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Modeling Gas and Brine Migration for Assessing Compliance of the Waste Isolation Pilot Plant

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ABSTRACT

The U.S. Department of Energy (DOE) is developing the Waste Isolation Pilot Plant (WIPP) in southeastern New Mexico as a facility for the long-term disposal of defense-related transuranic (TRU) wastes. Use of the WIPP for waste disposal is contingent on demonstrations of compliance with applicable regulations of the U.S. Environmental Protection Agency (EPA). This paper addresses issues related to modeling gas and brine migration at the WIPP for compliance with both EPA 40 CFR 191 (the Standard) and 40 CFR 268.6 (the RCRA).

At the request of the WIPP Project Integration Office (WPIO) of the DOE, the WIPP Performance Assessment (PA) Department of Sandia National Laboratories (SNL) has completed preliminary uncertainty and sensitivity analyses of gas and brine migration away from the undisturbed repository. This paper contains descriptions of the numerical model and simulations, including model geometries and parameter values, and a summary of major conclusions from sensitivity analyses.

Because significant transport of contaminants can only occur in a fluid (gas or brine) medium, two-phase flow modeling can provide an estimate of the distance to which contaminants can migrate. Migration of gas or brine beyond the RCRA "disposal-unit boundary" or the Standard's accessible environment constitutes a potential, but not certain, violation and may require additional evaluations of contaminant concentrations.

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ACKNOWLEDGMENTS

The authors wish to recognize the technical reviews of this report by David Gallegos and Mel Marietta (6342) of Sandia National Laboratories.

PREFACE

This SAND report is a reproduction of the identically titled paper published in:

American Nuclear Society and American Society of Civil Engineers. *High-Level Waste Management: Proceedings of the Fourth Annual International Conference in Las Vegas, NV, April 26 - 30, 1993*. American Nuclear Society, La Grange, IL; American Society of Civil Engineers, New York, NY.

MODELING GAS AND BRINE MIGRATION FOR ASSESSING COMPLIANCE
OF THE WIPP

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ABSTRACT

The U.S. Department of Energy (DOE) is developing the Waste Isolation Pilot Plant (WIPP) in southeastern New Mexico as a facility for the long-term disposal of defense-related transuranic (TRU) wastes. Use of the WIPP for waste disposal is contingent on demonstrations of compliance with applicable regulations of the U.S. Environmental Protection Agency (EPA).^{1,2} This paper addresses issues related to modeling gas and brine migration at the WIPP for compliance with both EPA 40 CFR 191 (the Standard) and 40 CFR 268.6 (the RCRA).

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Because significant transport of contaminants can only occur in a fluid (gas or brine) medium, two-phase flow modeling can provide an estimate of the distance to which contaminants can migrate. Migration of gas or brine beyond the RCRA "disposal-unit boundary" or the Standard's accessible environment constitutes a potential, but not certain, violation and may require additional evaluations of contaminant concentrations.

PROBABILISTIC APPROACH AND METHODOLOGY

The methodology used in these analyses relies on a probabilistic approach to provide estimates based on a range of possible conditions.^{3,4} Multiple simulations use sampled values for selected input parameters, and permit analysis of the uncertainty in the outcomes. Probabilistic analyses of this sort provide information about the appropriate level of

confidence that should be attached to performance predictions, rather than an absolute, deterministic prediction.

The input sets associated with the simulations for this study are generated by a Monte-Carlo procedure. Three types of parameters make up the input to the model: 1) parameters that are held constant, 2) parameters that are Latin hypercube sampled, and 3) parameters that are derived from sampled parameters. In order to account for parameter uncertainty certain sampled parameters are described by probability distributions of possible values. The flow of brine and gas in and around the repository system is then simulated conditional on each of the input realizations using the numerical model BRAGFLO.³

MODEL CONCEPTUALIZATION

A brief conceptualization of multi-phase porous media flow presents some basic assumptions inherent in the BRAGFLO formulation. The porous media is assumed to be a solid continuum containing a network of interconnected void space. All fluids collectively occupy all of the void space. The fluids are immiscible and each is regarded as a continuum separated by an interface whose curvature and surface tension give rise to a capillary pressure difference across that interface. The equation of motion for each fluid in a multi-phase and multi-dimensional system is described by heuristic extensions of Darcy's Law, which empirically relates on a macroscopic scale flow rate linearly to flow-potential gradient.

