APPENDIX E
DESCRIPTION OF THE DESIGN ANALYSIS MODEL

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DESCRIPTION OF THE DESIGN ANALYSIS MODEL

1.0 DESIGN ANALYSIS (COUPLED PROCESSES) MODEL

The components of the Design Analysis Model (DAM) are defined according to the physical barriers that will exist following waste emplacement at the Waste Isolation Pilot Plant (WIPP). These barriers and modeling regions are:

- Host rock and panel seals surrounding the rooms and drifts—The seven rooms and the equivalent volume of five and one-half rooms existing in the access drifts within a panel (12.5 room equivalents), are modeled on a collective basis to most accurately approximate the conditions within a disposal panel at each time step. The modeling is done using the ROOM-SCALE component of the DAM.

- Shaft and panel seals—The permeabilities of the seals are obtained as a function of time using the SHAFT-SEAL component of the DAM.

The DAM considers the processes that are essential to predicting changes in performance resulting from the application of alternative repository designs, waste forms, and backfills. The simulation by the DAM of the processes described in Section 3.1 is summarized below.

- Creep Closure of the Surrounding Host Rock—The Chabannes (1982) equation has been combined with a nonlinear regression equation based on several years of measured closure rates at 30 locations in the WIPP to predict creep closure rates of the host rock as a function of time. This equation expresses creep closure rates at each time step as a function of the room height, the room width, and the difference between lithostatic stress (14.8 MPa) and the internal stress in the panel. The internal stress is the sum of the effective stress of the waste/backfill composite and the fluid pressure inside the panel.

- Hydrogen Generation by Anoxic Corrosion—The dominant corrosion reaction is assumed to be the reaction of iron, usually in the form of mild steel, with water via one of the following two reactions (SNL/NM, 1991):

  1) $Fe + 2H_2O \rightarrow Fe(OH)_2 + H_2$ E.1

  2) $3Fe + 4H_2O \rightarrow Fe_3O_4 + 4H_2$ E.2

  These two reactions have differing stoichiometry; therefore, an average stoichiometry is derived as:

$$Fe + \frac{4+2x}{3}H_2O \rightarrow \frac{4-x}{3}H_2 + xFe(OH)_2 + \frac{1-x}{3}Fe_3O_4 \qquad \text{E.3}$$

  where x mole fraction of iron is consumed by equation 1. The parameter x is assumed to have a uniform distribution between 0 and 1. The median value of parameter x is reported as 0.5 (SNL/NM, 1993), resulting in an average reaction which generates seven moles of hydrogen for every ten moles of water consumed.

At each time step, brine in a disposal room (if available) is assumed to react with iron (or steel) to generate hydrogen at a rate of 0 to 0.6 moles of hydrogen per drum per year, depending on the percent saturation within the disposal panel (Brush, 1995). Any brine remaining at the end of a given time step is available for corrosion during the following time step. This corrosion process continues as long as brine (water) and corrodible metal are present in the panel. The corrosion process is self-limiting since the hydrogen that is generated contributes to the pressurization of the room, which in turn inhibits brine inflow.

- Microbial and Radiolytic Gas Generation—Microbial activity by a potentially broad range of microbes, which may be aerobic, anaerobic, halophilic, or halotolerant, is assumed to consume cellulosic materials and perhaps other organic materials in the waste as well. Since microbial activity and radiolysis utilize the same organic substrates, gas generation rates are assumed to represent both microbial and radiolytic gas generation. The total potential for microbial gas generation, along with the rate of generation, have been modeled based on the data provided in Brush (1995). The is based on the following assumptions:

    - Brine inflow is also necessary to sustain significant gas generation from microbial degradation of organic waste. Water is required to foster microbe growth, but it is not known whether microbe activity consumes or creates water. Therefore, it is assumed that microbial degradation results in gas generation without any effect on brine accumulation (Brush, 1995).

    - The gases generated during biodegredation are assumed to be methane, carbon dioxide, and nitrogen in the ratio of 15:20:12 (Lappin et al., 1989).

    - Microbial gas generation rates are assumed to vary from 0.1 to 1.0 moles of gas per drum per year, depending on the percent saturation within the disposal panels (Brush, 1995).

    - Based on the median stoichiometry for microbial gas generation presented in Sandia National Laboratories/New Mexico (SNL/NM) (1993), it is assumed that 0.835 moles of gas are generated for every one mole of cellulosics that are consumed.

