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Impact of inventory changes on the Waste Isolation Pilot Plant Performance Assessment

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INTRODUCTION

The Waste Isolation Pilot Plant (WIPP), located in southeastern New Mexico, has been developed by the U.S. Department of Energy (DOE) for the geologic (deep underground) disposal of transuranic (TRU) waste. Containment of TRU waste at the WIPP is regulated by the U.S. Environmental Protection Agency (EPA) according to the regulations set forth in Title 40 of the Code of Federal Regulations (CFR), Part 191 [1].

The DOE must demonstrate that the WIPP facility complies with the containment requirements in Title 40 CFR Part 191 by means of performance assessment (PA) calculations. The waste inventory used in the WIPP PA is always scaled to the maximum volume allowed as specified by the Land Withdrawal Act (LWA) [2] and the Consultation and Cooperation (C&C) agreement [3]. However, the final scaled inventory used in the PA calculation is affected by the method for measuring the volume of waste (e.g., inner versus outer container volume) and by the inclusion of potential waste streams such as surplus plutonium or pit production waste.

WIPP PERFORMANCE ASSESSMENT

WIPP PA models releases from several pathways. Most releases in the WIPP PA model come from hypothetical inadvertent drilling events. The solid waste removed by a drill bit during an intrusion and the solid waste material eroded from the borehole by drilling fluids comprise releases due to cuttings and cavings. Direct brine releases are releases of mobile actinides dissolved in brine or sorbed onto colloids suspended in the brine that enter the wellbore and are transported to the surface during a drilling event. Spallings releases result when waste solids enter the borehole due to the release of waste-generated gas escaping into the lower-pressure borehole. Culebra releases are actinides that transport in the brine up the shaft or an abandoned wellbore to the Culebra member of the Rustler formation, then transport across the Culebra to the Land Withdrawal Boundary (LWB). WIPP PA also models actinide transport through the anhydrite marker beds in the Salado formation to the LWB, however this pathway never realizes significant releases.

WIPP PA breaks uncertainty into two categories, epistemic and aleatory. Epistemic uncertainty represents a lack of knowledge about parameters that are considered constants and represents a distribution of confidence. Epistemic uncertainty is implemented in WIPP PA by a Latin Hypercube Sampling (LHS) of 64 uncertain parameters. Each set of sampled parameter values, termed a vector, is then used as input to the process-level models to ultimately generate one CCDF of releases. The Latin Hypercube Sample size is 100, creating 100 vectors per Latin Hypercube Sampling called a replicate. A total of 3 replicates are created, giving 300 total vectors.

Aleatory uncertainty deals with unknown future events. In the process models for WIPP PA, aleatory uncertainty is represented by modeling defined future events (e.g., when and what type of drilling intrusions will occur). The process model results based on these defined futures are used to create look-up tables that can be used to predict releases from random drilling events using time-shifting and interpolation algorithms. For each realization of epistemic uncertainty, ten-thousand random futures are simulated. The releases from the ten thousand random futures are used to create a complementary cumulative distribution function (CCDF). The mean of all 100 CCDFs in a replicate is calculated, and the 3 replicate means are used to create a confidence interval around the overall mean CCDF. The mean CCDF is the primary metric for showing regulatory compliance for long-term performance.

The WIPP PA calculation is broken into several decoupled process models that predict conditions and releases from predefined scenarios. This first process model is the Salado flow model that models brine flow in and around the repository. The Salado Flow model is a two-phase porous media flow calculation with a number of specialized components such as creep closure of the Salado Halite, gas generation reactions, DRZ and markerbed fracturing, and other chemistry reactions.

Actinide solubility limit are calculated from baseline solubilities given by the thermodyamic model in EQ3/6 and derived solubility uncertainty distributions. Concentration limits of dissolved and colloidal actinides mobilizated in the brine are calculated through time by the PANEL code. The Salado transport process model calculated by the NUTS code builds an advective radionuclide transport solution on top of the flow solution found by BRAGFLO and the actinide mobilization limits found by PANEL. The Salado transport solution finds the amount of radionuclides entering the Culebra.

