

*Exceptional service in the national interest*



# WIPP Performance Assessment: Current Status and The Road Ahead

2015 P&RA CoP Annual Technical Exchange Meeting  
Richland, WA December 15-16, 2015

Todd R. Zeitler

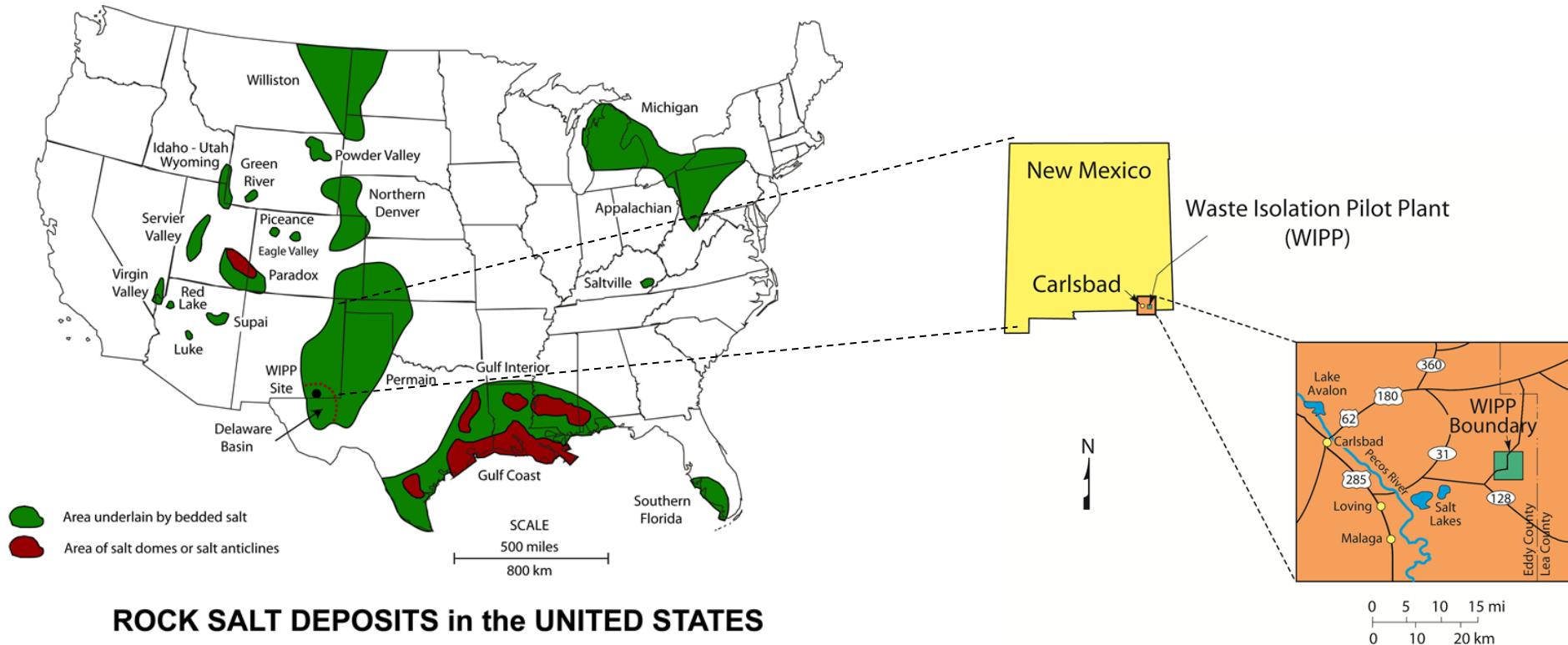


Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000. SAND NO. 2011-XXXXP. This research is funded by WIPP programs administered by the Office of Environmental Management (EM) of the U.S. Department of Energy.

# Outline

- WIPP Regulatory Requirements and PA
  - Release Mechanisms and Compliance Metric
- 2014 WIPP Compliance Recertification Application
  - Updates and Parameter Refinements
  - Approach and Results
- Future Changes to WIPP PA
  - PFLOTRAN as a Means to 3-D modeling
- Summary

