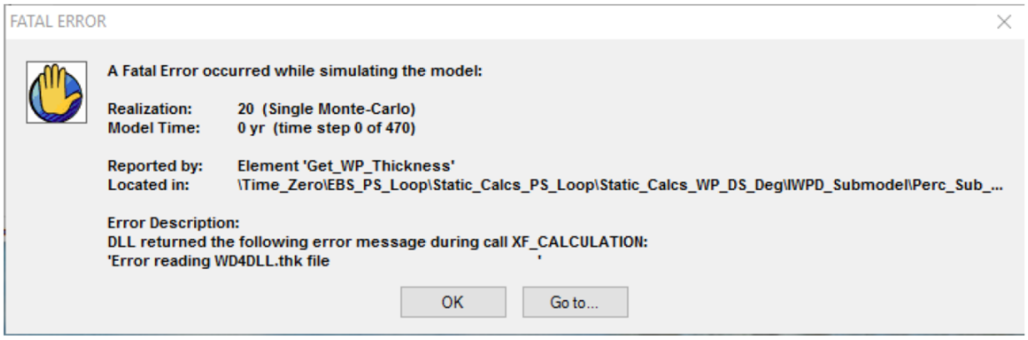
Realization	Start	Duration
#008	12:47:35	0:22:02
#047	13:09:37	0:22:27
#081	13:32:05	0:24:29
#115	13:56:34	0:23:33
#148	14:20:07	0:17:30
#172	14:37:37	0:23:47
#205	15:01:24	0:20:29
#234	15:21:53	0:16:24
#258	**15:38:17**	**0:24:06**
#291	**16:02:23**	**0:13:16**
#294	**16:15:39**	**0:02:45**
#298	**16:18:25**	**0:00:38**
#286	**16:19:03**	**0:00:10**
#296	**16:19:12**	**0:00:38**
#300	**16:19:51**	**0:00:05**

All failures on this and other slaves occurred 37 or 38 seconds after starting the realization. Note that realizations #286 and #300 presumably would have failed also on slave #16 if they had been able to run to 38 seconds. They were aborted before that point because the realizations either finished or failed on a separate slave.

Conclusions

Initially, our hypothesis was that a process from a previous, aborted realization was still holding onto the WD4DLL.thk file when a subsequent realization, assigned to the same slave, attempted to access the file. This would have led to a file access conflict and caused the realization to fail.

Later tests, however, suggested that this was not the case. These tests involved running the model in standalone (i.e. non-DP) mode with one realization. By aborting the standalone run during the time-zero initialization and then re-running the model, we were able to reproduce the same error ("*Error reading WD4DLL.thk file*"). Significantly, after shutting down and restarting the computer and re-running the simulation (with the same auxiliary files), the same error still occurred.



This behavior ruled out the possibility of a file access conflict since there was no process that could have been holding onto the .thk when we ran the model. One important thing we noted was that the .thk file was not empty. When re-running with this .thk file, we encountered the error. With a new, empty .thk file, the simulation completed successfully.

All of our observations seem consistent with the following conclusion:

Failures occur only after an aborted realization leaves the .thk file in a modified, rather than empty/new state. The designed behavior of GoldSim in managing the assignment of realizations to slaves significantly increases the likelihood that such conditions for failure will be satisfied when running the TSPA model with dozens or hundreds of realizations.

