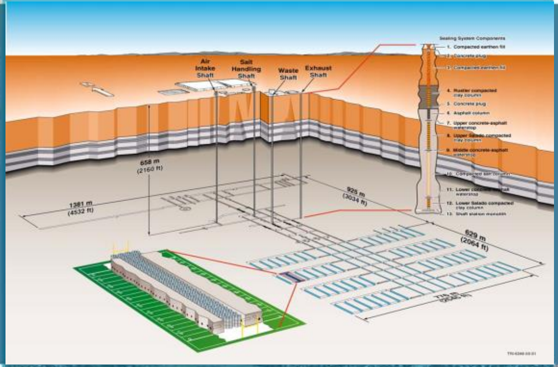
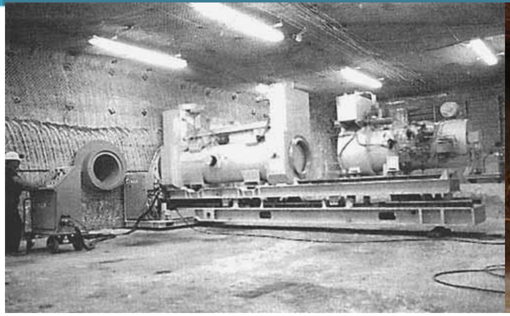
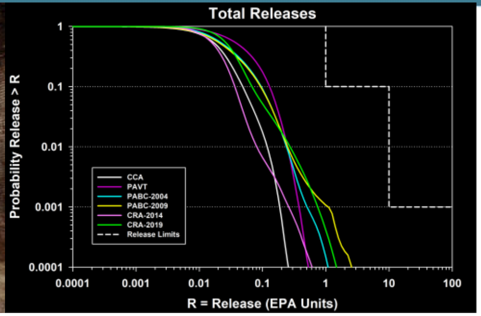
SAND2021-8604PE

Additional Panels Performance Assessment (APPA) Salado Flow Results







Seth King

July 2021

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525. This research is funded by WIPP programs administered by the Office of Environmental Management (EM) of the U.S. Department of Energy

SAND2021-8604 PE

Objectives

This presentation will describe the APPA Salado Flow model and results.

Outline:

- Conclusions
- Changes between CRA-2019 and APPA Salado Flow Models
- The Modeling Approach
  - Modeling Scenarios
  - Material Changes
- How the Salado Flow Model impacts releases
- Salado Flow Model Results
- Conclusions

This presentation is a summary of the results presented in the Analysis Package for Salado Flow in the Additional Panels Performance Assessment (King, 2021). The APPA calculation was done under AP-185 (Hansen, 2020).

Conclusions

The increased repository area has increased the DRZ, giving increased communication with the Salado formation. This allows more brine to flow into the repository.

- Increased brine in the repository and increased surface area of iron, has increased gas generation in scenarios without a Castile brine pocket intrusion.

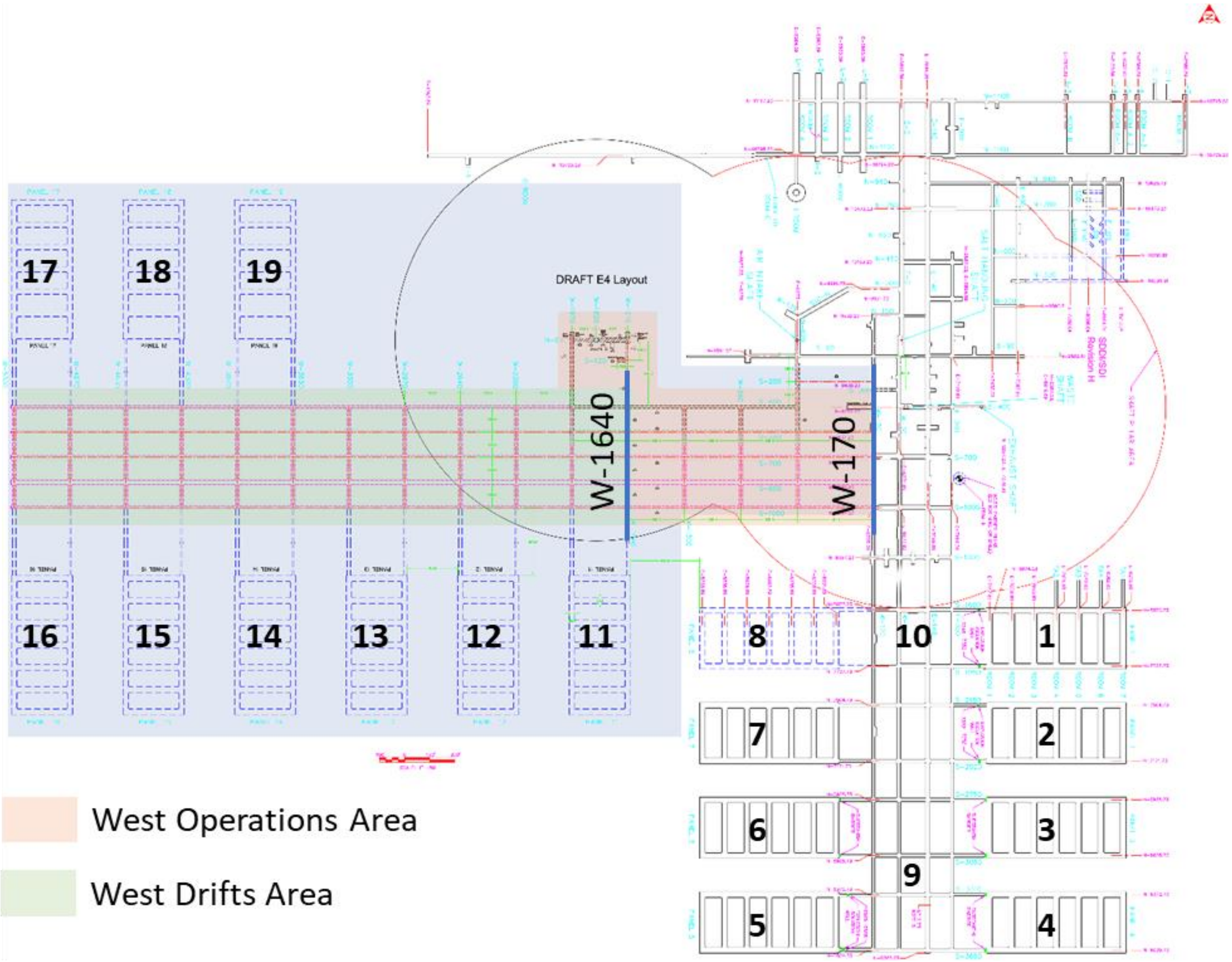
The additional repository volume and increased communication with the Salado has lowered the maximum pressures seen in the repository.

- Lower maximum pressures will reduce the drive for very large Spallings and DBR events.

Mean brine pressures and saturations have increased in Scenarios without a Castile brine pocket intrusion.

- This has led to an increased number of non-zero DBR events, and an increase in smaller spallings events as compared to the current configuration.

Modeling Approach - Repository Layout

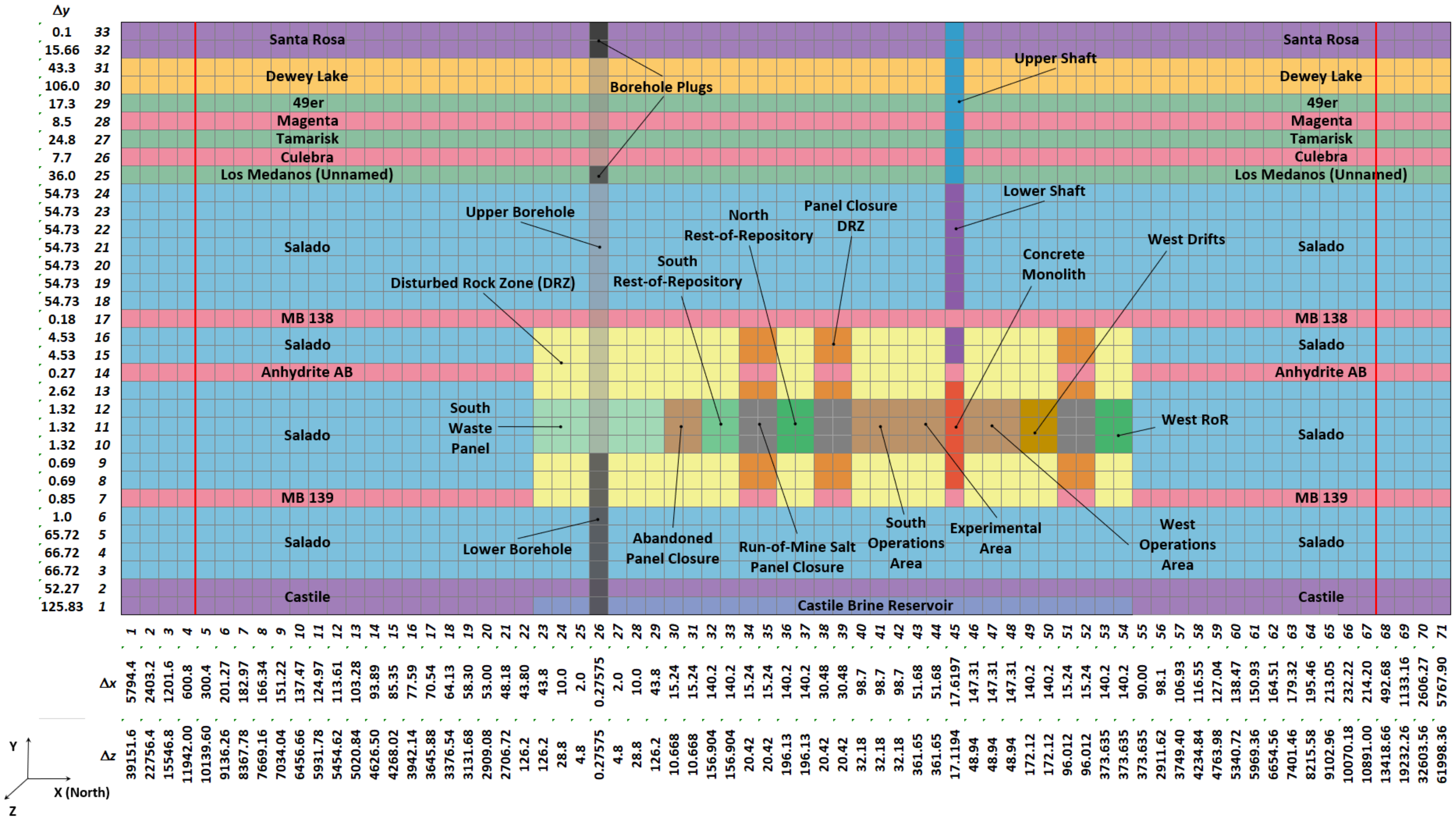


Current repository footprint and proposed additional waste panels (Hansen, 2020)

A 19 panel repository option is modeled. Panels 11 through 19 are modeled with similar dimensions to Panels 1 through 8, except that the abutment pillars (between the waste rooms and the access drifts) are increased from 61.0 m (200 ft) to 122 m (400 ft) and the isolation pillars (separating two panels) are increased from 61.0 m (200 ft) to 91.5 m (300 ft).

Five access drifts running east-west connect the new panels with the rest of the repository. The access drifts in the west are not modeled as containing waste. There are no plans for panel closures in the drifts that connect the west panels to the operations and experimental areas (Hansen, 2020).

Modeling Approach - BRAGFLO APPA Salado Flow Grid



Modeling Approach - Changes to the Salado Flow Calculation beyond the grid

Material	Property	CRA19 Value	APPA Value	Units	Reference
REFCON	VREPOS	438,406.08	819,834.21	m^3	Brunell, 2020
CAVITY_1	PRESSURE	128,039	115,610	Pa	King, 2020
CAVITY_2	PRESSURE	128,039	115,610	Pa	King, 2020
SOLMOD3	SOLSOH	1.63×10^{-7}	1.66×10^{-7}	moles/liter	Kim et al., 2020
SOLMOD3	SOLCOH	1.78×10^{-7}	1.90×10^{-7}	moles/liter	Kim et al., 2020

The repository volume change (in parameter values and in grid cells) is the most significant change.

The initial pressure (time=0 years) of the waste area is a function of CPR inventory and volume of the repository. Updated for new repository volume (not updated for CPR inventory). This is not an impactful change.

The (+III) baseline solubilities have been increased due to an error in the FM4 database. This is a minor change that effects the brine radiolysis model. This change has been shown to not be impactful (Kim et al., 2020).

Modeling Scenarios

The same 6 scenarios for Salado Flow as used in previous PA calculations.

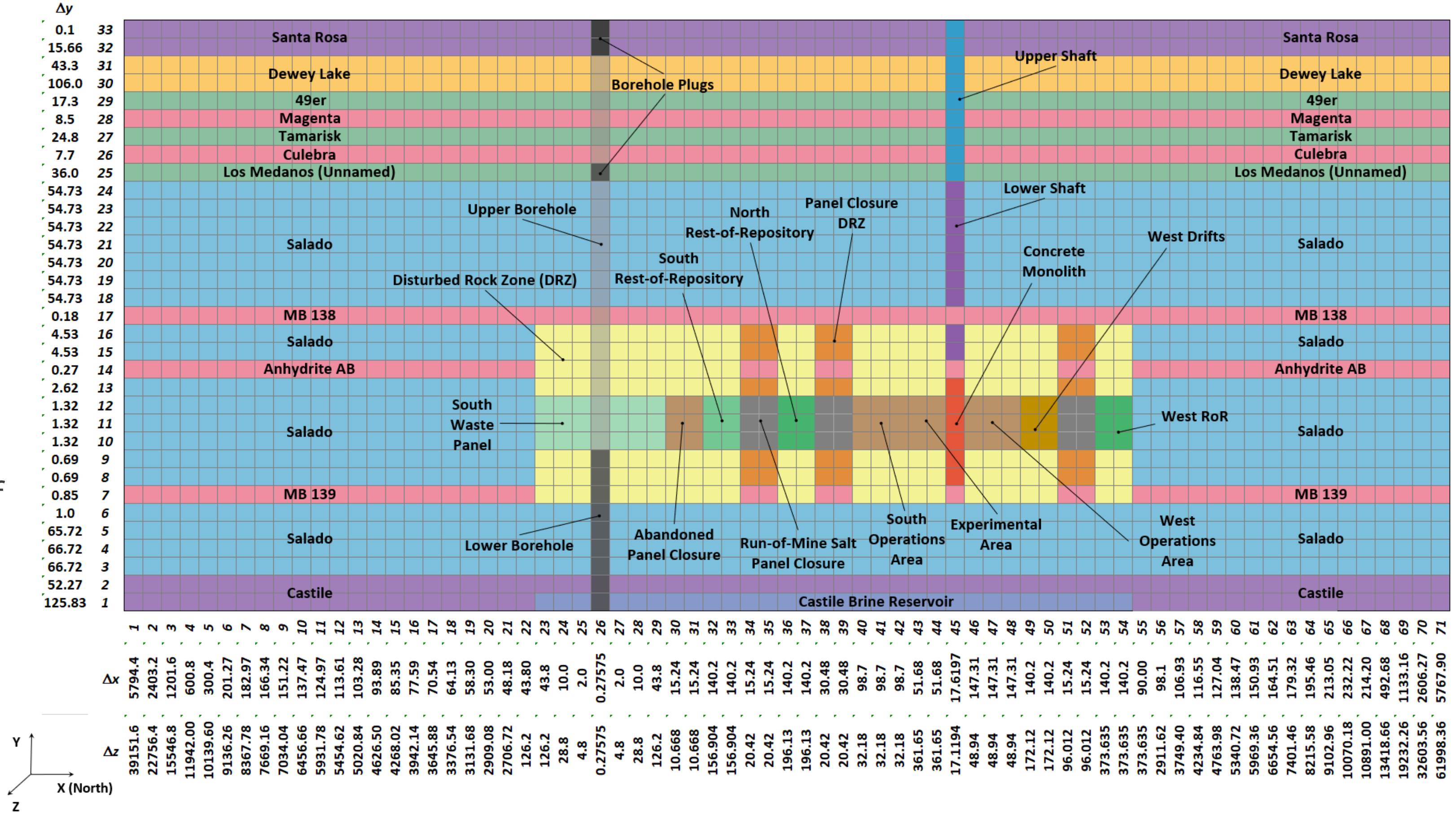
- E1 intrusions: Borehole intersects the repository and a pressurized brine pocket in the Castile.
- E2 intrusions: Borehole intersects the repository but not a pressurized brine pocket in the Castile.
- One representative borehole intrusion into a south panel (panel 5).
- Results for S3-BF and S5-BF closely follow the results for S2-BF and S4-BF with a shift in intrusion time, and therefore are not shown in this presentation. Results for S3-BF and S5-BF can be found in the supplemental material (King, 2021b).

