530631

Sandia National Laboratories

Operated for the U.S. Department of Energy by
Sandia Corporation

Joshua S. Stein Ph. D.
Performance Assessment & Decision Analysis Department
4100 National Parks Hwy., Carlsbad, NM 88220

P.O. Box 5800
Albuquerque, NM 87185-1395

Phone: (505) 234-0110 (Carlsbad)
Phone: (505) 845-0936 (Abq Direct Line)
Fax: (505) 234-0061
Internet: jsstein@sandia.gov

date: August 12, 2003

to: Mario Chavez (6820)

technical review: Cliff Hansen (6821) Clifford Hansen

management review: David Kessel (6821) (FOR DAVID KESSEL)

from: Joshua S. Stein (6821) Joshua S. Stein

subject: Page changes for ERMS# 525203

Typographical errors were discovered in the analysis report for the simplified shaft seal (James and Stein, 2003). The variable for pore compressibility COMP_POR was erroneously listed as COMP_RCK. These errors have been corrected by making page changes to pages 6 and 15. The updated pages are included with this memo.

Reference:

James, S.J., and Stein, J. 2003. "Analysis Report for the Development of a Simplified Shaft Seal Model for the WIPP Performance Assessment Rev 1." Carlsbad, NM: Sandia National Laboratories. ERMS# 525203.

WIPP:1.3.5.1.2.1:PA:QA-L:525186

the non-Salado seal components do not vary over time, a single equivalent permeability distribution for the simplified non-Salado shaft material was similarly obtained.

An analysis of the equivalent permeability data indicates that the distributions for 0–10, 10–25, and 25–50 years are nearly identical (with mean equivalent permeabilities decreasing by 5% and 42% at 10 and 25 years, respectively). After 50 years, permeability progressively decreases between time intervals 25–50, 50–100, 100–200, and 200–400 years (with mean equivalent permeabilities decreasing by 133%, 604%, and 2507% at 50, 100, and 200 years, respectively). The final change occurs at 400 years and results in a very slight increase in effective permeability (mean equivalent permeability increases by 31%) because of increases in concrete permeability assumed for the 400–10,000 year period.

The simplified shaft seal model comprises two composite materials (representing Salado and non-Salado components) instead of six distinct materials in ten layers (Figure 2) with changes to material properties occurring just once rather than six times. In addition, rather than requiring a pre-processing step to account for the effect of the DRZ (by first calculating effective permeabilities), equivalent permeability distributions are used directly.

The permeability of the simplified non-Salado composite material is sampled from an equivalent distribution derived from current baseline. This distribution is represented by the black curve in Figure 3. To capture the time-dependent behavior of the Salado composite material, there is a single permeability change at 200 years. A conservative choice for the distribution of the first 200 years is to average the distributions for the 0–10, 10–25, and 25–50 year intervals. Note that the 50–100 and 100–200 year intervals are not used. From 200 to 10,000 years, the distribution is defined as the average of the distributions from the 200–400 and 400–10,000 year intervals. Because only the highest permeability data from the first 50 years is used to constrain the model for 200 years, this approach overestimates the permeability during the first 200 years and is thereby conservative. Figure 4 shows the simplified equivalent permeability distributions for the new model.

The permeability distributions can be implemented in PA by fitting a cumulative distribution to the three empirical histograms shown in Figure 4 (Tierney, 1990). Figure 5 illustrates the cumulative distributions corresponding to the histograms in Figure 4 for the simplified non-Salado shaft as well as both time intervals for the simplified Salado shaft.

Volume weighted pore compressibility, COMP_POR, porosity, POROSITY, and initial brine saturation, SAT_IBRN, are presented in Table 2.

4 SUMMARY

A simplified version of the shaft seal model is derived. The new model reduces the number of materials from eight (in ten layers) to two composite materials: Salado and non-Salado. Additionally, the number of model restarts and material reassignments is reduced from six to one. Moreover, the preprocessing step required to calculate the effect of the DRZ on permeability (effective permeability) is incorporated into the parameter distributions. These

Table 2: Volume averaged rock compressibility, porosity, and initial brine saturation for the simplified shaft model.