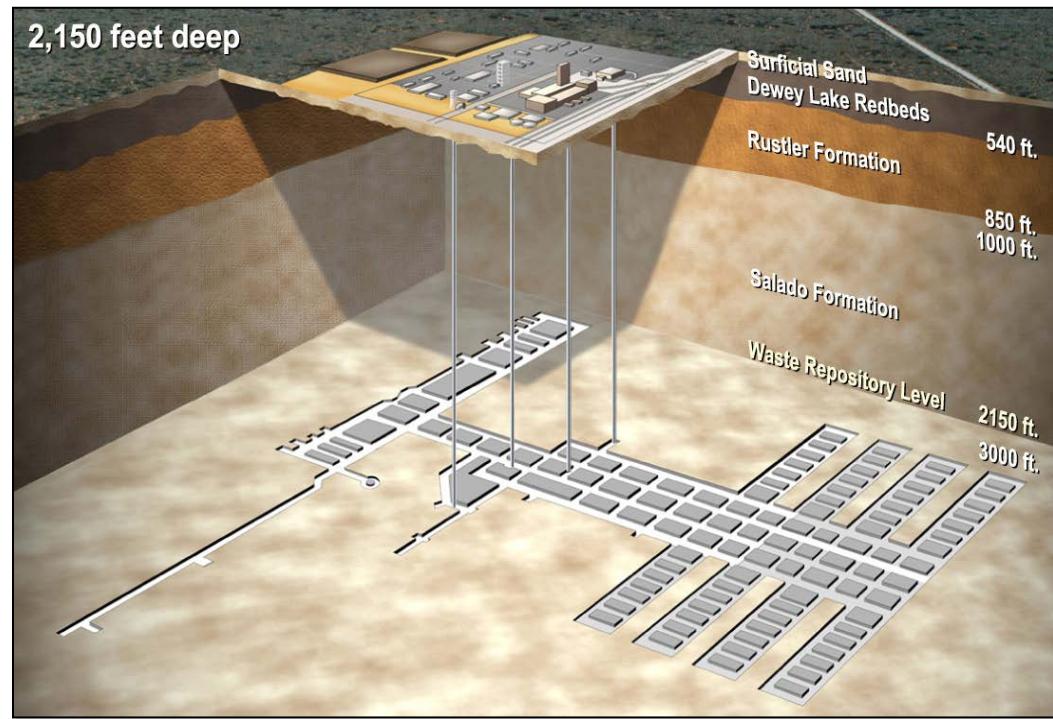
# Waste Isolation Pilot Plant Location



# About The WIPP

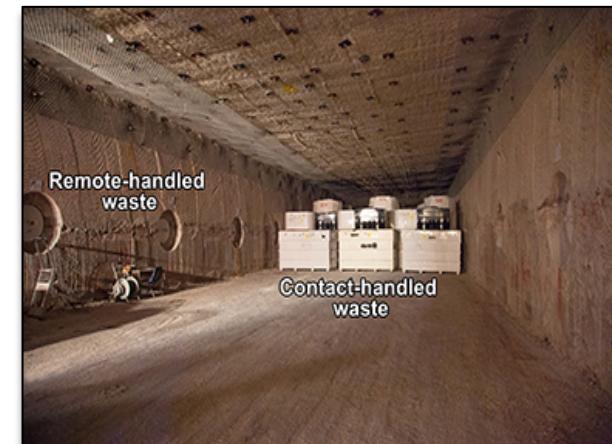
The WIPP is a permanent disposal facility for transuranic waste

- The nation's only licensed deep geologic repository for nuclear waste
- Operated by U.S. Department of Energy (**DOE**)
- Long-term performance regulated by U.S. Environmental Protection Agency (**EPA**)
- Waste is emplaced in a **salt formation** deep underground
- Long-term regulatory compliance is demonstrated via Performance Assessment (PA) undertaken by **SNL** Carlsbad



# Long-Term Regulatory Requirements

- Regulatory requirements guide the WIPP PA framework.
  - The WIPP must be designed to provide *reasonable expectation* that *cumulative releases* of radionuclides to the accessible environment for *10,000 years* after closure from all *significant processes and events* shall be less than specified *release limits*



# Regulatory Requirements

- Reasonable expectation: regulations acknowledge substantial uncertainties
- 10,000 years: PA must predict behavior for entire regulatory time period
- Significant processes and events: PA must include all of these, including the possibility of human intrusion

Radionuclide	Release limit per 1,000 MTHM or other unit of waste (see notes) (curies)
Americium-241 or -243 .....	100
Carbon-14 .....	100
Cesium-135 or -137 .....	1,000
Iodine-129 .....	100
Neptunium-237 .....	100
Plutonium-238, -239, -240, or -242 .....	100
Radium-226 .....	100
Strontium-90 .....	1,000
Technetium-99 .....	10,000
Thorium-230 or -232 .....	10
Tin-126 .....	1,000
Uranium-233, -234, -235, -236, or -238 .....	100
Any other alpha-emitting radionuclide with a half-life greater than 20 years .....	100
Any other radionuclide with a half-life greater than 20 years that does not emit alpha particles .....	1,000

From 40 CFR 191

$$R = \sum \frac{Q_i}{L_i} \left( \frac{1 \times 10^6 \text{ curies}}{C} \right)$$

**R** = Normalized release in “EPA units”

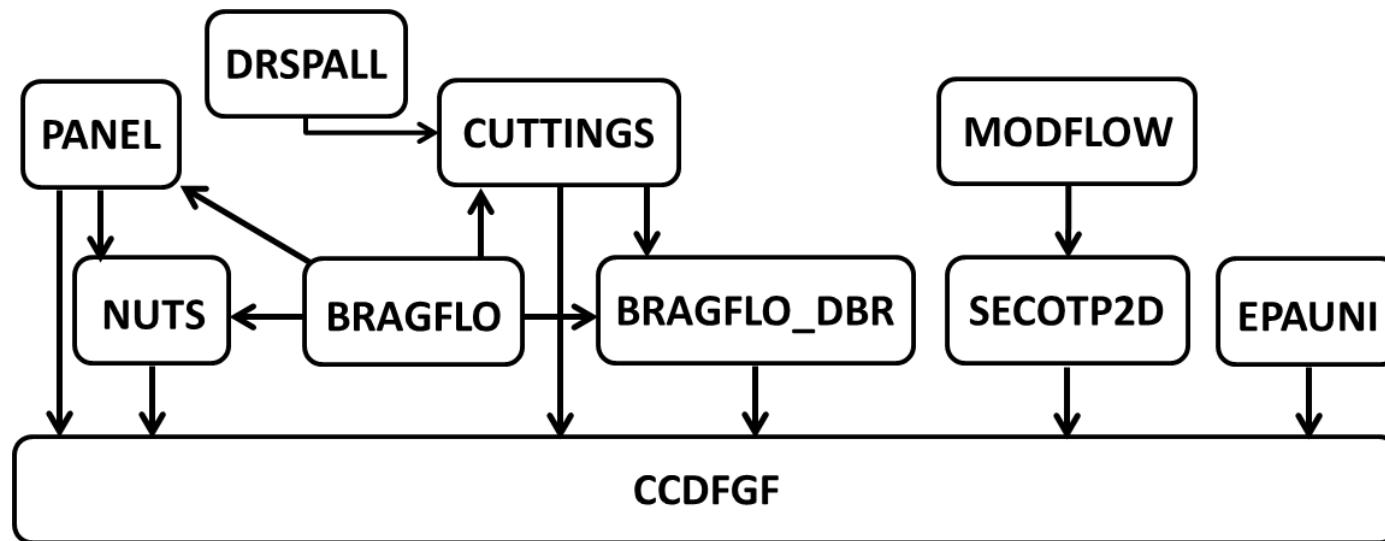
**Q<sub>i</sub>** = 10,000-year cumulative release (in curies) of radionuclide *i*

