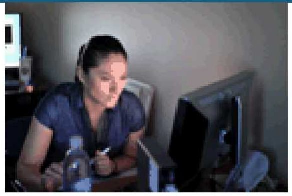
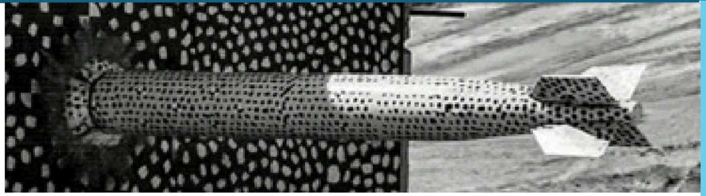
SAND2020-0921PE

CRA-2019 PA – Changes Since the CRA-2014 PA and Results





Todd R. Zeitler

December 12, 2019

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Outline

16 Changes Since the CRA-2014 PA

- Parameters
- Models
- Codes

CRA-2019 PA Results (CRA19 Analysis)

- CCDF results
- Some intermediate results

CRA19_CL Analysis

- Fully QA-qualified run of WIPP PA codes to investigate impact of closure rate for open areas
- Discussed in appendix to PA Summary Report (Zeitler et al. 2019)
- Not discussed in Appendix PA or in other CRA documentation

Changes Since CRA-2014 PA

1. Approach to Abandonment of Panel Closures in the South and No Waste in Panel 9
2. Additional Shaft and Associated Drifts
3. Brine Radiolysis as Part of Gas Generation Process Model
4. Refinement to the Probability of Encountering Pressurized Brine
5. Refinement to the Corrosion Rates of Steel
6. Refinement to the Effective Shear Strength of WIPP Waste
7. Refinement to Colloid Enhancement Parameters
8. Refinement to Hydromagnesite Conversion Rate
9. Removal of Iron Sulfidation Reactions
10. Correction to Length of Northernmost Panel Closure Representation
11. Updates to Drilling Rate and Plugging Pattern Parameters
12. Updates to WIPP Waste Inventory Parameters
13. Updates to Radionuclide Solubilities
14. Update to BH_OPEN:RELP_MOD Parameter
15. New Materials to Define Properties in DRZ Surrounding OPS, EXP, and Panel Closure Areas
16. Hardware and Computational Code Updates

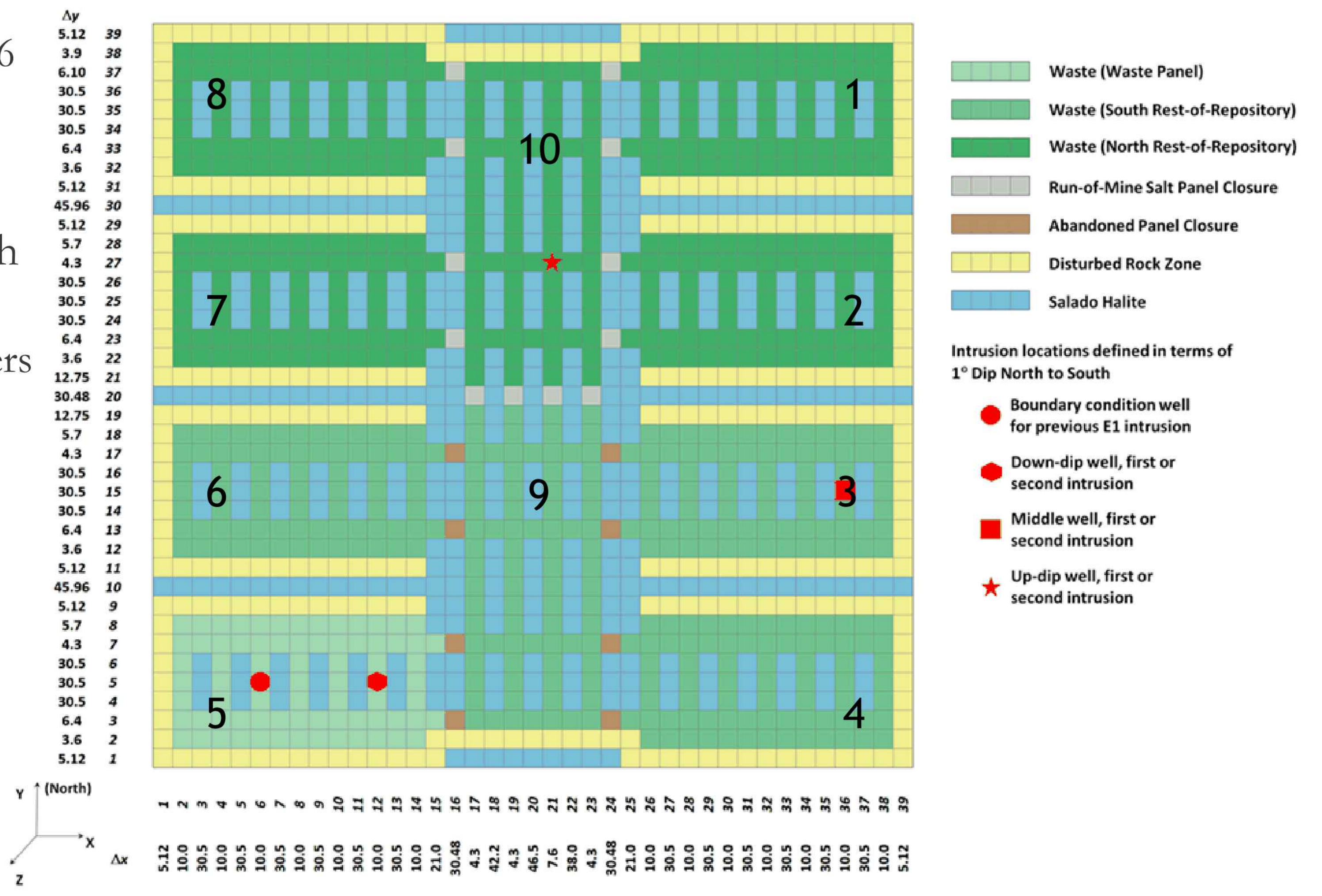
1. Approach to Abandonment of Panel Closures in the South and No Waste in Panel 9

Operational considerations

- No panel closures (PCS) in Panels 3, 4, 5, 6
- No waste in Panel 9

Carried forward approach used in Abandonment of Panel Closures in South End of Repository (APCS) Analysis

- Use of "open area" (OPS/EXP) parameters in southernmost (abandoned) panel closure—between waste panel and SROR
- Waste emplacement in Panel 9
- Reassessed panel neighboring



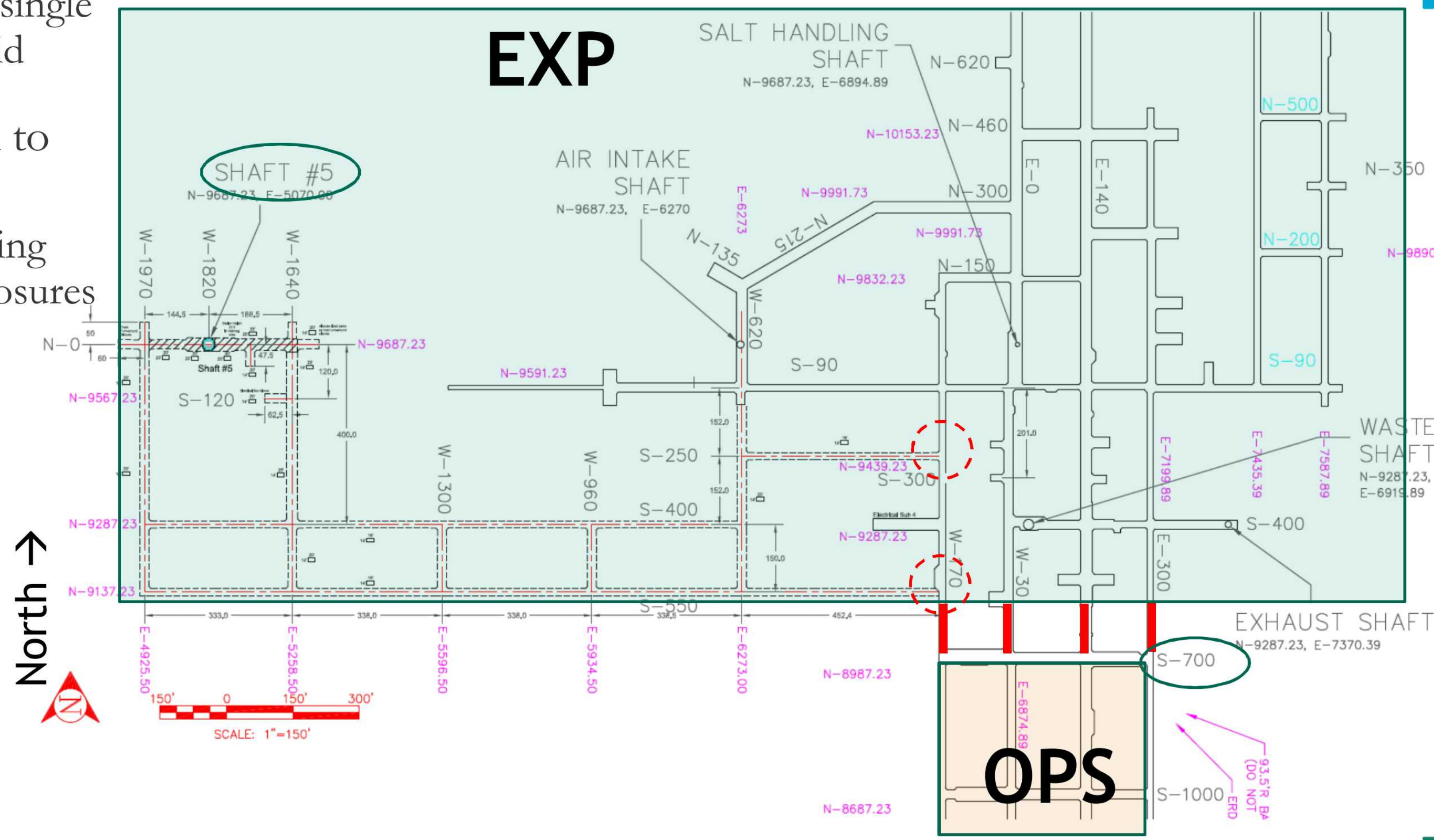
2. Additional Shaft and Associated Drifts

Fifth shaft added to shaft model

- Combined volumes of 5 shafts into a single shaft representation in BRAGFLO grid

Drifts associated with 5th shaft added to volume of experimental (EXP) area

- Design shows shafts intersecting existing drifts north of northernmost panel closures (S-700); shown in red



3. Brine Radiolysis as Part of Gas Generation Process Model

Day (2019) showed the potential impact of brine radiolysis on overall gas generation

Radiolytic gas generation screened in for CRA19

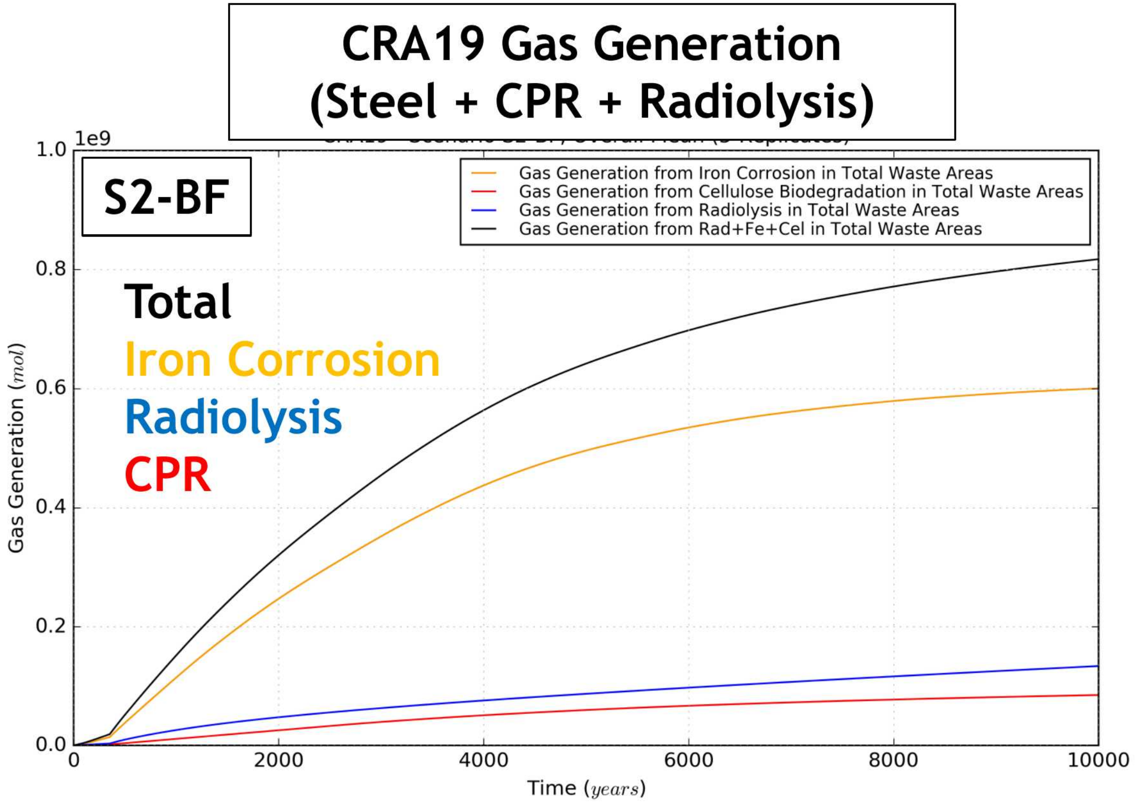
- Implemented in new version of BRAGFLO

Implementation included a new uncertain parameter

- GLOBAL:GDEPFAC -- energy deposition probability for wetted solid radionuclides
- Uniform distribution [0, 0.5]

