IMPORTANT NOTICE: The current official version of this document is available via the Sandia National Laboratories NWMP On-line Documents web site. A printed copy of this document may not be the version currently in effect.

Sandia National Laboratories
Waste Isolation Pilot Plant

Analysis Plan for Sensitivity Analyses: Compliance Recertification Application

AP-103

Task number
1.3.5.1.2.1

Effective Date: 06/24/03

Author: Cliff Hansen (6821) *Original signed by Clifford Hansen* *16 June 03*
Print Signature Date

Technical
Review: Christi Leigh (6821) *Original signed by Christi Leigh* *June 17, 2003*
Print Signature Date

Management
Review: David Kessel (6821) *Original signed by David Kessel* *6/17/03*
Print Signature Date

QA
Review: Mario Chavez (6820) *Original signed by Mario Chavez* *6/23/03*
Print Signature Date

TABLE OF CONTENTS

INTRODUCTION AND OBJECTIVES 3
APPROACH 3
SENSITIVITY ANALYSES FOR THE CRA 5
Sensitivity Analysis for Salado Flow 5
Sensitivity Analysis for Radionuclide Mobilization 6
Sensitivity Analysis for Salado Transport 6
Sensitivity Analysis for Culebra Transport 6
Sensitivity Analysis for Cuttings and Cavings 7
Sensitivity Analysis for DRSPALL 7
Sensitivity Analysis for Direct Brine Release 7
Sensitivity Analysis for Repository Performance 7
METHODOLOGY 8
Scatterplots 8
Regression Analysis 8
Standard Regression Coefficients 8
Partial Correlation Coefficients 9
Stepwise Regression Analysis 9
SOFTWARE LIST 9
SPECIAL CONSIDERATIONS 10
APPLICABLE PROCEDURES 10
REFERENCES 11

LIST OF TABLES

Table 1. Major Components of the 2003 WIPP PA. 4
Table 2. Variables Considered in the Sensitivity Analysis for BRAGFLO. 6
Table 3. Variables Considered in the Sensitivity Analysis for PANEL. 6
Table 4. Variables Considered in the Sensitivity Analysis for NUTS. 6
Table 5. Variables Considered in the Sensitivity Analysis for CCDFGF 8
Table 6. WIPP PA Software Qualified for Use in Sensitivity Analysis 9

LIST OF FIGURES

Figure 1. Sequence of Major Components of WIPP PA. 5

INTRODUCTION AND OBJECTIVES

In 1996 the Department of Energy (DOE) completed a performance assessment (PA) for the Waste Isolation Pilot Plant (WIPP). The PA was part of the Compliance Certification Application (CCA) submitted to the Environmental Protection Agency (EPA) to demonstrate compliance with the radiation protection regulations of 40 CFR 191 and 40 CFR 194. As required by the WIPP Land Withdrawal Act (Public Law 102-579), DOE is required to submit documentation to EPA for the recertification of the WIPP every five years following the first receipt of waste in order to continue operations at the site. This will require that a Compliance Recertification Application (CRA) be prepared and submitted to the EPA by March 26, 2004. The DOE expects to provide the CRA to the EPA during November 2003.

A new set of PA calculations will be included in the CRA submittal to EPA. Analysis Plan AP-105 (Leigh, 2003) presents the full set of PA calculations required for the CRA and lists the series of analysis plans that describe the specific details for each component model that will be run for the CRA. This analysis plan (AP-103) describes the sensitivity analyses that will conducted as part of the PA calculations, and the methodologies to be applied in these sensitivity analyses.

APPROACH

The performance assessment for the CRA involves a series of calculations to determine repository performance over the regulatory period. The PA incorporates both stochastic and subjective uncertainty; stochastic uncertainty describes the possible future states of the repository and incorporates random events such as drilling intrusions, while subjective uncertainty arises from incomplete knowledge about the physical systems affecting the repository, such as the presence or absence of brine pockets in the Castile. Consequently, the PA does not predict performance. Rather, the results of the PA are presented as cumulative complementary distribution functions (CCDFs) which show a family of probability distributions of releases. The distribution of releases represented in a single CCDF arises from the stochastic uncertainty about the future states of the repository. The family of CCDFs arises from subjective uncertainty about the repository system.

Stochastic uncertainty is evaluated by a random (Monte Carlo) sampling from the probability space of future repository states. For example, elements of this probability space can define the number and location of drilling intrusions during the regulatory period. Subjective uncertainty is evaluated by a structured sampling from the probability space of parameter values for the PA models. This structured sampling uses a Latin Hypercube sampling technique to ensure that extreme values for parameters are represented and to control correlations between individual parameters. Elements of the probability space for subjective uncertainty define the uncertain properties of physical materials, such as permeabilities, as well as the presence or absence of certain repository features, such as microbial activity in the waste.