Property	Non-Salado	Salado	
	0–10,000 years	0–200 years	200–10,000 years
COMP_POR	2.0491441×10^{-8}	4.2785786×10^{-9}	4.2785786×10^{-9}
POROSITY	0.29105080	0.11302095	0.11302095
SAT_IBRN	0.79638135	0.53412808	0.53412808

525203

Sandia National Laboratories
Waste Isolation Pilot Plant

Analysis Report for:
Development of a Simplified Shaft Seal Model for the WIPP Performance Assessment

Rev. 1

Author:	Scott James (6115)	Mario Chavez for	1/23/03
	Print	Signature	Date
Author:	Joshua Stein (6821)	Joshua S. Stein	1/23/03
	Print	Signature	Date
Technical Review:	Tom Pfeifle (6823)	Tom W. Pfeifle	1/23/03
	Print	Signature	Date
Management Review:	David Kessel (6821)	David Kessel	1/23/03
	Print	Signature	Date
QA Review:	Mario Chavez (6820)	Mario Chavez	1/23/03
	Print	Signature	Date

TABLE OF CONTENTS

1 INTRODUCTION AND OBJECTIVES

During conceptual model development for the Compliance Certification Application (CCA) and Performance Assessment Verification Test (PAVT), scientists speculated that the Waste Isolation Pilot Plant (WIPP) shaft seal system might influence repository performance by providing a preferential flowpath for escaped radionuclides (DOE, 1996, § 6.4.4). To examine this potential, a detailed representation of the shaft was implemented as a component of the repository system. However, performance assessment (PA) models demonstrated that the shaft seal prevents releases over the 10,000-year regulatory period. Both analyses of calculations supporting the shaft seal design effort (SNL, 1996; Statham et al., 1997; Statham et al., 1998) and the baseline PA calculations and sensitivity studies supporting WIPP certification (Helton et al., 1998) have concluded that the shaft seal prevents all releases up the shaft from the repository during the regulatory period.

Because the CCA and PAVT concluded that the shaft seals do not affect repository performance, the current implementation of the shaft seal system into the PA calculations is unnecessarily complicated. There are three sources for the complexity of the model:

1) The shaft seal is represented by 10 separate material layers (6 distinct materials), each requiring a unique set of PA parameters,
2) Several shaft seal materials are assigned time-dependent properties requiring flow models to be interrupted and then restarted with the new set of parameter values six times during each vector simulation,
3) Effective permeability values must be calculated for each shaft seal material within both the Salado Formation and the disturbed rock zone surrounding each seal material, requiring significant pre-processing. These calculations were originally intended to account for any possible upward flow between the shaft seal materials and the surrounding disturbed rock zone (DRZ).

Ultimately, the baseline shaft seal model requires over 400 parameters to be maintained in the database (see 1 and 2 above) and that expertise with the shaft seal material/DRZ effective permeability calculations (see 3 above) is available to set up and run BRAGFLO (WIPP, 2002) for the PA.

Because the shaft does not represent a viable release pathway at WIPP, it is not necessary to model it in such detail and PA efficiency would be significantly improved if the model were simplified. However, any simplification must accurately represent the shaft seal behavior as modeled in the baseline PA. This analysis report presents a simplified version of the shaft seal model and completes the work described in AP-094 (James and Stein, 2002). The simplification proposed here does not alter the conceptual models of the shaft seal components as described in SNL (1996). Rather, it will conservatively represent the behavior of seal components in the repository system model. Specifically, the 11 separate material layers will be reduced to two equivalent layers. Additionally, the six time intervals will also be reduced to two.

2 APPROACH

2.1 Permeabilities

The baseline shaft seal model is implemented in the BRAGFLO grid as a column of elements with vertical dimensions matching the thickness of the layers of the shaft seal materials. Figure 1~~Figure 1~~ shows the baseline logical grid and the shaft seal model used in the PAVT and CCA. Table 1~~Table 1~~ lists the material type, thickness, and database material names for each of the shaft seal materials at each time interval.

Materials used in the shaft seal model fall into two categories: non-Salado and Salado components. Materials used to seal the non-Salado formations (Rustler, Dewey Lake, and Santa Rosa Formations) have Latin-hypercube-sampled, time-invariant permeability values for the regulatory period that are not influenced by the DRZ. In general, materials used to seal the Salado Formation also have sampled permeability values; however, in contrast to the non-Salado seal materials, several of the Salado materials have permeabilities that vary with time. Furthermore, they are mathematically manipulated to yield effective permeabilities intended to account for any effects from the DRZ. Therefore, as shown in Figure 2~~Figure 2~~, two material layers, non-Salado and Salado, are used in a simplified shaft seal model, rather than the 10 material layers comprising the baseline shaft seal model.