Solution and other Recommendations

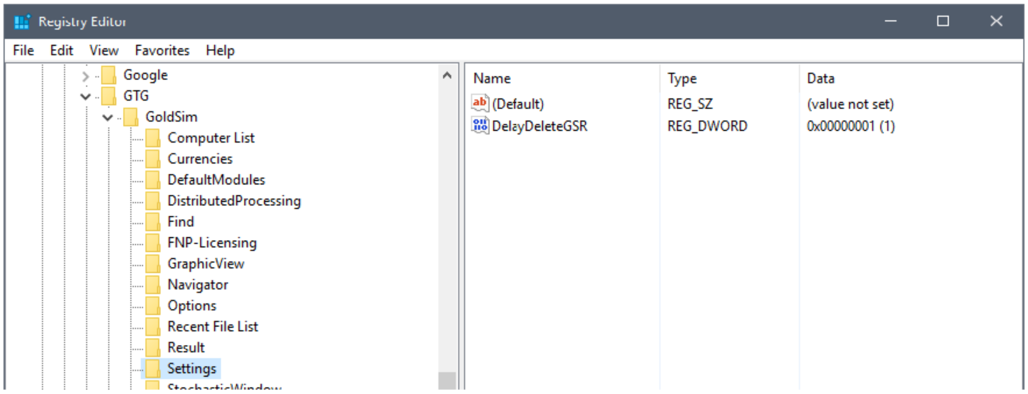
There is no direct or indirect way to change GoldSim's current management behavior during DP runs. The master re-assigns unfinished realizations to available slaves. The master also aborts realization runs on slaves if the realization was finished on another slave. Naturally, this means that a slave may be aborted during the time window in which the .thk state is changed. To resolve this, the author of the DLL responsible for altering the .thk file should ensure the valid structure of the .thk file during the XF_CLEANUP call made by GoldSim whenever a run ends. Whether the run is successfully completed or aborted, GoldSim always offers any initialized DLL a chance for cleanup. Implementing this correctly should resolve the issue that is causing aborted simulations to fail.

Mitigating Solutions

GoldSim offers a feature to resume a network run. Resuming/completing a network run consists of the following steps:

1. Configure master computer to not delete slave result files (.gsr)
2. Preserve original version of model files in edit mode.
3. Load model and start network run as usual. Then select import .gsr files and resume run.

1.The user must define a specific key in the computer's registry that instructs the DP master process to not immediately delete result files (.gsr) returned from slave processes. The registry key is shown in the screenshot below, and must be in place prior to starting a DP run:

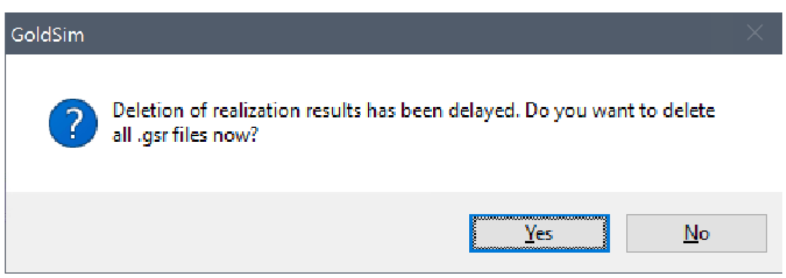


To add the key, do the following:

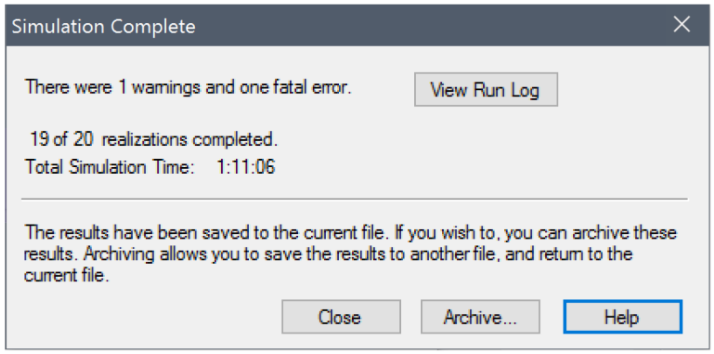
1. Open regedit.exe.
2. Find and expand the following path: `\HKEY_CURRENT_USER\SOFTWARE\GTG\GoldSim\Settings`
3. Right-click the blank background of the panel on the right and select `New`→`DWORD (32-bit) Value` from the context menu.
4. Name the key `DelayDeleteGSR`.
5. Double-click the key and set its value to `1`.

