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**Sandia National Laboratories
Waste Isolation Pilot Plant**

**Analysis Plan for Calculations of
Salado Flow and Transport:
Compliance Recertification Application**

AP-099

**Task number
1.3.5.1.2.1**

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1 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-099) describes the set of calculations that are run to simulate brine and gas flow and transport in and around the repository for 10,000 years.

2 APPROACH

Salado brine and gas flow is simulated using the BRAGFLO computer code while Salado transport is simulated using the computer codes PANEL and NUTS. BRAGFLO and NUTS use the same numerical grid. The numerical grid that will be used for the CRA simulations is different than what was used for the CCA and PAVT calculations. This grid is described in Section 2.1. In addition to grid changes, minor modifications have been made to the BRAGFLO source code for the CRA calculations. These code changes are described in Section 2.2.

Three LHS replicates each consisting of 100 vectors of sampled parameters will be generated using the LHS computer code. New random seeds will be used for the CRA calculations. Using new random seeds means that all comparisons to previous PA results can only be made on a replicate-by-replicate basis. No comparisons will be made on a vector-by-vector basis.

One undisturbed and five disturbed scenarios will be run for BRAGFLO. NUTS is used to calculate transport in all but one disturbed scenario (E2E1). Transport in this scenario is calculated by PANEL. These scenarios have not changed since the CCA and PAVT.

2.1 Numerical Grid

The numerical grid that will be used for the CRA BRAGFLO and NUTS calculations is shown in Figure 1. It is the same grid that was developed for the second meeting of the Salado Flow Peer Review and is described in detail in AP-106 (Stein and Zelinski, 2003).

The differences between the CRA grid and the grid used for the CCA and PAVT are listed below:

1. The CRA grid explicitly models the Option D panel closures. A final description of how these features are represented for the CRA is included in AP-106 (Stein and Zelinski, 2003). The material properties, CONC_PCS and DRZ_PCS are described in a separate memorandum (Stein, 2002).
2. A simplified shaft seal model is implemented for the CRA. This model and associated parameters is described in detail in the analysis plan AP-094 (James and Stein, 2002) and in the associated analysis report (James and Stein, 2003). This model includes the new materials: SHFTU, SHFTL_T1, and SHFTL_T2.
3. The fracture model will be applied to the upper and lower DRZ as was done in the PAVT.
4. CRA grid has more grid cells than the grid used in the CCA and PAVT PA. These additional grid cells were added to increase grid refinement and reduce numerical dispersion outside the repository along the transport pathways to the Land Withdrawal Boundary.

2.2 Salado Flow Calculations

2.2.1 BRAGFLO Version 5.0

A new version of BRAGFLO will be used for the CRA PA calculations. BRAGFLO version 5.0 differs from version 4.10, used for the PAVT calculations, only in the way it obtains some of the input parameters. These changes do not change the numerical functionality of the code. Version 5.0 has the following changes from version 4.10 (WIPP, 2003):

1. The creep closure “porosity surface” is read in from an external data file instead of being “hardwired” into data statements in the BRAGFLO source code. This change does not affect the porosity surface that will be used for the CRA calculations. This surface will be the same one used for the CCA and PAVT.
2. Additional “hardwired” parameters have been moved to the BRAGFLO input file. These parameters include molecular weights, equation of state parameters, and other constants that are now read in from the parameter database. Except for the molecular weight of cellulose (see section 2.2.2), these parameters have not changed since the CCA and PAVT.
3. An additional error check was added to the code to ensure that the number of waste areas is read in correctly.