**L<sub>i</sub>** = Release Limit for radionuclide *i*

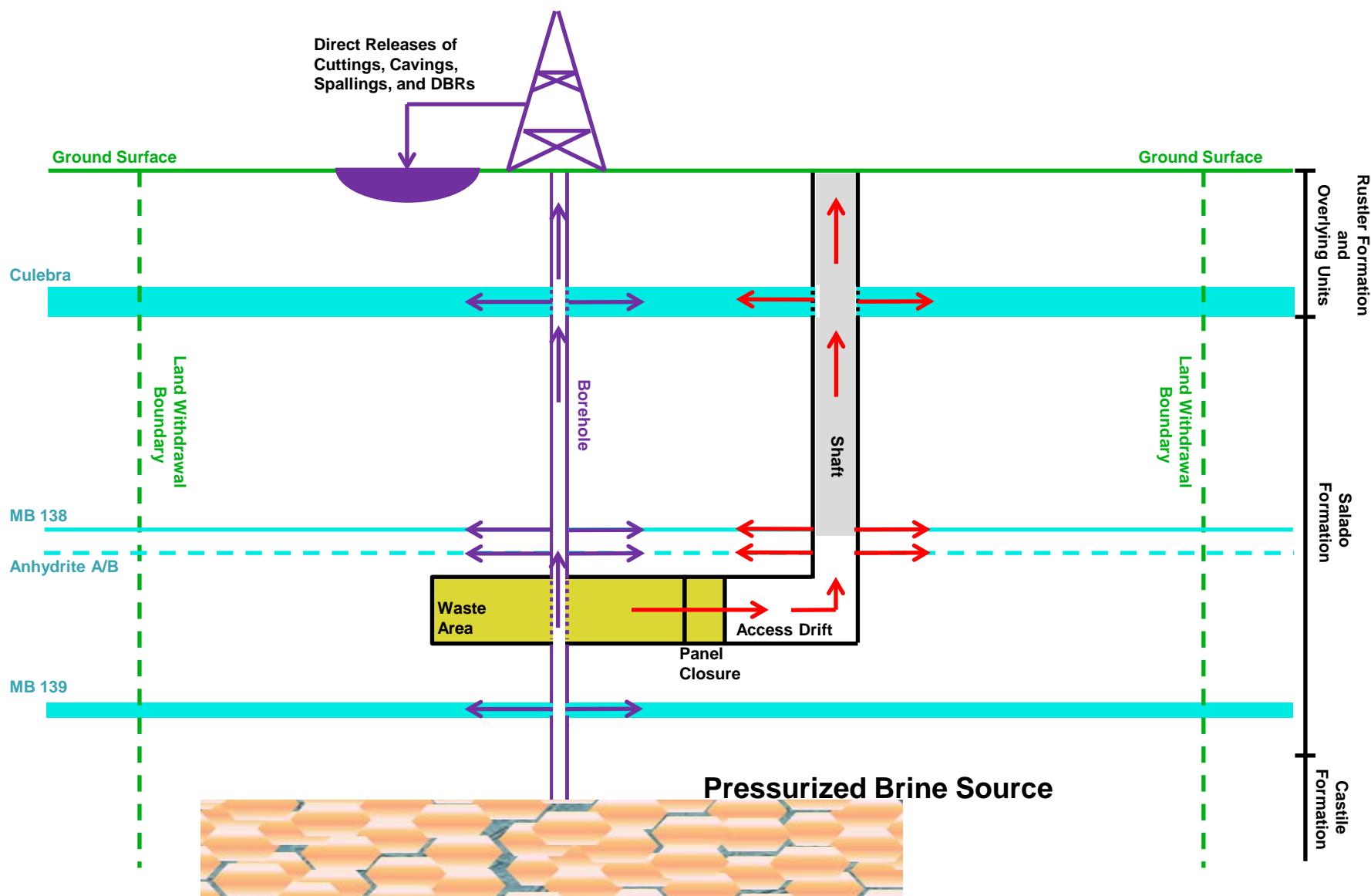
**C** = the total transuranic inventory (in curies of  $\alpha$  emitters w/halflives > 20 years)

# WIPP Performance Assessment

- PA calculations cover 24 peer-reviewed conceptual models
- PA codes include 10 principal codes and many utility codes