Scenario	Description
S1-BF	Undisturbed repository
S2-BF (E1)	E1 intrusion at 350 years in the Waste Panel
S3-BF (E1)	E1 intrusion at 1,000 years in the Waste Panel
S4-BF (E2)	E2 intrusion at 350 years in the Waste Panel
S5-BF (E2)	E2 intrusion at 1,000 years in the Waste Panel
S6-BF (E2E1)	E2 intrusion at 1,000 years; E1 intrusion at 2,000 years in the Waste Panel

Material Changes

Implementation of the Salado Flow modeling scenarios necessitates the modification of the grid material maps at different times. These changes include:

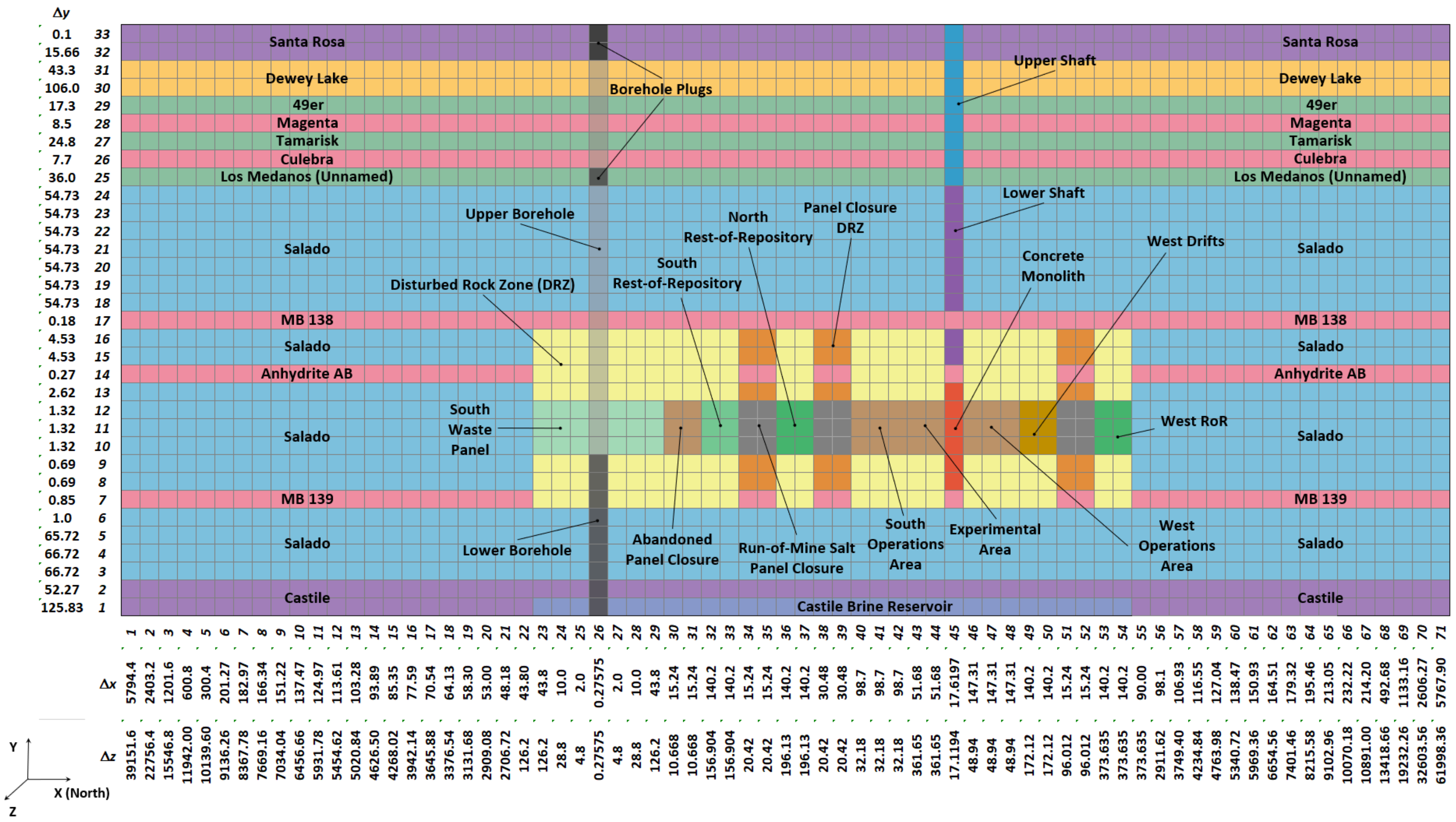
- **-5 years:** Initialization phase with open waste areas, panel closures, and shaft.
- **0 years:** Waste, panel closures, and shaft are emplaced. ROMPCS represented by material PCS_T1 with no healing of the DRZ above and below the panel closure and abandoned panel closure represented by material PCS_NO.
- **100 years:** ROMPCS material transitions from PCS_T1 to PCS_T2 with no healing of the DRZ above and below the panel closure.
- **200 years:** ROMPCS material transitions from PCS_T2 to PCS_T3 with healed regions of DRZ above and below the panel closure represented by material DRZ_PCS. Lower shaft material transitions from SHFTL_T1 to SHFTL_T2.



Material Changes

Implementation of the Salado Flow modeling scenarios necessitates the modification of the grid material maps at different times. These changes include:

- **E1 intrusion:** Borehole intrusion through the Waste Panel and into a hypothetical pressurized brine region in the underlying Castile Formation, with the borehole represented by material BH_OPEN. Concrete borehole plugs, represented by material CONC_PLG, immediately emplaced in the borehole below the Culebra and at the surface (unless previous intrusion).
- **E2 intrusion:** Borehole intrusion terminating at the floor of the Waste Panel, with the borehole represented by material BH_OPEN. Concrete borehole plugs, represented by material CONC_PLG, immediately emplaced in the borehole below the Culebra and at the surface.
- **200 years post-intrusion:** Borehole plugs fail, and the entire borehole is modeled as having properties equivalent to sand. The borehole, bottom to top, is represented by material BH_SAND.
- **1200 years post-E1 intrusion:** The permeability of the borehole between the repository and the Castile brine region decreases due to creep closure of the salt. The lower borehole is represented by material BH_CREEP.



How the Salado Flow Model impacts releases

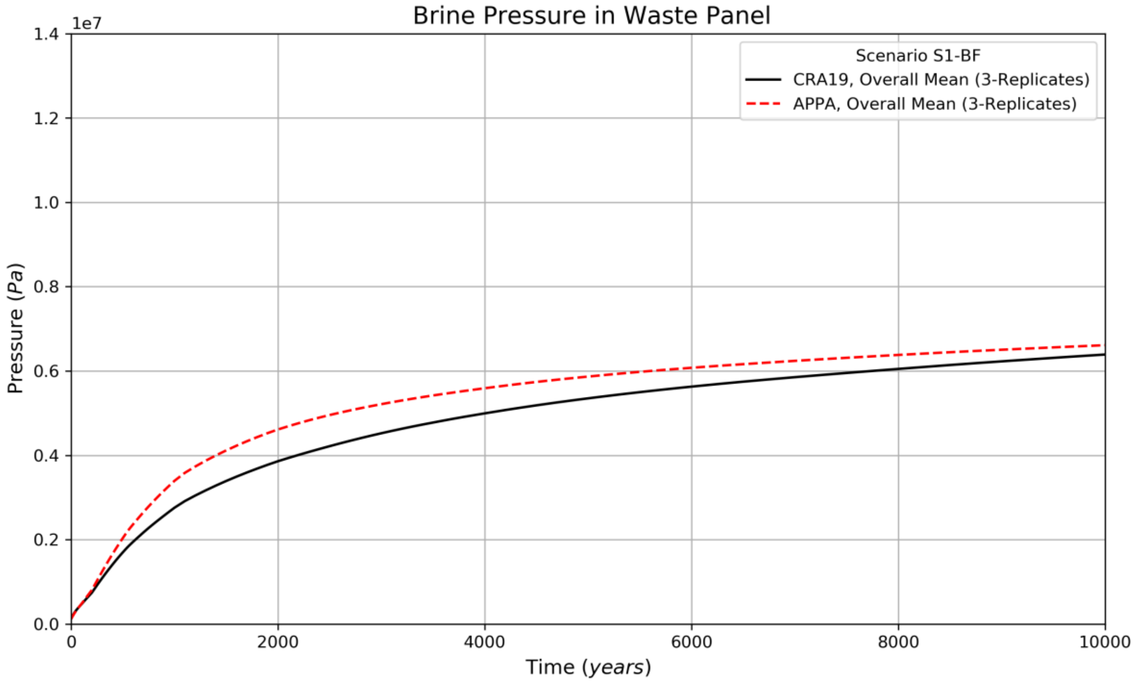
What Salado Flow results impact releases?

- **Cuttings and Cavings** are completely independent of the Salado flow modeling results.
- **Spallings** are determined by the brine pressure in the intruded waste area at the time of intrusion. The Salado Flow model is used to determine those brine pressures.
- **Direct Brine Release (DBR)** volumes are a function of the pressure drive (brine pressure) and available brine (brine saturation) in the intruded waste area at the time of intrusion. The Salado Flow model provides the brine pressures and saturations for the DBR volume calculation. Note that the brine pressure must be above 8 MPa and brine saturation must be above the residual saturation for a DBR event to occur.
- **Culebra Releases** are impacted by the radionuclide releases to the Culebra, which is a function of the brine flow up the borehole, and in the multi-intrusion case the amount of brine in the intruded waste panel (a function of brine saturation).*

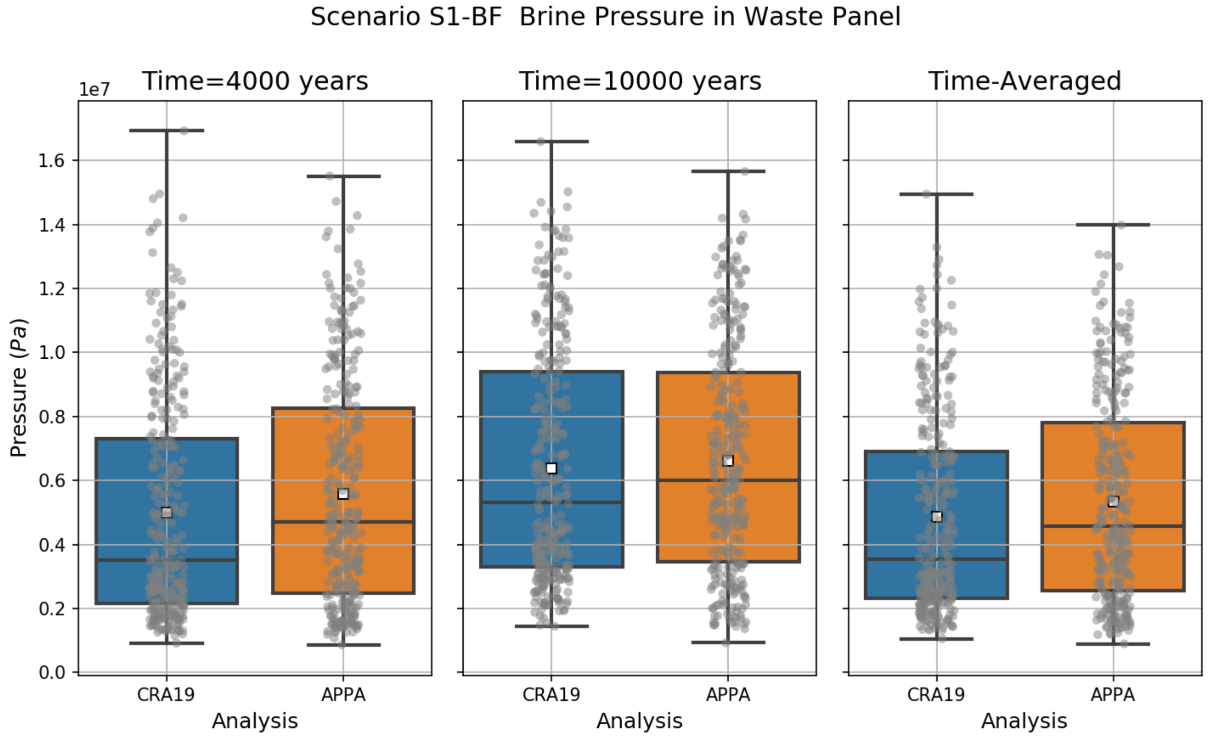
With this, brine pressure and saturation in the 4 waste areas and brine flows up the borehole will be the primary metrics of the Salado Flow results. Other metrics such as gas generation, waste porosity, and brine flows around the repository will be used to understand the evolution of these primary metrics.

*** In theory, long term releases could go through the marker beds, or up the shaft to the Culebra. These pathways do not provide significant releases, and are not focused on here.**

Salado Flow Modeling Results - Undisturbed pressures

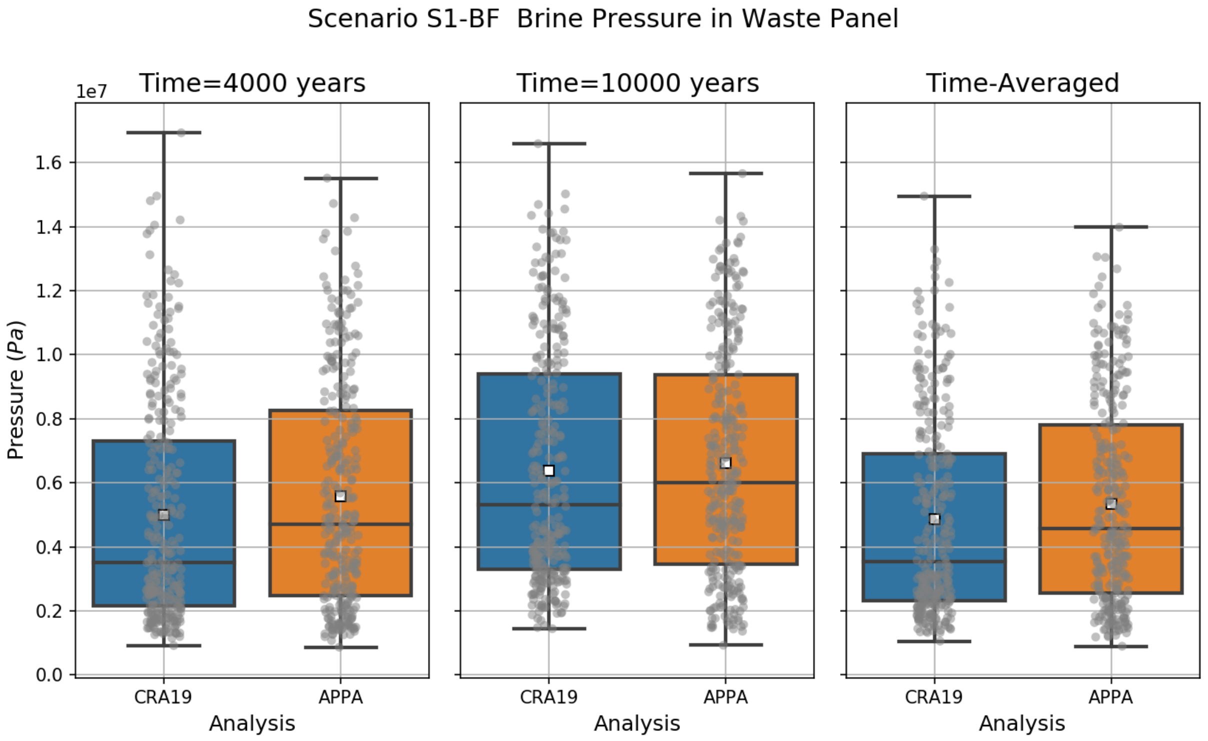


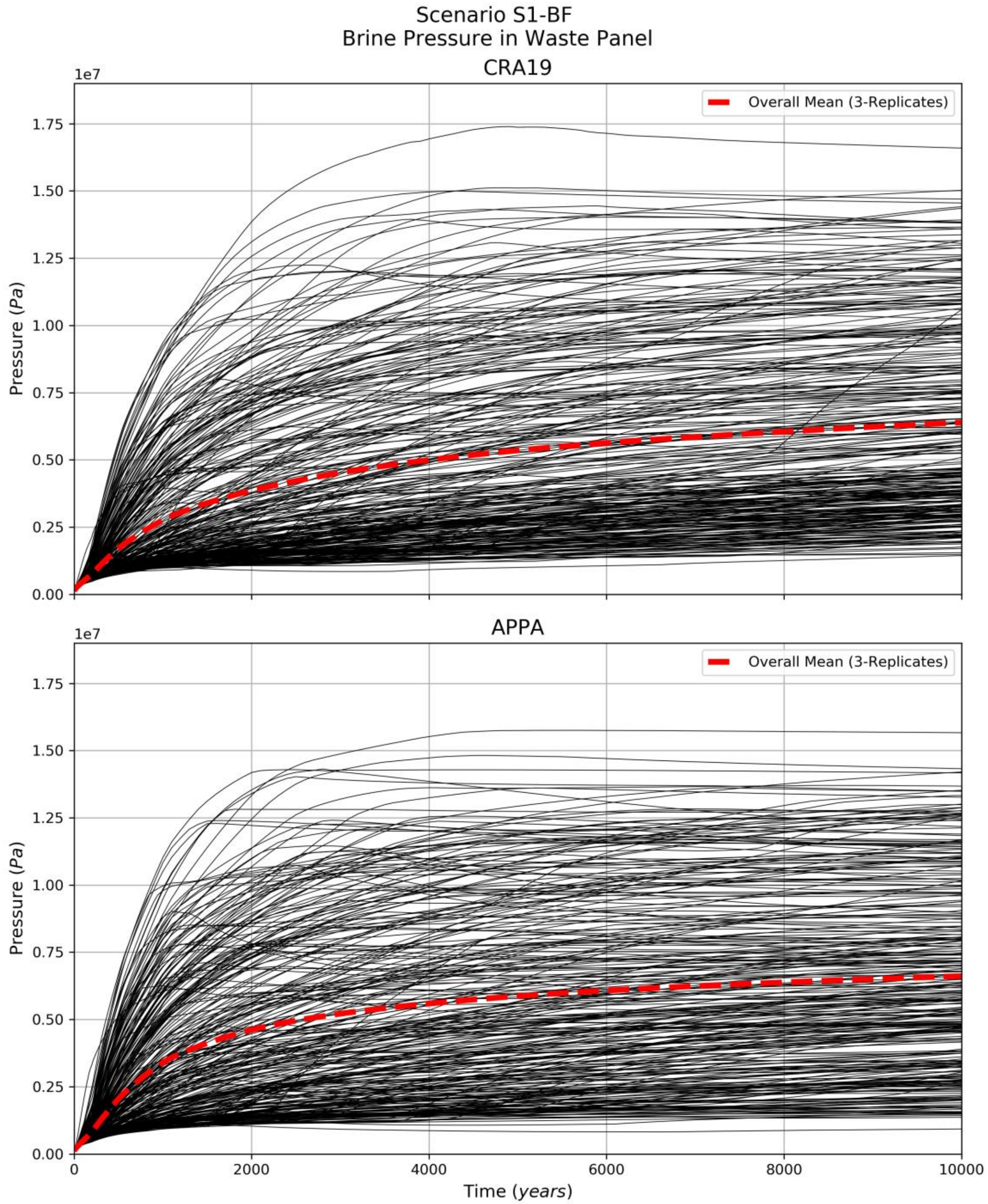
Compared to CRA19, in the undisturbed case mean pressure has increased; however, the maximum pressures (across vectors) has decreased. The range of pressures seen (across vectors) has decreased. This trend holds true for all excavated areas.



