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Sandia National Laboratories
Waste Isolation Pilot Plant

Analysis Plan for Calculations of Direct Brine Releases: Compliance Recertification Application

AP-104

Task number
1.3.5.1.2.1

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1 INTRODUCTION AND OBJECTIVES

In 1996 the Department of Energy (DOE) completed a performance assessment (PA) for the Waste Isolation Pilot Plant (WIPP). The PA was part of the Compliance Certification Application (CCA) submitted to the Environmental Protection Agency (EPA) to demonstrate compliance with the radiation protection regulations of 40 CFR 191 and 40 CFR 194. The WIPP Land Withdrawal Act (Public Law 102-579) requires DOE to submit documentation to EPA for the recertification of the WIPP every five years following the first receipt of waste in order to continue operations at the site. This will require that a Compliance Recertification Application (CRA) be prepared and submitted to the EPA by March 26, 2004. The DOE expects to provide the CRA to the EPA during November 2003.

A new set of PA calculations will be included in the CRA submittal to EPA. Analysis plan AP-105 (Leigh, 2003) presents the full set of PA calculations required for the CRA and lists the series of analysis plans that describe the specific details for each component model that will be run for the CRA. This analysis plan (AP-104) describes the set of calculations that are run to simulate direct brine releases that may result from future drilling intrusions into the repository during the 10,000 years following closure.

2 BACKGROUND

Direct brine releases (DBR) are releases of contaminated brine originating in the repository and flowing up an intrusion borehole during the period of drilling. In order for DBR to occur, two criteria must be met:

1. Pressures in the repository must exceed drilling fluid hydrostatic pressure (roughly 8 MPa).
2. Brine saturation in the repository must exceed the residual saturation of the waste material (sampled by LHS from a uniform distribution from 0.0 to 0.552).

If both of these criteria are met, DBR is calculated using the code BRAGFLO with a two dimensional, horizontally oriented grid, which represents the vicinity of the waste panels.

DBR releases are calculated from a well deliverability equation in BRAGFLO:

$$q_p(t) = J_p(P_p(t) - P_{wf}), \tag{1}$$

where $q_p(t)$ is the brine flux to the well as a function of time, J_p is the well productivity index, $P_p(t)$ is the repository pressure as a function of time, and P_{wf} is the flowing bottomhole pressure (assumed to be constant). The well productivity index quantifies how readily brine can enter the well and flow to the surface. It is calculated from the following equation:

$$J_p = \frac{2\pi k k_{rp} h}{\mu_p \left[\ln\left(\frac{r_e}{r_w}\right) + s - 0.5 \right]} \quad (2)$$

k = intrinsic permeability of the waste (constant: $10^{-12.6198}$ m^2)
k_{rp} = residual brine saturation of the waste (uniform distribution: 0 to 0.552)
h = crushed panel height ($h = h_i(1 - \phi_i) / (1 - \phi)$, where h_i is initial height (3.96 m), ϕ_i is the initial waste porosity (0.848) and ϕ is the waste porosity at the time of intrusion (calculated by BRAGFLO).
μ_p = brine viscosity (constant: 0.0018 Pa-s)
r_e = external drainage radius of the grid block containing the well ($r_e = \sqrt{(\Delta x)(\Delta y)/\pi}$) where Δx and Δy are the grid cell dimensions of the grid cell containing the well. For example, an intrusion into the down-dip panel (figure 1) would yield: $r_e = \sqrt{(10)(32.7)/\pi}$ = 10.2 m.
r_w = well radius (0.1156 m)
s = skin factor.

