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Sandia National Laboratories
Waste Isolation Pilot Plant

Analysis Plan for the Testing of a Proposed BRAGFLO Grid to be used for the Compliance Recertification Application Performance Assessment Calculations

AP-106

Task number
1.3.5.1.2.1

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1 INTRODUCTION AND OBJECTIVES

In May, 2002, the Salado Flow Peer Review panel met in Carlsbad to evaluate changes to conceptual models for the Performance Assessment (PA) of the Waste Isolation Pilot Plant (WIPP). These changes are detailed in a report by Hansen et al. (2002). To demonstrate the effects of these changes on BRAGFLO results a set of PA calculations (The Technical Baseline Migration (TBM)) was run. The peer review panel judged the changes to be "generally sound in their structure, reasonableness, and relationship to the original models," however the panel required that a total systems PA be run and complementary cumulative distribution functions (CCDFs) be generated before they would agree to the changes (Caporuscio et al., 2002). In response to this finding, Sandia National Laboratories has run a total system PA for the TBM and will present these results to the panel in February, 2003.

After the initial meeting of the Salado Peer Review panel in May 2002 the DOE received two letters from EPA (EPA, 2002a; 2002b) with a list of topics that EPA would like to be considered by in the PA calculations for the Compliance Recertification Application (CRA). In addition, additional issues and concerns were discussed in a series of technical exchange meetings with the EPA. Two of the topics discussed relate specifically to assumptions made for the TBM BRAGFLO calculations: (1) the presence or absence of the shaft in the BRAGFOL model grid, and (2) the move of the repository horizon up approximately 2 m to Clay seam "G" for panels 3, 4, 5, 6, and 9. These panels are located in the southern half of the waste disposal area.

The TBM calculations did not include an explicit model of the shaft seal system in the BRAGFLO grid. The shaft was removed because in all the previous calculations no significant flow occurred in this region and the shaft model required that nearly 1,000 separate parameters be defined. In subsequent discussions, SNL was led to believe that the presence of the shaft in the grid was considered important by EPA. Therefore SNL presented to EPA an approach for implementing a simplified shaft model with equivalent properties to the original detailed model. This work is described in AP-094 (James and Stein, 2002) and in the associated analysis report (James and Stein, 2003).

The second issue relates to a request by DOE to EPA to raise the repository horizon in panels 3, 4, 5, 6, and 9 so that the roof is at Clay seam "G" (DOE, 2000). EPA responded to the request in a letter (EPA, 2000) in which EPA agreed with DOE that the effects to long-term performance would be minimal. At the time, SNL considered the change minor enough not to warrant a full-scale impact assessment. However, in a subsequent letter from EPA the Agency indicated that "the conceptual model of the repository should reflect the change to raise the level of excavation to clay seam G. The conceptual change should be appropriately addressed in the modeling, if warranted" (EPA, 2002a). In response to this letter, SNL has initiated an effort to evaluate the effects, if any, on PA resulting from the move in the repository horizon. Specifically, SNL has initiated two sets of analyses:

1. The horizon change may influence the creep-closure porosity surface calculated by SANTOS and used by BRAGFLO. The SANTOS calculations are being repeated with the new horizon to test whether the response surface will change significantly. This work is in progress and is described in AP-093 (Park, 2002).
2. The thickness of upper and lower DRZ represented in the BRAGFLO grid may change due to the horizon change. This change may affect flow pathways around the Option D panel closures as well as the total pore volume represented in the DRZ above and below the waste rooms. Specifically, in the raised half of the repository, the distance from the panel floor to MB 139 will increase by 2.4 meters (based on site stratigraphy) and the roof of the raised repository will be flush with Anhydrite "B." These changes mean that in the event of high pressures, fracture flow around the Option D panel closures in the raised half of the repository may be more likely to occur through the Anhydrite "B" layer rather than only though the floor and MB 139 as was modeled in the TBM grid. A new grid has been developed to test whether these changes are significant and the present analysis plan describes this work.