The shaft seal is so effective because of its low overall hydraulic conductance. Hydraulic conductance is directly proportional to permeability and cross-sectional area and inversely proportional to flow length. A practical way of expressing hydraulic conductance for a layered hydrologic feature, such as the shaft seal system, is to define an 'equivalent' permeability that represents the cumulative hydraulic effects of all subcomponents (seal materials). This approach is valid for the shaft seal because the cross-sectional area is uniform for all shaft seal materials. The equivalent permeability for flow across multiple layers with varying permeabilities is defined as the weighted harmonic mean of the subcomponent permeabilities. The harmonic mean of permeability, k_{eq}, across i distinct layers is expressed as:

$$\frac{1}{k_{eq}} = \frac{1}{L}\sum_i \frac{\ell_i}{k_i}, \qquad (1)$$

where L is the total length of the simplified shaft seal material; and ℓ_i and k_i are the layer thickness and the (effective) permeability of each subcomponent, respectively (de Marsily, 1986). The harmonic mean of the permeability is the equivalent permeability value for a shaft seal constructed of a single material. In other words, given a certain pressure gradient, the total flow through the simplified (single material) shaft model with permeability k_{eq} would be equal to the flow through the original multicomponent shaft seal system.

The simplified shaft seal conservatively defines two equivalent permeability distributions for the portion of the shaft in the Salado – one for the first 200 years of operation and another for 200 to 10,000 years. One equivalent permeability distribution is defined for the shaft in the non-Salado formations.

2.2 *Other material properties*

While permeability is the most important parameter to consider when simplifying the shaft seal model, other parameters must also be evaluated.

2.2.1 Porosity and compressibility

Simplified shaft seal pore ~~compressibility~~compressibilities, porosity, and initial brine saturation are defined as the volume-weighted arithmetic mean of the values of each original shaft's subcomponents. This approach ensures that the total pore volume and the total effect of pressure transients do not change from their baseline model values. Although porosity and compressibility may change somewhat over the repository lifetime, in both the simplified and PAVT models, they are treated as constants. We are correcting a naming problem that is found in the parameter database for materials that were part of the baseline shaft seal model. For the original shaft seal materials the name COMP_RCK was used to represent pore compressibility values, but the parameter was described incorrectly as bulk compressibility. The value was used correctly in the PA modeling for the CCA and PAVT. To be consistent, we are changing the name of these parameters of the simplified shaft mode to COMP_POR.

2.2.2 Two-phase flow parameters

In the baseline model, the residual brine and gas saturations (SAT_RBRN and SAT_RGAS) and the Brooks-Corey pore distribution parameter (PORE_DIS) are sampled from the SALT_T1 distribution and these values are assigned to all shaft seal materials for all times. To remain consistent with the baseline, a similar practice is continued. Recall that the initial brine saturation in the simplified shaft is a volume-weighted average of the initial brine saturations in the original shaft's subcomponents. All other parameters related to two-phase flow (CAP_MOD, KPT, PC_MAX, PO_MIN, PCT_EXP, PCT_A, and RELP_MOD) are constant and uniform for all shaft seal materials. This practice will also be continued in the simplified model. The values for these parameters are listed in the Appendix.

3 RESULTS

The effective (DRZ corrected) permeabilities from the current baseline Replicate #1 (PAVT R1) for each shaft material are stored in the BRAGFLO output files (i.e. bf3_c97_r1_s1_v001.cdb) generated for the current baseline calculation and were extracted using the program SUMMARIZE version 2.0 (WIPP, 2002). For each of the 100 vectors of PAVT R1, Salado shaft-seal equivalent permeabilities are calculated. That is, 100 equivalent permeabilities are generated by substituting the eight effective permeabilities (non-shaded cells in Table 1~~Table 1~~) and corresponding thicknesses into Eq (1) for each of the seven constant-permeability time intervals (columns in Table 1~~Table 1~~). A histogram is generated to discretize the equivalent permeability distribution. Specifically, each of the 100 values is binned into a half-log interval (between –23 and –16) and the number that fell within each interval (frequency) is counted. These data are plotted for each time interval in Figure 3~~Figure 3~~.

Because the permeabilities of the non-Salado seal components do not vary over time, a single equivalent permeability distribution for the simplified non-Salado shaft material was similarly obtained.

An analysis of the equivalent permeability data indicates that the distributions for 0–10, 10–25, and 25–50 years are nearly identical (with mean equivalent permeabilities decreasing by 5% and 42% at 10 and 25 years, respectively). After 50 years, permeability progressively decreases between time intervals 25–50, 50–100, 100–200, and 200–400 years (with mean equivalent permeabilities decreasing by 133%, 604%, and 2507% at 50, 100, and 200 years, respectively). The final change occurs at 400 years and results in a very slight increase in effective permeability (mean equivalent permeability increases by 31%) because of increases in concrete permeability assumed for the 400–10,000 year period.

