Impact of Corrections to the Spallings Volume Calculation on Waste Isolation Pilot Plant Performance Assessment – 16135

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ABSTRACT

The numerical code DRSPALL (from direct release spallings) is written to calculate the volume of Waste Isolation Pilot Plant solid waste subject to material failure and transport to the surface (i.e., spallings) as a result of a hypothetical future inadvertent drilling intrusion into the repository. An error in the implementation of the DRSPALL finite difference equations was discovered and documented in a software problem report in accordance with the quality assurance procedure for software requirements. This paper describes the corrections to DRSPALL and documents the impact of the new spallings data from the modified DRSPALL on previous performance assessment calculations. Updated performance assessments result in more simulations with spallings, which generally translates to an increase in spallings releases to the accessible environment. Total normalized radionuclide releases using the modified DRSPALL data were determined by forming the summation of releases across each potential release pathway, namely borehole cuttings and cavings releases, spallings releases, direct brine releases, and transport releases. Because spallings releases are not a major contributor to the total releases, the updated performance assessment calculations of overall mean complementary cumulative distribution functions for total releases are virtually unchanged. Therefore, the corrections to the spallings volume calculation did not impact Waste Isolation Pilot Plant performance assessment calculation results.

INTRODUCTION

Software Problem Report (SPR) 13-001 [1] identifies an error in the implementation of the finite difference equations contained in DRSPALL source code file *wasteflowcalc.f90*. This paper documents the modifications to DRSPALL implemented in Version 1.22 to correct the finite difference equations and determines the impact of these modifications on Waste Isolation Pilot Plant (WIPP) performance assessment (PA) calculations.

A range of spallings volumes initially calculated using DRSPALL Version 1.10 [2] has been used in PA calculations beginning with the 2004 Compliance Recertification Application Performance Assessment Baseline Calculation (CRA-2004 PABC) and

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continuing through the 2014 Compliance Recertification Application (CRA-2014). This paper presents a new range of spallings volumes that will be used in future WIPP PA calculations and assesses the impact of applying the new spallings volumes (developed using DRSPALL Version 1.22) to previous WIPP PA calculations.

The conceptual model for spallings as documented by Lord et al. [3] has not changed. This conceptual model is implemented in the numerical Fortran code DRSPALL (from direct release spallings). DRSPALL is written to calculate the volume of WIPP spallings, which are defined as solid waste material subject to tensile stresses leading to mechanical failure and transported to the surface as a result of a hypothetical inadvertent drilling intrusion. The code calculates coupled repository and wellbore transient mixed-phase compressible fluid flow before, during, and after the drilling intrusion process. Mathematical models are included of bit penetration, mixed-phase (mud, salt, waste, and gas) fluid flow in the well, fluid expulsion at the surface, coupling of the well and the drilled repository, repository spalling (tensile) failure, fluidized bed transport of failed waste, and repository internal gas flow. The wellbore model is one-dimensional with linear flow, while the repository model is one-dimensional with either spherical or cylindrical radial flow. The spallings model domain is depicted in Fig. 1.

THE PERFORMANCE ASSESSMENT PROCESS

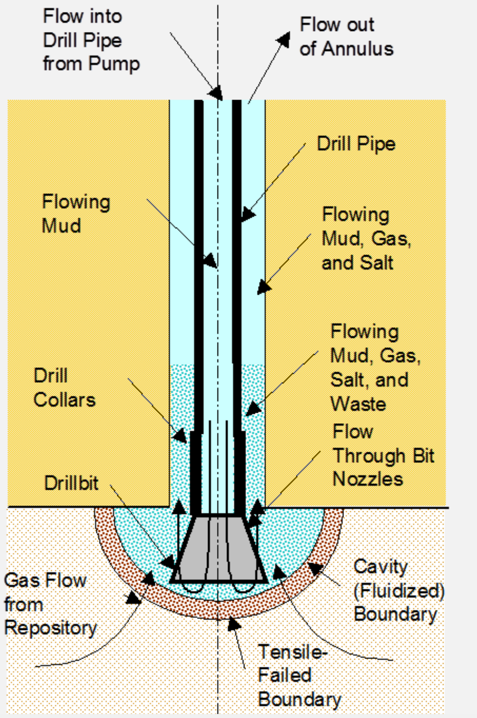
WIPP PA calculations estimate the probability and consequence of potential radionuclide releases from the repository to the accessible environment for a regulatory period of 10,000 years after facility closure. The PA models are updated with new information as part of a recertification process that occurs at five-year intervals following the receipt of the first waste shipment at the site in 1999. A new PA baseline was established by the 2009 Performance Assessment Baseline Calculation (PABC-2009) with recertification of the WIPP by the U.S. Environmental Protection Agency (EPA) in November 2010. The 2014 Compliance Recertification Application (CRA-2014) PA has been submitted to the EPA and is currently under review.

A significant amount of uncertainty is associated with characterizing the physical properties of geologic materials that influence potential releases. The WIPP PA methodology accommodates both aleatory (i.e., stochastic) and epistemic (i.e., subjective) uncertainty in its constituent models. Aleatory uncertainty pertains to unknowable future events such as intrusion times and locations that may affect repository performance. It is accounted for by the generation of random sequences of future events. Epistemic uncertainty concerns parameter values that are assumed to be constants, but the exact parameter values are uncertain due to a lack of knowledge about the system. An example of a parameter with epistemic uncertainty is the permeability of a material. Epistemic uncertainty is accounted for by sampling parameter values from assigned distributions. One set of sampled values required to run a WIPP PA calculation is termed a vector. In a performance assessment, models are executed for three replicates of 100 vectors, each vector providing model realizations resulting from a particular set of parameter values. Parameter values sampled in each PA were also used in the corresponding DRSPALL

