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Sandia National Laboratories
Waste Isolation Pilot Plant

Impact of the DRSPALL Modification on Waste Isolation Pilot Plant Performance Assessment Calculations

Revision 0

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NOMENCLATURE

CCDF	complementary cumulative distribution function
CRA-2004	2004 Compliance Recertification Application
CRA-2004 PABC	2004 Compliance Recertification Application Performance Assessment Baseline Calculation
CRA-2014	2014 Compliance Recertification Application
CVS	Concurrent Versions System
DBR	direct brine release
DPS	DRSPALL pressure scenario
DRZ	disturbed rock zone
EPA	U.S. Environmental Protection Agency
PA	performance assessment
PABC-2009	2009 Compliance Recertification Application Performance Assessment Baseline Calculation
SCMS	Software Configuration Management System
SPR	software problem report
WIPP	Waste Isolation Pilot Plant

1. INTRODUCTION

Software Problem Report (SPR) 13-001 (WIPP PA 2013a) identifies an error in the implementation of the finite difference equations contained in DRSPALL source code file *wasteflowcalc.f90*[1]. This report 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. DRSPALL Version 1.22 has been qualified for use in WIPP compliance calculations in accordance with Nuclear Waste Management Program Procedure NP 19-1 *Software Requirements* (Long 2014). The verification and validation testing of the DRSPALL code is documented in the *Verification and Validation Plan / Validation Document for DRSPALL Version 1.22* (WIPP PA 2015c).

A range of spallings volumes initially calculated using DRSPALL Version 1.10 (Vugrin 2005, Appendix D) has been used in PA calculations beginning with the 2004 Compliance Recertification Application Performance Assessment Baseline Calculation (CRA-2004 PABC) and continuing through the 2014 Compliance Recertification Application (CRA-2014). This impact assessment report documents a new range of spallings volumes (Appendix C) 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. (2006, Section 3) has not changed. This conceptual model is implemented in the numerical Fortran code DRSPALL (from **d**irect **r**elease **spall**ings). 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 an 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 Figure 1-1.

A description of the PA process, including the recent migration of PA codes to a new operating platform, is provided in Section 2. The modifications to the DRSPALL code are described in Section 3. The impact to WIPP PA calculations as a result of the DRSPALL modifications is provided in Section 4.

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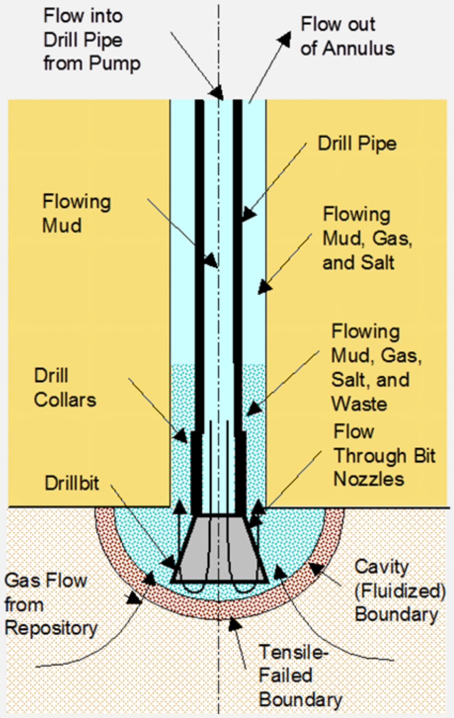
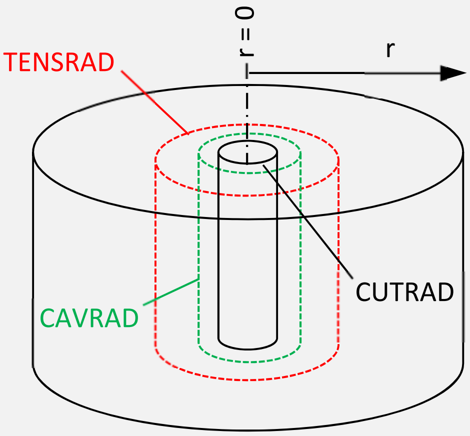
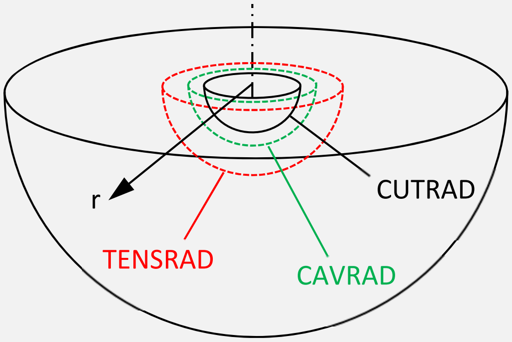
[1] Prior to Version 1.21, the DRSPALL source code file names contained the prefix “DRS_”. This prefix was removed from all source code file names in Version 1.21 and is not used in this document.



(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.

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 borehole intrusion of a pressurized waste room. The cavity in 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 (Figure 1-1a).

DRSPALL has the capability to model the repository 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 (Figure 1-1b). The origin for the spherical repository domain is a point where the axis of the drill bit first touches the top of the repository (Figure 1-1c). 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 Figure 1-1b and Figure 1-1c. 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. (2006) and the updated DRSPALL design document (WIPP PA 2015a).

Figure 1-1. Spallings Model Domain.

2. 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 maintained and 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.

2.1. Treatment of Uncertainty

There is a significant amount of uncertainty 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 impact assessment (Section 4), and are documented by Kirchner (2010 and 2013). 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, performance assessment results are presented as a distribution of CCDFs of releases (EPA 1996). 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.

2.2. Determination of Radionuclide Releases

Releases are quantified in terms of “EPA units”. Each radionuclide has a release limit prescribed to it. This limit is defined as the maximum allowable release (in curies) of that radionuclide per a waste amount containing 1×10^6 curies of alpha-emitting transuranic radionuclides with half-lives greater than 20 years. Releases in EPA units result from a normalization by radionuclide and the total inventory. For each radionuclide, the ratio of its 10,000 year cumulative release (in curies) to its release limit is calculated. The sum of these ratios is calculated across the set of radionuclides and normalized by the transuranic inventory (in curies) of α-emitters with half-lives greater than 20 years, as specified by regulation. Mathematically, the formula used to calculate releases in terms of EPA units is

$$R = \frac{1\times10^6 \, curies}{C} \sum_i \frac{Q_i}{L_i} \tag{2-1}$$

where R is the normalized release in EPA units. Quantity Q_i is the 10,000 year cumulative release (in curies) of radionuclide i. Quantity L_i is the release limit for radionuclide i, and C is the total transuranic inventory (in curies) of α-emitters with half-lives greater than 20 years. Note that the definition of the release limit L_i results in a constant value of 1×10^6 curies being factored out of the summation.

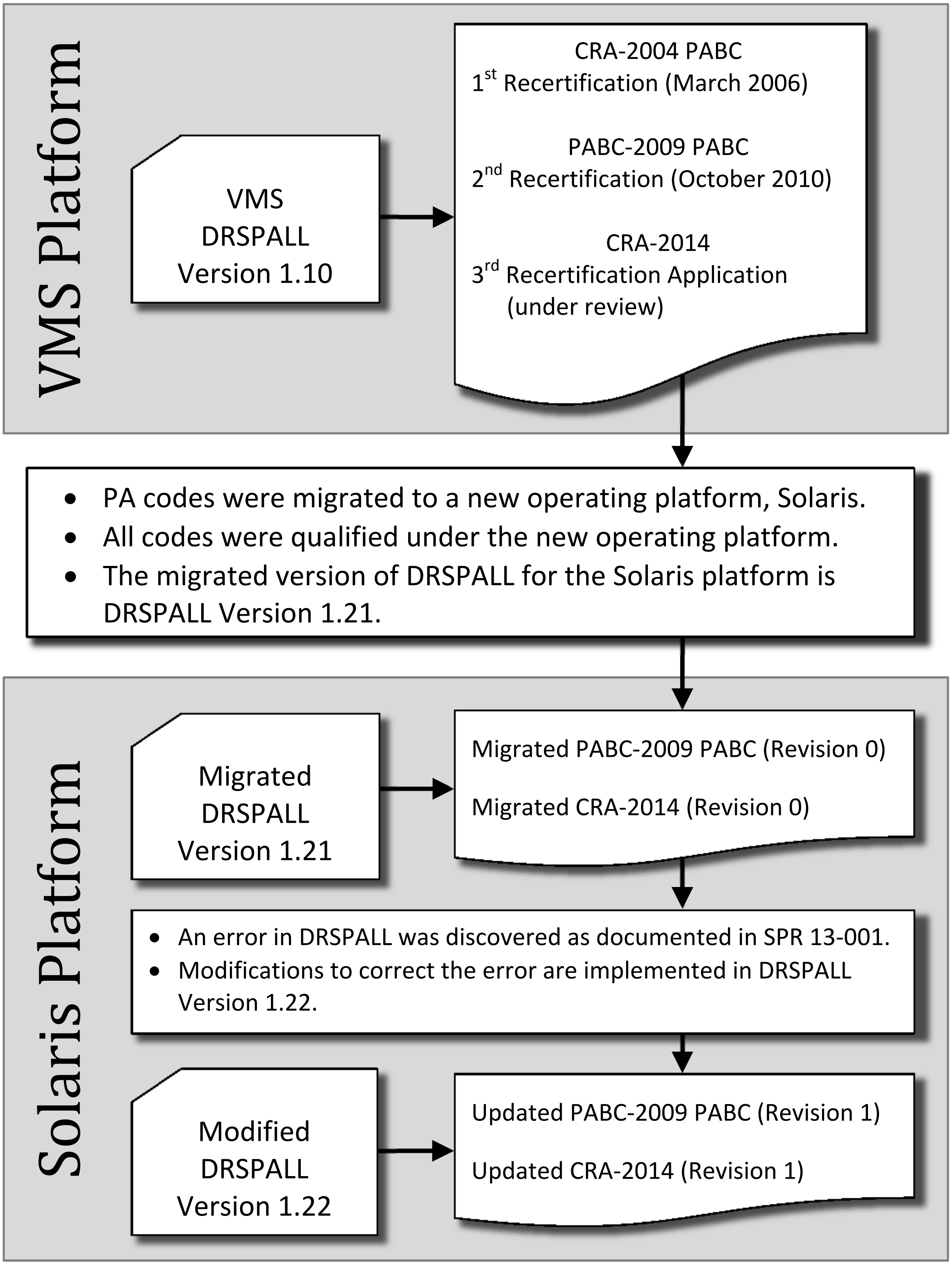
2.3. Migration of the WIPP Performance Assessment Codes

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 using DRSPALL Version 1.10 (Figure 2-1).

After the 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 (Figure 2-1).

As part of the migration, both the PABC-2009 calculations (Clayton et al. 2010) and the CRA-2014 calculations (Camphouse et al. 2013), 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 (Kirchner, Gilkey, and Long 2013). 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 as presented in Section 4 (see Sections 4.1.2.2, 4.1.2.3, and 4.1.2.4). 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 (Figure 2-1). The modified DRSPALL Version 1.22 was run solely on the Solaris platform. The impact assessment presented in Section 4 uses a new set of DRSPALL 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 (Kirchner, Gilkey, and Long 2015). The updated PAs (Revision 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.



- 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.

Figure 2-1. Migration of WIPP PA Codes and the DRSPALL Modification.

3. MODIFICATIONS TO THE DRSPALL CODE

SPR 13-001 (WIPP PA 2013a) states that the DRSPALL source code file *wasteflowcalc.f90* contains an error in the implementation of the finite difference equations. This source code file contains three Forchterm equations (for the first cell, the interior cell, and the last cell), with each Forchterm equation as follows:

$$Forchterm = \frac{k'(i+1) - k'(i)}{4k'(i)\Delta r(i)} \tag{3-1}$$

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

However, in accordance with the previous version of the DRSPALL design document (WIPP PA 2004a; WIPP PA 2013b), which is based on a centered-difference discretization, the correct equation should be:

$$Forchterm = \frac{k'(i+1) - k'(i-1)}{4k'(i)\Delta r(i)} \tag{3-2}$$

In response to SPR 13-001, the finite difference solution to the DRSPALL waste flow equation was evaluated. In addition to the error identified in SPR 13-001, it was found that the derivation of the constant zone size equations was also incorrect. The derivation of Equation 4.6.2 in the previous design document (WIPP PA 2004a) was incorrect because k' was treated as a constant in the denominator, despite it being a variable in the numerator. The approach for modifying the DRSPALL code was to start from design document Equation 4.3.10 (WIPP PA 2015a, Section 4.3), which is equivalent to Equation A-1, and clarify the original design document Equation 4.6.1 (WIPP PA 2004a, Section 4.6), shown by Equation A-5. This essentially results in a simplification of the original Equation 4.6.1 to include a natural log term, as shown in Equation A-5. The original Equation 4.6.2 in the previous design document (WIPP PA 2004a, Section 4.6) was re-derived as shown by Equation A-6.

The finite difference discretization is then performed for zones of constant size. Appendix A provides a simplified version of the final derivation (Equation A-7), which is in fact identical to the previous design document Equation 4.6.3 (WIPP PA 2004a, Section 4.6), except that the coefficient terms α_1 and α_2 are different due to the correction for the spatial variability of k', which results in the natural log term.

A variable zone size implementation was described based on the previous DRSPALL design document (WIPP PA 2004a, Section 4.6; WIPP PA 2013b). However, this was done incorrectly, as a simple substitution of variable zone sizes into the equation derived for a constant zone size is not valid. The derivation of an equation similar to Equation A-6 for a variable zone size would require a complete re-derivation, which was determined unnecessary because current computing resources allow for reasonably fast computational times even for a greater number of zones, such that an increasing zone size is not needed. So it was decided to run DRSPALL exclusively with a constant zone size (it will now fail in source code file *A1main_drspall.f90* if a growth rate other than 1.0 is input).

These changes are made in the CalculateWasteFlowImplicit routine of the source code file *wasteflowcalc.f90* in the calculation of 'Forchterm' for first, interior, and last cell coefficients. In correcting the calculation of 'Forchterm', the indexing of the second permeability() term was also corrected to be 'i-1' instead of 'i'. The coefficients for the last cell (i=numReposZones) have changed: aa(i) has been changed from '-alpha1' to '-alpha1-alpha2' and bb(i) has been changed from '1.0+alpha1' to '1.0+alpha1+alpha2'.

It should be noted that since a constant zone size is used exclusively, values for both 'reposDR(i)' (distance between zone edges) and 'reposDRH(i)' (distance between zone centers) will now be the same.

3.1. Boundary Conditions

In the CalculateWasteFlowImplicit routine of *wasteflowcalc.f90*, the index of the "first cell coefficients" (i) has been changed from 'firstIntactZone' to 'firstIntactZone+1', since any values for the boundary ('firstIntactZone') would be constant and fixed by the specified pressure (Dirichlet) boundary condition in the cavity. That is, the boundary nodes are not included in the coefficient matrix, so there should be no aa(i), bb(i), cc(i) coefficients for 'firstIntactZone'. The effect of the boundary node (firstIntactZone) is included in the b-vector of the linear system of equations. Consequently, the indexing for the "interior cell coefficients" now begins at 'firstIntactZone+2' instead of 'firstIntactZone+1'. Also, as a consequence of this, the indexing of the matrix inversion has changed (lines 230-245). The boundary pressure is now assigned to 'reposPres(firstIntactZone)' instead of 'reposPres(0)'. Because of that, 'exitPoreVelocity' is now calculated using a centered-difference approximation, which leads to 'reposPres(firstIntactZone+1)' being used instead of 'reposPres(firstIntactZone)'.

Previously, the permeability of the 'firstIntactZone-1' zone was set to the value of the 'firstIntactZone'. This was changed by eliminating that assignment (line 32 of *wasteflowcalc.f90*) because the permeability of the 'firstIntactZone-1' is no longer used. Also, where previously the array element 'psi(firstIntactZone-1)' was calculated from the gas viscosity and boundary pressure, this assignment has been made applicable to 'psi(firstIntactZone)' (line 37 of *wasteflowcalc.f90*), since the 'firstIntactZone' is the boundary.

3.2. Summary of Code Changes

A summary of the changes to the source code files for DRSPALL Version 1.22 is described in Appendix B along with source code excerpts from DRSPALL Versions 1.21 and 1.22 showing the change. Changes were made in the following DRSPALL source code files:

- *A1main_drspall.f90*
- *globals.F90*
- *maincalc.f90*
- *parameters.f90*
- *setupcalc.f90*
- *vmsfilewrite.f90*
- *wasteflowcalc.f90*

- *wastestresscalc.f90*
- *wellborecalc.f90*

Source code files *cdbcontrol.f90*, *cdbglobals.F90*, and *vmsoutputcontrol.f90* were not modified in DRSPALL Version 1.22.

4. 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 was the same as that used in the corresponding PA. PA-calculated results impacted by the change in spallings volume were updated (Kirchner, Gilkey, and Long 2015), while the results from previous PAs were used for individual numerical codes not affected by these changes. The updated PAs (Revision 1) utilized 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.

4.1. Spallings

There are two procedures 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 (10, 12, 14, and 14.8 MPa). Then the code CUTTINGS_S interpolates between DRSPALL volumes based on repository pressures calculated (by the code BRAGFLO) for a set of discrete times and locations.

4.1.1. Calculation of Spall Volumes by DRSPALL

Four initial repository pressures are considered for DRSPALL calculations. These pressures correspond to what 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 1200 separate runs. Based on a zone size sensitivity study, the following zone size parameters have been selected as the standard configuration for DRSPALL calculations (Kicker 2015):

- Repository zone size, $\Delta r = 0.004$ m
- Characteristic length, $L_t = 0.04$ m
- Wellbore zone size, $\Delta z = 2.0$ m.

4.1.1.1. Output Variables

A complete list of DRSPALL variables and their definitions is given in WIPP PA (2015a, 2004b, 2013c, 2015b). The discussion of the following variables is required for comprehension of this document:

- Drilled radius (DRILLRAD) - this variable represents the contribution of the cavity radius in the repository that is due to drill cuttings. This variable is a function of time and is bounded by the variable CUTRAD, the maximum equivalent cuttings radius.

- Maximum equivalent cuttings radius (CUTRAD) - this variable represents the length of the radius of the hemisphere (or cylinder, depending on choice of geometric model) with the same amount of surface area as the lateral surface area of a cylinder with height equal to the repository height and diameter equal to the drill-bit diameter. This variable is constant with respect to time.

- Cavity radius (CAVRAD) - this variable represents the length of the radius of the cavity and includes contributions from drill cuttings and spallings. This variable changes with time.

- Repository thickness (REPOSTCK) - this variable represents the thickness of the repository. This variable is constant with respect to time.

- SPLVOL2 – this variable represents the accumulated uncompacted spall volumes. This variable changes with time and is the major variable of interest.

4.1.1.2. Exception Runs — Increased Run Time

The DRSPALL input control file allows the user to specify the length of time of the drilling intrusion (WIPP PA 2004b, 2013c, 2015b). All DRSPALL calculations were initially run for a 600-second drilling intrusion time, which is generally long enough to capture all drilling and spalling activity.

CAVRAD is a non-decreasing quantity, and two processes can occur that result in an increase of CAVRAD. The first process that causes CAVRAD to increase is the passage of the drill bit through the repository, and as drilling occurs, the radius of the equivalent cavity increases. Secondly, if spalling is occurring, the cavity radius will increase, and the quantity CAVRAD increases. When the drill bit reaches the bottom of the repository and spallings have ceased, CAVRAD does not increase.

CAVRAD is used as an indicator to determine when the system has stabilized and the spallings process has ceased. If CAVRAD has increased at a time close to the end of the simulation, the spallings process may not have finished, and the run time for the simulation needs to be increased to ensure that all of the spallings volume has been calculated. All runs that had an increase in CAVRAD after 500 seconds indicate that cavity growth was occurring in the final 100 seconds of the DRSPALL simulation, and thus were rerun with an increased "maximum run time" and "stop drilling time" of 1500 seconds.

4.1.1.3. Repository — Spherical and Cylindrical Geometries

The spallings model domain is divided into two regions that are coupled. The first is the wellbore domain, and this document does not discuss the details associated with flow in the wellbore. For a thorough discussion of the wellbore domain, see Sandia Report SAND2004-

0730 (Lord et al. 2006) and the DRSPALL design document (WIPP PA 2015a). This section briefly discusses the geometries associated with the repository domain.

DRSPALL has the capability to model the repository using either the cylindrical model or the spherical model as discussed in the zone size sensitivity study (Kicker 2015, Section 1.2). When the user specifies the cylindrical model, the repository and cavity are modeled as a cylinder of constant height equal to the constant REPOSTCK. The calculation of REPOSTCK is discussed in Section 4.1.1.4. All spallings executions were begun using the spherical model. Certain exception runs required restarting the code with the cylindrical model. These exception runs are discussed in further detail in the following section.

4.1.1.4. Exception Runs

The repository thickness at the time of intrusion, represented by the variable REPOSTCK, is determined from the repository porosity ϕ (the sampled parameter SPALLMOD:REPIPOR), the height of the repository at burial time, H_o, and porosity ϕ_o of a waste-filled room prior to closure:

$$REPOSTCK = \frac{(1-\phi_0)H_0}{1-\phi}. \tag{4-1}$$

WIPP PA assigns the values of H_o = 3.96 m (BLOWOUT:HREPO) and ϕ_o = 0.85 (BLOWOUT:INPORO). By the end of some DRSPALL simulations, the cavity radius exceeded the height of the repository. In an actual intrusion, this would correspond to spalling occurring into the disturbed rock zone (DRZ) below the repository. Lord et al. (2003) state that "the unsteady porous flow and stress equations that describe the repository in hemispherical geometry do not address the presence of the lower DRZ." When the cavity radius reaches the height of the repository, the cavity no longer expands vertically and cavity growth can only result from lateral expansion, thus the DRSPALL calculation proceeds in the cylindrical mode from that point forward. For the DRSPALL cylindrical exception runs, the height of the cylinder remains equal to the height of the repository while the radius of cylinder increases as spalling occurs. An initial radius for the cylindrical cavity was specified to be the height of the repository. This initial radius was specified to account for the cavity calculated when DRSPALL was executed in spherical mode. The initial radius is set equal to the repository thickness so that the initial cylindrical cavity has a lateral surface area equivalent to the surface area of the hemispherical cavity at the time when the hemispherical cavity reaches the base of the repository. The volume of spalled material (SPLVOL2) from the cylindrical run was added to the volume of spalled material (SPLVOL2) at the time step when CAVRAD first exceeded the repository height during the spherical run, and this total volume is used by CUTTINGS_S.

The procedure for implementing each exception run was as follows:

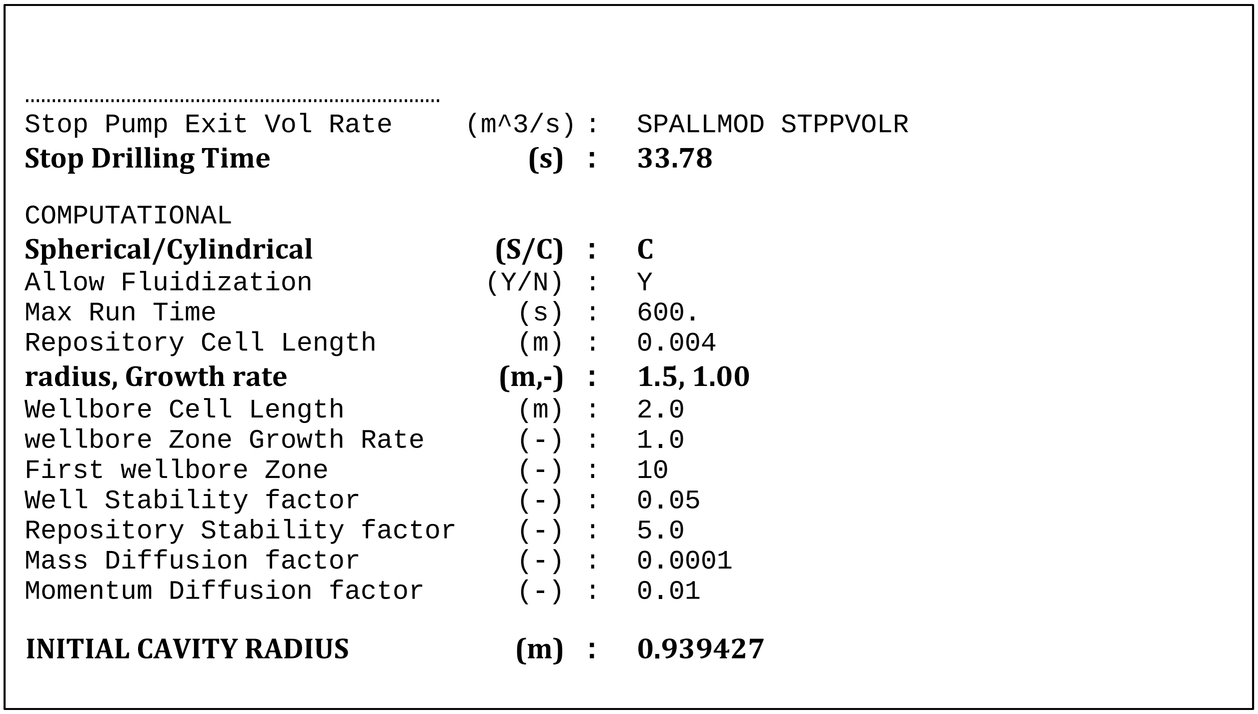
1) DRSPALL was run for all vectors and DPSs with a maximum run time of 600 seconds.
2) All DRSPALL runs were examined to determine in which runs CAVRAD exceeded REPOSTCK.