Undisturbed pressures (horsetails)

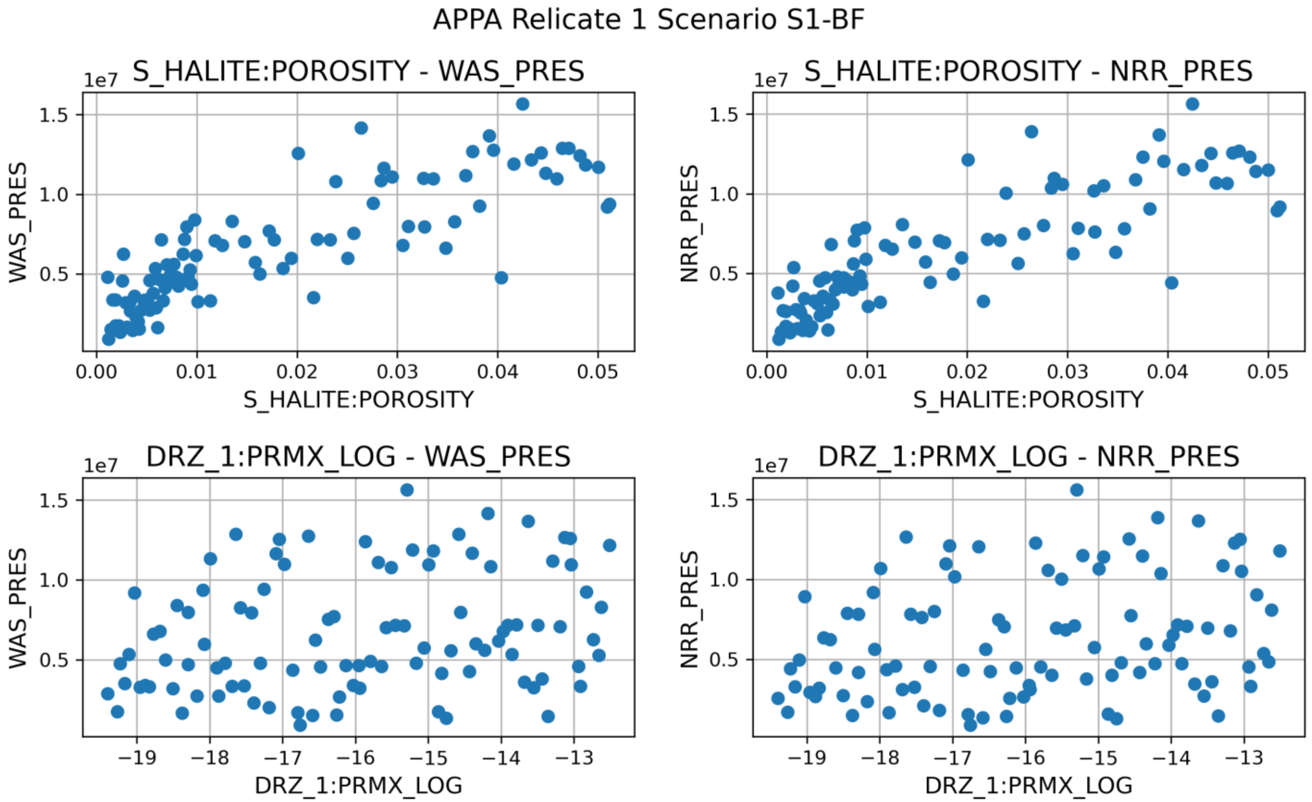
In the undisturbed case mean pressure has increased; however, the maximum pressures (across vectors) has decreased. The range of pressures seen (across vectors) has decreased. This trend holds true for all excavated areas.





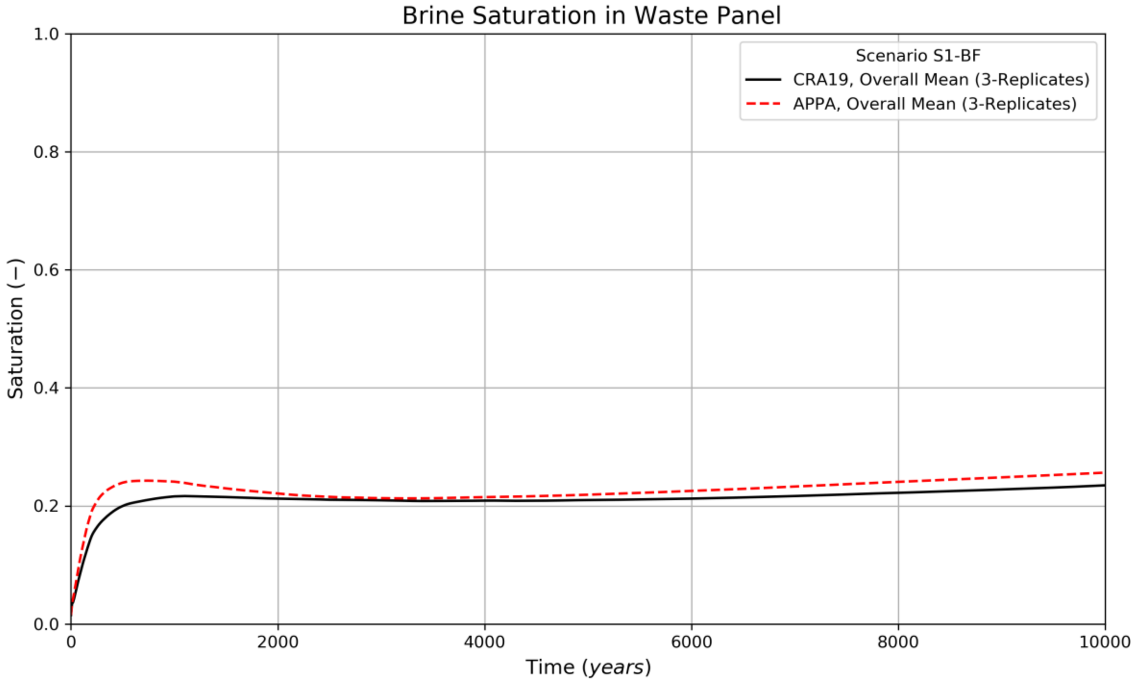
Undisturbed Pressure Sensitivity Analysis

In the undisturbed case long-term (measured at time=10,000 years) pressure in the repository is most sensitive to the porosity of intact halite (S_HALITE:POROSITY). Porosity in the intact halite controls 70-76% of the variability in the pressure response in the Waste Panel in Scenario S1-BF of the APPA, an increase from the 42-67% control of variability the porosity had on the Waste Panel pressure in CRA-2019. Permeabilities in the DRZ and marker beds (DRZ_1:PRMX_LOG, DRZ_PCS:PRMX_LOG, and S_MB139:PRMX_LOG) that provide communication between the repository and intact Salado also have impacts on the pressure response in the undisturbed case.

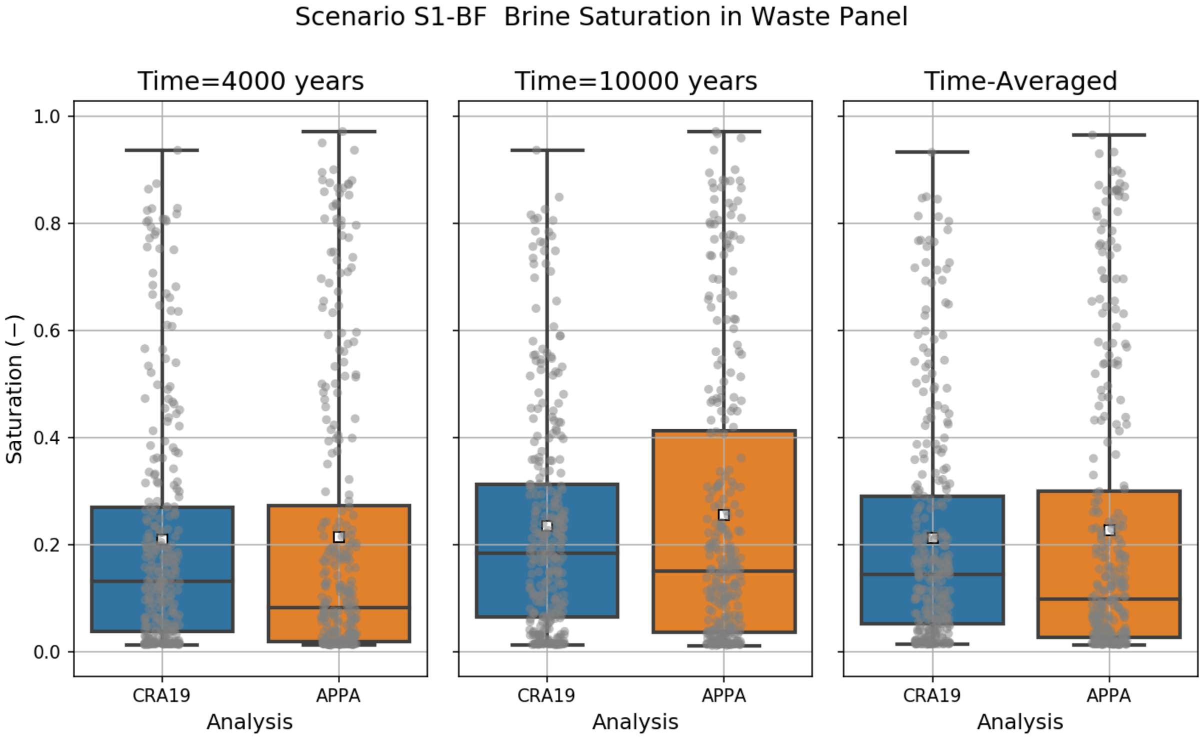


More details of the sensitivity analysis on Salado Flow results provided in Appendix A of King (2021).

Salado Flow Modeling Results - Undisturbed brine saturations

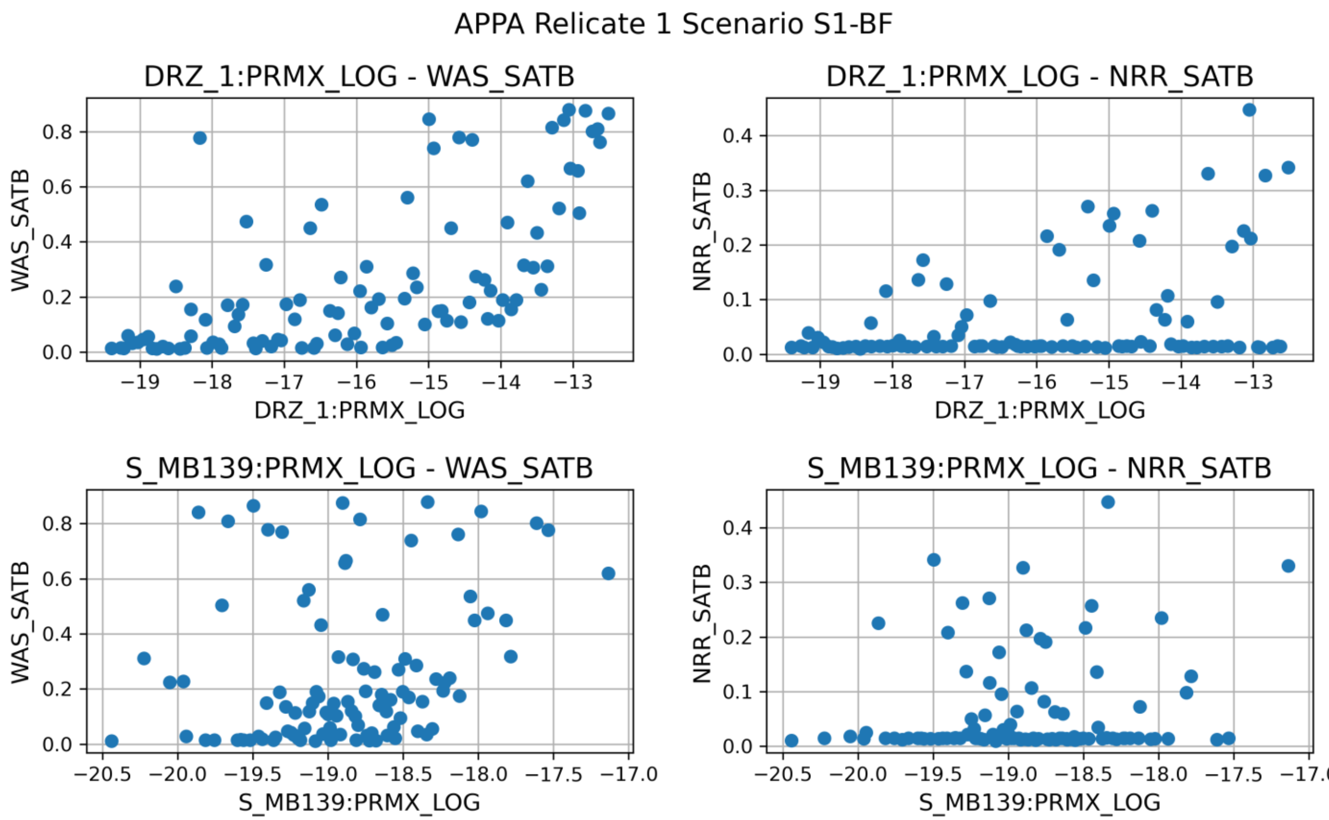


In the undisturbed case mean and maximum brine saturations have increased. The range of brine saturations seen (across vectors) has increased. This trend holds true for all excavated areas.



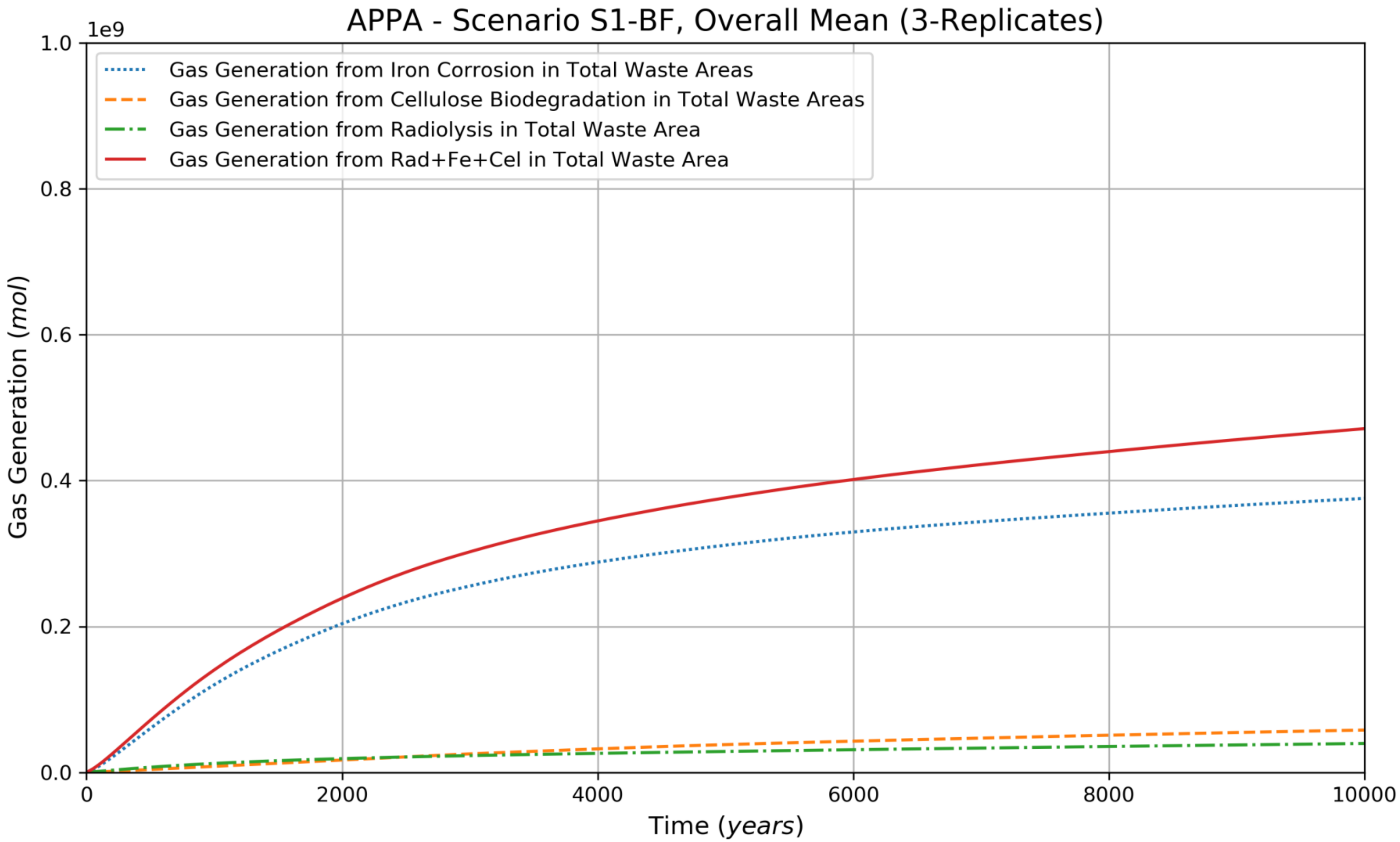
Undisturbed Brine Saturation Sensitivity Analysis

In the undisturbed case, the long-term (measured at time=10,000 years) variability in brine saturation in the waste panel is controlled by the long term DRZ permeability (DRZ_1:PRMX_LOG), followed by the marker bed permeability (S_MB139:PRMX_LOG). For APPA, the DRZ permeability controls 41-52% of the waste panel brine saturation variability in Scenario S1-BF, an increase from the 33-43% seen in CRA-2019. Waste areas farther up-dip are more sensitive to the intact halite porosity (S_HALITE:POROSITY) than the DRZ permeability.