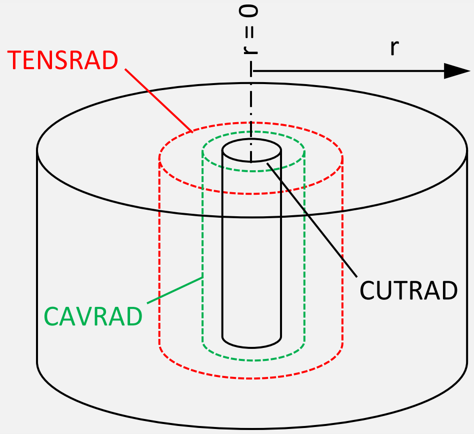
The spallings model is a dynamic simulation of fluid flow and mechanical stresses near the borehole during the few minutes immediately prior to and then after a hypothetical borehole intrusion of a pressurized waste room. A cavity in a waste room will grow axisymmetrically due to drilling and/or spalling. Radioactive solids failed by a tensile stress mechanism, fluidized in the cavity, and ejected from the borehole are considered spallings releases (Fig. 1a).

DRSPALL has the capability to model the repository in two different ways. When the user specifies the cylindrical model, the repository and cavity are modeled as a cylinder of constant height equal to the repository thickness. The radius of the cylindrical cavity, CAVRAD, increases with drilling time and as spalling occurs. When the user specifies the spherical model, the repository and cavity are hemispherical where the cavity radius, CAVRAD, is also a function of time and increases for the same reasons.

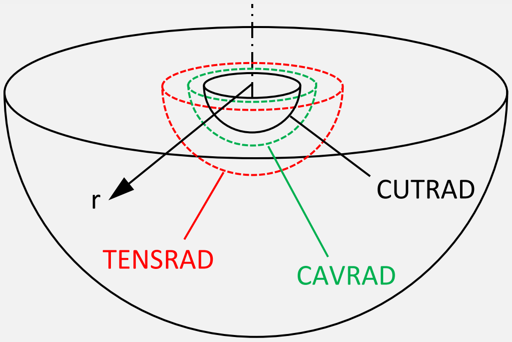
The origin for the cylindrical geometry is a line down the center of the borehole denoting the axis of symmetry (Fig. 1b). The origin for the spherical repository domain is the point where the axis of the drill bit first touches the top of the repository (Fig. 1c). The three primary radial variables in DRSPALL output are the drill cuttings radius (CUTRAD), cavity radius (CAVRAD), and the tensile-failed radius (TENSRAD). The relationship among these three is demonstrated in Fig. 1b and Fig. 1c. The cuttings radius represents the position of the drill-bit face in the repository. Typically drilling is the only mechanism that expands the cavity radius, so the drill radius and cavity radius will overlay. In the event of spallings, however, the cavity radius may grow larger than the drilled radius. A third radial variable, tensile-failed radius, identifies solid material that has failed due to the stress state but has not mobilized into the flow stream. This may or may not be larger than the cavity radius, but it can never be smaller. A thorough discussion of the DRSPALL spallings model is provided by Lord et al. [3] and the updated DRSPALL design document [4].



(a) Schematic diagram of flow geometry after repository penetration. Spherical case is shown.



(b) Schematic diagram of cylindrical geometry.



(c) Schematic diagram of spherical geometry.

Fig. 1. Spallings Model Domain.

impact assessment, and are documented by Kirchner [5, 6]. A sample size of 10,000 possible sequences of future events is used in PA calculations to address aleatory uncertainty. The releases for each of 10,000 possible sequences of future events are tabulated for each of the 300 vectors, totaling 3,000,000 possible futures.

For a random variable, the complementary cumulative distribution function (CCDF) provides the probability of the variable being greater than a particular value. By regulation, PA results are presented as a distribution of CCDFs of releases [7]. Each individual CCDF summarizes the likelihood of releases across all futures for one vector of parameter values. The uncertainty in parameter values results in a distribution of CCDFs.