3) For each run in which CAVRAD exceeded REPOSTCK, a new DRSPALL input control file was created. This control file differed from the control file that was used for the initial run in the following ways (Figure 4-1):

   a. The flag indicating use of the spherical model was changed from “S” to “C” to indicate that the cylindrical model is used.

   b. “INITIAL CAVITY RADIUS” is specified to a length equal to the height of the repository.

   c. To assist in establishing “true” initial conditions from the inputted approximate initial conditions for restarting the run in cylindrical mode, the drill bit is started 0.15 m above the repository with a velocity of 0.00444 m/s. At 33.78 seconds, the drill bit is at the top of the repository. “STOP DRILLING TIME” was changed from “1.0000E+03” to “33.78.” At this point, sufficient initial conditions have been re-established and the code proceeds with the normal coupled wellbore/repository calculations without drilling. Since the drilled volume was already determined in the spherical run, the drill bit is stopped before penetration, and spalling proceeds as determined by the model.



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.......................................................................
Stop Pump Exit Vol Rate     (m^3/s) :   SPALLMOD STPPVOLR
Stop Drilling Time              (s) :   33.78

COMPUTATIONAL
Spherical/Cylindrical         (S/C) :   C
Allow Fluidization            (Y/N) :   Y
Max Run Time                    (s) :   600.
Repository Cell Length          (m) :   0.004
radius, Growth rate           (m,-) :   1.5, 1.00
Wellbore Cell Length            (m) :   2.0
wellbore Zone Growth Rate       (-) :   1.0
First wellbore Zone             (-) :   10
Well Stability factor           (-) :   0.05
Repository Stability factor     (-) :   5.0
Mass Diffusion factor           (-) :   0.0001
Momentum Diffusion factor       (-) :   0.01

INITIAL CAVITY RADIUS           (m) :   0.939427
```

Figure 4-1. Excerpt of Modified DRSPALL Control File for Cylindrical Runs. Lines in bold differ from control files for spherical runs.

   d. “RADIUS, GROWTH RATE” was changed from “0.5, 1.00” to “1.5, 1.00.” “RADIUS” separates the region in the repository where zone size is constant from the region where zone size grows at "GROWTH RATE." Note that in DRSPALL Version 1.22, the zone size growth rate is always 1.00, which means the zone size remains constant. The value specified for "RADIUS" in the cylindrical runs results in about 0.5 m (1.5 - 1) outside the initial cavity radius. This assumes a repository height of approximately 1.0 m.

4) DRSPALL was run using the new input control file.

5) SPLVOL2 at time 600 seconds from the cylindrical run was added to the spherical SPLVOL2 value at the first time when CAVRAD exceeded REPOSTCK. This procedure is discussed in greater detail in Section 4.1.1.5. Note that for all cylindrical DRSPALL runs, CAVRAD attained a steady state value within 500 seconds, and thus it was not necessary to increase the run time as described in Section 4.1.1.2.

The code does not have the capability to start with an arbitrary pressure profile within the repository or fluid/solid distribution in the wellbore, and, therefore, a uniform pressure distribution and mud-filled column are used for the initial conditions at the beginning of the cylindrical run (end of the run in spherical geometry). Thus, the cylindrical calculations start with a similar initial pressure difference between the wellbore and repository as the spherical calculations.

4.1.1.5. Creation of the Spallings Data File for CUTTINGS_S

The code CUTTINGS_S calculates spall volumes for the PA drilling intrusion scenarios from the DRSPALL calculated spall volumes. A spall volume is calculated for each PA vector and at each of a set of discrete times and locations (unique pressure) within the repository for each drilling intrusion scenario.

CUTTINGS_S requires an input file that contains the spallings volumes calculated by DRSPALL for each vector and DPS for one replicate (WIPP PA 2004c). This section details how this spallings data file was created for a PA calculation.

The first step involved a series of SUMMARIZE runs. The code SUMMARIZE was run using the DRSPALL data from the spherical runs, once per DPS and replicate combination. As an example, the SUMMARIZE input file for replicate 1, DPS 1 is provided by Vugrin (2005, Appendix B, Figure 21) for the CRA-2004 PABC and has not changed for the PABC-2009 and subsequent PAs. A fragment of the corresponding output table from the migrated PABC-2009 is shown in Figure 4-2. The entire file, *sum_drs_PABC09_sphere_r1_p1.tbl*, is stored in the Concurrent Versions System (CVS) repository at /nfs/data/CVSLIB/WIPP_ARCHIVES/PABC09/SUMMARIZE/Output.

The output file (Figure 4-2) contains data for the variables REPOSTCK, CAVRAD, and SPLVOL2 at a set of discrete set of times for each vector of a DPS. The output contains two header lines followed by a blank line. The first header line lists the CAMDAT variable names of the data contained in the file: vector, time, REPOSTCK, CAVRAD, and SPLVOL2. The second header line contains information pertaining to the type of CAMDAT variable listed in line 1. The data following the header lines are grouped in sections containing 100 lines and five columns. The first column contains the vector number of the DRSPALL run, the second column contains a time (multiples of 2 seconds), the third column contains the repository height for each vector (constant for all times), the fourth column contains the value of CAVRAD calculated by DRSPALL at the time in the second column for the vector in the first column, and the fifth column contains the value of SPLVOL2 calculated by DRSPALL for the same time and vector. Each group of 100 lines has the same time value. The structure of the output file for spherical runs has not changed for the PABC-2009 and subsequent PAs.

A second set of SUMMARIZE runs was performed using the output from the DRSPALL cylindrical exception runs. SUMMARIZE was run once per DPS and replicate combination that produced spallings in the spherical runs. The output from these runs contained the accumulated spall volume, SPLVOL2, calculated at 600 seconds for the cylindrical exception DRSPALL runs. As an example, Figure 4-3 shows the output for Replicate 1, DPS 3 for the migrated PABC-2009. The structure of the output file for cylindrical runs has not changed for the PABC-2009 and subsequent PAs.

```
vector,time REPOSTCK CAVRAD   SPLVOL2
 ,[P:9],[H],[H]
     .
     .
     .
  95  0.000000E+00  1.143436E+00  0.000000E+00  0.000000E+00
  96  0.000000E+00  1.326540E+00  0.000000E+00  0.000000E+00
  97  0.000000E+00  1.035864E+00  0.000000E+00  0.000000E+00
  98  0.000000E+00  1.232377E+00  0.000000E+00  0.000000E+00
  99  0.000000E+00  1.728078E+00  0.000000E+00  0.000000E+00
 100  0.000000E+00  1.010622E+00  0.000000E+00  0.000000E+00

   1  2.000000E+00  1.520442E+00  1.100081E-01  0.000000E+00
   2  2.000000E+00  1.071487E+00  1.100081E-01  0.000000E+00
   3  2.000000E+00  1.092032E+00  1.100081E-01  0.000000E+00
   4  2.000000E+00  9.150674E-01  1.100081E-01  0.000000E+00
   5  2.000000E+00  1.242655E+00  1.100081E-01  0.000000E+00
     .
     .
     .
```

Figure 4-2. Fragment of SUMMARIZE Output File for Spherical DRSPALL Run – Migrated PABC-2009 (Revision 0) Replicate 1, DPS 1.

```
vector,time SPLVOL2
  ,[H]