Conceptually, the PA models can be regarded as a mapping from a set of input parameters into a set of model results. A sensitivity analysis explores this mapping to determine how the uncertainty in the input parameters induces uncertainty in the output results. In particular, the sensitivity analyses for the WIPP PA help to identify which of the parameters in the space for subjective uncertainty are significant in the uncertainty in PA results.

Sensitivity analyses will be conducted for each of the major components of the PA. The sensitivity analysis for each component will consider all uncertain parameters used as input for that component. Table 1 lists the major components of the PA and the associated computer codes; Figure 1 shows the sequence in which the major codes are run. With the exception of DRSPALL, each code's results will be documented in an analysis package. Sensitivity analyses will be documented along with the analysis package for each component.

Table 1. Major Components of the 2003 WIPP PA.

Process or Event	Computer Code
Salado Flow (Brine and Gas)	BRAGFLO
Radionuclide Mobilization	PANEL
Radionuclide Transport in the Salado (except for multiple intrusions)	NUTS
Radionuclide Transport in the Salado (multiple intrusions only)	PANEL
Radionuclide Transport in the Culebra	SECOTP2D
Direct Releases - Cuttings and Cavings	CUTTINGS_S
Direct Releases – Spallings	DRSPALL
Direct Brine Releases	BRAGFLO
Repository Performance	CCDFGF

A new conceptual model for spallings releases is currently under development. The code DRSPALL implements the new conceptual model, and may be used to compute the volume of solid material brought to the surface as spallings from a drilling intrusion. If DRSPALL results are used in the CRA, these results will be documented in an analysis package and will be accompanied by the sensitivity analysis of DRSPALL results.

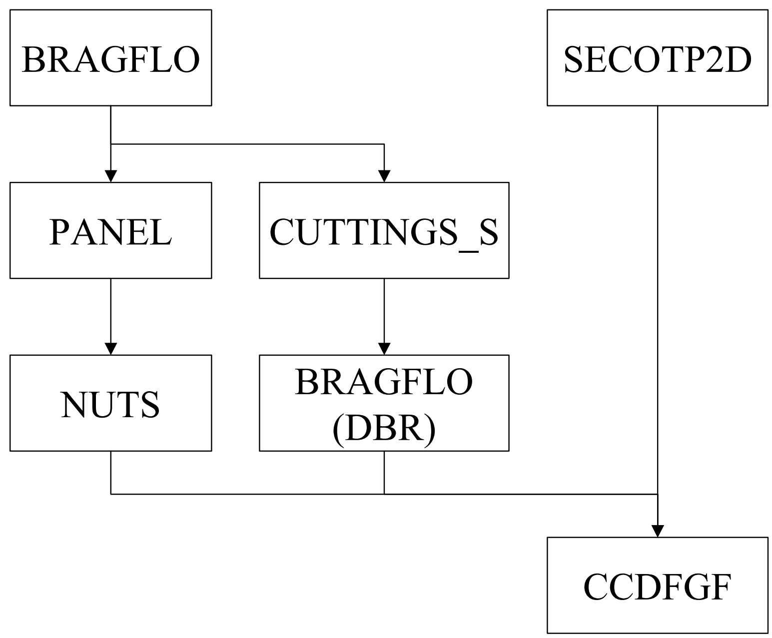

Figure 1. Sequence of Major Components of WIPP PA.

SENSITIVITY ANALYSES FOR THE CRA

The following sections identify the sensitivity analysis that will be included in the documentation of each code's results. Additional analysis can be included at the discretion of the analysts responsible for each code's analysis package. The CRA calculations will include 3 replicates with 100 realizations each from the space of subjective uncertainty. Sensitivity analyses will be done for replicate 1 for all codes except CCDFGF. Sensitivity analysis for CCDFGF will be done on a pooled sample of all 300 realizations.

Sensitivity Analysis for Salado Flow

BRAGFLO computes brine pressures, saturations and brine flows that are used as initial conditions for the subsequent models. BRAGFLO is run for a single undisturbed scenario, and for both E1 and E2 intrusion scenarios. Although BRAGFLO results are intermediate in the context of the PA, analysis of these results can yield insights into processes that may be significant to repository performance.

The sensitivity analysis for BRAGFLO will identify which uncertain input parameters are important to the uncertainty of the BRAGFLO output variables listed in Table 2. Variable names in Table 2 are taken from the set of variables computed by the code ALGEBRA when applied to the output of the code POSTBRAG, which in turn consolidates the output of the code BRAGFLO.

Table 2. Variables Considered in the Sensitivity Analysis for BRAGFLO.

