570325

Sandia National Laboratories

Operated for the United States Department of Energy
by National Technology and Engineering Solutions
of Sandia, LLC.

Albuquerque, New Mexico 87185-0101
Livermore, California 94551-0969

date: September 6, 2018

to: WIPP Records Center

from: Brad Day *BD*

subject: Impact Analysis for BRAGFLO 6.03 Software Problem Report, SPR 18-002

Three software errors associated with BRAGFLO 6.03 were identified for correction. All three errors were related to the calculation of capillary pressure as detailed on SPR 18-002. Due to the fundamental impact of capillary pressure on 2-phase flow modeled with BRAGFLO and the fact that these software errors have been in place since the earliest revisions of BRAGFLO and potentially affect all the previous Performance Assessment (PA) analyses performed for WIPP, an assessment of the impact of these errors was performed with a corrected version of the BRAGFLO code. This memorandum summarizes the very minor impact to WIPP repository pressures, saturations, and flows up the borehole due to the capillary pressure corrections implemented for the relative permeability models invoked by setting the BRAGFLO input parameter, KRP, equal to 1, 2, 5, 6, 7, or 8. It is concluded that resolution of the software errors have a negligible impact on PA calculations and that the error is appropriately identified as “Minor” such that all previous PA calculations are appropriately used “As-Is.”

The analysis utilized as a baseline to perform the impact assessment with the corrected version of BRAGFLO was the most recent sensitivity study performed in support of CRA-2014, namely CRA14_SEN4 [Zeitler and Day, 2016]. The comparative analysis performed with the corrected version of BRAGFLO was named SER18002 and was modeled/parameterized identical to CRA14_SEN4 with one minor exception. One of the corrections to BRAGFLO was to the capillary pressure function for KRP=5, a linear model that was documented and intended to allow the capillary pressure to vary linearly over the range of saturations. The error in BRAGFLO 6.03 (and previous versions) caused the capillary pressure to be zero. The KRP=5 model was employed in the Salado Flow model as the capillary pressure function for the BH_OPEN material to represent the open borehole. With the software error, it was serendipitously physically appropriate to utilize KRP=5 because an open borehole would not likely exhibit 2-phase flow with capillary pressure. So, with the correction to the KRP=5 model, activation of a linearly-varying capillary pressure is inconsistent with the anticipated physical conditions within the open borehole. As such, the SER18002 model was modified from CRA14_SEN4 to employ KRP=11, which is specifically designed to model flow within an open area and have zero capillary pressure (BRAGFLO User’s Manual, Camphouse 2012).

An assessment of the impacts of the capillary pressure code corrections on the overall WIPP repository flow simulation was performed by evaluating the 300-vector by 6-scenario (1800 run) results to compare the southernmost waste panel brine pressures and saturations between CRA14_SEN4 and SER18002. In addition, flow up the borehole for Castile reservoir intrusion cases (scenarios 2, 3, and 6) were compared. Finally, total repository releases are compared to confirm the minor impact of the changes.

Details of the code errors, code revisions to correct, and justification are also provided below.

Waste Area Brine Pressures:

Average waste panel brine pressures for 300 realizations in each of the six BRAGFLO scenarios are provided in Figure 1 through Figure 6. As shown, the average brine pressures in the waste area most important to releases are imperceptibly different as a result of the code corrections.