Cuttings, cavings, and spallings volumes are found by the CUTTING_S code using the repository conditions from the Salado Flow simulations. Spallings volumes are interpolated from tables of spallings volumes by repository pressures output from the DRSPALL code. The DBR process model again uses BRAGFLO for a flow solution to find the brine volume that would enter an intruding wellbore given the repository conditions from the Salado Flow solution for various times and scenarios. The brine volume from the DBR calculation is combined with actinide mobilization to calculate releases from the DBR event.

Steady-state flow in the Culebra member is simulated with MODFLOW2000. Radionuclide transport in the Culebra is modeled using the dual porosity code SECOTP2D and the steady-state flow solution.

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TABLE I. Inventory Data

Inventory	Activity (Ci)	Waste Unit Factor (-)	Iron Mass (kg)	CPR Mass (kg)
Inventory 1	6.14×10^6	3.30	6.31×10^7	1.78×10^7
Inventory 2	8.14×10^6	7.28	8.32×10^7	2.42×10^7
Inventory 3	1.98×10^7	16.18	1.11×10^8	3.56×10^7

Given the complexity of a full WIPP PA calculation, a complete description is out of the scope of this paper. A more through explanation of WIPP PA can be found in [4] and Appendix PA of [5].

Performance Metrics

WIPP PA calculates cumulative releases over the 10,000 year post-closure regulatory time period. Releases are measured in EPA Units. An EPA Unit is a relative metric to the total activity of alpha-emitting TRU waste with half-lives longer than 20 years emplaced in WIPP. The sum of all releases in a 10,000-year future is expressed by:

$$R_j = \frac{1}{f_w}\left\{\frac{Q_{1j}}{L_1} + \frac{Q_{2j}}{L_2} + \cdots + \frac{Q_{nRj}}{L_{nR}}\right\} \tag{1}$$

where:

R_j is the total normalized release (in EPA Units) for the j^{th} future

f_w is the Waste Unit Factor (WUF) = $\frac{\sum W_i}{10^6 Ci}$

W_i is the activity in Ci for α-emitting radionuclide i having a half-life ($T_{\frac{1}{2}}$) ≥ 20 years

Q_{ij} is the cumulative release for radionuclide i and future j.

L_i is the EPA release limit for radionuclide i (see Table 1 of section 191.13 in [1])

nR is the number of radionuclides contributing to the release

Releases for 10,000 futures are ordered by value and displayed as a complementary cumulative distribution function (CCDF) for each vector. The mean CCDF is calculated by taking a mean probability value of all vectors for each release value. Post-closure compliance is measured against the mean CCDF for total releases.

INVENTORIES

Changes to the waste inventory and to the procedures for estimating the waste volume represented in PA (termed here the WIPP inventory) can affect the outcome of the WIPP PA. WIPP has a legislated capacity of 175,564 m^3 of waste [2], and all PA calculations use an inventory that is scaled to that volume [6]; however the method of calculating volume of the waste in a container has been changed from the outer container volume to the inner container volume [7]. The shift to inner container volume allows a more accurate accounting of the waste emplaced in WIPP to best utilize the legislated capacity.

The second change to dramatically shift the content of the WIPP inventory is the inclusion of surplus plutonium in WIPP [8]. Surplus plutonium has a higher level of activity than most WIPP waste streams, so the inclusion of surplus plutonuim in the WIPP waste inventory can significantly increase the total activity of the inventory. As incremental quantities of the surplus plutonium are approved for disposition in WIPP, the activity of the waste inventory increases.

