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Sandia National Laboratories
Carlsbad Programs Group

Waste Isolation Pilot Plant

Analysis Plan for Completion of the Spallings Model for WIPP Recertification

Task 1.3.5.1.2.1

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1. INTRODUCTION AND OBJECTIVES

During the period July 1996 to April 1997, the 24 conceptual models that comprise the Waste Isolation Pilot Plant Performance Assessment (WIPP PA) underwent peer review according to 40 CFR Part 194.27 as part of the process of qualifying them for use in compliance calculations. While the peer review panel ultimately accepted 23 of these models, it found the spallings model inadequate to represent future states of the repository (Wilson et al., 1997). Despite the inadequacies of spallings conceptual model, the total system performance assessment was accepted by the US Environmental Protection Agency (US EPA) in the May 1998 Final Rule (EPA, 1998) because the spallings release volumes presented in the Compliance Certification Application (CCA) (DOE, 1996) were deemed conservative.

Much of the supporting work that led to the conclusion that CCA spallings release volumes were reasonable and conservative was encompassed in a new mechanistically based model, called the Cavity Growth Model, documented in Hansen et al. (1997). While several approaches were explored, the primary computational model used to generate quantitative results in Hansen at al. (1997) was GASOUT. This code successfully calculated bounding releases for spallings within expected ranges of boundary conditions and input parameters. The peer review panel identified limitations, however, which led to an initiative to increase the model's range of robustness and applicability. At the direction of the US Department of Energy (US DOE), Sandia National Labs (SNL) attempted to improve the GASOUT code under AP-048, Analysis Plan for Development of Improved Spall Failure Physical Model and Computational Methodology (Schatz, 1998). The work was undertaken from May, 1998 to November, 1999, and therein the GASOUT model evolved into DR_SPALL. AP-048 was subsequently recalled, though it serves as a starting point for outlining where the model was in 1998-1999, and what work remains.

According to the WIPP Land Withdrawal Act of 1992 (Public Law 102-579, 1992), the US Department of Energy (US DOE) must submit documentation demonstrating continued compliance with federal environmental regulations every five years in order to continue operating the site. This will require that a compliance re-certification application (CRA) be prepared and submitted to the EPA by November 2003. In a guidance letter sent from EPA headquarters in Washington, DC to the US DOE Carlsbad Field Office on August 6, 2002, the EPA indicated that they "expect the CRA PA will implement a new spallings conceptual model." (EPA, 2002). This analysis plan outlines the steps necessary to produce a fully verified and validated, peer-reviewed spallings model for the WIPP recertification PA.

2. APPROACH

The starting point for this analysis is with the DR_SPALL model that resulted from work documented by Hansen et al. (1997) and Schatz (1998). DR_SPALL estimates spallings releases to the surface using repository gas flow, wellbore hydraulics, and tensile failure models coupled by a cavity growth region. While the model is currently operational, it was never successfully peer-reviewed and qualified for use in the WIPP PA. There are several steps required to prepare the model for peer review and implementation in the total system PA.

Key task areas include:

1. Submit Software Design Package
2. Model testing, verification, and validation
3. Qualification of input parameters
4. Submission of software QA package
5. Implementation in CRA PA

2.1 Submit Software Design Package

The initial deliverable, a software design package, will comprise the following items:

- Analysis Plan for Completion of the Spallings Model for WIPP Recertification
- Software Quality Assurance Plan for DR_SPALL
- Requirements Document for DR_SPALL
- Design Document for DR_SPALL

2.2 Model Testing, Verification, and Validation

There are no "standard" spallings models against which to compare DR_SPALL output. As such, results will be validated against field analogs or analytical solutions for specific processes. The current conceptual model couples several processes including (1) radial, compressible gas flow through porous media, (2) tensile failure of a continuous medium due to effective stresses including seepage forces, (3) fluidization of tensile-failed material in a growing cavity region, and (4) multiphase wellbore flow.

