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Waste Isolation Pilot Plant

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

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1 INTRODUCTION AND OBJECTIVES

During conceptual model development for the Compliance Certification Application (CCA) and Performance Assessment Verification Test (PAVT), it was 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 prospect, a detailed representation of the shaft was implemented as a component of the repository system. However, these performance assessment (PA) models demonstrated that the shaft seal design effectively prevents releases via the shafts 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.

With knowledge that the shaft seals do not affect repository performance, the current implementation of the shaft seal system into the PA calculations is overly complicated. There are three sources for the inordinate complexity of the model:

1) The shaft seal is represented by 11 separate material layers (9 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 for WIPP, it is not necessary to model it in detail and PA efficiency would be significantly improved if the model were simplified. Nevertheless, any simplification must accurately represent the shaft seal behavior as modeled in the baseline PA. 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 shows the baseline logical grid and the shaft seal model used in the PAVT and CCA. 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, two material layers, non-Salado and Salado, are proposed for use in a simplified shaft seal model, rather than the 11 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). 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 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 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) generated for the current baseline calculation and were extracted using the program SUMMARIZE (WIPP, 2002). For each of the 100 vectors of PAVT R1, Salado shaft-seal equivalent permeabilities must first be calculated. That is, 100 equivalent permeabilities were generated by substituting the nine effective permeabilities (non-shaded cells in Table 1) and corresponding thicknesses into (1) for each of the seven constantpermeability time intervals (columns in Table 1). To discretize the equivalent permeability distribution, a histogram was generated. Specifically, each of the 100 values was binned into a half-log interval (between –23 and –16) and the number that fell within each interval (frequency) was counted. These data are plotted for each time interval in Figure 2. Because the permeability of the non-Salado seal components does 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%, 602%, and 2500% 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 proposed simplified shaft seal model comprises two composite materials (representing Salado and non-Salado components) instead of nine materials in eleven layers (Figure 3) 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 will be used directly.

The permeability of the non-Salado composite material will be sampled from the equivalent distribution calculated from current baseline. This distribution is represented by the black curve in Figure 2. To capture the time-dependent behavior of the Salado composite material, a single permeability change at 200 years is suggested. A conservative choice for the distribution of the first 200 years is to average the distributions for the 0–10, 10–25, 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 proposed for the new model.

The permeability distributions can be implemented in PA by fitting a cumulative distribution to the two empirical ones shown in Figure 4. If the simplified shaft seal model is adopted, the distributions will be derived in accordance with NP 9-2 and detailed in a subsequent memorandum or routine calculation.

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 porosity and compressibility will be 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.

2.2.2 Two-phase flow parameters

In the baseline model, the residual brine and gas saturations 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, this practice will be continued. All other parameters related to two-phase flow (e.g., pore-size distribution parameter and variables used to calculate Brooks-Corey or van Genuchten characteristic curves) are uniform for all shaft seal materials. This practice will also be continued in the simplified model.

3 SUMMARY

A simplified version of the shaft seal model is outlined. The proposed model reduces the number of materials from nine (in eleven layers) to two and reduces the number of model restarts and material reassignments from six to one. Additionally, the preprocessing step required to calculate the effect of the DRZ on permeability is incorporated into the parameter distributions. These modifications result in a simpler model that conservatively represents the shaft seals in the WIPP PA.

4 SOFTWARE LIST

Permeability values from PAVT R1 are tabulated using the program SUMMARIZE version 2.20 (WIPP, 2002). All calculations will be performed in a spreadsheet per NP 9-1 for routine calculations.

5 TASKS

1. Parameter values must be tabulated from the PAVT R1 CDB files that were generated by POSTBRAG (WIPP, 2002) and which are stored in the Configuration Management System (CMS).
2. Equivalent simplified shaft seal material parameter values will be calculated in a spreadsheet and will be documented as a routine calculation. The methodology is described in this Analysis Plan (AP).
3. Parameter distributions will be defined for the new simplified shaft seal materials.
4. Parameter distributions will be qualified according to NP 9-2 QA standards and proper documentation will be produced.

5. The new parameters will be entered into the WIPP parameter database so they are available for PA calculations.

6 SPECIAL CONSIDERATIONS

In order that the simplified shaft seal model parameters are qualified and available for the CRA calculations, this work must be completed before the CRA BRAGFLO calculations begin.

