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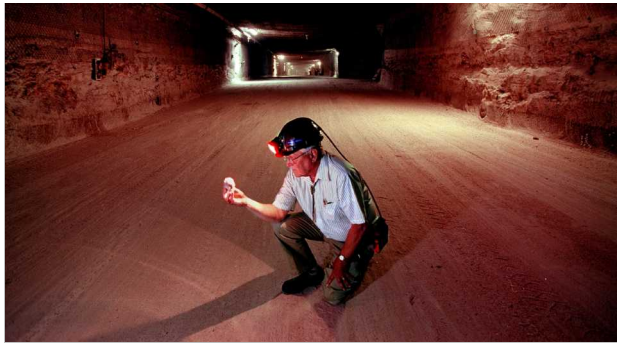

2/2/2016

Impact of the DRSPALL Modification on WIPP PA Calculations

Dwayne C. Kicker

Stoller Newport News Nuclear, Inc.

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U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

Outline

I. The software problem

II. Background on DRSPALL

III. DRSPALL modifications

IV. Impact on WIPP PA calculations

V. Summary

The Software Problem

- An error in the implementation of the DRSPALL finite difference equations was discovered and documented in Software Problem Report (SPR) 13-001.
- DRSPALL uses the Darcy flow equation with a Forchheimer correction to account for high gas flow rates (the variable 'Forchterm').
- The original *wasteflowcalc.f90* source code file contained three 'Forchterm' equations (for the first cell, the interior cells, and the last cell), having the form:

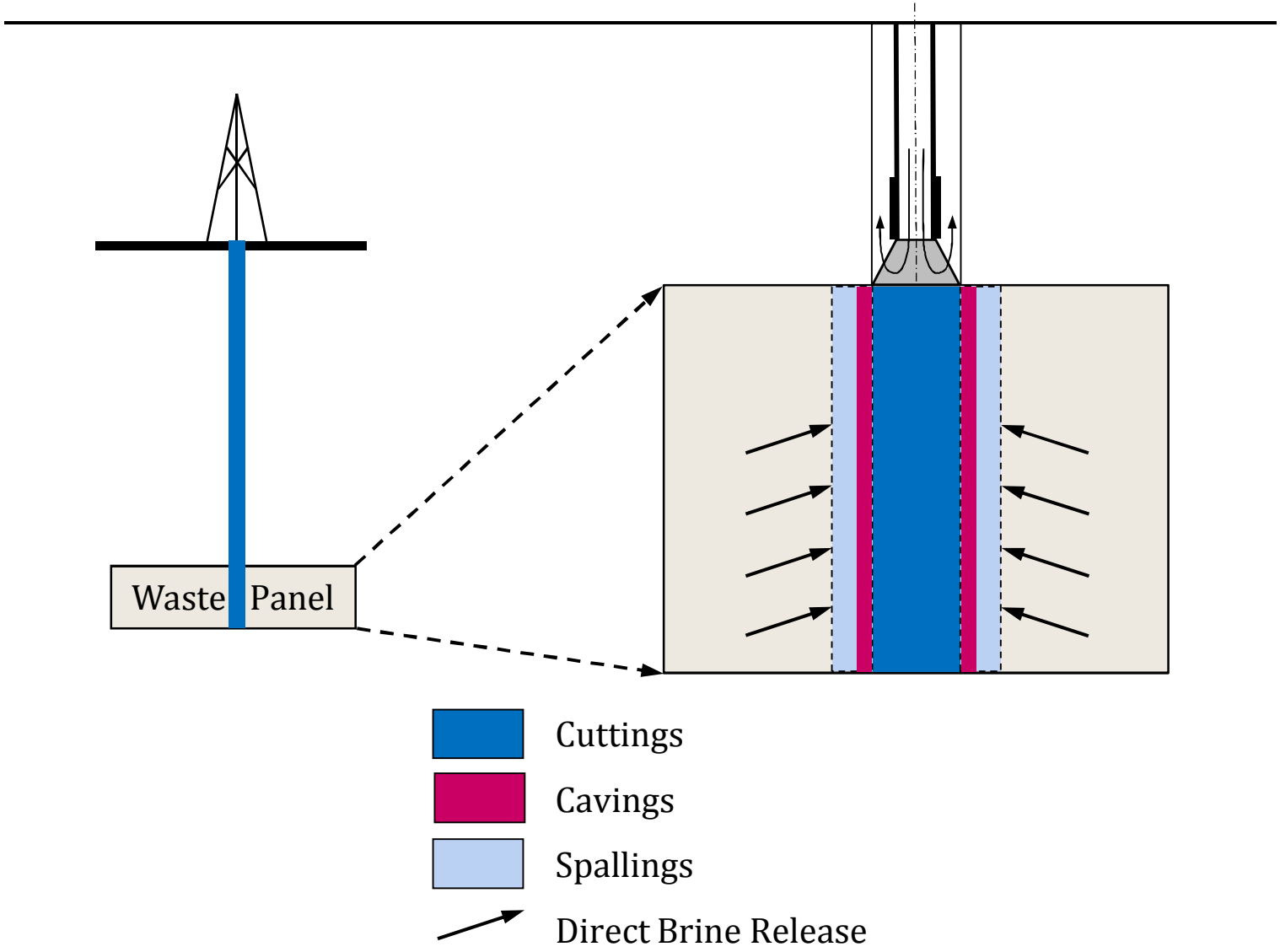
$$Forchterm = \frac{k'(i+1) - k'(i)}{4\,k'(i)\Delta r(i)}$$

where k' = velocity dependent permeability (m^2)
Δr = repository zone size (m)
i = finite differencing zone index.