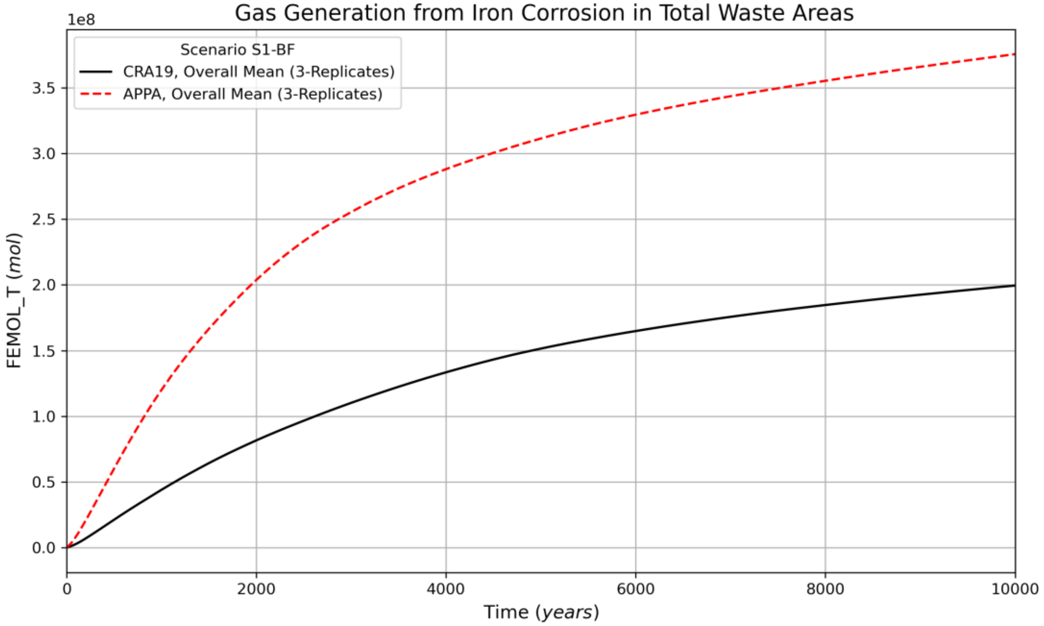
More details of the sensitivity analysis on Salado Flow results provided in Appendix A of King (2021).

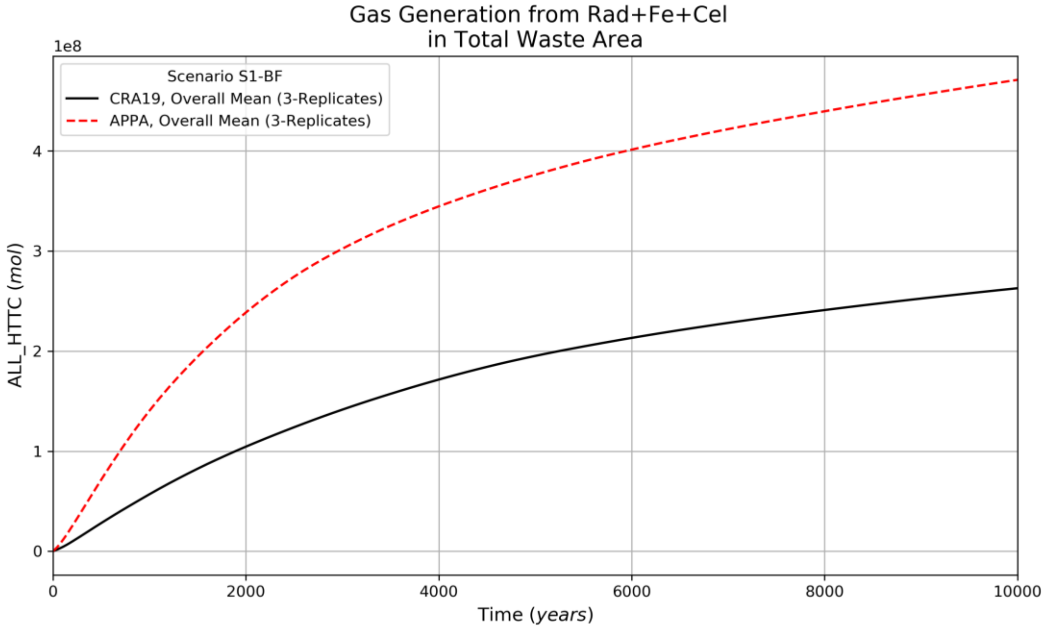
Salado Flow Modeling Results - Undisturbed Gas Generation



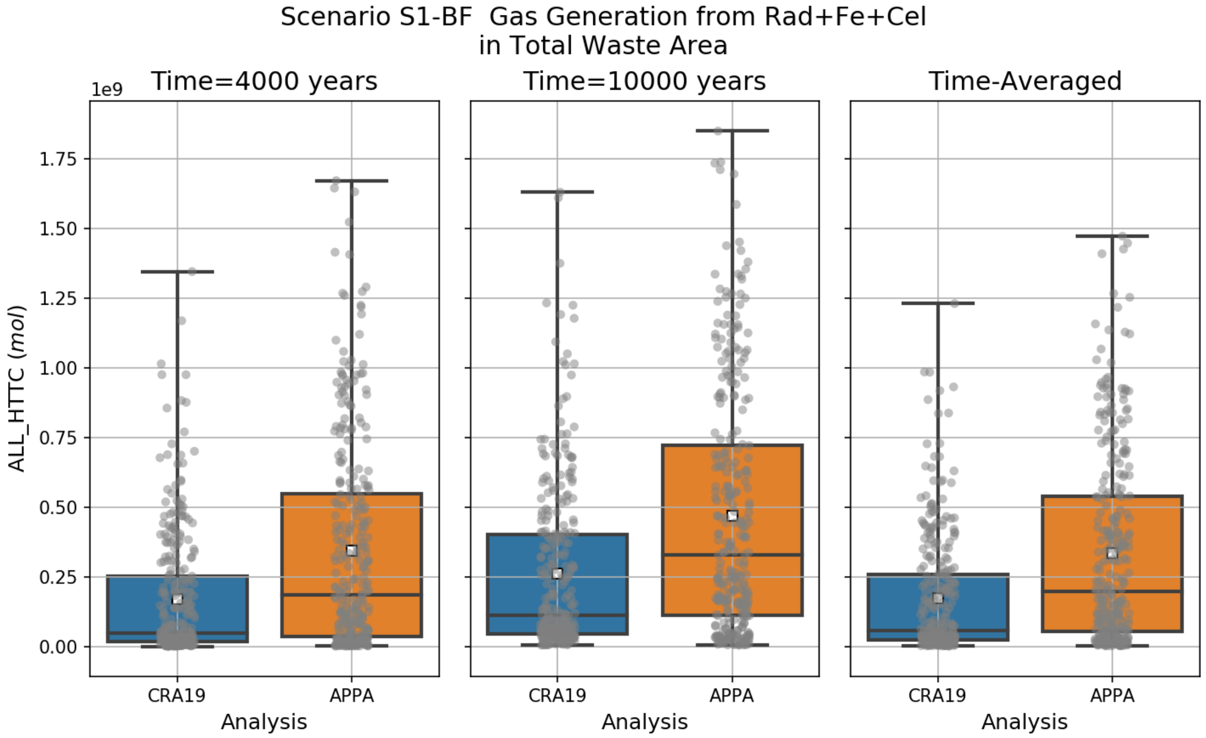
There are three gas generating reactions in the Salado flow model, iron corrosion, microbial biodegradation of CPR materials, and radiolysis of brine. Iron corrosion continues to be the dominating reaction

Salado Flow Modeling Results - Undisturbed Gas Generation





Iron surface area is calculated as a function of repository volume (assuming optimal loading). Doubling the repository volume has doubled the iron surface area. The increased brine saturation has increased gas generation in all 3 reactions. Together these two effects have increased gas generation.



Iron corrosion rate

The iron corrosion rate that goes into BRAGFLO is specified in units of (moles/(m^3s)). This rate is calculated with:

- CORRMCO2 (K_{CR}) – Sampled iron corrosion rate in m/s (inundated and humid).
- $D_{N,Fe}$ - Density of iron (7870 kg/m^3).
- Mw_{Fe} - Molecular Weight of iron (0.055847 kg/mole).
- ASDRUM (A_d) – Surface area of iron per drum (6 m^2/drum).
- DRROOM (n_d) – Drums per room (6804 drums/room).
- VROOM (V_R) – Volume of a room (3644.37 m^3).

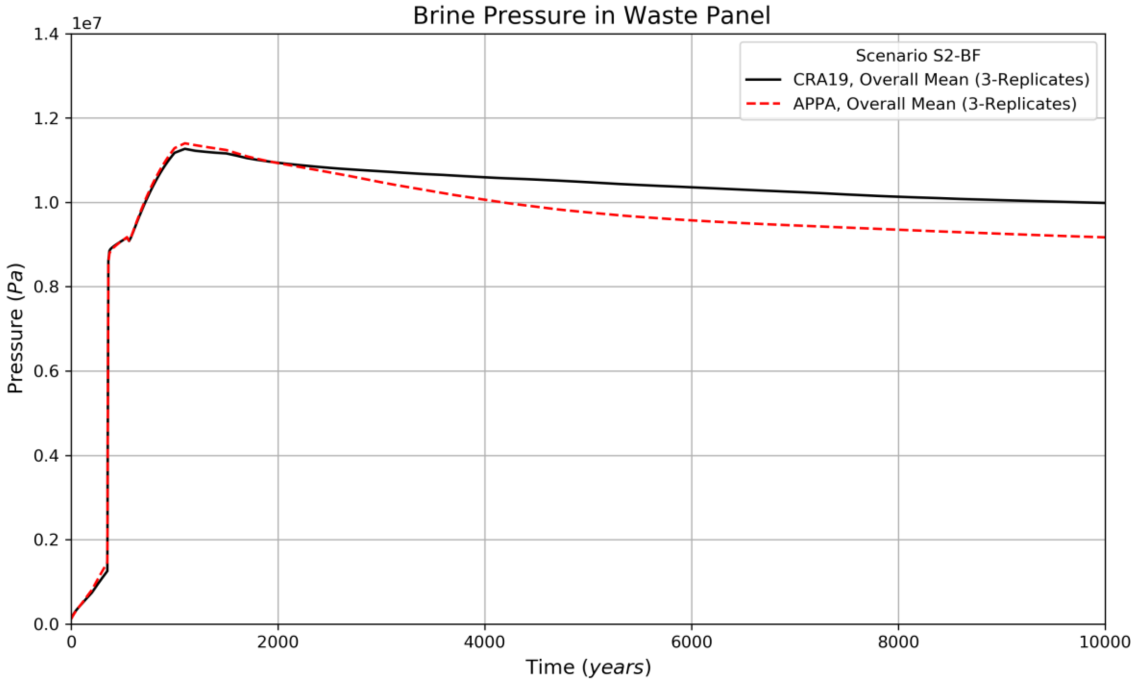
$$Gratcor\left(\frac{i}{h}\right) = K_{CR}\frac{D_{N,Fe}}{Mw_{Fe}}A_d\frac{n_d}{V_R}moles/(m^3s)$$

The coefficient D_s is the steel surface area per unit volume of repository, defined as:

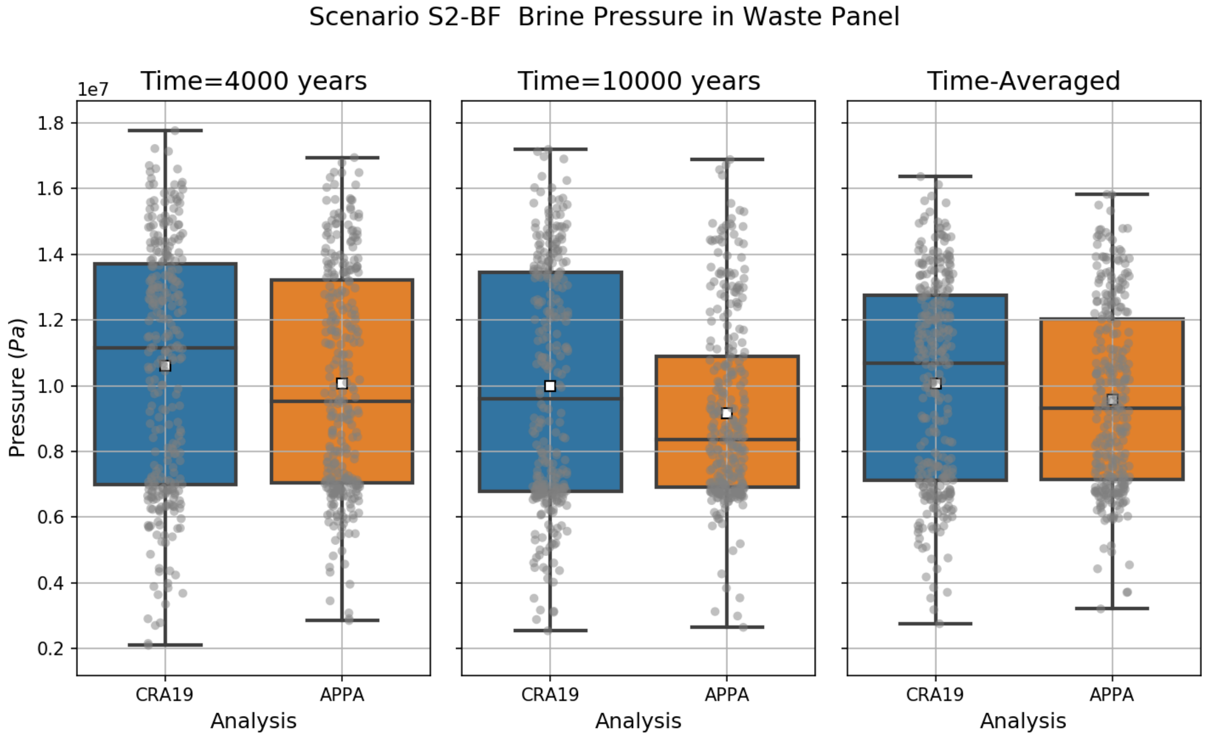
$$D_s = \frac{A_d n_d}{V_R} = 11.2\ \frac{m^2}{m^3}$$

Day (2015) evaluated the surface area of iron as a function of repository volume. There is no connection between the iron inventory mass and iron surface area, and therefore no connection between the iron inventory and iron corrosion rate, except iron corrosion will stop when the iron inventory is exhausted.

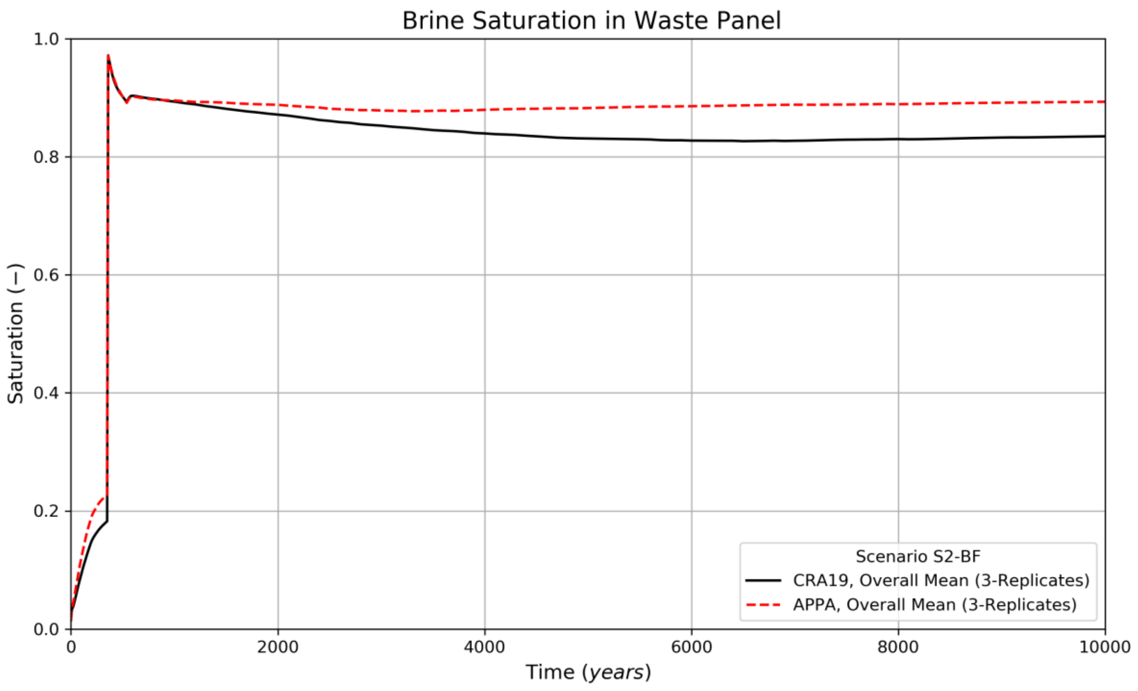
Salado Flow Modeling Results - S2-BF (E1) pressures



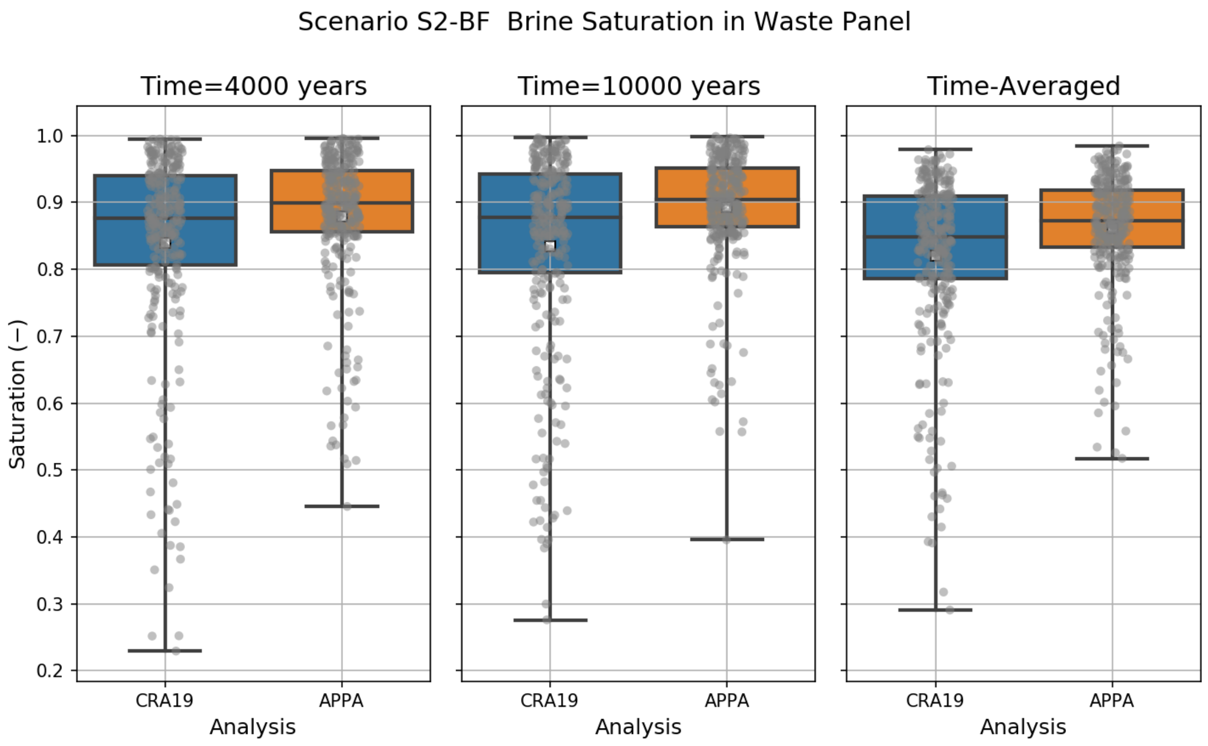
In the E1 case mean and maximum pressures have decreased at most time points. The range of pressures seen (across vectors) has decreased. This trend holds true for all excavated areas.