7 APPLICABLE PROCEDURES

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

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 the Compaq Alpha using Open VMS AXP, Version 7.2-1.

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.

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Baseline Grid

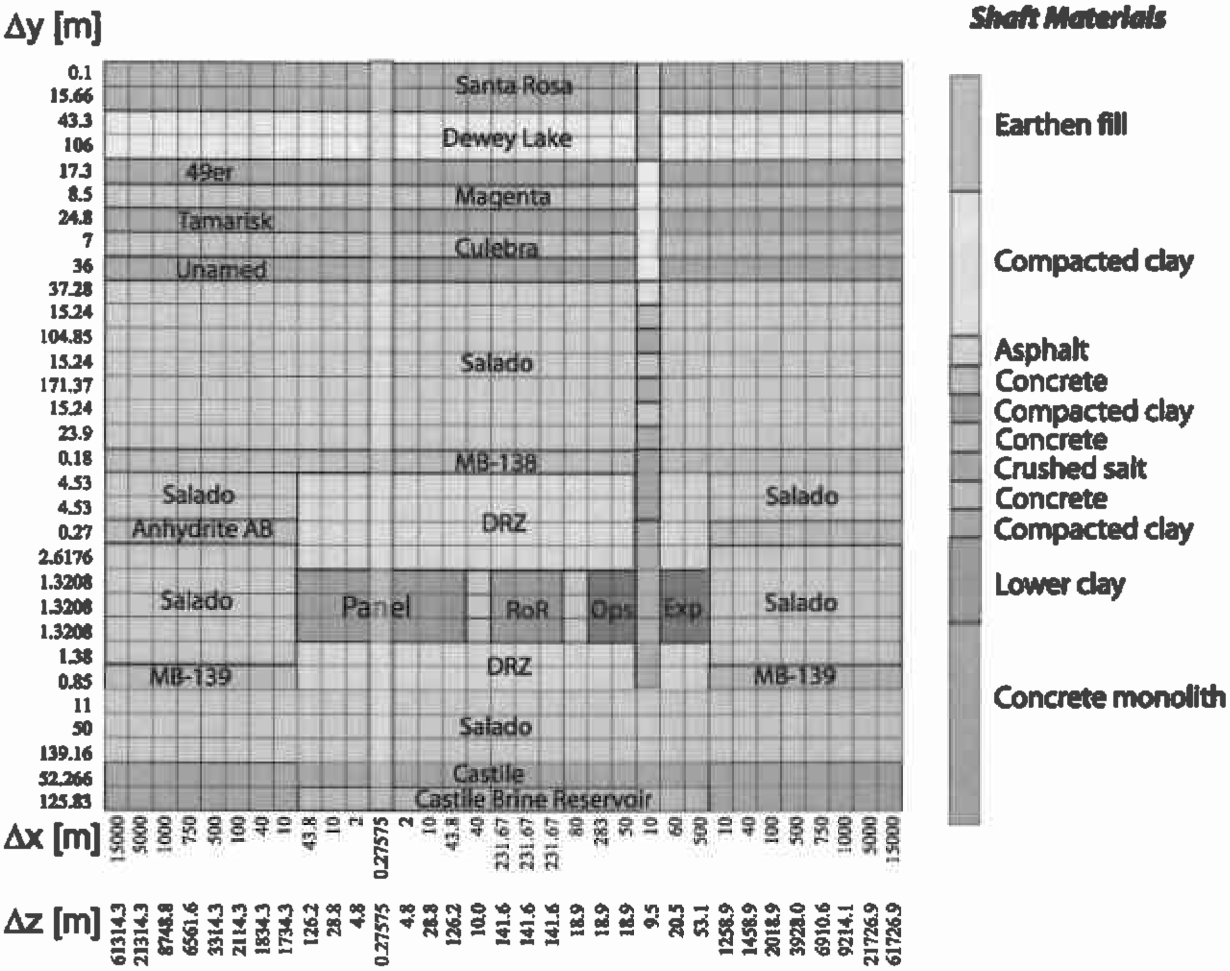

Figure 1. Baseline BRAGFLO logical grid showing the location of the shaft. The shaft is enlarged to the right and the materials used in the baseline model are labeled.