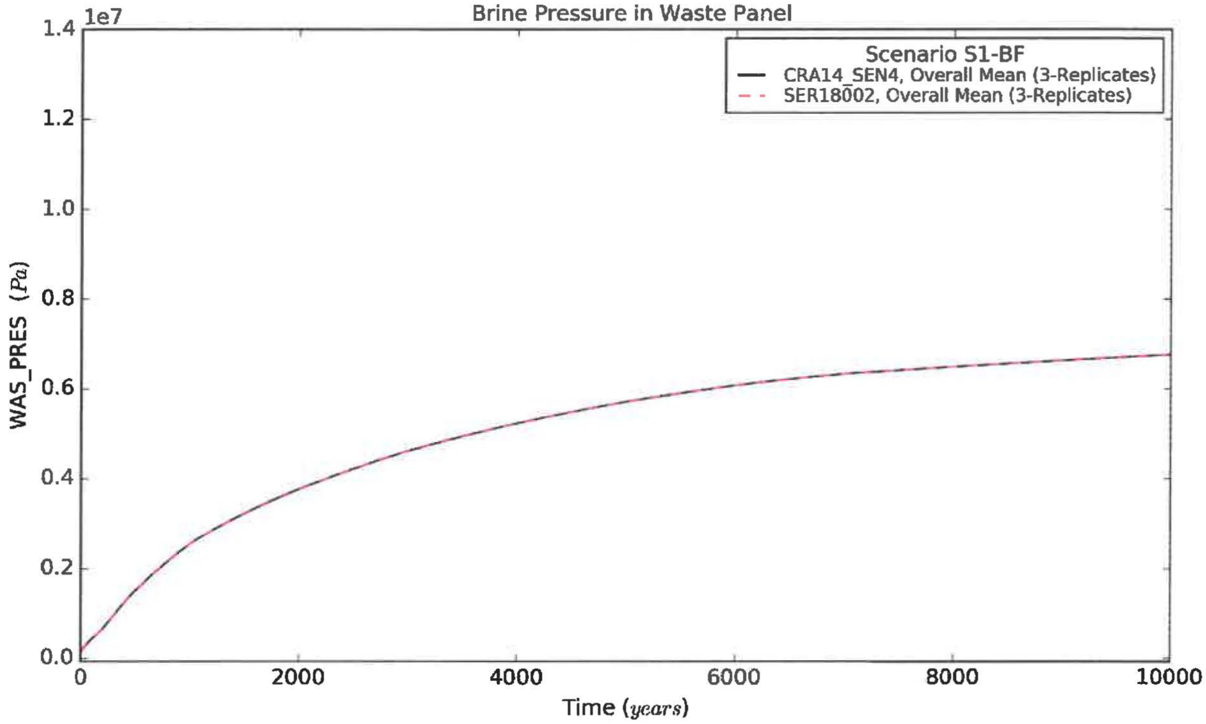


Figure 1 – Scenario 1 Brine Pressure

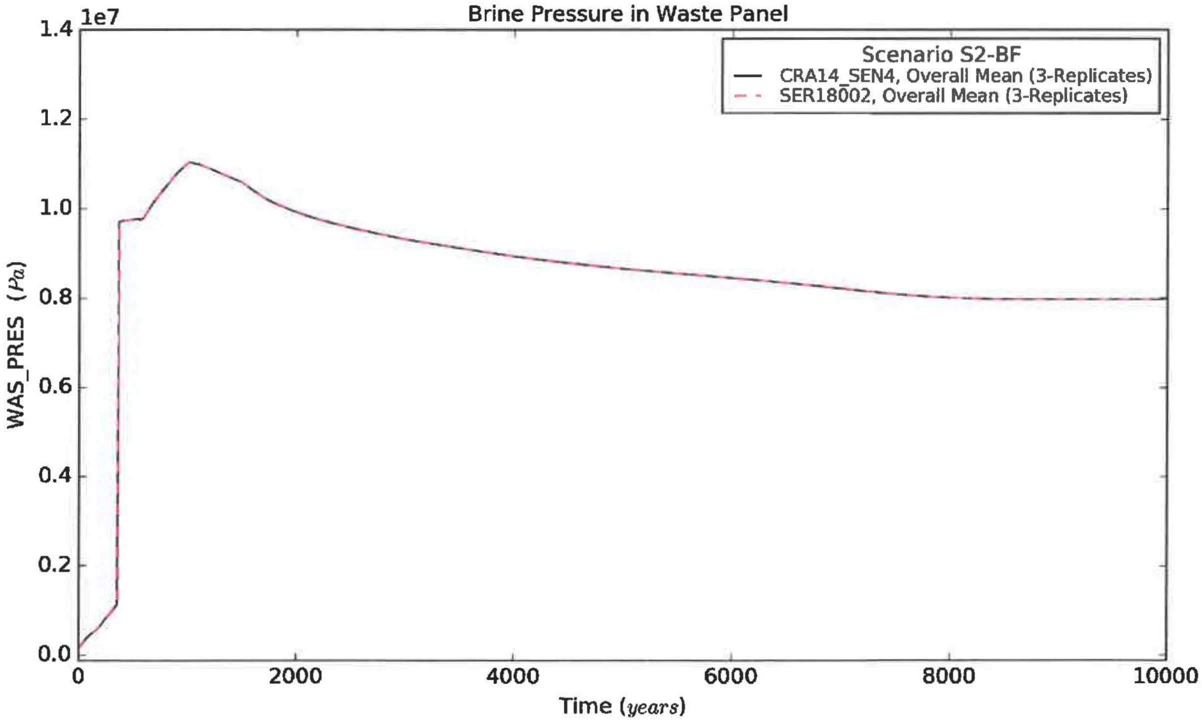


Figure 2 – Scenario 2 Brine Pressure

Information Only

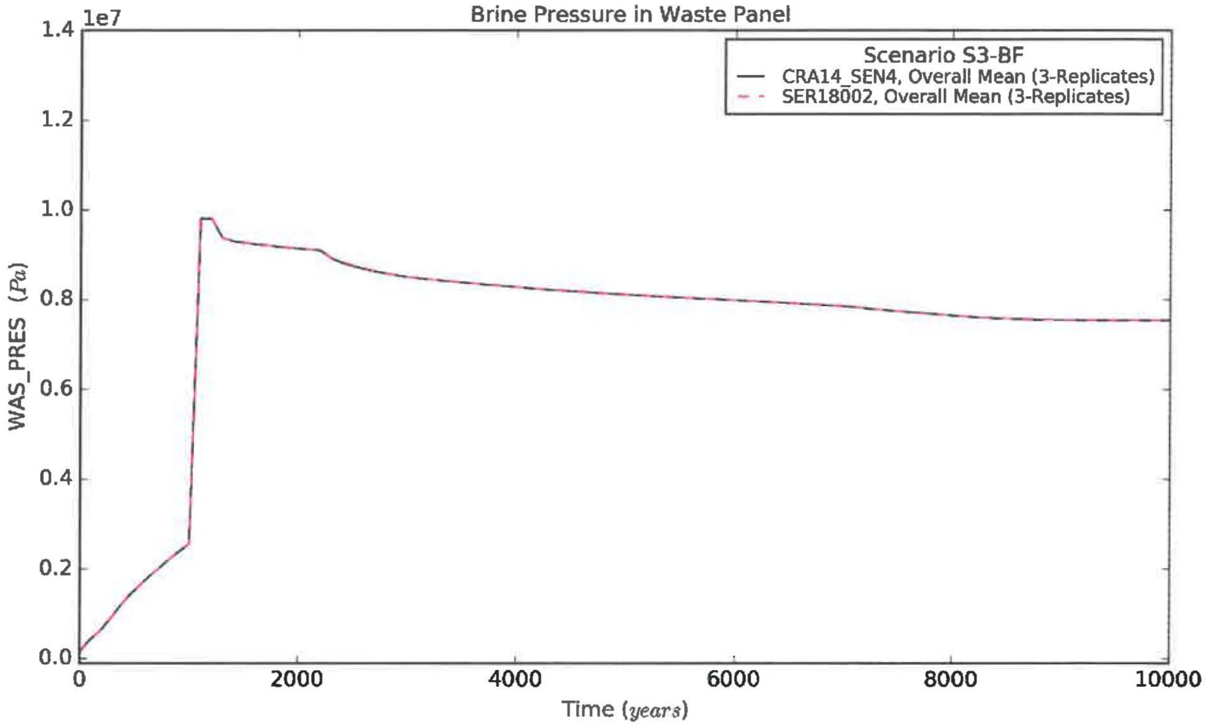


Figure 3 – Scenario 3 Brine Pressure

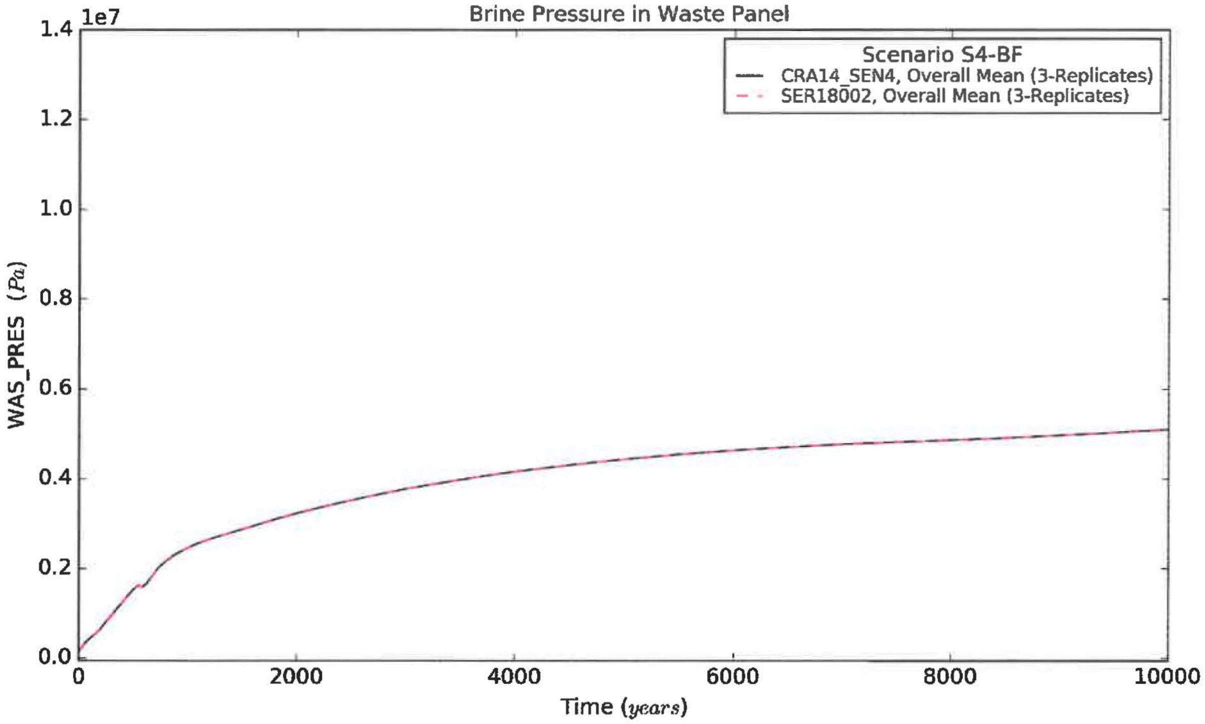


Figure 4 – Scenario 4 Brine Pressure

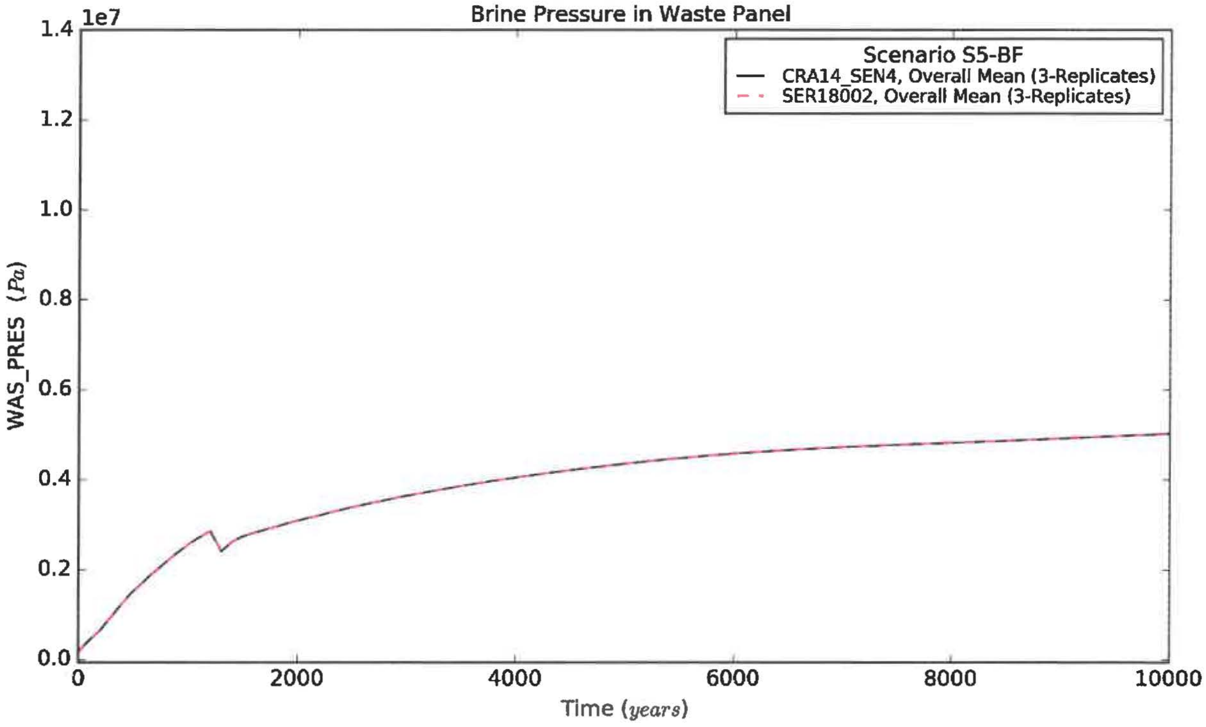


Figure 5 – Scenario 5 Brine Pressure