For inventory scaling to the legislated capacity, WIPP waste is broken into 3 categories; emplaced (already shipped to WIPP), stored (already generated), and projected (not yet generated). When the total inventory is less than the legislated capacity, a scaling factor is applied to projected waste to increase the inventory to the legislated capacity. The scaling factor is only applied to projected waste. Using the inner volume of the waste containers decreases the volume of the waste streams, resulting in an increase of the applied scaling factor. Since the surplus plutonium waste stream is included in the projected waste category, it is included as a part of the inventory that is scaled up to the LWA volume. The combination of the increase of the scaling factor due to the change in the volume of record and the scaling up of the surplus Pu waste streams results in a compounding effect on the WIPP PA inventory.

In this study 3 inventories are used. The first inventory is based on [6], which includes 6 metric tons of surplus plutonium and uses the outer waste container volume. The scaling factor for contact-handled (CH) waste is 1.58, and the scaling factor for remote-handled waste is 12.7. The total activity of the waste at repository closure is $6.14 \times 10^6 Ci$ with a waste unit factor of 3.30.

The second inventory uses the inner waste container volume and increases the projected surplus plutonium to 13.1 metric tons. Because of the volume of record change, the scaling factor for this inventory increases to 3.11 for CH waste. Several RH waste streams were added to this inventory reducing the RH scaling factor to 5.99. With this increase in scaling factor and increase in surplus plutonium, the activity of the waste at repository closure is $8.14 \times 10^6 Ci$, with a waste unit factor of 7.28 [9].

The final inventory uses the inner waste container volume and the full 42.2 metric tons of surplus plutonium under consideration for disposal at WIPP. The scaling factor the CH waste is 2.97, and the scaling factor for the RH waste is 6.96. The activity of the waste is increased to $1.98 \times 10^7 Ci$, with a waste unit factor of 16.18 [10]. More details of the three inventories used are listed in Table I.

RESULTS

Results for the PA calculations using each of the three inventories will now be shown.

Actinide Solubilities

TABLE II. Baseline Solubilities in Castile Brine

Inventory	+III Actinide Solubility (*moles/liter*)	+IV Actinide Solubility (*moles/liter*)	+V Actinide Solubility (*moles/liter*)
Inventory 1	1.90×10^{-7}	5.44×10^{-8}	1.2×10^{-6}
Inventory 2	1.94×10^{-7}	5.44×10^{-8}	1.18×10^{-6}
Inventory 3	1.70×10^{-7}	5.44×10^{-8}	9.81×10^{-7}

The mass of iron, lead, and organic ligands in the inventory impacts the calculated baseline solubilities. Table II contains the recalculated baseline solubilities for the Castile brine in the minimum brine volume for a DBR release. Baseline solubilities were also calculated for 4 other brine volumes, and for the Salado brine at the same five brine volumes.

Salado Flow

The Salado Flow calculation is a two-phase flow simulation over the 10,000 year post-closure regulatory time period to determine the conditions of the repository and the surrounding area. The output brine pressures, brine saturations, and brine flow serve as inputs for downstream PA codes. To cover the aleatory uncertainty, several scenarios with different drilling intrusions are simulated in the Salado Flow calculation. Scenario S1-BF is the undisturbed repository with no drilling intrusions. Scenario S2-BF has a drilling intrusion at 350 years post-closure that also intersects a pressurized brine pocket in the Castile formation. Scenario S4-BF has a drilling intrusion at 350 years post closure that does not intersect a brine pocket in the Castile. Scenario S6-BF has a drilling intrusion at 1000 years that does not intersect a brine pocket, then a subsequent intrusion at 2000 years that does intersect a brine pocket in the Castile.

In the Salado Flow calculation inventory primarily impacts gas generation from iron corrosion, the biodegradation of cellulose, plastic, and rubber (CPR), and brine radiolysis. The mean (across 300 vectors) cumulative gas generation from all mechanisms is shown in Figure 1. Scenarios with a drilling intrusion that also intersects a brine pocket in the Castile formation tend to flood the repository with brine from the Castile, leading to an increase in brine saturation that greatly increases gas generation. In Scenarios with a Castile intrusion the difference between the three inventories is most dramatic, with an increase in cumulative gas generation at 10,000 years between 70 to 87% from inventory 1 to inventory 3. Table I shows that the mass of iron, mass of CPR, and activity of the waste increases for each inventory, which leads to an increase in all three of the gas generation mechanisms. Iron corrosion is primary increased where the iron inventory is depleted in scenarios with high saturation such as Castile brine reservoir intrusions. The increase in CPR mass leads to a increase in gas generation from CPR bio-degradation in most scenarios. The most dramatic change in gas generation comes from brine radiolysis due to the increase in waste activity.