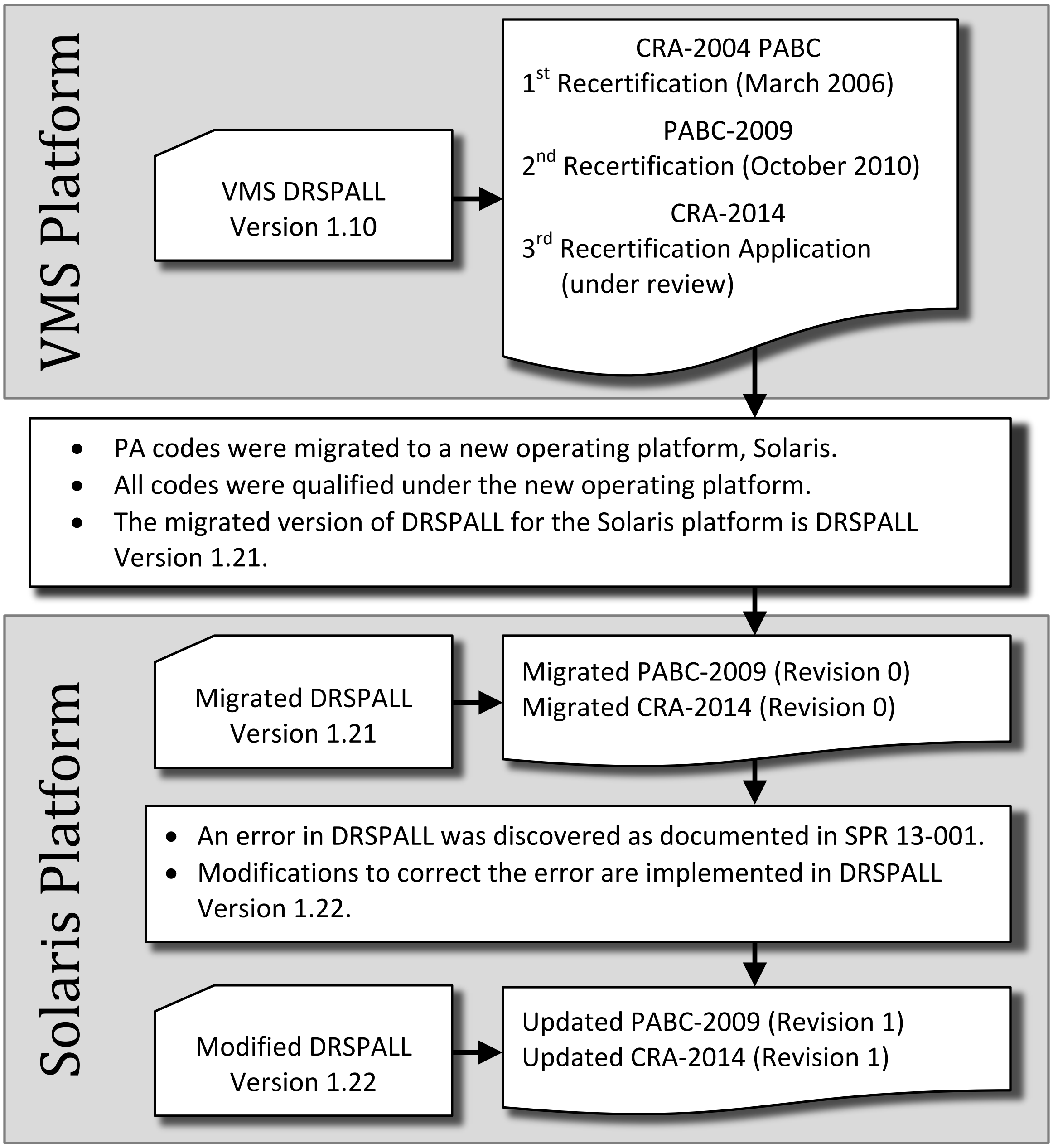
The original DRSPALL results were developed for the CRA-2004 PABC on an Alpha OpenVMS platform using DRSPALL Version 1.10. These results were used for all subsequent PAs continuing through the CRA-2014. These are referred to as “VMS” results (Fig. 2). After submittal of the CRA-2014, PA codes have been migrated to a Sun Solaris Blade Server using a UNIX operating system as part of a planned update to an aging operating system. The migration process includes qualifying PA codes on the new platform. The version of DRSPALL that was implemented and qualified on the Solaris platform is Version 1.21. It is referred to as the “migrated” version (Fig. 2).

As part of the migration, both the PABC-2009 calculations [8] and the CRA-2014 calculations [9], which were originally run on the VMS platform, were rerun on the Solaris platform and the releases projected from analyses on the two platforms were compared [10]. While slight differences in spallings volumes exist between the VMS DRSPALL (Version 1.10) and the migrated DRSPALL (Version 1.21), the cumulative distributions are essentially indistinguishable. The PA calculations performed on the Solaris platform using DRSPALL Version 1.21 are referred to as migrated PABC-2009 (Revision 0) and migrated CRA-2014 (Revision 0).

The modifications to DRSPALL described in this document were applied to the migrated DRSPALL Version 1.21 to create DRSPALL Version 1.22, which is subsequently referred to as the “modified” version (Fig. 2). The modified DRSPALL Version 1.22 was run solely on the Solaris platform. The impact assessment uses a new set of spallings results using DRSPALL Version 1.22 that have been applied to both the PABC-2009 and CRA-2014 PAs to produce the updated PABC-2009 (Revision 1) and the updated CRA-2014 (Revision 1) PA results [11]. The updated PAs (Revisions 1) are compared to the current baseline (i.e., the VMS PABC-2009), the migrated PABC-2009 (Revision 0), the VMS CRA-2014, and the migrated CRA-2014 (Revision 0) to assess the impact of modified spallings data on PA results.

MODIFICATIONS TO THE DRSPALL CODE

SPR 13-001 [1] states that the DRSPALL source code file *wasteflowcalc.f90* contains an error in the implementation of the finite difference equations. DRSPALL uses the Darcy flow equation with a Forchheimer correction to account for high gas flow



- PA codes were migrated to a new operating platform, Solaris.
- All codes were qualified under the new operating platform.
- The migrated version of DRSPALL for the Solaris platform is DRSPALL Version 1.21.

- An error in DRSPALL was discovered as documented in SPR 13-001.
- Modifications to correct the error are implemented in DRSPALL Version 1.22.

Fig. 2. Flowchart of the Migration of WIPP PA Codes and DRSPALL Modifications.

rates [4], which is defined using the variable ‘Forchterm’. The *wasteflowcalc.f90* source code file contains three ‘Forchterm’ equations (for the first cell, the interior cell, and the last cell), with each equation as follows:

$$Forchterm = \frac{k'(i+1)-k'(i)}{4k'(i)\Delta r(i)} \qquad \text{(Eq. 1)}$$

where k' = velocity-dependent permeability (m^2), and
Δr = repository zone size (m).