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) formation. 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
Concrete monolith	2.89	**CONC_MON**	CONC_MON	CONC_MON	CONC_MON	CONC_MON	CONC_MON	CONC_MON

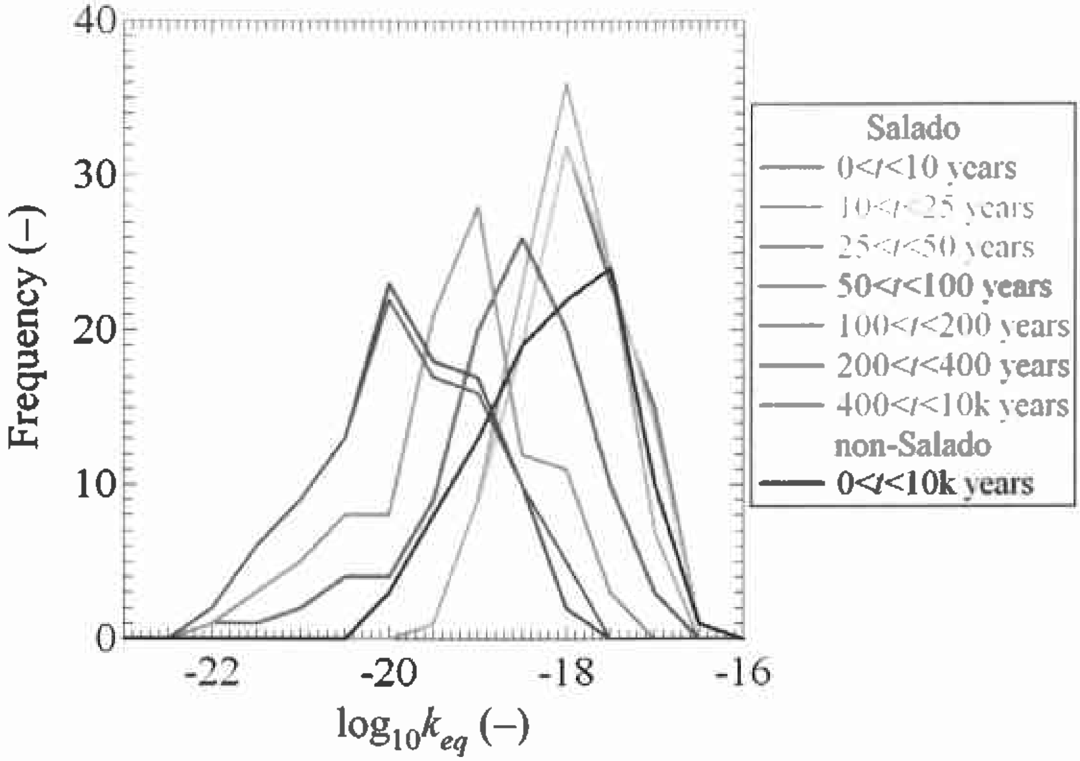

Figure 2. Distribution of equivalent permeabilities for the R1 PAVT shaft. Note that change in color represents the distribution of equivalent permeabilities over a different time interval.