  32  6.000000E+02  1.915924E+00
  36  6.000000E+02  6.617699E-01
  42  6.000000E+02  0.000000E+00
```

Figure 4-3. SUMMARIZE Output file for DRSPALL Cylindrical Run – Migrated PABC-2009 (Revision 0) Replicate 1, DPS 3.

The final step in the creation of the spallings data files (one for each DPS) was execution of the utility MERGESPALL to combine the "summarized" results from the spherical and cylindrical runs. This utility was developed for the CRA-2004 PABC (Vugrin 2005, Appendix C). MERGESPALL works in the following manner:

1) MERGESPALL reads a SUMMARIZE output file containing the DRSPALL data from the spherical calculations for a single DPS. For each vector, MERGESPALL reads through all the times and finds the first time where CAVRAD exceeds REPOSTCK and writes the value of SPLVOL2 at that time to an intermediate text file. If CAVRAD does not exceed REPOSTCK, MERGESPALL records the value of SPLVOL2 at the final time. For all vectors, MERGESPALL also writes the final time listed in the SUMMARIZE output file.

2) MERGESPALL reads the SUMMARIZE output file containing SPLVOL2 quantities from the cylindrical exception runs for the same DPS (if the file exists). For all of the vectors whose CAVRAD value exceeded its REPOSTCK value, MERGESPALL adds the SPLVOL2 quantity from the cylindrical run to the corresponding spherical SPLVOL2 quantity. If MERGESPALL does not find a SPLVOL2 value for a vector that requires one, an error message is logged in the log output file.

3) MERGESPALL checks the output directory to see if a file already exists with the user specified output file name. If one does exist, it appends the data to the end of that file. MERGESPALL writes 3 columns: the vector number, a time, and the spall volume for the vector. Otherwise, MERGESPALL creates a new text output file with a three line header. The first line contains the number of vectors, the second line contains the number of DPSs, and the third line contains the initial repository pressures used for each DPS. MERGESPALL assumes four pressure scenarios with initial pressures of 10, 12, 14, and 14.8 MPa. After writing the header, MERGESPALL writes the spall data to the new output text file.

For the CRA-2004 PABC, MERGESPALL was executed four times per replicate (data for the 4 DPSs are merged) for a total of three separate spallings data files (one for each replicate). The CRA-2004 PABC MERGESPALL files were developed using DRSPALL Version 1.10. Note that DRSPALL Version 1.10 used a variable zone size with a zone size growth rate of 1.5. DRSPALL Version 1.22 uses a constant zone size (i.e., a growth rate of 1.0) as described in Section 3.

4.1.2. DRSPALL Results

The VMS DRSPALL results (i.e., the MERGESPALL spallings data files developed using DRSPALL Version 1.10) were produced as part of the CRA-2004 PABC, and provided input for all subsequent PAs including the CRA-2014. With the migration of PA codes to a new operating platform (see Section 2.3), a new set of DRSPALL results were developed on Solaris for PABC-2009 using DRSPALL Version 1.21. Both the VMS DRSPALL (Version 1.10) and the migrated DRSPALL (Version 1.21) used zone size parameters $\Delta r = 0.004$ m, $L_t = 0.02$ m, and $\Delta z = 2.0$ m as recommended by Lord et al. (2006, Section 5.7) with a variable zone size.

Using the calculation procedure described in Section 4.1.1, the final spallings volumes calculated for PABC-2009 using DRSPALL Version 1.22 (using a constant zone size with zone size parameters Δr = 0.004 m, L_t = 0.04 m, and Δz = 2.0 m as recommended by Kicker 2015) are listed in Appendix C (Tables C-1, C-2, and C-3). The tables correspond to the spallings data files *mspall_drs_PABC09_r1.out*, *mspall_drs_PABC09_r2.out*, and *mspall_drs_PABC09_r3.out*, respectively, and are located in the CVS repository at /nfs/data/CVSLIB/WIPP_ANALYSES/ PABC09/DRSPALL/Output. These volumes were calculated by the procedures outlined in Sections 4.1.1.4 and 4.1.1.5. All spallings volumes statistics presented in the following sections were calculated using these volumes, which represent the volumes after processing by MERGESPALL and not the volumes listed in the DRSPALL output files.

4.1.2.1. DPS 1 Results

For DPS 1, the initial repository pressure was set to 10 MPa. All DPS 1 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 et al. (2003) 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 can occur.

4.1.2.2. DPS 2 Results

For DPS 2 the initial repository pressure was set to 12 MPa. Table 4-1 lists the DRSPALL volume statistics from the modified DRSPALL (Version 1.22), the migrated DRSPALL (Version 1.21), and the VMS DRSPALL (Version 1.10). They are separated by replicate, and the pooled statistics (combined replicates 1, 2, and 3) are presented, as well. Of the modified DRSPALL replicates, replicate 1 has the largest individual spall volume (9.68 m^3) and the largest mean volume (0.360 m^3). All three replicates yield similar percentages of nonzero spall volume vectors (66% to 68%), and the percentages of large spall volume vectors are also similar, ranging from 3% to 5%.

The modified DRSPALL mean spall volume exceeds the VMS DRSPALL mean spall volume by approximately 86% (0.15 m^3). The largest DPS 2 spall volume from the VMS DRSPALL is 7.71 m^3, and the largest DPS 2 spall volume from the modified DRSPALL is 9.68 m^3. The modified DRSPALL have a much higher percentage of nonzero spall vectors (67% versus 21%), while both the modified and VMS DRSPALL vectors yield a similar percentage of spall volumes greater than 1 m^3 (4%). Note that while the migrated DRSPALL (Version 1.21) maximum and mean spall volumes are lower than the VMS DRSPALL (Version 1.10), their cumulative distributions are essentially identical as shown in Figure 4-4.

4.1.2.2.1. Exception Runs – Increased Run Times

As discussed in Section 4.1.1.2, the cavity radius (CAVRAD) is the key indicator for determining when the spallings process has ceased. Table 4-2 lists the vectors that have CAVRAD values that increased after 500 seconds of the DRSPALL simulation, and Figures 4-5, 4-6, and 4-7 plot the DPS 2 cavity radii for all vectors versus time for the modified DRSPALL

(Version 1.22). As shown in these figures, all vectors are no longer increasing after 600 seconds.

Table 4-1. Statistics for DRSPALL Volumes: DPS 2.

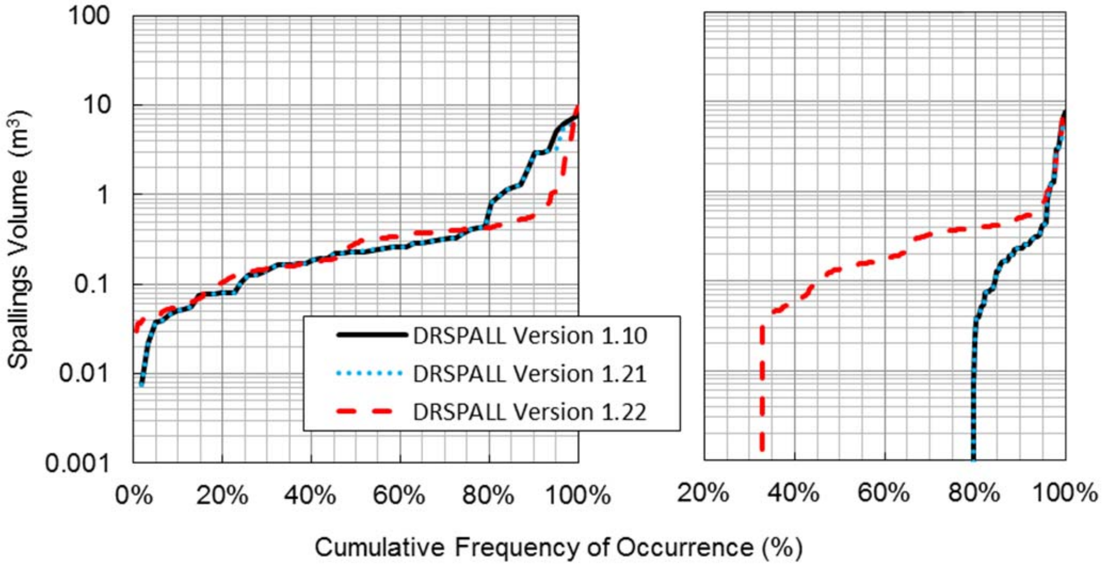
Replicate	**Maximum (m^3)**	**Mean (m^3)**	**Median (m^3)**	**% of Vectors with Volumes > 0 m^3**	**% of Vectors with Volumes > 1 m^3**
Modified DRSPALL[1], Version 1.22 (combined R1, R2, and R3)	9.68	0.320	0.138	67	4
Modified DRSPALL – R1	9.68	0.360	0.145	68	5
Modified DRSPALL – R2	7.07	0.262	0.128	68	3
Modified DRSPALL – R3	7.96	0.338	0.108	66	5
Migrated DRSPALL[2], Version 1.21 (combined R1, R2, and R3)	5.99	0.156	0.000	21	4
Migrated DRSPALL – R1	5.99	0.179	0.000	21	4
Migrated DRSPALL – R2	5.83	0.140	0.000	21	3
Migrated DRSPALL – R3	5.97	0.148	0.000	20	4
VMS DRSPALL[3], Version 1.10 (combined R1, R2, and R3)	7.71	0.172	0.000	21	4
VMS DRSPALL – R1	7.71	0.196	0.000	21	4
VMS DRSPALL – R2	6.27	0.163	0.000	21	3
VMS DRSPALL – R3	6.86	0.157	0.000	20	4

NOTES:

[1] Modified DRSPALL (Version 1.22) spallings volumes are listed in Appendix C and correspond to data files *mspall_drs_PABC09_r1.out*, *mspall_drs_PABC09_r2.out*, and *mspall_drs_PABC09_r3.out*, which are stored in the CVS repository at /nfs/data/CVSLIB/WIPP_ANALYSES/PABC09/DRSPALL/Output.

[2] Migrated DRSPALL (Version 1.21) spallings volumes are described by Kirchner, Gilkey, and Long (2013). Spallings data (files *mspall_drs_PABC09_r1.out*, *mspall_drs_PABC09_ r2.out*, and *mspall_drs_PABC09_r3.out*) are stored in the CVS repository at /nfs/data/CVSLIB/WIPP_ARCHIVES/PABC09/DRSPALL/Output (Revision 0).

[3] VMS DRSPALL (Version 1.10) spallings volumes are from Vugrin (2005, Appendix D) and correspond to the spallings data files *MERGESPALL_DRS_CRA1BC_R1.OUT*, *MERGESPALL_DRS_CRA1BC_R2.OUT*, and *MERGESPALL_DRS_CRA1BC_R3.OUT*, which are stored in the SCMS library PACMS2:[CMS_CRA1BC.CRA1BC_DRS] in the class CRA1BC-0.



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

b. All spallings results — includes simulations with no spallings

Figure 4-4. The Cumulative Distributions of DRSPALL Spallings Volumes for Replicates 1, 2, and 3 at a Repository Pressure of 12 MPa (DPS 2).

Table 4-2. Vectors with Increasing CAVRAD Values after 500 s: DPS 2.

Replicate 1 Vectors	Replicate 2 Vectors	Replicate 3 Vectors
V032	V041	V025

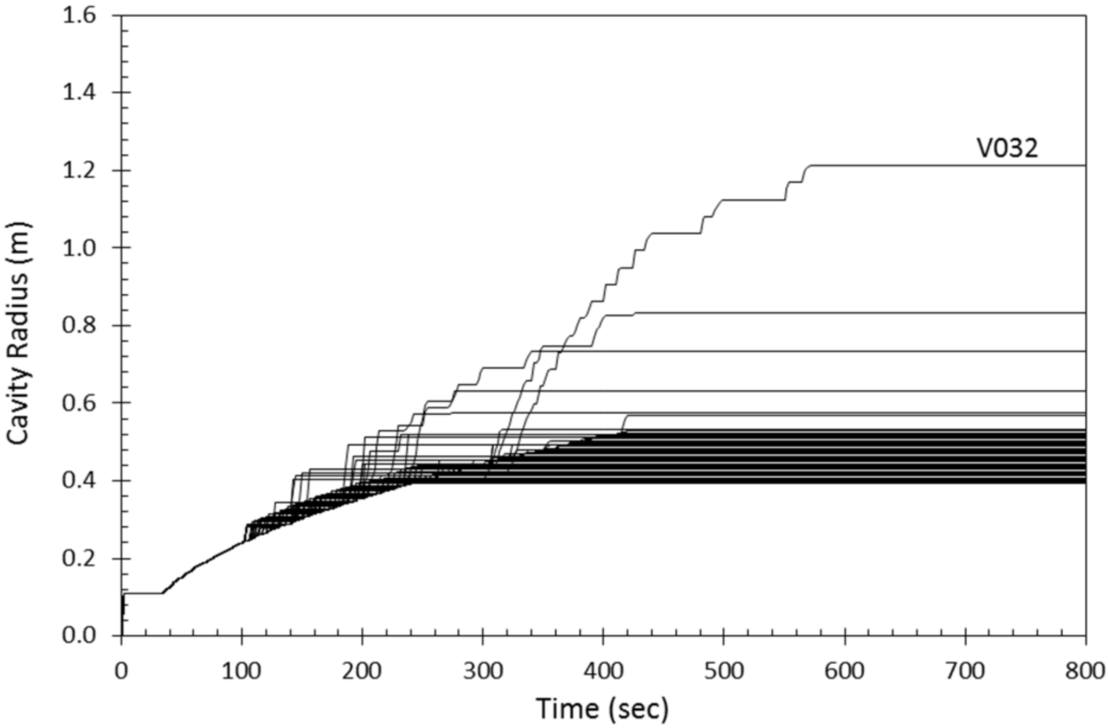


Figure 4-5. Cavity Radius Versus Time: Replicate 1, DPS 2.

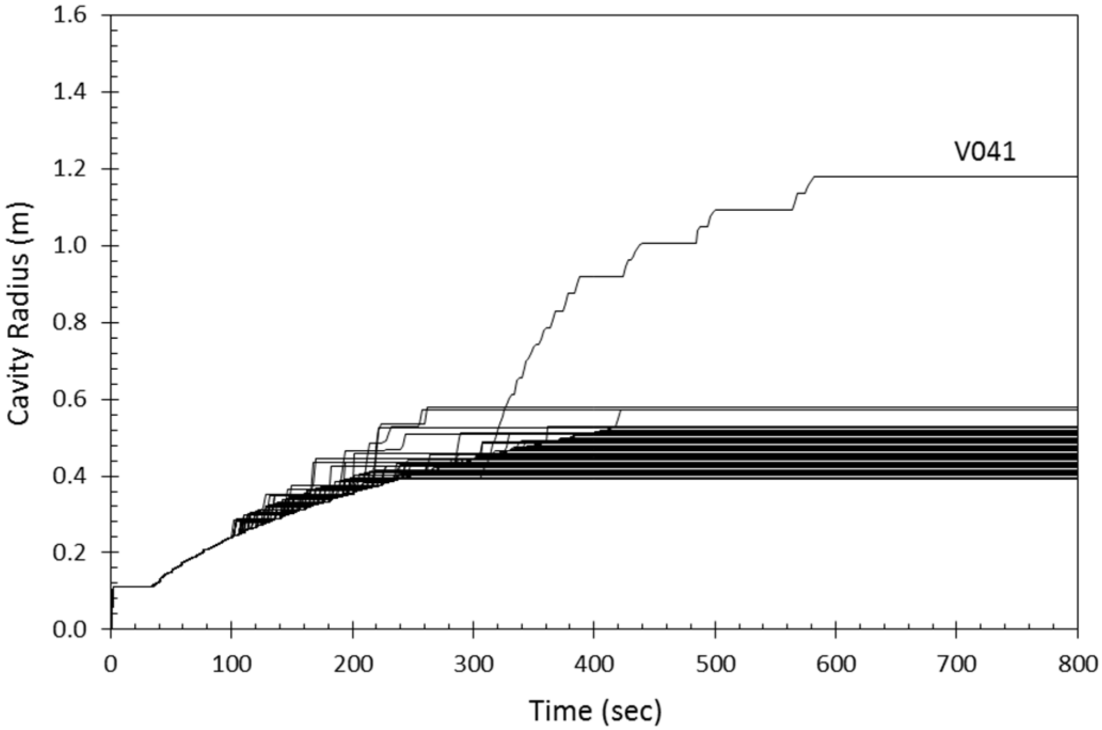


Figure 4-6. Cavity Radius Versus Time: Replicate 2, DPS 2.

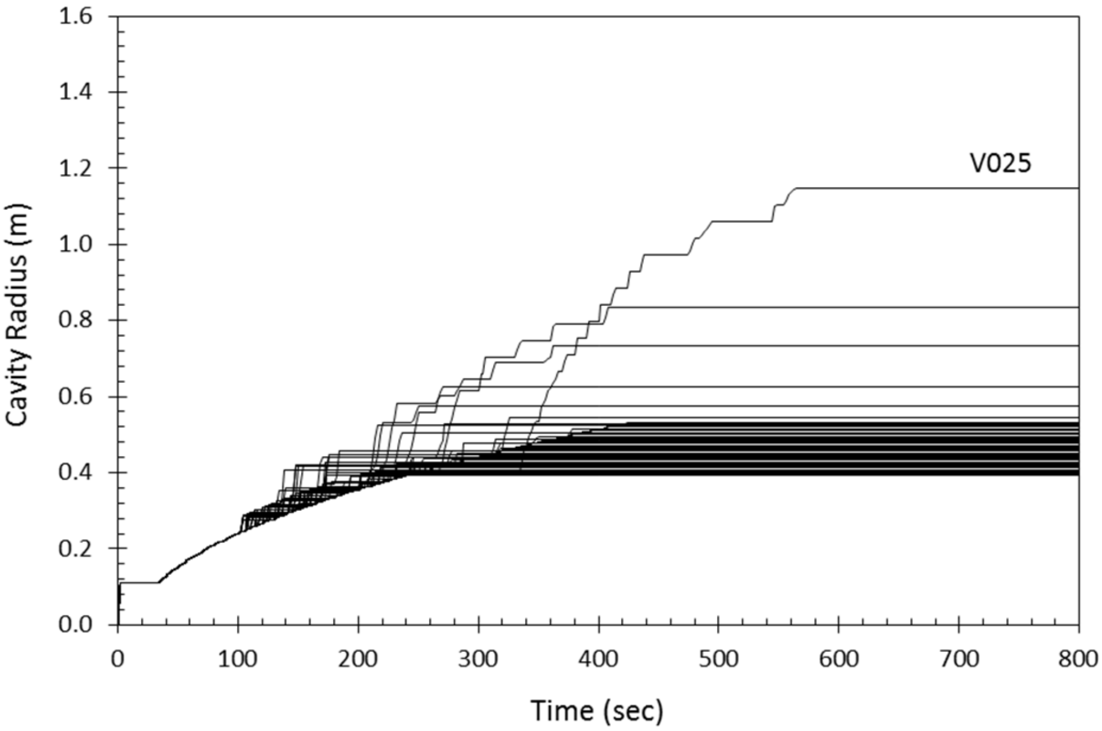


Figure 4-7. Cavity Radius Versus Time: Replicate 3, DPS 2.

4.1.2.2.2. Exception Runs – Cylindrical Model Restarts

Table 4-3 lists the vectors that were restarted using the cylindrical model and the values of REPOSTCK and CAVRAD after 600 seconds using the spherical model for the modified DRSPALL (Version 1.22). Additionally, the final spall volume calculated for each vector is broken down into the contributions from the spherical model run and the cylindrical model restart.

Table 4-3. DPS 2 Cylindrical Model Restarts.

Replicate - Vector	REPOSTCK (m)	Final CAVRAD (m)	Spherical Volume (m^3)	Cylindrical Volume (m^3)	Total Volume (m^3)
R1-V032	1.10	1.21	9.676	0.000	9.676
R2-V041	0.92	1.18	7.070	0.000	7.070
R3-V025	0.99	1.15	7.958	0.000	7.958

4.1.2.3. DPS 3 Results

For DPS 3 the initial repository pressure was set to 14 MPa. Table 4-4 lists the DRSPALL volume statistics from the modified DRSPALL (Version 1.22), the migrated DRSPALL (Version 1.21), and the VMS DRSPALL (Version 1.10). They are separated by replicate, and the pooled statistics (combined replicates 1, 2, and 3) are presented, as well. Of the modified DRSPALL replicates, replicate 3 has the largest individual spall volume (10.18 m^3), while replicate 1 has the largest mean volume (1.243 m^3). All three replicates yield similar percentages of nonzero spall volume vectors (approximately 74%), and the percentages of large spall volume vectors are also similar, ranging from 23% to 28%.

The modified DRSPALL mean spall volume exceeds the VMS DRSPALL mean spall volume by approximately 64% (0.42 m^3). The largest DPS 3 spall volume from both the VMS and migrated DRSPALL is 11.83 m^3, and the largest DPS 3 spall volume from the modified DRSPALL is 10.18 m^3. Both the VMS and migrated DRSPALL have a slightly higher percentage of nonzero spall vectors compared to the modified DRSPALL (76% versus 74%), and 13% of the VMS and migrated DRSPALL vectors yield spall volumes greater than 1 m^3, whereas 26% of the modified DRSPALL vectors result in spall volumes exceeding 1 m^3.

Table 4-4. Statistics for DRSPALL Volumes: DPS 3.

Replicate	Maximum (m^3)	Mean (m^3)	Median (m^3)	% of Vectors with Volumes > 0 m^3	% of Vectors with Volumes > 1 m^3
Modified DRSPALL[1], Version 1.22 (combined R1, R2, and R3)	10.18	1.089	0.599	74	26
Modified DRSPALL – R1	10.00	1.243	0.643	74	28
Modified DRSPALL – R2	9.43	0.928	0.592	74	23
Modified DRSPALL – R3	10.18	1.097	0.548	74	28
Migrated DRSPALL[2], Version 1.21 (combined R1, R2, and R3)	11.83	0.657	0.160	76	13
Migrated DRSPALL – R1	11.83	0.745	0.162	76	13
Migrated DRSPALL – R2	7.11	0.507	0.156	77	11
Migrated DRSPALL – R3	8.86	0.718	0.166	76	16
VMS DRSPALL[3], Version 1.10 (combined R1, R2, and R3)	11.83	0.665	0.160	76	13
VMS DRSPALL – R1	11.83	0.745	0.162	76	13
VMS DRSPALL – R2	7.72	0.530	0.156	77	11
VMS DRSPALL – R3	8.86	0.721	0.166	76	16

NOTES:

[1] Modified DRSPALL (Version 1.22) spallings volumes are listed in Appendix C and correspond to data files *mspall_drs_PABC09_r1.out*, *mspall_drs_PABC09_r2.out*, and *mspall_drs_PABC09_r3.out*, which are stored in the CVS repository at /nfs/data/CVSLIB/WIPP_ANALYSES/PABC09/DRSPALL/Output.

[2] Migrated DRSPALL (Version 1.21) spallings volumes are described by Kirchner, Gilkey, and Long (2013). Spallings data (files *mspall_drs_PABC09_r1.out*, *mspall_drs_PABC09_ r2.out*, and *mspall_drs_PABC09_r3.out*) are stored in the CVS repository at /nfs/data/CVSLIB/WIPP_ARCHIVES/PABC09/DRSPALL/Output (Revision 0).

[3] VMS DRSPALL (Version 1.10) spallings volumes are from Vugrin (2005, Appendix D) and correspond to the spallings data files *MERGESPALL_DRS_CRA1BC_R1.OUT*, *MERGESPALL_DRS_CRA1BC_R2.OUT*, and *MERGESPALL_DRS_CRA1BC_R3.OUT*, which are stored in the SCMS library PACMS2:[CMS_CRA1BC.CRA1BC_DRS] in the class CRA1BC-0.

The cumulative distributions of DRSPALL spallings volumes for DPS 3 (repository pressure of 14 MPa) are shown in Figure 4-8.

4.1.2.3.1. Exception Runs – Increased Run Times

As discussed in Section 4.1.1.2, the cavity radius (CAVRAD) is the key indicator for determining when the spallings process has ceased. Table 4-5 lists the vectors that have CAVRAD values that increased after 500 seconds of the DRSPALL simulation, and Figures 4-9, 4-10, and 4-11 plot the DPS 3 cavity radii for all vectors versus time for the modified DRSPALL (Version 1.22). As shown in these figures, all vectors are no longer increasing after 600 seconds.

4.1.2.3.2. Exception Runs – Cylindrical Model Restarts

Table 4-6 lists the vectors that were restarted using the cylindrical model and the values of REPOSTCK and CAVRAD after 600 seconds using the spherical model for the modified DRSPALL (Version 1.22). Additionally, the final spall volume calculated for each vector is broken down into the contributions from the spherical model run and the cylindrical model restart.

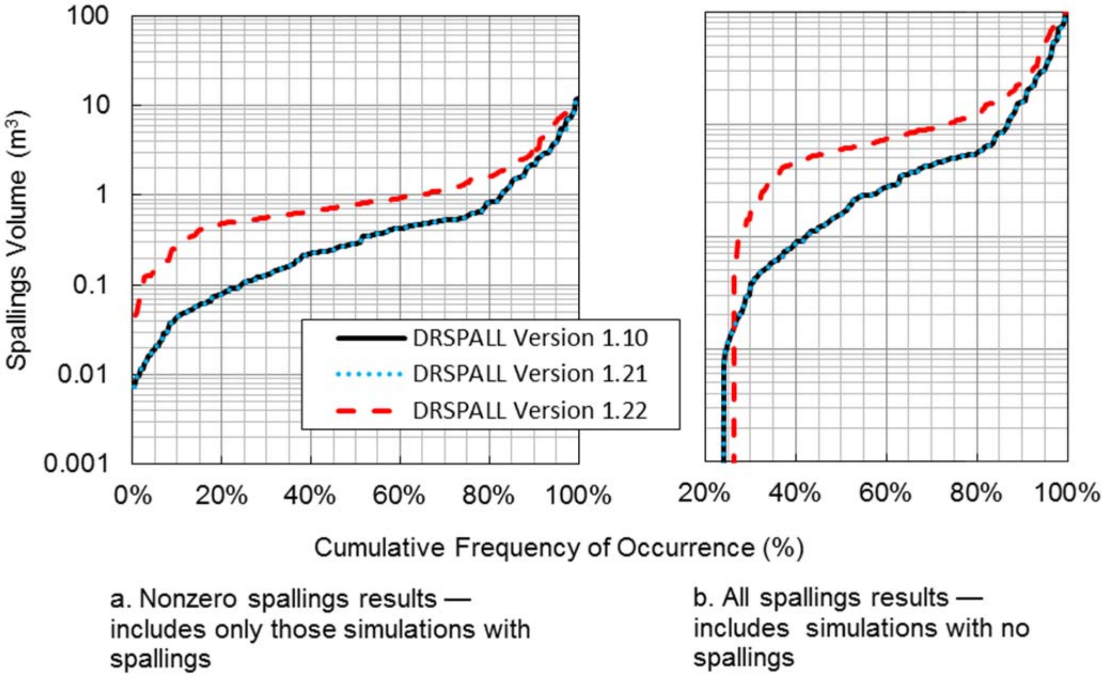


Figure 4-8. The Cumulative Distributions of DRSPALL Spallings Volumes for Replicates 1, 2, and 3 at a Repository Pressure of 14 MPa (DPS 3).

Table 4-5. Vectors with Increasing CAVRAD Values after 500 s: DPS 3.

Replicate 1 Vectors	Replicate 2 Vectors	Replicate 3 Vectors
V032	V041	V025

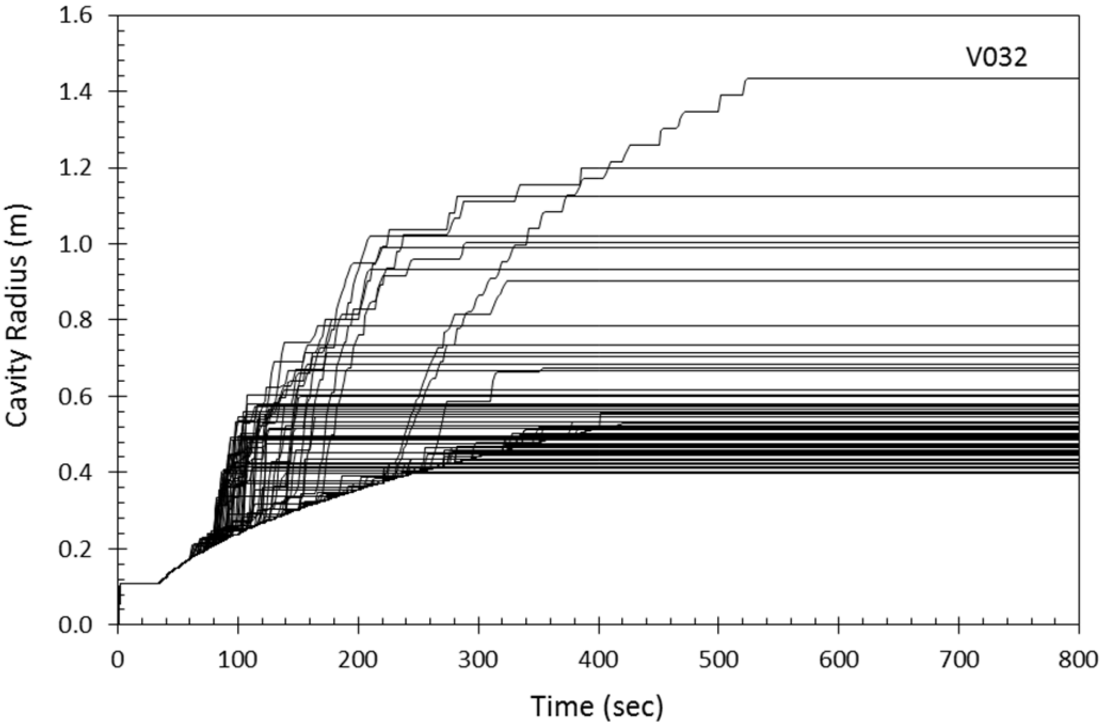


Figure 4-9. Cavity Radius Versus Time: Replicate 1, DPS 3.

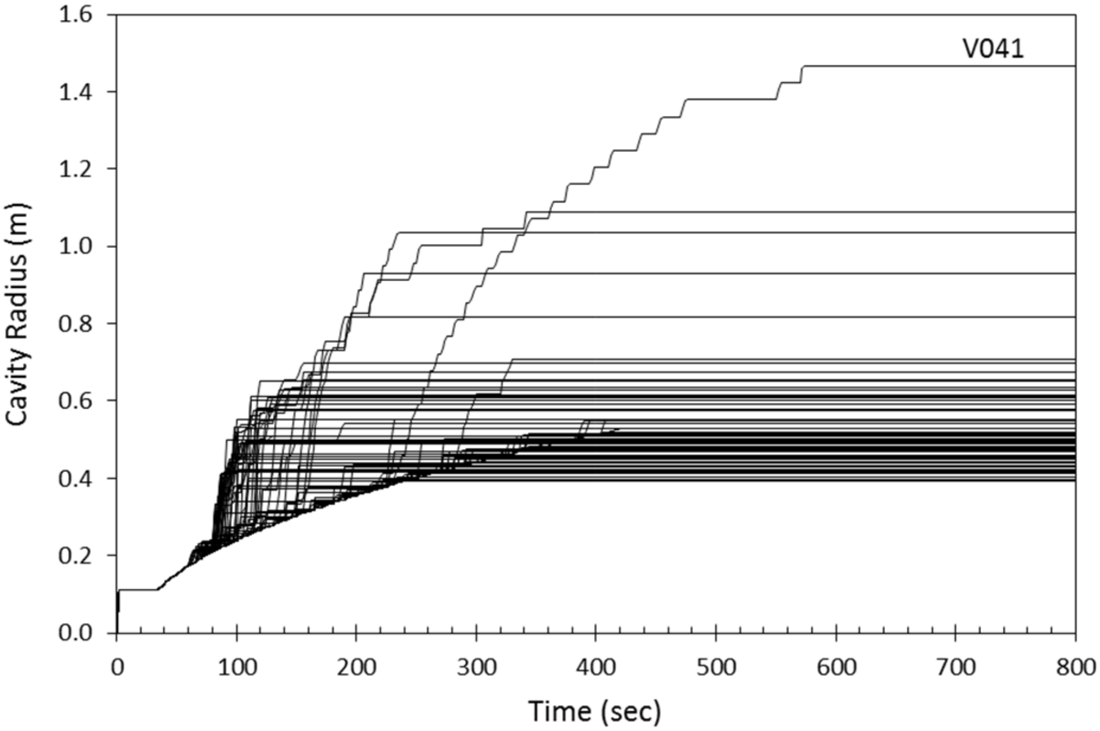


Figure 4-10. Cavity Radius Versus Time: Replicate 2, DPS 3.

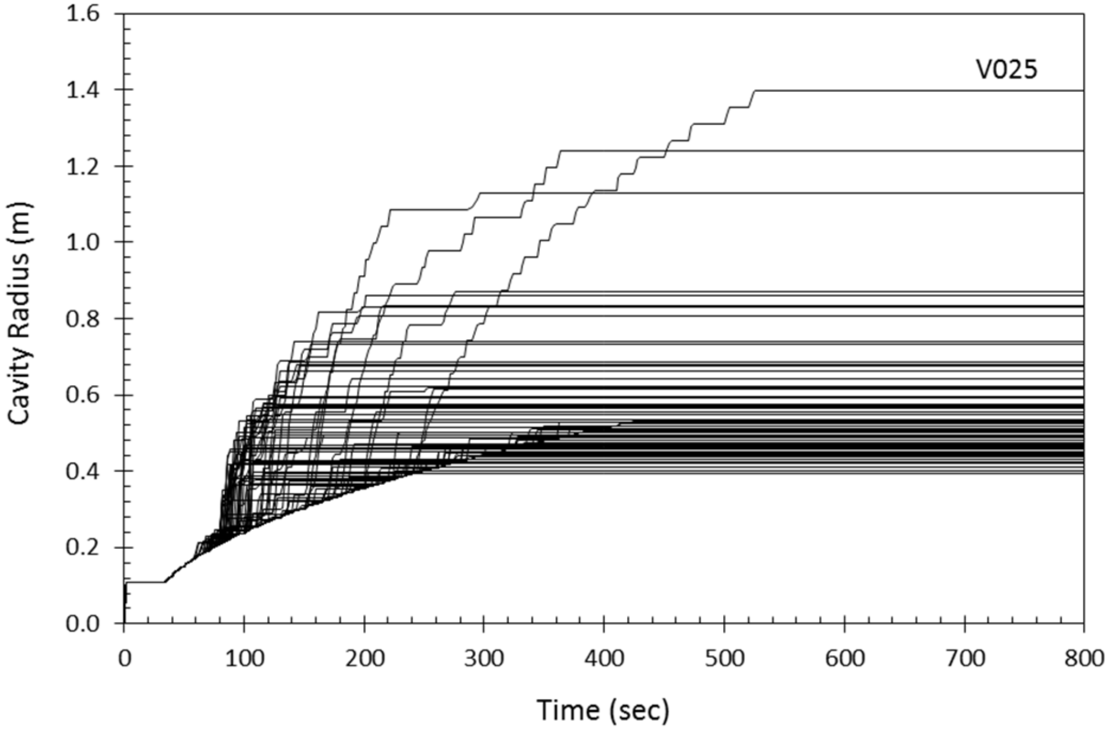


Figure 4-11. Cavity Radius Versus Time: Replicate 3, DPS 3.

Table 4-6. DPS 3 Cylindrical Model Restarts.

Replicate - Vector	REPOSTCK (m)	Final CAVRAD (m)	Spherical Volume (m^3)	Cylindrical Volume (m^3)	Total Volume (m^3)
R1-V032	1.10	1.43	9.996	0.000	9.996
R1-V059	1.06	1.20	9.262	0.000	9.262
R2-V041	0.92	1.47	6.749	0.000	6.749
R2-V071	0.92	0.93	7.027	0.000	7.027
R2-V086	0.95	1.04	7.663	0.000	7.663
R3-V001	0.94	1.24	7.486	0.996	8.482
R3-V025	0.99	1.40	8.018	0.000	8.018

4.1.2.4. DPS 4 Results

For DPS 4 the initial repository pressure was set to 14.8 MPa. Table 4-7 lists the DRSPALL volume statistics from the modified DRSPALL (Version 1.22). For comparison, the statistics from the VMS DRSPALL (Version 1.10) and migrated DRSPALL (Version 1.21) are also included. Of the modified DRSPALL replicates, replicate 2 has the largest individual spall volume (15.82 m^3), and replicate 1 has the largest mean volume (1.672 m^3). All three replicates yield similar percentages of nonzero spall volume vectors (approximately 75%), and the percentages of large spall volume vectors range from 35% to 45%.

Table 4-7. Statistics for DRSPALL Volumes: DPS 4.

Replicate	Maximum (m^3)	Mean (m^3)	Median (m^3)	% of Vectors with Volumes > 0 m^3	% of Vectors with Volumes > 1 m^3
Modified DRSPALL[1], Version 1.22 (combined R1, R2, and R3)	15.82	1.471	0.772	75	40
Modified DRSPALL – R1	10.81	1.672	0.811	75	45
Modified DRSPALL – R2	15.82	1.321	0.744	75	40
Modified DRSPALL – R3	13.33	1.420	0.753	74	35
Migrated DRSPALL[2], Version 1.21 (combined R1, R2, and R3)	14.54	0.968	0.318	79	20
Migrated DRSPALL – R1	14.54	1.076	0.320	79	22
Migrated DRSPALL – R2	9.89	0.764	0.327	79	16
Migrated DRSPALL – R3	11.90	1.065	0.312	78	23
VMS DRSPALL[3], Version 1.10 (combined R1, R2, and R3)	14.54	0.978	0.318	79	20
VMS DRSPALL – R1	14.54	1.077	0.320	79	22
VMS DRSPALL – R2	9.89	0.789	0.327	79	16
VMS DRSPALL – R3	11.90	1.068	0.312	78	23

NOTES:

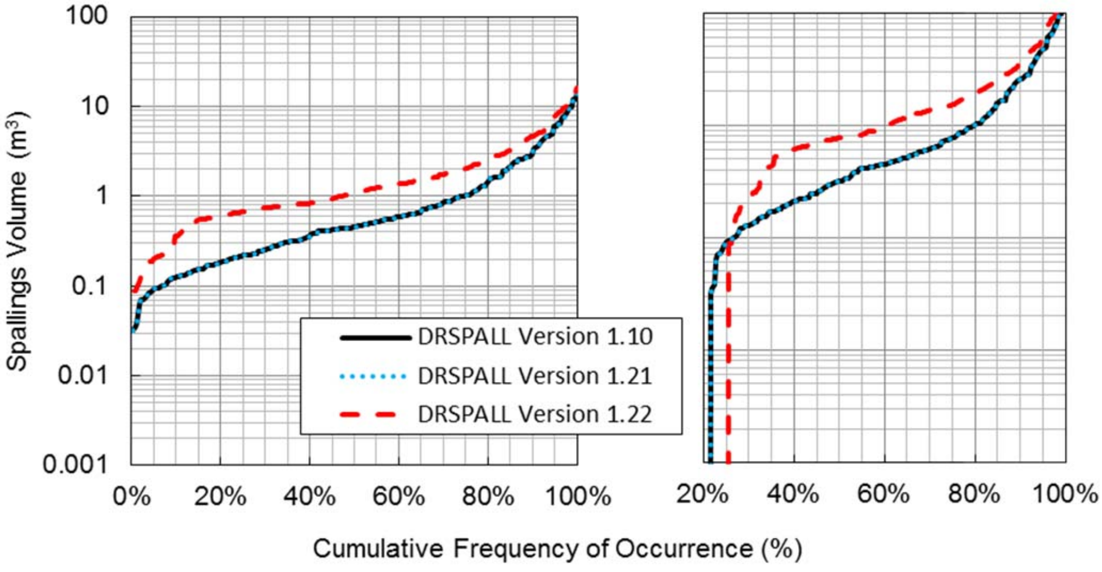
[1] Modified DRSPALL (Version 1.22) spallings volumes are listed in Appendix C and correspond to data files *mspall_drs_PABC09_r1.out*, *mspall_drs_PABC09_r2.out*, and *mspall_drs_PABC09_r3.out*, which are stored in the CVS repository at /nfs/data/CVSLIB/WIPP_ANALYSES/PABC09/DRSPALL/Output.