However, in accordance with the previous version of the DRSPALL design document [12, 13], which is based on a centered-difference discretization, the correct equation should be:

$$Forchterm = \frac{k'(i+1) - k'(i-1)}{4k'(i)\Delta r(i)} \qquad \text{(Eq. 2)}$$

In response to SPR 13-001, the finite difference solution to the DRSPALL waste flow equation was evaluated. DRSPALL assumes a Darcy flow of an isothermal ideal gas in a porous medium, which allows the simplifying pseudopressure approach to be taken, as is commonly done in the field of petroleum reservoir engineering. The approach for modifying the DRSPALL code was to re-derive the governing equations and the finite difference discretization, resulting in the following equation for pseudopressure:

$$\psi_j^n = -\alpha_1 \psi_{j-1}^{n+1} + (1+2\alpha)\psi_j^{n+1} - \alpha_2 \psi_{j+1}^{n+1} \qquad \text{(Eq. 3)}$$

where

$\psi_j^n =$ pseudopressure (Pa/s) at cell j and timestep n

$$\alpha = \frac{D_j^n \Delta t}{(\Delta r)^2}$$

$$\alpha_1 = \frac{D_j^n \Delta t}{\Delta r}\left(\frac{1}{\Delta r} - \frac{(m-1)}{2r_j} - Forchterm\right)$$

$$\alpha_2 = \frac{D_j^n \Delta t}{\Delta r}\left(\frac{1}{\Delta r} + \frac{(m-1)}{2r_j} + Forchterm\right)$$

$$Forchterm = \frac{\ln\left({k'}_{j+1}^{n+1} \big/ {k'}_{j-1}^{n+1} \right)}{4\Delta r}$$

t = time (s)
r = radius of cavity (m)
m = geometry exponent (m=2 for cylindrical, m=3 for spherical)

$$D_j^n = \frac{k'p}{\phi\eta}$$

p = pressure in gas (Pa)
ϕ = porosity of waste
η = viscosity of gas (Pa·s).

The re-derivation of Eq. 3 resulted in the same original equation except that the coefficient terms α_1 and α_2 are different due to a correction in the spatial variability of k', which produced a modified ‘Forchterm’ that uses the natural log. Additional details of the modifications to the DRSPALL code are provided by Kicker, Herrick, and Zeitler [14].

IMPACT TO WIPP PERFORMANCE ASSESSMENT CALCULATIONS

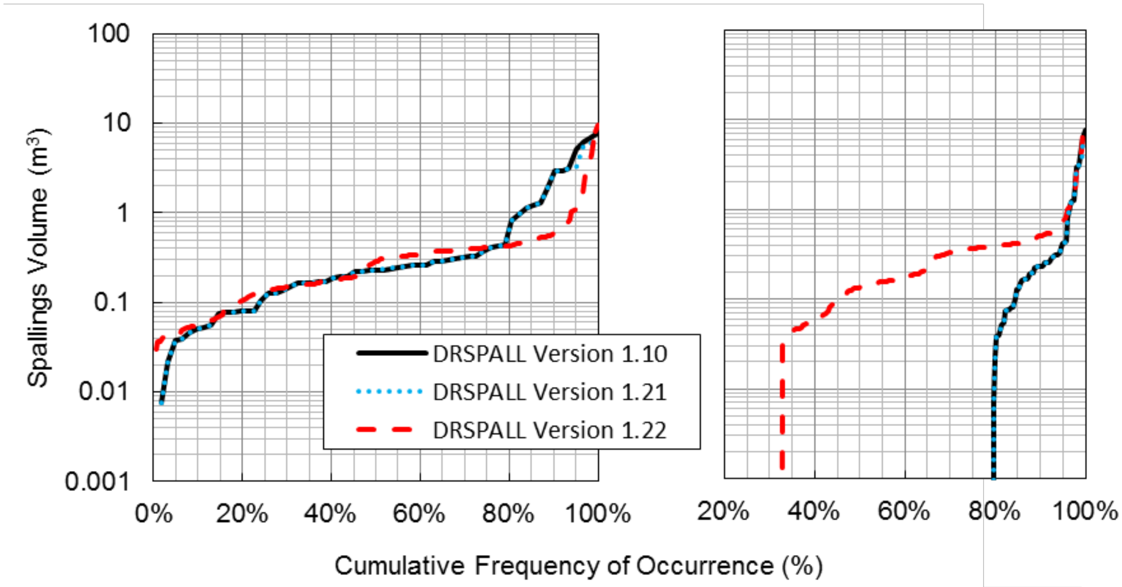
This DRSPALL impact assessment was developed to assess the impact of modified spallings data on four PA calculations, including the VMS PABC-2009, the migrated PABC-2009 (Revision 0), the VMS CRA-2014, and the migrated CRA-2014 (Revision 0). The structure of calculations performed herein is the same as that used in corresponding PAs. The first step for this impact assessment was to run DRSPALL Version 1.22 to produce a modified set of spallings volumes. Next, only those PA codes impacted by the change in spallings volume were rerun, including CUTTINGS_S, BRAGFLO_DBR, and CCDFGF. The output from the remaining PA codes (EPAUNI, LHS, BRAGFLO, NUTS, PANEL, and SECOTP2D) was unchanged, so their Revision 0 results were used in this impact assessment [11]. The updated PAs (Revision 1) use the same waste inventory information, drilling rate and plugging pattern parameters, and radionuclide solubility parameters as were used in the corresponding VMS and migrated PAs.

Spallings

Two procedures are used to calculate the volume of solid waste material released to the surface from a single drilling intrusion into the repository due to spallings. First, the code DRSPALL calculates the spallings volumes at four values of repository pressure, which are referred to as DRSPALL pressure scenarios (DPSs). DPS 1 has an initial repository pressure of 10.0 MPa, DPS 2 has an initial repository pressure of 12.0 MPa, DPS 3 has an initial repository pressure of 14.0 MPa, and DPS 4 has an initial repository pressure of 14.8 MPa. DRSPALL was executed once for each vector and scenario combination, resulting in 1,200 separate runs. Then the code CUTTINGS_S interpolates between DRSPALL volumes based on calculated (by the code BRAGFLO) repository pressures for a set of discrete times and locations.