The additional gas generated tends to be driven out of the repository leading to little increase in brine pressure despite the increase in gas generation. Figure 2 shows the mean brine pressure in the representative waste panel for each inventory. The increase in iron corrosion and brine radiolysis does consume more brine reducing the brine saturation as the inventory increases. The mean brine saturation for the representative waste panel is shown in Figure 3.

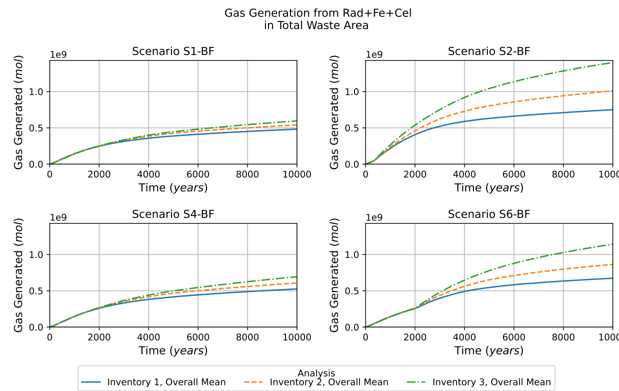

Fig. 1. Mean Cumulative Gas Generation from all mechanisms

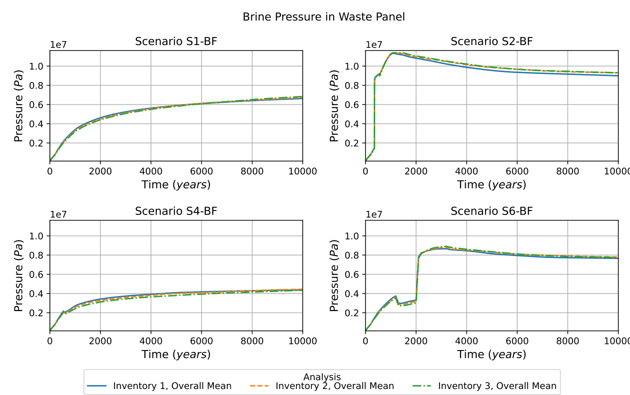

Fig. 2. Mean Waste Panel Brine Pressure

Releases

Cuttings and cavings are composed of the solid waste removed by the drillbit during a drilling intrusion and the solid waste eroded from the borehole by the drilling fluid. Cuttings and cavings dominate total release CCDFs at high probability. The mean cuttings and cavings CCDF curves are shown in Figure 4. For the first inventory the cuttings and cavings slope is fairly smooth. For the second inventory, the cuttings and cavings CCDF has a plateau around the 50% probability, which is the probability of a future having at least one drilling intrusion that intersects the surplus plutonium waste stream. The third inventory shows the same plateau in the cuttings and cavings release CCDF, however the plateau is at a higher

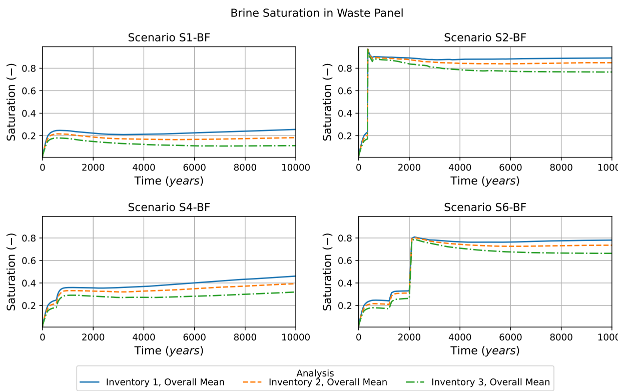

Fig. 3. Mean Waste Panel Brine Saturation

(90%) probability due to the increased volume of the surplus plutonium waste stream. Both the second and third inventories show increased cuttings and cavings releases at the compliance probabilities (10% and 0.1%).