2 APPROACH

This analysis will run a full replicate consisting of three BRAGFLO scenarios (S1, S3, and S5) using a modified version of the TBM BRAGFLO grid, which hereafter is referred to as the PreCRA grid. In addition a limited set of vectors will be run with "adjusted" DRZ porosity to evaluate the significance of the reduced pore volume in the upper DRZ and the increased pore volume in the lower DRZ in the raised half of the repository. The PreCRA grid is described below in detail. It is essentially the TBM grid with the simplified shaft model, modifications to allow fracture flow "around" the Option D panel closures both above and below the closure concrete through the DRZ and marker beds, and a minor error correction relating to the volume of the rest of the repository regions in the TBM grid (Stein, 2002). The PreCRA grid used in this analysis is shown as a logical grid in Figure 1. For comparison, the TBM grid is shown in Figure 2.

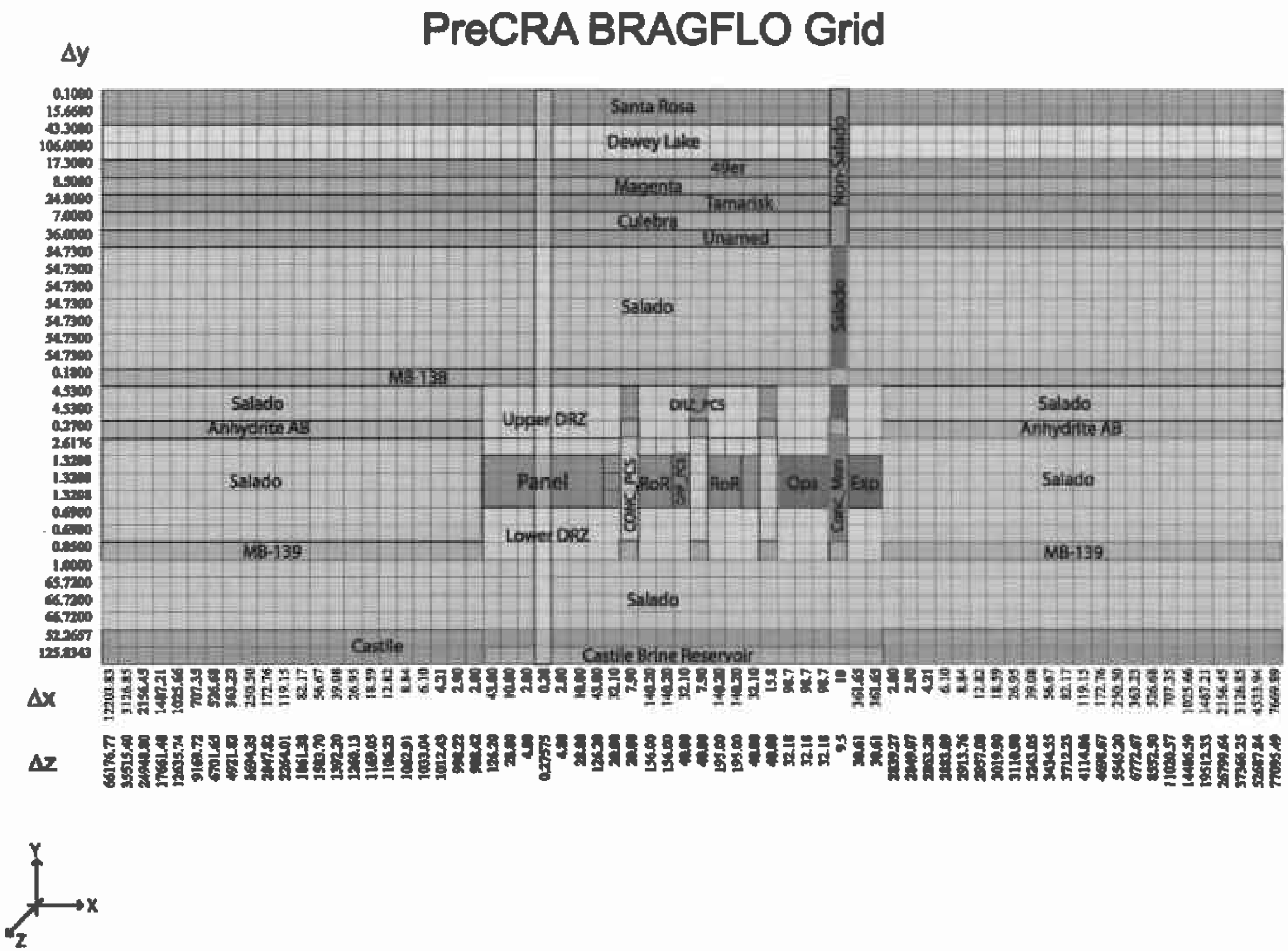

Figure 1. The PreCRA logical BRAGFLO grid. Dimensions in red indicate changes from the TBM grid.