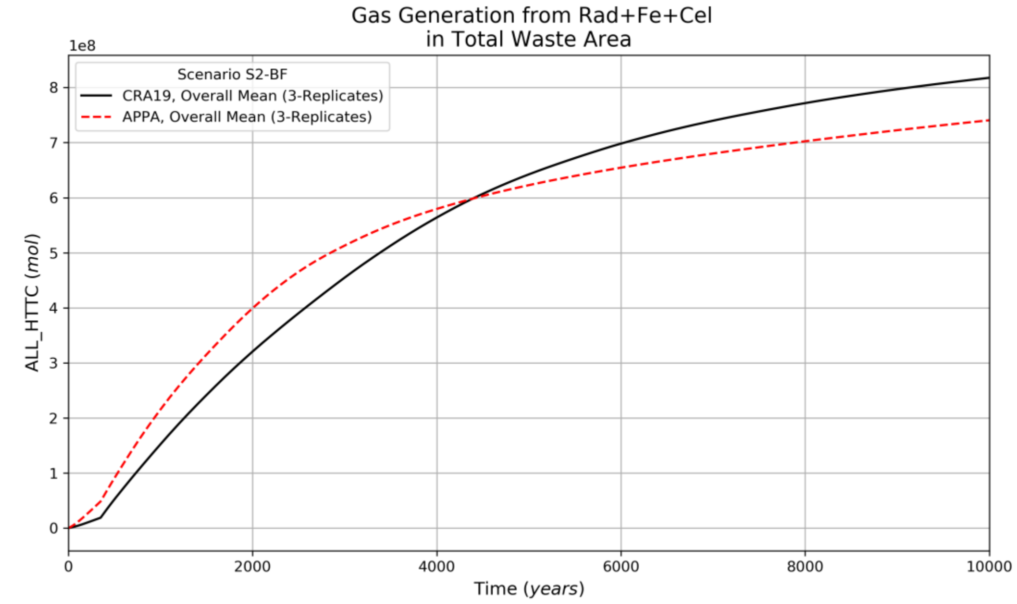
Salado Flow Modeling Results - S2-BF (E1) brine saturations

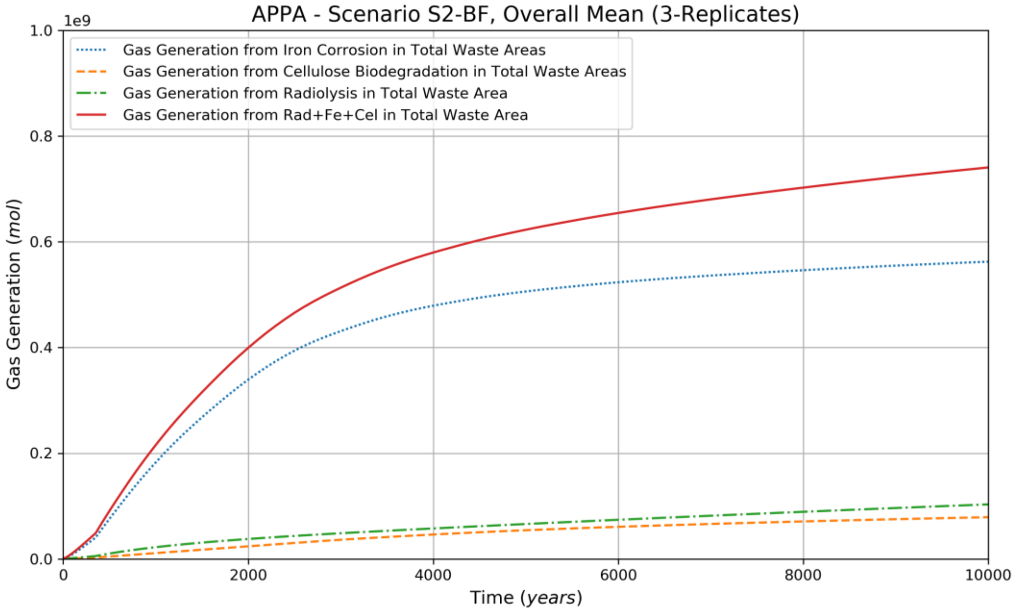


In the E1 case mean brine saturations have increased. The range of brine saturations seen (across vectors) has decreased. This trend holds true for all excavated areas.

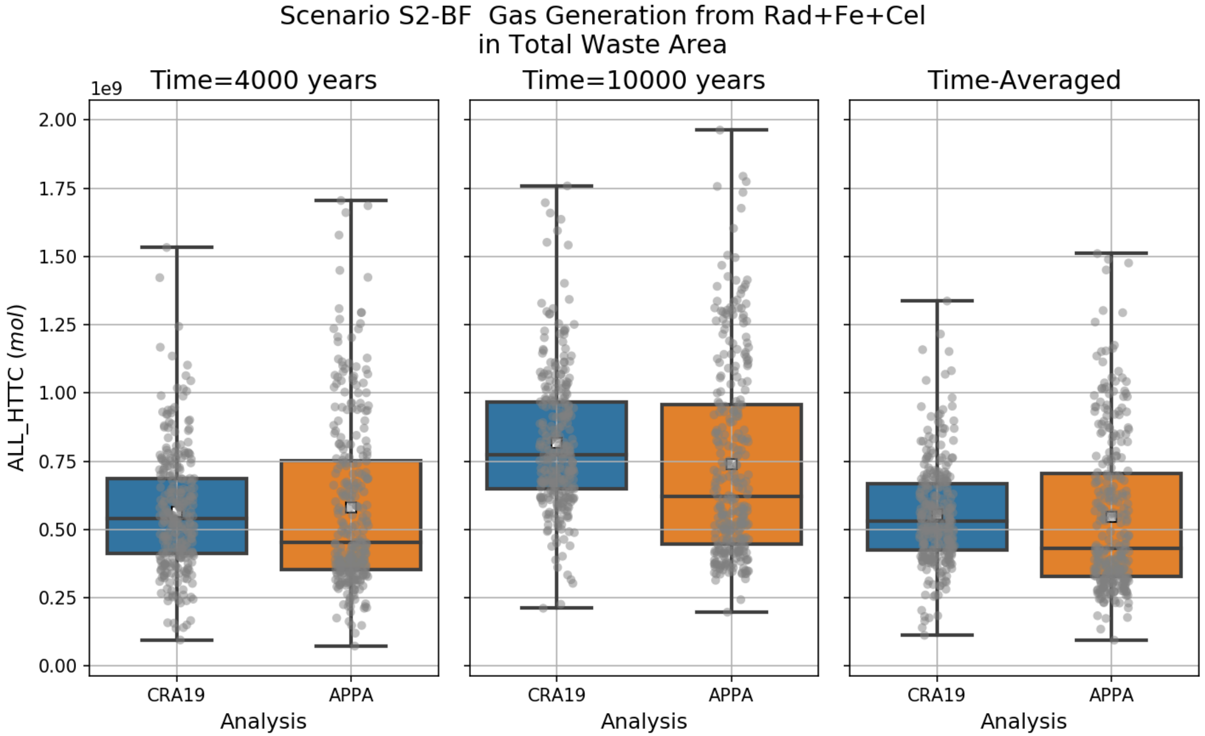


Salado Flow Modeling Results - S2-BF (E1) gas generation

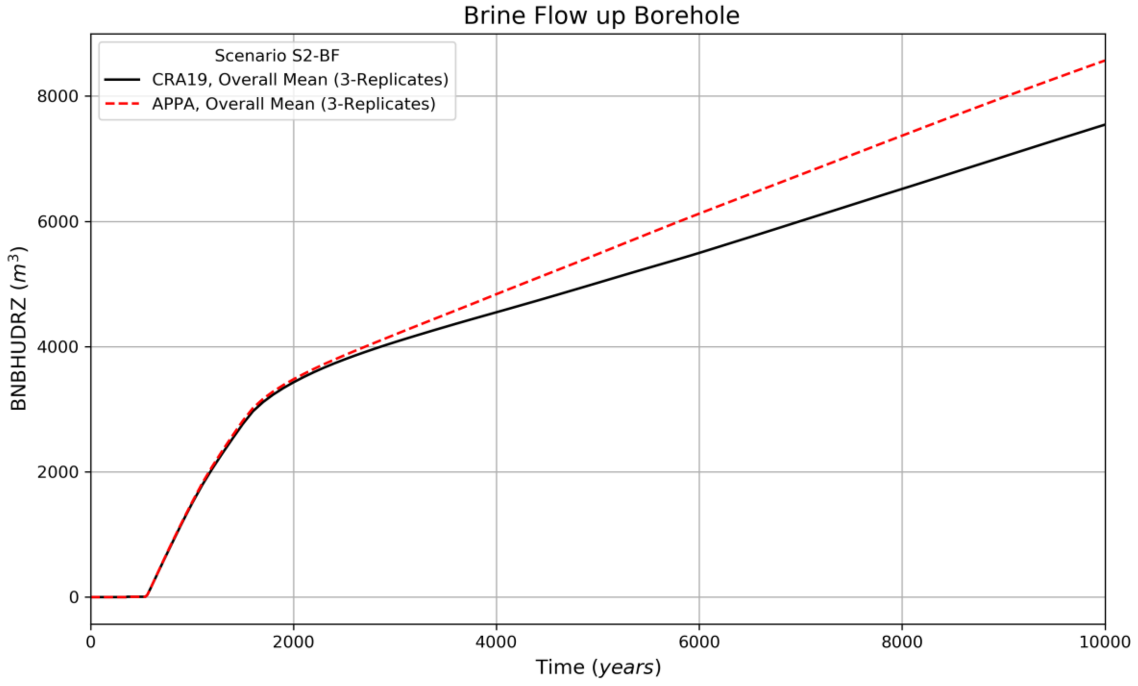




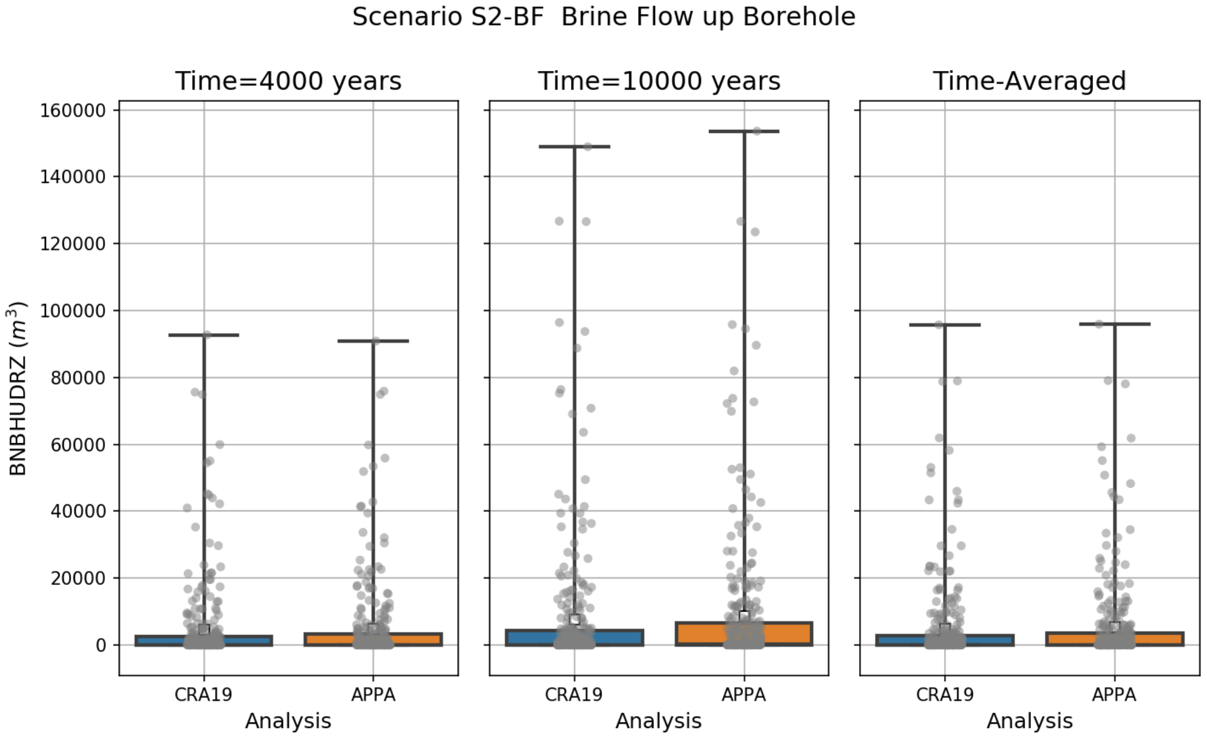
In the E1 case early gas generation has increased, however late gas generation has decreased. The range of gas generation seen (across vectors) has increased. Waste being moved up-dip farther away from the intrusion location is the reason behind lower total gas generation in these cases even with the increased brine saturations and Fe surface area.



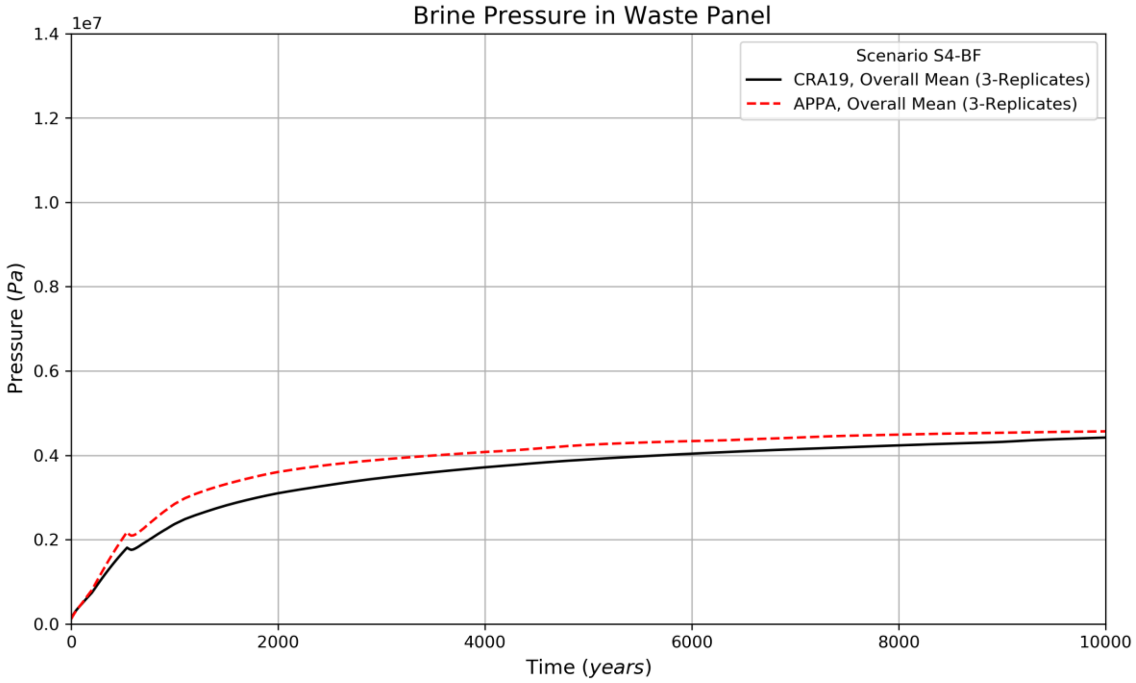
Salado Flow Modeling Results
S2-BF (E1) brine flow up the borehole



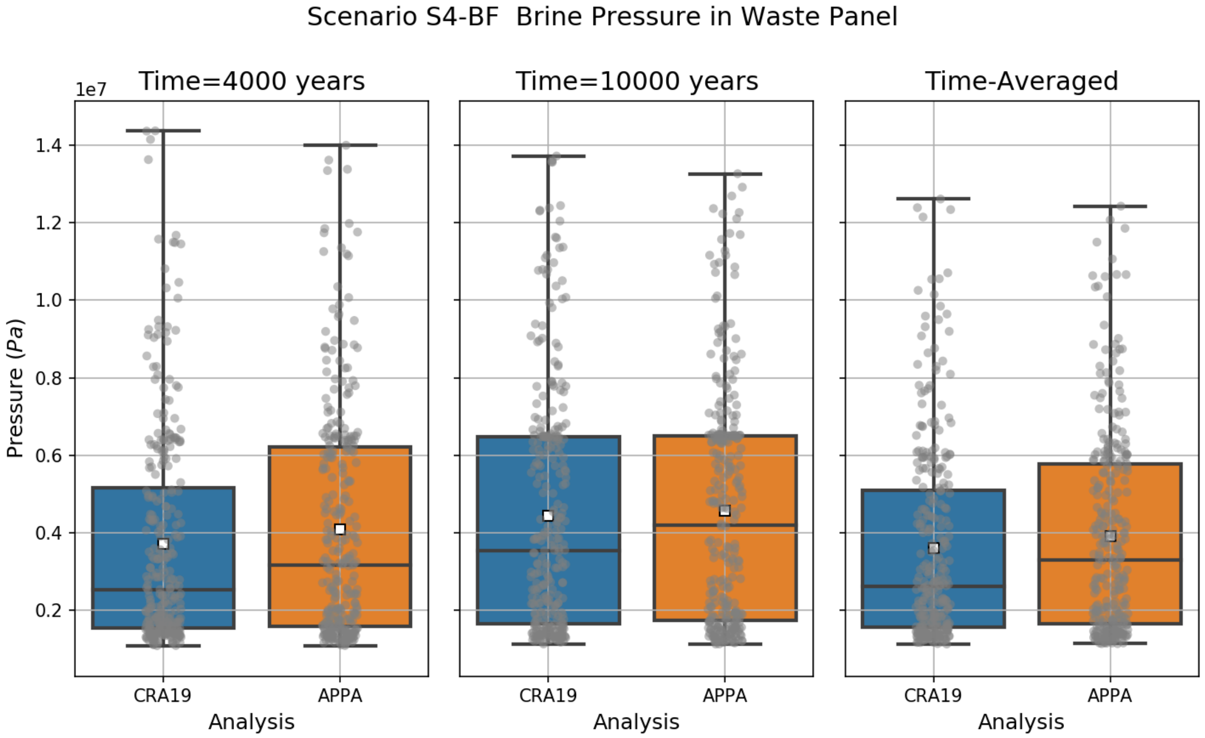
In the E1 case mean brine flow up the borehole has increased at later times.