For DPS 1, all DRSPALL calculations resulted in no spalling. These modified results (DRSPALL Version 1.22) are identical to what was observed in both the VMS DRSPALL (Version 1.10) and migrated DRSPALL (Version 1.21). Lord, Rudeen, and Hansen [15] explain this phenomenon by noting that the initial pressure difference between the repository and the wellbore (hydrostatic pressure of approximately 7.8 MPa) is not large enough to cause tensile failure of the waste material. As a result, no spalling occurs for DPS 1. The cumulative distributions of DRSPALL spallings volumes for DPSs 2, 3, and 4 are shown in Figs. 3, 4, and 5, respectively.

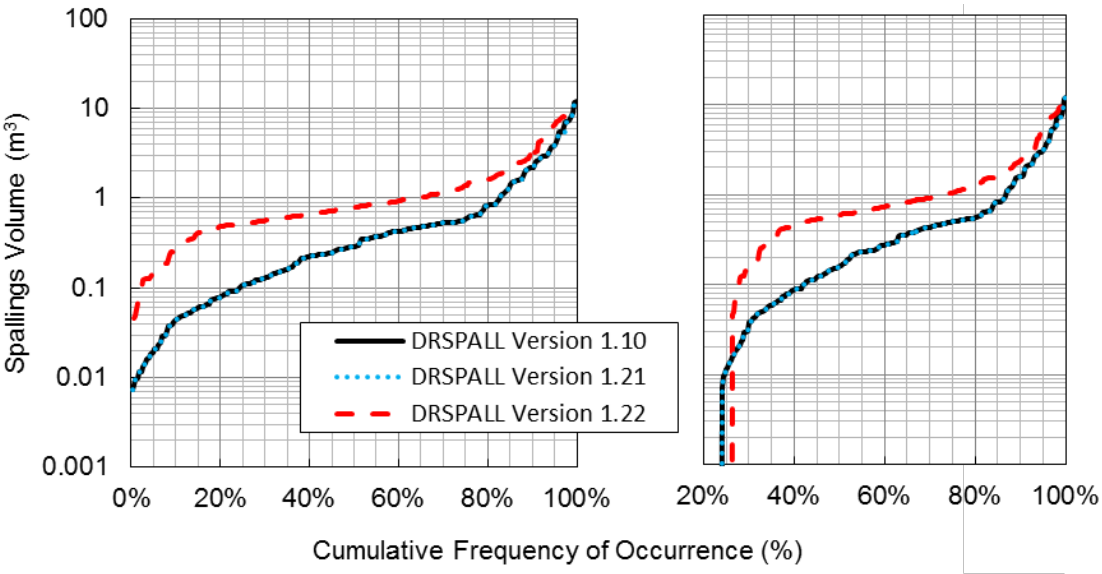
The spallings volume for a given vector is determined in CUTTINGS_S by linearly interpolating between volumes calculated by DRSPALL based on the pressure calculated by BRAGFLO in each realization. Using the spallings volumes calculated by DRSPALL and the repository pressures calculated by BRAGFLO, the impact of DRSPALL Version 1.22 output on repository spallings volumes for PABC-2009 can be determined. The cumulative frequency of occurrence of spallings volumes (for



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

b. All spallings results — includes simulations with no spallings

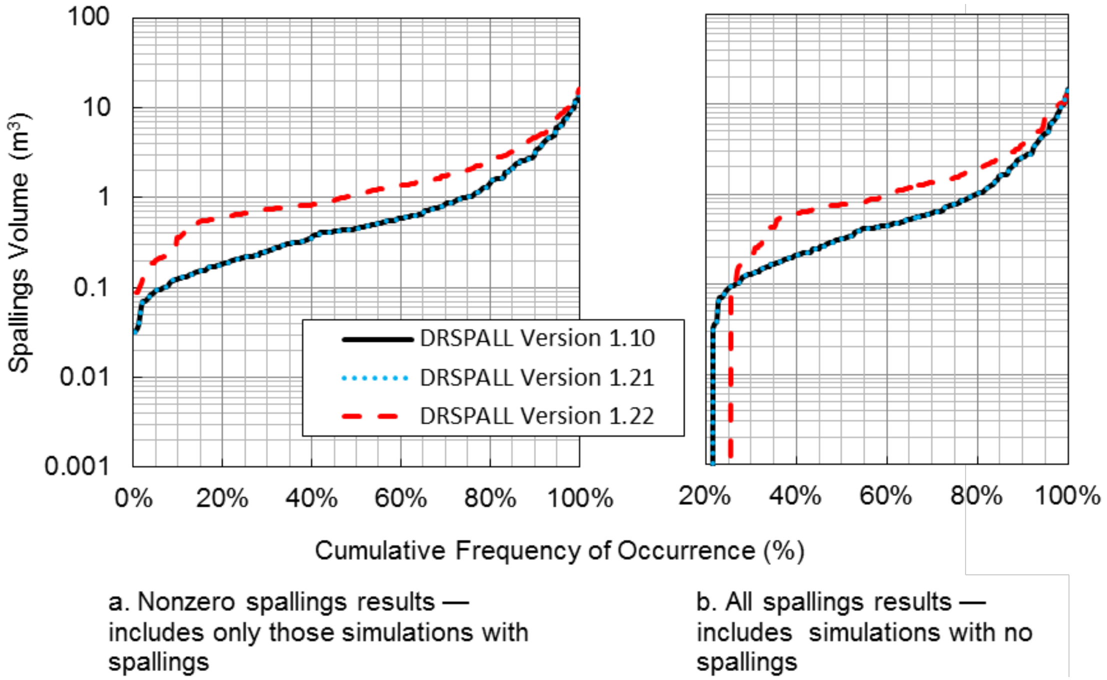
Fig. 3. Cumulative Distributions of DRSPALL Spallings Volumes for Pooled Vectors (Replicates 1, 2, and 3 Combined) at a Repository Pressure of 12 MPa (DPS 2).