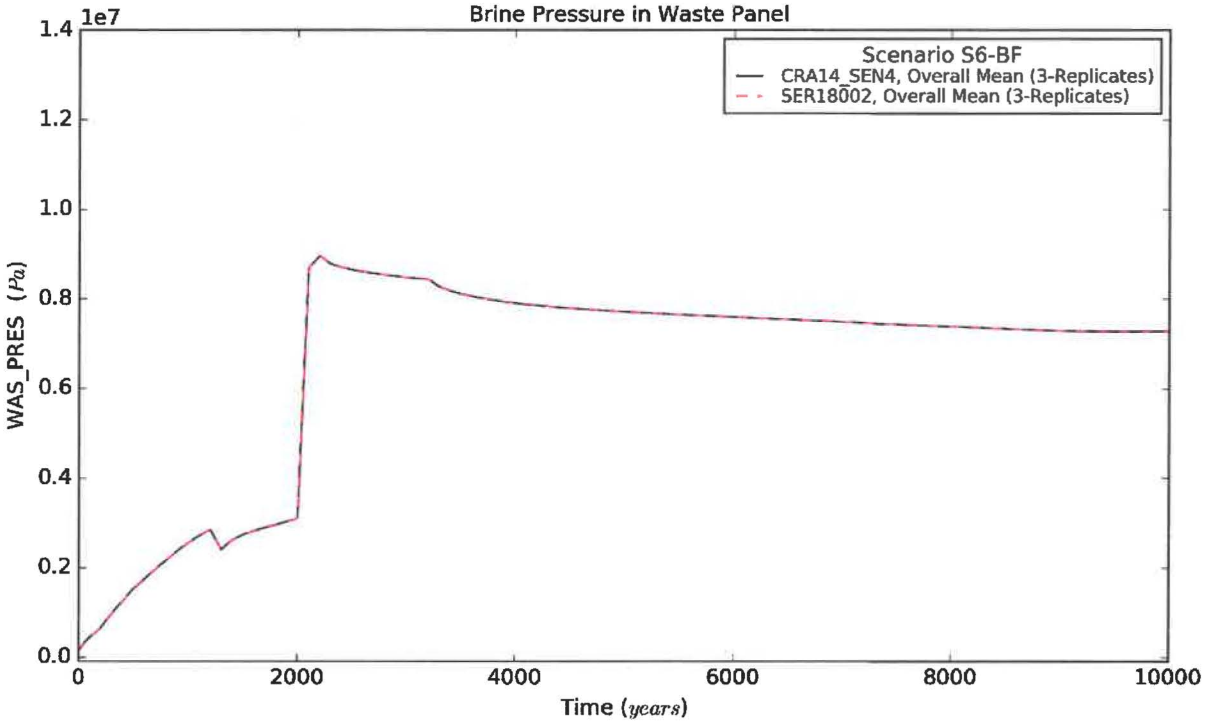


Figure 6 – Scenario 6 Brine Pressure

Waste Area Brine Saturations:

Average waste panel brine saturations for 300 realizations in each of the six BRAGFLO scenarios are provided in Figure 7 through Figure 12. As shown, the average brine saturations in the waste area most important to releases are imperceptibly different as a result of the code corrections.