Inventory assessment (Kicker 2019a) determined which radionuclides will participate in radiolysis based on decay heats

- ^{241}Am, ^{238}Pu, ^{239}Pu, ^{240}Pu, and ^{242}Pu



4. Refinement to the Probability of Encountering Pressurized Brine

Updated distribution for GLOBAL:PBRINE parameter

Cumulative distribution

Based on EPA-derived distribution developed from TDEM data (TSD)

Same as used in CRA14_SEN4 analysis

Generally increased probability of intersecting brine compared to CRA-2014

- Increased probability of E1 intrusions

Parameter	Units	Description	Distribution Type	Default Value	Source
GLOBAL:PBRINE	none	Prob. that Drilling Intrusion In Excavated Area Encounters Pressurized Brine	Cumulative	0.26345	Peake 2018, Veal 2017, U.S. EPA 2017a

5. Refinement to the Corrosion Rates of Steel

Updates to inundated (STEEL:CORRMCO2) and humid (STEEL:HUMCORR) iron corrosion rates

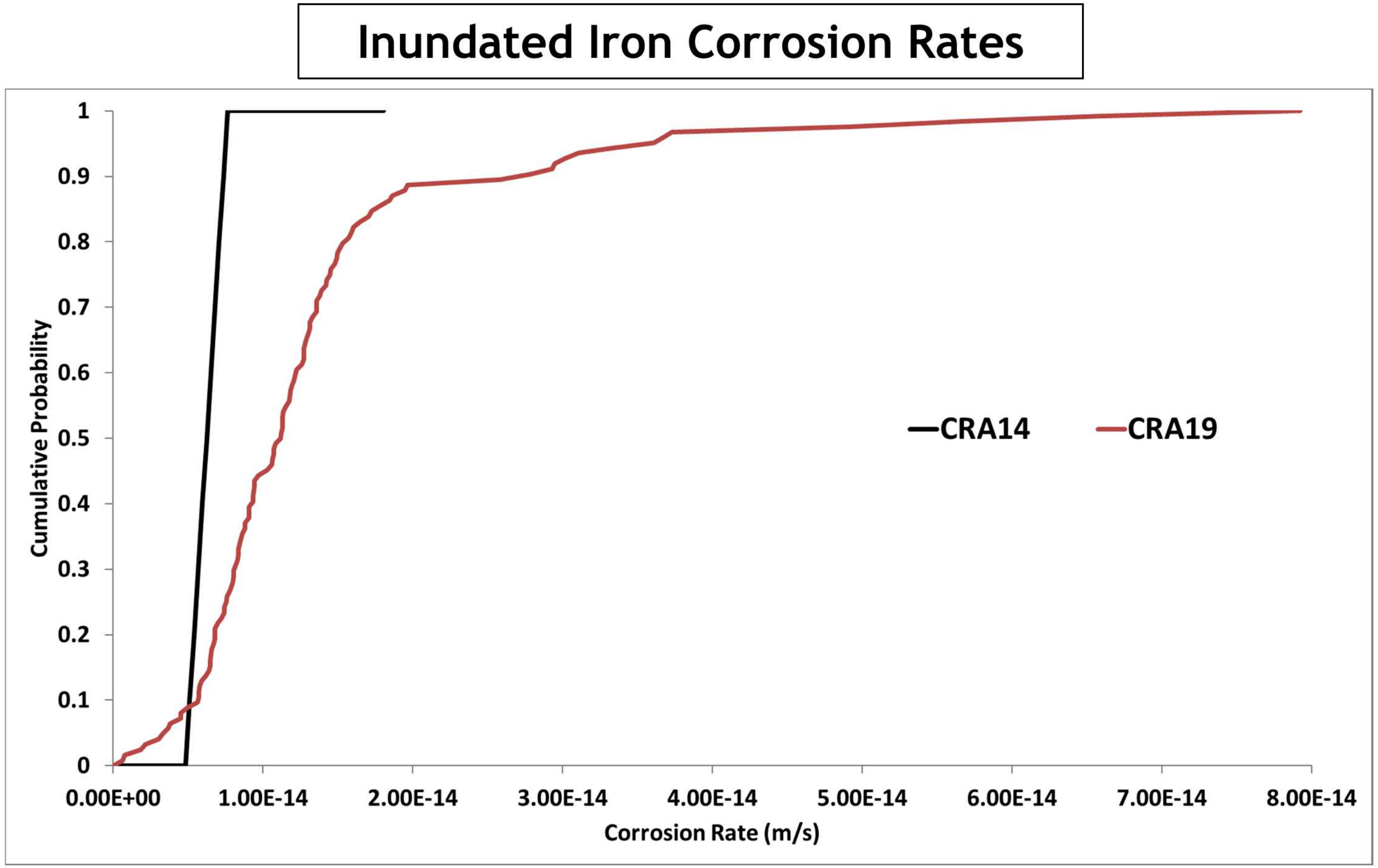
Includes TSD-recommended use of expanded set of Roselle (2013) data

Includes factor 2x applied to inundated rates recommended in TSD

Cumulative distributions

Increased rates compared to CRA-2014 PA

Humid rate is non-zero for first time in a compliance calculation



6. Refinement to the Effective Shear Strength of WIPP Waste

Updated distribution for BOREHOLE:TAUFAIL distribution

Based on EPA recommendation (TSD)

Uniform distribution

Decreased lower end of distribution

- Leads to increased cavings releases

Same as used in CRA14_SEN4 analysis

Parameter	Units	Description	Distribution Type	Distribution Parameters	Default Value	Source
BOREHOLE:TAUFAIL	Pa	Effective shear strength for erosion	Uniform	Min = 1.60 Max = 77 Mean = 39.3	39.3	Peake 2018, Veal 2017, U.S. EPA 2017c

7. Refinement to Colloid Enhancement Parameters

Based on new laboratory and literature data

Humic colloid proportionality constants (Mariner 2019)
- III and IV radionuclides
- Salado and Castile brine (PHUMSIM and PHUMCIM)

Microbial colloids (Reed et al. 2019)
- Max concentration (CAPMIC): Am, Np, Pu, Th, U
- Proportionality parameter (PROPMIC): Am, Np, Pu, Th, U

Intrinsic colloids (Reed et al. 2019)
- Mobile concentration (CONCINT): Am, Np, Pu, Th, U

Colloid Enhancement Parameters Used in CRA-2019

Actinide	Actinide Source Term Colloid Enhancement Parameters						
	Intrinsic	Mineral	Microbial		Humic		
	CONCINT (M)	CONCMIN (M)	CAPMIC (M)	PROPMIC	PHUMSIM	PHUMCIM	CAPHUM (M)
Thorium	4.3×10^{-8}	2.6×10^{-8}	3.8×10^{-8}	0.21	0.01	0.01	1.1×10^{-5}
Uranium[1]	1.4×10^{-6}	2.6×10^{-8}	3.8×10^{-8}	0.21	0.01 / 0.12	0.01 / 0.51	1.1×10^{-5}
Neptunium[2]	4.3×10^{-8}	2.6×10^{-8}	3.8×10^{-8}	0.21	0.01 / 9.1×10^{-4}	0.01 / 7.4×10^{-3}	1.1×10^{-5}
Plutonium[3]	4.3×10^{-8}	2.6×10^{-8}	3.8×10^{-8}	0.21	0.2 / 0.01	0.2 / 0.01	1.1×10^{-5}
Americium	9.5×10^{-9}	2.6×10^{-8}	2.3×10^{-9}	0.03	0.2	0.2	1.1×10^{-5}

1 - for uranium, humic colloid parameters are oxidation-state specific. Data are for U(IV) / U(VI)
2 - for neptunium, humic colloid parameters are oxidation-state specific. Data are for Np(IV) / Np(V)
3 - for plutonium, humic colloid parameters are oxidation-state specific. Data are for Pu(III) / Pu(IV)

Highlighted values have been updated for CRA19

8. Refinement to Hydromagnesite Conversion Rate

Update to WAS_AREA:HYMAGCON distribution

Based on TSD-recommended rates

Uniform distribution

Includes potential for no conversion (rate of zero)

Parameter	Units	Description	Distribution Type	Distribution Parameters	Default Value	Source
WAS_AREA:HYMAGCON	mol kg^{-1} sec^{-1}	Rate of conversion of hydromagnesite to magnesite	Uniform	Min = 0 Max = 3.4×10^{-10} Mean = 1.7×10^{-10}	1.7×10^{-10}	Peake 2018, U.S. EPA 2017d

9. Removal of Iron Sulfidation Reactions

Removal of iron sulfidation reactions from BRAGFLO water balance

- Set stoichiometric coefficients to zero

Same as used in CRA14_SEN4 analysis

Based on TSD recommendations

Parameter	Units	Description	Value	Source
REFCON:STCO_31	none	FeOH2 Sulfidation: H2 Stoichiometric Coefficient	0	Peake 2018, U.S. EPA 2017d
REFCON:STCO_32	none	FeOH2 Sulfidation: H2O Stoichiometric Coefficient	0	Peake 2018, U.S. EPA 2017d
REFCON:STCO_35	none	FeOH2 Sulfidation: FeOH2 Stoichiometric Coefficient	0	Peake 2018, U.S. EPA 2017d
REFCON:STCO_36	none	FeOH2 Sulfidation: FeS Stoichiometric Coefficient	0	Peake 2018, U.S. EPA 2017d
REFCON:STCO_43	none	Metallic Fe Sulfidation: Fe Stoichiometric Coefficient	0	Peake 2018, U.S. EPA 2017d
REFCON:STCO_46	none	Metallic Fe Sulfidation: FeS Stoichiometric Coefficient	0	Peake 2018, U.S. EPA 2017d

10. Correction to Length of Northernmost Panel Closure Representation

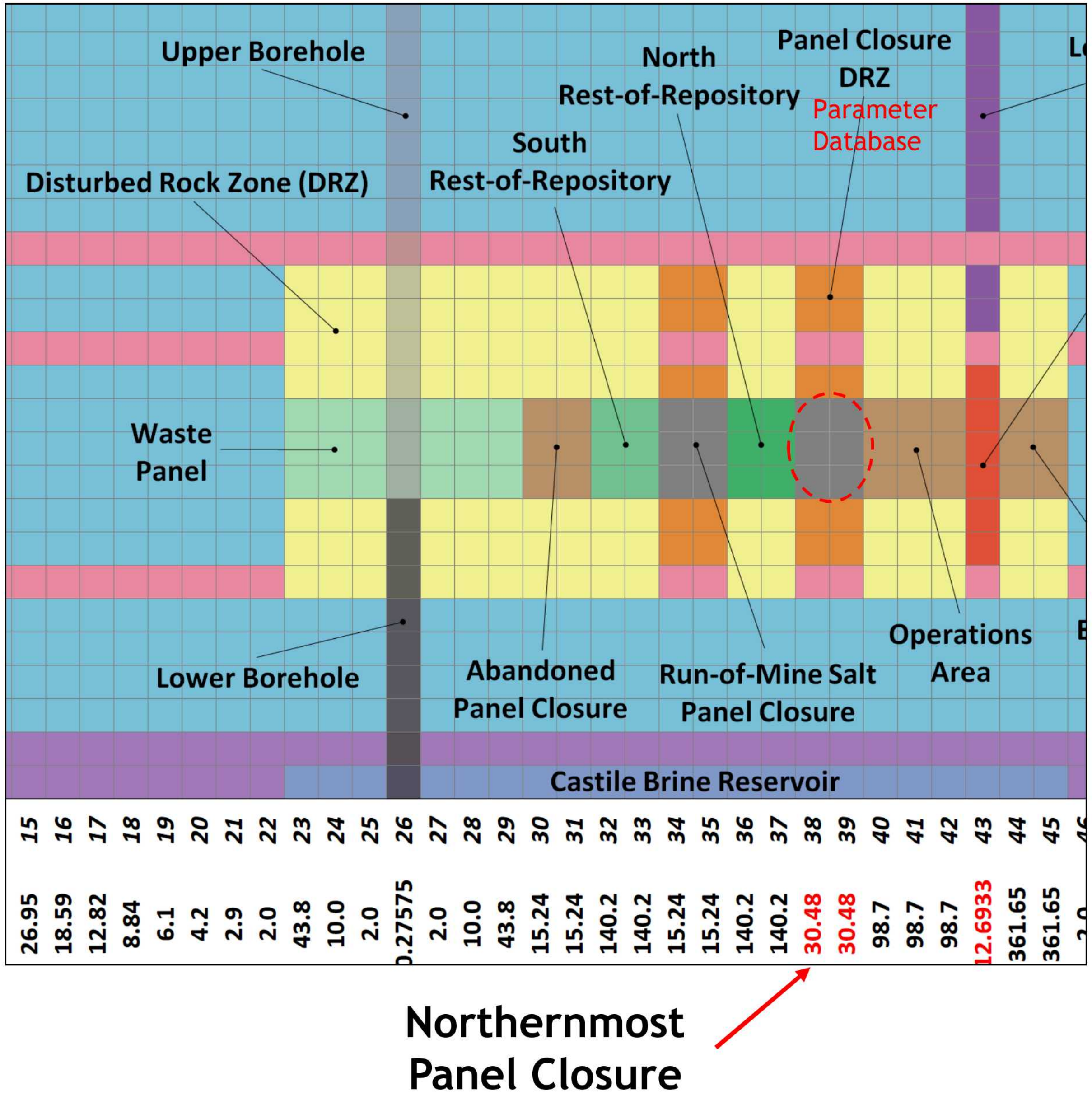
Error in the length of the northernmost panel closure BRAGFLO representation