The skin factor is calculated by

$$s = \left(\frac{k}{k_s} - 1\right) \ln\left(\frac{r_s}{r_w}\right), \quad (3)$$

where k is the permeability of the waste, k_s is the permeability of an open channel as a result of spallings releases (assumed to be infinite) and r_s is the effective radius of the well bore with the spallings volume (V_i) removed ($r_s = \sqrt{A_i/\pi}$), where A_i is an equivalent areal spallings release ($A_i = V_i/h_i$). In application, because k_s is assumed to be infinite, equation 3 can be simplified to:

$$s = (-1)\ln\left(\frac{r_s}{r_w}\right)$$

For the CCA, DBR releases were calculated using the code DBR_BRAGFLO using a two-dimensional horizontal grid. Five scenarios were employed, including one "first" intrusion scenario and four "second" or subsequent intrusion scenarios. In each scenario a borehole intruded the repository and provided a conduit to the surface for repository brine, if present. In two scenarios an additional borehole was simulated which connected the repository to the Castile brine pocket and provided a source of brine, which could flow through the repository and up the intrusion borehole to the surface. Two drilling locations were considered: and up-dip location and a down-dip location. The well deliverability equation (equation 1) was used by the model to calculate a source or sink for brine at the location of the well in the grid.

It was assumed that flow within the well was instantaneous. The model was run for a maximum of 11 days and the total volume of brine that reached the well connected to the surface was used to calculate the DBR release. The details of the DBR calculations for the CCA are described in Appendix MASS Attachment 16-2 (Stoelzel and O'Brien, 1996).

For the PAVT, the BRAGFLO code was used for the DBR calculations. However, several parameters were changed from the CCA. Specifically, the permeability of the waste was increased from 1.7×10^{-13} m^2 to 2.4×10^{-13} m^2. The permeability of the DRZ was changed from a constant value of 10^{-15} m^2 to a sampled value (uniform distribution: $10^{-19.4}$ to $10^{-12.5}$ m^2). To implement this sampled permeability for the PAVT the pillars between rooms were assigned the initial sampled permeability while the DRZ surrounding the repository was assigned the permeability at the time of intrusion (possibly enhanced due to fracturing).

Following the PAVT an error in the well productivity index was identified. The 2π term in the numerator (equation 2) was added (Hadgu and others, 1999).

3 APPROACH

The DBR calculations for the CRA will include several changes from the CCA and PAVT approach. These change include:

1. Implementation of Option D panel closures in the DBG calculations.
2. Redefine material map to reduce the extent of the DRZ into the walls of the repository.
3. Correction of the way the external drainage radius, r_e, is calculated.
4. Assumption of a constant value for the skin factor.
5. Adjustments of the way initial conditions (pressure and saturation) are assigned.
6. Addition of a "middle" drilling location.
7. Additional calculation sets as a result of the new drilling location.

These changes are described in the following sections.

3.1 Option D Panel Closures

In the CCA, the DOE presented four options for panel closure designs (A-D). The EPA as a condition for certification mandated the implementation of Option D, which is designed to provide the tightest closure between panels. For the CRA we plan to implement a panel closure model which represents the Option D panel closure. This model was reviewed and accepted by the Salado Flow Peer Review panel (Caporuscio and others, 2003).

For the CCA and PAVT the material used to represent the panel closures (PAN_SEAL) had a constant permeability of 10^{-15} m^2. For the DBR calculations in the CRA, the permeability of the panel closures will be calculated as the equivalent permeability of the various panel closure materials in series or in parallel depending on the orientation of the panel closures in the grid. The method we will use in the CRA to define the permeability in each direction is described in an earlier analysis plan for the Technical Baseline Migration DBR calculations (Hadgu, 2002). This is the approach that was presented to the Salado Flow Peer Review Panel during their February 2003 meetings and was judged to be an adequate representation (Caporuscio and others, 2003).

3.2 Material Maps

The numerical grid and scenarios to be used for the CRA calculations will be the same as were used for the CCA and PAVT. However, the mapping of materials to the grid will change as a result of the conceptual model changes associated with representing the Option D panel closures in the PA.