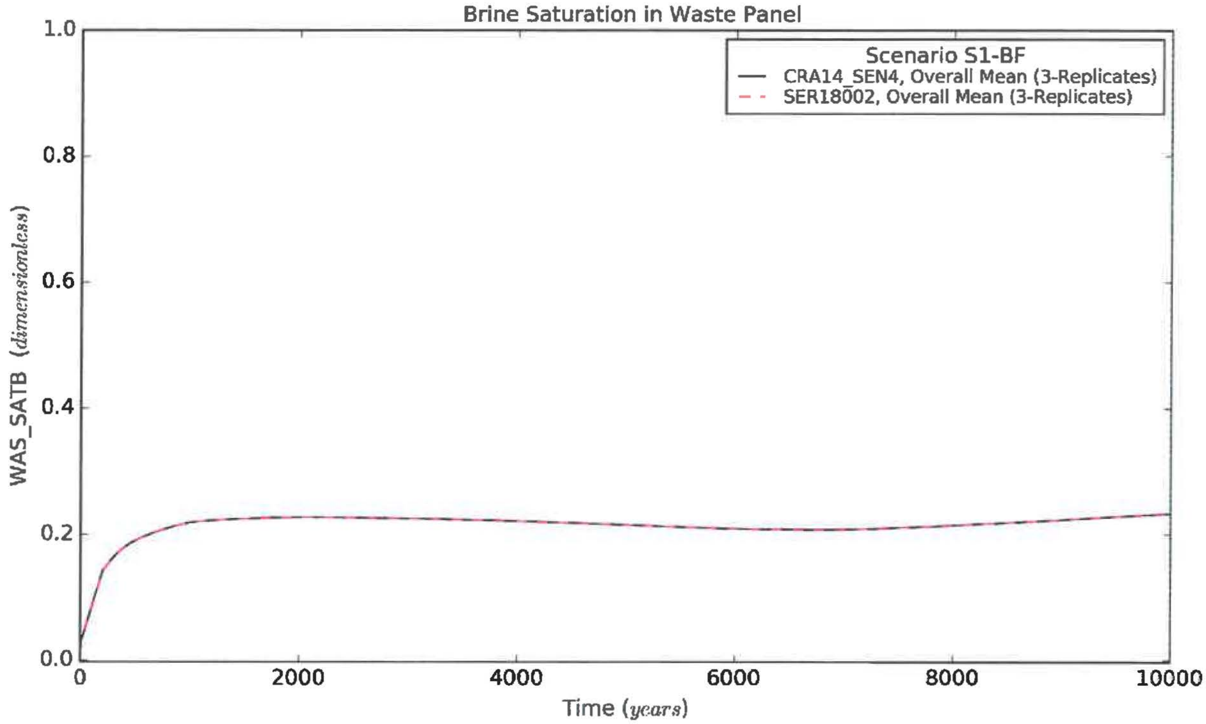


Figure 7 – Scenario 1 Brine Saturation

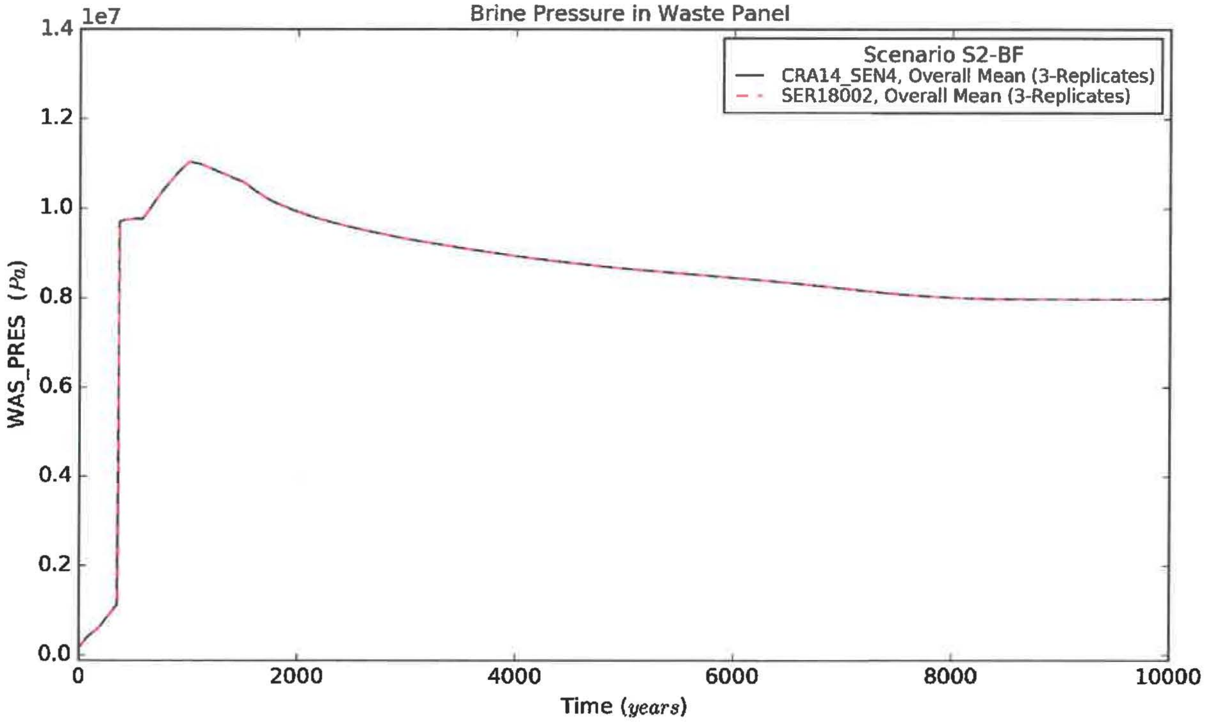


Figure 8 – Scenario 2 Brine Saturation

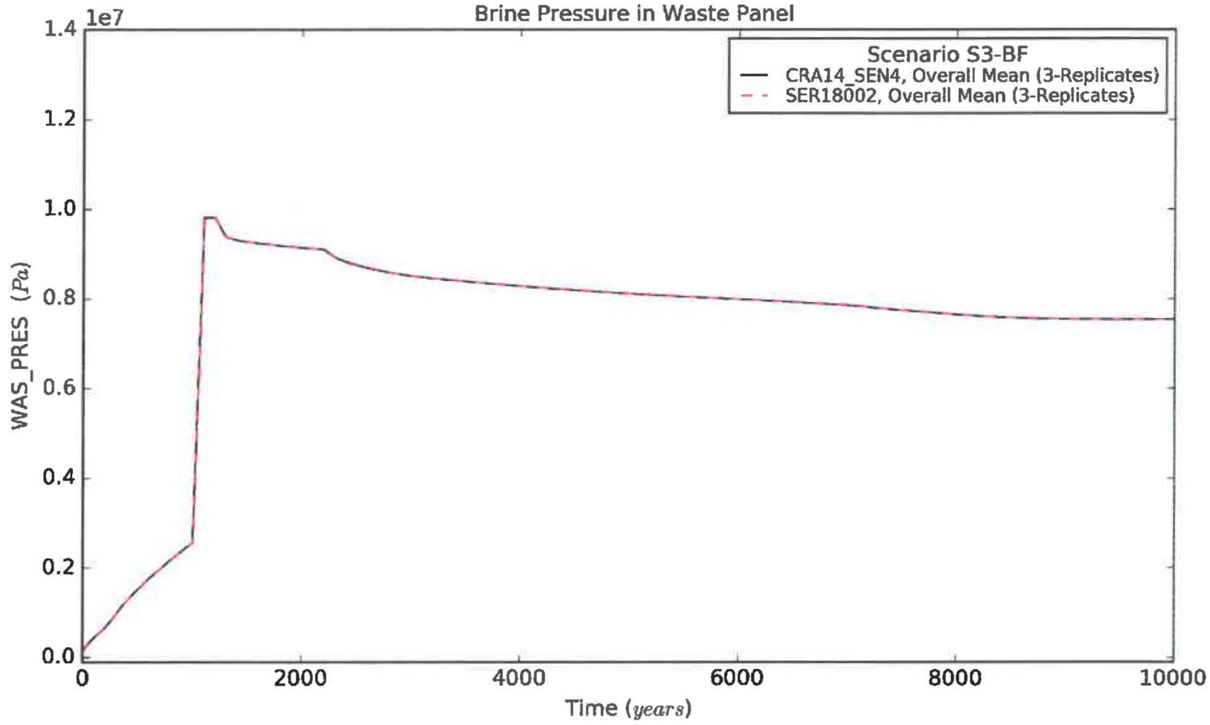


Figure 9 – Scenario 3 Brine Saturation

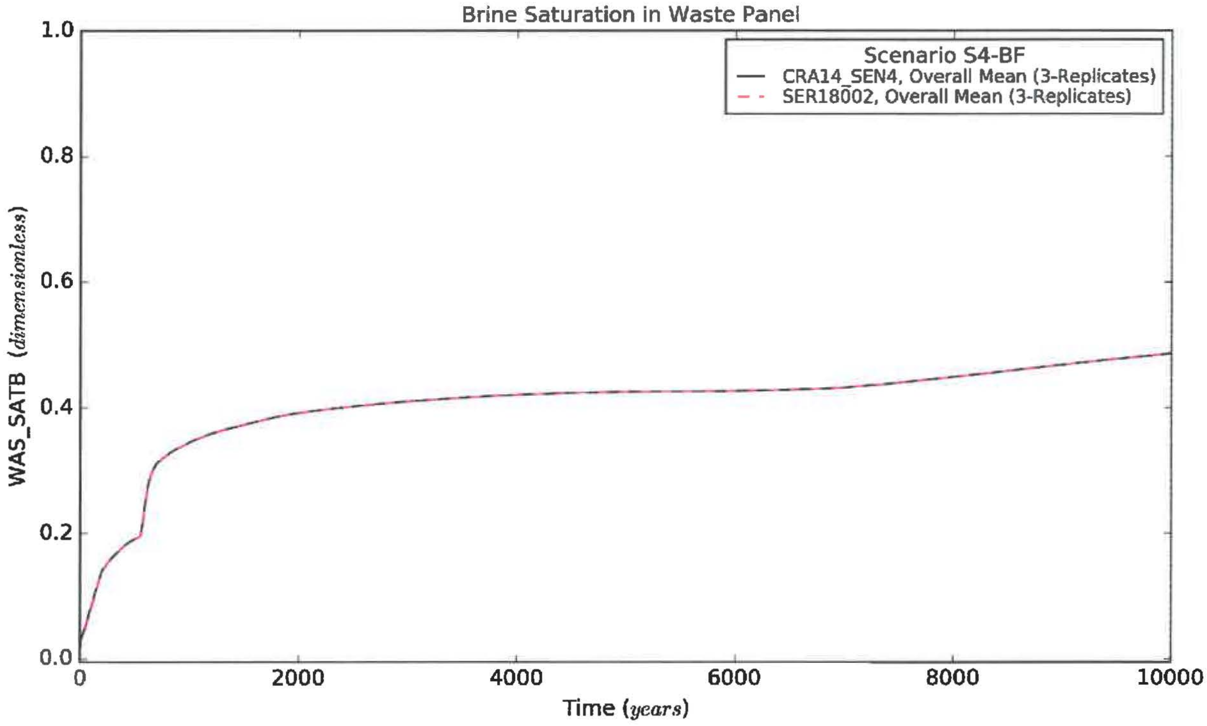


Figure 10 – Scenario 4 Brine Saturation

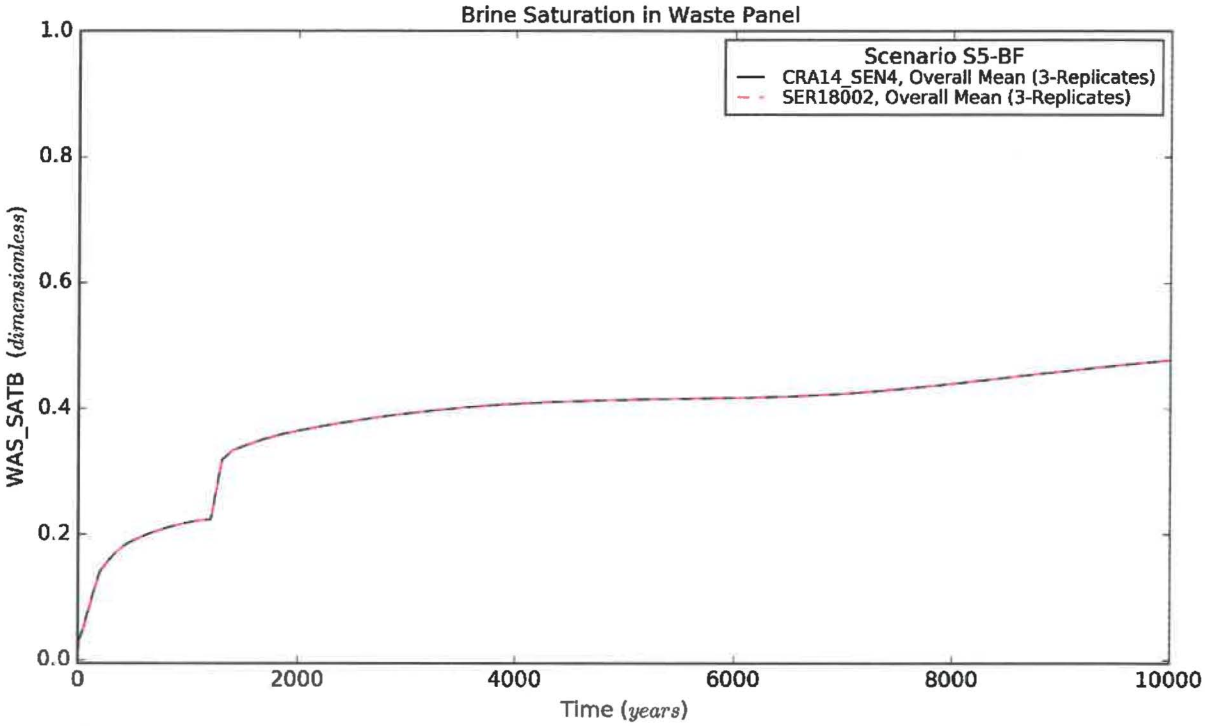


Figure 11 – Scenario 5 Brine Saturation