MODEL DESCRIPTION

BRAGFLO simultaneously solves the partial differential equations (PDE's) that describe the mass conservation of each mobile component (gas and brine) in one, two, or three dimensions along with appropriate initial and boundary conditions. Four additional constraints

complete the description: 1) the phase saturations (volume fraction of voids) are constrained so the volumes of the fluids occupy all of the void space, 2) the brine phase consists of only brine and dissolved gas, 3) the brine and gas phase pressures differ by the capillary pressure, and 4) the amount of dissolved gas varies with gas pressure. This system of equations is solved for the six different variables: two phase saturations, two phase pressures, and two mass fractions in the brine phase.

For application to WIPP, additional attention is given to the gas generation processes occurring in the waste. The rates of corrosion and biodegradation vary with brine saturation. Brine and ferrous metal and/or cellulose are consumed and gas is produced.

The numerical techniques in BRAGFLO are based on a fully implicit finite difference representation of the non-linear PDE's which are solved using a modified Newton-Raphson iteration technique with adaptive time-stepping. The numerical methods have been chosen for their robustness with respect to stability and convergence.

REPOSITORY CONCEPTUALIZATION

The WIPP is located 657 m below the surface in halite of the Salado Formation. More permeable subhorizontal anhydrite interbeds also exist in the Salado above and below the excavation and provide the dominant path for the lateral migration of brine and gas. A disturbed rock zone (DRZ) surrounds the excavation and provides communication between the repository and the anhydrite layers. The Rustler Formation approximately 390 m above the repository contains the nearest aquifer. The RCRA boundaries are assumed to be the Salado/Rustler interface and the 2.5-km land-withdrawal boundary.

Two representations of the repository have been selected for analysis. The cases use the BRAGFLO two-phase flow code,³ developed for WIPP performance assessment, and differ significantly in their two-dimensional approximations of the three-dimensional disposal system and in the parameter values used to describe selected material properties. Each model was used to examine different aspects of fluid migration and repository performance. Human intrusion is not considered and the simulations model the undisturbed performance of the repository over a 10,000-year period. Thus, the simulations are directly relevant to the RCRA, which addresses only undisturbed performance, and the "base-case" scenario for the Standard,⁵ which also is undisturbed performance for the WIPP.

Lateral migration of gas and brine from the repository is investigated in Case 1, which uses cylindrical model geometry, Figure 1. The axisymmetric geometry approximates the equivalent volume of a single isolated waste-disposal panel (including the intact pillars within a panel), and assumes perfect shaft sealing.

Case 2 investigates the flow of gas and brine using rectangular north-south cross-sections to approximate the entire repository, including drifts and shafts, Figure 2. Flow is allowed in two dimensions, horizontally in the north-south plane and vertically. In-the-page depth varies to preserve the volume of repository regions and accounts for far-field radial flow.

Case 2 is designed to examine flow to the RCRA disposal-unit boundary both laterally and up the shaft. In Case 2, with the exception of a 10-m-thick low-permeability seal in the shaft, other low-permeability barriers to fluid flow associated with panel seals, drift seals, or shaft backfill do not exist.

INPUT PARAMETERS

The values of the unsampled parameters are summarized in Table 1 while the ranges of possible values for the sample parameters are given in Table 2. More parameters are sampled in Case 2 including the two-phase flow parameters used in the Brooks/Corey relative permeability and capillary pressure sub-model. As indicated in Table 2, Case 2 is characterized by less permeable halite, a more permeable DRZ, and the presence of an intermediate permeability transition zone.

RESULTS

A total of 60 Case 1 simulations and 60 Case 2 simulations was performed for this study. Lagrangian particle tracking analysis indicates that during undisturbed conditions no contaminated brine migrates in 10,000 years beyond the thin DRZ that surrounds the excavation.