- Identified during completeness determination period for CRA-2014 PA

Northernmost panel closure should represent the length of two panel closures

Grid lengths doubled in BRAGFLO grid for northernmost PCS grid cells

- Total length increased: 30.48 m to 60.96 m



11. Updates to Drilling Rate and Plugging Pattern Parameters

Typical CRA updates

Based on 2018 Delaware Basin Monitoring Annual Report

Drilling rate increase

- Increased number of repository intrusions

Plugging patterns used in scenario selection

ONEPLG (full plug) increased

- E0 scenario

TWOPLG decreased

- E1 or E2 scenario (depends on PBRINE)

THREEPLG decreased

- E2 scenario

Material	Property	Description	Units	CRA14 Value	CRA19 Value
GLOBAL	LAMBDAD	Drilling rate per unit area	km^{-2} yr^{-1}	6.73×10^{-3}	9.90×10^{-3}
GLOBAL	ONEPLG	Probability of having Plug Pattern 1 (full plug)	(-)	0.04	0.403
GLOBAL	TWOPLG	Probability of having Plug Pattern 2	(-)	0.594	0.331
GLOBAL	THREEPLG	Probability of having Plug Pattern 3	(-)	0.366	0.266

12. Updates to WIPP Waste Inventory Parameters

Typical CRA updates

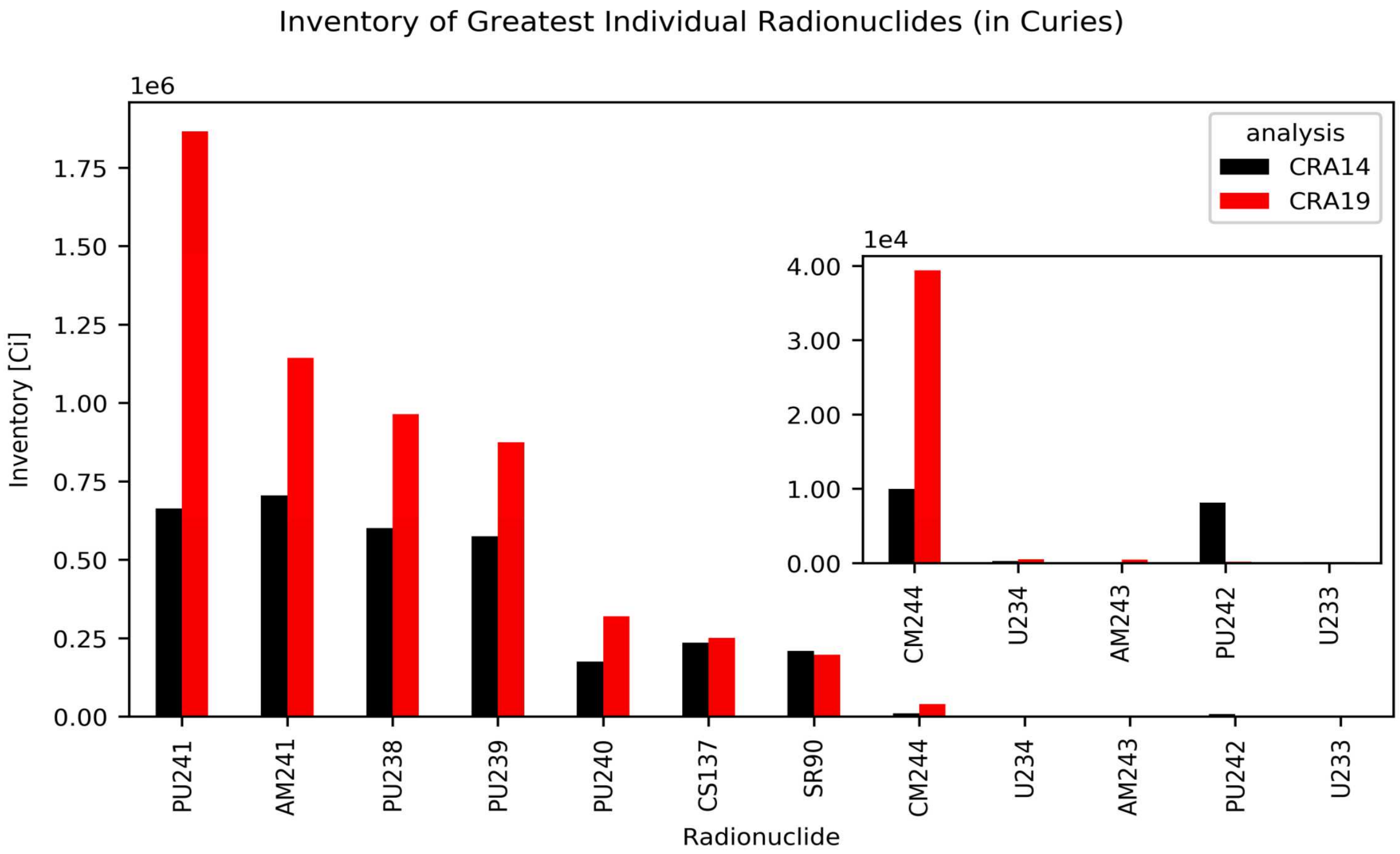
Waste parameters
- CH and RH waste
- 30 RNs + 5 lumped RNs

Non-waste parameters
- Includes waste and container materials
- Iron
- CPR
- Nitrate and sulfate

Lead inventory is not parameterized
- Greatly increased for CRA19, but screened-out as a contributor to gas generation

Waste unit factor (WUF)
- Increased from 2.06 to 3.30

Updated CH and RH waste stream volumes and concentrations for solids releases



13. Updates to Radionuclide Solubilities

Typical CRA updates

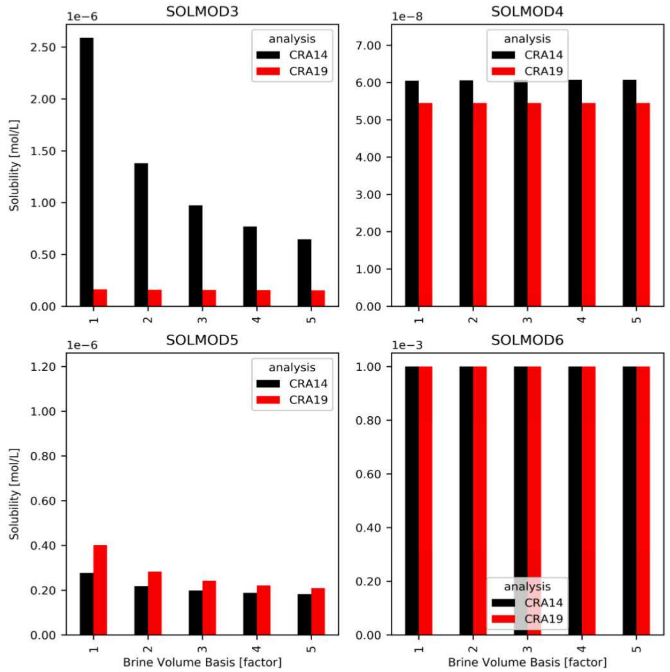
Updated thermodynamic database DATA0.FM4

Updated organic ligand concentrations

Baseline solubility (SOLSOH, SOLCOH) parameters updated for III, IV, and V radionuclides in Salado and Castile brine for 5 brine volumes

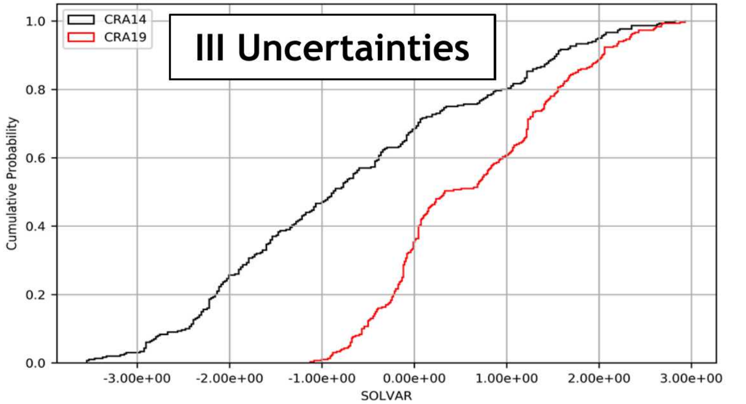
Solubility uncertainty (SOLVAR) parameters updated for III and IV radionuclides

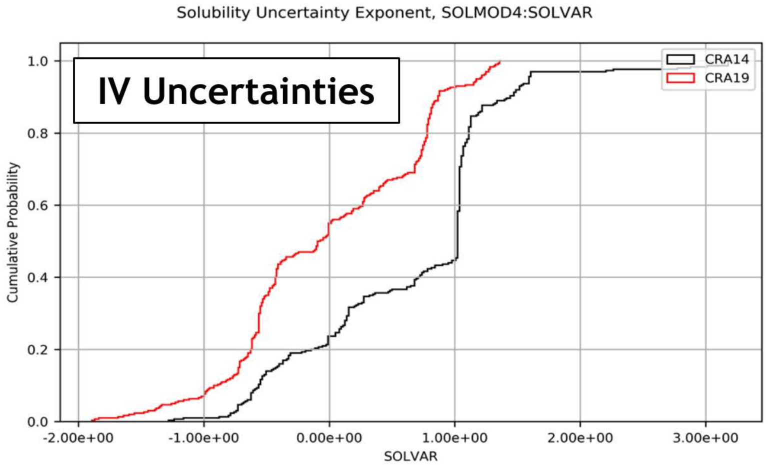
Baseline Solubilities (Salado Brine)



CRA14
CRA19

Solubility Uncertainties





14. Update to BH_OPEN:RELP_MOD Parameter

Minor error found in BRAGFLO code related to calculation of capillary pressure

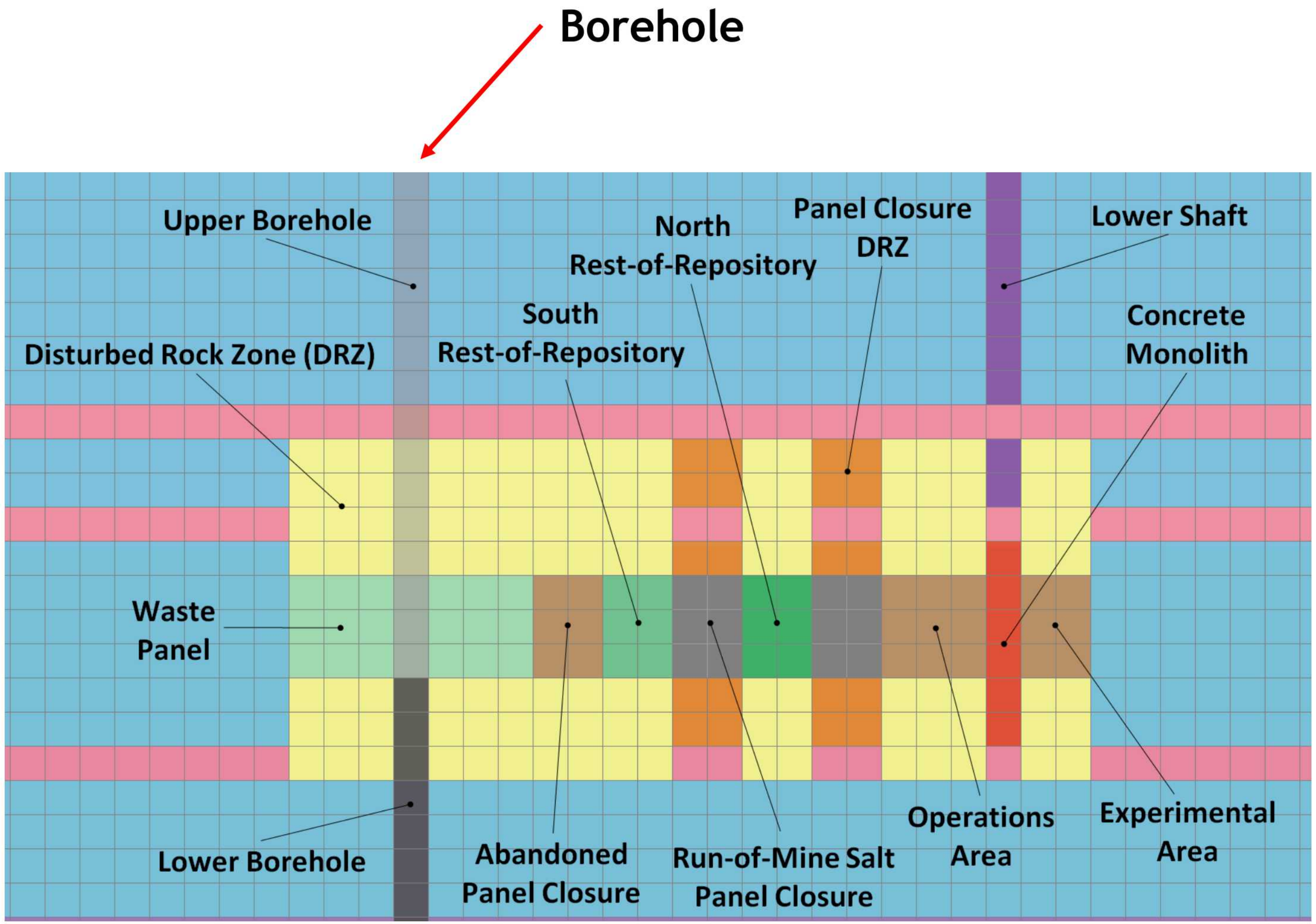
- Insignificant effect on PA results

Necessity to revise BH_OPEN:RELP_MOD

- BRAGFLO input parameter for the relative permeability and capillary pressure function that is used to model an open borehole