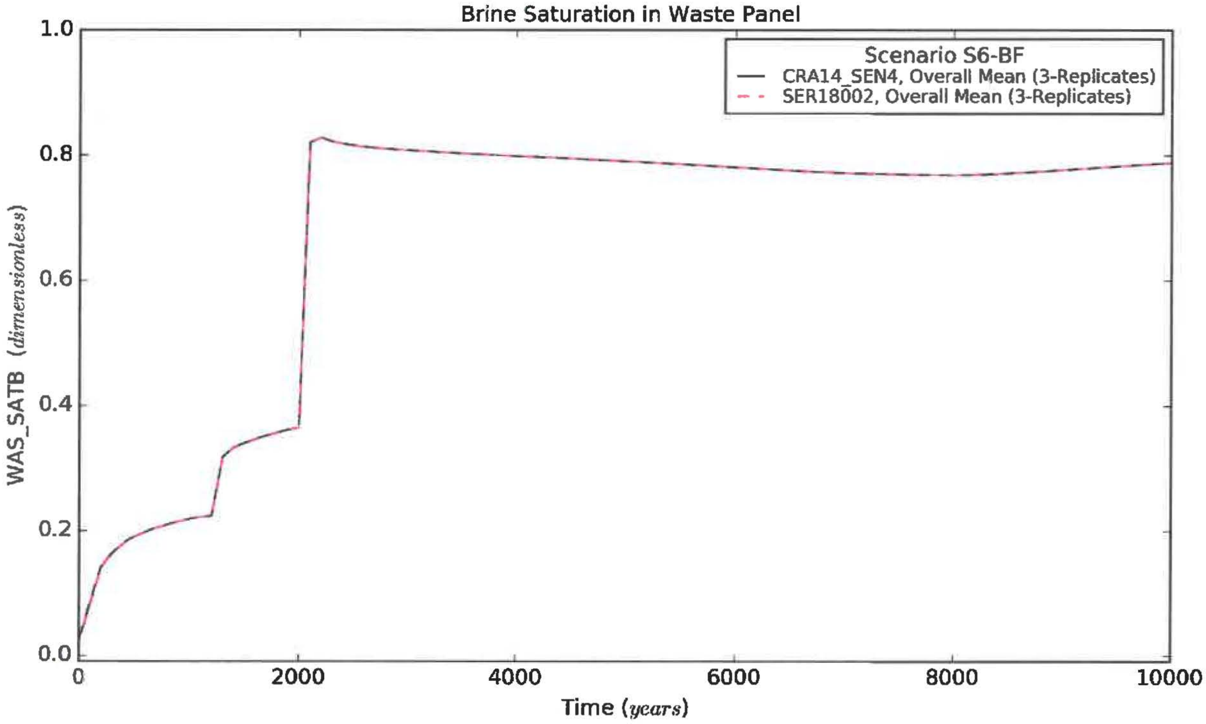


Figure 12 – Scenario 6 Brine Saturation

Brine Flow up the Borehole for Castile Intrusions:

Average brine flow up the borehole for 300 realizations in the Castile-intruded BRAGFLO scenarios are provided in Figure 13 through Figure 15. By observation, the brine flows are imperceptibly different as a result of the code corrections.