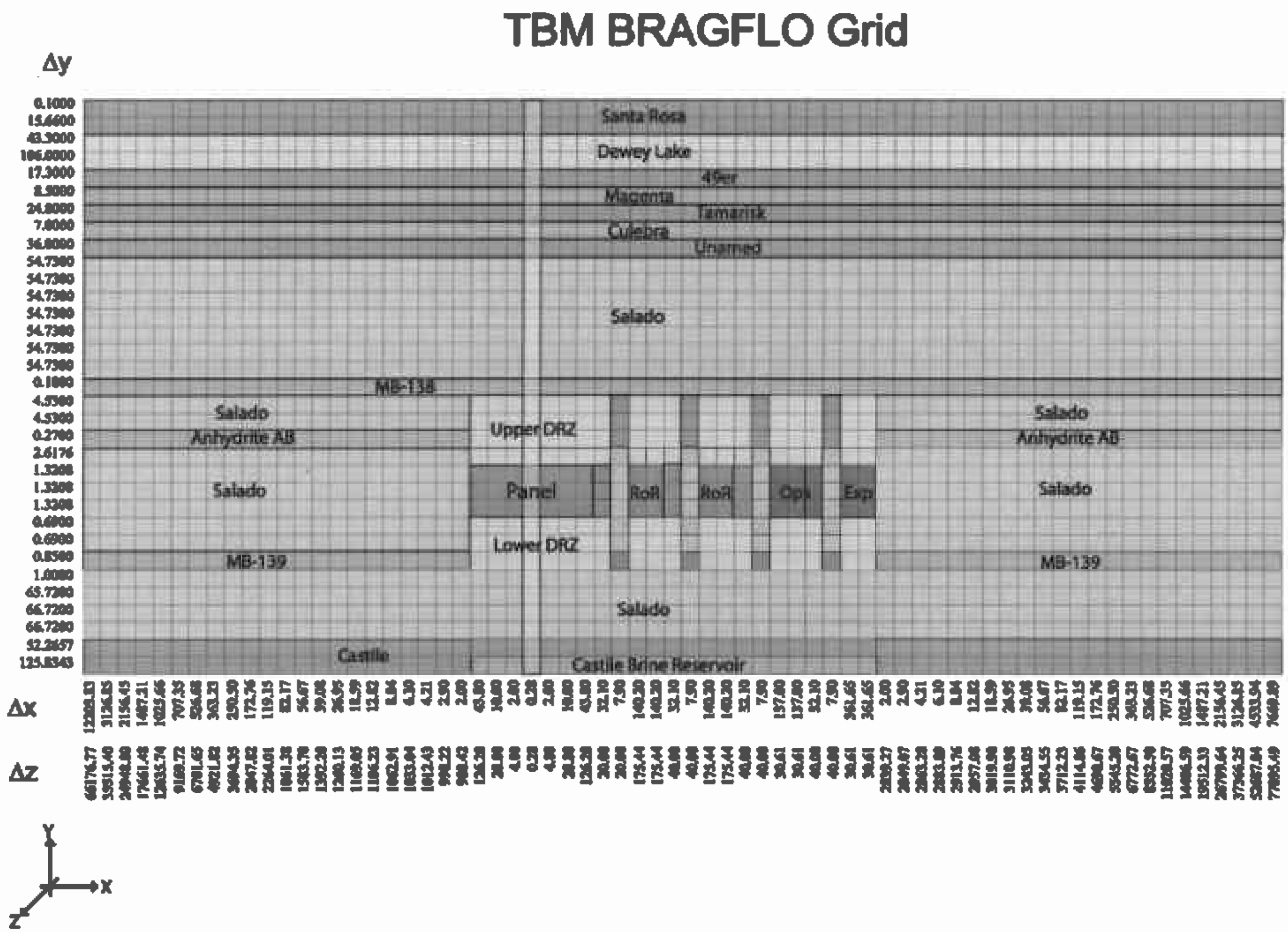

Figure 2. Technical Baseline Migration (TBM) Grid.