RELP_MOD parameter revised from 5 (used in CRA-2014 PA) to 11 to resolve issue where code correction resulted in positive capillary pressure within the open borehole under RELP_MOD=5, which is both physically unrealistic and numerically unstable

RELP_MOD = 11 for the BH_OPEN material is consistent with the relative permeability and (zero) capillary pressure implemented for other "open" repository areas (OPS, EXP)



15. New Materials to Define Properties in DRZ Surrounding OPS, EXP, and Panel Closure Areas

Zero impact to results

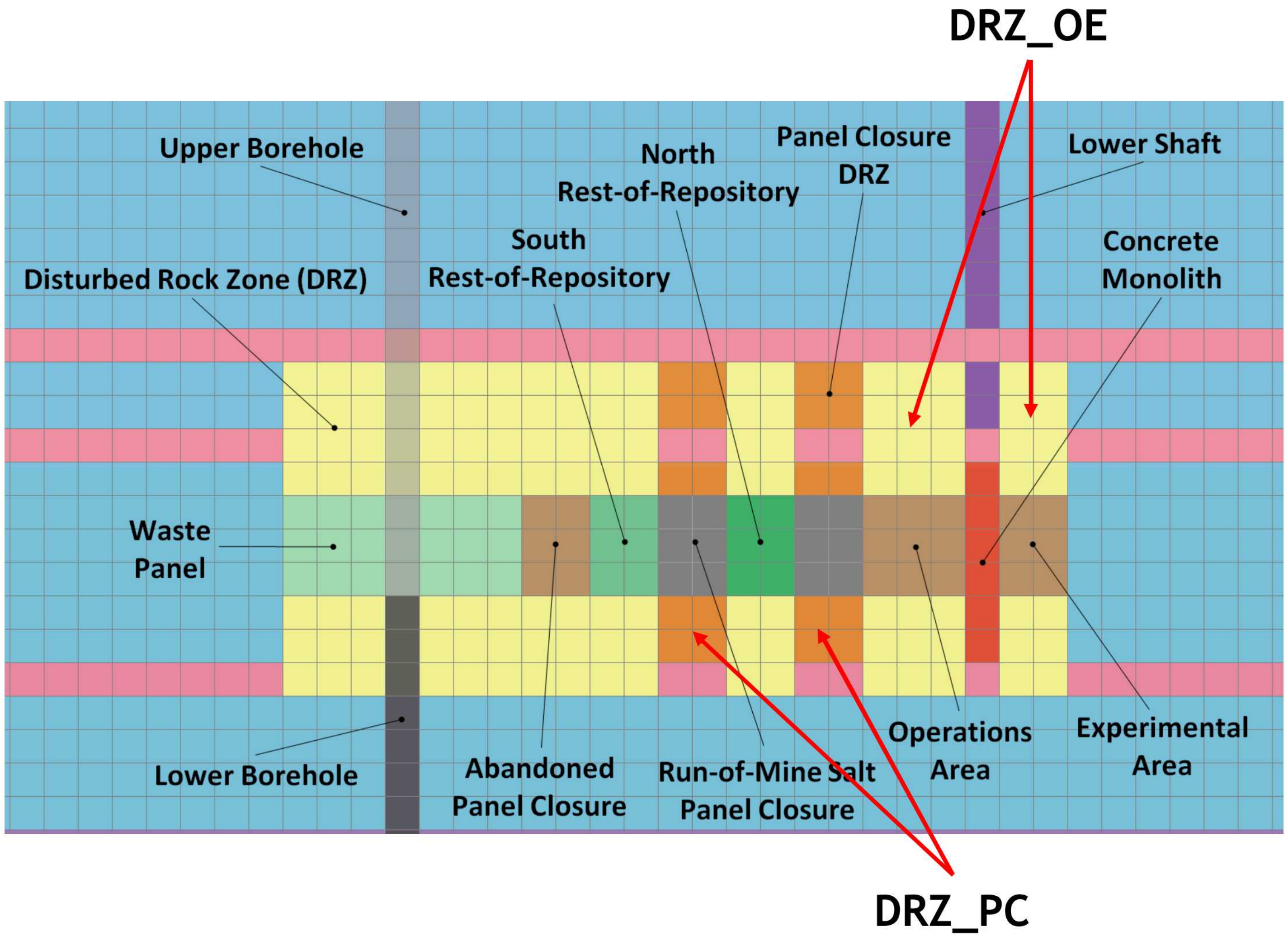
New material names used that introduce flexibility in specifying material properties independently across areas for which material properties were previously identical

- Ability to specify OPS/EXP/PCS DRZ separately from other DRZ

Flexibility of managing material properties

New materials: DRZ_OE_0, DRZ_OE_1, DRZ_PC_1, DRZ_PC_0, and CAVITY_5 (PCS area from -5 to 0 yrs)

Material names representing these areas of the BRAGFLO grid have changed, properties for those areas have not changed

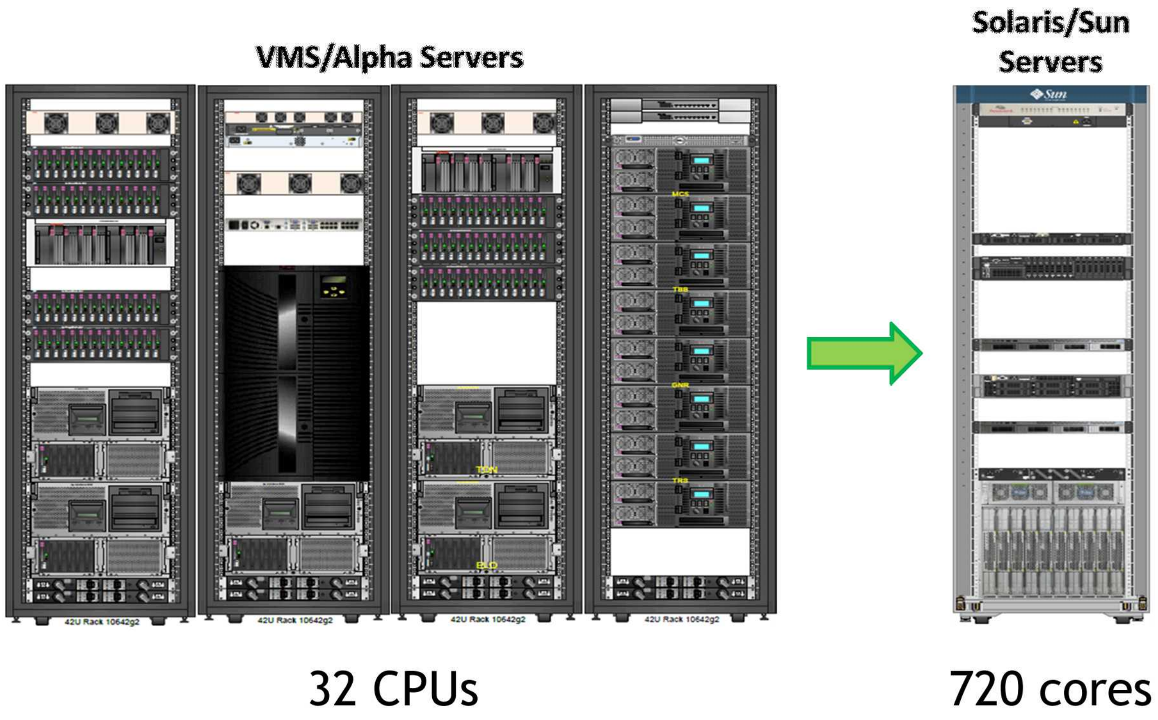


16. Hardware and Computational Code Updates

PA codes migrated to Solaris Cluster (2014, 2015)
- Recompilation, retesting, requalification
- Rerun of CRA-2014 PA

Additional code changes since migration
- Bug fixes (e.g., DRSPALL, BRAGFLO)
- Added code functionality (e.g., BRAGFLO)

Addition of two codes to baseline list
- SCREEN_NUTS – previously a utility code to screen NUTS results
- CCDFVECTORSTATS – CCDF statistics previously calculated by Access database as a post-processing step when across-vector means were calculated



CRA-2019 PA (CRA19 Analysis)

CRA14 results used as baseline

FEPs reassessment (Kirkes)

Inventory analysis (Kicker)

CRA19 running of codes (Long)

Parameter report (Kim/Feng)

Analysis reports:

- LHS (Zeitler)
- EPAUNI (Kicker)
- CUTTINGS_S/DRSPALL (Kicker)
- PANEL/NUTS (Sarathi)
- BRAGFLO (Day)
- BRAGFLO_DBR (Bethune)
- CCDFGF (Brunell)
- STEPWISE (Zeitler)

Summary PA report (Zeitler et al. 2019)

CRA documentation:

- Appendix SCR
- Appendix MASS
- Appendix PA

All references part of December 2019 submittal

CRA19 Results:

- Mean releases increased for all release mechanisms
- Total mean releases increase at all probabilities
- Cuttings and cavings releases continue to dominate at high probabilities
- DBRs continue to dominate at low probabilities

CRA-2019 PA – Parameter Sampling

64 sampled parameters

Same random seeds used as for CRA-2014 PA

Same parameter correlations applied

2 newly sampled parameters

- GLOBAL:GDEPFAC – used in radiolysis
- STEEL:HUMCORR – previously constant value

1 parameter sampled from CRA-2014 PA is now constant

- PHUMOX3:PHUMCIM – humic colloid parameter

Sampled Parameters with Updated Distributions Since the CRA-2014 PA

Material	Property	Description
GLOBAL	PBRINE	Prob. That drilling intrusion in excavated area encounters pressurized brine
STEEL	CORRMCO2	inundated corrosion rate for steel
BOREHOLE	TAUFAIL	Effective shear strength for erosion
WAS_AREA	HYMAGCON	Rate of conversion of hydromagnesite to magnesite
SOLMOD3	SOLVAR	Solubility multiplier, oxidation state III
SOLMOD4	SOLVAR	Solubility multiplier, oxidation state IV

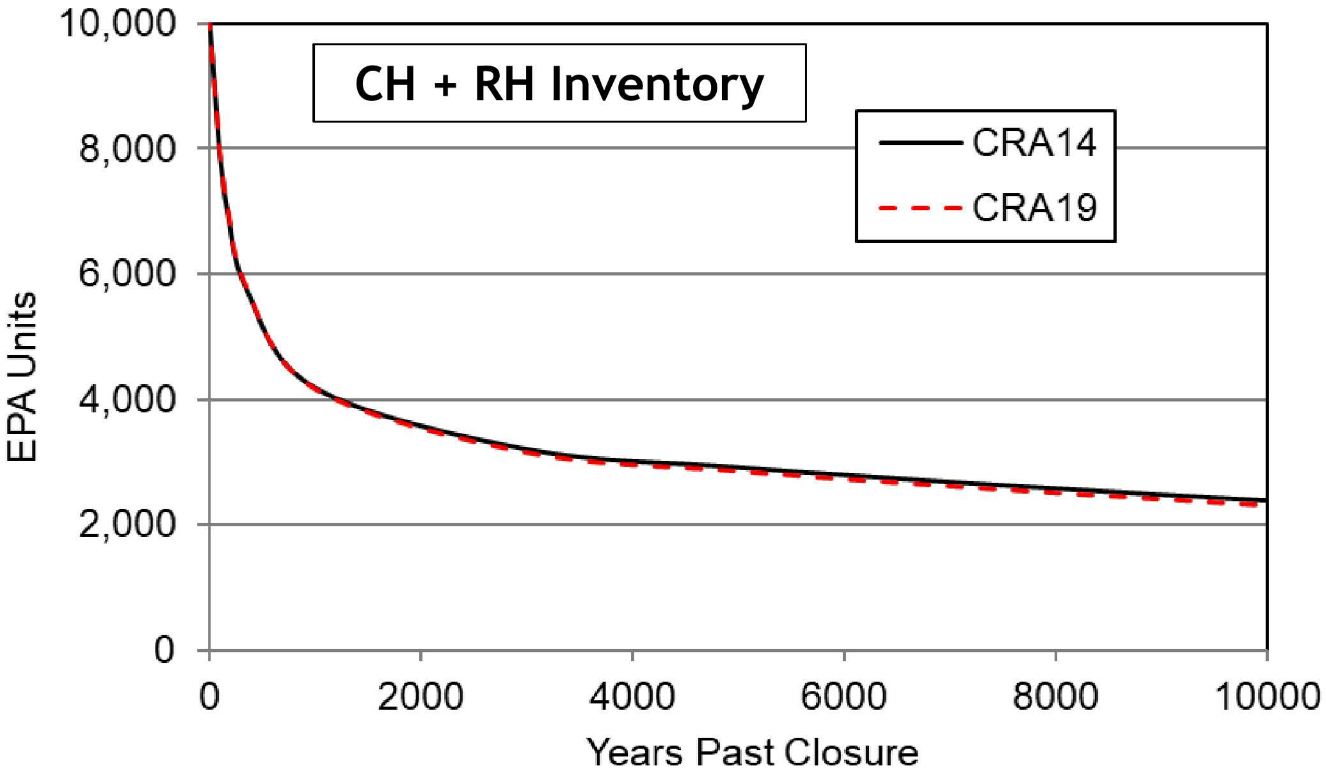
CRA-2019 PA – Inventory

	CRA14	CRA19
No. CH Waste Streams	451	510
No. RH Waste Streams	77	97
Waste Unit Factor (WUF)	2.06	3.30