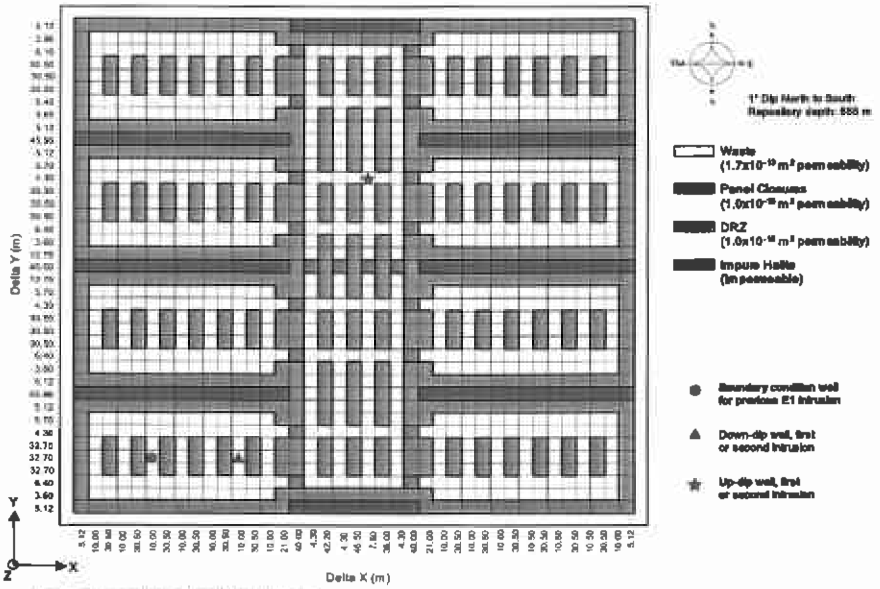
For the CCA and PAVT the DRZ material was used to represent nearly all the unexcavated salt within the bounds of the waste panels. This mapping was reasonable in the CCA because the DRZ permeability was constant (10^{-15} m^2) and low enough not to allow DBR drilling intrusions to influence panels other than the intruded panel. For the PAVT, the permeability of the DRZ was changed from a constant value to a sampled value (uniform distribution: $10^{-19.4}$ to $10^{-12.5}$ m^2). As a result of this change and the material mapping in the DBR grid used in the PAVT, vectors with high DRZ permeability displayed pressure perturbations in panels outside the intruded panel.

For the CRA we will convert many of the grid cells originally mapped as DRZ to Salado halite. This change ensures that each panel is relatively confined during a DBR intrusion and that little to no gas or brine can flow around the panel closures during the brief (11 days) runs (Hadgu, 2002). This change was presented to and accepted by the Salado Flow Peer Review panel Caporuscio and others, 2003).

Figures 1 and 2 compare the original and new material maps. The change from DRZ to Salado halite is consistent with the updated conceptual models of repository fluid flow that hold that Option D panel closures are relatively effective barriers to brine and gas flow between different panels, especially for the short time periods considered by DBR calculations. The total amount of brine available in the pores of the DRZ will continue to be conserved between the Salado BRAGFLO runs and the DBR BRAGFLO runs.