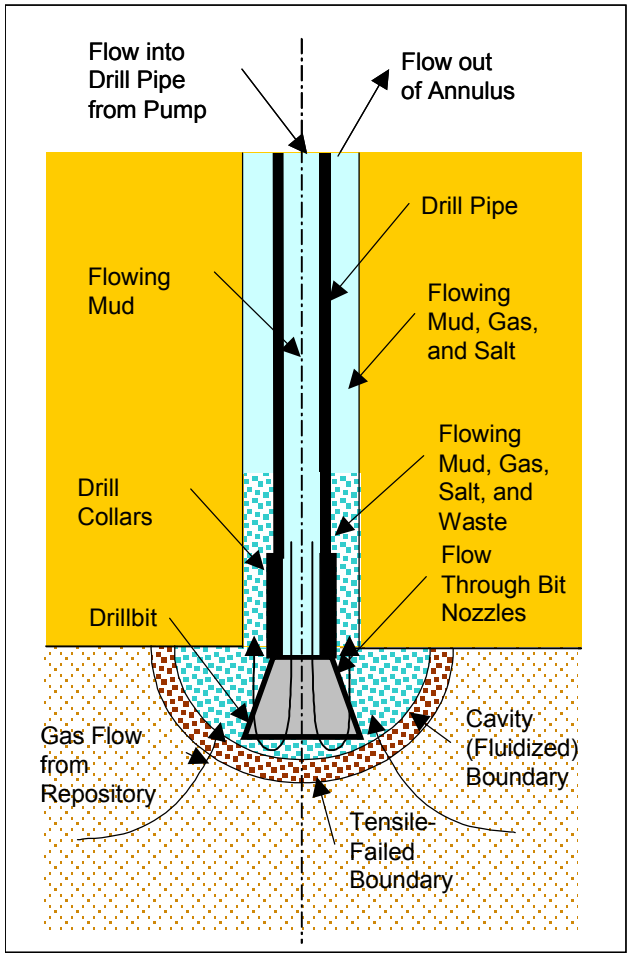
- However, the DRSPALL Design Document was based on a centered-difference discretization, and indicated the correct equation should be:

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

Schematic of Direct Releases



Conceptual Model Description



- The spallings model is a dynamic simulation of fluid flow and mechanical stresses near the borehole during a hypothetical borehole intrusion of a pressurized waste room.
- The cavity in waste room will grow axisymmetrically due to the spalling process.
- Radioactive solids failed by a tensile stress mechanism, fluidized in the cavity, and ejected from the borehole are considered spallings releases.

Modifications to DRSPALL

- DRSPALL assumes a Darcy flow of an isothermal ideal gas in a porous medium, which allows a simplifying pseudopressure approach to be taken.
- The approach for modifying the DRSPALL code was to re-derive the governing equations and the finite difference discretization, resulting in the following equation for pseudopressure:

$$\psi_j^n = -\alpha_1 \psi_{j-1}^{n+1} + (1+2\alpha)\psi_j^{n+1} - \alpha_2 \psi_{j+1}^{n+1}$$

where

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

new Forchterm

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

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

ψ = pseudopressure (Pa/s) at cell j and timestep n

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

k' = velocity-dependent permeability (m^2)

m = geometry exponent (m=2 for cylindrical, m=3 for spherical)

p = pressure in gas (Pa)

r = radius of cavity (m)

t = time (s)

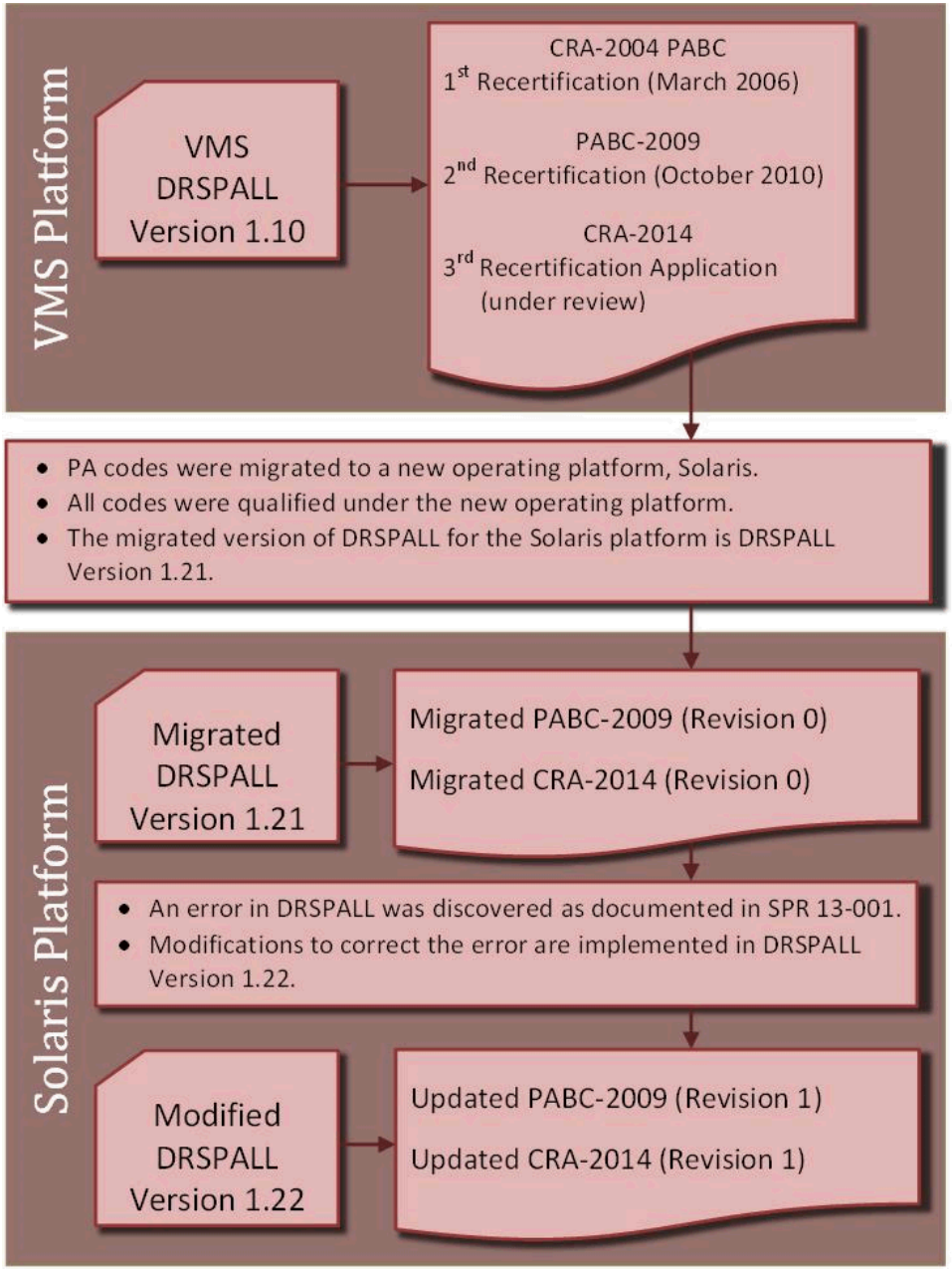
η = viscosity of gas (Pa·s)