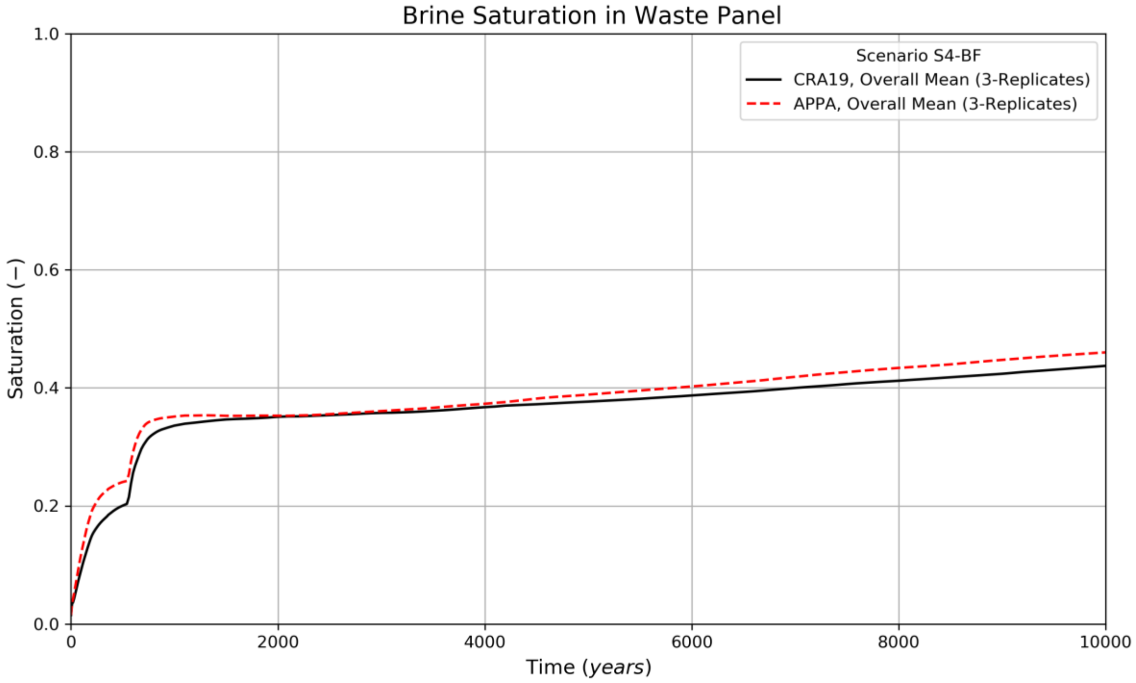
Salado Flow Modeling Results - S4-BF (E2) pressures



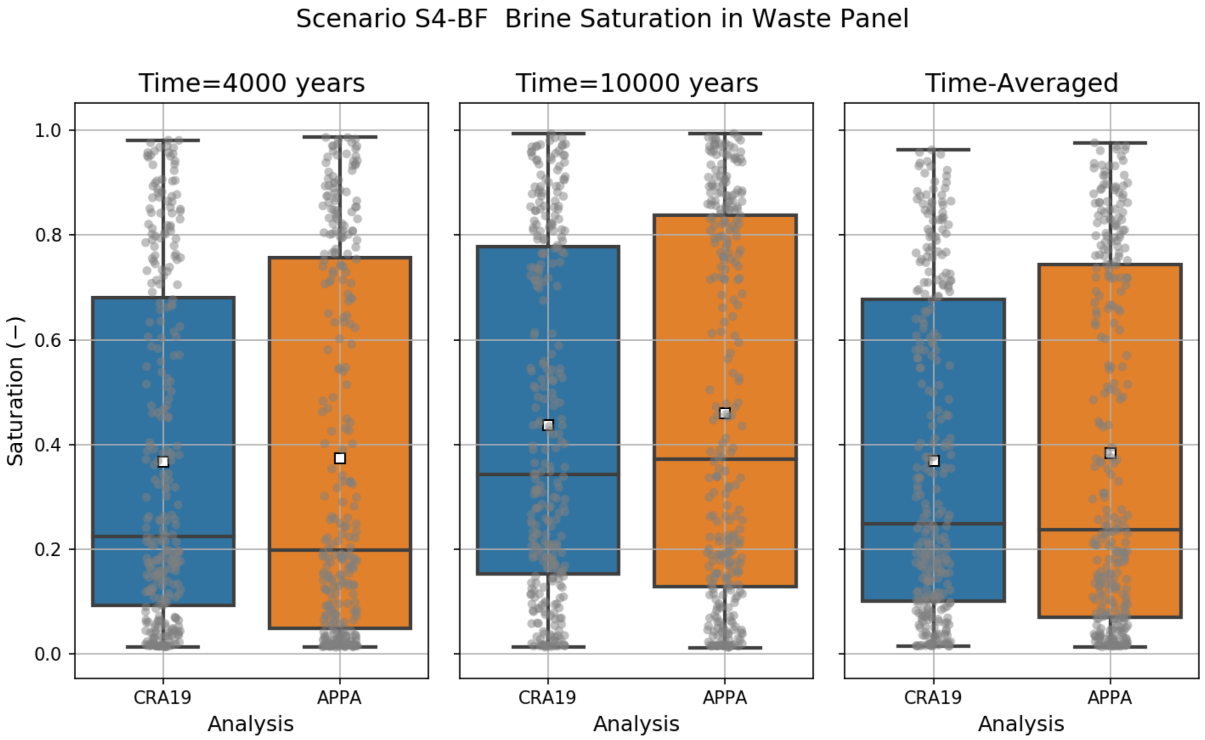
In the E2 case mean pressures have increased, however maximum pressures have decreased. The range of pressures seen (across vectors) has decreased. This trend holds true for all excavated areas.



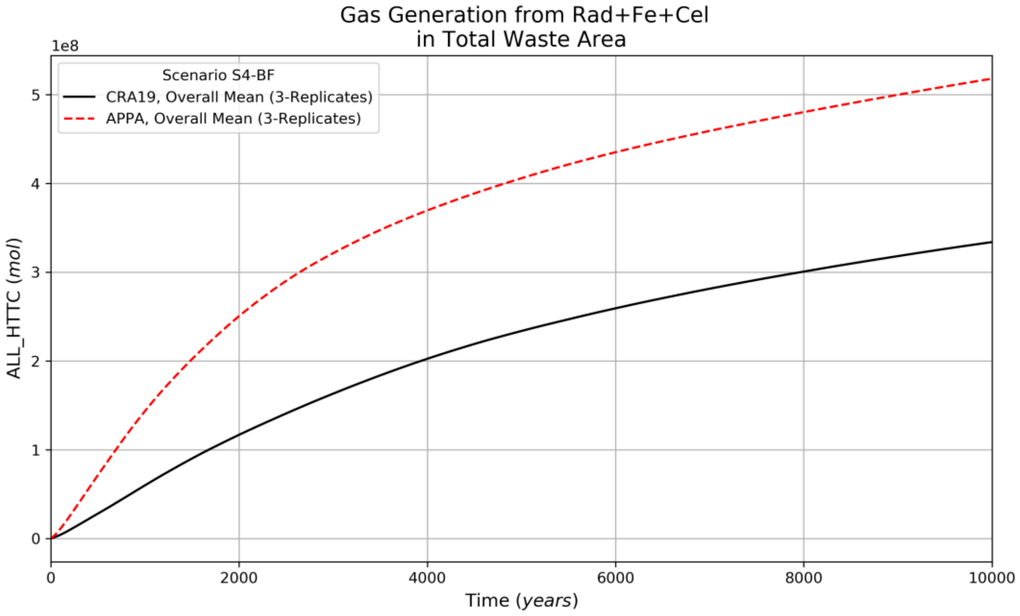
Salado Flow Modeling Results - S4-BF (E2) brine saturations

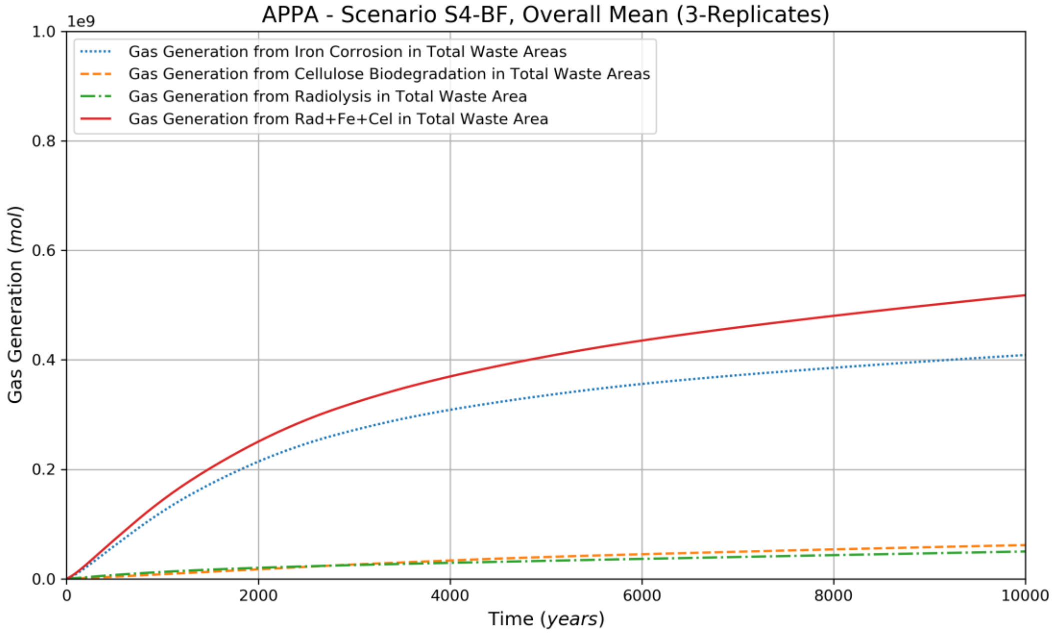


In the E2 case the brine saturation has a wider range of values, with fewer vectors at a mid-value and more vectors at the extremes. Up-dip waste areas have seen an increase in brine saturations.

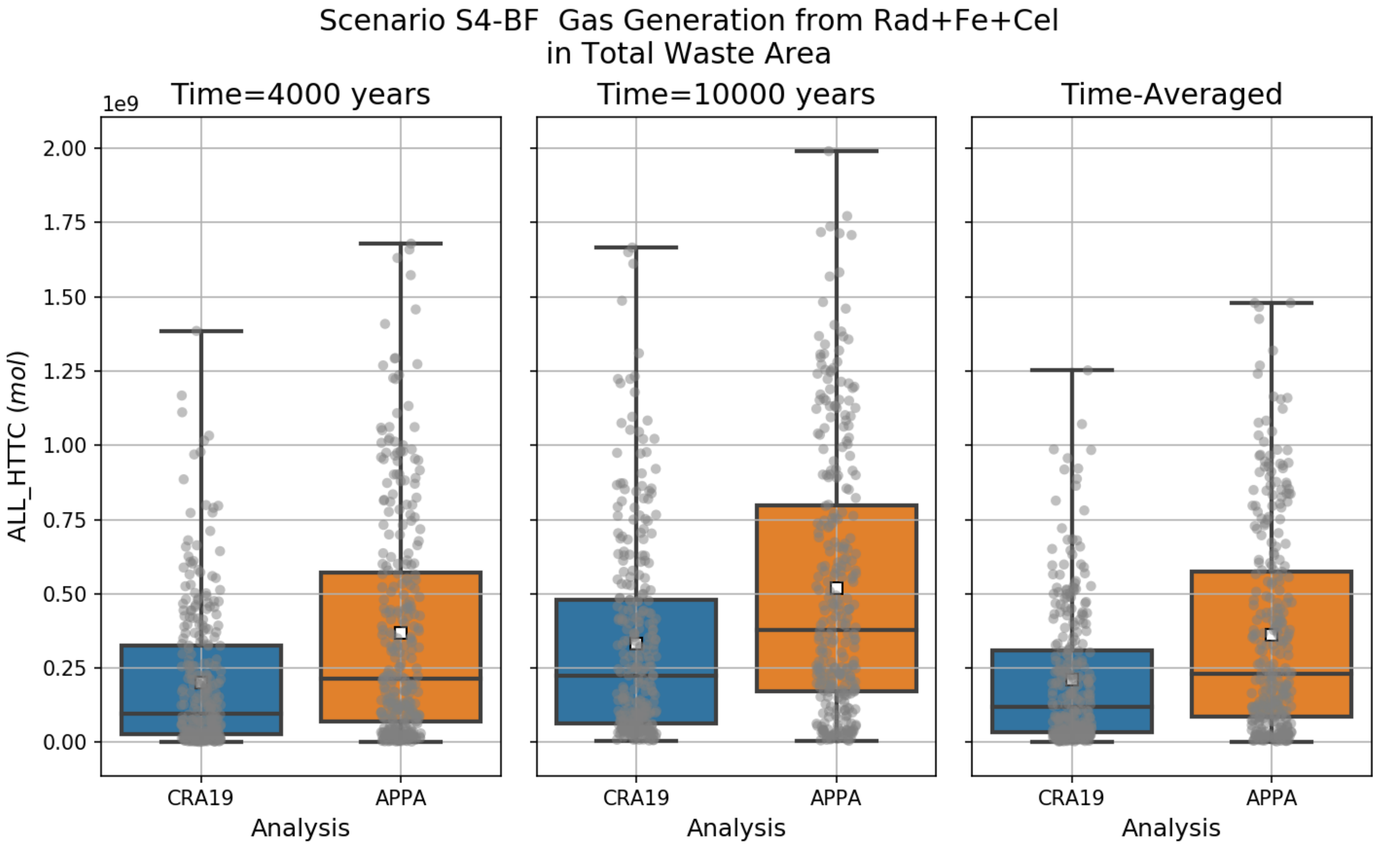


Salado Flow Modeling Results - S4-BF (E2) gas generation

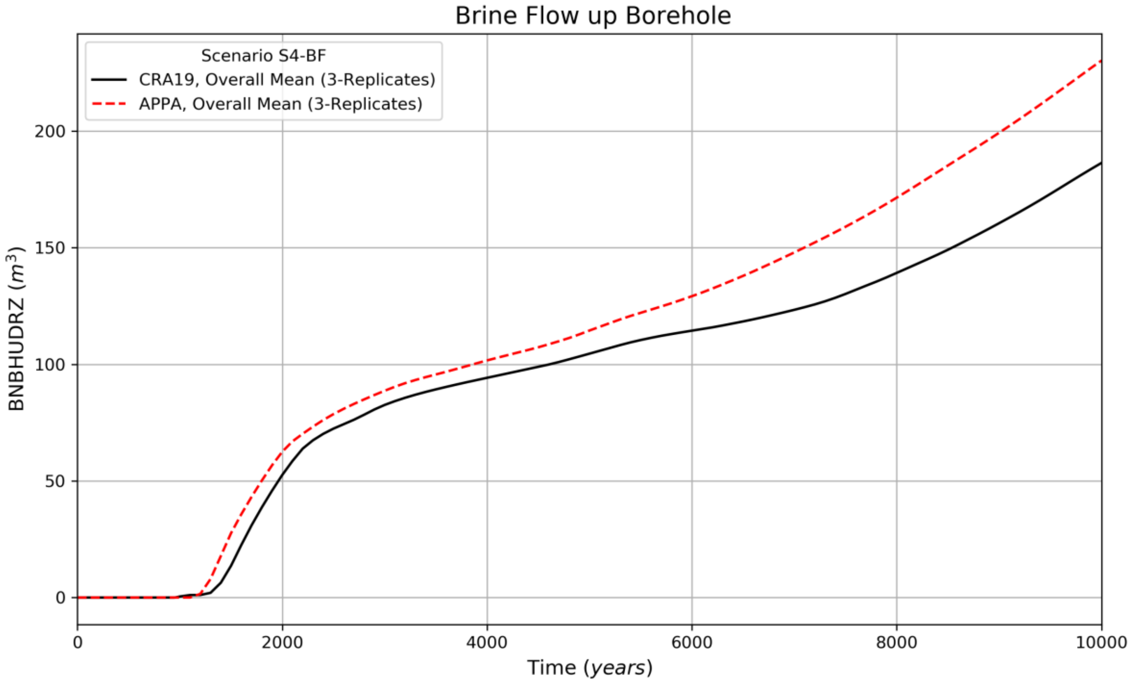




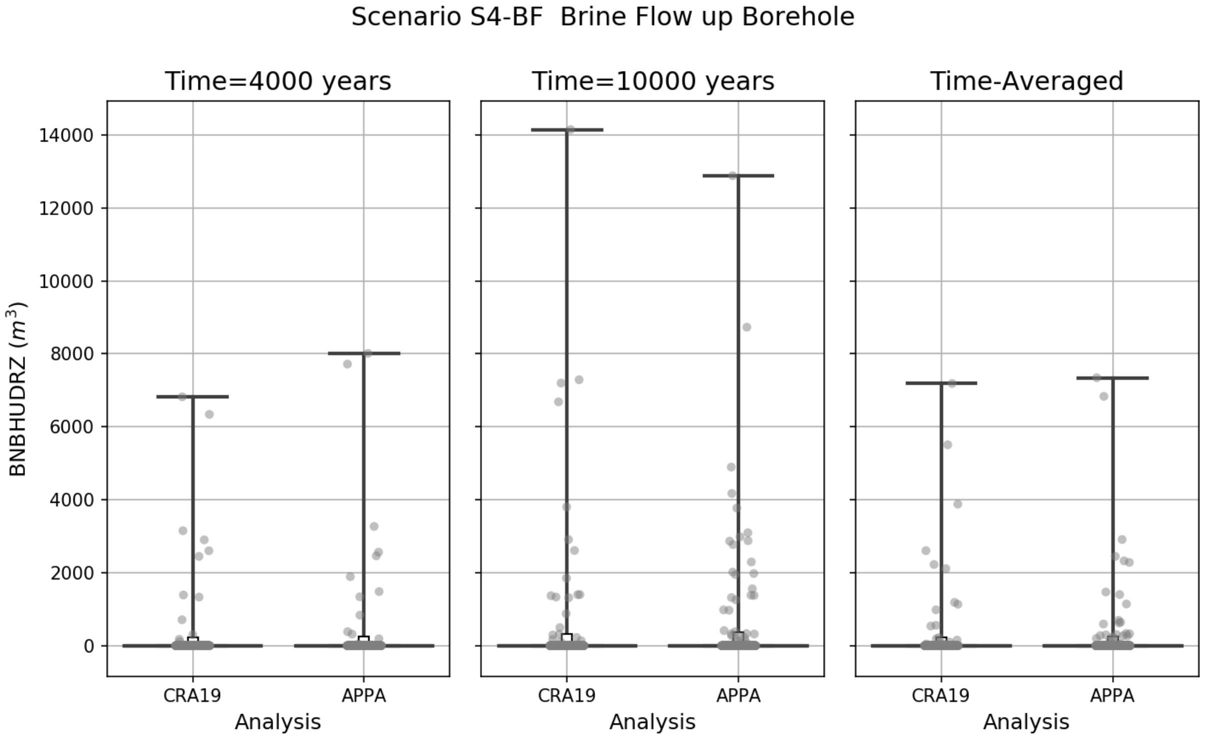
The increase in iron surface area and brine saturation has increased gas generation.