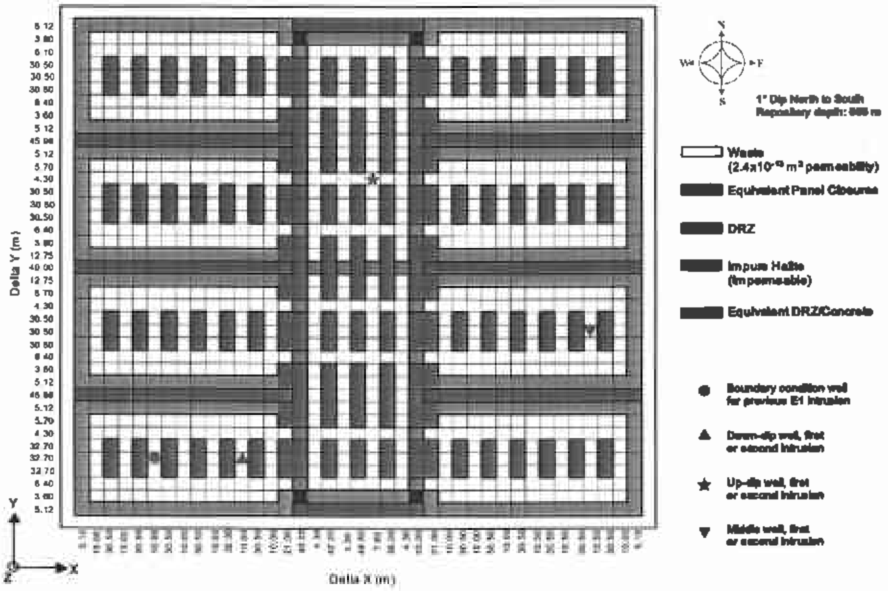
3.3 External Drainage Radius

For the CCA and the PAVT the external drainage radius, r_e, was calculated using the grid cell dimensions for the down-dip well only (10 x 32.7). The resulting value was then applied to up-dip well, which has a different grid cell dimension (7.6 x 4.3 m). To correct this error in the CRA we will calculate the external drainage radius for each of the wells separately and apply the appropriate value depending on the grid cell dimensions of the cell containing the well.



Note: Model cells are not to scaled. The actual dimensions of the grid blocks are indicated along the edge of the diagram.

Figure 1. CCA and PAVT DBR Material Map (logical grid)



Note: Model cells are not to scaled. The actual dimensions of the grid blocks are indicated along the edge of the diagram.

Figure 2. CRA DBR Material Map (logical grid)

3.4 Skin Factor

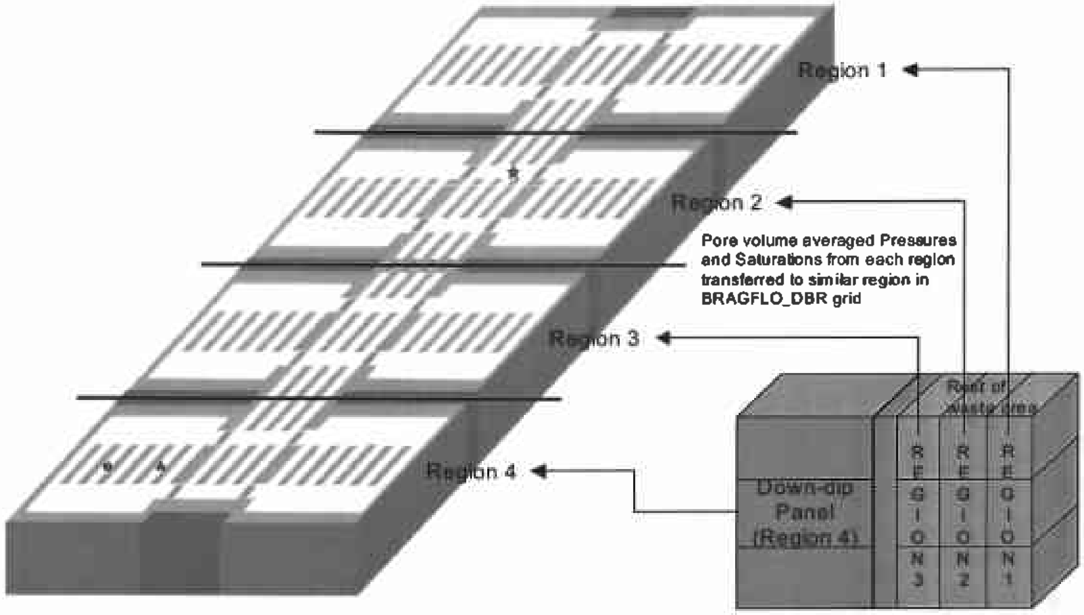
The skin factor (equation 3) depends on the spall volume though the effective radius, r_s. For the CCA and PAVT the spall volume was calculated by the CUTTINGS_S code. This dependence required that the CUTTINGS_S code and the DBR simulations be run in sequence.

For the CRA calculations we will sever the connection between DBR and CUTTINGS_S (spallings releases) and instead assume a constant, conservative value for the skin factor. The lowest value of the skin factor is conservative because it results in the highest value for the well productivity index (equation 2), which will conservatively overestimate the amount of brine that flows up the borehole during a DBR calculation (equation 1). The lowest skin factor is associated with the maximum spallings release volume (equation 3).

A revised spallings model is being developed and is planned for inclusion in the CRA PA assuming it is accepted by a peer review panel. Until approval of the new spall model, we will continue to use the PAVT spall model. In the PAVT, the spallings release volume was sampled between 0.5 and 4.0 m^3 .A spallings volume of 4 m^3 corresponds to the minimum skin factor $s = -1.3$. We will assume this value to be constant for all DBR calculations in the CRA. This change will result in an increase in the well productivity index for most vectors and a corresponding increase in the volume of DBR releases and is therefore a conservative assumption.