ϕ = porosity of waste

- The re-derivation of the pseudopressure equation resulted in the same original equation form except that the coefficient terms α_1 and α_2 are different due to a correction in the spatial variability of k', which produced a modified 'Forchterm'.

Flowchart of DRSPALL Versions

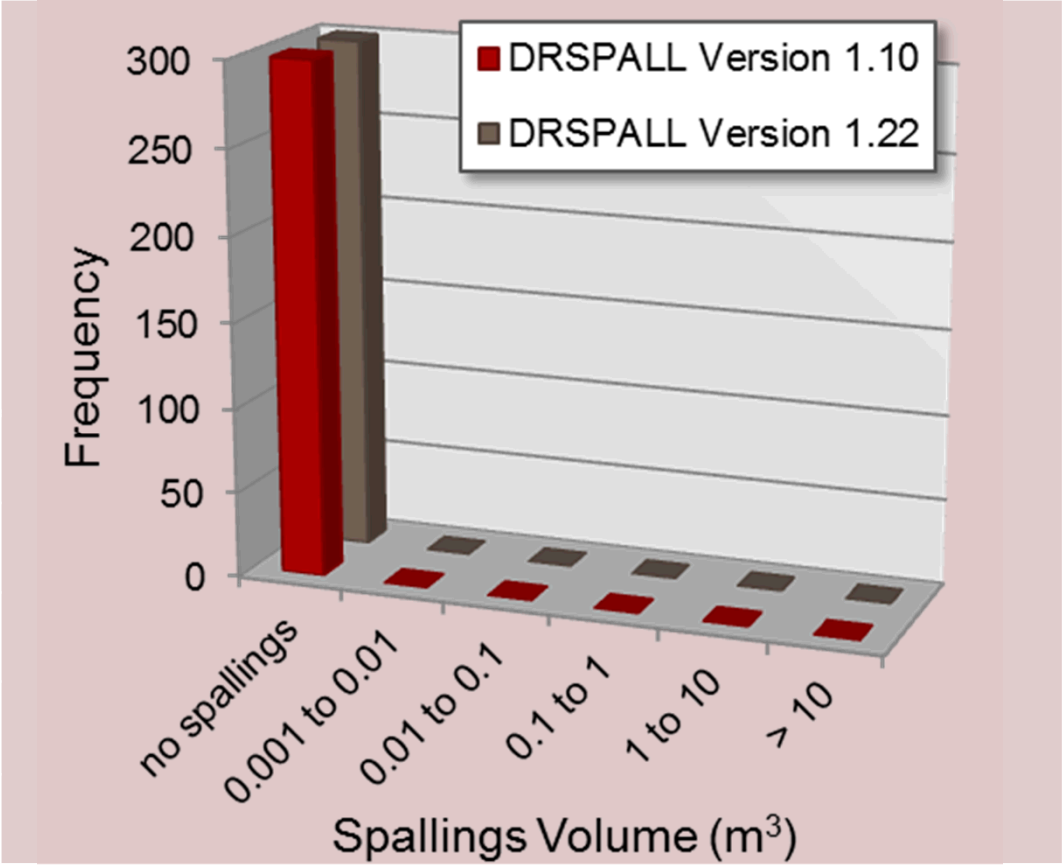
- Both the current PA baseline calculations (PABC-2009) and the CRA-2014 calculations were run on an Alpha OpenVMS platform.
- After the submittal of the CRA-2014, PA calculations have been migrated to a Sun Solaris Blade Server.