2.2.1 Code testing for stability and sensitivity

The code will be tested for stability and sensitivity over a range of input variables and boundary conditions that are deemed reasonable for the WIPP system. Several preliminary "response surfaces" will be generated that represent the results of a number calculations using a variety of input parameter values.

2.2.2 Code verification using analytical solutions

Where possible, sub-models will be tested against analytical solutions to verify that the mathematics are solved correctly. For example, the accuracy of the solution of the porous media equations in the repository gas flow model may be tested against solutions shown in Gilding and Goncerzewicz (2000) and Chan et al. (1989). This will require modification of initial conditions and boundary conditions specific to the test problems. Implementation will include insertion of parameters into the production code that instruct the code to control boundary conditions and geometry specific to the test problem. Normal execution of the code for production runs will operate with these parameters inactivated.

2.2.3 Validation against field analogs

Several field analogs from the petroleum industry exhibit sufficient similarity to the WIPP spallings event that a suitable quantitative comparison may be possible. In particular, well blowouts, coalbed methane, and sanding scenarios all incorporate processes analogous to a spalling event. Well blowout, and in particular, gas kick data may have application in validating the wellbore flow model in DR_SPALL. Moreover, coalbed methane production by dynamic openhole cavitation may provide some direct observation of spalling volumes. Finally, sanding in hydrocarbon production wells is a commonly-encountered problem, and some data are available to provide a basis for comparison of cavity growth and solids transport in the cavity and wellbore.

2.2.4 Code modifications

It is possible that the testing and validation stage of this analysis will identify problems with the model that require code modifications. Any code modifications will be followed by adequate testing and verification before implementation in the WIPP PA.

2.3 Qualification of input parameters

Parameter qualification will first require a review of all the parameters in the DR_SPALL model to identify those that already exist in the WIPP PA database. Parameters that do not already exist will have to be created and documented.

An initial review of the DR_SPALL input parameter set indicates that about 60 parameters are needed to execute the model. A full listing of the parameters is given in Appendix A. 30 of these parameters currently exist in the WIPP PA database, while another 15 are used to control computational processes, leaving 15 that require full QA pedigree.

2.3.1 Review of WIPP PA Parameter Database for applicable parameters

A preliminary review of the current version of DR_SPALL identified 31 parameters that currently exist in the WIPP PA database. The definition and value of each parameter will be examined to assure applicability to the new spallings model. In the event that a parameter value requires an update due to new information, it may be changed according to NP 9-2. It is anticipated that the waste tensile strength will require an update based on the measurements of Hansen et al. (1997).

2.3.2 Creation and documentation of new parameters

Table I lists the new parameters in the DR_SPALL model. Parameter types include those describing the repository, waste properties, and drilling. Repository properties may be derived from repository geometry and published literature. Waste properties will be derived from mechanical property measurements on surrogate wastes from (Hansen et al. ,1997), and documented in a parameter justification report that details the experimental approach and applicability of the measurements for use as parameters in the spallings model. Drilling parameters will be obtained from the database of current drilling practices in the Delaware Basin compiled for the CRA.

Table I. Parameters for the DR_SPALL model that are not currently in the WIPP PA database.

	Parameter Name	**Units**	**Type**
1	Outer Radius	m	Repository
2	Biot Beta	-	Waste Property
3	Poisson's Ratio	-	Waste Property
4	Cohesion	Pa	Waste Property
5	Friction Angle	deg	Waste Property
6	Particle Diameter	m	Waste Property
7	Max. Solids Vol. Fraction	-	Drilling
8	Solids Viscosity Exponent	-	Drilling
9	DDZ Thickness	m	Drilling
10	DDZ Permeability	m^2	Repository
11	Stop Drilling Exit Vol Rate	m^3/s	Drilling
12	Stop Pumping Exit Vol rate	m^3/s	Drilling
13	Shape Factor	-	Waste Property
14	Choke Efficiency	-	Drilling