3.5 Initial Conditions

Volume averaged pressures and brine saturations are calculated from the 10,000 year BRAGFLO simulations at the time of intrusion and transferred to the DBR simulations as initial conditions. For the CCA and PAVT the waste regions in the 10,000 year BRAGFLO grid and the DBR grid were each divided into four regions and volume averaged pressure and saturations were transferred from corresponding regions in the 10,000 year BRAGFLO grid to the DBR grid (figure 3).



Refined BRAGFLO_DBR grid geometry

Representation of waste area in BRAGFLO grid (not to scale)

Figure 3. Regions used to transfer initial pressure and saturation between the 10,000 year BRAGFLO grid and the DBR grid for the CCA and PAVT.

For the CRA DBR calculations we will use three regions instead of four. These regions correspond to the single waste panel, south RoR, and north RoR. This method ensures that the relative volume of these regions is preserved between the 10,000 year BRAGFLO runs and the DBR runs. Figure 4 illustrates the method to be used for the CRA.

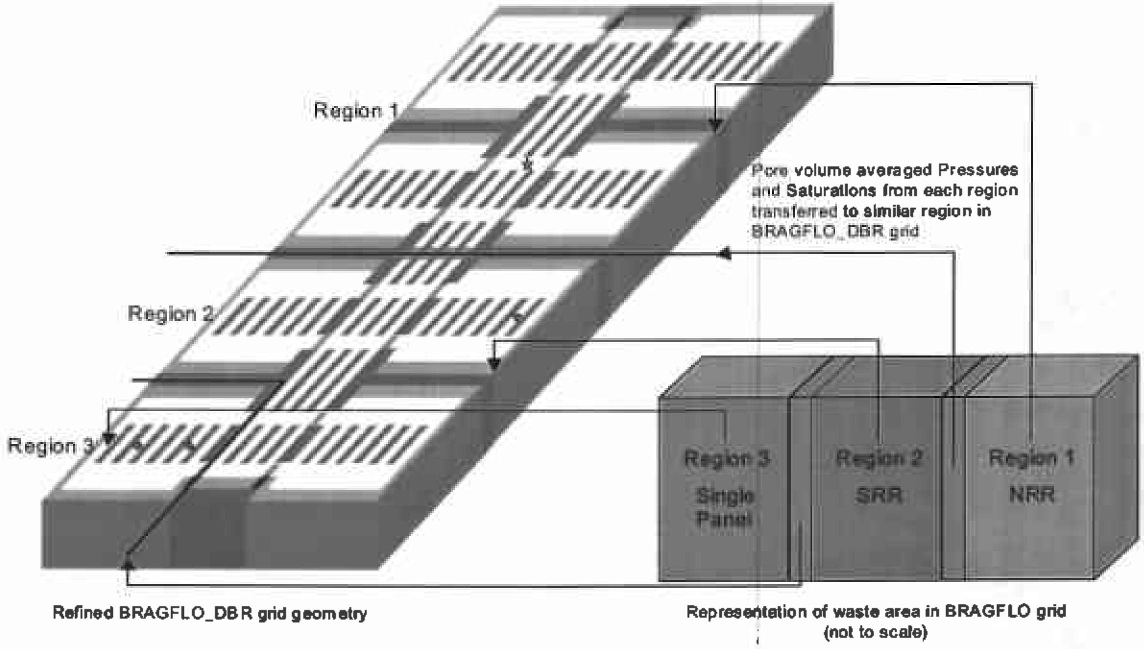


Figure 4. Regions to be used to transfer initial pressure and saturation between the 10,000 year BRAGFLO grid and the DBR grid for the CRA.