The simplified shaft seal model comprises two composite materials (representing Salado and non-Salado components) instead of six distinct materials in ten layers (Figure 2) with changes to material properties occurring just once rather than six times. In addition, rather than requiring a pre-processing step to account for the effect of the DRZ (by first calculating effective permeabilities), equivalent permeability distributions are used directly.

The permeability of the simplified non-Salado composite material is sampled from an equivalent distribution derived from current baseline. This distribution is represented by the black curve in Figure 3~~Figure 3~~. To capture the time-dependent behavior of the Salado composite material, there is a single permeability change at 200 years. A conservative choice for the distribution of the first 200 years is to average the distributions for the 0–10, 10–25, and 25–50 year intervals. Note that the 50–100 and 100–200 year intervals are not used. From 200 to 10,000 years, the distribution is defined as the average of the distributions from the 200–400 and 400–10,000 year intervals. Because only the highest permeability data from the first 50 years is used to constrain the model for 200 years, this approach overestimates the permeability during the first 200 years and is thereby conservative. Figure 4~~Figure 4~~ shows the simplified equivalent permeability distributions for the new model.

The permeability distributions can be implemented in PA by fitting a cumulative distribution to the three empirical histograms shown in Figure 4~~Figure 4~~ (Tierney, 1990). Figure 5~~Figure 5~~ illustrates the cumulative distributions corresponding to the histograms in Figure 4~~Figure 4~~ for the simplified non-Salado shaft as well as both time intervals for the simplified Salado shaft.

Volume weighted compressibility, COMP_RCK, porosity, POROSITY, and initial brine saturation, SAT_IBRN, are presented in Table 2~~Table 2~~.

4 SUMMARY

A simplified version of the shaft seal model is derived. The new model reduces the number of materials from eight (in ten layers) to two composite materials: Salado and non-Salado. Additionally, the number of model restarts and material reassignments is reduced from six to one. Moreover, the preprocessing step required to calculate the effect of the DRZ on permeability (effective permeability) is incorporated into the parameter distributions. These modifications result in a simpler model that conservatively represents the shaft seals in the WIPP PA.

5 CMS AND SOFTWARE INFORMATION

In deriving the parameter values for the new shaft model (according to AP-094), the program SUMMARIZE version 2.0 was run using the BRAGFLO CDB files from PAVT R1 as input. These files may be found on the WIPP VMS cluster in the CMS library: LIB_APS_AP094. Output from SUMMARIZE was imported into an Excel spreadsheet with routine calculations performed according to NP 9-1. There is an additional excel file that contains the distribution information for all shaft material parameters. These two excel files have been placed in the CMS library: LIB_APS_AP094.

6 REFERENCES

de Marsily, G. 1986. *Quantitative Hydrogeology: Groundwater Hydrology for Engineers*. San Diego: Academic Press.

U.S. DOE (U.S. Department of Energy). 1996. *Title 40 CFR Part 191 Compliance Certification Application for the Waste Isolation Pilot Plant*. DOE/CAO-1996-2184. Carlsbad, NM: U.S. Department of Energy, Waste Isolation Pilot Plant, Carlsbad Area Office.

Helton, J.C., Bean, J.E., Berglund, J.W., Davis, F.J., Garner, J.W., Johnson, J.D., MacKinnon, R.J., Miller, J., O'Brien, D.G., Ramsey, J.L., Schreiber, J.D., Shinta, A., Smith, L.N., Stoelzel, D.M., Stockman, C., and Vaughn, P. 1998. *Uncertainty and Sensitivity Analysis Results Obtained in the 1996 Performance Assessment for the Waste Isolation Pilot Plant*. SAND98-0365. Albuquerque, NM: Sandia National Laboratories.

SNL. 1996. *Waste Isolation Pilot Plant Shaft Sealing System compliance submittal design report*. SAND96-1326. Albuquerque, NM: Sandia National Laboratories.

Statham, W.H., Kelley, V.A., and Knowles, M.K. 1997. *Fluid Flow Analysis of the Lower Salado Components of the Waste Isolation Pilot Plant Shaft Sealing System Design*. Report for Sandia National Laboratories by Duke Engineering and Services.

Statham, W.H., Fryar, D.H., Reeves, M., and Knowles, M.K. 1998. *Evaluating Seal Performance and Parameter Sensitivity with a Full-Shaft Model*. Report for Sandia National Laboratories by Duke Engineering and Services.