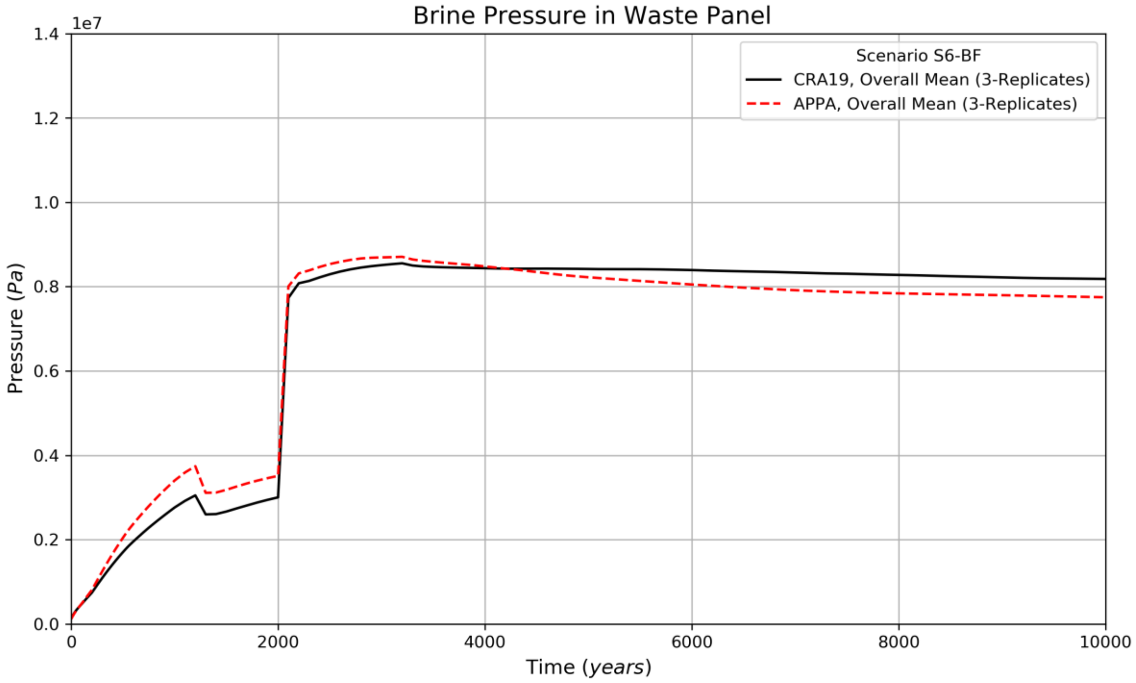
Salado Flow Modeling Results
S4-BF (E2) brine flow up the borehole



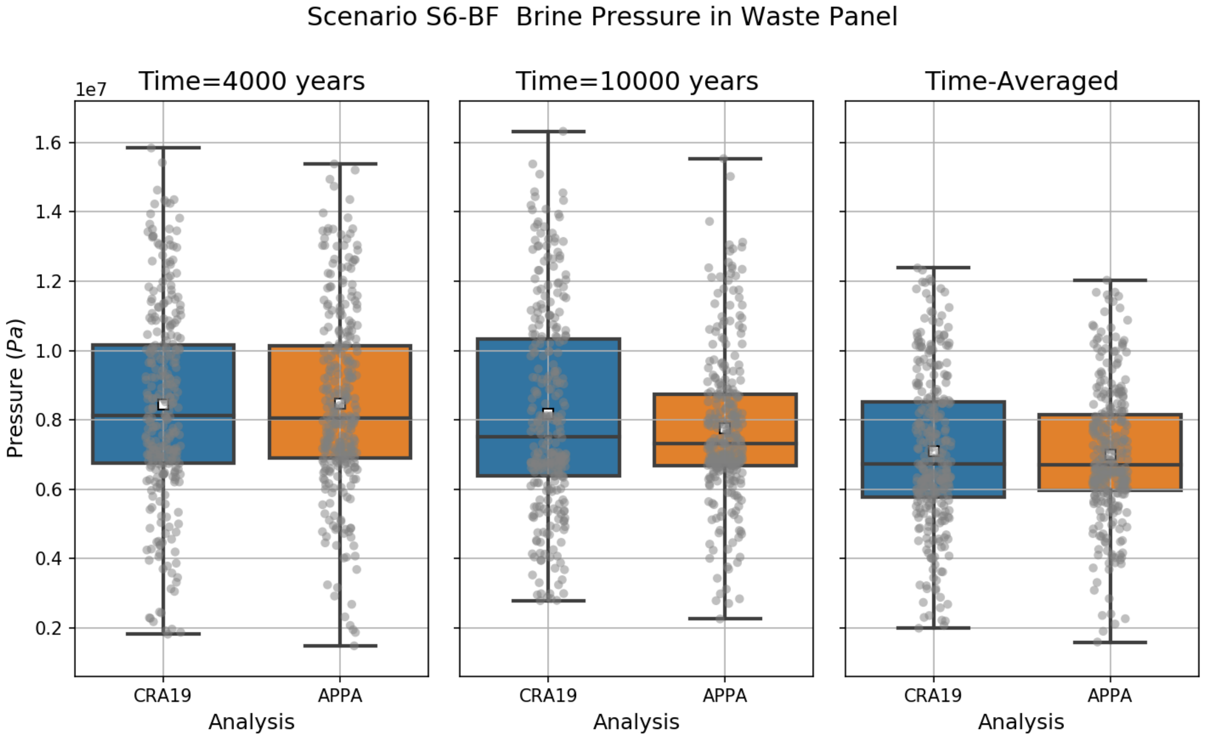
In the E2 case mean brine flow up the borehole has increased, though the maximum cumulative flow up the borehole has decreased.



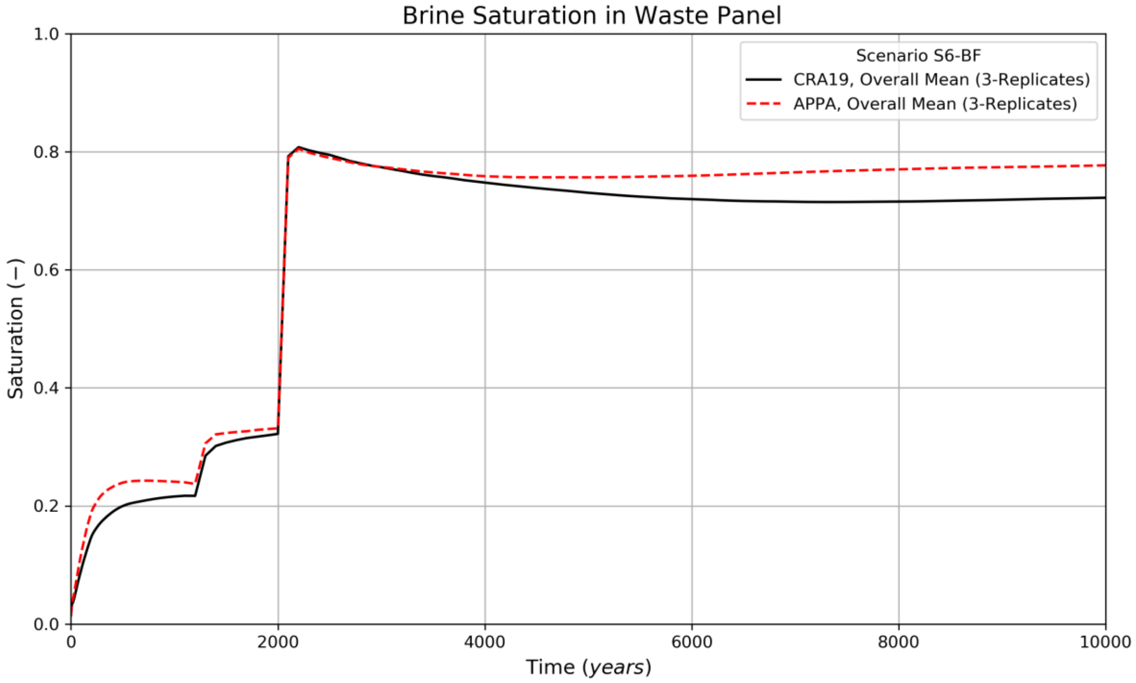
Salado Flow Modeling Results - S6-BF (E2E1) pressures



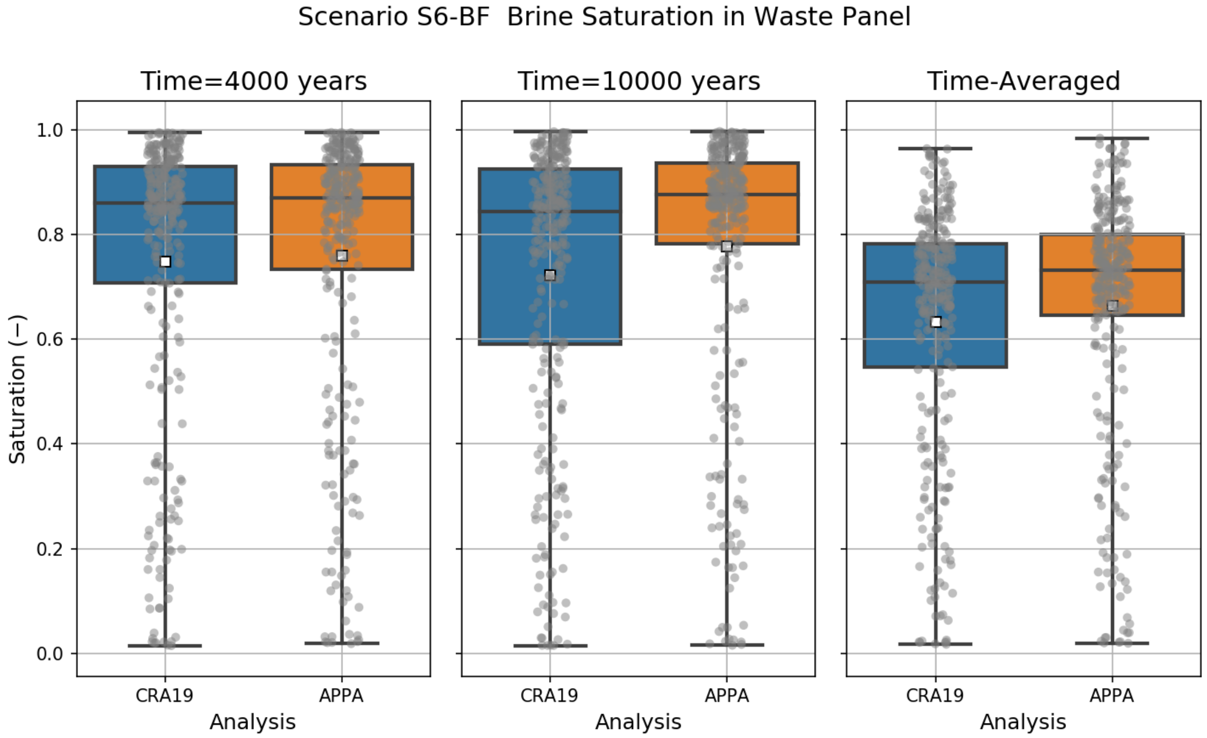
In the E2E1 case mean pressures show a slight increase in early time and a slight decrease in late time. Minimum and maximum pressures have slightly decreased at most time points. This trend holds true for all excavated areas.



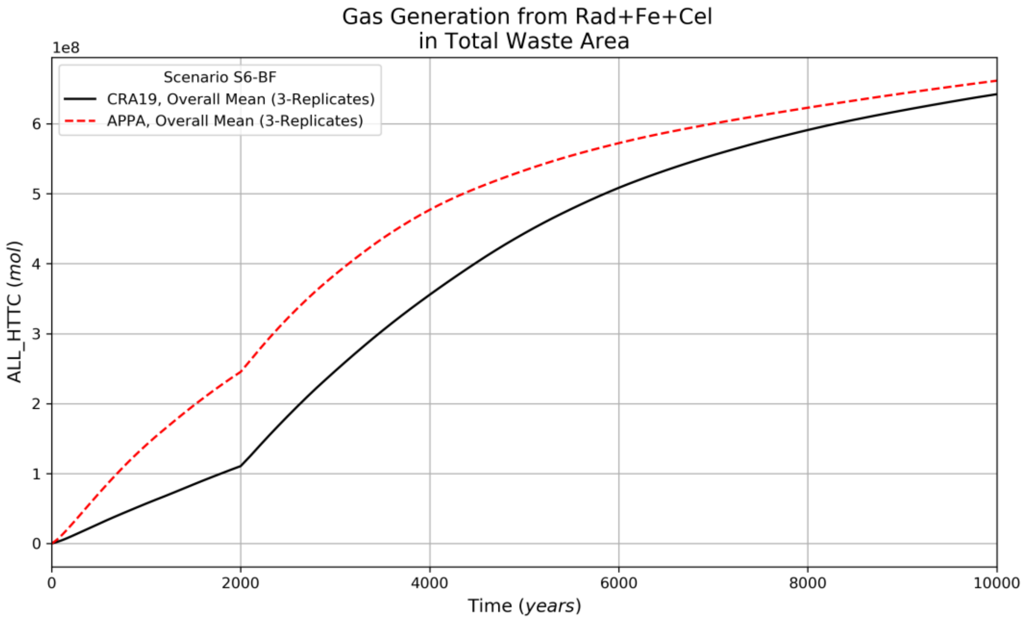
Salado Flow Modeling Results - S6-BF (E2E1) brine saturations

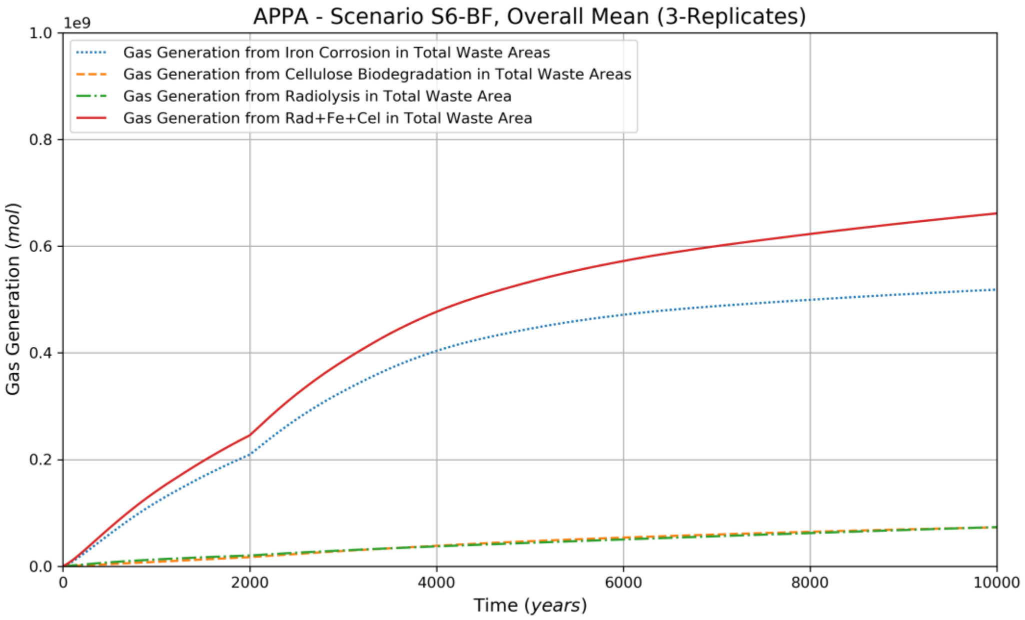


In the E2E1 case the brine saturation have increased, with more vectors at very high saturation values and less vectors at the mid and low saturation values. Up-dip waste areas have seen an increase in brine saturations.