- Dissolution of Gases in Brine—The moles of hydrogen, oxygen, and carbon dioxide dissolved in the brine present in a panel are evaluated at each time step. The moles of gas dissolved are calculated from phase equilibria relations using Henry's Law constants in brine (Reid et al., 1987). The Henry's Law constants and gas solubilities are evaluated from experimental correlations. The dissolution of nitrogen and methane is not considered since the brine already contains significant amounts of these gases (DOE, 1983).

- Brine Inflow—The following assumptions are made regarding brine flow into the disposal facility:

- An initial brine inflow rate of 0.597 cubic meters (m^3) per panel per year (Deal et al., 1994) is assumed. This is based on a constant room pressure of 1 atmosphere.

- The rate of brine inflow is assumed to linearly decrease as fluid (brine and gas) pressure in the room increases, and approaches zero when the pressure in the room reaches lithostatic pressure (14.8 MPa). Lithostatic rather than hydrostatic pressure is used since measurements of far-field pore pressures exceed hydrostatic (Lappin et al, 1989). This approach couples brine inflow to creep closure and gas generation, because all of these processes affect fluid pressure in the room, which in turn affects brine inflow.

- CO_2/Brine/Cement Interactions—Carbon dioxide (CO_2) generated by microbial or radiolytic processes will partition into any brine present in the room. This dissolved CO_2 will then react with portlandite to produce calcite plus water according to the reaction shown below. Portlandite is a major phase in Portland cement and is present in cementitious waste materials as well as sludges.

  - Carbon dioxide will react with portlandite (if present) to yield calcite and water according to the reaction:

$$CO_2 + Ca(OH)_2 = CaCO_3 + H_2O \qquad \text{E.4}$$

  - The reaction rate is assumed to be proportional to the volume of free brine in the room, and the reaction stops when either all of the portlandite or the brine/water in the room is consumed.

  - At each time step, water that is generated by the above reaction is added to the total number of moles of water in the room, and portlandite that is destroyed by the above reaction is subtracted from the number of moles of portlandite in the room.

- Diffusion of Gases into the Host Formation—Since undisturbed Salado brines at lithostatic pressure have significant amounts of dissolved N_2 and CH_4 (DOE, 1983), it is assumed that diffusion of these gases is negligible due to the lack of concentration gradients necessary to drive diffusive transport. Diffusion H_2 and CO_2 into the host rock are considered.

- Advection of Gases into the Host Formation, Across Seals, and into the Overlying and Underlying Anhydrite Beds—The host formation, panel and shaft seals, and the intact anhydrite beds are modeled as parallel routes for the advection of gases out of the panel. The following assumptions and information are being used for modeling purposes:

  - The permeability of the intact halite ranges from 1×10^{-23} m^2 to 1×10^{-18} m^2 with an expected permeability of 3.4×10^{-21} m^2 (Rechard et al., 1990).

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- The permeability of the intact anhydrite beds is estimated to be 2 to 3 orders of magnitude greater than the halite (10^{-18} m^2), and as such is assumed to be the most probable pathway for gas advection (Lappin et al., 1989).

Other assumptions include:

- The halite between each room and the anhydrites is fractured such that there is hydrological communication between the rooms and the disturbed anhydrite units.

- The anhydrite beds above and below the repository are extensively fractured due to excavation of the drifts and panels, and therefore all rooms and drifts within each panel are in equilibrium with respect to gas pressure.

- The disturbed anhydrites above and below the repository are assumed to be saturated with brine at the time of WIPP decommissioning.

- The intact anhydrites, and the halite layers above and below the repository (outside the disturbed rock zone), are assumed to be saturated with brine at pore pressures of 10.36 MPa (70% of lithostatic) and 14.8 MPa (lithostatic), respectively. The pressures in the intact Salado are chosen to provide the largest driving force for brine migration as a modeling assumption. Since there are measured values of the pore pressure approaching lithostatic, it has been chosen as the value for the far-field pressure of the brine.

- When the panel fluid pressure exceeds the assumed intact anhydrite pore pressure, the brine in the disturbed anhydrite is assumed to be driven into the undisturbed anhydrite.

- The flow of brine from the disturbed anhydrites to the intact anhydrites and Salado layers, is assumed to be governed by Darcy's equation of flow through porous media.

- The volume from which the brine is expelled is assumed to provide an additional void volume for panel gases to occupy.