Variable
Volume-averaged pressure in the repository
Volume-averaged brine saturation in the repository
Brine flow out of the repository

Sensitivity Analysis for Radionuclide Mobilization

PANEL computes mobilized concentrations of radionuclides, both as dissolved actinides and as colloids, in both Salado and Castile brines. PANEL also computes the amount of radionuclides transported to the Culebra for the representative multiple intrusion scenario. The sensitivity analysis for PANEL will identify which uncertain input parameters are important to the uncertainty of the PANEL outputs listed in Table 3.

Table 3. Variables Considered in the Sensitivity Analysis for PANEL.

Variable
Mobilized concentration of each radionuclide
Amount of each radionuclide transported to the Culebra in multiple intrusion scenario

Sensitivity Analysis for Salado Transport

NUTS computes the amount of radionuclides transported through the Salado to the land withdrawal boundary (LWB) and to the Culebra, for all scenarios except the multiple intrusion scenario. PANEL computes transport to the Culebra in the multiple intrusion scenario. The sensitivity analysis for NUTS will identify which uncertain input parameters are important to the uncertainty of the NUTS outputs listed in Table 4.

Table 4. Variables Considered in the Sensitivity Analysis for NUTS.

Variable
Total radionuclides transported through marker beds to the LWB
Total radionuclides transported to the Culebra through boreholes
Total radionuclides transported to the Culebra through the shaft seals

Sensitivity Analysis for Culebra Transport

SECOTP2D computes the amount of radionuclides transported through the Culebra to the land withdrawal boundary (LWB) from a source placed above the repository 100 years after closure. Radionuclides from this source reached the LWB in only one of the 300 realizations for the CCA. (Helton et al, 1998) Consequently, no detailed sensitivity analyses were conducted. If ten or more realizations of the CRA show transport to the LWB, then sensitivity analyses will be conducted to identify which uncertain input parameters are important to the uncertainty of the SECOTP2D output. The sensitivity analyses will consider the total amounts of each radionuclide transported to the LWB.

Sensitivity Analysis for Cuttings and Cavings

CUTTINGS_S computes the volume of solid material brought to the surface from a drilling intrusion as cuttings and cavings. The sensitivity analysis for CUTTINGS_S will identify which uncertain input parameters are important to the uncertainty in the volume of solid material released as cuttings and cavings.

Sensitivity Analysis for DRSPALL

A new conceptual model for spallings releases is currently under development. The code DRSPALL implements the new conceptual model, and may be used to compute the volume of solid material brought to the surface as spallings from a drilling intrusion. A sensitivity analysis will be done in conjunction with the peer review of DRSPALL. The sensitivity analysis for DRSPALL will identify which uncertain input parameters are important to the uncertainty in the volume of solid material released as spallings.

Sensitivity Analysis for Direct Brine Release

BRAGFLO computes the volume of brine that may be released to the surface during a drilling intrusion. Direct brine releases are calculated for three representative drilling locations, for both undisturbed conditions and for E1 and E2 intrusions. The sensitivity analysis for the direct brine release calculations from BRAGLO will identify which uncertain input parameters are important to the uncertainty of the volume of brine released during a drilling intrusion.

Sensitivity Analysis for Repository Performance

CCDFGF computes the probability distributions of releases from the repository. CCDFGF employs random sampling to determine future events at the repository, and uses the results of the other PA codes to determine the release for each future. The sensitivity analysis for CCDFGF will identify which uncertain input parameters are important to the uncertainty of the CCDFGF outputs listed in Table 5. Sensitivity analyses will be conducted for spallings releases only if DRSPALL results are used. The current model for spallings uses a single sampled parameter to determine the volume of material releases; therefore no sensitivity analysis is needed.

Table 5. Variables Considered in the Sensitivity Analysis for CCDFGF.

Variable
Total releases from the repository
Direct releases : cuttings and cavings
Direct releases : spallings (if DRSPALL is used)
Direct brine releases
Releases by transport in the Culebra (if any releases are observed.)
Releases by transport in the Salado (if any releases are observed.)

METHODOLOGY

WIPP PA employs two basic techniques for sensitivity analyses: scatterplots and regression analysis. An overview of the theory behind each technique is provided in Helton et al, 1998. The choice of techniques employed for the sensitivity analysis of each component of PA is left to the discretion of the analysts responsible for each package.

Scatterplots

Scatterplots provide the simplest and most direct method to illustrate the relationship between a single uncertain input variable and a single output variable. When there are only a few uncertain input parameters that can be significant in the variability of the output, scatterplots can completely reveal the relationships between input and output. In other circumstances, scatterplots are often a good technique to illustrate relationships identified by regression analysis. Scatterplots can help in identifying non-linear relationships which are not necessarily detected by regression techniques.

Regression Analysis

Regression analysis can identify linear relationships between input and output variables. Conceptually, a regression analysis attempts to find a linear relationship between the input and output variables that minimizes some quantity, which is usually the sum of the differences between the linear model and the actually data. Regression analyses are most useful when there are many input parameters that may contribute to variability in the output. The results of a regression analysis aid in identifying which of the many input variables have the most influence in the uncertainty of an output variable.