2.1 Simplified Shaft Model

The shaft seal model is included in the PreCRA grid but it is implemented in a simpler fashion to that used for the CCA and PAVT. A detailed description of the model and its parameters are discussed in AP-094 (James and Stein, 2002) and the resulting analysis report (James and Stein, 2003). The new model does not alter the conceptual model of the shaft seal components as described in SNL (1996). Rather, it conservatively represents the behavior of seal components in the repository system model. Specifically, the original 11 separate material layers that defined the shaft model for the CCA will be reduced to two layers each with properties equivalent to the original materials combined in series. Additionally, the six time intervals that were used to represent the evolution of the shaft seal materials over time are reduced to two intervals.

2.2 Fracturing in the Upper DRZ

In the TBM conceptualization of the DRZ, the permeability and porosity in the DRZ were represented as they were for the PAVT. However, SNL determined that fracturing should not be allowed in the DRZ above the repository. The upper DRZ was allowed to fracture in the PAVT in order to provide a gas path in the case of unrealistically high repository pressures. The PAVT analysis did not find unrealistic pressures in the repository; hence Sandia determined that the upper DRZ fracturing was not necessary for the TBM analysis since a fracture path was available in the lower DRZ. The argument made for allowing the lower DRZ to fracture was as follows. There is only a 1.4 m section of Salado halite between the repository floor and MB 139. As rooms close the floor heaves and fractures, and in the presence of higher gas pressures, fractures are not expected to heal thereby maintaining a hydraulic connection to MB 139. For this reason, fracturing was allowed only in the DRZ *below* the repository.

The proposed move of the repository horizon up 2.4 meters to Clay seam "G" and a closer examination of hydrofracture studies conducted in the WIPP underground in salt (Wawersik and Stone, 1989) requires the assumptions about allowing (or not allowing) fracturing in the grid elements representing the DRZ be reevaluated. Figure 3 compares the raised and unraised repository configurations in relation to the surrounding stratigraphy. Specifically, in the raised half of the repository, the distance through the DRZ from the repository floor to MB 139 will increase from 1.4 m to approximately 3.8 m. This change means that fracturing associated with floor heave will likely be reduced in this part of the repository. In addition, the raised waste rooms will have ready access to the Anhydrite "B" layer which will now be excavated to define the ceilings for the raised waste rooms. Anhydrite "B" is a thin (~6 cm-thick), layer that is present directly above Clay seam G. In the event of high repository pressures it is just as likely that a fracture pathway might form (1) parallel to the roof of the repository via Anhydrite "B", (2) vertically through the 2 m-thick DRZ to Anhydrite "A", (3) perhaps all the way to MB 138 or, 3.8 m into the floor to MB 139. In addition, an examination of hydraulic fracturing tests performed in WIPP salt 3-100 meters from excavated rooms (Wawersik and Stone, 1989) indicates that the pressures at which hydraulic fracturing initiated fall in a similar range as for hydrofracture tests done in anhydrite Marker Beds 139 and 140. Fracture initiation pressures for the anhydrite tests ranged from 7.36 to 12.46 MPa with an average initiation pressure of 10.5 MPa (Wawersik et al., 1997) while the fracture initiation pressures for the salt tests ranged from 4.14 to 17.24 MPa with an average initiation pressure of 11.98 MPa (Wawersik and Stone, 1989). One important difference in the fracture behavior of intact salt is that because it is so impermeable, fractures in WIPP salt will tend to stop at more permeable anhydrite marker beds and change direction, moving along the bed rather than fracturing across beds (Wawersik et al., 1997). These data indicate that fractures in both materials will typically initiate at pressures below lithostatic and thus repository pressures significantly above lithostatic are unjustified and unexpected. Because the data support the application of the fracture model to intact salt in addition to the Marker Beds, we will allow fracturing in both the upper and lower DRZ in this analysis. This approach is reasonable because the dimensions of the DRZ are modest and fractures would not have to extend very far before intersecting a marker bed. The parameters used by the BRAGFLO fracture model and applied to the Marker Beds materials and the DRZ are justified because they do not allow repository pressures to significantly exceed lithostatic.