[2] Migrated DRSPALL (Version 1.21) spallings volumes are described by Kirchner, Gilkey, and Long (2013). Spallings data (files *mspall_drs_PABC09_r1.out*, *mspall_drs_PABC09_r2.out*, and *mspall_drs_PABC09_r3.out*) are stored in the CVS repository at /nfs/data/CVSLIB/WIPP_ARCHIVES/PABC09/DRSPALL/Output (Revision 0).

[3] VMS DRSPALL (Version 1.10) spallings volumes are from Vugrin (2005, Appendix D) and correspond to the spallings data files *MERGESPALL_DRS_CRA1BC_R1.OUT*, *MERGESPALL_DRS_CRA1BC_R2.OUT*, and *MERGESPALL_DRS_CRA1BC_R3.OUT*, which are stored in the SCMS library PACMS2:[CMS_CRA1BC.CRA1BC_DRS] in the class CRA1BC-0.

The modified DRSPALL mean spall volume exceeds both the VMS and migrated DRSPALL mean spall volumes by approximately 50% (0.49 m^3). The largest DPS 4 spall volume from both the VMS and migrated DRSPALL is 14.54 m^3, and the largest DPS 4 spall volume from the modified DRSPALL is 15.82 m^3. Both the VMS and migrated DRSPALL have a slightly higher percentage of nonzero spall vectors compared to the modified DRSPALL (79% versus 75%), and 20% of the VMS and migrated DRSPALL vectors yield spall volumes greater than 1 m^3, whereas 40% of the modified DRSPALL vectors result in spall volumes exceeding 1 m^3.

The cumulative distributions of DRSPALL spallings volumes for DPS 4 (repository pressure of 14.8 MPa) are shown in Figure 4-12.



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

b. All spallings results — includes simulations with no spallings

Figure 4-12. The Cumulative Distributions of DRSPALL Spallings Volumes for Replicates 1, 2, and 3 at a Repository Pressure of 14.8 MPa (DPS 4).

4.1.2.4.1. Exception Runs – Increased Run Times

Table 4-8 lists the vectors that have CAVRAD values that continued to increase after 500 seconds of the DRSPALL simulation, and Figures 4-13, 4-14, and 4-15 plot the DPS 4 cavity radii for all vectors versus time for the modified DRSPALL (Version 1.22). As shown in these figures, all vectors are no longer increasing after 600 seconds. For each of the vectors listed in Table 4-8, their respective CAVRAD values exceed their respective repository height (REPOSTCK) values within the first 600 seconds of the simulation. These vectors were restarted with the cylindrical model and are addressed in Section 4.1.2.4.2.

Table 4-8. Vectors with Increasing CAVRAD Values after 500 s: DPS 4.

Replicate 1 Vectors	Replicate 2 Vectors	Replicate 3 Vectors
V032	V041	V025

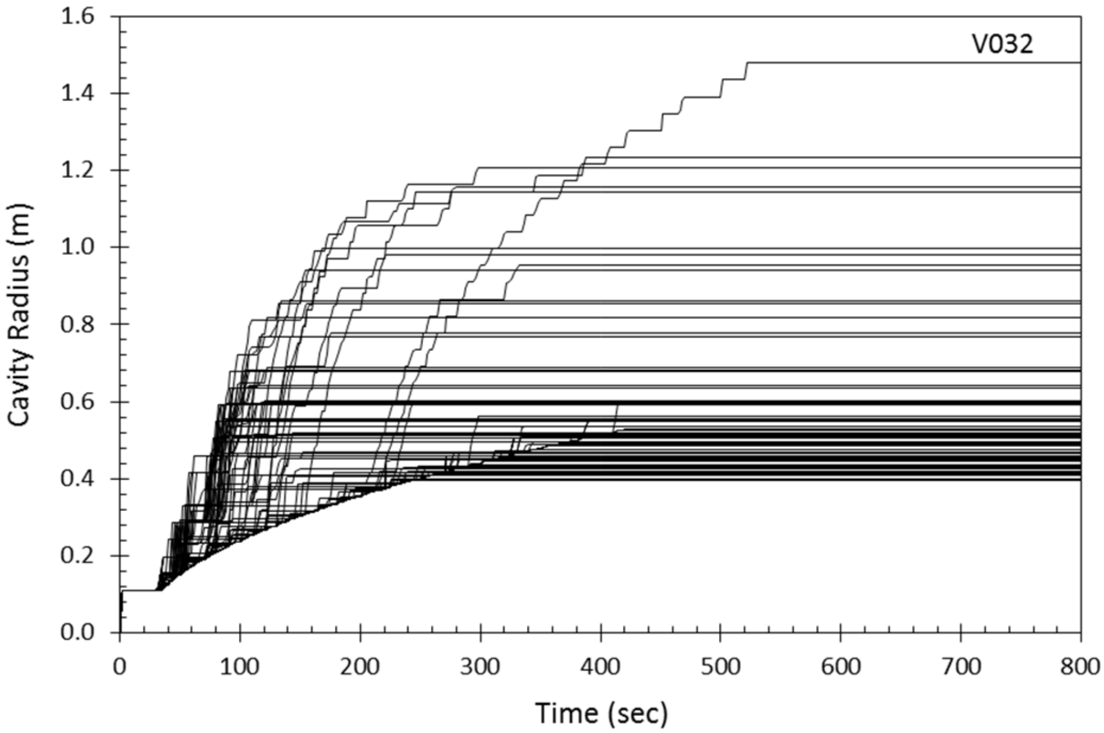


Figure 4-13. Cavity Radius Versus Time: Replicate 1, DPS 4.

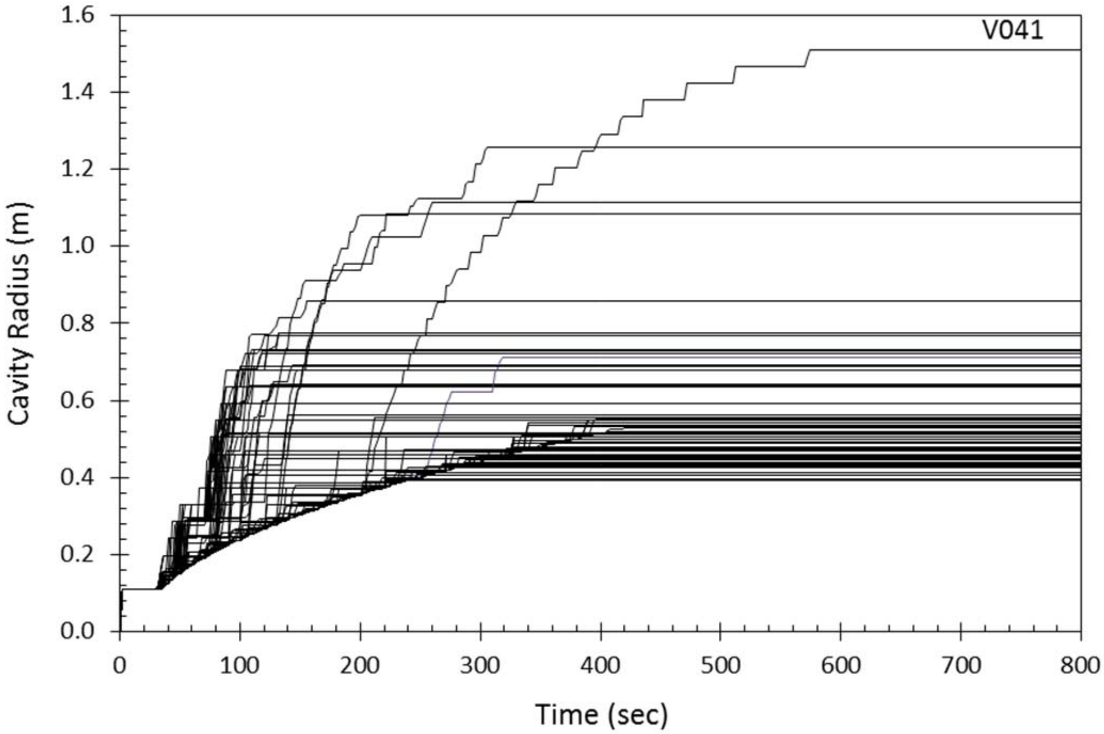


Figure 4-14. Cavity Radius Versus Time: Replicate 2, DPS 4.

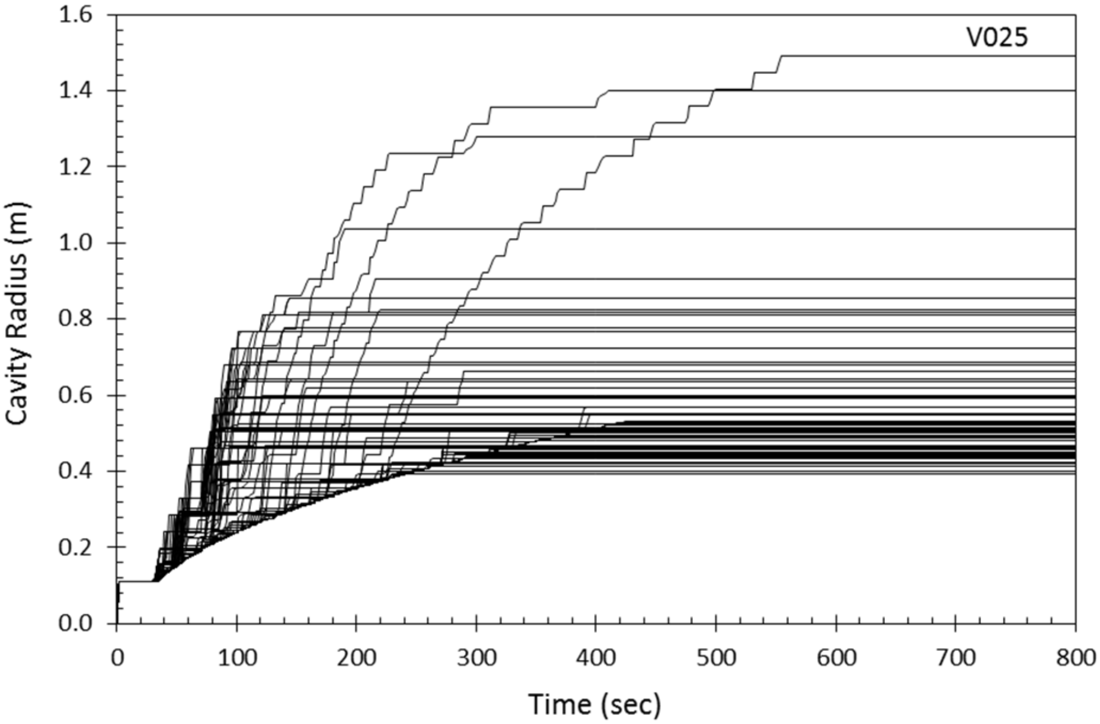


Figure 4-15. Cavity Radius Versus Time: Replicate 3, DPS 4.

4.1.2.4.2. Exception Runs – Cylindrical Model Restarts

Table 4-9 lists the DPS 4 vectors that were restarted using the cylindrical model and the values of REPOSTCK and CAVRAD after 600 seconds using the spherical model for the modified DRSPALL (Version 1.22). Additionally, the spall volume for each vector is broken down into the contributions from the spherical model run and the cylindrical model restart.

Table 4-9. DPS 4 Cylindrical Model Restarts.

Replicate - Vector	REPOSTCK (m)	Final CAVRAD (m)	Spherical Volume (m^3)	Cylindrical Volume (m^3)	Total Volume (m^3)
R1-V002	1.07	1.16	9.682	1.129	10.811
R1-V028	0.92	0.94	7.473	0.000	7.473
R1-V032	1.10	1.48	10.229	0.000	10.229
R1-V059	1.06	1.23	9.426	0.000	9.426
R2-V025	1.11	1.11	10.183	0.000	10.183
R2-V041	0.92	1.51	6.748	9.069	15.817
R2-V071	0.92	1.08	7.051	0.000	7.051
R2-V086	0.95	1.26	8.045	1.010	9.055
R3-V001	0.94	1.40	7.698	0.996	8.694
R3-V025	0.99	1.49	8.036	0.000	8.036
R3-V067	1.15	1.28	12.123	1.204	13.326
R3-V068	0.92	1.04	7.668	0.000	7.668

It should be noted that vector 32 of replicate 1, vector 41 of replicate 2, and vector 25 of replicate 3 were restarted with the cylindrical model for DPSs 2, 3, and 4. If DRSPALL recorded SPLVOL2 values at the precise time the CAVRAD equaled REPOSTCK, the spherical volumes in Tables 4-3, 4-6, and 4-9 for the corresponding vectors should be equal because the hemispherical cavities that contribute to the spalling calculations would have the same radii (REPOSTCK) for DPS2, DPS3, and DPS4. However, SPLVOL2 is recorded only at discrete times, so spherical volumes are not precisely equal. This analysis handles this limitation in a conservative manner. When determining the volume contribution from the spherical run, MERGESPALL selected the SPLVOL2 value at the first time when CAVRAD *exceeded* REPOSTCK and then added the volume contribution from the cylindrical run. Thus, the SPLVOL2 volumes reported are actually slightly larger than the volume of the cavity when CAVRAD equals REPOSTCK.

4.1.2.5. Scenario 4 Scatter Plots

This section presents scatter plots of DPS 4 spall volumes calculated by the modified DRSPALL (Version 1.22) versus the uncertain sampled parameters waste porosity, waste permeability, waste particle diameter, and waste tensile strength. The sampled values of the uncertain parameters used in the modified DRSPALL calculations have not changed from the sampled values used in the VMS DRSPALL and are provided by Kicker (2015, Table 4). The final SPLVOL2 values have been pooled and are plotted against each input variable on a vector by vector basis. The final SPLVOL2 numbers correspond to numbers given in Tables C-1, C-2, and C-3 in Appendix C and the sampled parameters match the values provided by Vugrin (2005, Appendix A, Tables 11, 12, and 13). Scatter plots can give a rough visual indication of how these parameters affect the resulting spall volumes. DPS 4 plots are shown because the high pressure results in more vectors that contain spallings compared to the lower pressures. Scatter plots for DPS 3 yield similar conclusions.

Figure 4-16 indicates that the largest spall volumes occur when waste permeability is less than 1.00E-13 m^2, but larger permeability values result in a higher frequency of nonzero spall volumes. This observation can be explained as follows: the higher permeability values that were sampled result in less tensile stresses and less tensile failure but promote fluidization. Lower permeability leads to greater tensile stresses and tensile failure, but failed material may not be able to fluidize at this low permeability. Smaller particle diameter values (see Figure 4-17) tend to result in larger spall volumes and higher frequency of nonzero spall volumes. This can be explained by the particle diameter’s impact on fluidization velocities: smaller particle diameters lead to lower minimum fluidization velocities (Lord et al. 2006). No obvious correlations could be established between waste tensile strength and spall volume over the small sampled range of tensile strengths (Figure 4-18); Lord et al. (2003) reached this same conclusion. Lord et al. (2003) concluded that lower waste porosity values tended to correlate with larger spallings volumes for the 2004 Compliance Recertification Application (CRA-2004). For the modified DRSPALL results, a similar correlation is observed (Figure 4-19). The conclusions in this section using spallings volumes from the modified DRSPALL (Volume 1.22) are consistent with those made in Lord et al. (2003).

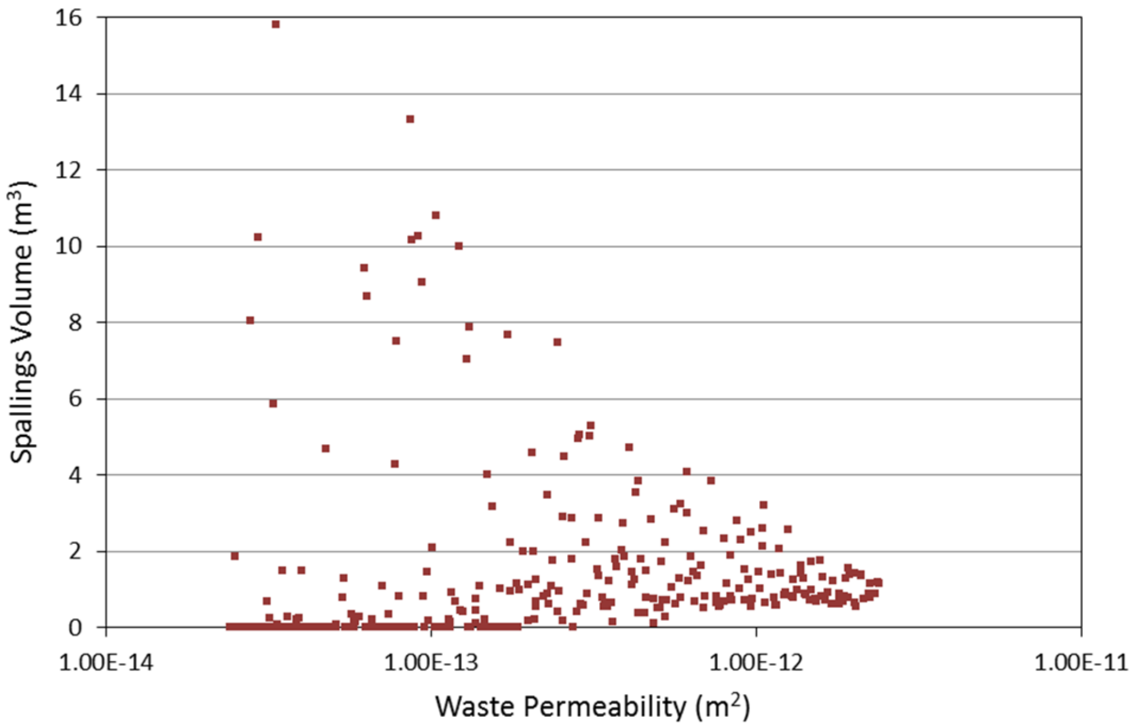


Figure 4-16. Scatter Plot of Pooled Vectors: Waste Permeability vs SPLVOL2.

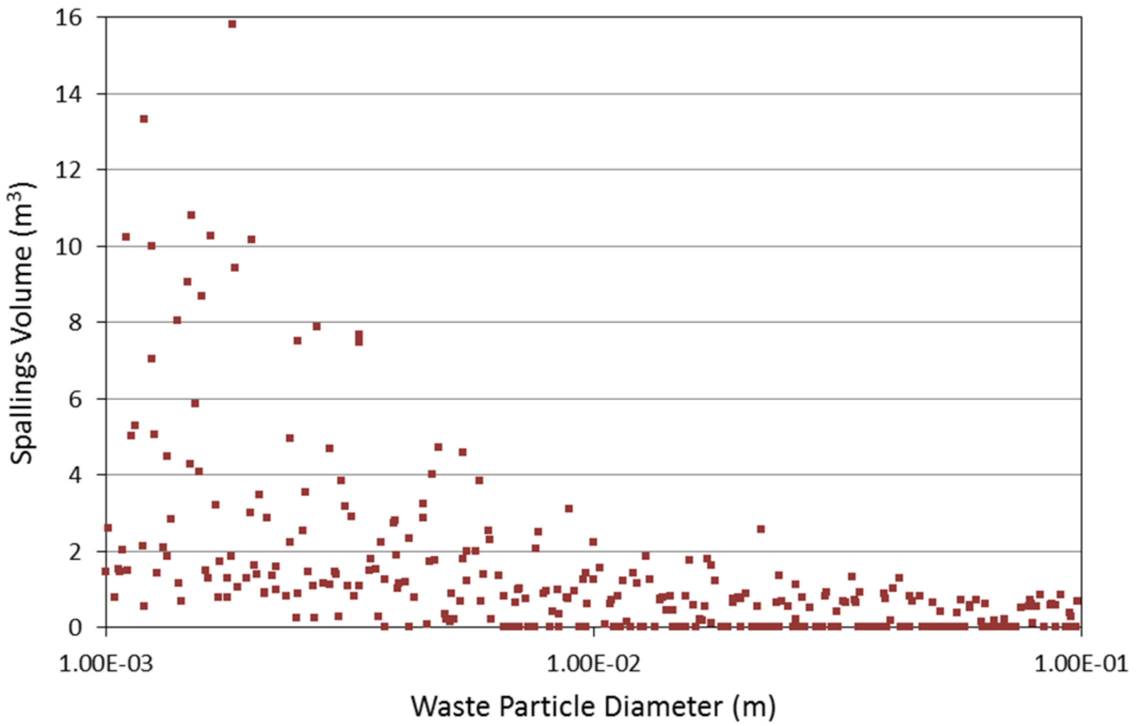


Figure 4-17. Scatter Plot of Pooled Vectors: Waste Particle Diameter vs SPLVOL2.

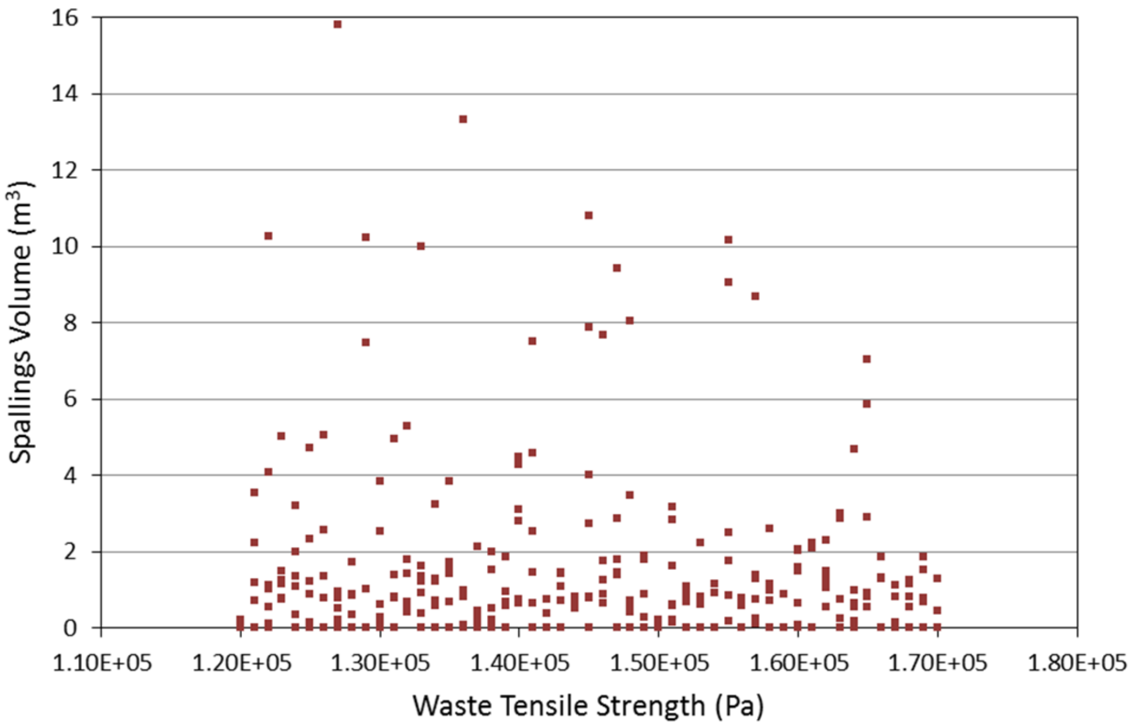


Figure 4-18. Scatter Plot of Pooled Vectors: Waste Tensile Strength vs SPLVOL2.

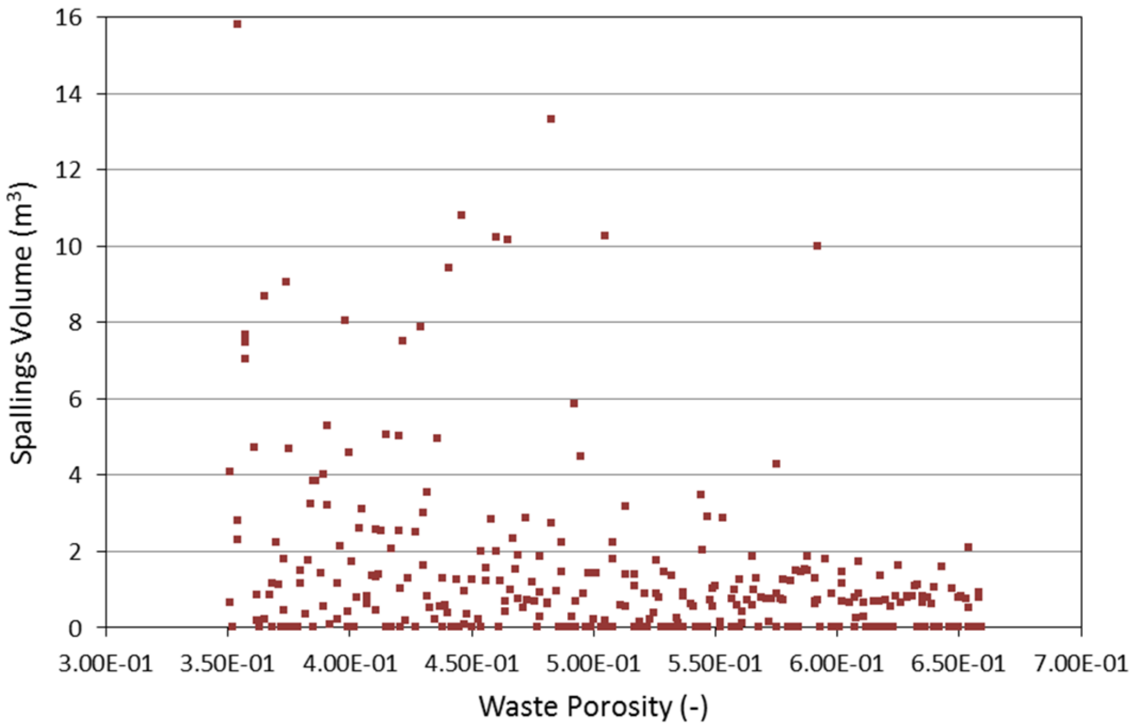


Figure 4-19. Scatter Plot of Pooled Vectors: Waste Porosity vs SPLVOL2.

4.1.3. Calculation of Repository Spall Volumes in CUTTINGS_S

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 in each realization by BRAGFLO. DRSPALL volumes used in the VMS PABC-2009, the migrated PABC-2009, the VMS CRA-2014, and the migrated CRA-2014 have been updated based on the modified DRSPALL code (Version 1.22) as described in Section 4.1.2 and listed in Appendix C.

PA code CUTTINGS_S is also used as a transfer program between the BRAGFLO Salado flow calculation and the BRAGFLO direct brine release (DBR) calculation. Results obtained by BRAGFLO for each realization in scenarios S1-BF to S5-BF (Camphouse 2013b) are used to initialize the flow field properties necessary for the calculation of DBRs. This requires that results obtained on the BRAGFLO grid be mapped appropriately to the DBR grid. Code CUTTINGS_S is used to transfer the appropriate scenario results obtained with BRAGFLO to the DBR calculation. These transferred flow results are used as initial conditions in the calculation of DBRs. As a result, intrusion scenarios and times used in the calculation of spallings volumes correspond to those used in the calculation of DBRs. Five intrusion scenarios are considered in the DBR calculations, and are listed in Table 4-10.

Table 4-10. PA Intrusion Scenarios Used in Calculating Direct Solids Releases.

Scenario	Conditioning (or 1st) Intrusion Time (year) and Type	Intrusion Times – Subsequent (year)
S1-DBR	None	100, 350, 1000, 3000, 5000, 10000
S2-DBR	350, E1	550, 750, 2000, 4000, 10000
S3-DBR	1000, E1	1200, 1400, 3000, 5000, 10000
S4-DBR	350, E2	550, 750, 2000, 4000, 10000
S5-DBR	1000, E2	1200, 1400, 3000, 5000, 10000

While CUTTINGS_S uses these standard DBR scenarios as a basis for its calculations, it does so to provide flow field results (generated with BRAGFLO) as initial conditions to the DBR calculation at each subsequent intrusion time. CUTTINGS_S does not model the intrusion scenario itself. Scenario S1-DBR corresponds to an initial intrusion into the repository, with repository flow conditions at the time of intrusion transferred from BRAGFLO scenario S1-BF results. Scenarios S2-DBR through S5-DBR are used to model an intrusion into a repository that has already been penetrated. The times at which intrusions are assumed to occur for each scenario are outlined in the last column of Table 4-10; six intrusion times are modeled for scenario S1-DBR, while five times are modeled for each of scenarios S2-DBR through S5-DBR.

4.1.3.1. PABC-2009 Spallings Volumes

Utilizing 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. Summary statistics of spallings volumes for the intrusion scenarios considered by CUTTINGS_S are shown in Table 4-11 for the PABC-2009

Table 4-11. Summary of PABC-2009 Spallings Volumes by Scenario.

		Scenarios					Total
		S1-DBR	S2-DBR	S3-DBR	S4-DBR	S5-DBR	
Updated PABC-2009 (Revision 1) Using DRSPALL Version 1.22							
R1	**Maximum [m^3]**	7.47	9.73	9.70	7.47	7.47	9.73
	Average nonzero volume [m^3]	0.84	0.73	0.80	0.77	0.78	0.79
	Number of nonzero volumes	244	225	232	107	166	974
	Percent of nonzero volumes	13.6%	15.0%	15.5%	7.1%	11.1%	12.5%
R2	**Maximum [m^3]**	2.53	2.24	2.23	2.03	2.07	2.53
	Average nonzero volume [m^3]	0.38	0.29	0.28	0.34	0.32	0.32
	Number of nonzero volumes	257	225	228	106	150	966
	Percent of nonzero volumes	14.3%	15.0%	15.2%	7.1%	10.0%	12.4%
R3	**Maximum [m^3]**	4.68	5.23	4.52	3.55	4.52	5.23
	Average nonzero volume [m^3]	0.61	0.41	0.34	0.38	0.41	0.44
	Number of nonzero volumes	222	214	228	103	150	917
	Percent of nonzero volumes	12.3%	14.3%	15.2%	6.9%	10.0%	11.8%
R1, R2, R3 Pooled	**Maximum [m^3]**	7.47	9.73	9.70	7.47	7.47	9.73
	Average nonzero volume [m^3]	0.61	0.48	0.48	0.50	0.51	0.52
	Number of nonzero volumes	723	664	688	316	466	2857
	Percent of nonzero volumes	13.4%	14.8%	15.3%	7.0%	10.4%	12.2%
Migrated PABC-2009 (Revision 0) Using DRSPALL Version 1.21							
R1	**Maximum [m^3]**	2.24	6.84	6.38	1.67	1.67	6.84
	Average nonzero volume [m^3]	0.37	0.51	0.46	0.30	0.37	0.42
	Number of nonzero volumes	142	118	111	59	76	506
	Percent of nonzero volumes	7.9%	7.9%	7.4%	3.9%	5.1%	6.5%
R2	**Maximum [m^3]**	2.36	2.76	1.86	2.29	1.96	2.76
	Average nonzero volume [m^3]	0.32	0.38	0.36	0.49	0.47	0.38
	Number of nonzero volumes	168	120	123	59	84	554
	Percent of nonzero volumes	9.3%	8.0%	8.2%	3.9%	5.6%	7.1%
R3	**Maximum [m^3]**	4.90	6.19	2.62	1.47	1.49	6.19
	Average nonzero volume [m^3]	0.53	0.39	0.28	0.30	0.28	0.38
	Number of nonzero volumes	156	114	119	45	71	505
	Percent of nonzero volumes	8.7%	7.6%	7.9%	3.0%	4.7%	6.5%
R1, R2, R3 Pooled	**Maximum [m^3]**	4.90	6.84	6.38	2.29	1.96	6.84
	Average nonzero volume [m^3]	0.40	0.42	0.37	0.37	0.38	0.39
	Number of nonzero volumes	466	352	353	163	231	1565
	Percent of nonzero volumes	8.6%	7.8%	7.8%	3.6%	5.1%	6.7%

Table 4-11. Summary of PABC-2009 Spallings Volumes by Scenario. (Continued)

		Scenarios					Total
		S1-DBR	S2-DBR	S3-DBR	S4-DBR	S5-DBR	
VMS PABC-2009 Using DRSPALL Version 1.10							
R1	Maximum [m^3]	2.24	8.29	7.97	1.67	1.67	8.29
	Average nonzero volume [m^3]	0.37	0.54	0.50	0.30	0.37	0.43
	Number of nonzero volumes	142	117	111	59	77	506
	Percent of nonzero volumes	7.9%	7.8%	7.4%	3.9%	5.1%	6.5%
R2	Maximum [m^3]	2.36	2.76	1.86	2.26	1.93	2.76
	Average nonzero volume [m^3]	0.32	0.39	0.37	0.50	0.47	0.39
	Number of nonzero volumes	168	122	122	57	84	553
	Percent of nonzero volumes	9.3%	8.1%	8.1%	3.8%	5.6%	7.1%
R3	Maximum [m^3]	4.91	6.23	2.62	1.47	1.49	6.23
	Average nonzero volume [m^3]	0.53	0.39	0.28	0.30	0.28	0.38
	Number of nonzero volumes	156	113	118	45	72	504
	Percent of nonzero volumes	8.7%	7.5%	7.9%	3.0%	4.8%	6.5%
R1, R2, R3 Pooled	Maximum [m^3]	4.91	8.29	7.97	2.26	1.93	8.29
	Average nonzero volume [m^3]	0.40	0.44	0.38	0.37	0.38	0.40
	Number of nonzero volumes	466	352	351	161	233	1563
	Percent of nonzero volumes	8.6%	7.8%	7.8%	3.6%	5.2%	6.7%

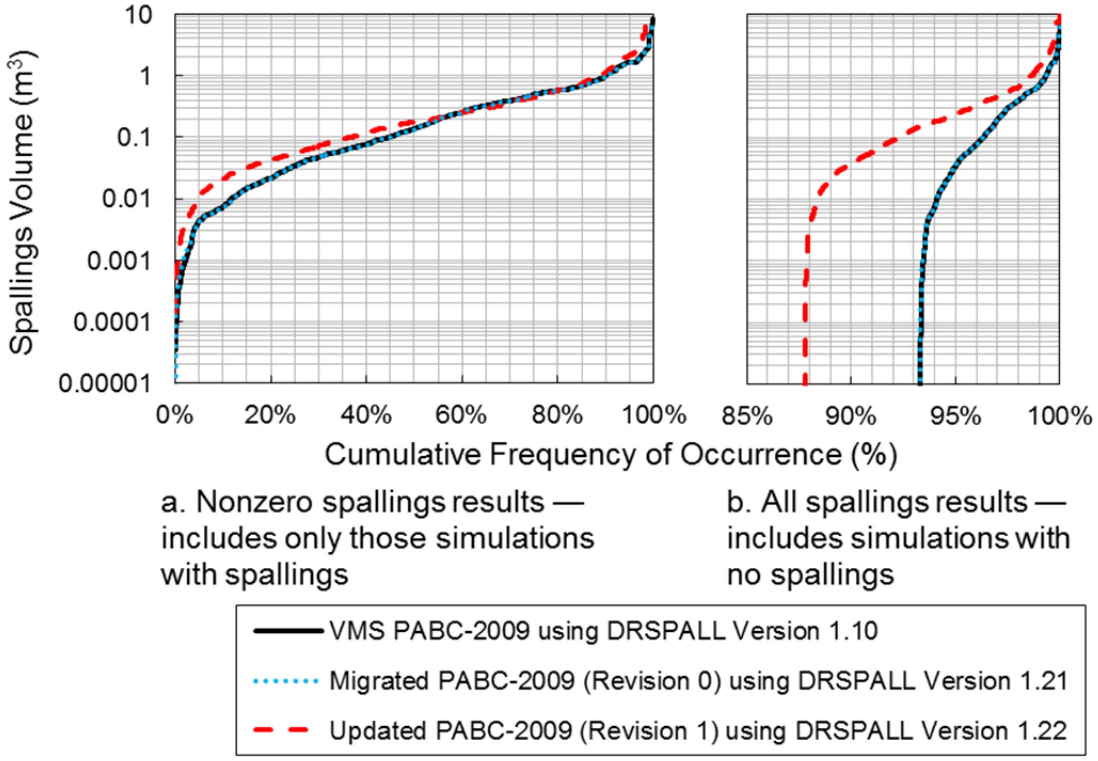
NOTES: The notation Rr stands for Replicate *r*. Summary results for the updated PABC-2009 (Revision 1) and the migrated PABC-2009 (Revision 0) are provided in file *CUTTINGS_PABC09.xlsx*, which is stored in the CVS repository at /nfs/data/CVSLIB/WIPP_ANALYSES/PABC09/CUTTINGS_S/Auxiliary. The VMS PABC-2009 results using DRSPALL Version 1.10 are provided by Ismail (2010).

using spallings output from DRSPALL Version 1.22, DRSPALL Version 1.21, and DRSPALL Version 1.10. The VMS PABC-2009 results (using DRSPALL Version 1.10 output) reported in Table 4-11 are provided by Ismail (2010). As seen in Table 4-11, values obtained using the DRSPALL Version 1.22 output are similar for many of the scenarios when compared to those obtained using DRSPALL Version 1.10. In replicate R1, the updated PABC-2009 using DRSPALL Version 1.22 output result in higher maximum spallings volumes, average spallings volumes, and number of nonzero spallings for all five scenarios. In replicate R2, the updated PABC-2009 produces slightly higher maximum for scenarios S1-DBR, S3-DBR, and S5-DBR, while average spallings volumes generally are slightly lower than the VMS PABC-2009 data. In replicate R3, the updated PABC-2009 produces higher maximum spallings volumes for scenarios S3-DBR, S4-DBR, and S5-DBR, with slightly higher average spallings volumes across all five scenarios compared to the VMS PABC-2009 data. For the updated PABC-2009 (using DRSPALL Version 1.22), there is a higher percentage of vectors resulting in nonzero spallings volumes for all replicates and scenarios compared to both the VMS PABC-2009 (using DRSPALL Version 1.10) and the migrated PABC-2009 (using DRSPALL Version 1.21).

The cumulative frequency of occurrence of spallings volumes (for replicates R1, R2, and R3 combined) for PABC-2009 is shown in Figure 4-20. This figure provides a summary of all spallings data from all scenarios, repository regions, and times. Figure 4-20 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). Figure 4-20a 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. Figure 4-20b 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 (Figure 4-20b) is the result of more simulations with nonzero spallings.

4.1.3.2. CRA-2014 Spallings Volumes

Utilizing the spallings volumes calculated by DRSPALL for 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. Summary statistics of spallings volumes for the intrusion scenarios considered by CUTTINGS_S are shown in Table 4-12 for the CRA-2014 using spallings output from DRSPALL Version 1.22, DRSPALL Version 1.21, and DRSPALL Version 1.10.



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

b. All spallings results — includes simulations with no spallings