DRSPALL Volumes: DPS 1

(initial repository pressure = 10.0 MPa)

Summary of Statistics for DRSPALL Spallings Volumes	VMS DRSPALL (Version 1.10)	Modified DRSPALL (Version 1.22)
Maximum (m^3)	0	0
Mean (m^3)	0	0
Median (m^3)	0	0
% of Vectors with Volumes > 0 m^3	0	0
% of Vectors with Volumes > 1 m^3	0	0

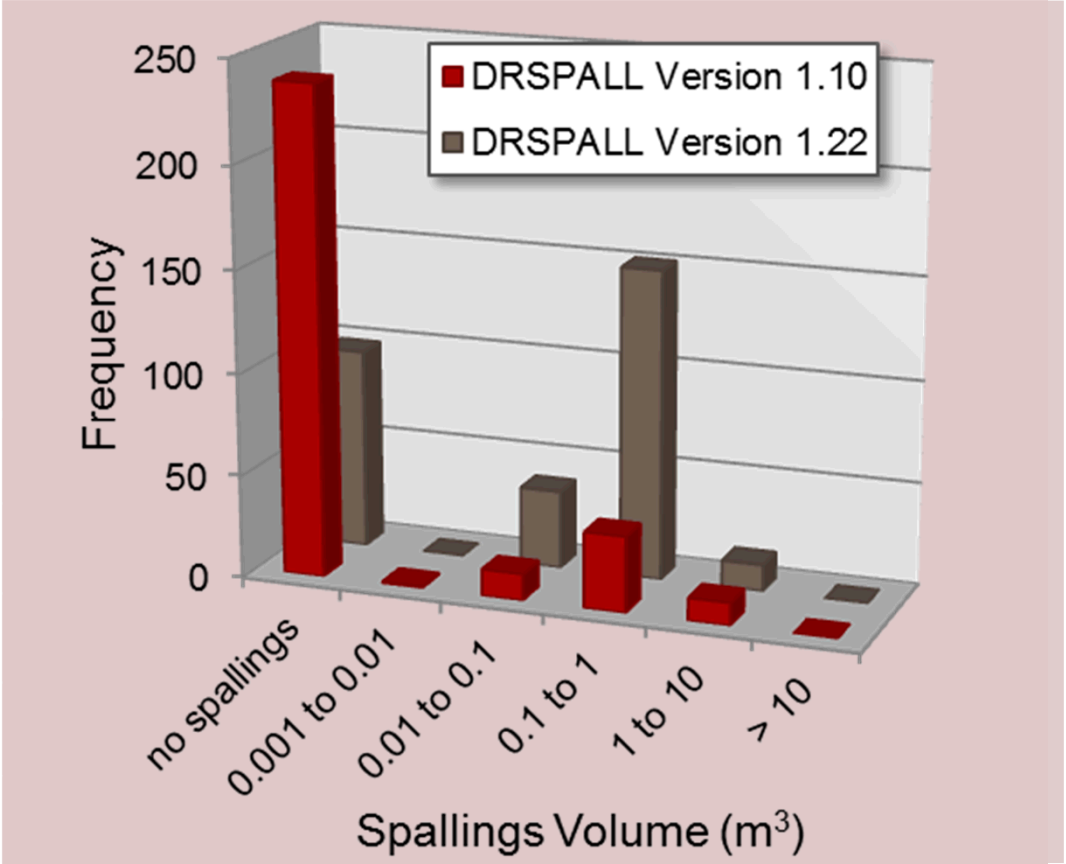


DPS = DRSPALL pressure scenario

DRSPALL Volumes: DPS 2

(initial repository pressure = 12.0 MPa)

Summary of Statistics for DRSPALL Spallings Volumes	VMS DRSPALL (Version 1.10)	Modified DRSPALL (Version 1.22)
Maximum (m^3)	7.71	9.68
Mean (m^3)	0.172	0.320
Median (m^3)	0.000	0.138
% of Vectors with Volumes > 0 m^3	21	67
% of Vectors with Volumes > 1 m^3	4	4