3.6 DBR Drilling Locations

To calculate DBR releases for the CCA and PAVT two drilling locations were considered: an up-dip and a down-dip location. These locations corresponded to the two waste filled regions in the Salado flow BRAGFLO grid (waste panel and rest of repository (RoR)). For the CRA the Salado flow BRAGFLO grid has three waste filled regions (waste panel, south RoR, and north RoR). To represent these regions in the DBR calculations for the CRA we will add an additional drilling location in the south RoR. The new "middle" drilling location will be in panel 3 (figure 2).

3.7 Calculations

The following DBR calculations will be performed for the CRA PA:

- Scenario 1: Upper, Middle, and Lower intrusions will be modeled at 550, 750, 1000, 3000, 5000, and 10000 years (18 calculations X 100 vectors = 1800 calculations per replicate).
- Scenario 2: Upper, Middle, and Lower intrusions will be modeled at 100, 350, 2000, 4000 and 10000 years (15 calculations X 100 vectors = 1500 calculations per replicate).
- Scenario 3: Upper, Middle, and Lower intrusions will be modeled at 1200, 1400, 3000, 5000 and 10000 years (15 calculations X 100 vectors = 1500 calculations per replicate).

- Scenario 4: Upper, Middle, and Lower intrusions will be modeled at 100, 350, 2000, 4000 and 10000 years (15 calculations X 100 vectors = 1500 calculations per replicate).
- Scenario 5: Upper, Middle, and Lower intrusions will be modeled at 1200, 1400, 3000, 5000 and 10000 years (15 calculations X 100 vectors = 1500 calculations per replicate).

4 SOFTWARE LIST

The major codes to be used for the CRA DBR calculations are listed in Table 1. Calculations will be performed on qualified ES-40, ES-45, and 8400 Compaq ALPHA computers running Open VMS Version 7.3-1 (SNL, 2003).

Table 1. Codes to be used in the CRA Direct Brine Releases Analysis.

Code	Version	Code Function
ALGEBRACDB	2.35	Data processor
BLOTCDB	1.37	Plotting
BRAGFLO	5.00	Brine and gas flow
GENMESH	6.08	Grid generation
ICSET	2.22	Sets initial conditions
MATSET	9.10	Sets material parameters
POSTBRAG	4.00	BRAGFLO postprocessor
PREBRAG	7.00	BRAGFLO preprocessor
RELATE	1.43	Grid data processor
SPLAT	1.02	Plotting
SUMMARIZE	2.20	Data interpolation

5 TASKS

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

Table 2. Tasks and responsibilities.

Estimated Date	Task(s)	Responsible Individual
May 1-May 9, 2003	Prepare input files	Joshua Stein
May 12- May 16, 2003	Begin DBR calculations	Rodger Coman
May 16, 2003	Begin analysis of DBR results	Joshua Stein
June 13, 2003	Final DBR Analysis Package Completed	Joshua Stein

6 SPECIAL CONSIDERATIONS

None.

7 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 fully qualified ES-40, ES-45, and/or 8400 DEC ALPHA computers 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.

8 REFERENCES

Caporuscio, F., Gibbons, J., and Oswald, E. 2003. *Waste Isolation Pilot Plant: Salado Flow Conceptual Models Final Peer Review Report.* Report prepared for the U.S. Department of Energy, Carlsbad Area Office, Office of Regulatory Compliance. ERMS# 526879.

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.

Hadgu, T. 2002. "Analysis Plan for the Analysis of Direct Releases Part of the Technical Baseline Migration." AP-085. Carlsbad, NM: Sandia National Laboratories. ERMS# 522634.

Hadgu, T., Vaughn, P., Bean, J.E., Johnson, D., Johnson, J., Aragon, K., and Helton, J. 1999. "Modifications to the 96 CCA direct brine release calculations." Memorandum to Melvin Marietta on November 2, 1999. Albuquerque, NM: ERMS# 511276.

SNL. 2003. Analysis Package for Upgrade of Operation System to OpenVMS 7.3-1 and Hardware to HP Alpha ES45. ERMS# 523490.

Stoelzel, D.M., and O'Brien, D.G. 1996. *Conceptual Model Description of BRAGFLO Direct Brine Release Calculations to Support the Compliance Certification Application (CCA MASS Attachment 16-2)*. Carlsbad, NM: U.S. DOE (U.S. Department of Energy).

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