Figure 4-20. Cumulative Frequency of Spallings Volumes in the PABC-2009 for Pooled Vectors (Replicates R1, R2, and R3 Combined).

Table 4-12. Summary of CRA-2014 Spallings Volumes by Scenario.

		Scenarios					Total
		S1-DBR	S2-DBR	S3-DBR	S4-DBR	S5-DBR	
Updated CRA-2014 (Revision 1) Using Modified DRSPALL Version 1.22							
R1	**Maximum [m^3]**	7.47	9.84	9.80	7.47	7.47	9.84
	Average nonzero volume [m^3]	1.05	0.78	0.90	0.98	1.09	0.90
	Number of nonzero volumes	69	161	114	31	38	413
	Percent of nonzero volumes	3.8%	10.7%	7.6%	2.1%	2.5%	5.3%
R2	**Maximum [m^3]**	2.02	4.18	1.90	1.79	1.79	4.18
	Average nonzero volume [m^3]	0.28	0.32	0.28	0.32	0.31	0.30
	Number of nonzero volumes	77	168	116	34	43	438
	Percent of nonzero volumes	4.3%	11.2%	7.7%	2.3%	2.9%	5.6%
R3	**Maximum [m^3]**	4.73	5.26	5.04	2.93	2.71	5.26
	Average nonzero volume [m^3]	0.59	0.53	0.43	0.57	0.44	0.50
	Number of nonzero volumes	54	144	99	21	28	346
	Percent of nonzero volumes	3.0%	9.6%	6.6%	1.4%	1.9%	4.4%
R1, R2, R3 Pooled	**Maximum [m^3]**	7.47	9.84	9.80	7.47	7.47	9.84
	Average nonzero volume [m^3]	0.63	0.54	0.54	0.62	0.61	0.57
	Number of nonzero volumes	200	473	329	86	109	1197
	Percent of nonzero volumes	3.7%	10.5%	7.3%	1.9%	2.4%	5.1%
Migrated CRA-2014 (Revision 0) Using DRSPALL Version 1.21							
R1	**Maximum [m^3]**	1.67	8.89	8.08	1.67	1.67	8.89
	Average nonzero volume [m^3]	0.41	0.54	0.65	0.42	0.41	0.52
	Number of nonzero volumes	41	95	60	16	23	235
	Percent of nonzero volumes	2.3%	6.3%	4.0%	1.1%	1.5%	3.0%
R2	**Maximum [m^3]**	1.24	2.76	1.97	0.64	0.65	2.76
	Average nonzero volume [m^3]	0.28	0.30	0.23	0.22	0.25	0.27
	Number of nonzero volumes	41	100	64	23	26	254
	Percent of nonzero volumes	2.3%	6.7%	4.3%	1.5%	1.7%	3.3%
R3	**Maximum [m^3]**	0.96	6.13	4.87	0.49	0.43	6.13
	Average nonzero volume [m^3]	0.25	0.41	0.44	0.17	0.16	0.35
	Number of nonzero volumes	30	86	46	16	17	195
	Percent of nonzero volumes	1.7%	5.7%	3.1%	1.1%	1.1%	2.5%
R1, R2, R3 Pooled	**Maximum [m^3]**	1.67	8.89	8.08	1.67	1.67	8.89
	Average nonzero volume [m^3]	0.32	0.41	0.44	0.26	0.28	0.38
	Number of nonzero volumes	112	281	170	55	66	684
	Percent of nonzero volumes	2.1%	6.2%	3.8%	1.2%	1.5%	2.9%

Table 4-12. Summary of CRA-2014 Spallings Volumes by Scenario. (Continued)

		Scenarios					Total
		S1-DBR	S2-DBR	S3-DBR	S4-DBR	S5-DBR	
VMS CRA-2014 Using DRSPALL Version 1.10							
R1	**Maximum [m^3]**	1.67	9.69	9.13	1.67	1.67	9.69
	Average nonzero volume [m^3]	0.41	0.58	0.70	0.42	0.41	0.55
	Number of nonzero volumes	41	95	60	16	23	235
	Percent of nonzero volumes	2.3%	6.3%	4.0%	1.1%	1.5%	3.0%
R2	**Maximum [m^3]**	1.23	2.76	1.96	0.64	0.64	2.76
	Average nonzero volume [m^3]	0.28	0.31	0.23	0.22	0.25	0.27
	Number of nonzero volumes	41	98	64	23	26	252
	Percent of nonzero volumes	2.3%	6.5%	4.3%	1.5%	1.7%	3.2%
R3	**Maximum [m^3]**	0.96	6.14	4.91	0.48	0.43	6.14
	Average nonzero volume [m^3]	0.25	0.41	0.44	0.17	0.16	0.35
	Number of nonzero volumes	30	85	46	16	17	194
	Percent of nonzero volumes	1.7%	5.7%	3.1%	1.1%	1.1%	2.5%
R1, R2, R3 Pooled	**Maximum [m^3]**	1.67	9.69	9.13	1.67	1.67	9.69
	Average nonzero volume [m^3]	0.32	0.43	0.45	0.26	0.28	0.39
	Number of nonzero volumes	112	278	170	55	66	681
	Percent of nonzero volumes	2.1%	6.2%	3.8%	1.2%	1.5%	2.9%

NOTES: The notation Rr stands for Replicate *r*. Summary results for the updated CRA-2014 (Revision 1) and the migrated CRA-2014 (Revision 0) are provided in file *CUTTINGS_CRA14.xlsx*, which is stored in the CVS repository at /nfs/data/CVSLIB/WIPP_ANALYSES/CRA14/CUTTINGS_S/Auxiliary. The VMS CRA-2014 results using DRSPALL Version 1.10 are provided by Kicker (2013).

There are four cases for CRA-2014, which are denoted CRA14BL, CRA14BV, CRA14TP, and CRA14-0 (Camphouse 2013a). Case CRA14-0 includes all changes from cases CRA14BL, CRA14BV, and CRA14TP, as well as refinements to the steel corrosion rate and a water balance that includes MgO hydration. Case CRA14-0 represents the new baseline for CRA-2014 and is the only case evaluated in this impact assessment.

The VMS CRA-2014 results (using DRSPALL Version 1.10 output) reported in Table 4-12 are provided by Kicker (2013). As seen in Table 4-12, values obtained using DRSPALL Version 1.22 output are similar for many of the scenarios when compared to those obtained using DRSPALL Version 1.10. In replicates R1 and R3, the updated CRA-2014 using DRSPALL Version 1.22 output results in higher maximum spallings volumes, average spallings volumes, and number of nonzero spallings for all five scenarios. In replicate R2, the updated CRA-2014 generally produces higher maximum spallings volumes for all scenarios, while average spallings volumes are similar. For the updated CRA 2014 (using DRSPALL Version 1.22), there is a higher percentage of vectors resulting in nonzero spallings volumes for all replicates and scenarios compared to both the VMS CRA-2014 (using DRSPALL Version 1.10) and the migrated CRA-2014 (using DRSPALL Version 1.21).

The cumulative frequency of spallings volumes for CRA-2014 (replicates R1, R2, and R3), is shown in Figure 4-21. This figure provides a summary of all spallings data from all scenarios, repository regions, and times. Figure 4-21a 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. Figure 4-21b 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 CRA-2014 results. The shift in the cumulative frequency of occurrence curve for the updated CRA-2014 spallings volumes (Figure 4-21b) is the result of more simulations with nonzero spallings.

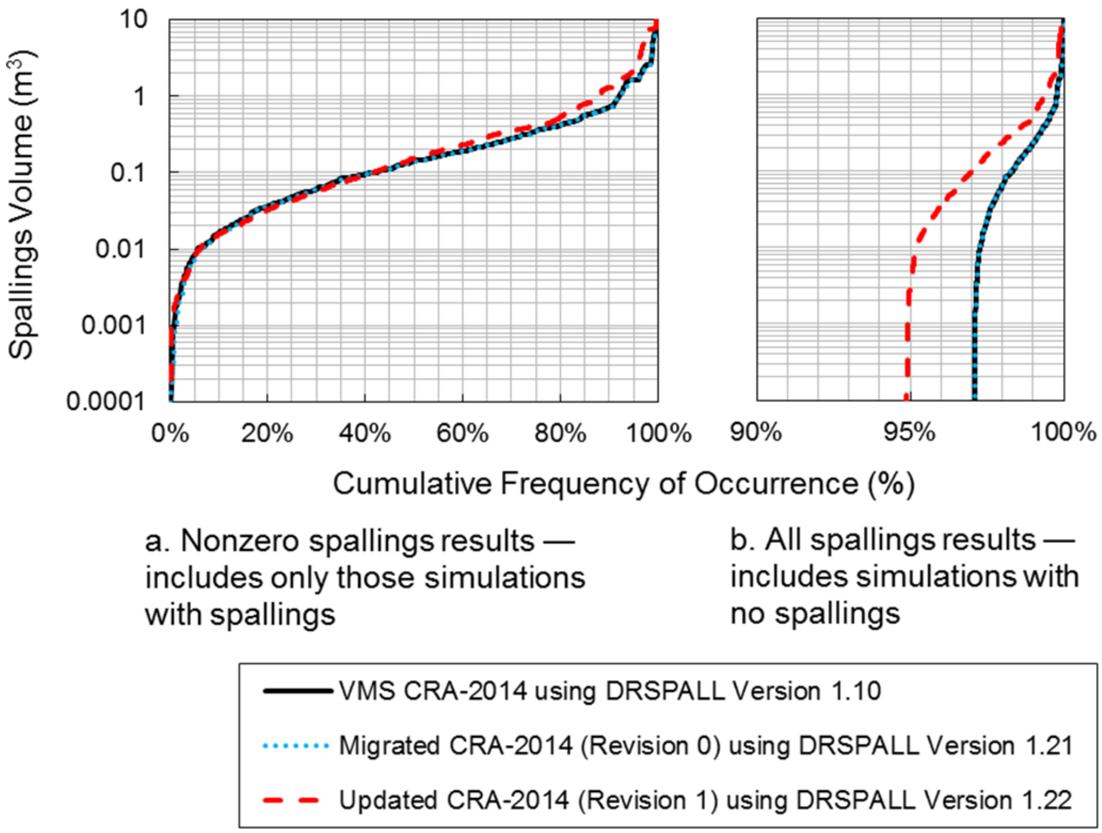


Figure 4-21. Cumulative Frequency of Spallings Volumes in the CRA-2014 for Pooled Vectors (Replicates R1, R2, and R3 Combined).

4.2. 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 Figure 4-22 for pooled vectors (replicates R1, R2, and R3 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 translate 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 Figure 4-23 for pooled vectors (replicates R1, R2, and R3 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 translate to an increase in spallings releases as all analyses use the same waste inventory.

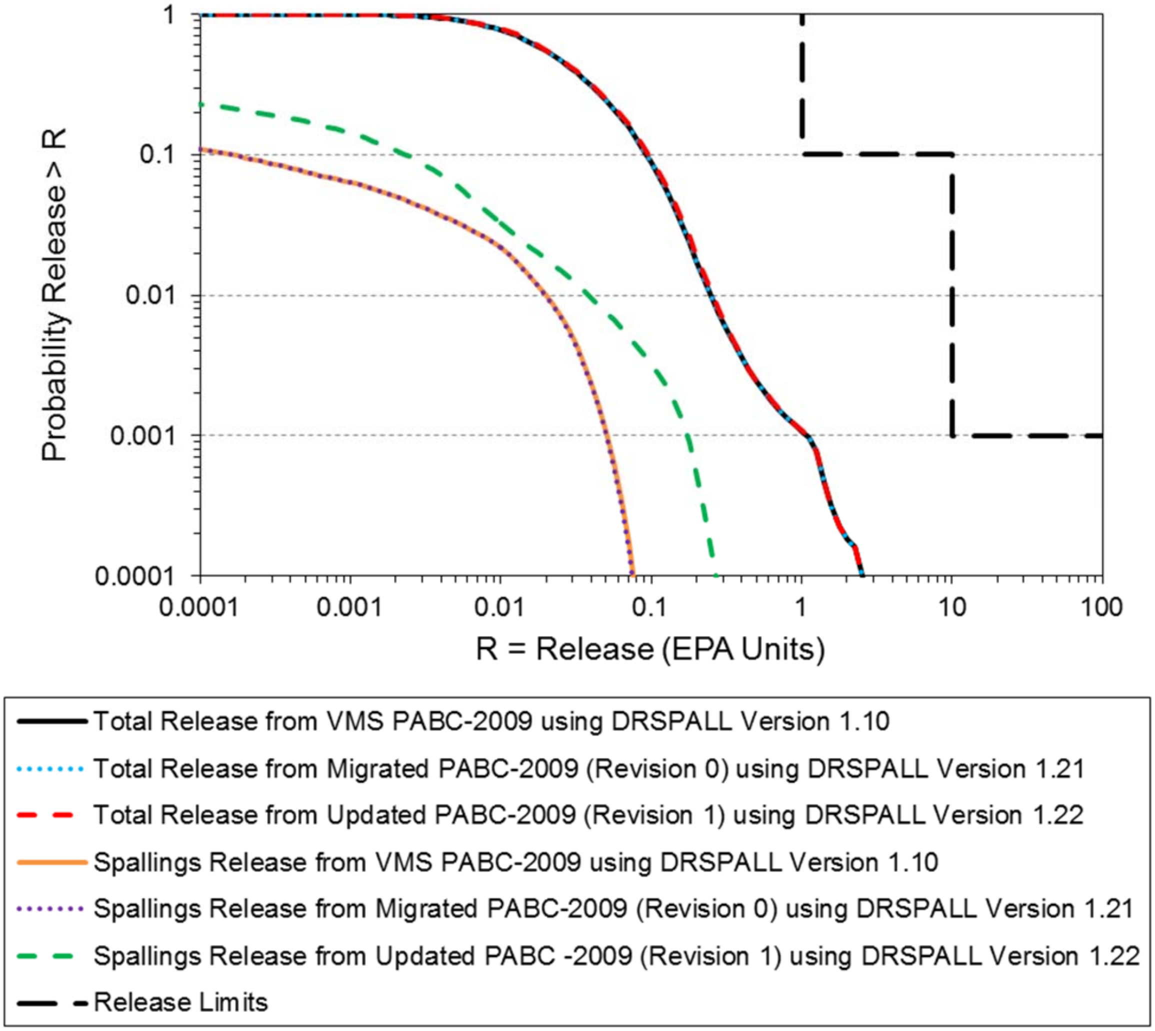


Figure 4-22. Impact of DRSPALL Version 1.22 Output on the PABC-2009 Overall Mean CCDFs for Normalized Radionuclide Releases for Pooled Vectors.

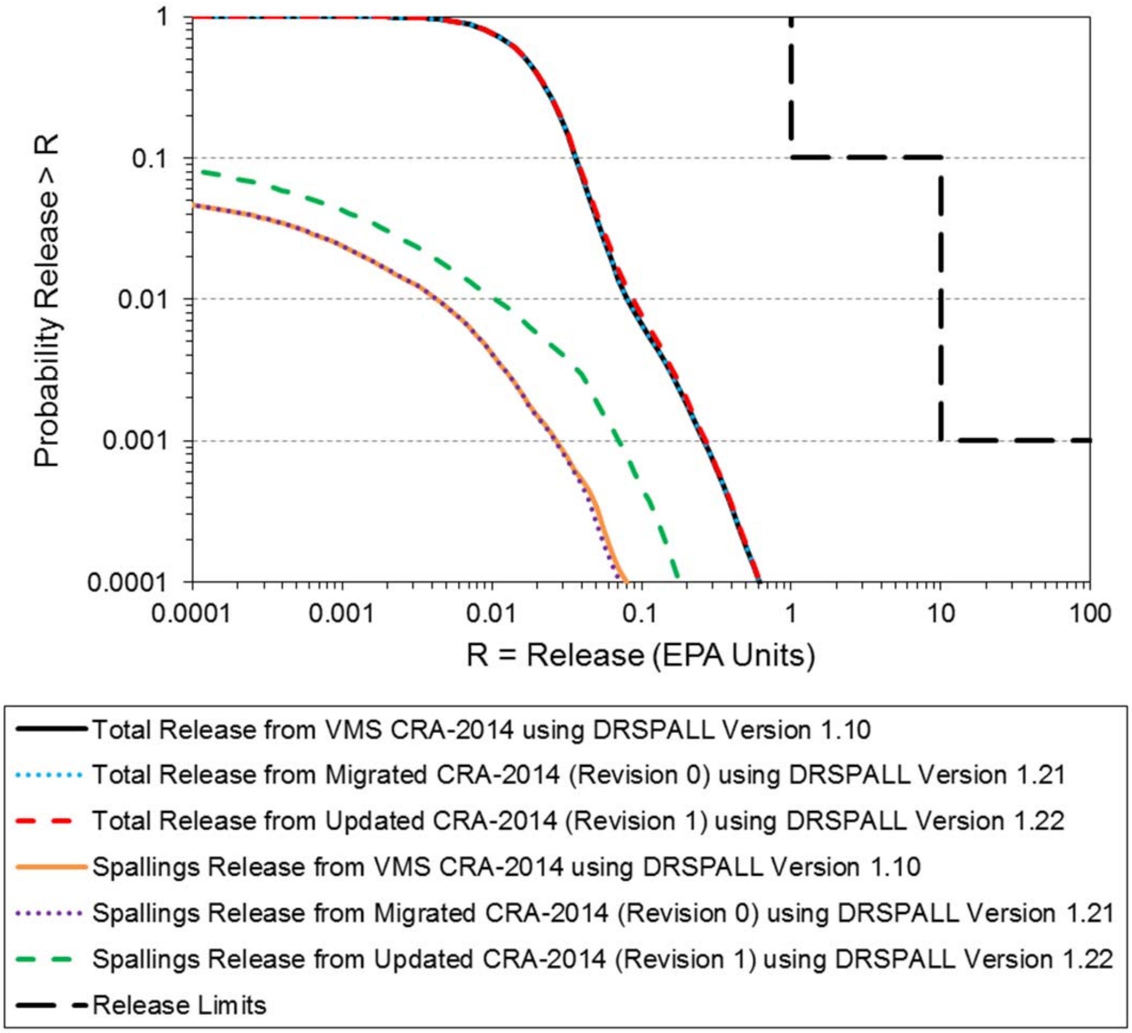


Figure 4-23. Impact of DRSPALL Version 1.22 Output on the CRA-2014 Overall Mean CCDFs for Normalized Radionuclide Releases for Pooled Vectors.

Total normalized releases using DRSPALL Version 1.22 output are also presented in Figures 4-22 and 4-23 for the PABC-2009 and CRA-2014, respectively 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 (Clayton et al. 2010, Section 6.5; Camphouse et al. 2013, Section 6.9.5). 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 (Figures 4-22 and 4-23).

5. SUMMARY AND CONCLUSIONS

In response to SPR 13-001 (WIPP PA 2013a), modifications were implemented in DRSPALL Version 1.22 to correct the finite difference equations contained in the source code file *wasteflowcalc.f90*. The errors identified in DRSPALL have been resolved, and this document provides the basis for closing SPR 13-001. Based on the assessment provided in this document, there is no impact to WIPP PA total radionuclide release calculations resulting from the modification to DRSPALL. Updated DRSPALL output is listed in Appendix C, which provides spallings data input for future PA calculations. The corresponding spallings data files are located in the CVS repository at /nfs/data/CVSLIB/WIPP_ANALYSES/PABC09/DRSPALL/Output.

The primary modifications to DRSPALL include:

- Forchterm

  The 'Forchterm' was corrected in three sections of the code as identified in SPR 13-001. In addition to the error identified in SPR 13-001, it was found that the derivation of the constant zone size equations were also incorrect. The derivation of Equation 4.6.1 in the design document (WIPP PA 2004a) was incorrect because k' was treated as a constant in the denominator, despite it being a variable in the numerator.

  In correcting the calculation of 'Forchterm', the indexing of the second permeability() term was also corrected to be 'i-1' instead of 'i'. The coefficients for the last cell (i=numReposZones) have changed: aa(i) has been changed from '-alpha1' to '-alpha1-alpha2' and bb(i) has been changed from '1.0+alpha1' to '1.0+alpha1+alpha2'.

- Constant zone size

  Previously, a variable zone size implementation was described based on the DRSPALL design document (WIPP PA 2004a, Section 4.6; WIPP PA 2013b). However, this was done incorrectly, as a simple substitution of variable zone sizes into the equation derived for a constant zone size is not valid. The derivation of an equation similar to design document Equation 4.6.2 for a variable zone size would require a complete re-derivation, which was determined unnecessary because current computing resources allow for reasonably fast computational times even for a greater number of zones. It was decided to run DRSPALL exclusively with a constant zone size. The following zone size parameters have been selected as the standard configuration for DRSPALL calculations:

  - Repository zone size, $\Delta r = 0.004$ m
  - Characteristic length, $L_t = 0.04$ m
  - Wellbore zone size, $\Delta z = 2.0$ m.

- Boundary conditions

  The index of the "first cell coefficients" (i) has been changed from 'firstIntactZone' to 'firstIntactZone+1', since any values for the boundary ('firstIntactZone') would be constant and fixed by the specified pressure (Dirichlet) boundary condition in the cavity. That is, the boundary nodes are not included in the coefficient matrix, so there should be no aa(i), bb(i), cc(i) coefficients for ‘firstIntactZone’. The effect of the boundary node (firstIntactZone) is included in the b-vector of the linear system of equations. Consequently, the indexing for the “interior cell coefficients” now begins at ‘firstIntactZone+2’ instead of ‘firstIntactZone+1’. Also, as a consequence of this, the indexing of the matrix inversion has changed. The boundary pressure is now assigned to ‘reposPres(firstIntactZone)’ instead of ‘reposPres(0)’. Because of that, ‘exitPoreVelocity’ is now calculated using a centered-difference approximation, which leads to ‘reposPres(firstIntactZone+1)’ being used instead of ‘reposPres(firstIntactZone)’.

Previously, the permeability of the ‘firstIntactZone-1’ zone was set to the value of the ‘firstIntactZone’. This was changed because the permeability of the ‘firstIntactZone-1’ is no longer used. Also, where previously the array element ‘psi(firstIntactZone-1)’ was calculated from the gas viscosity and boundary pressure, this assignment has been made applicable to ‘psi(firstIntactZone)’, since the ‘firstIntactZone’ is the boundary.

- Fluidization limit

  Unrealistic values of ‘fractionFluidized’ could be calculated in the source code file *wellborecalc.f90*. Previously, ‘fractionFluidized(i)’ was set to 1.0 only if ‘i’ was for the ‘firstIntactZone’. Otherwise, the ‘fractionFluidized’ could increase to values much higher than 1.0, which are not physically reasonable, and led to problems in calculating ‘permeability’ in *wasteflowcalc.f90*. An ‘elseif’ statement was added to set ‘fractionFluidized(i)’ to a number slightly larger than 1.0, such that the ‘if’ statement will be satisfied for zone ‘i’ in a later step.

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 MPa, 14.0 MPa, and 14.8 MPa show higher spallings volumes compared to both the VMS DRSPALL (Version 1.10) and migrated DRSPALL (Version 1.21) (Figures 4-4, 4-8, and 4-12).

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 (Figures 4-20a and 4-21a). Figures 4-20b and 4-21b 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 difference arises 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 (Figure 4-22). The CCDF of spallings releases obtained in the CRA-2014 was 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 (Figure 4-23).

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 (Figures 4-22 and 4-23). 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.

6. REFERENCES

Camphouse, R.C. 2013a. *Analysis Plan for the 2014 Compliance Recertification Application Performance Assessment*. AP-164. Carlsbad, NM: Sandia National Laboratories. ERMS 559198.

Camphouse, R.C. 2013b. *Analysis Package for Salado Flow Modeling Done in the 2014 Compliance Recertification Application Performance Assessment (CRA-2014 PA)*. Carlsbad, NM: Sandia National Laboratories. ERMS 559980.

Camphouse, R.C., D.C. Kicker, S. Kim, T.B. Kirchner, J.J. Long, B. Malama, and T.R. Zeitler 2013. *Summary Report for the 2014 WIPP Compliance Recertification Application Performance Assessment*. Carlsbad, NM: Sandia National Laboratories. ERMS 560252.

Clayton, D.J., R.C. Camphouse, J.W. Garner, A.E. Ismail, T.B. Kirchner, K.L. Kuhlman, and M.B. Nemer. 2010. *Summary Report of the CRA-2009 Performance Assessment Baseline Calculation*. Carlsbad, NM: Sandia National Laboratories. ERMS 553039.

EPA (U.S. Environmental Protection Agency) 1996. 40 CFR Part 194: Criteria for the Certification and Recertification of the Waste Isolation Pilot Plant's Compliance with the 40 CFR Part 191 Disposal Regulations; Final Rule. Federal Register, Vol. 61, 5223-5245.

EPA 2010. 40 CFR Part 194 Criteria for the Certification and Recertification of the Waste Isolation Pilot Plant's Compliance With the Disposal Regulations: Recertification Decision, Federal Register No. 222, Vol. 75, pp. 70584-70595, November 18, 2010.

Ismail, A.E. 2010. *Analysis Package for Cuttings, Cavings, and Spallings: CRA-2009 Performance Assessment Baseline Calculation*. Carlsbad, NM: Sandia National Laboratories. ERMS 552893.

Kicker, D.C. 2013. *Analysis Package for Cuttings, Cavings, and Spallings: 2014 Compliance Recertification Application Performance Assessment (CRA-2014 PA)*, Revision 0. Carlsbad, NM: Sandia National Laboratories. ERMS 560060.

Kicker, D.C. 2015. *DRSPALL Zone Size Sensitivity Study*, Revision 0. Carlsbad, NM: Sandia National Laboratories. ERMS 564427.

Kirchner, T.B. 2010. *Generation of the LHS Samples for the AP-145 (PABC09) PA Calculations*. Carlsbad, NM: Sandia National Laboratories. ERMS 552905.

Kirchner, T.B. 2013. *Generation of the LHS Samples for the CRA-2014 (AP-164) Revision 0 PA Calculations*. Carlsbad, NM: Sandia National Laboratories. ERMS 559950.

Kirchner, T., A. Gilkey, and J. Long 2013. *Summary Report on the Migration of the WIPP PA Codes From VMS to Solaris, AP-162*. Carlsbad, NM: Sandia National Laboratories. ERMS 561457.

Kirchner, T., A. Gilkey, and J. Long 2015. *Addendum to the Summary Report on the Migration of the WIPP PA Codes From VMS to Solaris, AP-162*. Carlsbad, NM: Sandia National Laboratories. ERMS 564675.

Long, J. J. 2014. Nuclear Waste Management Procedure NP 19-1 Software Requirements, Revision 16. Carlsbad, NM: Sandia National Laboratories. ERMS 562870.

Lord, D., D. Rudeen, and C. Hansen 2003. *Analysis Package for DRSPALL: Compliance Recertification Application, Part I – Calculation of Spall Volumes*. Carlsbad, NM: Sandia National Laboratories. ERMS 532766.

Lord, D.L., D.K. Rudeen, J.F. Schatz, A.P. Gilkey, and C.W. Hansen 2006. *DRSPALL: Spallings Model for the Waste Isolation Pilot Plant 2004 Recertification*. SAND2004-0730. Albuquerque, NM: Sandia National Laboratories.

Özişik, M.N. 1993. *Heat Conduction*. Second Edition. New York, NY: John Wiley & Sons.

Vugrin, E. 2005. *Analysis Package for DRSPALL, CRA-2004 Performance Assessment Baseline Calculation*. Carlsbad, NM: Sandia National Laboratories. ERMS 540415.

WIPP PA (Waste Isolation Pilot Plant Performance Assessment) 2004a. *Design Document for DRSPALL Version 1.10*. Carlsbad, NM: Sandia National Laboratories. ERMS 533149.

WIPP PA 2004b. *User's Manual for DRSPALL Version 1.10*. Carlsbad, NM: Sandia National Laboratories. ERMS 533151.

WIPP PA 2004c. *Design Document for CUTTINGS_S (Version 6.00)*. Carlsbad, NM: Sandia National Laboratories. ERMS 537038.

WIPP PA 2013a. *Software Problem Report (SPR) 13-001 for DRSPALL Versions 1.10 and 1.21*. Carlsbad, NM: Sandia National Laboratories. ERMS 561524.

WIPP PA 2013b. *Addendum to Design Document (ERMS# 533149) for DRSPALL Version 1.21*. Carlsbad, NM: Sandia National Laboratories. ERMS 560045.

WIPP PA 2013c. *Addendum to User's Manual for DRSPALL Version 1.21*. Carlsbad, NM: Sandia National Laboratories. ERMS 560048.