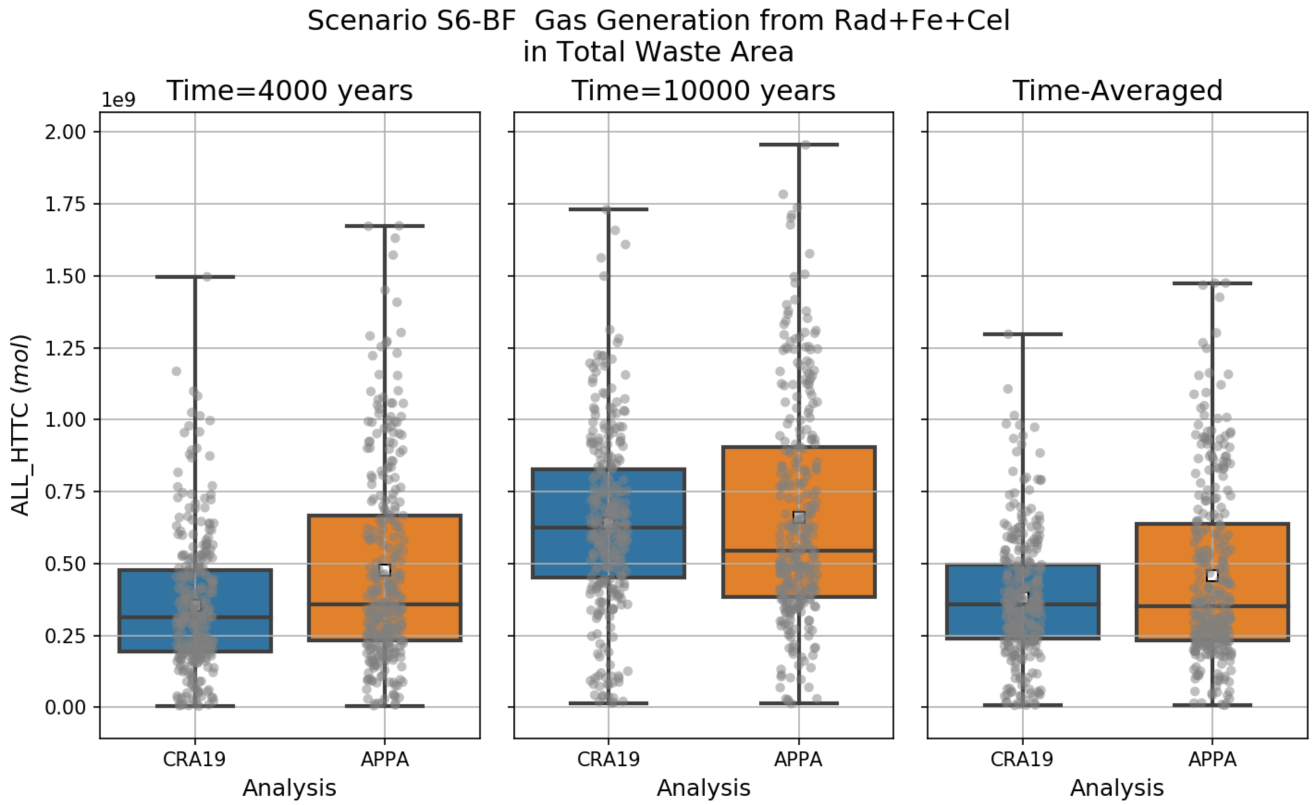


Salado Flow Modeling Results - S6-BF (E2E1) gas generation

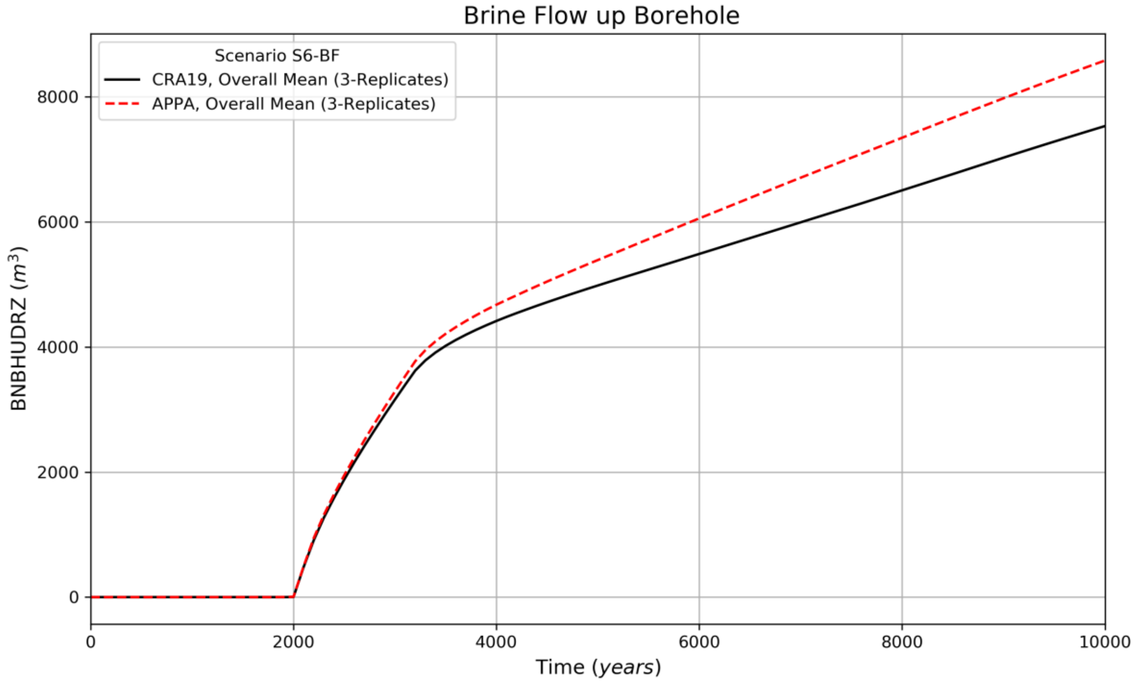




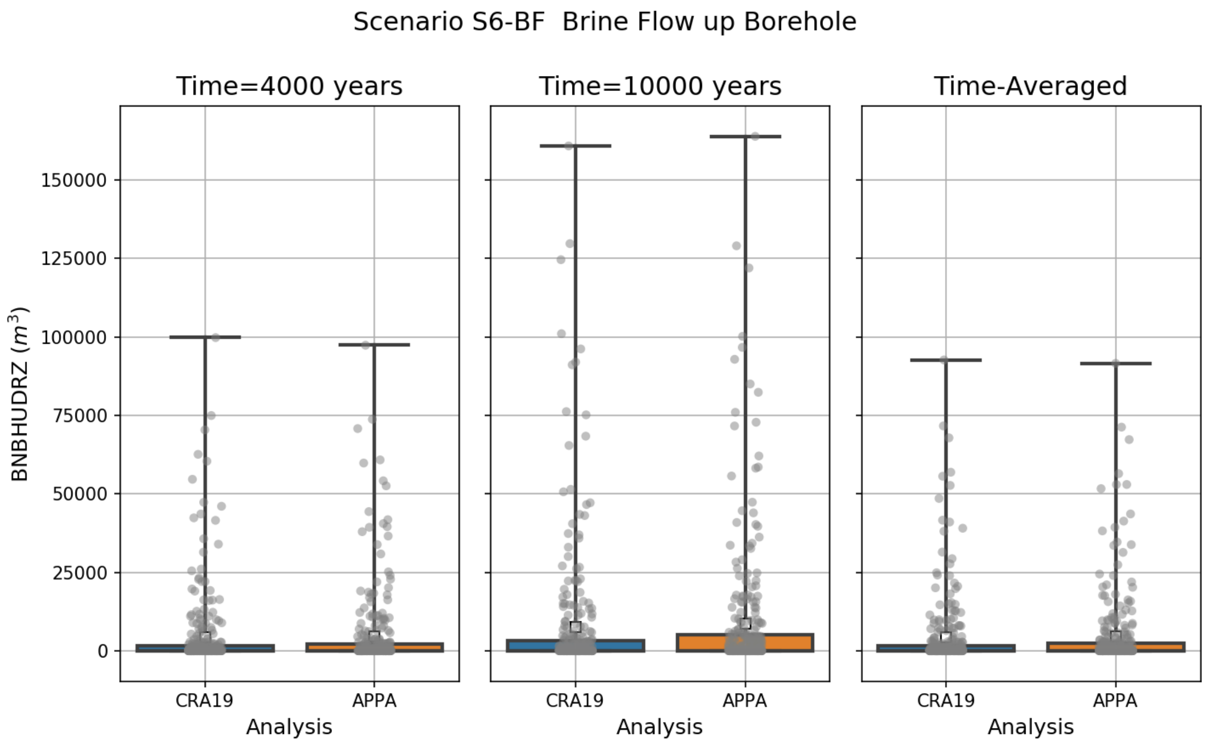
In the E2E1 case, the increase in iron surface area and brine saturation has increased gas generation.



Salado Flow Modeling Results
S6-BF (E2E1) brine flow up the borehole

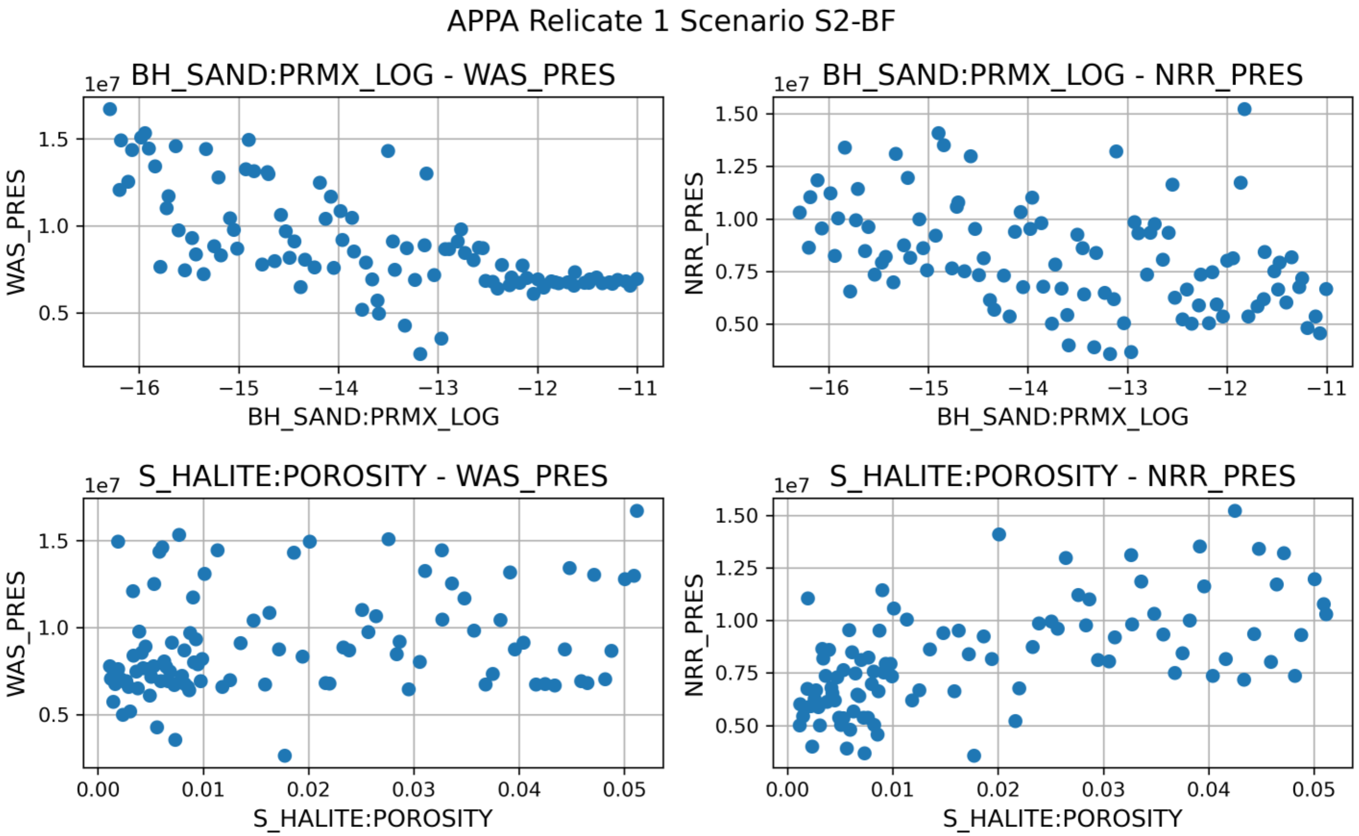


In the E2E1 case mean brine flow up the borehole has increased at later times.



Salado Flow Modeling Results
Intruded Pressure Sensitivity Analysis

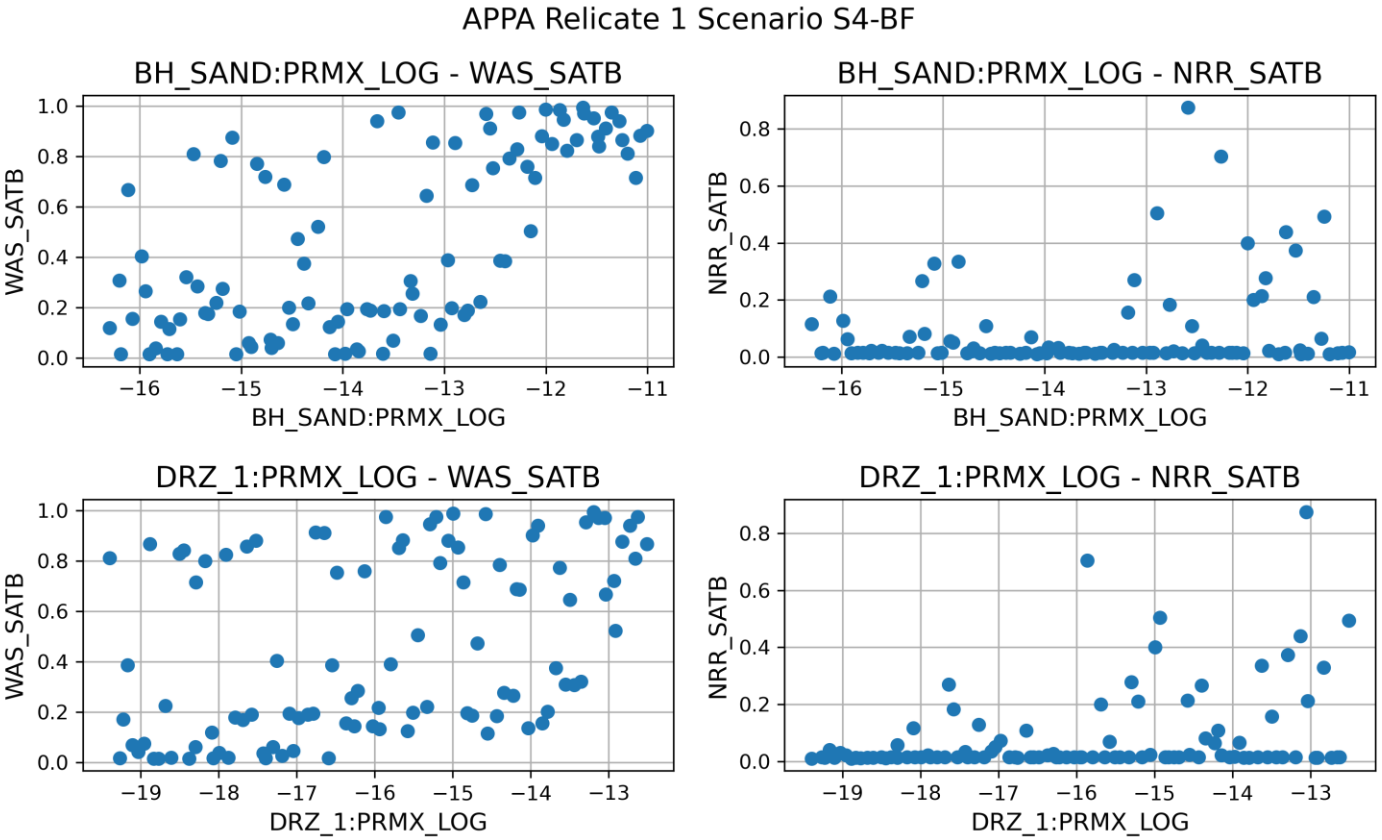
In scenarios with a borehole intrusion, the long-term permeability of the borehole (BH_SAND:PRMX_LOG) becomes an impactful parameter on the long-term repository brine pressure. In Scenario S2-BF, the borehole permeability controls 50-59% of the variability in the Waste Panel brine pressure, a decrease from the 66-67% seen in CRA-2019. The borehole permeability has less impact on the brine pressures in S4-BF and S6-BF and in waste areas farther away from the intrusion (such as the North Rest-of-Repository and West Rest-of-Repository), often less important than the significant parameters of the undisturbed performance



More details of the sensitivity analysis on Salado Flow results provided in Appendix A of King (2021).

Salado Flow Modeling Results
Intruded Brine Saturation Sensitivity Analysis

In Scenario S2-BF, many vectors reach complete brine saturation in the waste panel; in this case the brine saturation becomes a function of the sampled residual gas saturation. In the other scenarios with an intrusion the long-term borehole permeability (BH_SAND:PRMX_LOG) controls much of the variability in brine saturation along with the parameters mentioned for other scenarios.



More details of the sensitivity analysis on Salado Flow results provided in Appendix A of King (2021).

Conclusions

The increased repository area has increased the DRZ, giving increased communication with the Salado formation. This allows more brine to flow into the repository.

- Increased brine in the repository and increased surface area of iron, has increased gas generation in scenarios without a Castile brine pocket intrusion.

The additional repository volume and increased communication with the Salado has lowered the maximum pressures seen in the repository.

- Lower maximum pressures will reduce the occurrence of very large Spallings and DBR events.

Mean brine pressures and saturations have increased in Scenarios without a Castile brine pocket intrusion.

- This has led to an increased number of non-zero DBR events, and an increase in smaller spallings events as compared to the current configuration.

References

Brunell, S. 2020. Calculation of Parameter Values for the Additional Panels Performance Assessment (APPA). Sandia National Laboratories. Carlsbad, NM. ERMS 574030.

Day, B. 2015. Review of the Technical Basis for REFCON:ASDRUM, DRROOM, and VROOM Performance Assessment Analysis Parameters with Comparison to the Currently Emplaced Steel Surface Area per Unit Volume in the WIPP Repository. Carlsbad, NM: Sandia National Laboratories. ERMS 564670.

Day, B. 2019. Analysis Package for Salado Flow in the 2019 Compliance Recertification Application Performance Assessment (CRA-2019 PA). Sandia National Laboratories. Carlsbad, NM. ERMS 571368. https://wipp.energy.gov/library/CRA/CRA-2019/D%20-%20H/Day%20%202019%20%20ERMS%20571368.pdf

Hansen, C. 2020. Analysis Plan for the Additional Panels Performance Assessment. Sandia National Laboratories, Carlsbad, NM. ERMS 573557.

Kim, S., P. S. Domski, L. M. Feng. 2020. Impact Analysis of Corrected Actinide (III) Baseline Solubility Parameters on Performance Assessments. Sandia National Laboratories. Carlsbad, NM. ERMS 572507.

King, S. 2021. Analysis Package for Salado Flow in the Additional Panels Performance Assessment (APPA). Sandia National Laboratories. Carlsbad, NM. ERMS 574497.

King, S. 2021b. Supplemental APPA Salado Flow Results. Sandia National Laboratories. Carlsbad, NM.

King, S. 2020. Initial Waste Area Pressure for the Additional Panels Performance Assessment. Sandia National Laboratories. Carlsbad, NM. ERMS 574357.