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

b. All spallings results — includes simulations with no spallings

Fig. 4. Cumulative Distributions of DRSPALL Spallings Volumes for Pooled Vectors (Replicates 1, 2, and 3 Combined) at a Repository Pressure of 14 MPa (DPS 3).



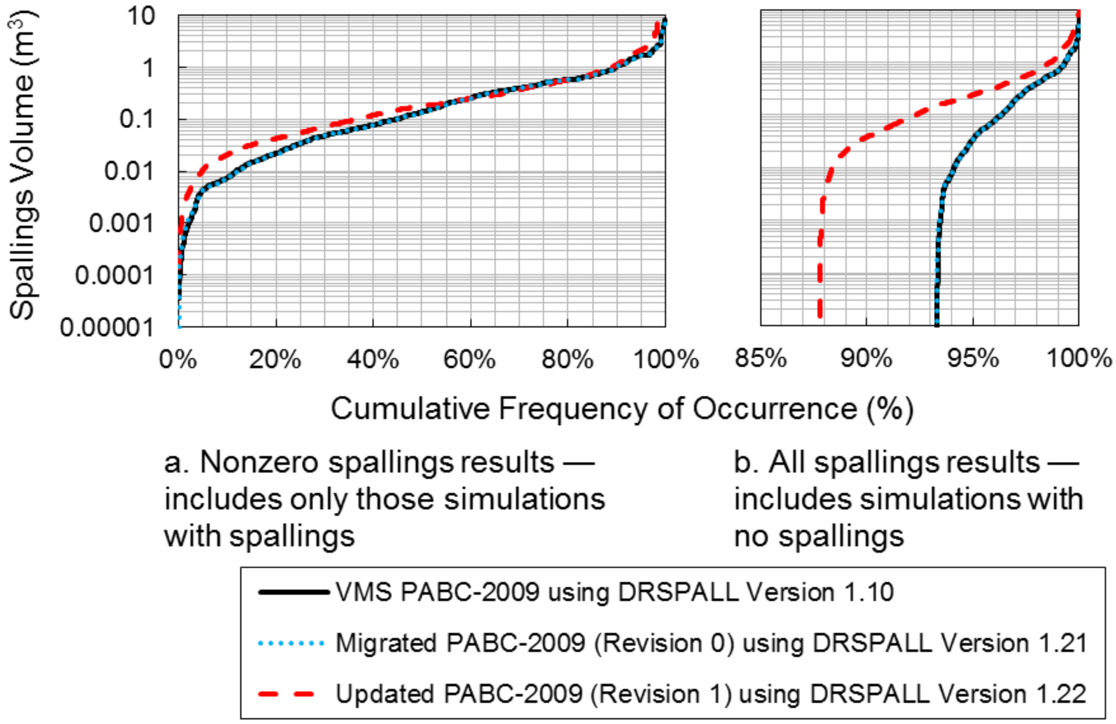
a. Nonzero spallings results — includes only those simulations with spallings

b. All spallings results — includes simulations with no spallings

Fig. 5. Cumulative Distributions of DRSPALL Spallings Volumes for Pooled Vectors (Replicates 1, 2, and 3 Combined) at a Repository Pressure of 14.8 MPa (DPS 4).

replicates 1, 2, and 3 combined) for PABC-2009 is shown in Fig. 6. This figure provides a summary of spallings data from all scenarios, repository regions, and times. Fig. 6 shows that the cumulative distributions of spallings volumes are essentially identical for the VMS PABC-2009 (using DRSPALL Version 1.10) and the migrated PABC-2009 (run on Solaris using DRSPALL Version 1.21). Fig. 6a considers only those simulations in which spallings occur. The cumulative distribution of spallings volumes from the updated PABC-2009 (run on Solaris using DRSPALL Version 1.22) is similar to the VMS and migrated PABC-2009. Fig. 6b is the same plot except that all spallings results are used, including those simulations where no spallings occur. In this case the cumulative distribution of spallings volumes from the updated results is quite different than those from the VMS and migrated PABC-2009 results. The shift in the cumulative frequency of occurrence curve for the updated PABC-2009 spallings volumes (Fig. 6b) is the result of more simulations with nonzero spallings.