WIPP PA 2015a. *Design Document for DRSPALL Version 1.22*. Carlsbad, NM: Sandia National Laboratories. ERMS 562640.

WIPP PA 2015b. *Addendum to User's Manual for DRSPALL Version 1.22*. Carlsbad, NM: Sandia National Laboratories. ERMS 562642.

WIPP PA 2015c. Verification and Validation Plan / Validation Document for DRSPALL Version 1.22. Carlsbad, NM: Sandia National Laboratories. ERMS 562643.

APPENDIX A. FINITE DIFFERENCE SOLUTION TO DRSPALL WASTE FLOW EQUATION

The derivation provided in this appendix follows that given in the DRSPALL design document (WIPP PA 2015a, Section 4.6). Throughout this appendix, reference is made to both the DRSPALL design document and the related Sandia Report SAND2004-0730 (Lord et al. 2006). The nomenclature for the equations presented in this appendix is provided in Table A-1.

Table A-1. Nomenclature for Equations in Appendix A.

Symbol	Definitions	Units
j, N	Zone indices	—
k'	Velocity dependent permeability	m^2
m	Geometry exponent (m=3 for spherical, m=2 for cylindrical)	—
p	Pressure in gas	Pa
r	Radius	m
t	Time	sec
n	Timestep index	—
η	Viscosity of gas	Pa·sec
ϕ	Current repository porosity	—
ψ	Pseudopressure	Pa/sec

A-1. Governing Equation Simplification

Start with DRSPALL design document Equation 4.3.10 (WIPP PA 2015a). This equation is not given in the Sandia Report (Lord et al. 2006).

$$\frac{\partial \psi}{\partial t} = \frac{D(\psi)}{r^{m-1}} \frac{\partial}{\partial r}\left(r^{m-1} \frac{\partial \psi}{\partial r} \right) + \frac{D(\psi)}{k'} \frac{\partial k'}{\partial r} \frac{\partial \psi}{\partial r} \qquad \text{(A-1)}$$

where

$$D(\psi) = \frac{k'}{\phi}\sqrt{\frac{\psi}{\eta}} = \frac{k'p}{\phi\eta}$$

Note that

$$\frac{\partial \ln k'}{\partial r} = \frac{1}{k'} \frac{\partial k'}{\partial r} \qquad \text{(A-2)}$$

Substituting Equation A-2 into Equation A-1 yields:

$$\frac{\partial \psi}{\partial t} = \frac{D(\psi)}{r^{m-1}} \frac{\partial}{\partial r}\left(r^{m-1} \frac{\partial \psi}{\partial r} \right) + D(\psi) \frac{\partial \ln(k')}{\partial r} \frac{\partial \psi}{\partial r} \tag{A-3}$$

Expand first term on right-hand side of Equation A-3:

$$\begin{aligned}
\frac{D(\psi)}{r^{m-1}} \frac{\partial}{\partial r}\left(r^{m-1} \frac{\partial \psi}{\partial r} \right) &= D(\psi)\left[\frac{1}{r^{m-1}} \frac{\partial}{\partial r}\left(r^{m-1} \frac{\partial \psi}{\partial r} \right) \right] \\
&= D(\psi)\left[\frac{1}{r^{m-1}} r^{m-1} \frac{\partial}{\partial r}\left(\frac{\partial \psi}{\partial r} \right) + \frac{\partial \psi}{\partial r} \frac{1}{r^{m-1}} \frac{\partial\left(r^{m-1}\right)}{\partial r} \right] \\
&= D(\psi)\left[\frac{\partial^2 \psi}{\partial r^2} + \frac{\partial \psi}{\partial r} \frac{1}{r^{m-1}} (m-1)\left(r^{m-2}\right) \frac{\partial r}{\partial r} \right] \\
&= D(\psi)\left[\frac{\partial^2 \psi}{\partial r^2} + \frac{(m-1)}{r} \frac{\partial \psi}{\partial r} \right]
\end{aligned} \tag{A-4}$$

Substituting Equation A-4 into Equation A-3 gives:

$$\frac{\partial \psi}{\partial t} = D(\psi)\left[\frac{\partial^2 \psi}{\partial r^2} + \frac{(m-1)}{r} \frac{\partial \psi}{\partial r} + \frac{\partial \ln(k')}{\partial r} \frac{\partial \psi}{\partial r} \right] \tag{A-5}$$

Equation A-5 is nonlinear due to the dependence of the parameter D on the state variable ψ. Hence, its numerical solution requires use of an iterative scheme such as the Newton-Raphson method. However, as explained in the next section, D is treated as independent of ψ in DRSPALL calculations, so an iterative Newton-Raphson scheme is not necessary here.

A-2. Finite Difference Discretization

Using an implicit scheme, Equation A-5 can be represented in finite difference form by using the central difference method to discretize the right-hand side and the forward difference method to discretize the left-hand side (Özişik 1993, Chapter 12, "Implicit Method").

This gives:

$$\begin{aligned}
\frac{\psi_j^{n+1} - \psi_j^n}{\Delta t} = D\left(\psi_j^{n+1}\right)\Bigg[& \frac{\psi_{j+1}^{n+1} - 2\psi_j^{n+1} + \psi_{j-1}^{n+1}}{(\Delta r)^2} + \frac{(m-1)}{r_j} \frac{\left(\psi_{j+1}^{n+1} - \psi_{j-1}^{n+1}\right)}{2\Delta r} \\
& + \frac{\left(\ln\left(k_{j+1}'^{n+1}\right) - \ln\left(k_{j-1}'^{n+1}\right)\right)}{2\Delta r} \frac{\left(\psi_{j+1}^{n+1} - \psi_{j-1}^{n+1}\right)}{2\Delta r} \Bigg]
\end{aligned} \tag{A-6}$$

As discussed in Lord et al. (2006), $D(\psi)$ is assumed constant over a zone, which simplifies the numerical implementation. Using its zone centered value at the current time, the linearizing approximation $D(\psi) \approx D(\psi_j^{n+1}) \approx D(\psi_j^n) \approx D_j^n$ is made. Equation A-6 becomes.

$$\frac{\psi_j^{n+1} - \psi_j^n}{\Delta t} = D_j^n \left[\frac{\psi_{j+1}^{n+1} - 2\psi_j^{n+1} + \psi_{j-1}^{n+1}}{(\Delta r)^2} + \frac{\left(\psi_{j+1}^{n+1} - \psi_{j-1}^{n+1}\right)}{2\Delta r} \left(\frac{(m-1)}{r_j} + \frac{\left(\ln\left(k_{j+1}'^{n+1}\right) - \ln\left(k_{j-1}'^{n+1}\right)\right)}{2\Delta r} \right) \right]$$

Solve for ψ_j^n and collect similar terms

$$\begin{aligned}
\psi_j^n &= \psi_j^{n+1} - D_j^n \Delta t \left[\frac{\psi_{j+1}^{n+1} - 2\psi_j^{n+1} + \psi_{j-1}^{n+1}}{(\Delta r)^2} + \frac{\left(\psi_{j+1}^{n+1} - \psi_{j-1}^{n+1}\right)}{2\Delta r} \left(\frac{(m-1)}{r_j} + \frac{\left(\ln\left(k_{j+1}'^{n+1}\right) - \ln\left(k_{j-1}'^{n+1}\right)\right)}{2\Delta r} \right) \right] \\
&= -D_j^n \Delta t \left[\frac{1}{(\Delta r)^2} - \frac{1}{2\Delta r} \left(\frac{(m-1)}{r_j} + \frac{\left(\ln\left(k_{j+1}'^{n+1}\right) - \ln\left(k_{j-1}'^{n+1}\right)\right)}{2\Delta r} \right) \right] \psi_{j-1}^{n+1} + \left[1 + \frac{2D_j^n \Delta t}{(\Delta r)^2} \right] \psi_j^{n+1} \\
&\quad - D_j^n \Delta t \left[\frac{1}{(\Delta r)^2} + \frac{1}{2\Delta r} \left(\frac{(m-1)}{r_j} + \frac{\left(\ln\left(k_{j+1}'^{n+1}\right) - \ln\left(k_{j-1}'^{n+1}\right)\right)}{2\Delta r} \right) \right] \psi_{j+1}^{n+1} \\
&= -\frac{D_j^n \Delta t}{\Delta r} \left[\frac{1}{\Delta r} - \frac{(m-1)}{2r_j} - \frac{\left(\ln\left(k_{j+1}'^{n+1}\right) - \ln\left(k_{j-1}'^{n+1}\right)\right)}{4\Delta r} \right] \psi_{j-1}^{n+1} + \left[1 + \frac{2D_j^n \Delta t}{(\Delta r)^2} \right] \psi_j^{n+1} \\
&\quad - \frac{D_j^n \Delta t}{\Delta r} \left[\frac{1}{\Delta r} + \frac{(m-1)}{2r_j} + \frac{\left(\ln\left(k_{j+1}'^{n+1}\right) - \ln\left(k_{j-1}'^{n+1}\right)\right)}{4\Delta r} \right] \psi_{j+1}^{n+1}
\end{aligned}$$

Noting that $\ln\left(k_{j+1}'^{n+1}\right) - \ln\left(k_{j-1}'^{n+1}\right) = \ln\left(k_{j+1}'^{n+1} \middle/ k_{j-1}'^{n+1} \right)$

$$\begin{aligned}
\psi_j^n &= -\frac{D_j^n \Delta t}{\Delta r} \left(\frac{1}{\Delta r} - \frac{(m-1)}{2r_j} - \frac{\ln\left(k_{j+1}'^{n+1} \middle/ k_{j-1}'^{n+1} \right)}{4\Delta r} \right) \psi_{j-1}^{n+1} + \left(1 + \frac{2D_j^n \Delta t}{(\Delta r)^2} \right) \psi_j^{n+1} \\
&\quad - \frac{D_j^n \Delta t}{\Delta r} \left(\frac{1}{\Delta r} + \frac{(m-1)}{2r_j} + \frac{\ln\left(k_{j+1}'^{n+1} \middle/ k_{j-1}'^{n+1} \right)}{4\Delta r} \right) \psi_{j+1}^{n+1}
\end{aligned}$$

Rewriting the equation:

$$\psi_j^n = -\alpha_1 \psi_{j-1}^{n+1} + \left(1 + 2\alpha\right)\psi_j^{n+1} - \alpha_2 \psi_{j+1}^{n+1} \tag{A-7}$$

where

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

$$\alpha_1 = \frac{D_j^n \Delta t}{\Delta r}\left(\frac{1}{\Delta r} - \frac{\left(m-1\right)}{2r_j} - \frac{\ln\left(k_{j+1}'^{n+1} \big/ k_{j-1}'^{n+1}\right)}{4\Delta r}\right)$$

$$\alpha_2 = \frac{D_j^n \Delta t}{\Delta r}\left(\frac{1}{\Delta r} + \frac{\left(m-1\right)}{2r_j} + \frac{\ln\left(k_{j+1}'^{n+1} \big/ k_{j-1}'^{n+1}\right)}{4\Delta r}\right)$$

and *j* and *n* are the cell and timestep indices, respectively. Equation A-7 is the same as Equation 4.6.3 in the previous version of the DRSPALL design document (WIPP PA 2004a) and Sandia Report Equation 4.3.4 (Lord et al. 2006) except that the coefficient terms α_1 and α_2 are different.

Also:

$$\begin{aligned}
\alpha_1 + \alpha_2 &= \frac{D_j^n \Delta t}{\Delta r}\left(\frac{1}{\Delta r} - \frac{\left(m-1\right)}{2r_j} - \frac{\ln\left(k_{j+1}'^{n+1} \big/ k_{j-1}'^{n+1}\right)}{4\Delta r}\right) + \frac{D_j^n \Delta t}{\Delta r}\left(\frac{1}{\Delta r} + \frac{\left(m-1\right)}{2r_j} + \frac{\ln\left(k_{j+1}'^{n+1} \big/ k_{j-1}'^{n+1}\right)}{4\Delta r}\right) \\
&= \frac{D_j^n \Delta t}{\Delta r}\left(\frac{1}{\Delta r} + \frac{1}{\Delta r}\right) \\
&= 2\frac{D_j^n \Delta t}{\left(\Delta r\right)^2} \\
\alpha_1 + \alpha_2 &= 2\alpha.
\end{aligned}$$

A-3. Boundary Conditions

For the boundary condition at the inner radius we use the method given in Thomas (1995, Section 1.6.3, "Cell Centered Grids") for cell centered grids. Using this method the difference equation is derived on the second cell in the usual, here central difference, manner. The first intact zone is the zone closest to the borehole and is indexed as 1. The boundary condition is implemented by noting that for the first intact cell ($j - 1 = 1$), ψ_1^{n+1} is the cavity psuedo pressure, ψ_{cav}^{n+1}, which is known. Therefore, $\psi_1^{n+1} = \psi_{cav}^{n+1}$ can be moved to the left-hand side of Equation A-7.

Using $j = 2$, the second cell, Equation A-7 gives:

$$\psi_2^n + \alpha_1 \psi_{cav}^{n+1} = (1+2\alpha)\psi_2^{n+1} - \alpha_2 \psi_3^{n+1} \tag{A-8}$$

The far-field boundary condition is a zero gradient condition. Mathematically this is:

$$\left.\frac{\partial \psi}{\partial r}\right|_{r=\infty} = 0 \tag{A-9}$$

Discretizing using a second-order central difference formulation:

$$\begin{gathered} \frac{\psi_{N+1}^{n+1} - \psi_{N-1}^{n+1}}{2\Delta r} = 0 \\ \psi_{N+1}^{n+1} = \psi_{N-1}^{n+1} \end{gathered} \tag{A-10}$$

Using this to eliminate the fictitious point in the domain discretization Equation A-7, at node point $j = N$ (i.e., the final cell):

$$\begin{aligned} \psi_N^n &= -\alpha_1 \psi_{N-1}^{n+1} + (1+2\alpha)\psi_N^{n+1} - \alpha_2 \psi_{N+1}^{n+1} \\ &= -\alpha_1 \psi_{N-1}^{n+1} + (1+2\alpha)\psi_N^{n+1} - \alpha_2 \psi_{N-1}^{n+1} \\ &= -(\alpha_1 + \alpha_2)\psi_{N-1}^{n+1} + (1+2\alpha)\psi_N^{n+1} \end{aligned}$$

Using $\alpha_1 + \alpha_2 = 2\alpha$, the final condition can be simplified to:

$$\psi_N^n = -(2\alpha)\psi_{N-1}^{n+1} + (1+2\alpha)\psi_N^{n+1} \tag{A-11}$$

In the previous version of the DRSPALL design document (WIPP PA 2004a, which was prepared for DRSPALL Version 1.10), a forward difference formulation was applied to the boundary condition Equation A-9. Özişik (1993) shows that the error involved with the central difference representation is second-order accurate, i.e., $O\left((\Delta r)^2\right)$; whereas the error involved with the forward difference representation is first-order accurate, i.e., $O(\Delta r)$. Therefore, the central difference formulation, Equation A-11, is used because it decreases numerical discretization errors and provides a more accurate numerical approximation to the exact solution.

A-4. Summary of Recommended Finite Difference Equations

The recommended tri-diagonal linear system of equations is:

$$
\begin{aligned}
\psi_j^n &= -\alpha_1 \psi_{cav}^{n+1} + (1+2\alpha)\psi_j^{n+1} - \alpha_2 \psi_{j+1}^{n+1} && \text{for } j = 2 \\
\psi_j^n &= -\alpha_1 \psi_{j-1}^{n+1} + (1+2\alpha)\psi_j^{n+1} - \alpha_2 \psi_{j+1}^{n+1} && \text{for } j = 3,\ldots, N-1 \\
\psi_j^n &= -(2\alpha)\psi_{j-1}^{n+1} + (1+2\alpha)\psi_j^{n+1} && \text{for } j = N
\end{aligned}
\qquad \text{(A-12)}
$$

where

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

$$
\alpha_1 = \frac{D_j^n \Delta t}{\Delta r}\left(\frac{1}{\Delta r} - \frac{(m-1)}{2r_j} - \frac{\ln\left(k'^{n+1}_{j+1} \big/ k'^{n+1}_{j-1} \right)}{4\Delta r} \right)
$$

$$
\alpha_2 = \frac{D_j^n \Delta t}{\Delta r}\left(\frac{1}{\Delta r} + \frac{(m-1)}{2r_j} + \frac{\ln\left(k'^{n+1}_{j+1} \big/ k'^{n+1}_{j-1} \right)}{4\Delta r} \right)
$$

Figure A-1 illustrates the expansion point (*j*, *n*+1) and the surrounding finite-difference molecules.

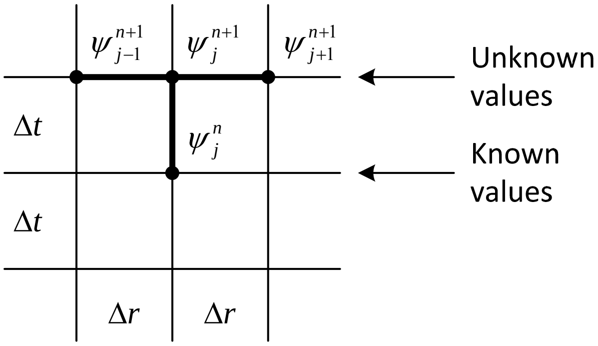


Figure A-1. Finite Difference Molecules for the Implicit Scheme Using Constant Zone Sizes.

APPENDIX B. SUMMARY OF CODE CHANGES

A summary of DRSPALL code changes is provided in Table B-1, which shows excerpts of source code from DRSPALL Versions 1.21 and 1.22, highlighting the changes to DRSPALL Version 1.22. A description of the changes is also provided in Table B-1.

Table B-1. Summary of DRSPALL Code Changes.

DRSPALL Version 1.21	**DRSPALL Version 1.22 (changes shown in red)**	**Description of Change**
Excerpts from source code file *A1main_drspall.f90*		
fluidizationValidationFileID = 122 expulsionValidationFileID = 123 ! test case #5, wellboreValidationFileID = 125	fluidizationValidationFileID = 122 expulsionValidationFileID = 123 fluidizationTimeValidationFileID = 124 !trz ! test case #5, wellboreValidationFileID = 125	An additional output file, *fluidization_time.dat*, was included as part of test case #4. This new output file provides the fluidization time for each zone to improve the ability to verify the DRSPALL fluidization time calculation. Specific changes to this source code file include: – Added file id for *fluidization_time.dat* – Added definition of filename of *fluidization_time.dat* – Added opening of *fluidization_time.dat* – Added writing of QA information to *fluidization_time.dat*

TC4EjectFileName =
trim(validationFilePrefix)//'_expulsion.dat' !apg
 	
Open(fluidizationValidationFileID, FILE=
TC4Fluidfilename, RECL=2048, FORM='FORMATTED',
STATUS=status)
Open(expulsionValidationFileID, FILE= TC4Ejectfilename,
RECL=2048, FORM='FORMATTED', STATUS=status)
	TC4EjectFileName =
	trim(validationFilePrefix)//'_expulsion.dat' !apg
	TC4FluidTimeFileName =
	trim(validationFilePrefix)//'_fluidization_time.dat' !trz
	
	Open(fluidizationValidationFileID, FILE=
	TC4Fluidfilename, RECL=2048, FORM='FORMATTED',
	STATUS=status)
	Open(expulsionValidationFileID, FILE= TC4Ejectfilename,
	RECL=2048, FORM='FORMATTED', STATUS=status)
	Open(fluidizationTimeValidationFileID, FILE=
	TC4FluidTimefilename, RECL=2048,
	FORM='FORMATTED', &
	STATUS=status) !trz	

! expulsion file CALL QAPAGE (expulsionValidationFileID,blank) write(expulsionValidationFileID,'(1x,a)') trim(TC4Ejectfilename) !apg new !apg CALL QABANNER(expulsionValidationFileID,blank,blank,blank) !apg CALL QADOEDIS(expulsionValidationFileID,'*') endif	! expulsion file CALL QAPAGE (expulsionValidationFileID,blank) write(expulsionValidationFileID,'(1x,a)') trim(TC4Ejectfilename) !apg new !apg CALL QABANNER(expulsionValidationFileID,blank,blank,blank) !apg CALL QADOEDIS(expulsionValidationFileID,'*') ! fluidization time file CALL QAPAGE (fluidizationTimeValidationFileID,blank) write(fluidizationTimeValidationFileID,'(1x,a)') trim(TC4FluidTimefilename) !trz endif	

Table B-1. Summary of DRSPALL Code Changes. (Continued)

DRSPALL Version 1.21	DRSPALL Version 1.22 (changes shown in red)	Description of Change
Excerpts from source code file *A1main_drspall.f90* (continued)		

string = READCFA(parameterFileID,'radius,growthRate')
read(string,*)reposRadius1, growthRate
initialWellZoneSize = READCF (parameterFileID,initialWellZoneSize,'initialWellZoneSize')
wellGrowthRate = READCF (parameterFileID,wellGRowthRate,'wellGRowthRate')
firstWellZone = READCF (parameterFileID,dble(firstWellZone),'firstWellZone')
	string = READCFA(parameterFileID,'radius,growthRate')
	read(string,*)reposRadius1, growthRate
	if (growthRate < 1.0 .or. growthRate > 1.0) then !trz
	call QAABORT ('Growth rate must be 1.0') !trz
	endif !trz
	initialWellZoneSize = READCF (parameterFileID,initialWellZoneSize,'initialWellZoneSize')
	wellGrowthRate = READCF (parameterFileID,wellGRowthRate,'wellGRowthRate')
	if (wellGrowthRate < 1.0 .or. wellGrowthRate > 1.0) then !trz
	call QAABORT ('Well growth rate must be 1.0') !trz
	endif !trz
	firstWellZone = READCF (parameterFileID,dble(firstWellZone),'firstWellZone')
		Checks of ‘growthRate’ and ‘wellGrowthRate’ were added to make sure they are set to ‘1.0’ in the input file, since the code will now be run exclusively with constant zone sizes. If not, the code exits with an error.

Excerpts from source code file *globals.F90*		
Character(255) TC1chanFileName, TC4couplefilename, TC4stressfilename, & TC4Fluidfilename, TC4Ejectfilename, TC5Wellfilename	Character(255) TC1chanFileName, TC4couplefilename, TC4stressfilename, & TC4Fluidfilename, TC4Ejectfilename, TC4FluidTimefilename, TC5Wellfilename	As a result of the new output file for test case #4, new definitions are required to pass values between subroutines. Specifically, *TC4FluidTimefilename* and *fluidizationTimeValidationFileID* variables were added.