The Shaft Seal Model Representations

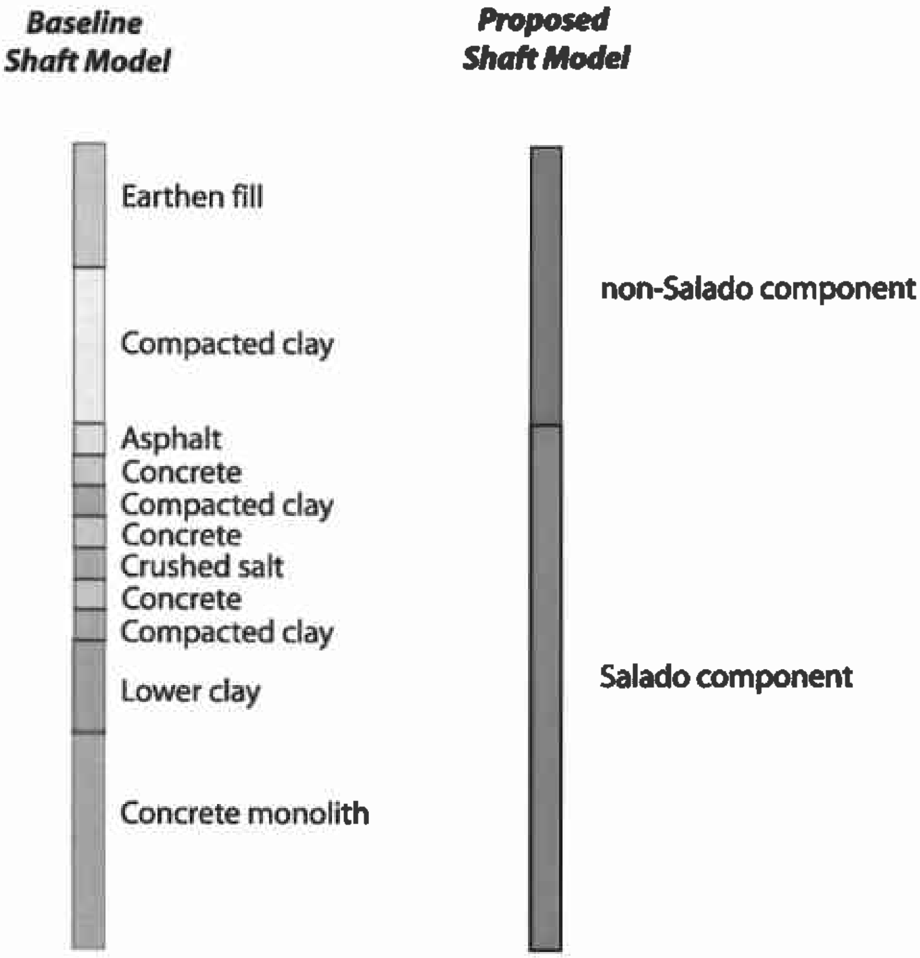

Figure 3. Representation of the baseline shaft seal model contrasted with the proposed simplified model.

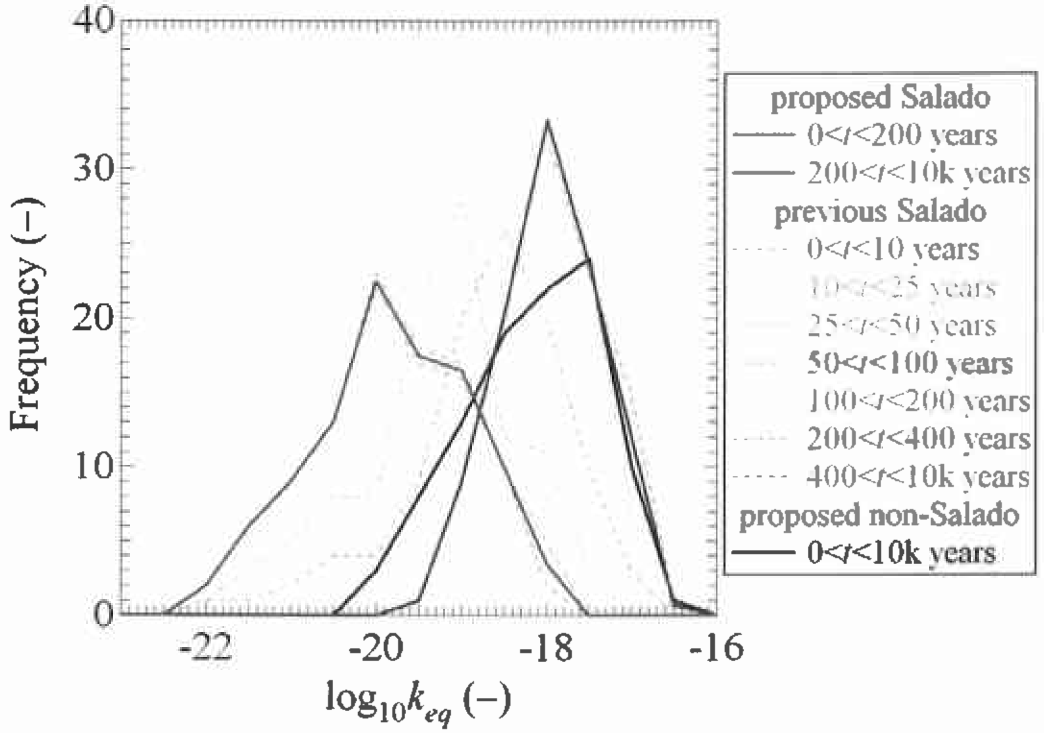

Figure 4. Thick lines show the proposed distributions for the simplified shaft model. The simplified model would include only one material property change at 200 years for the Salado component of the seal. The permeability distribution proposed for non-Salado material is simply the equivalent permeabilities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

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