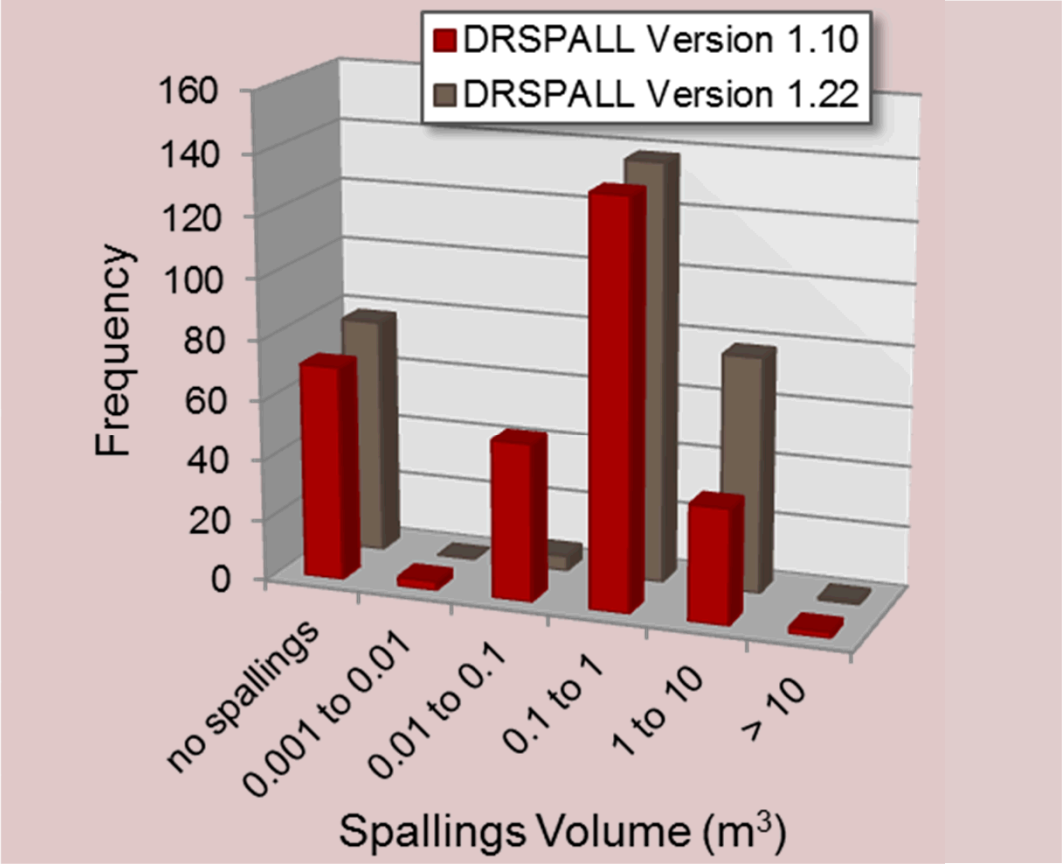


DPS = DRSPALL pressure scenario

DRSPALL Volumes: DPS 3

(initial repository pressure = 14.0 MPa)

Summary of Statistics for DRSPALL Spallings Volumes	VMS DRSPALL (Version 1.10)	Modified DRSPALL (Version 1.22)
Maximum (m^3)	11.83	10.18
Mean (m^3)	0.665	1.089
Median (m^3)	0.160	0.599
% of Vectors with Volumes > 0 m^3	76	74
% of Vectors with Volumes > 1 m^3	13	26