Overall activity (in EPA units) with time is similar

SR-KAC-PuOX waste stream comprises:

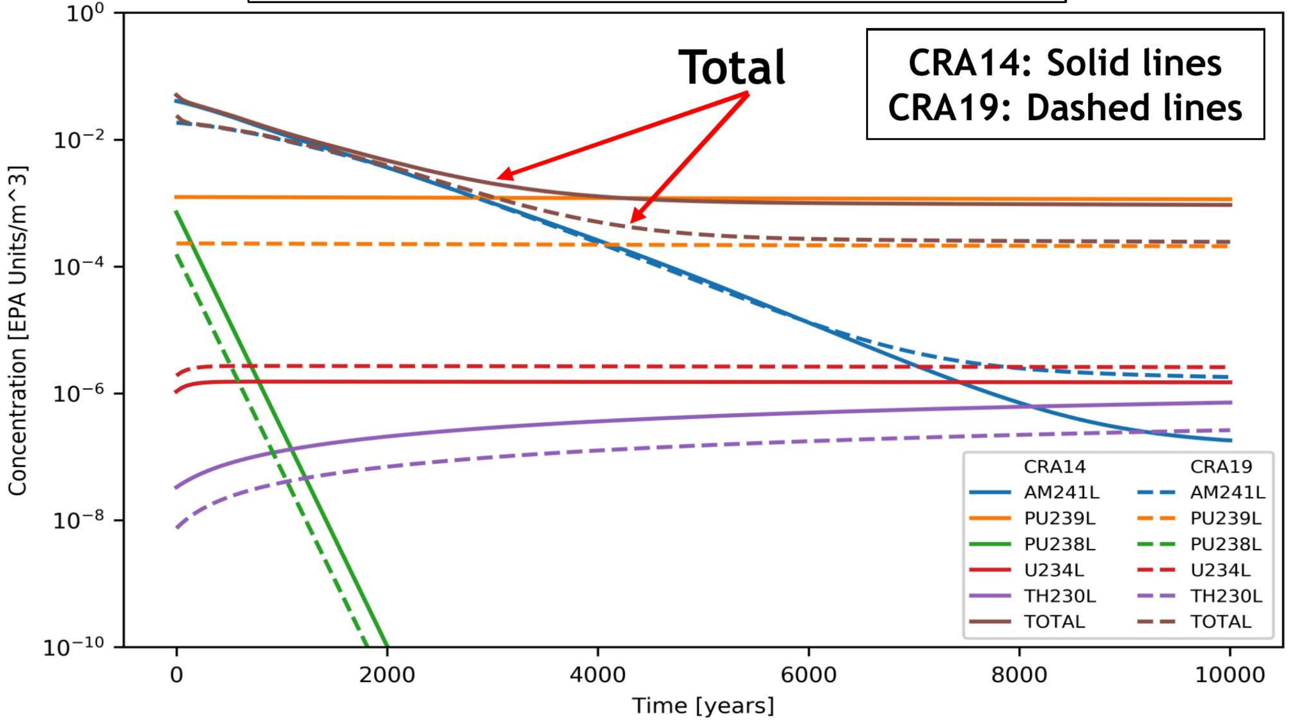
- 3.5% of total waste stream volume
- 29 % of total EPA Units at closure

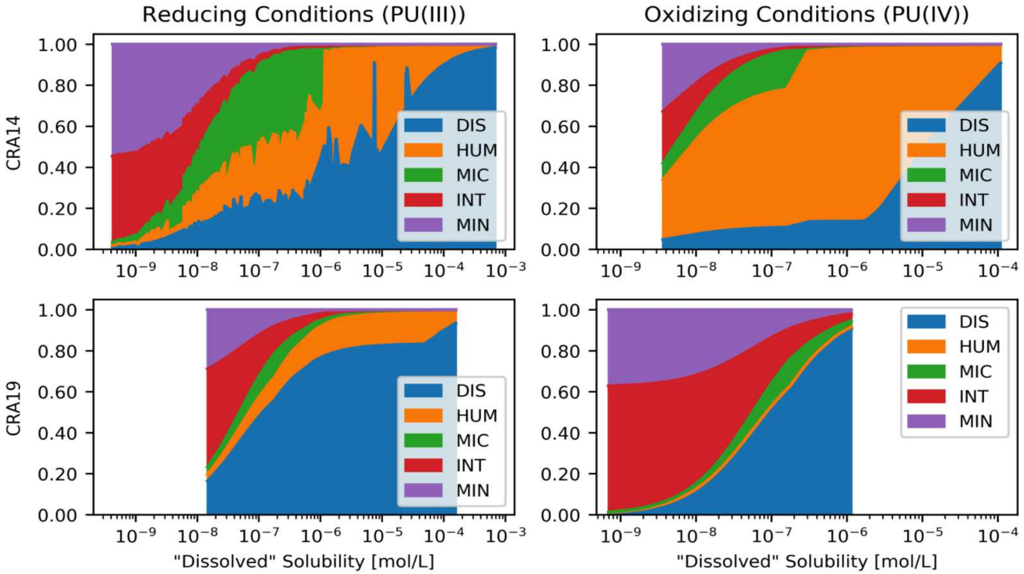


CRA-2019 PA – Mobilized Concentrations

- Mobilized radionuclide concentration in waste panels over time
- Include dissolved and colloidal contributions
- Mean total concentration decreased compared to CRA14
  - Reduction in the An(III) and An(IV) concentration limits

Mean Concentrations (Castile Brine)





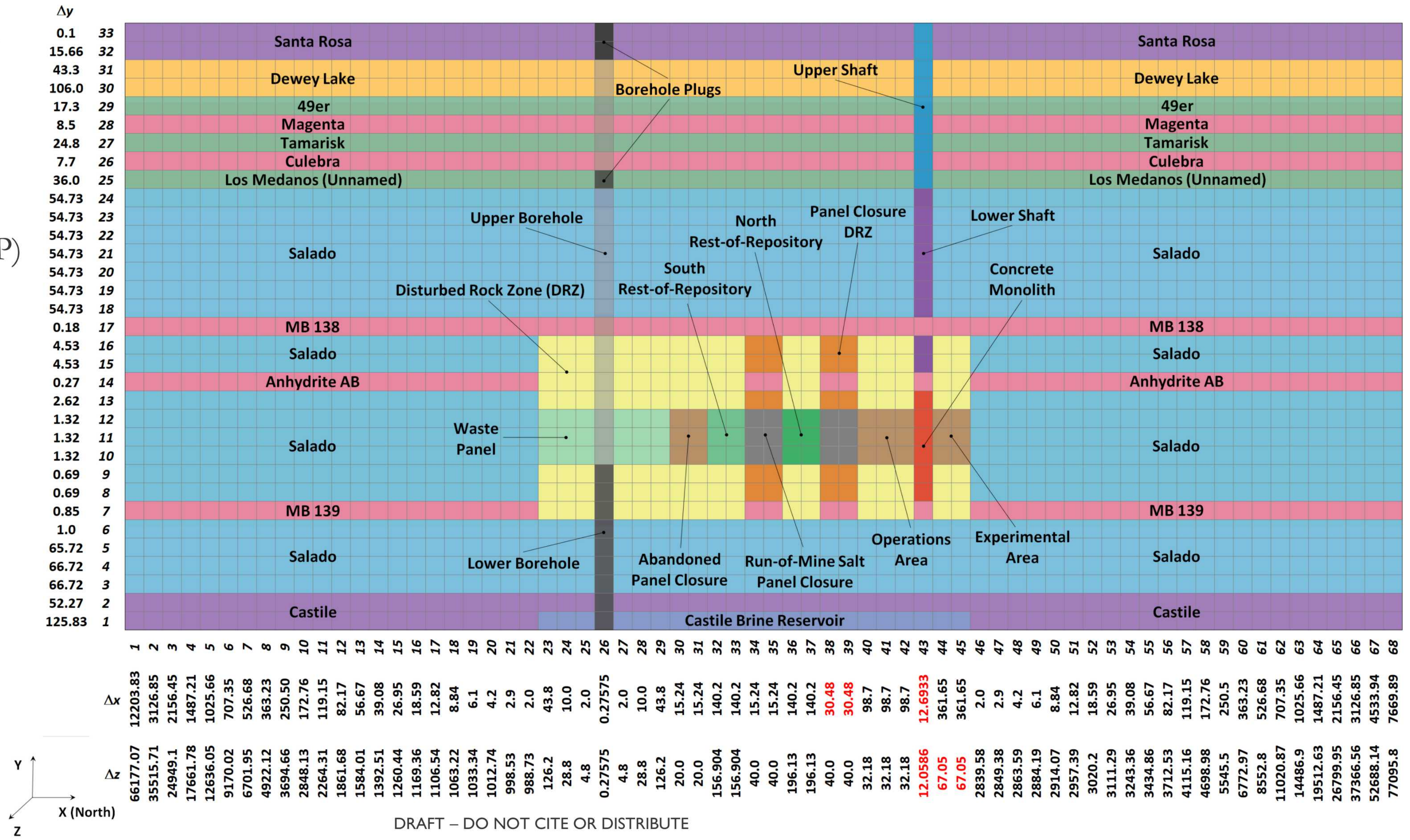
Fractional Colloidal Contributions to Mobilization Potential, Pu

CRA19 BRAGFLO Grid

Similar to CRA14 grid

Changes for CRA19:

- Abandoned southernmost PCS (above and below are treated like OPS/EXP)
- Corrected length of northernmost PCS
- Updated shaft dimensions
- Updated EXP dimensions (due to drifts associated with new shaft)