Spallings releases are the solid waste entrained in flows out of the wellbore during a drilling intrusion. Mean spalling release CCDFs are shown in Figure 5. Spallings releases are increased because of the increase in repository pressure and the increase in waste activity.

Both cuttings and cavings releases and spallings releases are increased with the increasing inventories, despite being measured in the relative metric of EPA Units. While Spallings can be impacted by changing repository conditions, the volume of cuttings and cavings is the same for all three calculations, so the increase in releases is due to the inventory activity concentrations in those release volumes. EPA Units are relative to the inventory activity at repository closure. Through time, the relatively long half-life of plutonium means the inventories will decay differently. The inventories with more plutonium will decay slower in terms of EPA Units, leading to higher concentrations at later times. This is shown in Figure 6. This leads to the higher cumulative solids releases seen in the CCDF curves.

Direct brine releases (DBRs) are the mobile actinides that enter the drilling fluid during a drilling event. For a DBR to occur there must be mobile brine in the repository and enough brine pressure to overcome the weight of the drilling fluid (set to 8 MPa for WIPP). Mean direct brine release CCDFs are shown in Figure 7. Direct brine releases decrease with the increase in inventory because of two reasons. First, the increased gas generation driving lower brine saturation leads to fewer DBR events meeting the requirement of having mobile brine and less brine available for a DBR event when one occurs. Second, most of the time mobile actinides in the brine are solubility limited rather than inventory limited, so a solubility limited release will be similar release in curies but a smaller release in the relative metric of EPA Units. With the first inventory DBRs are greater than spallings and control total releases at low probabilities. In the second and third inventories spallings releases are greater than DBRs leading to spallings driving total releases at low probabilities.

Total releases are the sum of all release mechanisms. Mean total release CCDFs are shown in Figure 8. The increase in cuttings and cavings releases at 10% probability leads to increased total releases for inventories 2 and 3 over inventory 1. There is very little change from inventory 2 to inventory 3. At the 0.1% probability compliance point, all three mean CCDFs are very similar.