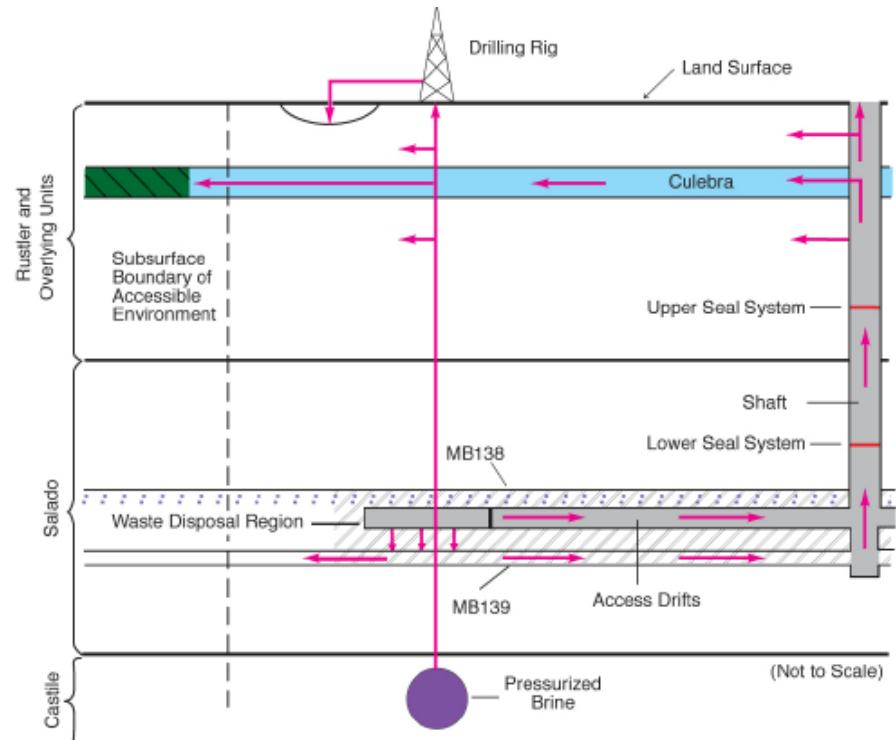
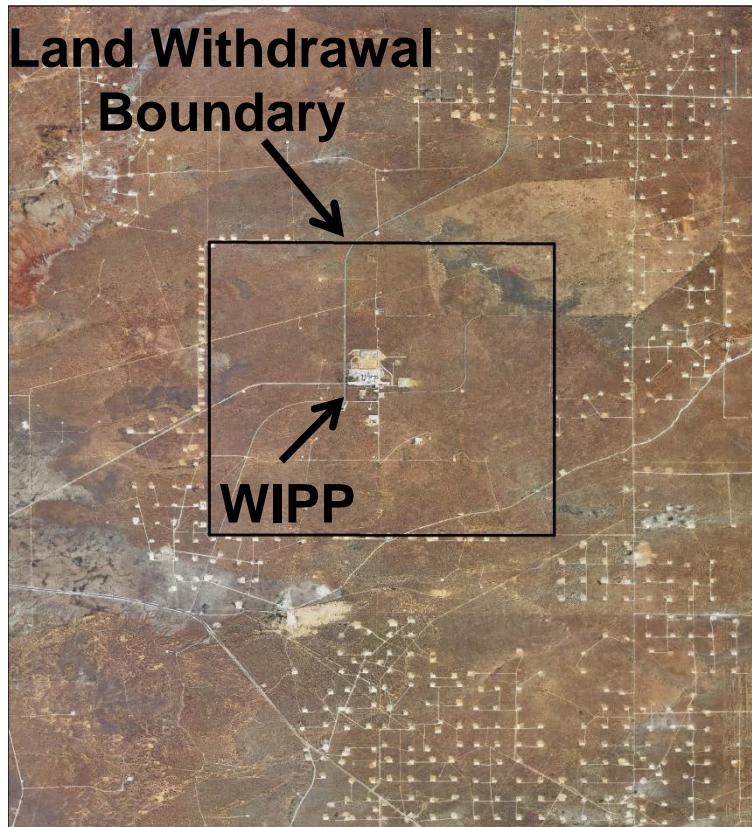


# Release Pathways



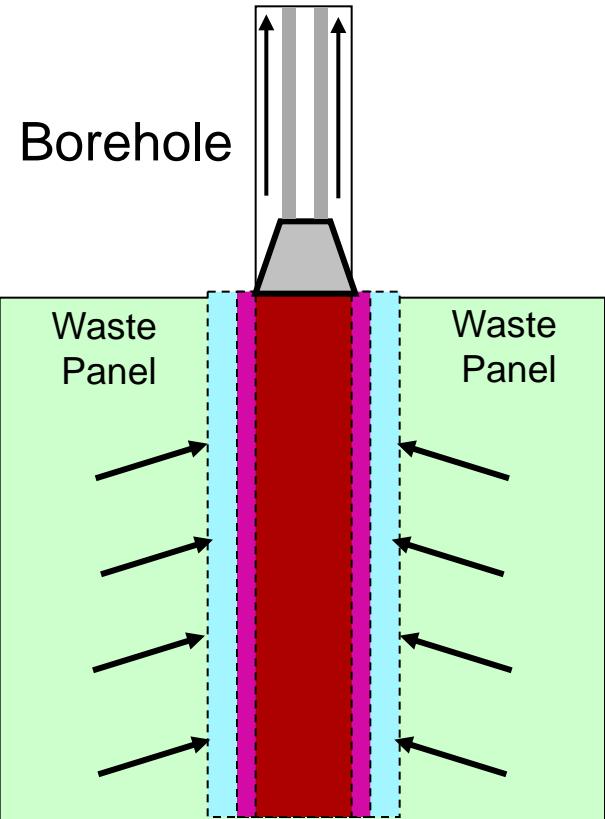
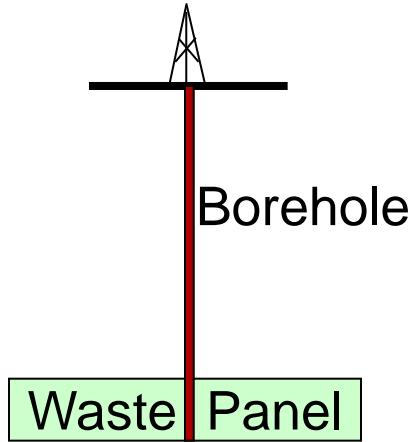
# Long-Term Release Mechanisms Considered in WIPP PA