Tierney, M.S. 1990. *Construction of Probability Distributions of Uncertain Variables in Models of the Performance of the Waste Isolation Pilot Plant: The 1990 Performance Simulations*. SAND90-2510. Albuquerque, NM: Sandia National Laboratories.

WIPP. 2002. Baseline software list, ERMS# 248640.

7 APPENDIX: EXCEL SPREADSHEETS

There are two excel spreadsheet files that make up the appendix to this document. They are in the CMS Library: LIB_APS_AP094.

Baseline Grid

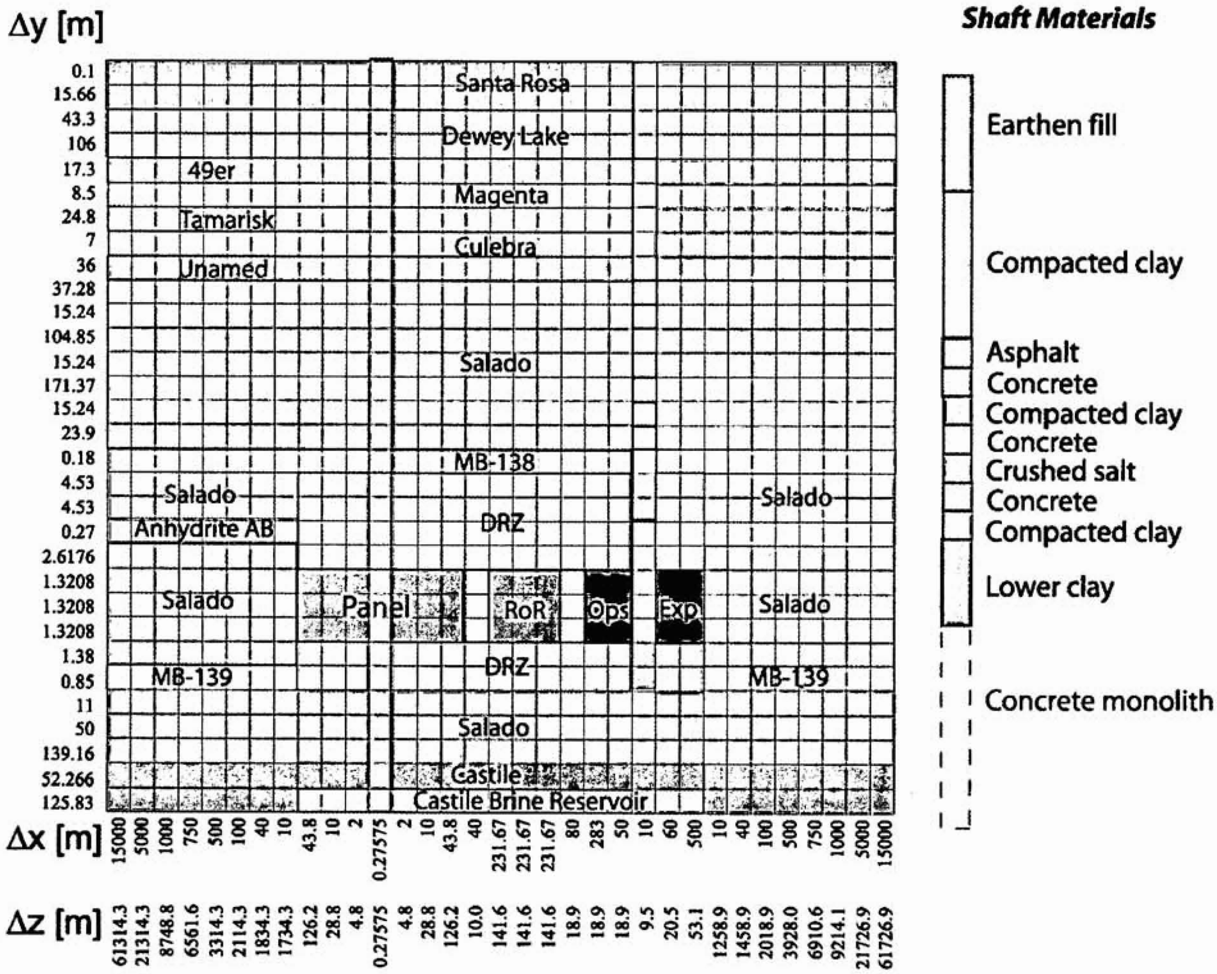

Figure 1: Baseline BRAGFLO logical grid showing the location of the shaft. The shaft is enlarged to the right and the materials used in the baseline model are labeled.