In the PreCRA grid we represent regions where the Option D panel closures and the shaft intersect a Marker Bed as isolated marker bed material. This representation is warranted for two reasons.

1. First, the marker bed material has a very similar permeability distribution (10^{-21} to $10^{-17.1}$ m^2) as the concrete portion of the Option D panel closures ($10^{-20.699}$ to 10^{-17} m^2) and thus calling this material marker bed in the model has essentially the same effect as calling it concrete as long as pressures are below the fracture initiation pressure.
2. Second, in the case of high pressures (near lithostatic) it is expected that fracturing may occur in the marker beds and flow could go "around" the panel closures out of the 2-D plane considered in the model. In this case the flow would be through the marker bed material that is already allowed to fracture. Therefore assigning these isolated cells as Marker Bed materials is appropriate.

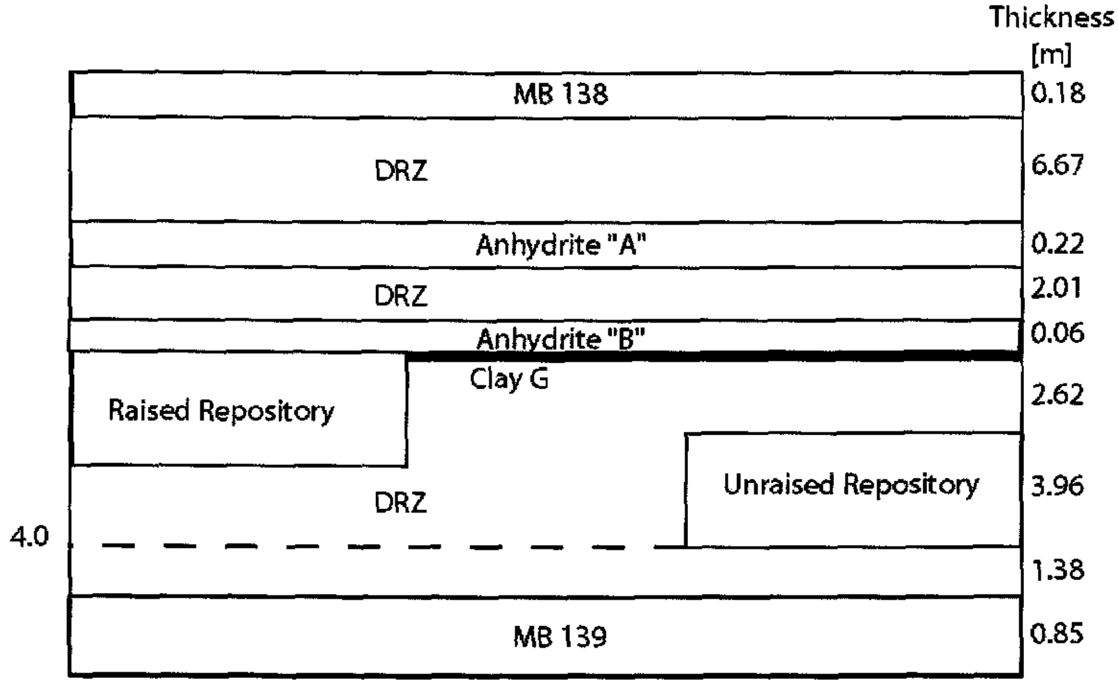

Figure 3. Schematic of the stratigraphy surrounding the raised and unraised sections of the repository. Not to scale.

2.3 Other changes

In the TBM grid, a panel closure was included between the operations area and the experimental area. In the PreCRA grid, this panel closure was replaced by the material CONC_MON to represent where the shaft intersects the repository. This was the same approach used for the CCA and PAVT calculations. To account for the presence of that panel closure south of the shaft, the concrete portion of the panel closure located between the northern rest of repository and the operations area has been set to represent two panel closures (double thickness: 7.9 x 2 = 15.8 m).