Radionuclide Transport through Groundwater Comprise  
Long-Term Releases



# Direct Release Mechanisms Considered in WIPP PA

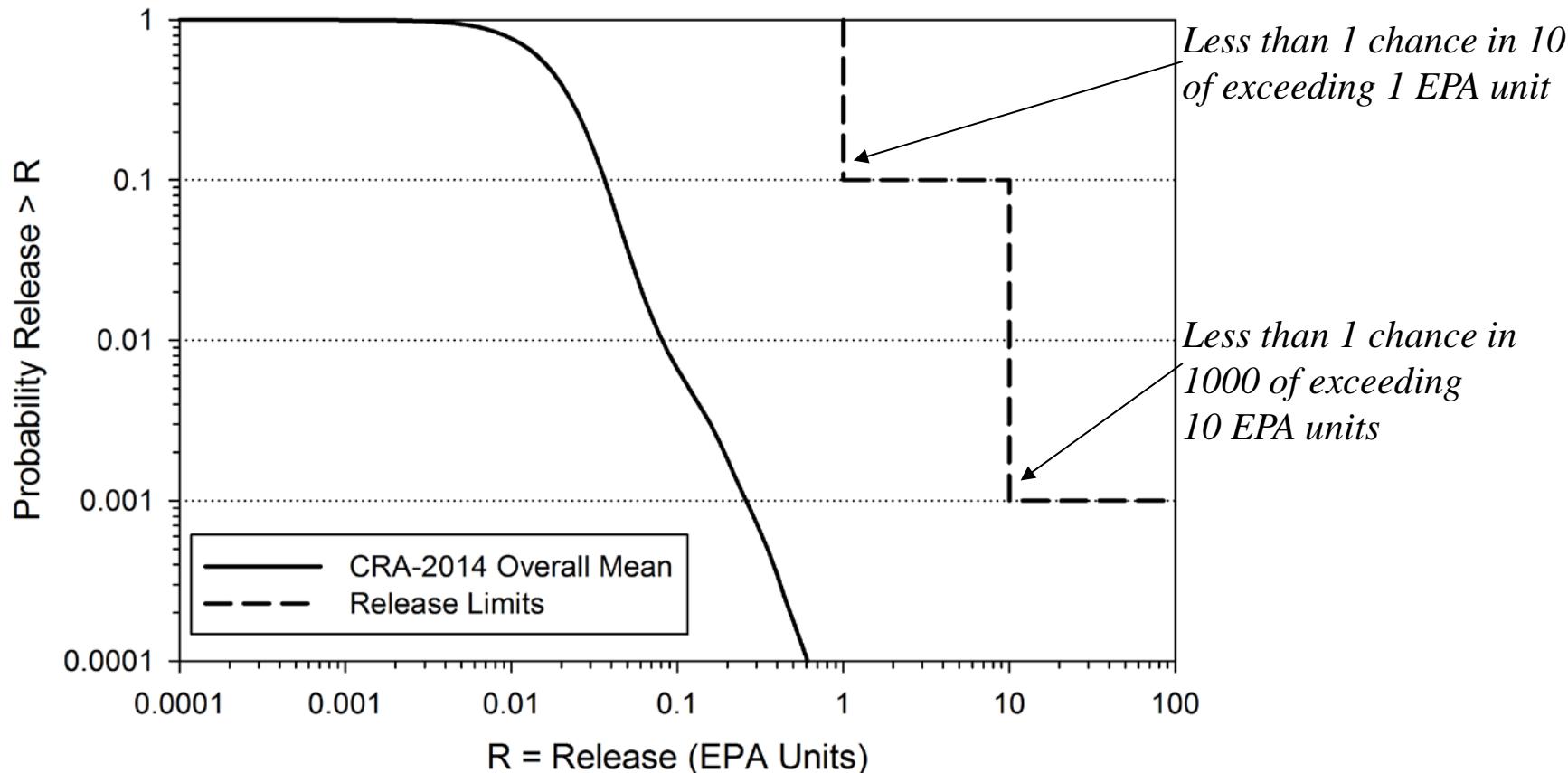
Direct Releases Dominate Total Releases



- Cuttings (Solids from Drilling)
- Cavings (Solids from Drilling)
- Spallings (Solids from Pressure Release)
- ↗ Direct Brine Release (DBR) (Brine from Pressure Release)