Of the 60 Case 1 realizations, 13 result in gas migration beyond the DRZ through the more-permeable anhydrite interbeds that exist in the Salado Formation halite that hosts the repository, Table 3. One realization results in gas migration into the numerical grid block containing the 2.5-km land-withdrawal boundary.

Anhydrite permeability and its related capillary threshold pressure are important in limiting the lateral migration of gas. In Table 3, it is seen that 12 of the 13 Case 1 input realizations that result in lateral gas migration had values of anhydrite permeability in the upper one-third of the sampled range. Table 4 presents

Table 1. Fixed Parameter Values.

Parameter	Case	
	1	2
Formation Parameters		
Permeability (m ²)		
Intact Halite/Anhydrite*	S	S
DRZ Halite	10-20	S
DRZ Anhydrite	D	S
Transition Zone	N	S
Waste	10-13	10-13
Culebra	10-13	10-13
Seals	N	S
Shaft	N	10-13
Backfill	N	10-13
Porosity (% Formation Volume)		
Intact Halite	1.0	S
Intact Anhydrite	1.0	S
DRZ Halite	6.0	S
DRZ Anhydrite	5.5	S
Transition Zone	N	S
Waste	D	D
Culebra	14.0	14.0
Seals	N	7.5
Shaft	N	7.5
Backfill	N	7.5
Two-Phase Properties		
Residual Brine Saturation		
Salado Materials	0.20	S
Waste	0.28	0.28
Culebra	0.20	0.20
Other Excavations/Seals	N	S
Residual Gas Saturation		
Salado Materials	0.20	S
Waste	0.07	0.28
Culebra	0.20	0.20
Other Excavations/Seals	N	S
Pore-Size Distribution Parameter		
Salado Materials	0.7	S
Waste	2.9	2.9
Culebra	0.7	0.7
Other Excavations/Seals	N	S
Threshold Displacement Pressure (MPa)		
Intact Salado Materials	D	D
DRZ/Transition Zone	D	0.0
Waste	0.0	0.0
Culebra	0.01	0.01
Seals	N	0.0
Backfill	N	0.0
Shaft	N	0.0

* - Permeabilities of intact halite and anhydrite were rank correlated with $r = 0.8$
 S - Sampled
 D - Derived
 N - Not Used

information on the largest 10 gas generation realizations of Case 1. Only two realizations result in lateral gas migration. In the remaining 8 realizations, low anhydrite permeability and high threshold pressure are responsible for limiting gas migration.

Figure 3 presents the volume-average repository pressure history for all 60 Case 2 realizations. In all but one realization, generated gas is able to access sufficient pore space to keep repository pressures below lithostatic levels. Accounting for closure of the repository due to salt creep in future analyses is expected to reduce available void volume and produce larger repository pressures.

Figure 4 summarizes the migration of gas from the repository for Case 2. In 45 realizations gas flows past the 10-m-thick shaft seal (Figure 4A). A total of 6 realizations result in lateral gas migration into one or more of the

anhydrite interbeds. One realization results in the flow of gas into the grid block containing the 2.5-km land-withdrawal boundary. The large number of realizations producing gas flow past the shaft seal is in part due to the assumption that only a 10-m section of the 400 m length shaft provides resistance to flow and to the assumption that there is no capillary threshold pressure barrier for gas to overcome in entering the shaft or seal.

Neutral particle tracking conditioned on the brine phase velocity fields indicates that any contaminated brine leaving the repository is confined to the DRZ and backfill. Some brine, less than 60 m³, did flow upward past the shaft seal, but this brine is not believed to have been in contact with the waste. Its volume represents less than 5% of the available void space in the shaft between the seal and the top of the Salado, so it is unlikely that this brine reached the Salado/Rustler interface.