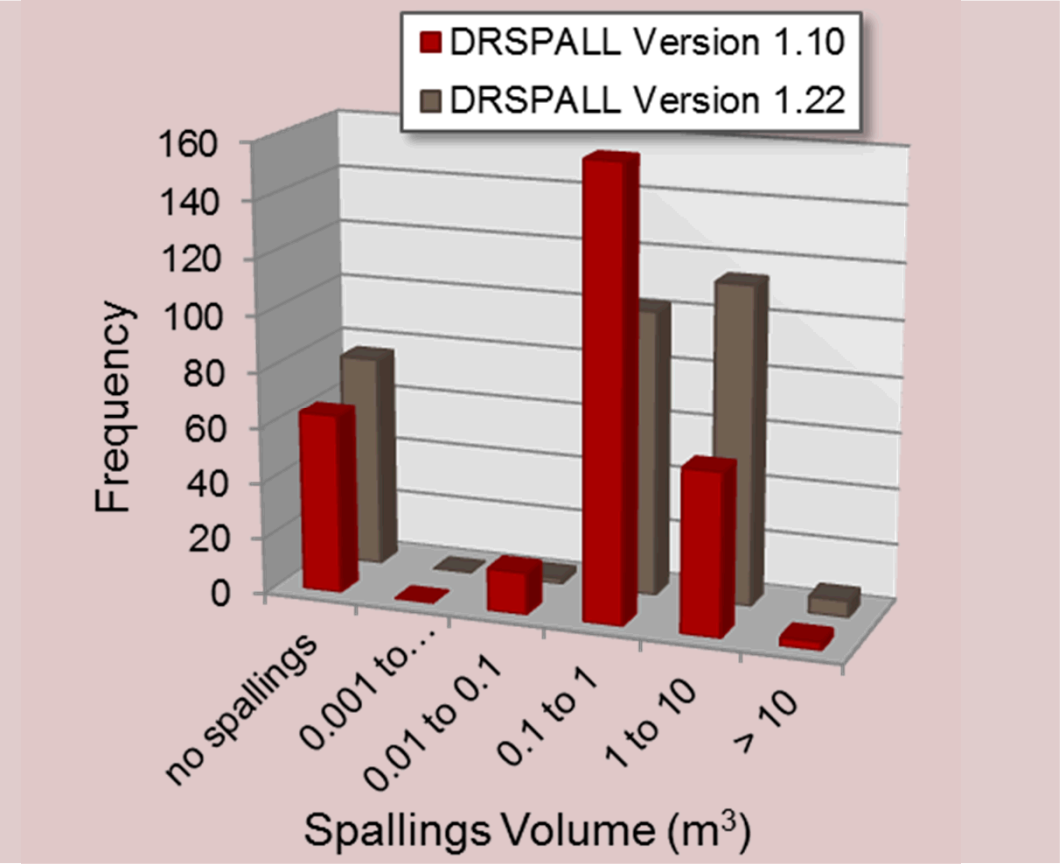


DPS = DRSPALL pressure scenario

DRSPALL Volumes: DPS 4

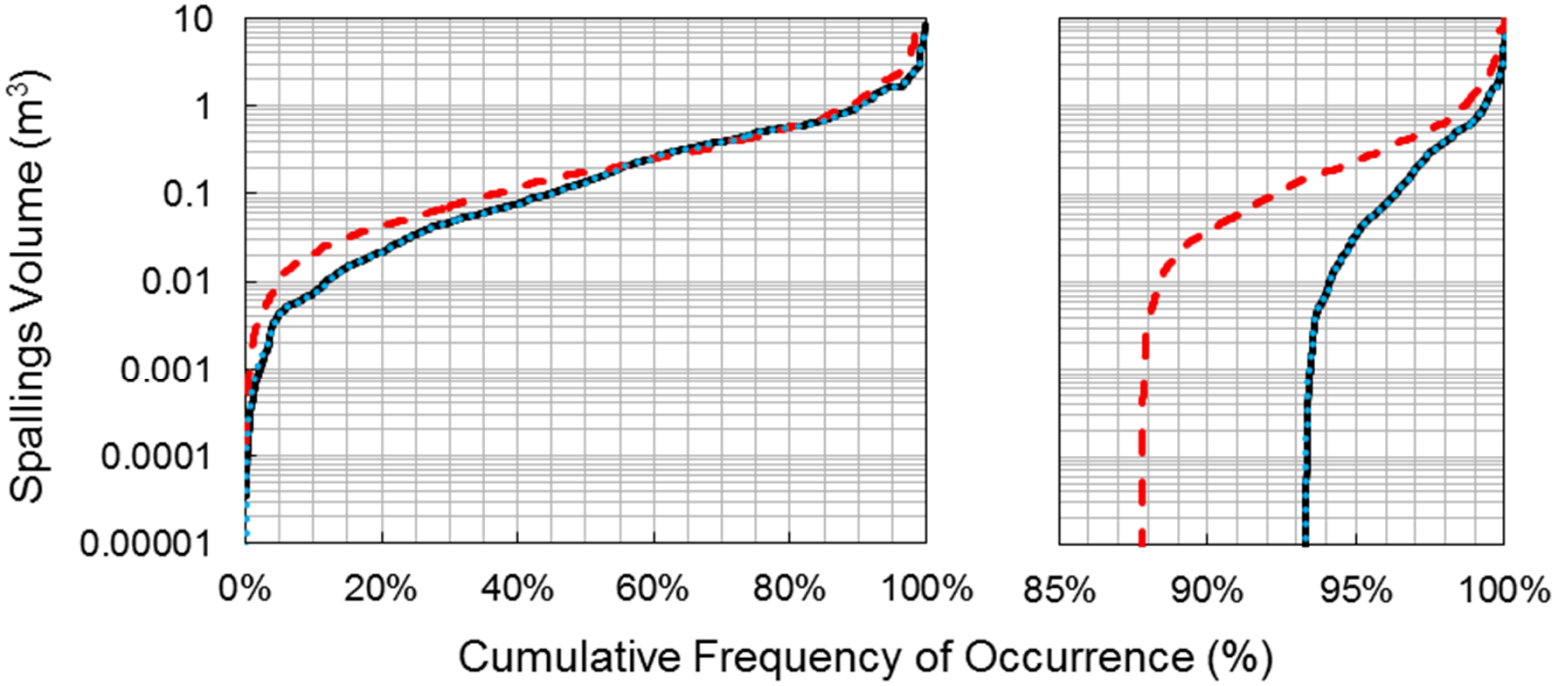
(initial repository pressure = 14.8 MPa)

Summary of Statistics for DRSPALL Spallings Volumes	VMS DRSPALL (Version 1.10)	Modified DRSPALL (Version 1.22)
Maximum (m^3)	14.54	15.82
Mean (m^3)	0.978	1.471
Median (m^3)	0.318	0.772
% of Vectors with Volumes > 0 m^3	79	75
% of Vectors with Volumes > 1 m^3	20	40



DPS = DRSPALL pressure scenario

PABC-2009 Spallings Volumes



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

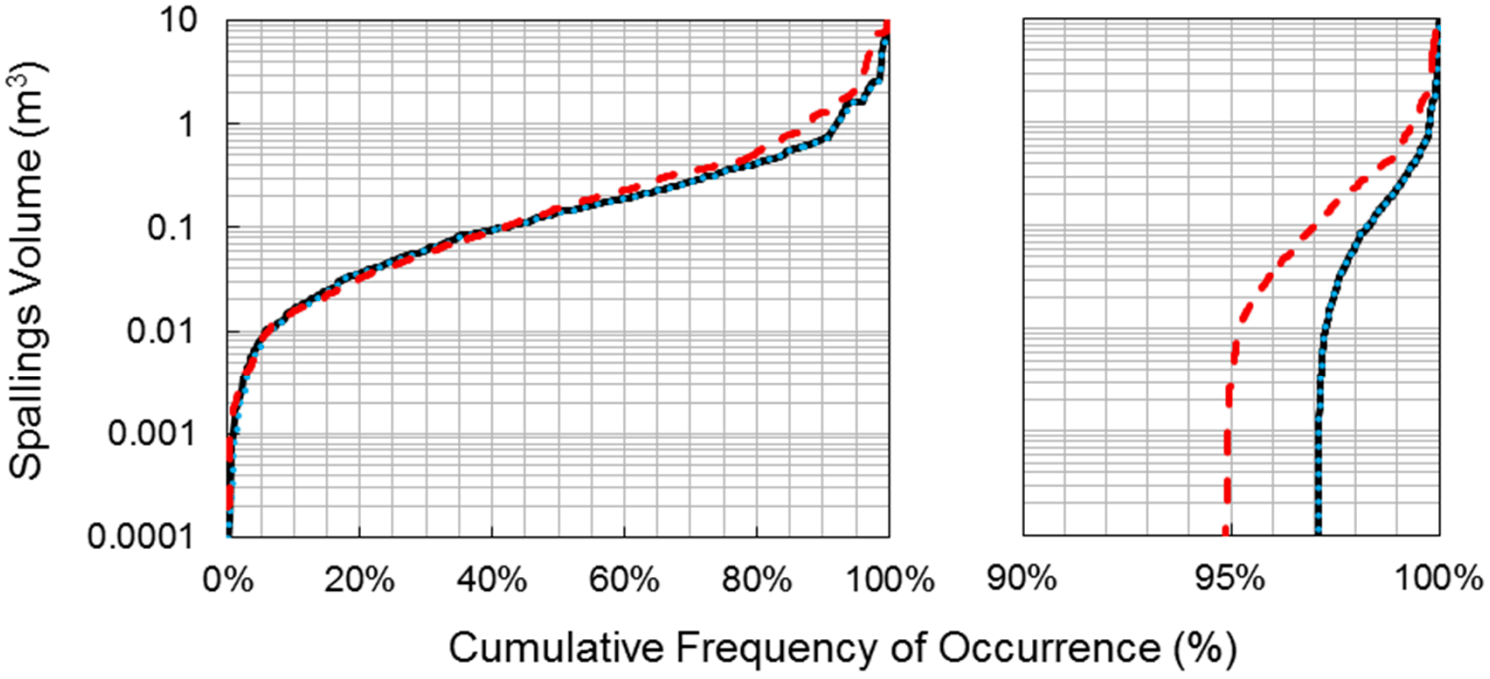
b. All spallings results — includes simulations with no spallings