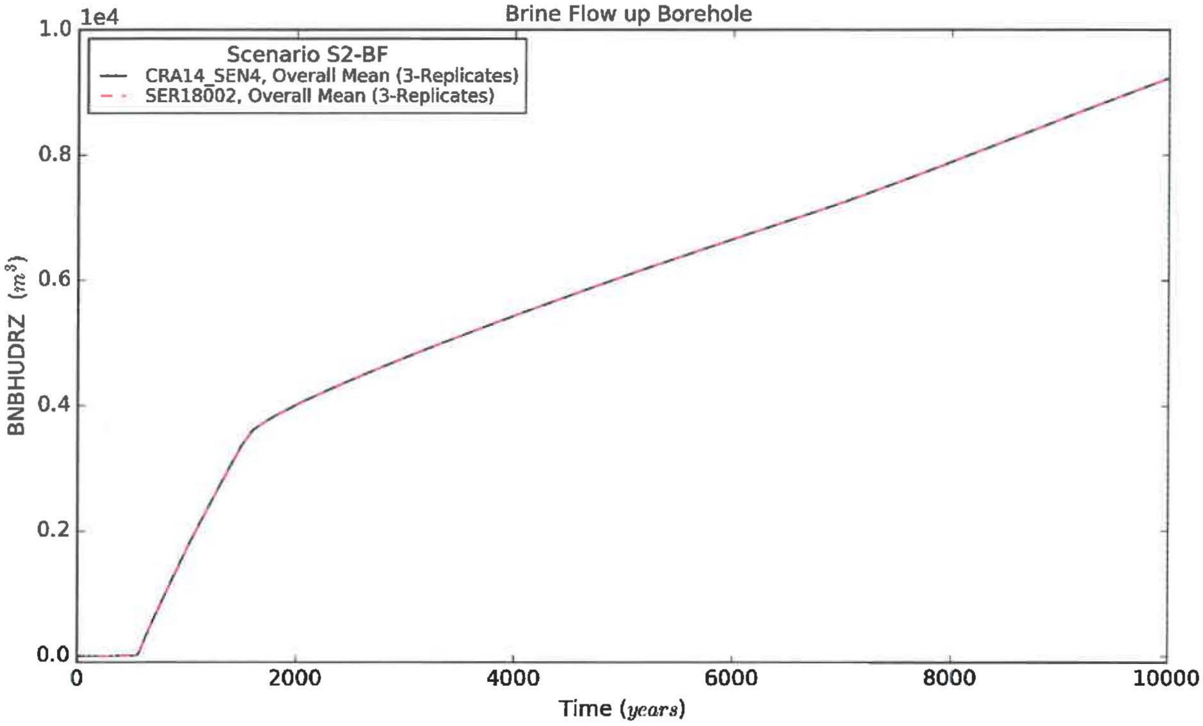


Figure 13 – Scenario 2 Brine Flow up the Borehole

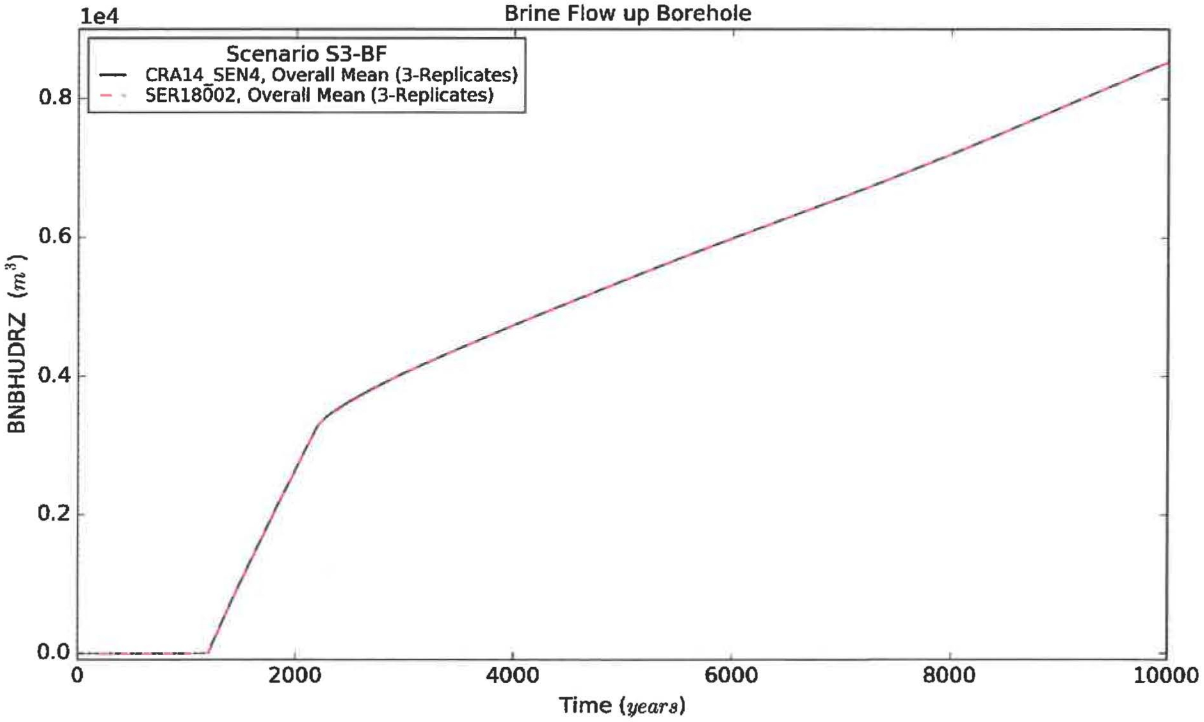


Figure 14 – Scenario 3 Brine Flow up the Borehole

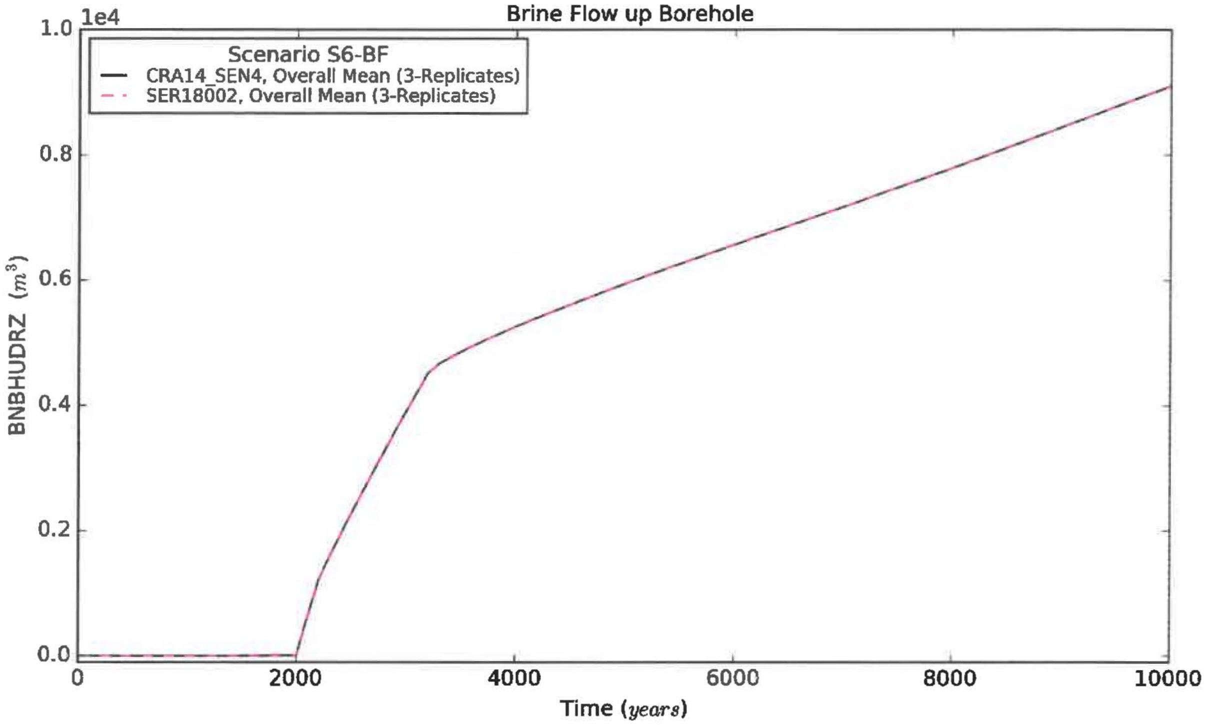
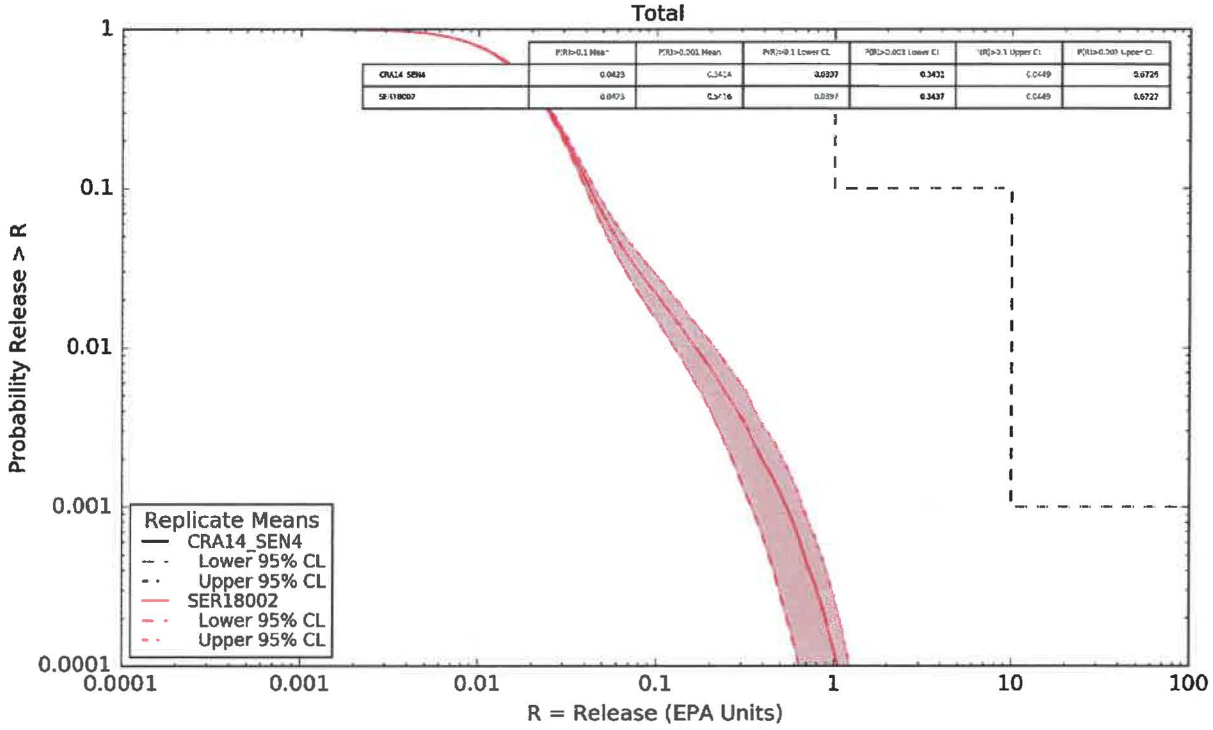