A minor error in the dimensions of the TBM grid was identified during the calculation and documented by Stein in a memo to M.K. Knowles (Stein, 2002). Fixing this error required adjusting the delta Z dimensions of the rest of repository blocks. This has been done for the PreCRA grid.

2.4 Modeling the effect of raising the repository horizon to Clay Seam "G"

SNL intends to determine whether the change in repository horizon warrants more detailed consideration in the model grid by evaluating two possible effects of this change to PA calculations. First, SNL is reevaluating the creep-closure porosity surface (Park, 2002). Second, there is a need to evaluate if this change might affect the flow of gas and brine in the repository. This evaluation is part of the present analysis plan and is described below.

One effect of moving the southern half of the repository up to Clay seam G is that the floor of this half of the repository will ramp up 2 meters. In the original BRAGFLO grid used for the CCA and PAVT the repository was at a single stratigraphic level, but it dipped to the south by 1 degree. From a permeability standpoint fluids were relatively free to communicate between panels and across permeable panel closures. As a result, brine tended to flow down dip and collected in the single waste panel represented at the south end of the repository in the model grid. This resulted in higher brine saturations in this panel than in the rest of the repository. As part of the changes incorporated for the TBM, Option D panel closures were added into the grid and had the result that fluids no longer were able to easily flow between panels due to the impermeable panel closures. The TBM conceptual model results in the repository being more segmented than in the open CCA/PAVT conceptual model and the undisturbed brine saturations in all the waste regions are essentially equivalent. Because the Option D panel closures are so effective in preventing brine from flowing between panels, adding a ramp up to the southern half of the repository will not affect brine flow patterns due to the 1-degree dip. For this reason SNL advises that the horizon change need not be included explicitly in the model grid.

Another effect of the horizon change is to change the thickness of the upper and lower DRZ. This was discussed in section 2.2 in relation to the justification for including fracturing in both the upper and lower DRZ. The thickness of the DRZ is important not only in relation to flow pathways, but also in relation to total pore volume in the DRZ, and brine availability to the waste. A significant portion of the brine that contacts the waste and allows gas generation reactions to proceed comes from the DRZ in the first couple of hundred of years (Hansen et al., 2002). In the raised repository, the upper DRZ will be 2.4 meters thinner and the lower DRZ will be thicker by 2.4 meters. It is unlikely this change will be important to performance, however, to test this we will run a full replicate of 100 vectors from the undisturbed scenario (S1). In these "excursion" runs the porosity of the upper and lower DRZ in the southern half of the repository will be adjusted to account for the effect of changing the DRZ thickness without actually changing the thickness. Specifically, we will reduce the porosity in the upper DRZ directly over the southern half of the waste areas (single waste panel and southern rest of repository blocks) so that the total pore volume in these grid cells is equal to the total pore volume expected in the thinner DRZ. A similar practice will be used in the lower DRZ, except that the porosity will be increased proportionally to the increase in thickness of this layer. Gas generation, pressure and brine saturation time histories will be compared to see if the change in thickness of the DRZ is important.

3 SOFTWARE LIST

The major codes to be used for these calculations are listed in Table 1. Calculations will be performed on the ES-40 DEC ALPHA running Open VMS Version 7.3-1

Table 1. Codes to be used in this analysis.

Code	Version
ALGEBRACDB	2.35
BLOTCDB	1.37
BRAGFLO	4.10.02
GENMESH	6.08
ICSET	2.22
LHS	2.41
MATSET	9.10
POSTBRAG	4.00
POSTLHS	4.07
PREBRAG	6.00
PRELHS	2.10
SPLAT	1.02
SUMMARIZE	2.20

4 TASKS

The schedule, tasks, and responsible individuals are outlined in Table 2.

Table 2. Tasks and responsibilities.

Date	Task(s)	Responsible Individual
Jan 13-28, 2003	Prepare input files	William Zelinski Joshua Stein
Jan 13-28, 2003	Finialize new parameters for simplified shaft model	Joshua Stein Scott James
Jan 29-Feb 3, 2003	BRAGFLO calculations	Roger Coman
Jan 29-Feb 10, 2003	Analysis of BRAGFLO results	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 the ES-40 DEC ALPHA 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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EPA. 2002b. "Letter from Mr. Marcinowski to Dr. Triay dated December 13, 2002."

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