Parameter sensitivity analysis is complicated by the nonlinear interaction of the sampled variables that influence gas migration. The migration of waste-generated gas through the interbeds toward the far-field boundary is affected by rock properties, the rate and amount of gas generated, the two-phase flow properties of a brine/gas system, and the far-field boundary pressure. Because the gas-generation process is dependent on the amount of brine available for corrosion and biodegradation, the instantaneous rate and amount of gas varies with saturation and consequently with time and space within the waste panel. The amount of brine available in the panel for reaction depends on the amount of brine initially present, the amount of brine that flows into or out of the panel, and the amount of brine consumed by the reactions. The rate at which brine flows into or out of the waste panel depends on the rock

Figure 3. Repository Pressure Histories for Case 2 Simulations.

Table 2. Sampled Parameter Value Ranges

Parameter	Case	
	1	2
Gas Generation Parameters		
Corrosion Rates $\left(\frac{\text{mol gas}}{\text{drum-yr}} \right)$		
Inundated Conditions	0.0 - 2.5	Same
Humid Conditions	0.0 - 1.0	Same
Biodegradation Rates $\left(\frac{\text{mol gas}}{\text{drum-yr}} \right)$		
Inundated Conditions	0.0 - 5.0	Same
Humid Conditions	0.0 - 1.0	Same
Corrosion Stoichiometry		
Gas Production (mol gas/mol Fe)	1.0 - 1.3	Same
Water Consumption (mol H ₂ O/mol Fe)	2.0 - 1.3	Same
Biodegradation Stoichiometry		
Gas Production (mol gas/mol CH ₂ O)	0 - 1.7	Same
Potential (volume % of waste)		
Wood	28 - 48	Same
Ferrous Metals	27 - 47	Same
Formation Parameters		
Permeabilities (m ²)		
Intact Halite	10-22 - 10-19	10-25 - 10-21
Intact Anhydrite	10-20 - 10-18	10-20 - 10-18
Disturbed Rock Zone	10-19 - 10-17	10-18 - 10-13
Transition Zone	N	10-21 - 10-19
Porosities (% Formation Volume)		
Intact Anhydrite	0.1 - 3.0	0.1 - 3.0
Disturbed Rock Zone	F	0.1 - 6.0
Transition Zone	N	0.1 - 6.0
Waste	47 - 62	47 - 62
Initial Conditions		
Initial Brine Saturation in Waste (% Void)	0 - 28	0 - 28
MB 139 Far Field Pore Pressure (MPa)	8 - 15	8 - 15
Two-Phase Properties (Salado Formation)		
Residual Brine Saturation (% Void)	F	0.0 - 0.4
Residual Gas Saturation (% Void)	F	0.0 - 0.4
Pore-Size Distribution Parameter	F	0.2 - 10.0
Threshold Pressure Correlated to Permeability	D	D
Excavation Fill/Engineered Barriers		
Permeability (m ²)		
Shaft Seal	N	10-21 - 10-18
Lower Shaft	N	F
Middle Shaft	N	F
Upper Shaft	N	F
Backfill	N	F
Length (m)		
Shaft Seal	N	F

F - Fixed

N - Not Used

D - Derived

Table 3. Non-Zero Lateral Gas Migration Realizations for Case 1 Simulations.

Input Set	Migration Distance		Permeability	
	Upper Anhydrite	Lower Anhydrite	Value (m^2)	Rank
11	4700	500	1.3×10^{-18}	54
41	1500	500	2.8×10^{-19}	43
25	1500	0	1.8×10^{-18}	60
24	1500	0	1.7×10^{-18}	59
2	1500	0	1.5×10^{-18}	57
7	1500	50	1.0×10^{-18}	51
1	1500	0	1.1×10^{-18}	52
39	500	150	2.0×10^{-19}	42
19	500	0	6.6×10^{-19}	47
54	150	15	6.8×10^{-19}	16
46	150	150	1.6×10^{-18}	58
31	15	6	8.2×10^{-20}	40
42	1	0	8.9×10^{-19}	50

Table 4. Top Ten Gas Generation Realizations for Case 1 Simulations.