A program simulating two-phase flow is used to derive a parametric equation for the advection rate into the intact anhydrites when the panel fluid pressure exceeds 11.3 MPa [brine pore pressure of 10.36 MPa plus a threshold pressure of 0.94 MPa (Davies, 1989)]. Concurrently with gas advection into the anhydrites, the advection of panel gases into the four shaft seals (conductance varying with time) is also simulated. A viscosity correlation which is valid at both low and high pressures is used to estimate the viscosity of the gas mixture for use in the advection calculations.

- Gas Compressibility—The Lee-Kessler Equation of State (Reid et al., 1987) is used to estimate the compressibility of the gas mixture in a panel at each time step based in the mole fractions of each gas present. The fluid pressure is updated at each time step based on the resulting value of compressibility. The fluid pressure is then used to estimate molar advection rates of gases, volume of brine inflow, creep closure rates, and gas solubilities in brine during the next time step.

- Waste/Backfill Composite Compaction and Resulting Mechanical Resistance to Closure—Stress/density relationships have been obtained for each waste form and backfill material from literature and experimental data. For each engineered alternative, an average density (based upon the mass fraction and density of each component) is calculated at various stress levels of compaction. The density of the waste/backfill composite is evaluated at each time step. The effective stress corresponding to this density is evaluated using the stress/density relationships of the composite. This effective stress is then used as input to the Chabannes equation (see discussion on creep closure above) as the mechanical component of resistance to creep closure.

- Development of a Zone of Enhanced Porosity Surrounding the Panel—The creep of the host rock creates an additional void volume within a zone of enhanced porosity which the panel gases will occupy. The rate and extent of creep closure will govern the magnitude of this void volume. This void volume is calculated at each time step as the product of the porosity of the Intact Salado (0.001) (Marietta et al., 1989, Table 3-9) and the difference between the initial panel volume and the panel volume at the current time step.

  - It is assumed that the zone of enhanced porosity does not contain brine.

  - It is assumed that all the pores in this zone are interconnected.

- Future Human Intrusion Into the Repository—Three human intrusion events (reference figure if there is one included in the report) were evaluated to determine the relative effectiveness of each engineered alternative in reducing radionuclide releases. The three scenarios, the modeling procedure for each scenario, and the assumptions behind them are described as follows:

  - The E1 scenario (Marietta et al., 1989) (see Figure 4-2) (SNL/NM, 1993) assumes a borehole penetration through a waste-filled panel and continuing into or through a pressurized brine pocket existing in the underlying Castile Formation. This event was modeled using a parametric equation relating flow rate through the waste/backfill composite to the hydraulic conductivity of the composite. This equation was developed by statistically regressing data resulting from a series of computer runs using the flow and transport code SWIFT III (Reeves et al., 1986).

    The modeling associated with the E1 scenario is performed on a room basis, since only the area surrounding the actual borehole allows the brine to come in contact with the waste. In order to verify this, the SWIFT III was used to determine the velocities of the fluid flow through the waste/backfill composite. A bounding brine velocity was chosen such that in 5,000 years a fluid particle would not be able to move a distance equal to the height of the room. This velocity defined a radius of influence used to calculate an effective wash-through volume. This volume was simulated as an ellipsoid, with the major axis along the borehole and the other axes into the room. If the conductivity of the waste/backfill composite was such that the effective radius was greater than the width of the room, the width of the room was chosen for one of the axes since the halite was considered to be impermeable. The other axis was allowed to continue to the edge of the room, but in no case did the effective radius exceed half of the length of one room. The assumption of an infinite reservoir of brine in the Castile allows a constant pressure of 16 MPa to be prescribed for the brine pocket.

- The E2 scenario (Marietta et al., 1989) (see Figure 4-3) (SNL/NM, 1993) is one in the report for intrusion scenarios) assumes a borehole just penetrating into the repository, not passing through. This scenario is modeled using an analytical solution to the radial flow equation through a porous media, simulating the borehole and the panel as concentric circles. The halite is considered to be an impermeable boundary that is located at a sufficient distance to allow the volume of the cylinder to be the volume of a panel. Simplifying assumptions regarding the flow of gas and brine are made. In actuality, the gas phase would be located towards the top of the panel and the brine phase would be located towards the bottom of the panel. In fact, the amount of brine predicted by the model to be present in the panel at 5,000 years would not be enough to fill the borehole to reach the Culebra. The gas being less viscous and towards the top of the panel, would tend to escape preferentially to the brine, thereby reducing the room pressure.