Figure 15 – Scenario 6 Brine Flow up the Borehole

Total Releases:

Total mean releases are compared for CRA14_SEN4 and SER18002 as shown in Figure 16 for 300 realizations (3 replicates). As shown, the high-probability mean releases are unchanged to 3 significant digits and the low-probability releases are minimally increased by less than 0.05%. These results are expected due to the minimal changes to repository waste area pressures, saturations, and brine flows up the borehole.



	P(R)>0.1 Mean	P(R)>0.001 Mean	P(R)>0.1 Lower CL	P(R)>0.001 Lower CL	P(R)>0.1 Upper CL	P(R)>0.001 Upper CL
CRA14_SEN4	0.0423	0.5414	0.0397	0.3432	0.0449	0.6726
SER18002	0.0423	0.5416	0.0397	0.3437	0.0449	0.6727

Figure 16 – Total Releases

SER18002 Analysis Details:

All analysis input and output files are located on Solaris cluster (santana.sandia.gov) in the folder /nfs/data/CVSLIB/WIPP_SPECIAL_ANALYSES/SER18002

SPR 18-002 Issue Summary and Assessment:

Issue #1

Calculation of the reference pressure (P_o) for the modified van Genuchten-Parker (KRP=1) capillary pressure model uses an incorrect equation. The reference pressure should be based on equating capillary pressure to 2nd modified Brooks-Corey (KRP=4) model with effective saturation equal to 0.5 (as documented in Appendix PA of CRA-2014, and illustrated below).

The current implementation is to invoke the same equation for both KRP=1 and KRP=8 which for KRP=8 is derived below.

$$P_c = P_o\left(S_{e_1}^{-1/m} - 1\right)^{1-m} \quad \text{Original van Genuchten-Parker (KRP=8)}$$

$$P_c = \frac{P_t}{S_{e_2}^{1/\lambda}} \quad \text{2}^{\text{nd}} \text{ Modified Brooks-Corey (KRP=4)}$$

where

$$m = \frac{\lambda}{1+\lambda}$$

$$S_{e_1} = \frac{S_w - S_{wr}}{1 - S_{wr}}$$

$$S_{e_2} = \frac{S_w - S_{wr}}{1 - S_{gr} - S_{wr}} = 0.5$$

Solving for S_w from given value for S_{e_2} gives

$$S_w = S_{wr} + 0.5\left(1 - S_{gr} - S_{wr}\right)$$

Substituting into S_{e_1} gives

$$S_{e_1} = \frac{S_{wr} + 0.5\left(1 - S_{gr} - S_{wr}\right) - S_{wr}}{1 - S_{wr}}$$

Equating P_c, solving for P_o, substituting S_{e_1} and S_{e_2}, and simplifying gives

$$P_o\left(S_{e_1}^{-1/m} - 1\right)^{1-m} = \frac{P_t}{S_{e_2}^{1/\lambda}}$$

$$P_o = \frac{P_t}{\left(S_{e_1}^{-1/m} - 1\right)^{1-m} S_{e_2}^{1/\lambda}}$$

$$= P_t S_{e_2}^{-1/\lambda}\left(S_{e_1}^{-1/m} - 1\right)^{m-1}$$

$$= P_t\, 0.5^{-1/\lambda}\left(\left[\frac{0.5(1 - S_{gr} - S_{wr})}{1 - S_{wr}}\right]^{-1/m} - 1\right)^{m-1}$$

$$= P_t\, 2^{1/\lambda}\left(\left[\frac{0.5(1 - S_{gr} - S_{wr})}{1 - S_{wr}}\right]^{-1/m} - 1\right)^{m-1}$$

The correct derivation for KRP=1 is provided as follows:

$$P_c = P_o\left(S_{e_2}^{-1/m} - 1\right)^{1-m} \quad \text{Modified van Genuchten-Parker (KRP=1)}$$

$$P_c = \frac{P_t}{S_{e_2}^{1/\lambda}} \quad 2^{\text{nd}} \text{ ModifiedBrooks-Corey (KRP=4)}$$

where

$$m = \frac{\lambda}{1+\lambda}$$

$$S_{e_2} = \frac{S_w - S_{wr}}{1 - S_{gr} - S_{wr}} = 0.5$$

Equating P_c, solving for P_o, substituting S_{e_2}, and simplifying gives

$$P_o\left(0.5^{-1/m} - 1\right)^{1-m} = \frac{P_t}{0.5^{1/\lambda}}$$

$$P_o = \frac{P_t}{\left(0.5^{-1/m} - 1\right)^{1-m} 0.5^{1/\lambda}}$$

$$= P_t 2^{1/\lambda}\left(0.5^{-1/m} - 1\right)^{m-1}$$

An example that illustrates the issue is to compare the currently implemented KRP=1 calculation of capillary pressure against the KRP=4 calculation. By definition, the capillary pressure for KRP=1 should be equal to KRP=4 when $S_{e2} = 0.5$ (or $S_w = 0.55$, when $S_{wr} = 0.3$ and $S_{gr} = 0.2$). As shown in Figure 17), the current implementation produces a capillary pressure for KRP=1 that does not intersect KRP=4 whereas the corrected implementation does intersect when $S_{e2} = 0.5$ (per App PA).