VMS PABC-2009 using DRSPALL Version 1.10

Migrated PABC-2009 (Revision 0) using DRSPALL Version 1.21

Updated PABC-2009 (Revision 1) using DRSPALL Version 1.22

CRA-2014 Spallings Volumes



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

b. All spallings results — includes simulations with no spallings

VMS CRA-2014 using DRSPALL Version 1.10

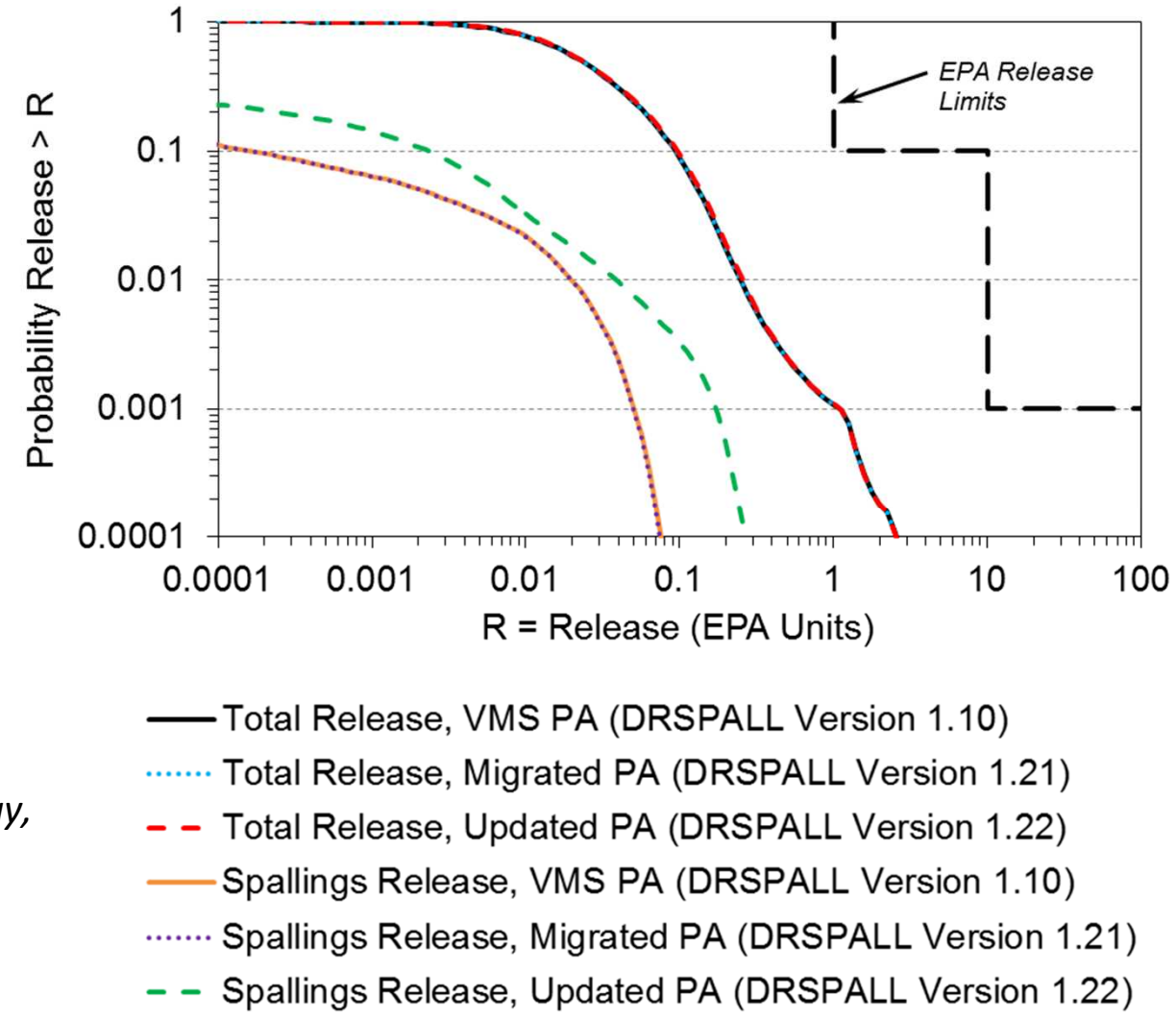
Migrated CRA-2014 (Revision 0) using DRSPALL Version 1.21

Updated CRA-2014 (Revision 1) using DRSPALL Version 1.22

PABC-2009 Normalized Radionuclide Releases

- Spallings Releases
  - VMS PABC-2009
  - Migrated PABC-2009
  - Updated PABC-2009 using DRSPALL v 1.22
- Total Releases
  - **VMS PABC-2009**
  - Migrated PABC-2009
  - Updated PABC-2009 using DRSPALL v 1.22