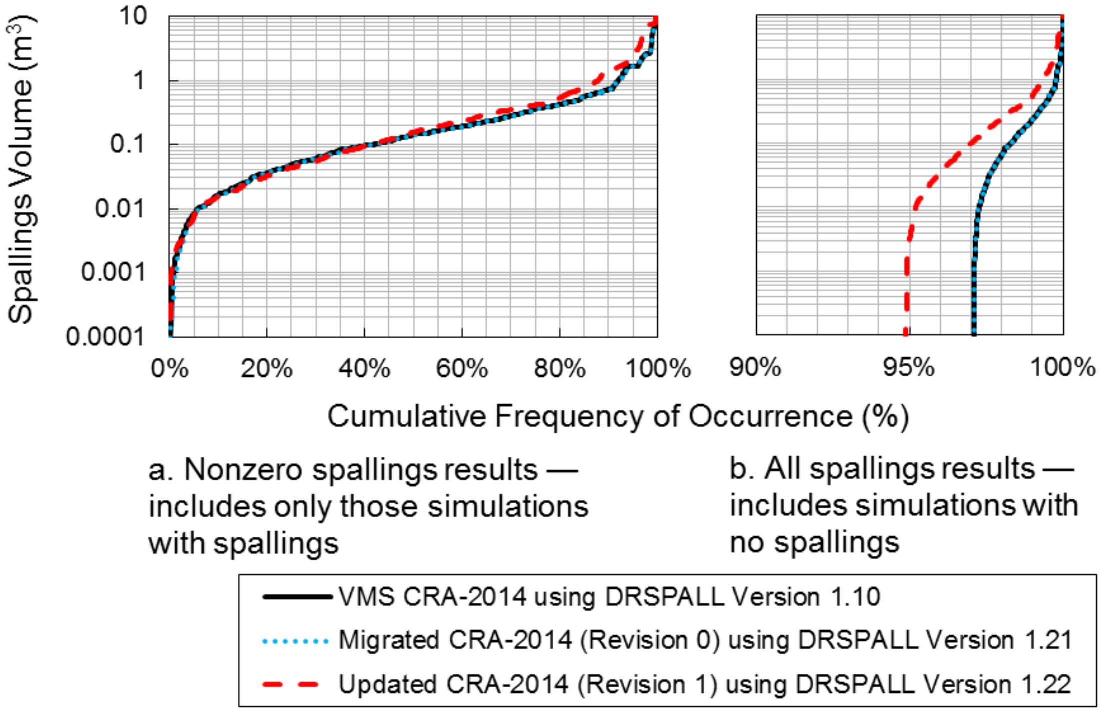
Using the spallings volumes calculated by DRSPALL for the updated PABC-2009 and the repository pressures calculated by BRAGFLO, the impact of DRSPALL Version 1.22 output on repository spallings volumes for CRA-2014 can be determined. The cumulative frequency of spallings volumes for CRA-2014 (replicates 1, 2, and 3 combined) is shown in Fig. 7. This figure provides a summary of spallings data from all scenarios, repository regions, and times. Fig. 7a considers only those simulations in which spallings occur. The cumulative distribution of spallings volumes from the updated CRA-2014 (run on Solaris using DRSPALL Version 1.22) is similar to the VMS and migrated CRA-2014. Fig. 7b is the same plot except that all spallings results are used, including those simulations where no spallings occur.



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

b. All spallings results — includes simulations with no spallings

Fig. 6. Cumulative Distributions of Spallings Volumes in the PABC-2009 for Pooled Vectors (Replicates 1, 2, and 3 Combined).



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

b. All spallings results — includes simulations with no spallings

Fig. 7. Cumulative Distributions of Spallings Volumes in the CRA-2014 for Pooled Vectors (Replicates 1, 2, and 3 Combined).

Again, as was the case for the PABC-2009 spallings volumes, the cumulative distribution of spallings volumes from the updated results is quite different than those from the VMS and migrated CRA-2014 results. The shift in the cumulative frequency of occurrence curve for the updated CRA-2014 spallings volumes (Fig. 7b) is the result of more simulations with nonzero spallings.

Normalized Radionuclide Releases

The impact of the changes in spallings volumes on the overall mean CCDF for normalized spallings releases obtained in the updated PABC-2009 developed using DRSPALL Version 1.22 output can be seen in Fig. 8a for pooled vectors (replicates 1, 2, and 3 combined). As seen in that figure, the CCDF of spallings releases obtained in the updated PABC-2009 is higher compared to both the VMS PABC-2009 (using DRSPALL Version 1.10) and the migrated PABC-2009 (using DRSPALL Version 1.21). The differences in spallings volumes and in the number of vectors that result in a nonzero spallings volume for the updated PABC-2009 correspond to an increase in spallings releases as all analyses use the same waste inventory.

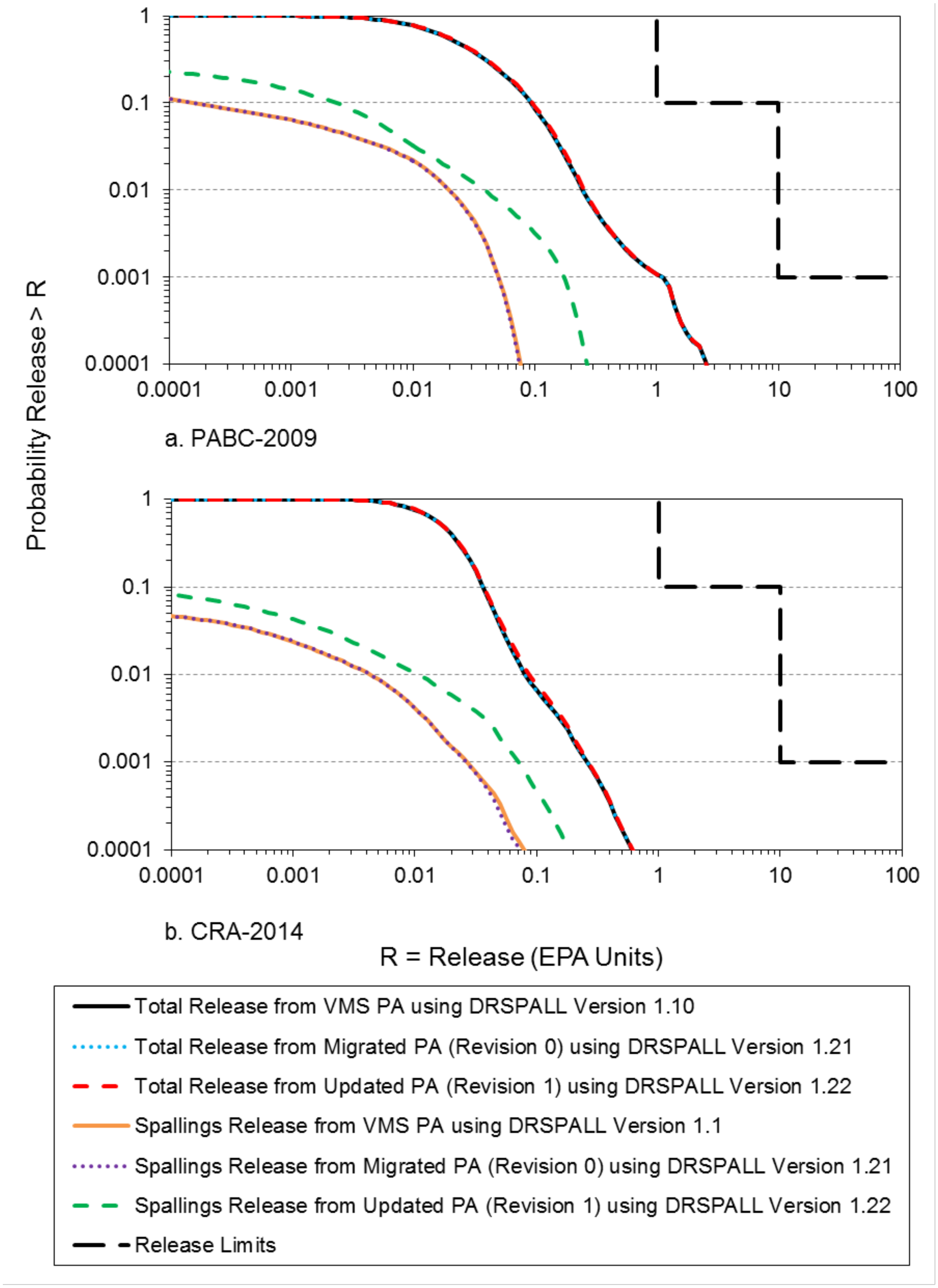
The impact of the changes in spallings volumes on the overall mean CCDF for normalized spallings releases obtained in the updated CRA-2014 developed using DRSPALL Version 1.22 output can be seen in Fig. 8b for pooled vectors (replicates 1, 2, and 3 combined). As seen in this figure, the CCDF of spallings releases obtained in the updated CRA-2014 is higher compared to both the VMS CRA-2014 (using DRSPALL Version 1.10) and the migrated CRA-2014 (using DRSPALL Version 1.21). The differences in spallings volumes and in the number of vectors that result in a nonzero spallings volume for the updated CRA-2014 correspond to an increase in spallings releases as all analyses use the same waste inventory.