!test case #4 couplingValidationFileID, stressValidationFileID, fluidizationvalidationFileID, & expulsionValidationFileID, & !test case #5	!test case #4 couplingValidationFileID, stressValidationFileID, fluidizationvalidationFileID, & expulsionValidationFileID, fluidizationTimeValidationFileID, & !test case #5	

Table B-1. Summary of DRSPALL Code Changes. (Continued)

DRSPALL Version 1.21	DRSPALL Version 1.22 (changes shown in red)	Description of Change
Excerpts from source code file *maincalc.f90*		

gasFac = DSqrt(invGasViscosity)
i = firstIntactZone
dCoeff(i) = permeability(i)*invPorosity(i)*gasFac*DSqrt(psi(i))
reposAllowedDeltaTime = reposDR(i)**2/DCoeff(i)
cellControl(2) = i
do i = firstIntactZone+1, numReposZones
	gasFac = DSqrt(invGasViscosity)
	!trz
	reposAllowedDeltaTime = maxTime !initialize with large time
	if (cavityPres /= 0.0) then !skip for test case #1
	i = firstIntactZone
	dCoeff(i) = permeability(i)*invPorosity(i)*gasFac*DSqrt(psi(i))
	reposAllowedDeltaTime = reposDR(i)**2/DCoeff(i)
	cellControl(2) = i
	endif
	!trz
	do i = firstIntactZone+1, numReposZones
		A check of the timestep calculation was added for the 'firstIntactZone' that will skip the calculation if 'cavityPres' is zero. Because of the changes to the boundary condition, this change was needed to run validation test case 1.

Excerpts from source code file *parameters.f90*		
ie = ie+ boundcheck('tensileStrength', tensileStrength, 1.0D4, 6.91D6) ie = ie+ boundcheck('Lt', Lt, -0.0001D0, 0.1D0) !dkr changed for QE0110 ie = ie+ boundcheck('particleDiameter',particleDiameter, 1.0D-3, 1.0D0)	ie = ie+ boundcheck('tensileStrength', tensileStrength, 1.0D4, 6.91D6) ie = ie+ boundcheck('Lt', Lt, -0.0001D0, 0.1D2) !dkr changed for QE0110 ie = ie+ boundcheck('particleDiameter',particleDiameter, 1.0D-3, 1.0D0)	The upper bound for characteristic length, L_t, was increased to 10 for zone size sensitivity testing.
Excerpts from source code file *setupcalc.f90*		
if(numwellzones2 > 0)Then wellArea(collarIndex-1) = .6667*collarAnnulusArea+0.3333*pipeAnnulusArea wellArea(collarIndex) = .3333*collarAnnulusArea+0.6667*pipeAnnulusArea wellVol (collarIndex-1) = wellArea(collarIndex-1)*wellZoneSize(collarIndex-1)	if(numwellzones2 > 0)Then wellArea(collarIndex-1) = (2d0/3d0)*collarAnnulusArea+(1d0/3d0)*pipeAnnulusArea !dkr v1.22, was .3333/.6667 wellArea(collarIndex) = (1d0/3d0)*collarAnnulusArea+(2d0/3d0)*pipeAnnulusArea !dkr v1.22, was .6667/.3333 wellVol (collarIndex-1) = wellArea(collarIndex-1)*wellZoneSize(collarIndex-1)	– The 'wellArea' array definition was updated to calculate fractions 2/3 and 1/3 instead of the given decimal values of 0.6667 and 0.3333. – The 'reposVol' array definition was updated to calculate fraction 2/3

Table B-1. Summary of DRSPALL Code Changes. (Continued)

DRSPALL Version 1.21	DRSPALL Version 1.22 (changes shown in red)	Description of Change
Excerpts from source code file *setupcalc.f90* (continued)		

`if (geometry == 'S') then`
`reposVol(i) = 0.666667d0*Pi*(reposRadiusH(i+1)**3 &`
`-reposRadiusH(i)**3)`
 	
`else`
	`if (geometry == 'S') then`
	`reposVol(i) = (2d0/3d0)*Pi*(reposRadiusH(i+1)**3 &`
	`-reposRadiusH(i)**3)  !dkr v1.22, was .666667`
	`else`
		instead of the given decimal value of 0.666667.
		– The 'numReposZones' definition was updated to work correctly with a constant zone size (added 1).
		– Updated the 'reposZoneSize' definition to work correctly with a constant zone size (subtracted 1 from denominator). The original code version failed when a constant zone size was selected.
		– Added call to QAABORT that exits out of the section of code that previously recalculated the number of zones based on a growth rate greater than 1.0.
		– In the definition of 'reposDR', the option to calculate its values using the cell growth rate was commented out, which ensures that 'reposDR' array values will all be the same (constant zone size).

`numReposZones = repositoryOuterRadius/initialReposZoneSize` `reposZoneSize = (repositoryOuterRadius-initialCavityRadius)/numReposZones`	`numReposZones = repositoryOuterRadius/initialReposZoneSize + 1 !trz` `reposZoneSize = (repositoryOuterRadius-initialCavityRadius)/(numReposZones - 1) !trz`	

`IF( reposRadius1 < (repositoryOuterRadius-initialCavityRadius) .and. GrowthRate > 1.00001) then`
 	
`!dkr 7/23 use brute force`
	`IF( reposRadius1 < (repositoryOuterRadius-initialCavityRadius) .and. GrowthRate > 1.00001) then`
	`call QAABORT ('Growth Rate should be 1.0 ')`
	`!dkr 7/23 use brute force`	

`endif`
 	
`if(reposRadius(i-1) > reposRadius1a)then`
`reposDR (i) = reposDR(i-1)*GrowthRate`
`if(reposRadius(i-1) < reposRadius2) Then`
`reposDR(i)= MIN(LT/minNumCells, reposDR (i))`
`endif`
 	
`else`
`reposDR (i) = reposDR(i-1)`
`endif`
`reposDRH(i) = 0.5*(reposDR(i) + reposDR(i-1))`
	`endif`
	
	`!trz  if(reposRadius(i-1) > reposRadius1a)then`
	`!trz    reposDR (i) = reposDR(i-1)*GrowthRate`
	`!trz    if(reposRadius(i-1) < reposRadius2) Then`
	`!trz      reposDR(i)= MIN(LT/minNumCells, reposDR (i))`
	`!trz    endif`
	`!trz`
	`!trz  else`
	`reposDR (i) = reposDR(i-1)`
	`!trz  endif`
	`reposDRH(i) = 0.5*(reposDR(i) + reposDR(i-1))`	

Table B-1. Summary of DRSPALL Code Changes. (Continued)

DRSPALL Version 1.21	DRSPALL Version 1.22 (changes shown in red)	Description of Change
Excerpts from source code file *vmsfilewrite.f90*		
Close(expulsionValidationFileID) ! test case #5	Close(expulsionValidationFileID) Close(fluidizationTimeValidationFileID) !trz ! test case #5	– Added closing of *fluidization_time.dat.* – Added writing of header data to *fluidization_time.dat.* – Increased output for stress validation file to indices less than 250. – Redefined when information is written to the fluidization.dat file. Previously, data was only written when the first intact zone was less than or equal to zone 20 (or between 100 and 150). Based on the other changes made to the code, the relevant output is now needed when the first intact zone is less than or equal to zone 70 (or between 100 and 150), so the 'if' statement has been modified.
write(expulsionValidationFileID, '(10A15)') '(sec)', 'Penetrated(T/F)', 'Removed(-)', 'Removed(kg)', & 'Store (kg)', 'In Well (kg)', 'Ejected (kg)', 'In Well (m)', 'Error (-)' endif	write(expulsionValidationFileID, '(10A15)') '(sec)', 'Penetrated(T/F)', 'Removed(-)', 'Removed(kg)', & 'Store (kg)', 'In Well (kg)', 'Ejected (kg)', 'In Well (m)', 'Error (-)' ! fluidization time file !trz Write(fluidizationTimeValidationFileID, '(A)') 'Program DR_SPALL - WIPP PA 2003' Write(fluidizationTimeValidationFileID, '(A)') 'ASCII Output file for Test Case #4' Write(fluidizationTimeValidationFileID, '(A)') '' Write(fluidizationTimeValidationFileID, '(A)') 'Zone Fluidization Time' endif	
if (maxTensileFailedIndex <= 20 .or. & (maxTensileFailedIndex > 100 .and. maxTensileFailedIndex <150)) then write(stressValidationFileID, '(A15)') ''	if (maxTensileFailedIndex <= 20 .or. & (maxTensileFailedIndex > 100 .and. maxTensileFailedIndex <250)) then write(stressValidationFileID, '(A15)') ''	
if (firstIntactZone <=20 .or. & (firstIntactZone >100 .and. firstIntactzone < 150)) then i = 0	if (firstIntactZone <=70 .or. & !trz (firstIntactZone >100 .and. firstIntactzone < 150)) then i = 0	

Table B-1. Summary of DRSPALL Code Changes. (Continued)

DRSPALL Version 1.21	**DRSPALL Version 1.22 (changes shown in red)**	**Description of Change**
Excerpts from source code file *vmsfilewrite.f90* (continued)		
end !--- ------------------------- ! test case #4 Subroutine WriteToCouplingValidationFile	end !--- ------------------------- ! test case #4 !trz Subroutine WriteToFluidizationTimeValidationFile(izone) Use Globals Implicit None Integer izone write (fluidizationTimeValidationFileID, 200) izone, fluidizationTime(izone) 200 FORMAT (I8, 1pE21.13) return end !--- ------------------------- ! test case #4 Subroutine WriteToCouplingValidationFile	Added subroutine WriteToFluidizationTimeValidationFile() that writes fluidization times to *fluidization_time.dat*.
Excerpts from source code file *wasteflowcalc.f90*		
Real(8) exitGasDen, exitGasArealFlux, boundaryPres, exitGasFlowRate, & deltaP, curGasDen, ForchNumber, temp, c1, c2, c3, c4, dr2 !if (repositoryPenetrated == .FALSE.) then boundaryPres = cavityPres	Real(8) exitGasDen, exitGasArealFlux, boundaryPres, exitGasFlowRate, & deltaP, curGasDen, ForchNumber, temp, c1, c2, c3, c4, dr2 Real(8) permEnhanceFactor !dkr !if (repositoryPenetrated == .FALSE.) then boundaryPres = cavityPres	– Added definition of 'permEnhanceFactor' and set value to 4.0; this results in no change, since the factor of 4.0 was already used, just not defined as a variable.

Table B-1. Summary of DRSPALL Code Changes. (Continued)

DRSPALL Version 1.21	DRSPALL Version 1.22 (changes shown in red)	Description of Change
Excerpts from source code file *wasteflowcalc.f90* (continued)		
!JFS3 add velocity dependent k (Forchheimer) do i = firstIntactZone, (numReposZones-1) curGasDen = 0.5d0*gasBaseDensity*reposPres(i)*invAtmosphericPressure ForchNumber = ABS(ForchBeta)*curGasDen*abs(superficialVelocity(i))* invGasViscosity*invPorosity(i) permeability(i) = repositoryInitialPerm*(1.0+4.0*fractionFluidized(i))/(1.0+ ForchNumber) enddo permeability(firstIntactZone-1) = permeability(firstIntactZone) !**	!JFS3 add velocity dependent k (Forchheimer) permEnhanceFactor = 4.0 !dkr V1.22, was 4.0 do i = firstIntactZone, numReposZones !trz curGasDen = gasBaseDensity*reposPres(i)*invAtmosphericPressure !trz ForchNumber = ABS(ForchBeta)*curGasDen*abs(superficialVelocity(i))* invGasViscosity*invPorosity(i) permeability(i) = repositoryInitialPerm*(1.0+permEnhanceFactor* fractionFluidized(i))/(1.0+ForchNumber) enddo !permeability(firstIntactZone-1) = permeability(firstIntactZone) !trz !**	– The factor of 0.5 was eliminated in the definition of 'curGasDen' to be consistent with the ideal gas law. – The definition of 'permeability(i)' was updated to include the variable 'permEnhanceFactor'. – The definition of 'permeability(firstIntact Zone-1)' was removed (commented out).
deltaP = reposPres(firstIntactZone) - boundaryPres psi(firstIntactZone-1) = invGasViscosity*(boundaryPres)**2 ! flow calculations	deltaP = reposPres(firstIntactZone) - boundaryPres psi(firstIntactZone) = invGasViscosity*(boundaryPres)**2 !trz !psi(firstIntactZone-1) = invGasViscosity*(boundaryPres)**2 !orig ! flow calculations	The index of 'psi()' was changed from 'firstIntactZone-1' to 'firstIntactZone'.

do i = firstIntactZone, numReposZones
 	
reposPres(i) = DSqrt(gasViscosity*psi(i))
 	
end do
	do i = firstIntactZone, numReposZones
	temp = gasViscosity*psi(i) !apg V1.22 temp for negative
	check
	IF(temp < 0.0) then !apg V1.22
	call QAABORT ('SQRT(-x) reposPres') !apg V1.22
	ENDIF !apg V1.22
	reposPres(i) = DSqrt(temp) !apg was
	DSqrt(gasViscosity*psi(i))
	end do
		The variable 'temp' (equal to 'gasViscosity*psi(i)') was created to use in a test to prevent the square root of a negative number. Inserted a QAABORT call if the code is about to take the square root of a negative number.

Table B-1. Summary of DRSPALL Code Changes. (Continued)

DRSPALL Version 1.21	**DRSPALL Version 1.22 (changes shown in red)**	**Description of Change**
Excerpts from source code file *wasteflowcalc.f90* (continued)		
!dkr used for zone in cavity on CDB reposPres(0) = boundaryPres	!dkr used for zone in cavity on CDB reposPres(firstIntactZone) = boundaryPres !trz !reposPres(0) = boundaryPres !orig	The boundary pressure (‘boundaryPres’) is set equal to ‘reposPres(firstIntact Zone)’ instead of ‘reposPres(0)’.
!dkr changed to improve centering => improved mass balance !exitPoreVelocity = 2.0d0*(reposPres(firstIntactZone)-boundaryPres) & exitPoreVelocity = (reposPres(firstIntactZone)-boundaryPres) &	!dkr changed to improve centering => improved mass balance !exitPoreVelocity = 2.0d0*(reposPres(firstIntactZone)-boundaryPres) & exitPoreVelocity = (reposPres(firstIntactZone+1)-boundaryPres) & !trz	The variable ‘exitPoreVelocity’ is defined using ‘(reposPres(firstIntact Zone+1)-boundaryPres)’ instead of ‘(reposPres(firstIntact Zone)-boundaryPres)’.
! First cell coefficients i = firstIntactZone compressibility = 1.0d0/reposPres(i)	! First cell coefficients i = firstIntactZone + 1 !trz compressibility = 1.0d0/reposPres(i)	Definition of ‘i’ is ‘firstIntactZone+1’, instead of ‘firstIntactZone’.

IF(forchBeta > 0.0)THEN
Forchterm = (permeability(i+1)-permeability(i)) &
/ (permeability(i)*4.0*reposDR(i))
ELSE
ForchTerm = 0.0
	IF(forchBeta > 0.0)THEN
	Forchterm = log(permeability(i+1)/permeability(i-1)) & !trz
	/ (4.0*reposDR(i)) !trz
	ELSE
	ForchTerm = 0.0
		The definition of ‘Forchterm’ is now
		‘Forchterm = log(permeability(i+1)/ permeability(i-1))/ (4.0*reposDR(i))’
		This is due to a re-derivation of an equation in the design document (WIPP PA 2015a; see the definition of the coefficient terms α_1 and α_2 in Section A-2) and is done in three sections of the code.

! Interior cell coefficients do i = (firstIntactZone+1), (numReposZones-1) compressibility = 1.0d0/reposPres(i)	! Interior cell coefficients do i = (firstIntactZone+2), (numReposZones-1) !trz compressibility = 1.0d0/reposPres(i)	Index of ‘i’ starts at ‘firstIntactZone+2’, instead of ‘firstIntactZone+1’.

Table B-1. Summary of DRSPALL Code Changes. (Continued)

DRSPALL Version 1.21	DRSPALL Version 1.22 (changes shown in red)	Description of Change
Excerpts from source code file *wasteflowcalc.f90* (continued)		

IF(forchbeta > 0.0)THEN
Forchterm = (permeability(i+1)-permeability(i)) &
/ (permeability(i)*4.0*reposDR(i))
ELSE
ForchTerm = 0.0
	IF(forchbeta > 0.0)THEN
	Forchterm = log(permeability(i+1)/permeability(i-1)) & !trz
	/ (4.0*reposDR(i)) !trz
	ELSE
	ForchTerm = 0.0
		The 'Forchterm' occurs at three locations in the source code. This is the second occurrence.

IF(forchbeta > 0.0)THEN
Forchterm = (permeability(i+1)-permeability(i)) &
/ (permeability(i)*4.0*reposDR(i))
ELSE
ForchTerm = 0.0
	IF(forchbeta > 0.0)THEN
	Forchterm = log(permeability(i)/permeability(i-1)) & !trz
	/ (4.0*reposDR(i)) !trz
	ELSE
	ForchTerm = 0.0
		The 'Forchterm' occurs at three locations in the source code. This is the third occurrence.

alpha1 = (DarcyTerm1 -Forchterm) *dPrime*deltaTime/reposDR(i) alpha2 = (DarcyTerm2 +Forchterm) *dPrime*deltaTime/reposDR(i) aa(i) = -alpha1 bb(i) = 1.0d0 + alpha1 rr(i) = psi(i) ! Perform inversion. bet = bb(firstIntactZone) psi(firstIntactZone) = rr(firstIntactZone)/bet do i = (firstIntactZone+1), numReposZones gam(i) = cc(i-1)/bet bet = bb(i)-aa(i)*gam(i) psi(i) = (rr(i)-aa(i)*psi(i-1))/bet end do !dkr changed from contant pressure to zero gradient !psi(numReposZones) = repositoryInitialPressure**2/gasViscosity !New BC - Comment next line****************** !psi(numReposZones) = reposPres(numReposZones- 1)**2/gasViscosity do i = (numReposZones-1), firstIntactZone, -1 psi(i) = psi(i)-gam(i+1)*psi(i+1)	alpha1 = (DarcyTerm1 -Forchterm) *dPrime*deltaTime/reposDR(i) alpha2 = (DarcyTerm2 +Forchterm) *dPrime*deltaTime/reposDR(i) aa(i) = -alpha1 - alpha2 !trz bb(i) = 1.0d0 + alpha1 + alpha2 !trz rr(i) = psi(i) ! Perform inversion. bet = bb(firstIntactZone+1) !trz psi(firstIntactZone+1) = rr(firstIntactZone+1)/bet !trz do i = (firstIntactZone+2), numReposZones !trz gam(i) = cc(i-1)/bet bet = bb(i)-aa(i)*gam(i) psi(i) = (rr(i)-aa(i)*psi(i-1))/bet end do !dkr changed from contant pressure to zero gradient !psi(numReposZones) = repositoryInitialPressure**2/gasViscosity !New BC - Comment next line****************** !psi(numReposZones) = reposPres(numReposZones- 1)**2/gasViscosity do i = (numReposZones-1), firstIntactZone+1, -1 !trz psi(i) = psi(i)-gam(i+1)*psi(i+1)	– Definition of 'aa(i)' is now '-alpha1-alpha2'. – Definition of 'bb(i)' is now '1.0d0 + alpha1 + alpha2'. – Definition of 'bet' is now 'bb(firstIntactZone+1)' instead of 'bb(firstIntactZone).' – The definition 'psi(firstIntactZone) = rr(firstIntactZone)/bet' has been replaced by 'psi(firstIntactZone+1) = rr(firstIntactZone+1)/bet' – Index of 'i' starts at 'firstIntactZone+2', instead of 'firstIntactZone+1'. – Index of 'i' ends at 'firstIntactZone+1', instead of 'firstIntactZone'.

Table B-1. Summary of DRSPALL Code Changes. (Continued)

Excerpts from source code file *wastestresscalc.f90*

DRSPALL Version 1.21