# Total Release CCDF is the Measure of Compliance

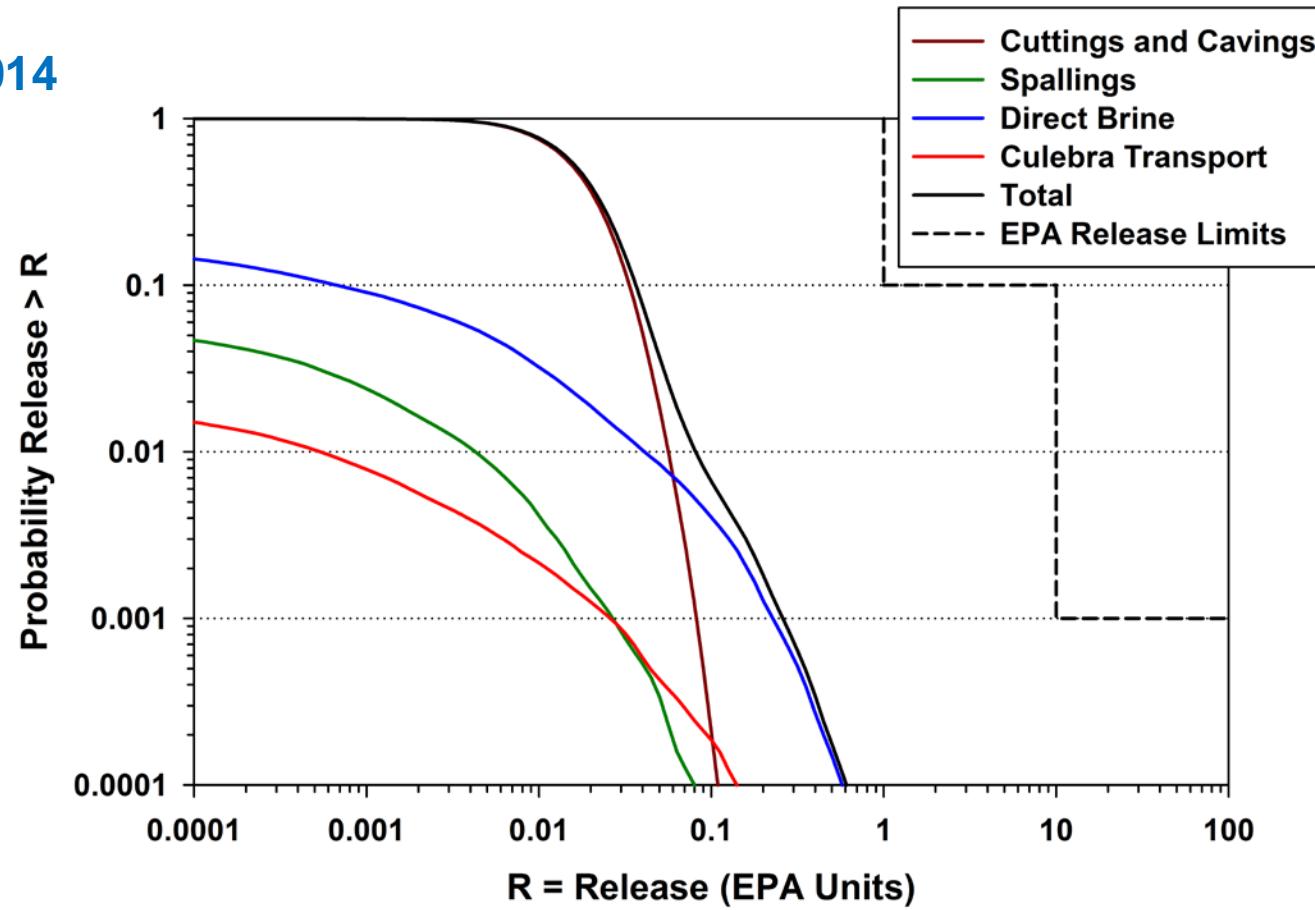
**Total releases from the repository are compared to regulatory release limits to determine compliance via a Complementary Cumulative Distribution Function (CCDF).**



# CCDFs for each Release Mechanism

Each Release Component is Quantified by a  
Complementary Cumulative Distribution Function (CCDF)