Input Set	10,000 yr Total Gas Generation		Anhydrite Permeability		Anhydrite Threshold Pressure		Anhydrite Gas Flow
	Value (m^3)	Rank	Value (m^2)	(Rank)	Value (MPa)	Rank	
36	1.43×10^8	60	7.03×10^{-20}	23	9.44	48*	No
21	1.36×10^8	59	7.67×10^{-20}	29	160.75	60*	No
17	1.35×10^8	58	2.60×10^{-20}	3*	0.36	14	No
24	1.30×10^8	57	1.66×10^{-18}	59	0.28	12	Yes
40	1.26×10^8	56	7.74×10^{-20}	30	4.21	39*	No
56	1.26×10^8	55	1.87×10^{-20}	2*	2.72	31	No
45	1.24×10^8	54	8.06×10^{-20}	37	6.59	44*	No
41	1.23×10^8	53	2.84×10^{-19}	43	0.23	10	Yes
37	1.22×10^8	52	7.84×10^{-20}	31	3.21	37*	No
43	1.21×10^8	51	5.97×10^{-20}	9*	0.68	18	No

* Indicates parameter inferred to control gas flow into anhydrite layers.

Figure 4. Gas Migration for Case 2 Simulations

properties of the surrounding media, the two-phase flow properties, and the instantaneous pressure gradient, the latter being itself a function of the pressure in the panel resulting from gas generation.

A formal sensitivity analysis using procedures based on partial correlation analysis and linear stepwise regression analysis was used to identify those parameters having the most influence on various repository performance measures. Such measures include amount of gas generated, repository pressure and saturation, and the cumulative release of brine and gas.

Some of the results of these analyses are presented in Table 5. For example, the sampled range of values for the initial brine saturation in the waste is able to account for 42% of the observed variability in total gas production. When the uncertainties in stoichiometry for corrosion and bio-degradation are included in the linear regression model, the three parameters account for 60% of the variability. A summary for other performance measures is included in Table 5.

The small sample size of non-zero values for lateral gas migration precludes analysis by linear stepwise regression; however, examination of the driving force that gives rise to flow provides some insight. The pressure gradient defined as the difference between the gas pressure in the DRZ and the sum of the brine pressure and capillary threshold pressure in the adjacent anhydrite interbed determines whether gas penetrates the initially brine-filled pores of the interbeds. A partial rank correlation

analysis indicates that the variability in this pressure gradient is dominated by anhydrite permeability and capillary threshold pressure and to a lesser extent by the anhydrite far-field or boundary pressure and the initial brine saturation of the waste.

CONCLUSIONS

Principal conclusions that can be drawn from these analyses are the following:

1. The methodology used for these analyses can provide quantitative probabilistic estimates of gas and brine migration as well as identifying dominant parameters influencing repository performance.
2. Gas generation parameters, shaft seal permeability, and anhydrite interbed permeability and capillary threshold pressure are important in determining gas migration. Including salt creep and interbed fracturing could increase gas migration.
3. Contaminated brine does not migrate horizontally to the 2.5 km land-withdrawal boundary or vertically to the top of the Salado formation if the repository remains undisturbed.
4. Many realizations result in the migration of gas to the Salado/Rustler interface. Fewer realizations result in any gas entering the interbeds, although in two realizations gas may have migrated past the land-withdrawal boundary.

Table 5. Dominant Parameters Influencing Various Repository Performance Measures.

<u>Performance Measure</u>	<u>Dominant Parameter</u>	<u>Cumulative % of Variability Accounted For</u>
1) Total gas production over 10,000 yr	Initial brine saturation in waste	42
	Stoichiometry of biodegradation	52
	Stoichiometry of corrosion	60
2) Repository pressure	Initial brine saturation in waste	59
	Transition Zone porosity	68
	Shaft seal permeability	74
3) Brine flow into waste	Halite/anhydrite porosity	39
	Anhydrite permeability	51
	Transition Zone porosity	60
	Initial brine saturation in waste	66
4) Total gas flow Through shaft seal over 10,000 yr	Initial brine saturation in waste	37
	Inundated corrosion rate	49
	Shaft seal permeability	60
	Transition Zone porosity	67

ACKNOWLEDGMENT

This work was performed for the United States Department of Energy under contract DE-AC04-76DP00789.

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