During a DP simulation slaves return a data file (.gsr) to the master after they finish an assigned realization. The file contains run log information (including any warnings and errors) and may contain raw realization results, if the realization was completed successfully. By default, GoldSim imports the .gsr files in sequence (by realization) and immediately deletes the files. Automatic deletion occurs because these files are typically no longer needed and to reclaim disk space (300 realizations in the TSPA model generate about 4GB of .gsr files).

With the above registry key in place, GoldSim no longer deletes the .gsr files after importing them. Instead, GoldSim prompts the user at the end of a DP run:

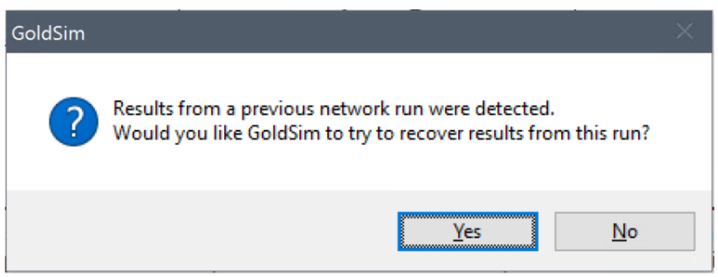


2. After a DP run completes with fatal error, immediately secure the original model file and all completed .gsr files (duplicate them to a different folder or compress them into a backup ZIP archive).

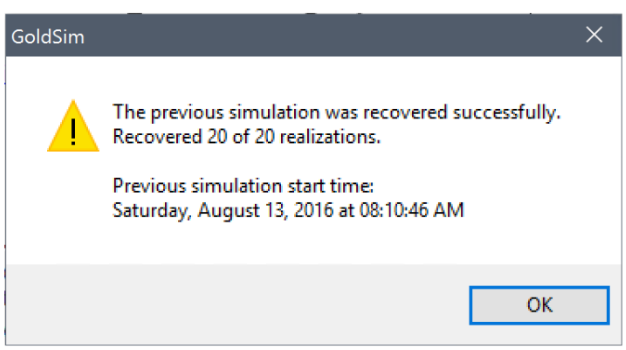


When asked, do not allow GoldSim to delete the .gsr files. Keep them in the same folder as the original model file. Close the Simulation Complete dialog. Do not save the model file as is. If you want to preserve the state of the incomplete simulation, save the model using a different file name.

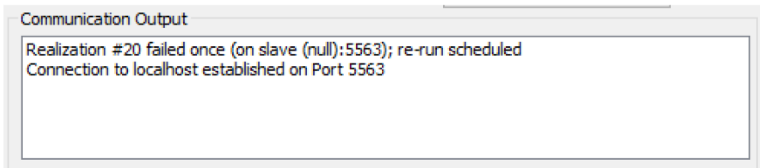
3. To resume a previously incomplete (failed) DP run, the original (Edit Mode) version of the model needs to be opened. When requesting *Run on Network* GoldSim finds the .gsr files in the model file folder location, and prompts the user as shown below:



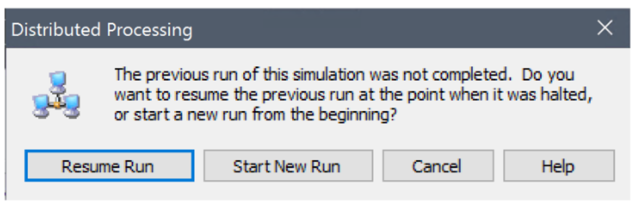
If Yes is clicked, GoldSim inspects the .gsr files and imports them. Afterwards the following status information is shown:



After closing the status message, GoldSim opens the Master Settings dialog. The Communication Output window shows additional information about realizations that previously failed:



The remaining realizations can now be simulated using an appropriate number of slaves. After activating and connecting to the required number of slaves, the simulation can be started by pressing the Run/Resume button. Doing so invokes the following prompt, from which Resume Run must be chosen:



With that, GoldSim resumes the DP simulation and carries out the remaining realizations. Of course, in the process it may encounter the same problem and stop the run prematurely. If so, this process can be repeated (starting with a larger number of previously completed realizations).

Page is intentionally blank

7. 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)

Sandia National Laboratories