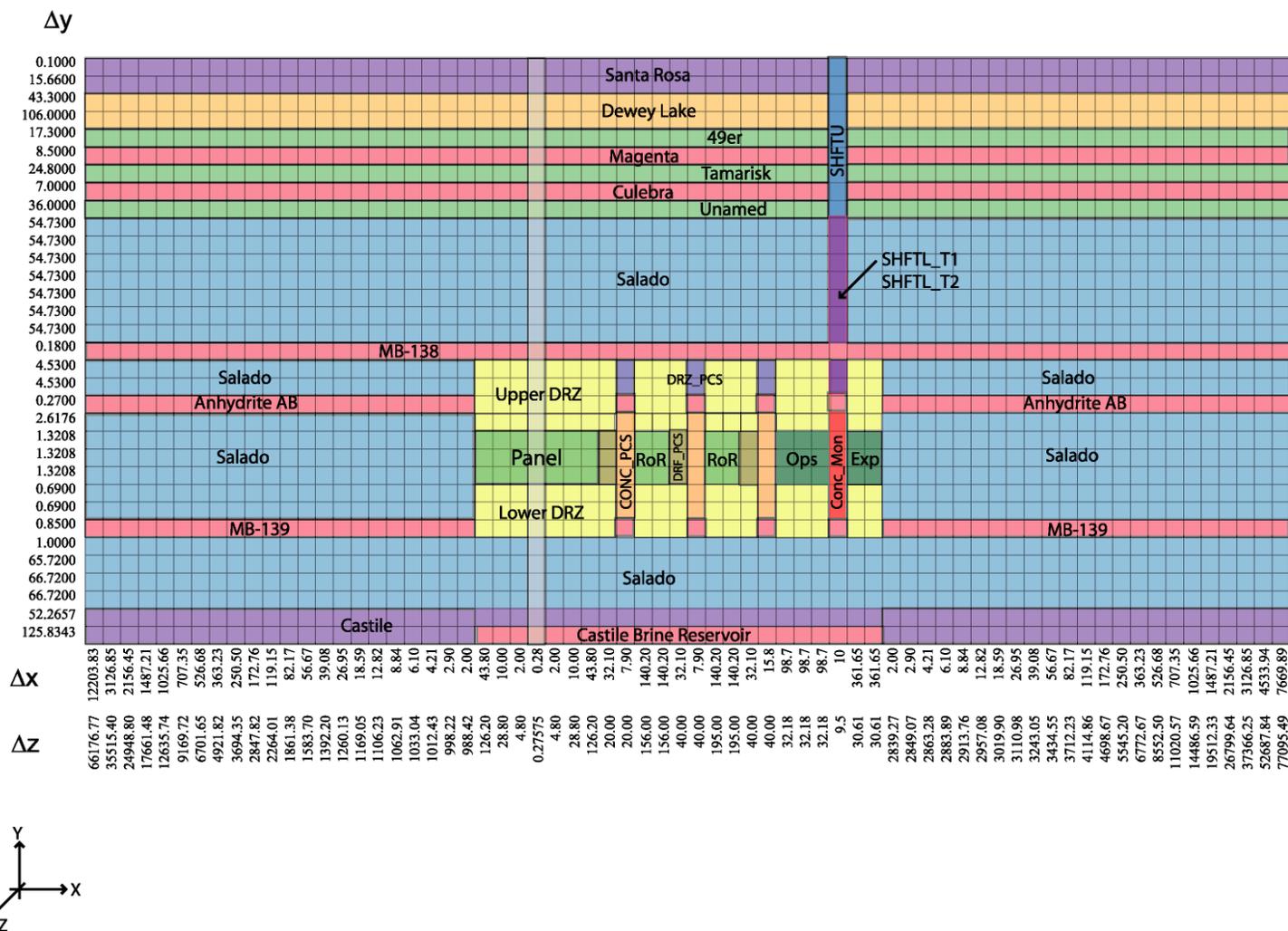


Figure 1. The numerical grid that will be used by BRAGFLO and NUTS for the CRA PA calculations of Salado flow and transport.

2.2.2 *New Parameters used in BRAGFLO Calculations*

Several parameters will change for the CRA Salado flow and transport calculations since the CCA and PAVT. These include the molecular weight of cellulose (new parameter) and inventory related parameters (new values). Table 1 lists the parameters that will change for the CRA. All parameter changes will be made and documented in accordance with QA procedure NP 9-2.

Table 1. Parameter Changes Affecting BRAGFLO Calculations for the CRA

<i>Material</i>	<i>Property</i>	<i>Description</i>
REFCON	MW_CELL (new parameter)	Carbon-normalized molecular weight of cellulose
WAS_AREA & REPOSIT	DCELLCHW	Average density of CH cellulose
WAS_AREA & REPOSIT	DCELLRHW	Average density of RH cellulose
WAS_AREA & REPOSIT	DIRNCCHW	Bulk density of iron containers in CH waste
WAS_AREA & REPOSIT	DIRNCRHW	Bulk density of iron containers in RH waste
WAS_AREA & REPOSIT	DIRONCHW	Average density of iron-based materials in CH waste
WAS_AREA & REPOSIT	DIRONRHW	Average density of iron-based materials in RH waste
WAS_AREA & REPOSIT	DPLASCHW	Average density of plastics in CH waste
WAS_AREA & REPOSIT	DPLASRHW	Average density of plastics in RH waste
WAS_AREA & REPOSIT	DPLSCCHW	Bulk density of plastic liners in CH waste
WAS_AREA & REPOSIT	DPLSCRHW	Bulk density of plastic liners in RH waste
WAS_AREA & REPOSIT	DRUBBCHW	Average density of rubber in CH waste
WAS_AREA & REPOSIT	DRUBBRHW	Average density of rubber in RH waste

2.2.2.1 Molecular Weight of Cellulose

In order to calculate gas generation by microbial degradation, the BRAGFLO code uses a single molecular weight for cellulosic material. At the time of the CCA, it was decided that the most appropriate representation for cellulosic materials that are present in that waste was in the form of $C_6H_{10}O_5$ (Wang and Brush, 1996; DOE, 1996: Appendix WCA.5.1). However, the BRAGFLO CCA calculations used the molecular weight of CH_2O (DOE, 1996: Appendix BRAGFLO 4.13). The CRA will reconcile this difference by using the $C_6H_{10}O_5$ model for cellulose. Specifically, the carbon-normalized molecular weight of cellulose represented by BRAGFLO in the CCA (CH_2O) was 30.026×10^{-3} kg/mol. This value has been changed for the CRA to 27.023×10^{-3} kg/mol, which corresponds to the molecular model $C_6H_{10}O_5$. This parameter value will be retrieved from the parameter database for the CRA calculations.