Table 1: Materials used in the baseline shaft model implemented in BRAGFLO. Bolded database material names indicate a change in parameter value from the previous time interval. The first two materials (gray shading) are used to seal the non-Salado (Rustler and above) units. The next nine layers (seven materials – note that concrete and compacted clay each appear twice) are used to seal the Salado Formation.

Material type	*Thickness [m]*	*0 to 10 yrs*	*10 to 25 yrs*	*25 to 50 yrs*	*50 to 100 yrs*	*100 to 200 yrs*	*200 to 400 yrs*	*400 to 10 k yrs*
Earthen fill	165.06	**EARTH**	EARTH	EARTH	EARTH	EARTH	EARTH	EARTH
Compacted clay	93.6	**CLAY_RUS**	CLAY_RUS	CLAY_RUS	CLAY_RUS	CLAY_RUS	CLAY_RUS	CLAY_RUS
Asphalt	37.28	**ASPHALT**	ASPHALT	ASPHALT	ASPHALT	ASPHALT	ASPHALT	ASPHALT
Concrete	15.24	**CONC_T1**	CONC_T1	CONC_T1	CONC_T1	CONC_T1	CONC_T1	**CONC_T2**
Compacted clay	104.85	**CL_M_T1**	**CL_M_T2**	**CL_M_T3**	**CL_M_T4**	CL_M_T4	CL_M_T4	CL_M_T4
Concrete	15.24	**CONC_T1**	CONC_T1	CONC_T1	CONC_T1	CONC_T1	CONC_T1	**CONC_T2**
Crushed salt	171.37	**SALT_T1**	**SALT_T2**	**SALT_T3**	**SALT_T4**	**SALT_T5**	**SALT_T6**	SALT_T6
Concrete	15.24	**CONC_T1**	CONC_T1	CONC_T1	CONC_T1	CONC_T1	CONC_T1	**CONC_T2**
Compacted clay	23.9	**CL_L_T1**	**CL_L_T2**	**CL_L_T3**	**CL_L_T4**	CL_L_T4	CL_L_T4	CL_L_T4
Lower clay	9.24	**CLAY_BOT**	CLAY_BOT	CLAY_BOT	CLAY_BOT	CLAY_BOT	CLAY_BOT	CLAY_BOT

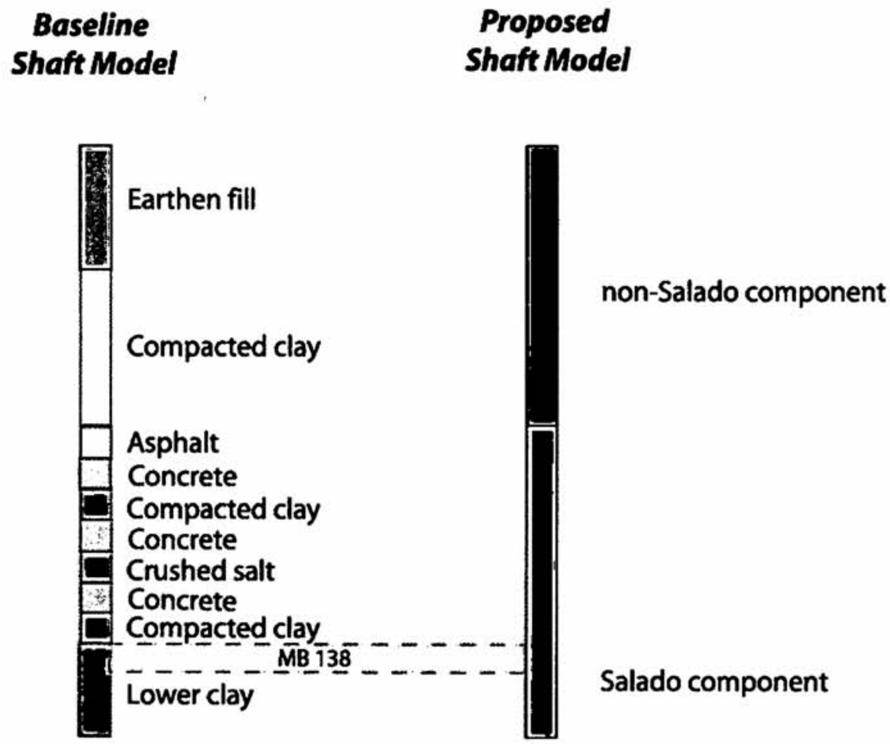

Figure 2: Representation of the baseline shaft seal model contrasted with the proposed simplified model.