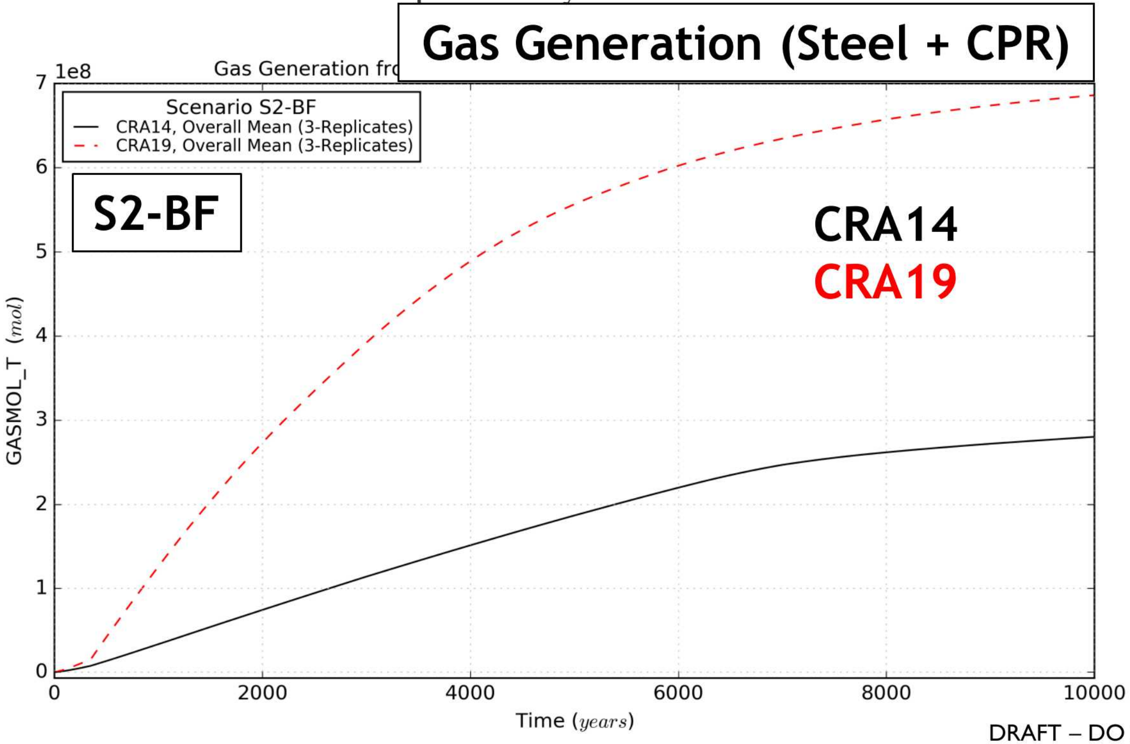
CRA-2019 PA – Salado Flow

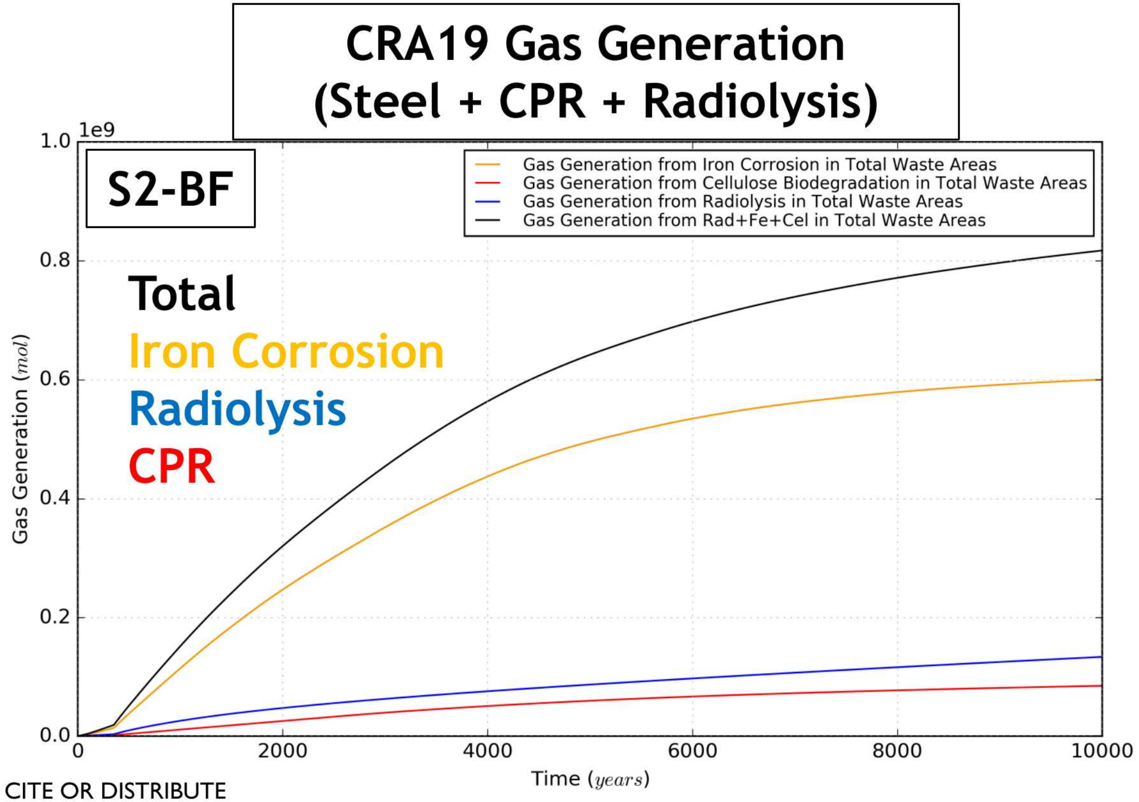
Increased waste area brine pressures and reduced saturations for intrusion scenarios that intersect a hypothetical brine reservoir (S2, S3, S6)

Increased total gas generation due to the availability of brine within the waste panel and south rest-of-repository

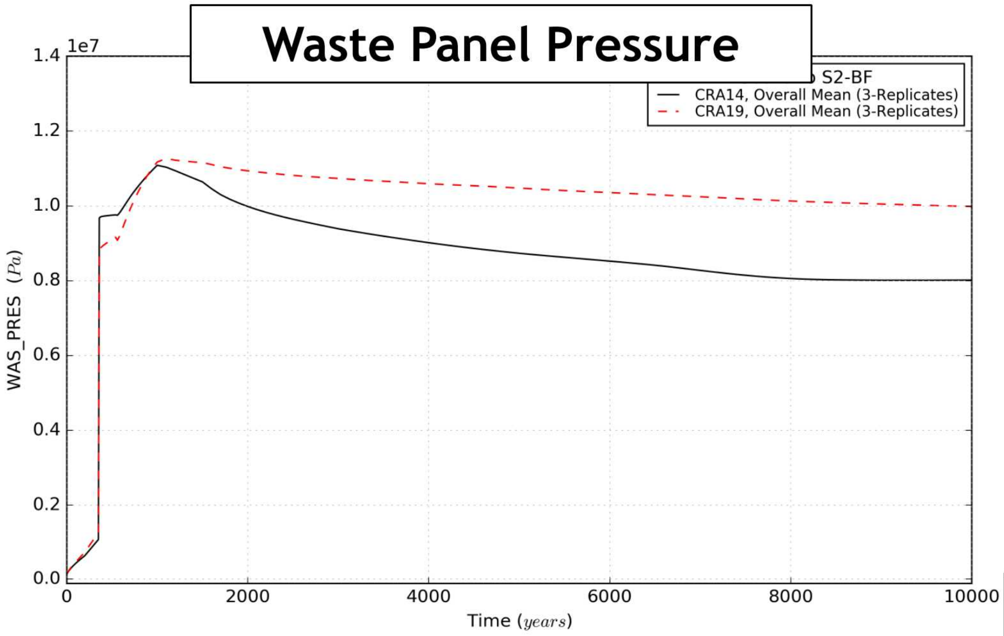
Introduction of radiolysis + increased steel corrosion

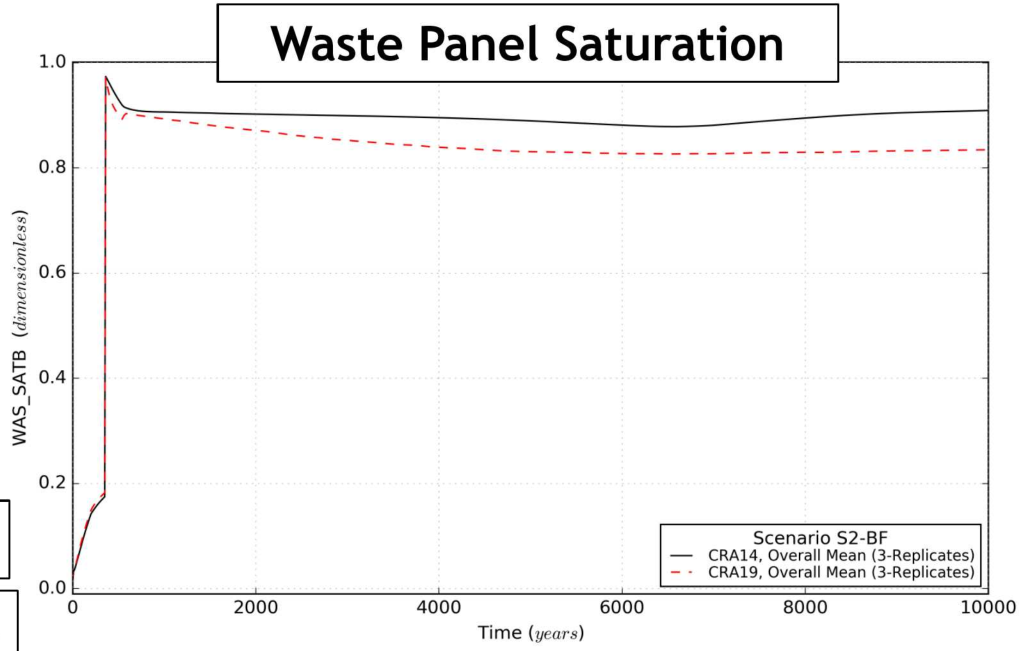
Mean radiolytic gas generation exceeds mean CPR gas generation