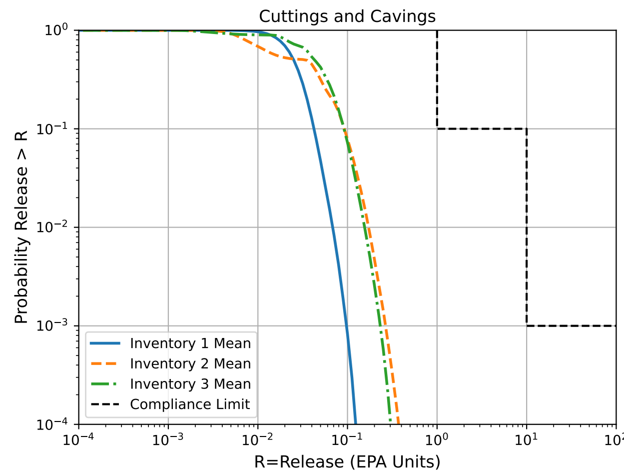

Fig. 4. Mean Cuttings and Cavings Release CCDFs

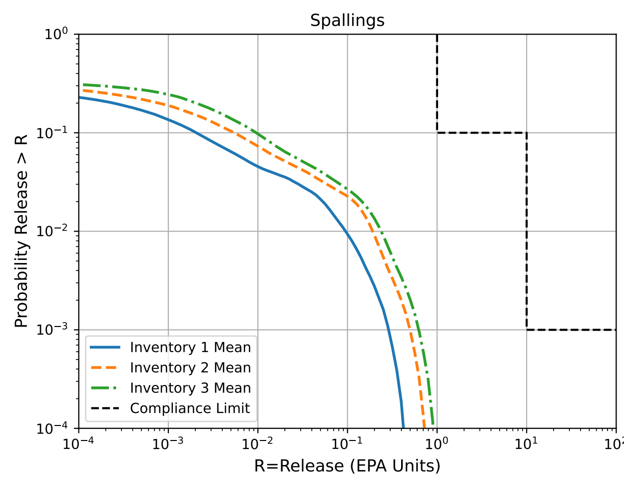

Fig. 5. Mean Spallings Release CCDFs

CONCLUSION

Inventory goes into many different aspects of the PA calculation for WIPP. As such, the PA calculation can be affected in many different ways from the changing inventory. Three inventories were used that increased the activity of the waste and the mass of waste components that go into the PA calculation. While some shifts were seen in intermediate outputs of the PA such as gas generation, the compliance metrics of mean CCDFs is not sensitive to the inventory changes.

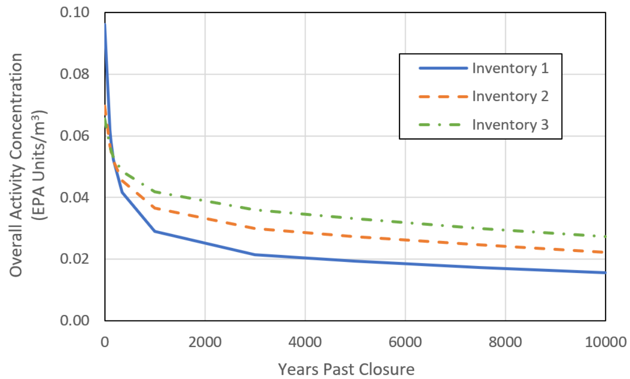

Fig. 6. Average Inventory Concentration through time

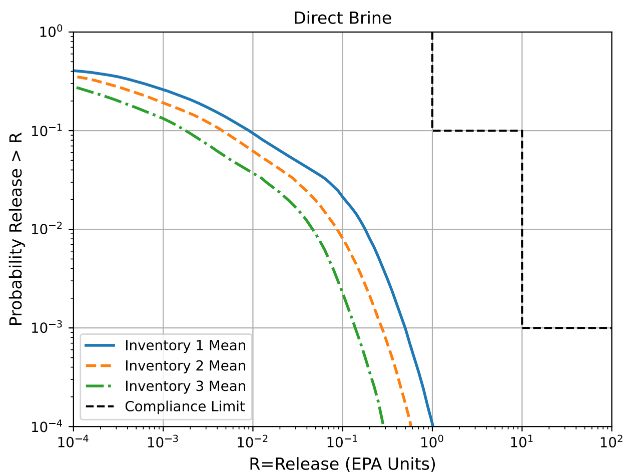

Fig. 7. Mean Direct Brine Release CCDFs

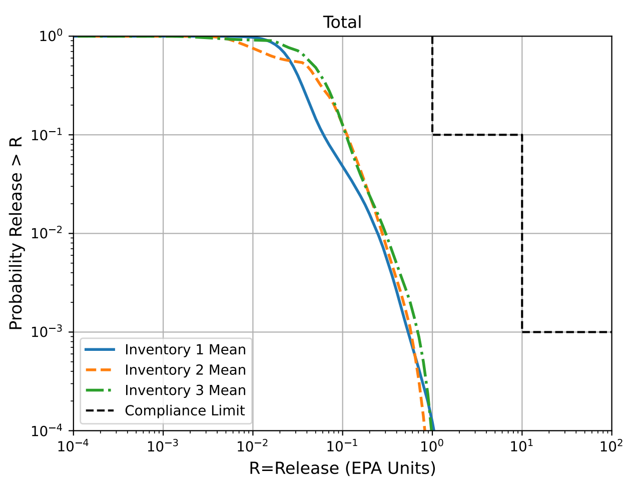

Fig. 8. Mean Total Release CCDFs

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