2.4 Qualification of code

Full documentation and testing will be completed in accordance with NP 19-1 prior to model implementation in the CRA. In addition to the design package (§ 2.1) and Parameter Justification Report (§ 2.3.2), this includes delivery of:

- Verification and Validation Plan
- Verification and Validation Report
- Software User's Manual

2.5 Implementation in WIPP PA

The need for thousands of realizations coupled with long execution times for the DR_SPALL model would create a prohibitive bottleneck in the flow of PA calculations. The proposed approach for alleviating this problem is to create look-up tables of spall volumes based on the repository pressure at the time of intrusion and several key parameters identified in the sensitivity calculations (§ 2.2.1). Using this strategy, fewer overall executions will be necessary, and the look-up table can be produced at any time before the output is needed, rather than in series with the production runs. The resolution of the look-up tables must consider the sensitivity of the output to the relevant input parameters so that interpolation errors do not unduly affect output. The objective from a practical perspective will be to minimize the number of independent parameters in the table without sacrificing critical accuracy of the model.

3. RESPONSIBLE STAFF

The personnel assigned to this project include:

1. David Lord, SNL org 6821, Principal investigator
2. John Schatz, John F. Schatz Research and Consulting, Technical consultant
3. David Rudeen, GRAM Inc., Analyst
4. Frank Hansen, SNL Org 6822, Parameter justification
5. Bill Thompson, Golder Associates, Technical consultant
6. Cliff Hansen, SNL Org 6821, Total System Performance Assessment Team Lead
7. James Garner, PIRU, Analyst
8. Kari Cox, SNL Org 6821, Student intern

4. SCHEDULE ESTIMATE

The primary driver for the schedule is the WIPP recertification PA, which must be executed, analyzed and delivered by Fall, 2003. PA calculations will start in March, 2003, and spallings results will be required by May, 2003. As such, a peer review must be completed by March, 2003, in order to proceed with creating the look-up tables to be ready for use in May and June. Table II lists the delivery dates for each of the major tasks.

Table II. Schedule of Tasks for the Spallings Model Development through Recertification

Task	Responsible personnel	Delivery Date
Submit Preliminary Design Package	David Lord, John Schatz, David Rudeen	Dec. 31, 2002
Model testing, verification, and validation	David Lord, John Schatz, David Rudeen, James Garner, Cliff Hansen	March 1, 2003
Qualification of input parameters	David Lord, Frank Hansen, Bill Thompson, Kari Cox	March 1, 2003
Qualification of code	David Lord, David Rudeen, James Garner	March 1, 2003
Implementation in WIPP PA	David Lord, David Rudeen, Cliff Hansen	May 1, 2003

5. SPECIAL CONSIDERATIONS

No special considerations have been identified for this analysis.

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 of NP-2-1, Qualification and Training.

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

Computer Codes: Computer codes used in the analysis will be qualified in accordance with NP19-1. The platform on which codes will be run is the Compaq ES 40 and ES45, Open VMS AXP, version 7.3.

Analysis and Documentation: Documentation will meet the applicable requirements in NP9-1 and NP17-1.

Reviews: Reviews will be conducted and documented in accordance with NP6-1 and NP9-1, as appropriate.

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Schatz, J.F., 1998. Analysis Plan for Development of Improved Spall Failure Physical Model and Computational Methodology, AP-048, ERMS#422027, Sandia National Laboratories, Carlsbad, NM.

Wilson, C., Porter, D., Gibbons, J., Oswald, E., Sjoblom, G., and F. Caporuscio, 1997. Conceptual Models Third Supplementary Peer Review Report, U.S. Department of Energy, Carlsbad Area Office, Office of Regulatory Compliance, April, 1997.