CRA-2019 PA – Salado Flow

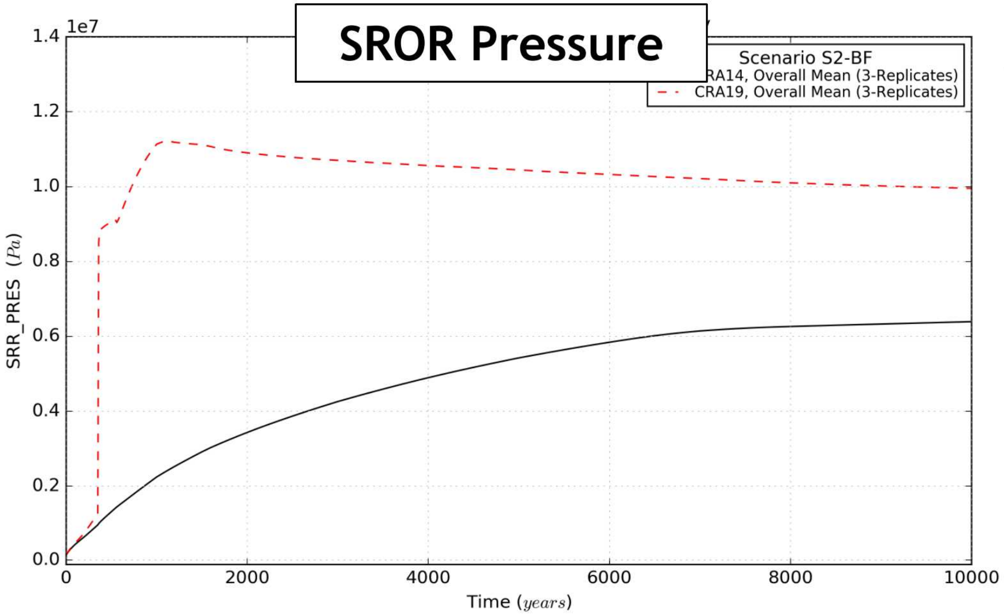


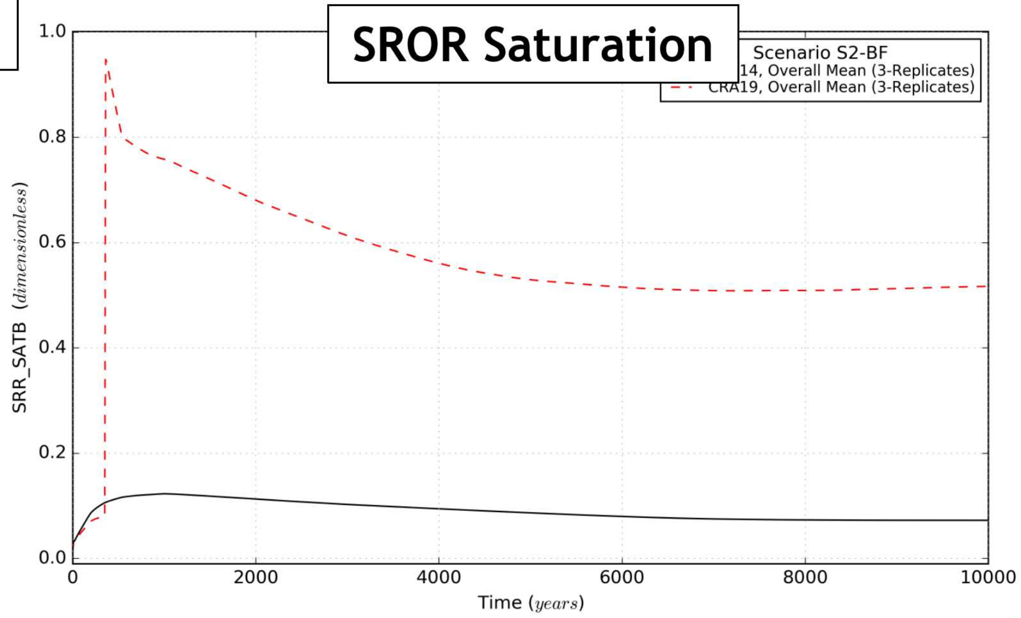


S2-BF

CRA14

CRA19

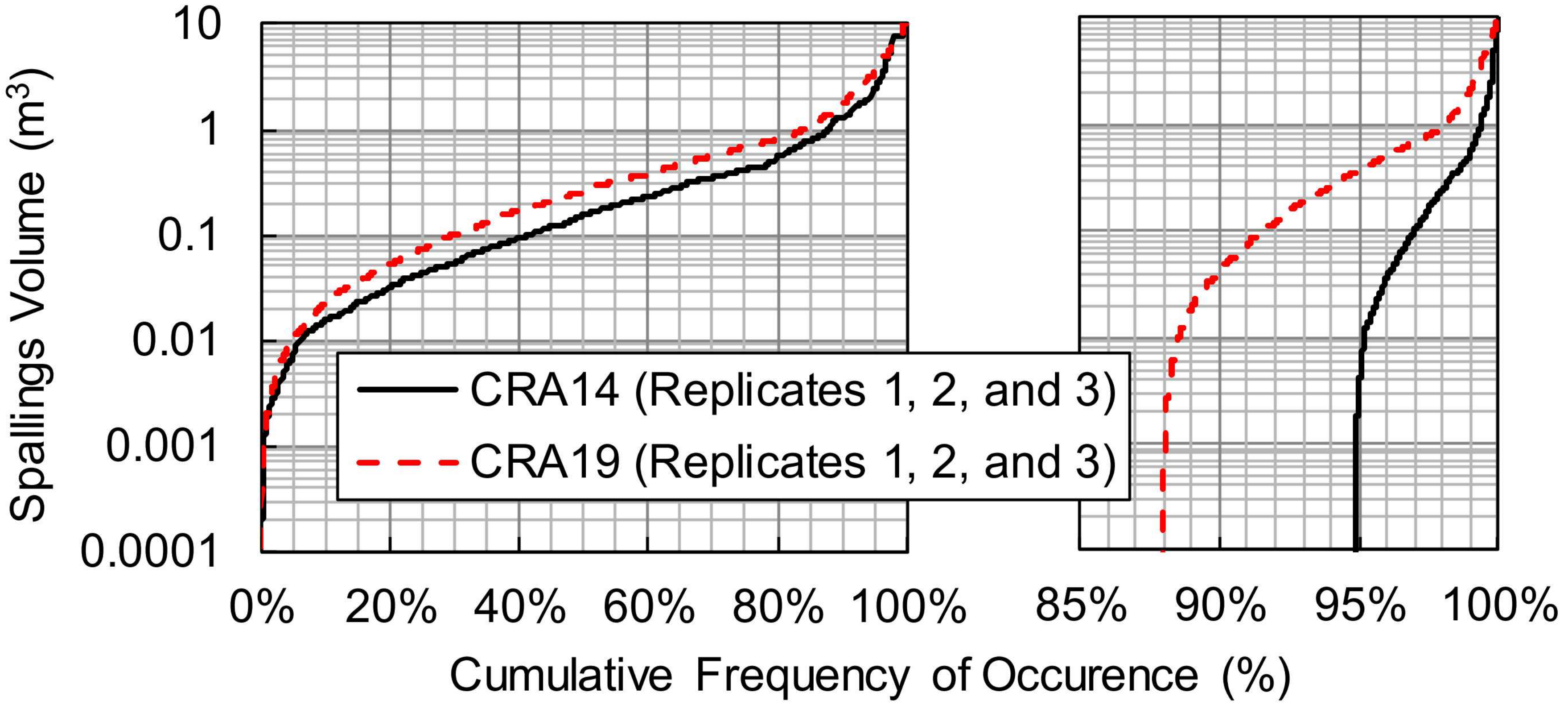




CRA-2019 PA – Spallings Volumes

Spallings volumes generally increased due to increased waste area pressures

Increased number of non-zero spallings volumes



a. Nonzero spallings results — includes only those simulations with spallings

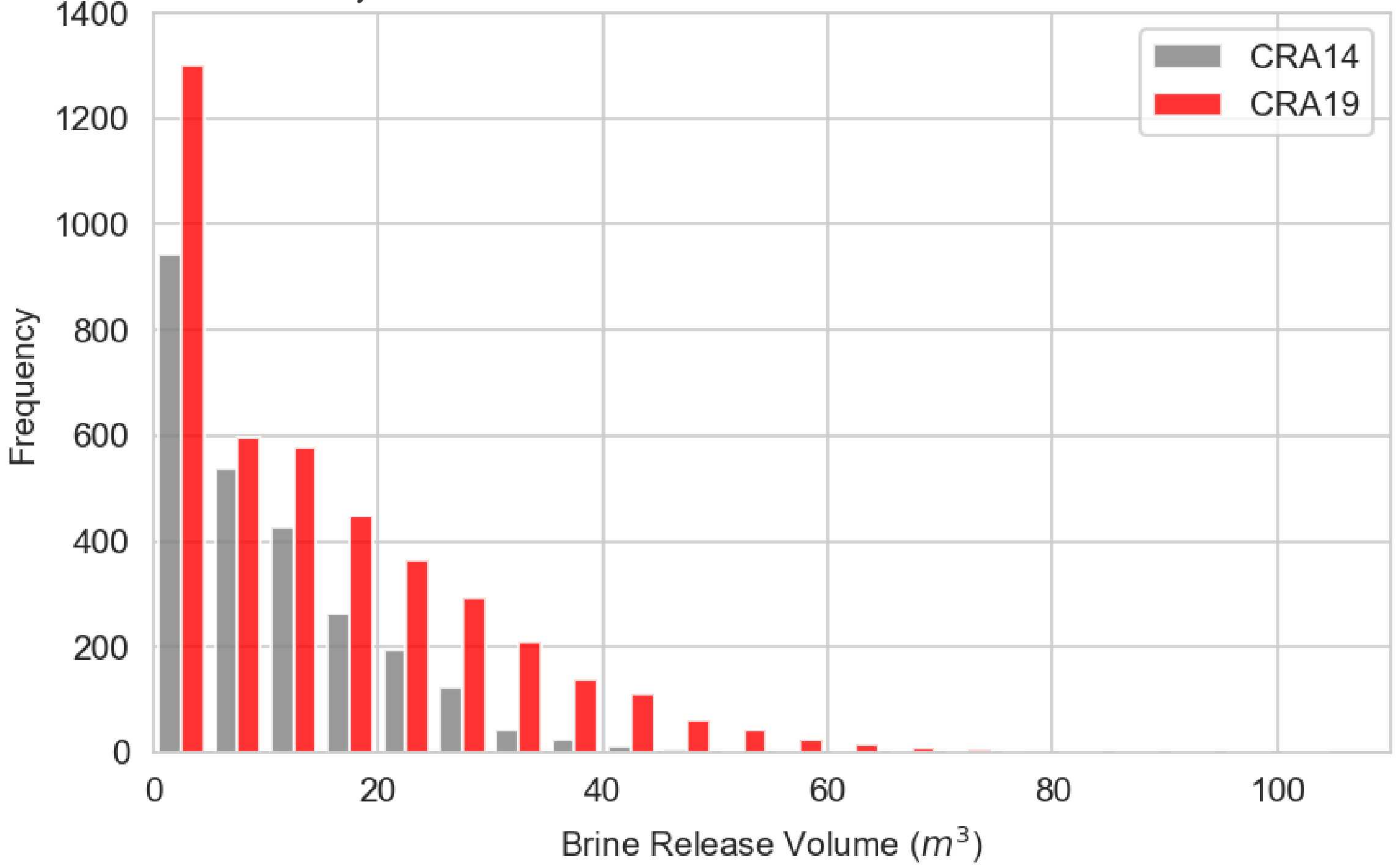
b. All spallings results — includes simulations with no spallings

CRA-2019 PA – DBR Volumes

DBR volume releases are generally increased

Increased number of non-zero DBR volumes

Middle release volumes substantially increased



CRA-2019 PA – Salado Transport

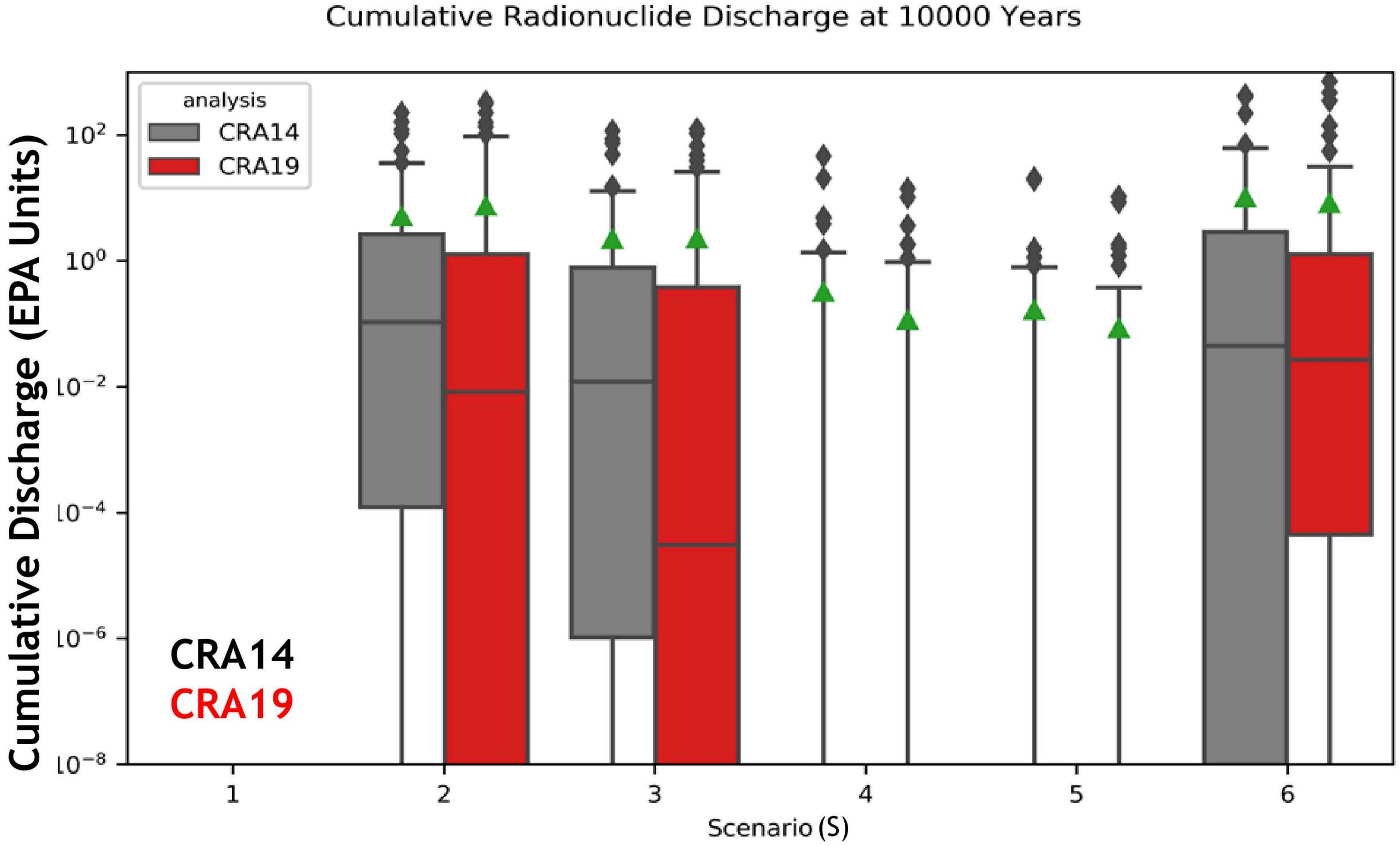
Undisturbed repository (S1) continues to show negligible long term releases up the shaft and through marker beds

Releases up borehole are generally decreased

Median release has decreased while the high-consequence outliers have increased

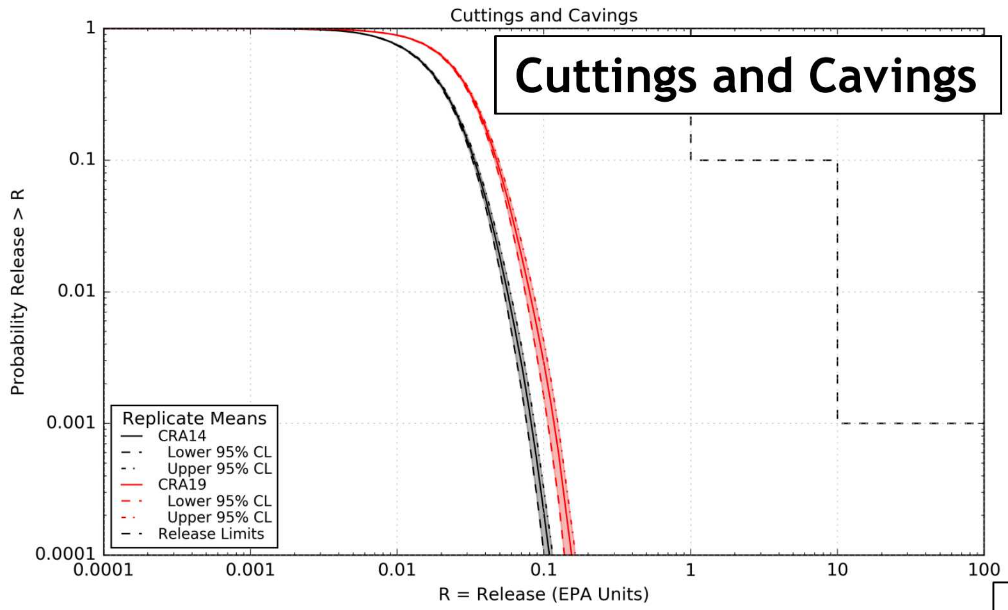
U234L cumulative discharges have increased due to the increase in its isotope-to-element mole fraction

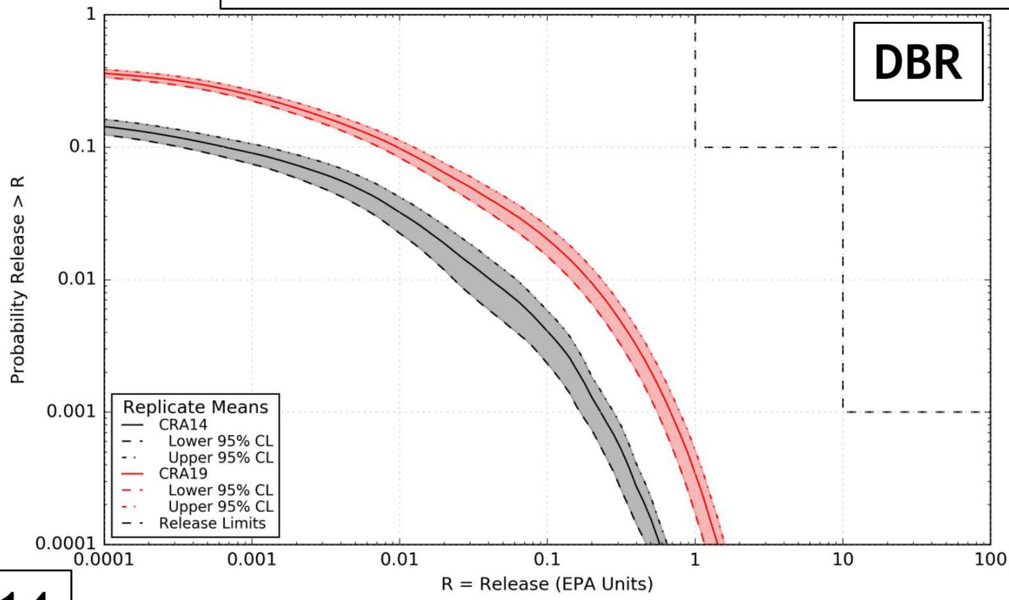
- U(VI) is assumed to have low adsorption (i.e., low linear matrix partition coefficient, K_D) in the Culebra