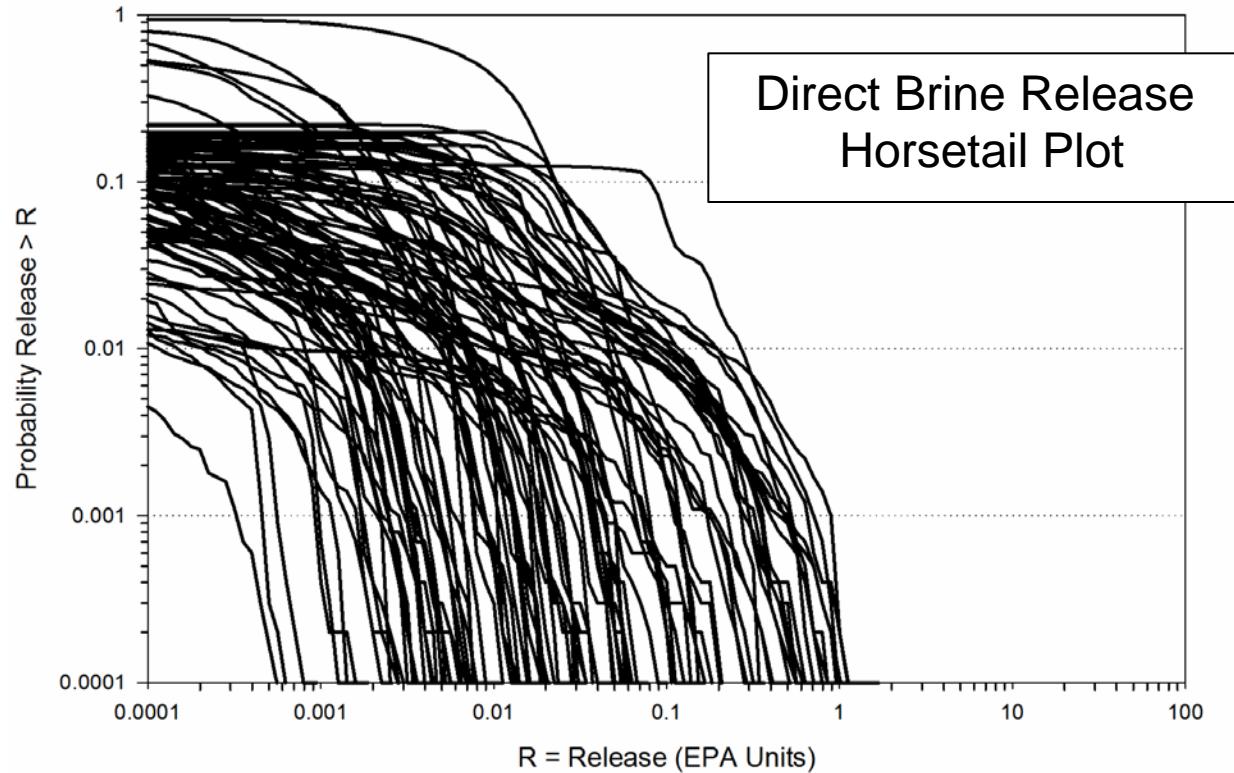
CRA-2014



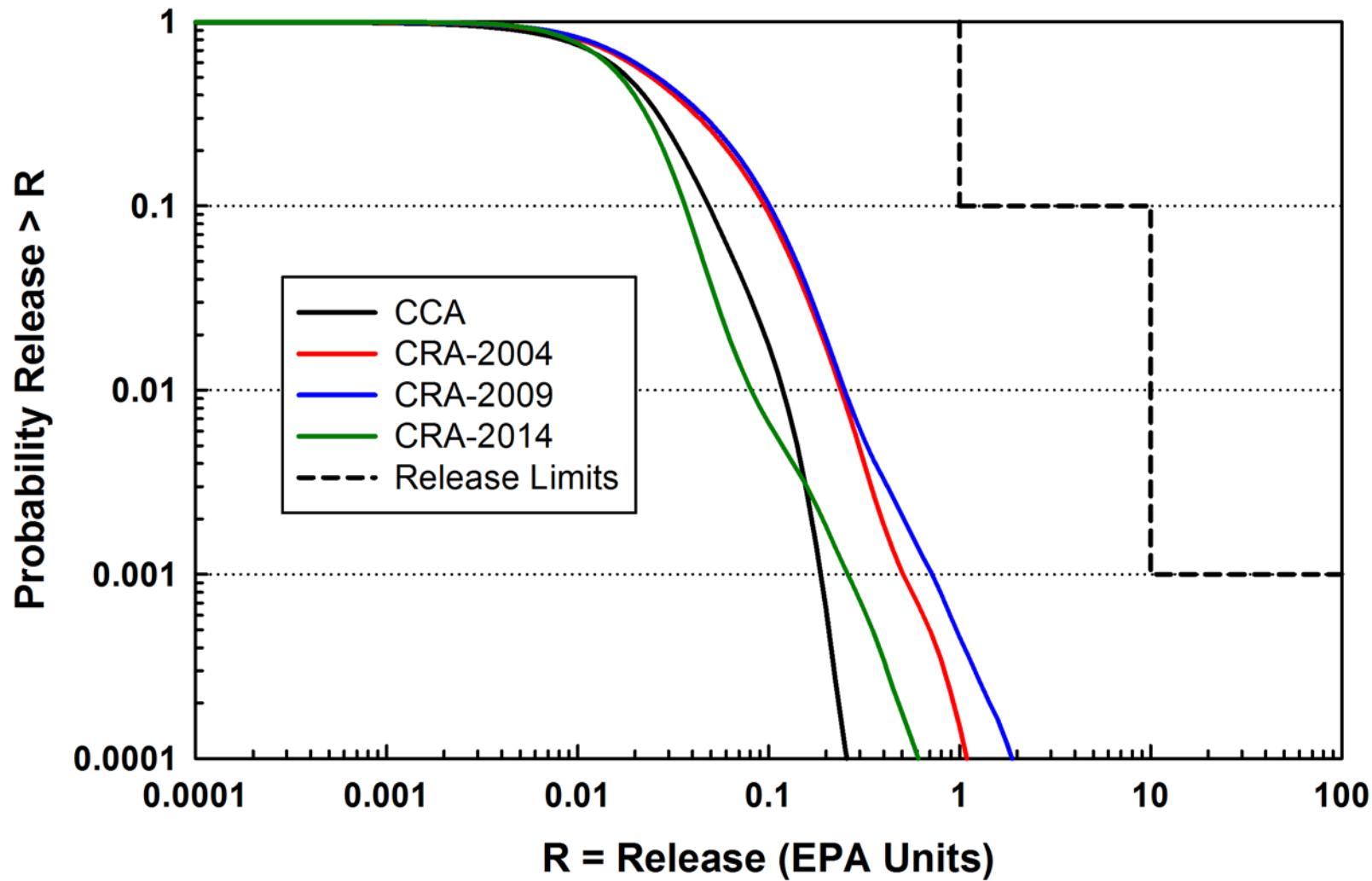
# CCDF Mean Assembly

Each mean CCDF is the average of 300 individual CCDFs obtained for each release component.

This is a way of considering aleatory (i.e., stochastic) uncertainty.



# Historical Results



# Outline

- WIPP Regulatory Requirements and PA
  - Release Mechanisms and Compliance Metric
- 2014 WIPP Compliance Recertification Application
  - Updates and Parameter Refinements
  - Approach and Results
- Future Changes to WIPP PA
  - PFLOTRAN as a Means to 3D modeling
- Summary