2.2.2.2 Non-Radioactive Inventory Parameters

A number of parameters related to the inventory of cellulose, plastics, and rubbers will likely change as a result of the revision of the transuranic waste inventory database being conducted by Los Alamos National Laboratory (Downes and Guerin, 2003). Table 1 lists these parameters.

2.3 Salado Transport Calculations

2.3.1 NUTS Calculations

The WIPP radioisotope mobilization and decay code NUTS version 2.05b will be used to simulate the transport of radionuclide isotopes through the Salado Formation for scenarios S1 through S5. This version of the code is identical to that used for the PAVT (2.05) except that it has been compiled with larger dimensions to accommodate the new grid. Two types of NUTS runs are made for the PA calculations. "Screening" runs determine if any radionuclides reach the accessible environment. "Non-screening" runs calculate the actual radionuclide transport for those vector/scenario combinations for which there is radionuclide transport to the accessible environment. NUTS "screening runs" require three input files for running a PA calculation. Two of the input files are associated with the BRAGFLO calculations (BRAGFLO input file and POSTBRAG binary file). These files provide NUTS with the flow fields needed for transport calculations. In addition, NUTS requires an input file containing run parameters and isotope decay data. NUTS "non-screening runs" require an additional binary input file that contains source term results from the code PANEL. In order for PANEL to be run, the updated radioactive inventory data must be available from Los Alamos National Laboratory (Downes and Guerin, 2003).

2.3.2 PANEL Calculations

The WIPP radioisotope mobilization and decay code PANEL version 4.02 will be used to simulate the transport of radionuclides through the Salado Formation for scenario S6. This scenario is the E2E1 scenario that has two intrusions that breach a single panel of the repository. The first intrusion (E2) hits only the repository at 1,000 years and a second intrusion (E1) passes through the repository and hits a brine pocket at 2,000 years. One of the input files needed for PANEL is the POSTALG binary file that is processed from the POSTBRAG binary file. The other input file contains solubility and inventory data derived from the parameter database.

PANEL version 4.02 has the source term calculation included in the code. In the CCA and PAVT, the source term calculation was done in ALGEBRA.

3 SOFTWARE LIST

The major codes to be used for the CRA calculations are listed in Table 2. Calculations will be performed on qualified ES-40 and ES-45 Compaq ALPHA computers running Open VMS Version 7.3-1 (SNL, 2003).

Table 2. Codes to be used in the CRA Salado Flow and Transport Analysis.

Code	Version	Code Function
ALGEBRACDB	2.35	Data processor
BLOTADB	1.37	Plotting
BRAGFLO	5.00*	Brine and gas flow
GENMESH	6.08	Grid generation
ICSET	2.22	Sets initial conditions
LHS	2.41	Latin hypercube sampler
MATSET	9.10	Sets material parameters
NUTS	2.05b	Salado transport
PANEL	4.02*	Salado transport
POSTBRAG	4.00	BRAGFLO postprocessor
POSTLHS	4.07	LHS postprocessor
PREBRAG	7.00*	BRAGFLO preprocessor
PRELHS	2.30	LHS preprocessor
SPLAT	1.02	Plotting
SUMMARIZE	2.20	Data interpolation

* Codes are not currently qualified for use under NP-19-1. These codes will be qualified before being run for the CRA.

4 TASKS

The schedule, tasks, and responsible individuals are outlined in Table 3.

Table 3. Tasks and responsibilities.

Estimated Date	Task(s)	Responsible Individual
March 1-March 31, 2003	Prepare input files	William Zelinski Joshua Stein
April 1, 2003	Begin BRAGFLO calculations	Roger Coman Steve Tisinger
April 15, 2003	Begin PANEL and NUTS calculations	Roger Coman Steve Tisinger
May 1, 2003	Begin analysis of BRAGFLO and NUTS results	Joshua Stein William Zelinski
June 1, 2003	Final Analysis Package Completed	Joshua Stein William Zelinski

5 SPECIAL CONSIDERATIONS

None.

6 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: New or revised computer codes that will be used in the analyses will be qualified in accordance with NP 19-1. All other codes unchanged since the PAVT are qualified under multi-use provisions of NP 19-1. Codes will be run on fully qualified ES-40 and/or ES-45 DEC ALPHA computers running Open VMS Version 7.3-1

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.

7 REFERENCES

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