  For the purposes of comparing EAs, a hypothetical "fluid" with the properties of brine is used. This fluid is comprised of the appropriate volumetric proportions of gas and brine, which are predicted by the model for each alternative. This fluid is assumed to saturate the room and be transported to the Culebra through the borehole. The amount of radionuclides within the brine portion of the fluid that is released are then compared for each alternative.

- The E1E2 scenario (Marietta et al., 1989) (see Figure 4-3) (SNL/NM, 1993) assumes a combination of the first two scenarios; two boreholes penetrate the repository in the same panel. One borehole provides a pathway for brine flow from the Castile brine pocket directly into the panel. This borehole is capped above the repository such that no brine can move vertically to the Culebra. The other borehole (occurring later in time) provides a pathway from the repository to the Culebra Dolomite. This pathway consists of a flow path through the panel from the E1 borehole to the E2 borehole. No credit is taken for any processes which may occur or change during the interim between the first and second boreholes. This scheme results in a pressurized flow path directly through a segment of the waste/backfill composite.

  The flow rate through the waste is obtained from an analytical solution to the one-dimensional flow equation through porous media, assuming the two boreholes are separated by the length of one room (300 feet [ft]; 91.44 m). Any effects of the pressure in the room being greater than the pressure of the Castile brine pocket, are neglected due to the assumption of an infinite brine pocket. It should be noted that the E2 scenario is a part of the E1E2 scenario. This happens when the second borehole breaches the repository, potentially releasing any gases and brine initially located there. This is neglected because the amount of brine originally located in the panel would be extremely small in comparison to the volume produced from the Castile brine pocket.

The following assumptions have been applied to all human intrusion scenarios:

- The intrusion occurs 5,000 years after decommissioning.

- The diameter of the borehole is 0.355 m based upon a survey of current standard drilling practices in the Delaware Basin (SNL/NM, 1993).

- The hydraulic conductivity of the waste/backfill composite is the weighted geometric mean of the properties of the three types of waste and backfill.

- The borehole conductivity is 1×10^{-3} m/second (clean sand/gravel) obtained from Freeze and Cherry (1979, Table 2-2).

- Waste element solubilities are assigned from Attachment 1 of Appendix G (the table is in the Appendix on Radionuclide Solubilities) based on the pH of any brine present in the disposal facility.

The activity of each radionuclide at the time of intrusion is computed using the solutions to differential equations that represent mass balances for each radionuclide. Based upon the radionuclide solubilities in brine and the volume of brine released, the cumulative activity of each radionuclide released to the Culebra was determined. The objective of these human intrusion simulations is to calculate a number which is similar in functional form to the U.S. Environmental Protection Agency (EPA) Summed Normalized Release (EPA, 1993 [40 CFR 191]); the difference being that the DAM calculates the cumulative release of radionuclides into the Culebra. Alternately, the EPA Summed Normalized Release specifies calculation of the cumulative activity of each radionuclide across the regulatory boundary, and in addition, employs scenario probability weighting to each release (EPA, 1993).

The DAM does not consider probabilities of occurrence of scenarios; the scenario is assumed to occur and the effectiveness measure is evaluated. The value generated by the DAM is the singular raw score for the effectiveness of each alternative design. Calculation of the measure of relative effectiveness is performed by dividing the effectiveness measure for the alternative by the effectiveness measure for the baseline case (see Section 3.1.2). The baseline case uses "as received" waste with no backfill. "As received" waste is defined as follows:

- Sludges with some cement added as solidifying agents [i.e., current processes at the Rocky Flats Environmental Technology Site (RFETS) for Content Code 111], but not a concreted monolith (DOE, 1994b).

- Solid organics and inorganics are in unshredded form, wrapped in multiple layers of plastic, inside a 90-mil rigid liner in a steel drum [i.e., current packaging at RFETS and most other sites (DOE, 1994b)].

The improvement resulting from a waste form modification or a repository design alteration is determined by comparison with the baseline case. For the baseline case, the assumptions are as follows:

- Each room is assumed to be filled to capacity (considered to be 6,421 drums) with "as received" waste no backfill.

- The initial room dimensions used in the calculations are 13 feet (3.96 m) high by 300 feet (91.44 m) long by 33 feet (10.06 m) wide (Lappin et al., 1989).

- A two-foot high clearance is assumed to be left above the waste/backfill composite in all rooms and drifts in the panel.

- The panel capacity (including the seven disposal rooms and the surrounding access drifts) is assumed to be approximately 12.5 times the capacity of one individual room.

- The panel and shaft seals are assumed to be in place.