11a
CDL 1/23/03

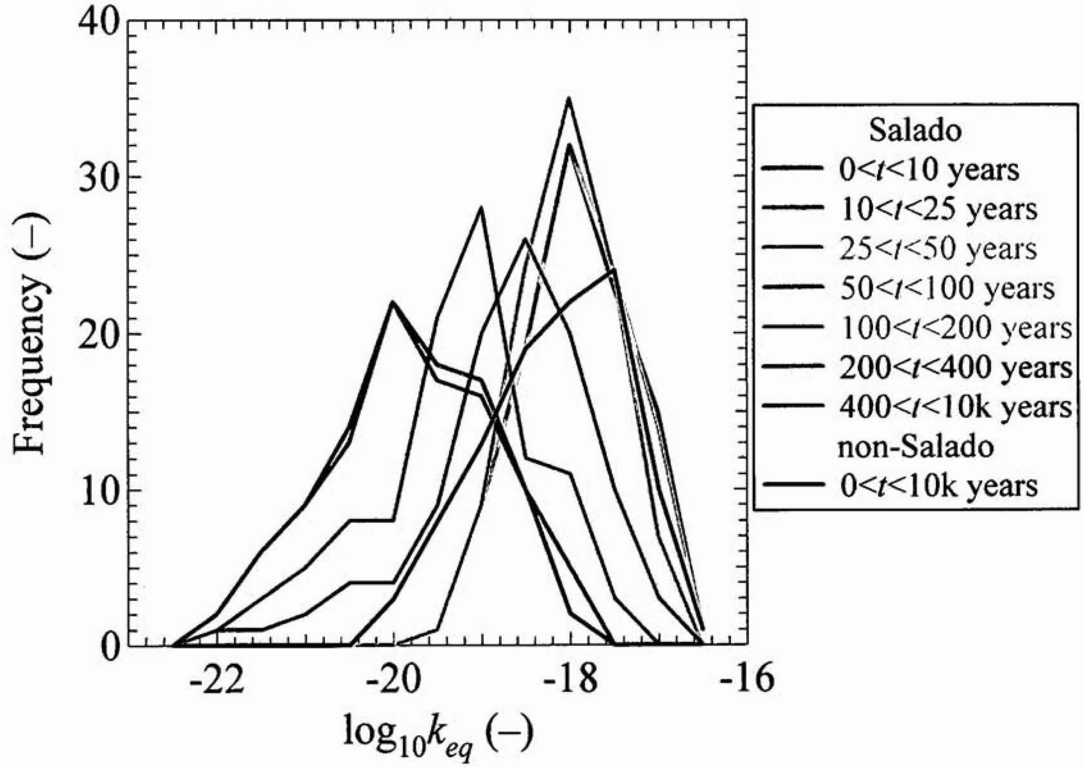

Figure 3: Distribution of equivalent permeabilities for the PAVT R1 shaft. Note that change in color represents the distribution of equivalent permeabilities over a different time interval.