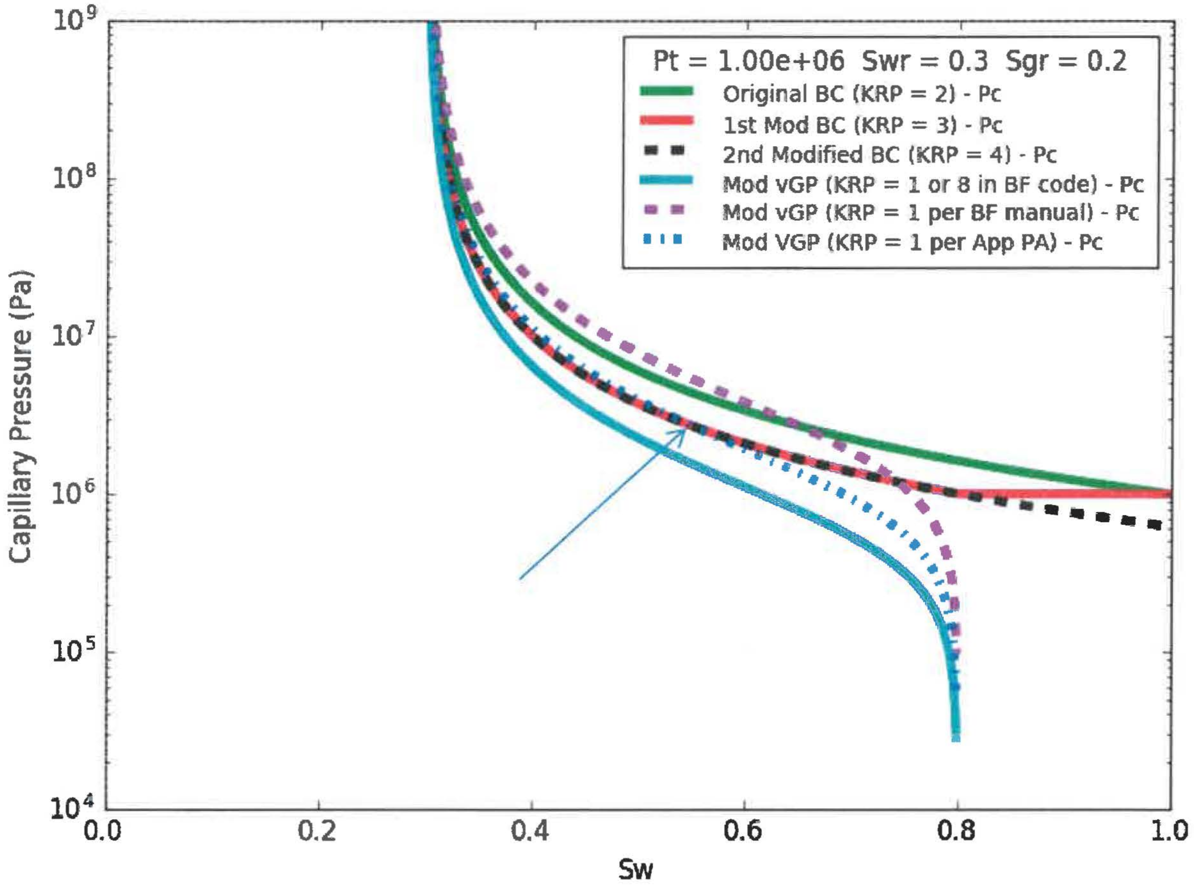


Figure 17 – Illustration of Capillary Pressure for KRP=1 Intersection with KRP=4

Correction of the error is accomplished by expanding the IF-THEN conditional in the PTHRESH subroutine to differentiate between KRP=1 and KRP=8 and using the above derived equation for the KRP=1 calculation as shown below.

```
PTHRESH
C
C BADAY 6/20/18 Revised conditionals to differentiate between
C               KRP1 and KRP8 to correct calculation of
C               threshold capillary pressure
C BADAY 6/20/18------- vG/P model pressure constant -- assumes Pc same
C BADAY 6/20/18-------   as Brooks-Corey Pc at Se=0.5
C
C BADAY 6/20/18      IF (KRP(MAT) .EQ. 1 .OR. KRP(MAT) .EQ.8) THEN
C BADAY 6/20/18         SEVGP = 0.5D0*(1.D0 - SGR(MAT) - SBR(MAT))*SETERM(MAT)
C BADAY 6/20/18         PTC    = PTC*2.D0**(1.D0/XLAMDA(MAT))*
C BADAY 6/20/18     1         (SEVGP**XLAM6(MAT) - 1.0D0)**(XLAM4(MAT)-1.0D0)
C BADAY 6/20/18      END IF
C
C------- vG/P model pressure constant -- assumes Pc equal to
C-------   2nd Modified Brooks-Corey at Se2=0.5
C
      IF (KRP(MAT) .EQ. 8) THEN
         SEVGP = 0.5D0*(1.D0-SGR(MAT)-SBR(MAT))*SETERM(MAT)
         PTC    = PTC*2.D0**(1.D0/XLAMDA(MAT))*
     1      (SEVGP**XLAM6(MAT)-1.0D0)**(XLAM4(MAT)-1.0D0)
      END IF
C
      IF (KRP(MAT) .EQ. 1 ) THEN
         SEVGP = 0.5D0
         PTC    = PTC*2.D0**(1.D0/XLAMDA(MAT))*
     1      (SEVGP**XLAM6(MAT)-1.0D0)**(XLAM4(MAT)-1.0D0)
```

Issue #2

Calculation of minimum effective saturation (S_{emin}) for the original van Genuchten-Parker (KRP=8) capillary pressure model uses an incorrect equation. The minimum effective saturation uses the Brooks-Corey (KRP=2,3,4) rather than the van Genuchten-Parker model (KRP=1,8) due to incorrect logic statement.

In the subroutine PTHRESH, the code logic statement evaluates for KRP > 1 OR < 5 such that KRP=8 satisfies the first logical and incorrectly gets evaluated along with the intended range of Brooks-Corey relations (KRP=2,3,4).

Correction of the error is accomplished by simply changing the conditional from "OR" to "AND" as shown below:

```
PTHRESH
C
C BADAY 6/20/18 Revised conditional from OR to AND such that
C               ELSE IF is executed when KRP=8
C BADAY 6/20/18            IF (KRP(MAT) .GT. 1 .OR. KRP(MAT) .LT. 5) THEN
C
            IF (KRP(MAT) .GT. 1 .AND. KRP(MAT) .LT. 5) THEN
```

Issue #3

Calculation of capillary pressure (P_c) for the linear models (KRP=5,6,7) use an incorrect equation. The capillary pressure should not be set to zero, but rather vary linearly between the maximum capillary pressure (P_{cmax}) and the threshold capillary pressure (P_t) for both capillary pressure conditions (KPC=1,2). Additionally, KRP=5 does not properly utilize a nonzero residual gas saturation in determination of the capillary pressure.

Correction of the error is accomplished by setting P_{cmax} for KRP=5,6,7 in the PTHRESH subroutine, adding KRP=5 to the list of models using a nonzero residual gas saturation to calculated capillary pressure in the RELPERM subroutine, and setting the capillary pressure for KRP=5,6,7 the same for KPC=1 and KPC=2 in the RELPERM subroutine as follows:

```
PTHRESH
C
C BADAY 6/20/18 Added conditional to fix zero Pc when KPC=1;
C               PCFIX not set otherwise for KRP5, KRP6, and KRP7
C
      IF (KRP(MAT) .GE. 5 .AND. KRP(MAT) .LE. 7) THEN
         PCFIX(MAT) = PCMAX(MAT)
      END IF
```

```
RELPERM
C
C BADAY 6/20/18 Revise to add KRP5 to list of models using
C               nonzero residual gas saturation to calc Pc
C BADAY 6/20/18         IF (KRP .EQ. 1 .OR. KRP .EQ. 3 .OR. KRP .EQ. 4 .OR.
C BADAY 6/20/18     1      KRP .EQ. 6) THEN
         IF (KRP .EQ. 1 .OR. KRP .EQ. 3 .OR. KRP .EQ. 4 .OR.
     1       KRP .EQ. 5 .OR. KRP .EQ. 6) THEN
```

```
RELPERM
C
C BADAY 6/20/18 Revise to set PC=PCNEW for KRP5, KRP6, and KRP7
C               to force equal treatment of capillary pressure
C               for KPC=1 and KPC=2
         ELSE IF (KRP .GE. 5 .AND. KRP .LE. 7) THEN
C
            PC = PCNEW
```

References:

Camphouse, C. 2012. *User's Manual for BRAGFLO Version 6.02.* Sandia National Laboratories, Carlsbad, NM. ERMS #558663.

Zeitler, T.R and B. Day. 2016. *CRA14_SEN4 Sensitivity Study, Rev. 1.* Sandia National Laboratories. Carlsbad, NM. ERMS 567505.

U.S. Department of Energy (DOE). 2014. Title 40 CFR Part 191 Compliance Recertification Application for the Waste Isolation Pilot Plant (March). DOE/WIPP 2014-3503. Carlsbad Field Office, Carlsbad, NM.

WIPP:4.5.1.1:SFT:QA-L:558349