```
do i = firstIntactZone, numReposZones
  ! Elastic Stresses
  temp1 = (reposRadius(firstIntactZone-1)/
reposRadius(i))**geomExponent
  radElasticStress(i) =  (cavityPres-farfieldStress)*temp1
+farfieldStress
```

DRSPALL Version 1.22 (changes shown in red)

```
do i = firstIntactZone, numReposZones
  ! Elastic Stresses
  temp1 = (reposRadius(firstIntactZone)/
reposRadius(i))**geomExponent
  radElasticStress(i) =  (cavityPres-farfieldStress)*temp1
+farfieldStress
```

Description of Change

In the definition of temp1, the index of reposRadius() was changed from: (firstIntactZone-1) to (firstIntactZone).

Excerpts from source code file *wellborecalc.f90*

DRSPALL Version 1.21

```
                                               ! used by test case #4
                                               fluidizationSaveTime =
runTime





     end if
```

DRSPALL Version 1.22 (changes shown in red)

```
                                               ! used by test case #4
                                               fluidizationSaveTime =
runTime
!trz
       if(validationTestCase == 4)then
          CALL WriteToFluidizationTimeValidationFile(i)
       endif
!trz
     end if
```

Description of Change

Added call to a new subroutine WriteToFluidizationTimeValidationFile(). This subroutine writes fluidization times to *fludization_time.dat*, which is an output file added for test case #4 to facilitate the verification of fluidization times.

DRSPALL Version 1.21

```
         firstIntactZone = i+1





       end if

     end if
     i = i + 1
   end do
```

DRSPALL Version 1.22 (changes shown in red)

```
         firstIntactZone = i+1

       elseif (fractionFluidized(i) > 1.0001) then !trz
         fractionFluidized (i) = 1.0001      !trz

       end if

     end if
     i = i + 1
   end do
```

Description of Change

Added 'elseif' possibility for 'fractionFluidized(i)' calculation. Previously, 'fractionFluidized(i)' was set to 1.0 only if 'i' was for the 'firstIntactZone'. Otherwise, the 'fractionFluidized' could increase to values much higher than 1.0, which are not physically reasonable, and led to problems in calculating 'permeability' in *wasteflowcalc.f90*. The 'elseif' statement was added to set 'fractionFluidized(i)' to a number slightly larger than 1.0 (1.0001), such that the 'if' statement will be satisfied for zone 'i' in a later step.

APPENDIX C. DRSPALL CALCULATED SPALL VOLUMES

Tables C-1, C-2 and C-3 list the spall volumes calculated by the modified DRSPALL code (Version 1.22) for all four pressure scenarios and for replicates 1, 2, and 3, respectively. These data are located in the CVS repository at /nfs/data/CVSLIB/WIPP_ANALYSES/PABC09/DRSPALL/Output (files *mspall_drs_PABC09_r1.out*, *mspall_drs_PABC09_r2.out*, and *mspall_drs_PABC09_r3.out*).

Table C-1. Modified Spall Volumes from DRSPALL Version 1.22: Replicate 1.

Vector	DPS1 10.0 MPa	DPS2 12.0 MPa	DPS3 14.0 MPa	DPS4 14.8 MPa
1	0.000	0.143	1.147	1.727
2	0.000	0.769	7.300	10.811
3	0.000	0.320	0.874	1.236
4	0.000	0.351	0.472	0.660
5	0.000	0.000	0.000	0.000
6	0.000	0.000	0.000	0.000
7	0.000	0.000	0.000	0.000
8	0.000	0.154	1.002	1.290
9	0.000	0.055	0.425	0.794
10	0.000	0.000	0.000	0.000
11	0.000	0.163	1.031	1.855
12	0.000	0.000	0.000	0.000
13	0.000	0.363	0.533	0.608
14	0.000	0.439	1.024	1.114
15	0.000	0.000	0.328	0.772
16	0.000	0.303	0.497	0.597
17	0.000	0.342	1.524	2.524
18	0.000	0.051	0.427	0.877
19	0.000	0.044	0.750	0.753
20	0.000	0.000	0.000	0.000
21	0.000	0.000	0.125	0.201
22	0.000	0.000	0.000	0.000
23	0.000	0.197	1.200	2.590
24	0.000	0.182	0.949	1.770
25	0.000	0.131	0.785	1.432
26	0.000	0.205	0.960	0.856
27	0.000	0.183	0.358	0.422
28	0.000	0.470	4.268	7.473
29	0.000	0.533	1.932	3.473
30	0.000	0.054	0.539	0.817
31	0.000	0.263	1.027	1.224
32	0.000	9.676	9.996	10.229
33	0.000	1.625	7.964	7.502

Table C-1. Modified Spall Volumes from DRSPALL Version 1.22: Replicate 1. (Continued)

Vector	DPS1 10.0 MPa	DPS2 12.0 MPa	DPS3 14.0 MPa	DPS4 14.8 MPa
34	0.000	0.426	3.292	5.283
35	0.000	0.540	2.289	3.558
36	0.000	3.509	4.819	5.864
37	0.000	0.175	0.462	0.701
38	0.000	0.104	0.618	0.639
39	0.000	0.000	0.000	0.000
40	0.000	0.425	0.901	1.005
41	0.000	0.186	1.139	1.856
42	0.000	0.745	2.199	1.482
43	0.000	0.133	0.835	1.360
44	0.000	0.305	1.143	2.231
45	0.000	0.549	0.793	1.020
46	0.000	0.000	0.000	0.000
47	0.000	0.378	2.485	4.502
48	0.000	0.145	0.691	1.261
49	0.000	0.000	0.000	0.000
50	0.000	0.048	0.618	0.655
51	0.000	0.000	0.000	0.142
52	0.000	0.176	0.896	2.073
53	0.000	0.379	1.632	2.809
54	0.000	0.159	0.884	1.251
55	0.000	0.207	0.350	0.436
56	0.000	0.644	0.673	0.931
57	0.000	0.395	0.536	0.709
58	0.000	0.000	0.000	0.000
59	0.000	2.651	9.262	9.426
60	0.000	0.000	0.000	0.000
61	0.000	0.000	0.000	0.000
62	0.000	0.000	0.000	0.000
63	0.000	0.000	0.000	0.000
64	0.000	0.328	1.127	1.368
65	0.000	0.503	6.320	7.880
66	0.000	0.360	1.510	1.812
67	0.000	0.000	0.142	0.223
68	0.000	0.000	0.000	0.000
69	0.000	0.000	0.000	0.000
70	0.000	0.000	0.000	0.000
71	0.000	0.150	0.942	1.421
72	0.000	0.000	0.047	0.090
73	0.000	0.000	0.000	0.000

Table C-1. Modified Spall Volumes from DRSPALL Version 1.22: Replicate 1. (Continued)

Vector	DPS1 10.0 MPa	DPS2 12.0 MPa	DPS3 14.0 MPa	DPS4 14.8 MPa
74	0.000	0.144	0.977	1.469
75	0.000	0.376	0.555	0.622
76	0.000	0.546	5.939	9.995
77	0.000	0.214	0.974	1.788
78	0.000	0.188	0.949	1.718
79	0.000	1.013	9.647	10.268
80	0.000	0.457	1.197	1.257
81	0.000	0.139	0.776	1.385
82	0.000	0.138	0.602	0.889
83	0.000	0.141	0.827	1.223
84	0.000	0.000	0.000	0.000
85	0.000	0.307	0.462	0.743
86	0.000	0.407	0.597	0.631
87	0.000	0.403	2.231	3.185
88	0.000	0.124	0.624	0.676
89	0.000	0.139	0.662	0.773
90	0.000	0.000	0.000	0.000
91	0.000	0.036	0.665	0.805
92	0.000	0.419	0.994	1.798
93	0.000	0.000	0.175	0.220
94	0.000	0.000	0.069	0.103
95	0.000	0.061	0.592	0.631
96	0.000	0.000	0.000	0.000
97	0.000	0.000	0.000	0.000
98	0.000	0.000	0.000	0.000
99	0.000	0.000	0.000	0.000
100	0.000	0.069	0.702	1.393

Table C-2. Modified Spall Volumes from DRSPALL Version 1.22: Replicate 2.

Vector	DPS1 10.0 MPa	DPS2 12.0 MPa	DPS3 14.0 MPa	DPS4 14.8 MPa
1	0.000	0.416	2.239	2.012
2	0.000	0.106	0.792	0.813
3	0.000	0.157	0.318	0.420
4	0.000	0.387	0.501	0.597
5	0.000	0.461	0.493	0.548
6	0.000	0.399	2.444	4.066
7	0.000	0.000	0.000	0.000

Table C-2. Modified Spall Volumes from DRSPALL Version 1.22: Replicate 2. (Continued)

Vector	DPS1 10.0 MPa	DPS2 12.0 MPa	DPS3 14.0 MPa	DPS4 14.8 MPa
8	0.000	0.000	0.142	0.254
9	0.000	0.381	0.701	0.792
10	0.000	0.000	0.000	0.000
11	0.000	0.327	1.835	2.887
12	0.000	0.000	0.189	0.253
13	0.000	0.000	0.169	0.184
14	0.000	0.000	0.000	0.000
15	0.000	0.000	0.000	0.000
16	0.000	0.366	1.991	3.121
17	0.000	0.414	1.077	1.110
18	0.000	0.000	0.125	0.190
19	0.000	0.000	0.000	0.000
20	0.000	0.000	0.000	0.000
21	0.000	0.000	0.000	0.000
22	0.000	0.609	0.627	0.877
23	0.000	0.000	0.178	0.208
24	0.000	0.098	0.683	1.143
25	0.000	1.103	9.431	10.183
26	0.000	0.146	1.254	1.491
27	0.000	0.397	2.603	4.953
28	0.000	0.000	0.000	0.000
29	0.000	0.000	0.000	0.000
30	0.000	0.199	1.191	2.148
31	0.000	0.000	0.000	0.000
32	0.000	0.369	1.869	3.851
33	0.000	0.123	0.834	1.629
34	0.000	0.680	2.521	2.104
35	0.000	0.150	0.711	1.477
36	0.000	0.094	0.273	0.365
37	0.000	0.000	0.000	0.089
38	0.000	0.000	0.000	0.000
39	0.000	0.182	0.855	1.525
40	0.000	0.157	0.909	1.344
41	0.000	7.070	6.749	15.817
42	0.000	0.093	0.253	0.362
43	0.000	0.309	0.433	0.551
44	0.000	0.030	0.337	0.645
45	0.000	0.536	1.276	1.749
46	0.000	0.408	1.806	2.244
47	0.000	0.373	0.878	1.264

Table C-2. Modified Spall Volumes from DRSPALL Version 1.22: Replicate 2. (Continued)

Vector	DPS1 10.0 MPa	DPS2 12.0 MPa	DPS3 14.0 MPa	DPS4 14.8 MPa
48	0.000	0.000	0.000	0.000
49	0.000	0.000	0.000	0.000
50	0.000	0.392	0.686	0.640
51	0.000	0.000	0.000	0.000
52	0.000	0.000	0.000	0.000
53	0.000	0.000	0.000	0.000
54	0.000	0.040	0.772	0.815
55	0.000	0.352	1.512	2.552
56	0.000	0.173	0.877	1.635
57	0.000	0.000	0.000	0.000
58	0.000	0.084	1.728	1.850
59	0.000	0.067	0.611	1.193
60	0.000	0.161	0.885	1.308
61	0.000	0.081	0.255	0.369
62	0.000	0.133	0.909	1.605
63	0.000	0.192	0.416	0.534
64	0.000	0.000	0.000	0.000
65	0.000	0.345	0.440	0.519
66	0.000	0.073	0.758	1.171
67	0.000	0.152	0.771	1.439
68	0.000	0.111	0.728	0.773
69	0.000	0.000	0.000	0.000
70	0.000	0.583	1.094	1.098
71	0.000	0.845	7.027	7.051
72	0.000	0.000	0.000	0.000
73	0.000	0.000	0.000	0.000
74	0.000	0.502	1.298	1.166
75	0.000	0.169	0.806	1.470
76	0.000	0.085	0.562	0.777
77	0.000	0.370	1.636	2.860
78	0.000	0.420	0.619	0.698
79	0.000	0.046	0.529	0.767
80	0.000	0.044	0.505	0.607
81	0.000	0.176	0.926	1.339
82	0.000	0.000	0.000	0.000
83	0.000	0.332	1.517	2.754
84	0.000	0.162	0.883	1.277
85	0.000	0.325	0.644	1.022
86	0.000	1.246	7.663	9.055
87	0.000	0.000	0.234	0.268

Table C-2. Modified Spall Volumes from DRSPALL Version 1.22: Replicate 2. (Continued)

Vector	DPS1 10.0 MPa	DPS2 12.0 MPa	DPS3 14.0 MPa	DPS4 14.8 MPa
88	0.000	0.151	0.821	0.923
89	0.000	0.158	0.327	0.427
90	0.000	0.000	0.000	0.000
91	0.000	0.064	0.634	1.559
92	0.000	0.271	0.551	0.678
93	0.000	0.154	0.712	0.730
94	0.000	0.046	0.540	0.755
95	0.000	0.338	1.529	2.921
96	0.000	0.042	0.574	0.732
97	0.000	0.302	0.610	0.886
98	0.000	0.000	0.000	0.000
99	0.000	0.422	0.499	0.564
100	0.000	0.000	0.000	0.000

Table C-3. Modified Spall Volumes from DRSPALL Version 1.22: Replicate 3.

Vector	DPS1 10.0 MPa	DPS2 12.0 MPa	DPS3 14.0 MPa	DPS4 14.8 MPa
1	0.000	3.009	8.482	8.694
2	0.000	0.409	3.209	5.072
3	0.000	0.046	0.386	0.758
4	0.000	0.000	0.350	0.560
5	0.000	1.174	3.262	4.298
6	0.000	0.279	1.614	1.523
7	0.000	0.000	0.000	0.000
8	0.000	0.389	0.822	0.970
9	0.000	0.397	3.136	5.032
10	0.000	0.000	0.000	0.000
11	0.000	0.571	0.784	0.950
12	0.000	0.186	0.976	0.848
13	0.000	0.440	2.772	2.241
14	0.000	0.302	0.417	0.549
15	0.000	0.513	1.393	1.104
16	0.000	0.114	0.625	0.819
17	0.000	0.054	0.554	0.920
18	0.000	0.000	0.000	0.000
19	0.000	0.342	0.487	0.521
20	0.000	0.052	0.487	0.703
21	0.000	0.476	1.081	1.492

Table C-3. Modified Spall Volumes from DRSPALL Version 1.22: Replicate 3. (Continued)

Vector	DPS1 10.0 MPa	DPS2 12.0 MPa	DPS3 14.0 MPa	DPS4 14.8 MPa
22	0.000	0.483	0.752	1.304
23	0.000	0.000	0.122	0.188
24	0.000	0.000	0.000	0.000
25	0.000	7.958	8.018	8.036
26	0.000	0.000	0.000	0.000
27	0.000	0.000	0.000	0.000
28	0.000	0.665	1.582	1.475
29	0.000	0.065	0.613	0.687
30	0.000	0.365	0.528	0.564
31	0.000	0.000	0.000	0.000
32	0.000	0.180	0.646	0.571
33	0.000	0.134	0.662	0.644
34	0.000	0.000	0.000	0.000
35	0.000	0.000	0.000	0.000
36	0.000	4.516	5.382	4.678
37	0.000	0.403	0.990	1.097
38	0.000	0.372	1.665	2.299
39	0.000	0.057	0.582	1.397
40	0.000	0.189	1.162	2.561
41	0.000	0.000	0.000	0.000
42	0.000	0.284	1.374	2.319
43	0.000	0.408	0.958	0.800
44	0.000	0.000	0.000	0.000
45	0.000	0.056	0.580	1.013
46	0.000	0.102	0.528	1.005
47	0.000	0.159	0.730	0.749
48	0.000	0.000	0.000	0.000
49	0.000	0.118	0.850	1.052
50	0.000	0.000	0.000	0.000
51	0.000	0.517	4.722	3.999
52	0.000	0.000	0.000	0.000
53	0.000	0.379	2.026	3.233
54	0.000	0.046	0.623	0.809
55	0.000	0.045	0.441	0.885
56	0.000	0.180	1.091	1.887
57	0.000	0.388	0.505	0.827
58	0.000	0.382	0.571	0.674
59	0.000	0.189	1.177	2.489
60	0.000	0.000	0.000	0.000
61	0.000	0.468	4.277	4.572

Table C-3. Modified Spall Volumes from DRSPALL Version 1.22: Replicate 3. (Continued)

Vector	DPS1 10.0 MPa	DPS2 12.0 MPa	DPS3 14.0 MPa	DPS4 14.8 MPa
62	0.000	0.071	0.723	1.143
63	0.000	0.054	0.539	0.780
64	0.000	0.000	0.099	0.158
65	0.000	0.089	0.288	0.395
66	0.000	0.000	0.000	0.000
67	0.000	1.048	10.177	13.326
68	0.000	0.523	5.610	7.668
69	0.000	0.417	2.723	4.726
70	0.000	0.000	0.000	0.000
71	0.000	0.000	0.000	0.000
72	0.000	0.000	0.126	0.273
73	0.000	0.000	0.000	0.000
74	0.000	0.400	0.845	0.834
75	0.000	0.156	0.319	0.452
76	0.000	0.000	0.000	0.000
77	0.000	0.052	0.543	0.986
78	0.000	0.331	1.249	2.991
79	0.000	0.149	0.756	0.736
80	0.000	0.000	0.000	0.000
81	0.000	0.055	0.175	0.281
82	0.000	0.219	0.422	0.818
83	0.000	0.055	0.674	0.718
84	0.000	0.000	0.000	0.000
85	0.000	0.000	0.050	0.110
86	0.000	0.339	0.520	0.581
87	0.000	0.290	1.116	2.045
88	0.000	0.000	0.000	0.000
89	0.000	0.000	0.000	0.000
90	0.000	0.000	0.181	0.216
91	0.000	0.129	0.682	0.735
92	0.000	0.000	0.000	0.000
93	0.000	0.342	1.534	2.843
94	0.000	0.321	1.508	3.194
95	0.000	0.000	0.090	0.165
96	0.000	0.420	1.478	1.989
97	0.000	0.000	0.185	0.213
98	0.000	0.000	0.000	0.000
99	0.000	0.037	0.477	0.888
100	0.000	0.396	2.573	3.848