APPENDIX A

The current version of DR_SPALL requires specification of 61 parameters and run control variables in order to execute. These may be subdivided into 6 general types: waste properties, repository properties, drilling practices, physical constants, computational, and post-processing parameters. Table 1 documents all these parameters along with the source of the value. The source may be identified as follows:

CCA	Value exists in CCA PA database
BRAGFLO	Value is an output variable from BRAGFLO
NEW	New parameter
N/A	Run control or computational parameter specified at run time

Table 1. Source and type of parameters in current DR_SPALL code

#	Name	Units	Source	type
1	Land Elevation	m	CCA	Repository
2	Repository Top	m	CCA	Repository
3	Total Thickness	m	CCA	Repository
4	DRZ Thickness	m	CCA	Repository
5	DRZ Permeability	m^2	CCA	Repository
6	Outer Radius	m	NEW	Repository
7	Initial Gas Pressure	Pa	BRAGFLO	Repository
8	Far-Field Pore Pressure	Pa	BRAGFLO	Repository
9	Far-Field In-Situ Stress	Pa	CCA	Repository
10	Porosity	-	CCA	Waste Property
11	Permeability	m^2	CCA	Waste Property
12	Perm. from Porosity?	Y/N	N/A	Waste Property
13	Biot Beta	--	NEW	Waste Property
14	Poisson's Ratio	--	NEW	Waste Property
15	Cohesion	Pa	NEW	Waste Property
16	Friction Angle	deg	NEW	Waste Property
17	Tensile Strength	Pa	CCA	Waste Property
18	Particle Diameter	m	NEW	Waste Property
19	Gas Density at STP	kg/m^3	CCA	Physical
20	Gas Viscosity	Pa-s	CCA	Physical
21	Mud Density	kg/m^3	CCA	Drilling
22	Mud Viscosity	Pa-s	CCA	Drilling
23	Wall Roughness	m	CCA	Drilling
24	Max. Solids Vol. Fraction	--	NEW	Drilling

25	Solids Viscosity Exponent	--	NEW	Drilling
26	Bit Diameter	m	CCA	Drilling
27	Pipe Diameter	m	CCA	Drilling
28	Collar Diameter	m	CCA	Drilling
29	Pipe Inside Diameter	m	CCA	Drilling
30	Collar Length	m	CCA	Drilling
31	Drilling Rate	m/s	CCA	Drilling
32	Bit Above Repository (Init.)	m	N/A	Computational
33	Mud Pump Rate	m^3/s	CCA	Drilling
34	DDZ Thickness	m	NEW	Drilling
35	DDZ Permeability	m^2	NEW	Repository
36	Stop Drilling Exit Vol Rate	m^3/s	NEW	Drilling
37	Stop Pumping Exit Vol rate	m^3/s	NEW	Drilling
38	Stop Drilling Time	S	N/A	Computational
39	Spherical/Cylindrical	S/C	N/A	Computational
40	Fluidization?	Y/N	N/A	Computational
41	Maximum Run Time	S	N/A	Computational
42	Repository Cell Length	m	N/A	Computational
43	Wellbore Cell Length	m	N/A	Computational
44	Maximum Plot Radius	m	N/A	Post-Processing
45	Minimum Plot Stress	Pa	N/A	Post-Processing
46	Maximum Plot Stress	Pa	N/A	Post-Processing
47	π	-	CCA	Physical
48	Atmospheric pressure	Pa	CCA	Physical
49	Gravitational constant	m/s^2	CCA	Physical
50	Water Compressibility	1/Pa	CCA	Physical
51	Mass Diffusion Factor	--	N/A	Computational
52	Momentum Diffusion Factor	--	N/A	Computational
53	Gas Constant	J/kmol C	CCA	Physical
54	Repository Temperature	ºC	CCA	Repository
55	Waste Density	kg/m^3	CCA	Waste Property
56	Salt Density	kg/m^3	CCA	Repository
57	Shape Factor	--	NEW	Waste Property
58	Failure propagation limit	m/s	N/A	Computational
59	Bit Nozzle Number	--	CCA	Drilling
60	Bit Nozzle Diameter	m	CCA	Drilling
61	Choke Efficiency	--	NEW	Drilling

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