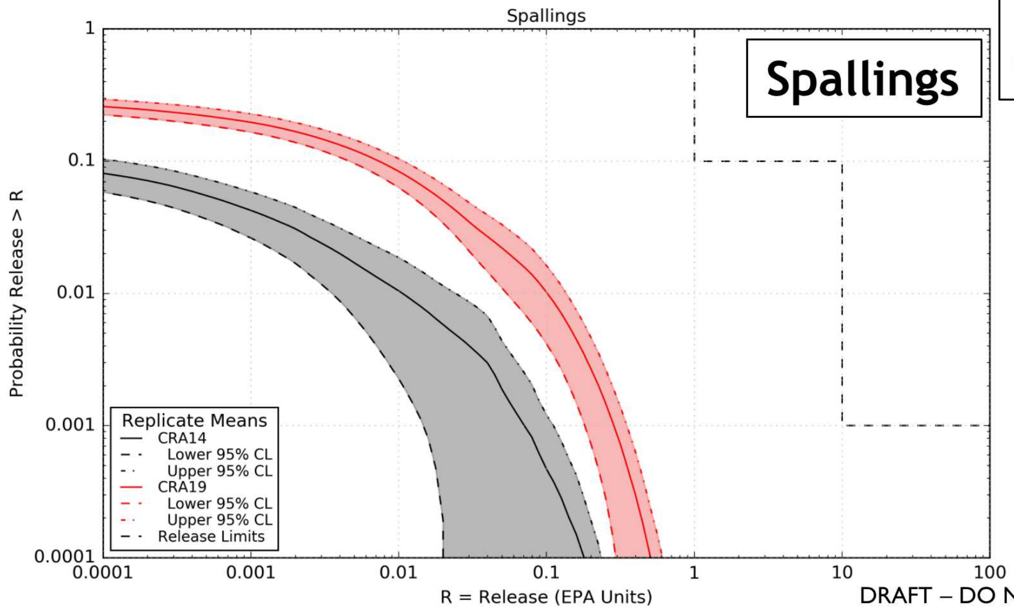
CRA-2019 PA (CRA19 Analysis) – CCDFs

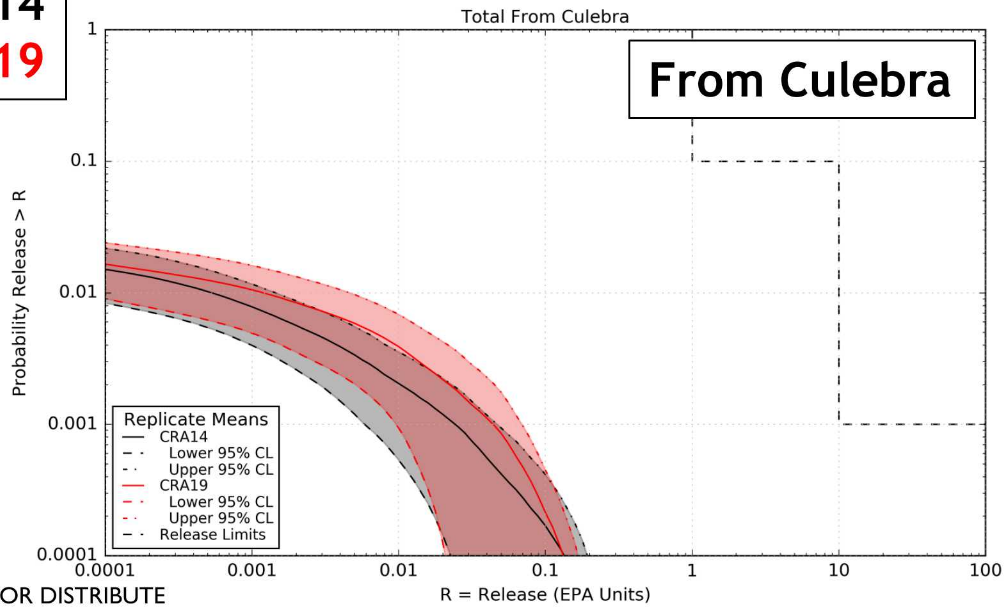
Means and 5%, 95% Confidence Limits





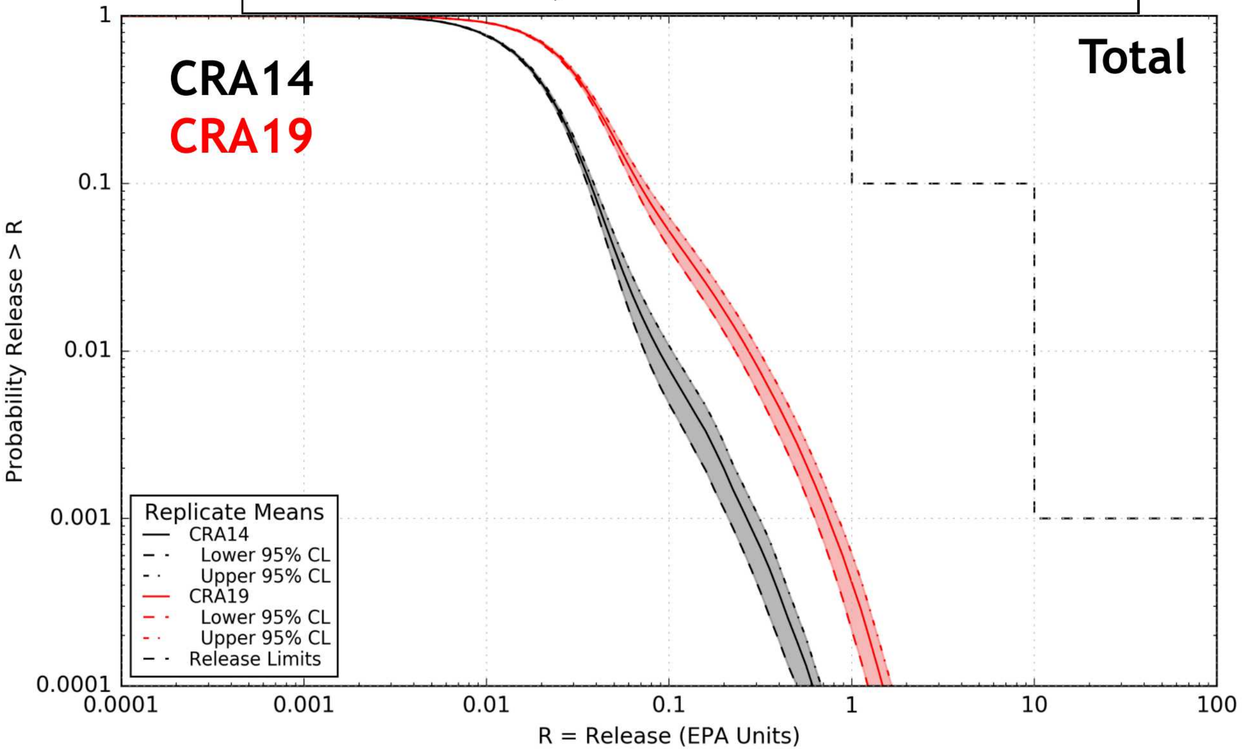
CRA14
CRA19



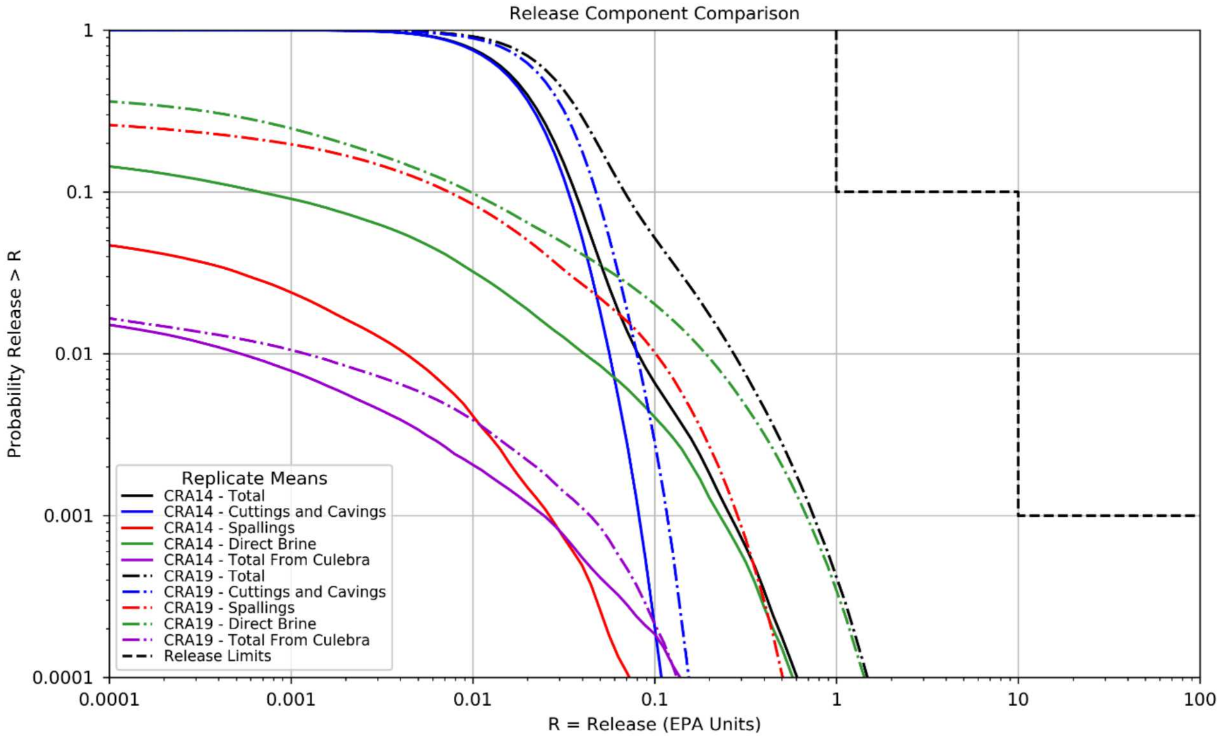


CRA-2019 PA (CRA19 Analysis) – CCDFs

Mean and 5%, 95% Confidence Limits



Release Component Mean Releases



Probability	Analysis	Mean Total Release	Lower 95% CL	Upper 95% CL	Release Limit
0.1	CRA14	0.0373	0.0355	0.0388	1
	CRA19	0.0685	0.0631	0.0745	
0.001	CRA14	0.2677	0.2124	0.3132	10
	CRA19	0.7505	0.6301	0.8501	

CRA14: Solid Lines
CRA19: Dashed Lines

Total
Cuttings & Cavings
Spallings
DBRs
From Culebra

CRA-2019 PA – Conclusions

Mean releases increased for all release mechanisms

Total mean releases increase at all probabilities

Cuttings and cavings releases continue to dominate at high probabilities

DBRs continue to dominate at low probabilities

Relatively impactful changes since CRA-2014:

- Waste panel and SROR pressures and saturations
  - Removal of southernmost panel closure
  - Iron corrosion rates
  - Radiolysis
- Panel concentrations
- Probability of intersecting brine
- Drilling rate
- Plugging patterns

CRA-2019 PA – Parameter Sensitivity

SOLMOD3:SOLVAR parameter (solubility multiplier for III oxidation states) is now the most dominant parameter contributing to variability in total releases in all three replicates

- Increased importance due in part to the shifting of the distribution mean to a higher value (thus making it more impactive on DBRs), as well as in part to the increased contribution of DBRs to total releases

Other dominant parameters with respect to total releases:

- BOREHOLE:TAUFAIL (waste shear strength)
- BH_SAND:PRMX_LOG (the logarithm of the permeability of the silty-sand-filled borehole)
- CASTILER:PRESSURE (Castile pressure)

STEEL:CORRMCO2 (inundated iron corrosion rate) has increased importance in the variability of DBRs, but the correlation with DBRs is negative

- Increased gas generation rates lead to decreased DBRs due to impact of repository pressure to reduce waste area saturations

Of the other sampled parameters that were changed or were new since the CRA14, none had any substantial impact on releases

- SOLMOD4:SOLVAR (solubility multiplier for IV oxidation states)
- GLOBAL:GDEPFAC (energy deposition probability for wetted solid radionuclides, which has a role in brine radiolysis)
- STEEL:HUMCORR (humid iron corrosion rate)
- WAS_AREA:HYMAGCON (hydromagnesite conversion rate)

CRA19_CL Analysis

Supplementary analysis documented in PA Summary Report (Zeitler et al. 2019)

3 replicates, 300 vectors

CRA19 used as baseline

Examine the impact from reducing the time to closure for areas in the repository modeled as "open" in the CRA19 analysis
- OPS/EXP/PCS_NO (abandoned PCS)

Intact halite properties assigned to those areas from 0-10,000 yrs

CRA19_CL results:
- Waste panel and SROR pressures and saturations decrease due to less brine inflow from Castile and less gas generation
- Spallings, DBRs, Culebra, and total releases **decrease**

CRA19 results show higher releases than the hypothetical case of immediate closure of open areas to halite properties