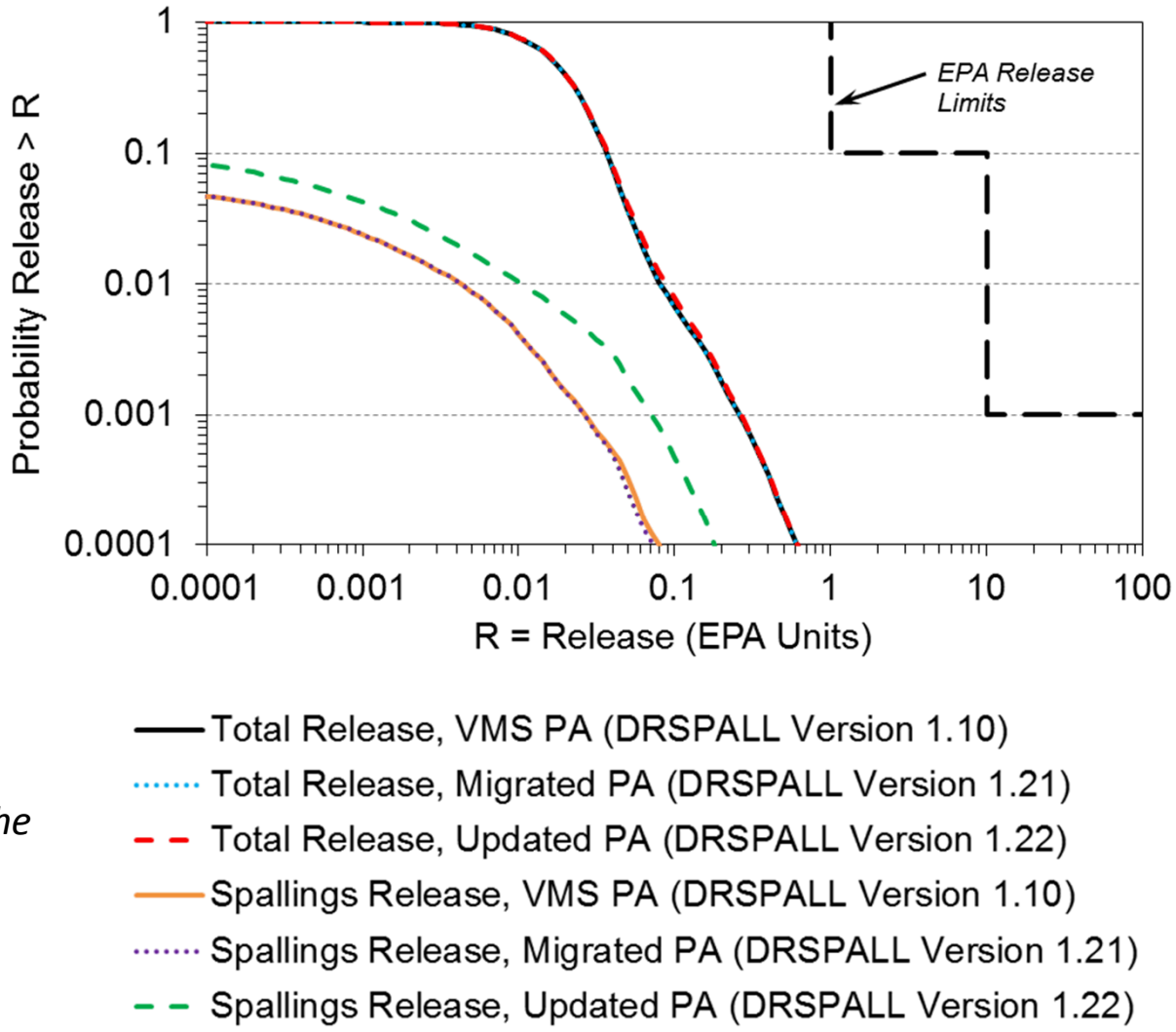
Total normalized releases are calculated by forming the summation of releases across each potential release pathway, namely cuttings and cavings releases, spallings releases, direct brine releases, and Culebra transport releases.



CRA-2014 Normalized Radionuclide Releases

- Spallings Releases
  - VMS CRA-2014
  - Migrated CRA-2014
  - Updated CRA-2014 using DRSPALL v 1.22
- Total Releases
  - **VMS CRA-2014**
  - Migrated CRA-2014
  - Updated CRA-2014 using DRSPALL v 1.22

Both the PABC-2009 and 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.



Summary

- In response to SPR 13-001, modifications were implemented in DRSPALL Version 1.22 to correct the finite difference equations contained in the source code file *wasteflowcalc.f90*.
- The modification to DRSPALL generally results in fewer simulations with no spallings and an increase in spallings volumes when it occurs.
- 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.
- The modifications to DRSPALL do not impact WIPP PA results for total releases.
- The spallings volume results from DRSPALL Version 1.22 will be used in the PABC-2014.

Bibliography of DRSPALL Modification Documents

Sandia National Laboratories

- Software Problem Report 13-001 (ERMS 561524)
- Implementation Document for DRSPALL Version 1.22 (ERMS 562641)
- Verification and Validation Plan / Validation Document for DRSPALL Version 1.22 (ERMS 562643)
- Design Document for DRSPALL Version 1.22 (ERMS 562640)
- Addendum to User's Manual for DRSPALL Version 1.22 (ERMS 562642)
- DRSPALL Zone Size Sensitivity Study (ERMS 564427)
- Impact of DRSPALL Modification on Waste Isolation Pilot Plant Performance Assessment Calculations (ERMS 564863)
- Software Problem Closure Report 13-001 (ERMS 564912)
- SAND Report — DRSPALL: Impact of the Modification of the Numerical Spallings Model on Waste Isolation Pilot Plant Performance Assessment (SAND2016-0231)
- WM2016 Conference — Impact of Corrections to the Spallings Volume Calculation on Waste Isolation Pilot Plant Performance Assessment (March 2016)