Total normalized releases using DRSPALL Version 1.22 output are also presented in Fig. 8 for the PABC-2009 and CRA-2014 for pooled vectors. Total releases are calculated by forming the summation of releases across each potential release pathway, namely cuttings and cavings releases, spallings releases, direct brine releases, and Culebra transport releases.

Both the VMS PABC-2009 and VMS CRA-2014 PAs have shown that spallings releases are a much less significant contributor to the total releases compared to the other potential release pathways [8, 9]. Because spallings releases are not a primary contributor to the total releases, the updated PA (using DRSPALL Version 1.22), the migrated PA (using DRSPALL Version 1.21), and the VMS PA (using DRSPALL Version 1.10) overall mean CCDFs for total releases are virtually identical (Fig. 8).

SUMMARY AND CONCLUSIONS

In response to SPR 13-001 [1], modifications were implemented in DRSPALL Version 1.22 to correct finite difference equations contained in the source code file *wasteflowcalc.f90*. The errors identified in DRSPALL have been resolved, and



a. PABC-2009

b. CRA-2014

Fig. 8. Impact of DRSPALL Version 1.22 Output on the PABC-2009 and CRA-2014 Overall Mean CCDFs for Normalized Radionuclide Releases for Pooled Vectors.

based on the assessment provided in this paper, there is no impact to WIPP PA total radionuclide release calculations resulting from the modification to DRSPALL.

The modifications to DRSPALL (Version 1.22) result in an increase in spallings volumes. The cumulative distributions of spallings volumes at repository pressures of 12.0, 14.0, and 14.8 MPa show higher spallings volumes compared to both the VMS DRSPALL (Version 1.10) and migrated DRSPALL (Version 1.21) (Figs. 3, 4, and 5).

When considering only those simulations in which spallings occur, the cumulative distributions of spallings volumes from the updated PAs (run on Solaris using DRSPALL Version 1.22) are similar to the VMS and migrated PAs (Figs. 6a and 7a). Figs. 6b and 7b show the same plots except that all spallings results are used, including those simulations where no spallings occur. In these cases, the cumulative distributions of spallings volumes from the updated results are quite different than those from the VMS and migrated PA results. The differences arise because the updated analyses yield more simulations with nonzero spallings.

The CCDF of spallings releases obtained in the PABC-2009 was updated using DRSPALL Version 1.22 output. Compared to both the VMS PABC-2009 (using DRSPALL Version 1.10) and the migrated PABC-2009 (using DRSPALL Version 1.21), there was an increase in the number of vectors that result in a nonzero spallings volume, which generally translates to an increase in spallings releases (Fig. 8a). The CCDF of spallings releases obtained in the CRA-2014 was also updated using DRSPALL Version 1.22 output. Similar to the PABC-2009, the update to CRA-2014 resulted in an increase in the number of vectors that result in a nonzero spallings volume, along with a corresponding increase in spallings releases (Fig. 8b).

Total normalized releases using DRSPALL Version 1.22 output were calculated for both the PABC-2009 and CRA-2014. The updated PA (using DRSPALL Version 1.22), the migrated PA (using DRSPALL Version 1.21), and the VMS PA (using DRSPALL Version 1.10) overall mean CCDFs for total releases are almost identical (Fig. 8). Although spallings releases increased as a result of the modification to DRSPALL, spallings releases are not a primary contributor to the total releases, and the updated PA calculations of overall mean CCDFs for total releases are virtually unchanged. Therefore, the corrections to the spallings volume calculation (implemented in DRSPALL Version 1.22) did not impact WIPP PA calculation results.

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