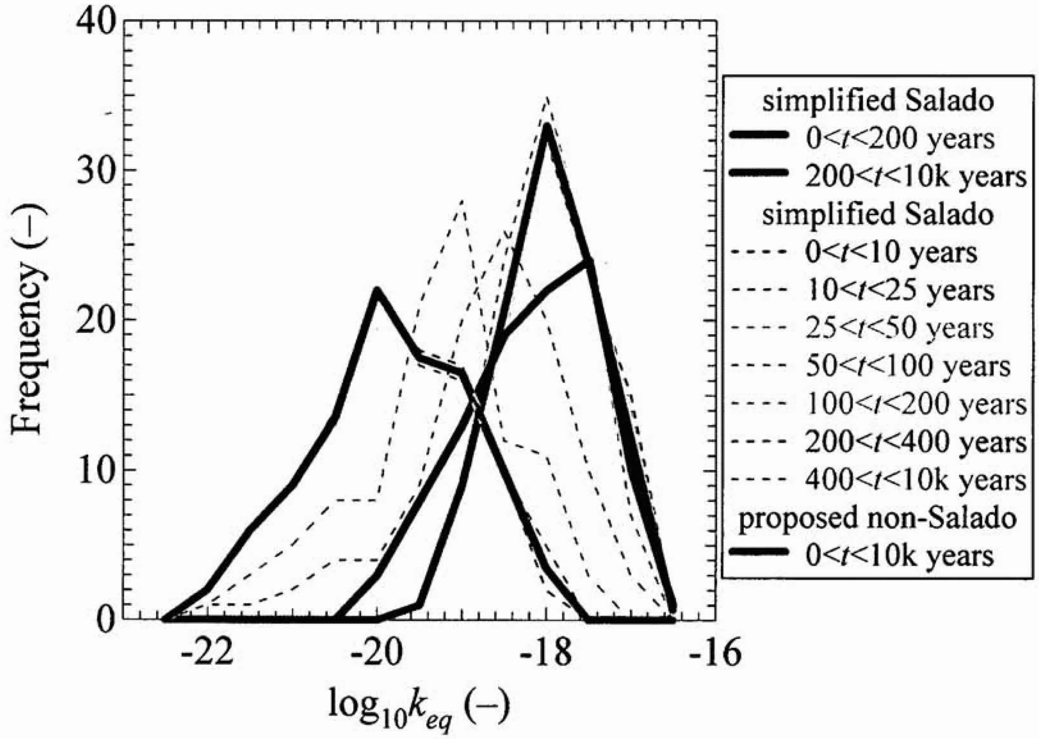

Figure 4: Thick lines show the proposed distributions for the simplified shaft model. The simplified model would include only one material property change at 200 years for the Salado component of the seal. The permeability distribution proposed for non-Salado material is simply the equivalent permeabilities from the baseline shaft seal model.

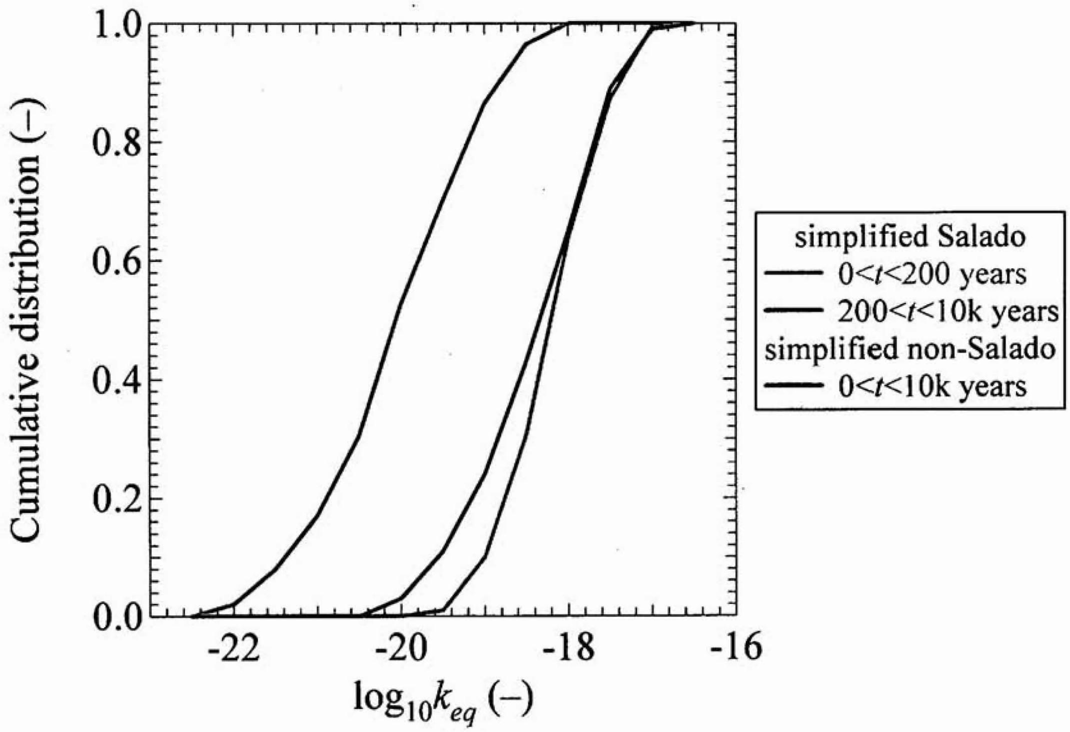

Figure 5: Cumulative distributions for the simplified shaft corresponding to the distributions in Figure 4~~Figure 4~~.

Information Only

Table 2: Volume averaged rock compressibility, porosity, and initial brine saturation for the simplified shaft model.

Property	Non-Salado	Salado	
	0–10,000 years	0–200 years	200–10,000 years
COMP_RCK	2.0491441×10^{-8}	4.2785786×10^{-9}	4.2785786×10^{-9}
POROSITY	0.29105080	0.11302095	0.11302095
SAT_IBRN	0.79638135	0.53412808	0.53412808