There are several variations of techniques that can be used to build linear models, including computing standard regression coefficients, partial correlation coefficients, and conducting stepwise regression analysis.

Standard Regression Coefficients

Standard regression coefficients (SRCs) are the simplest form of regression analysis. SRCs provide a simple ordering of the correlation coefficient of each input variable; the variables with the larger coefficients are more important in the uncertainty in the output variable. SRCs are computed by first normalizing the input variables to a mean of zero and standard deviation of one. Normalization eliminates any undue influence from each input variable's units and distribution and allows regression coefficients to be compared for input variables with greatly different ranges. The WIPP PA code PCCSRC can compute SRCs.

Partial Correlation Coefficients

Partial correlation coefficients (PCCs) provide a method of isolating the effects of each of the input variables. PCCs are computed by transforming both the input and output variables so that the PCC for each input variable measures the degree of correlation with the output variable, with the effects of the other input variables removed. The WIPP PA code PCCSRC can compute PCCs.

Stepwise Regression Analysis

When many input variables must be considered, stepwise regression analysis provides an alternative means of ordering the input variables in order of decreasing importance to the variability in the output variable. In a stepwise regression analysis, a sequence of linear models is constructed. First the analysis finds the single input variable with the largest absolute value for its SRC, and computes a one-variable linear model for the output data. Then the analysis transforms the output data to remove the effects of the first selected input variable, then repeats the analysis to find the second most important variable. Successive input variables are added to the regression model until the stopping criteria are satisfied. For more information on the theory behind a stepwise regression analysis, refer to Helton el al, 1998.

A stepwise regression analysis provides an ordered list of the input variables that are most significant to the variability in the output variable. In addition, the correlation coefficients provide a measure of the model's fit as each input variable is added to the model. When input variables are uncorrelated, the difference in successive correlation coefficients indicate the fraction of total uncertainty in the output variable that is accounted for by the latest additional input variable. The WIPP PA code STEPWISE can compute a stepwise regression analysis.

SOFTWARE LIST

Some sensitivity analyses, such as scatterplots, can be conducted with commercial software at the discretion of the analyst. The WIPP PA codes listed in Table 6 are qualified for sensitivity analysis on the ES-40, ES-45, and 8400 Compaq ALPHA computers running Open VMS Version 7.3-1 (SNL, 2003a, 2003b and 2003c). The code LHS2STEP is a preprocessor that is used with STEPWISE.

Table 6. WIPP PA Software Qualified for Use in Sensitivity Analysis

Code	Version	Code Function
PCCSRC	2.21	Computes SRCs and PCCs
STEPWISE	2.21	Computes stepwise regression analysis
SPLAT	1.02	Plotting
LHS2STEP	1.04	Preprocessor for STEPWISE

SPECIAL CONSIDERATIONS

None.

APPLICABLE PROCEDURES

Analyses will be conducted in accordance with the quality assurance (QA) procedures listed below.

Training: Training will be performed in accordance with the requirements in NP 2-1, Qualification and Training.

Parameter Development and Database Management: Selection and documentation of parameter values will follow NP 9-2. The database will be managed in accordance with relevant technical procedure.

Computer Codes: All software used in this analysis will be qualified in accordance with NP 19-1.

Analysis and Documentation: Documentation will meet the applicable requirements in NP 9-1.

Reviews: Reviews will be conducted and documented in accordance with NP 6-1 and NP 9-1, as appropriate.

REFERENCES

Helton, J.C., Bean, J.E., Berglund, J.W., Davis, F.J., Economy, K., Garner, J.W., Johnson, J.D, MacKinnon, R.J., Miller, J., O'Brien, D.G., Ramseq, J.L., Schreiber, J.D., Shinta, A., Smith, L.N., Stoelzel, D.M., Stockman, C., Vaughn, P. 1998. Uncertainty and Sensitivity Analysis Results Obtained in the 1996 Performance Assessment for the Waste Isolation Pilot Plant. Sandia National Laboratories. Albuquerque, N.M.

Leigh, C.D. 2003. Analysis Plan for Compliance Recertification Application Performance Assessment Calculations (AP-105). Sandia National Laboratories. Albuquerque, N.M.

WIPP PA (Performance Assessment). 2003a. "Analysis Report for the VMS 7.3-1 Regression Test." Sandia National Laboratories. Sandia WIPP Central Files Records Package # 525277.

WIPP PA (Performance Assessment). 2003b. "Analysis Report for the ES45 Regression Test." Sandia WIPP Central Files Records Package # 525278.

WIPP PA (Performance Assessment), 2003c. "Analysis Report for the A8400 Regression Test." Sandia WIPP Central Files Records Package # 525278.