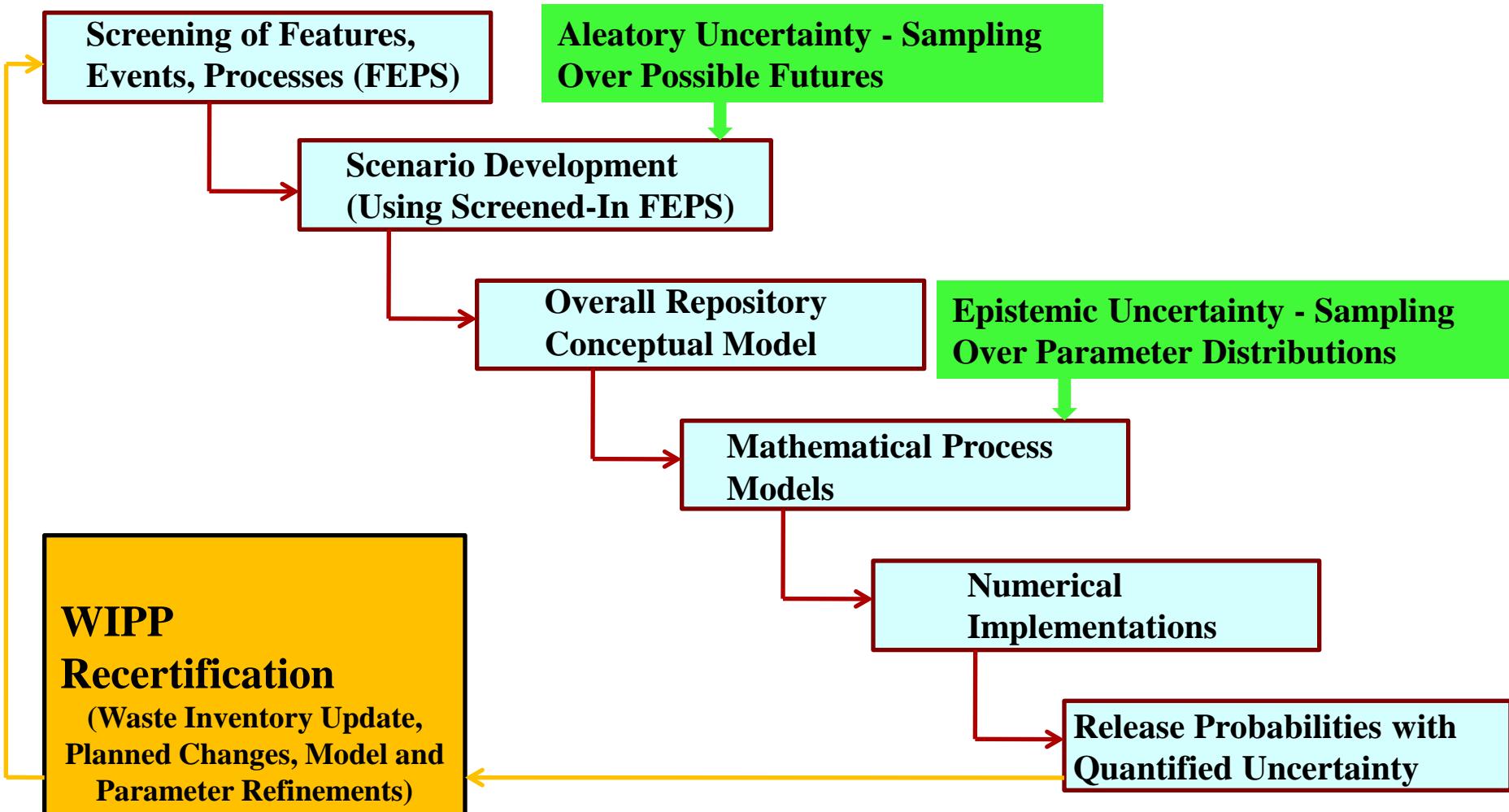
# WIPP Recertification



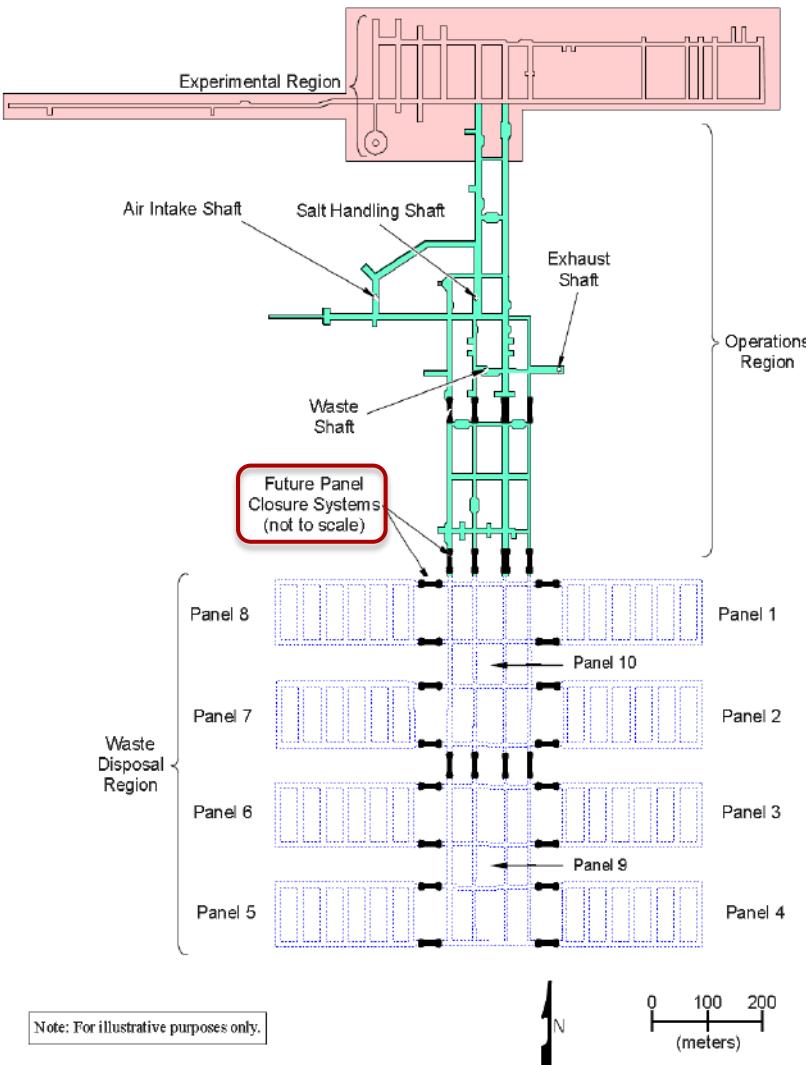
Federal regulations require that the WIPP be recertified **every five years** following the first waste shipment of 1999.

- The current regulatory baseline is that established by the 2009 Performance Assessment Baseline Calculation (PABC-2009).
- The 2014 Compliance Recertification Performance Assessment (CRA-2014 PA) demonstrates continued compliance of the WIPP with federal containment requirements.
- The CRA-2014 was submitted to the EPA in March, 2014.
- A number of changes/refinements are included in the CRA-2014 PA (e.g. incorporate new data and experimental results).

# WIPP PA Flow



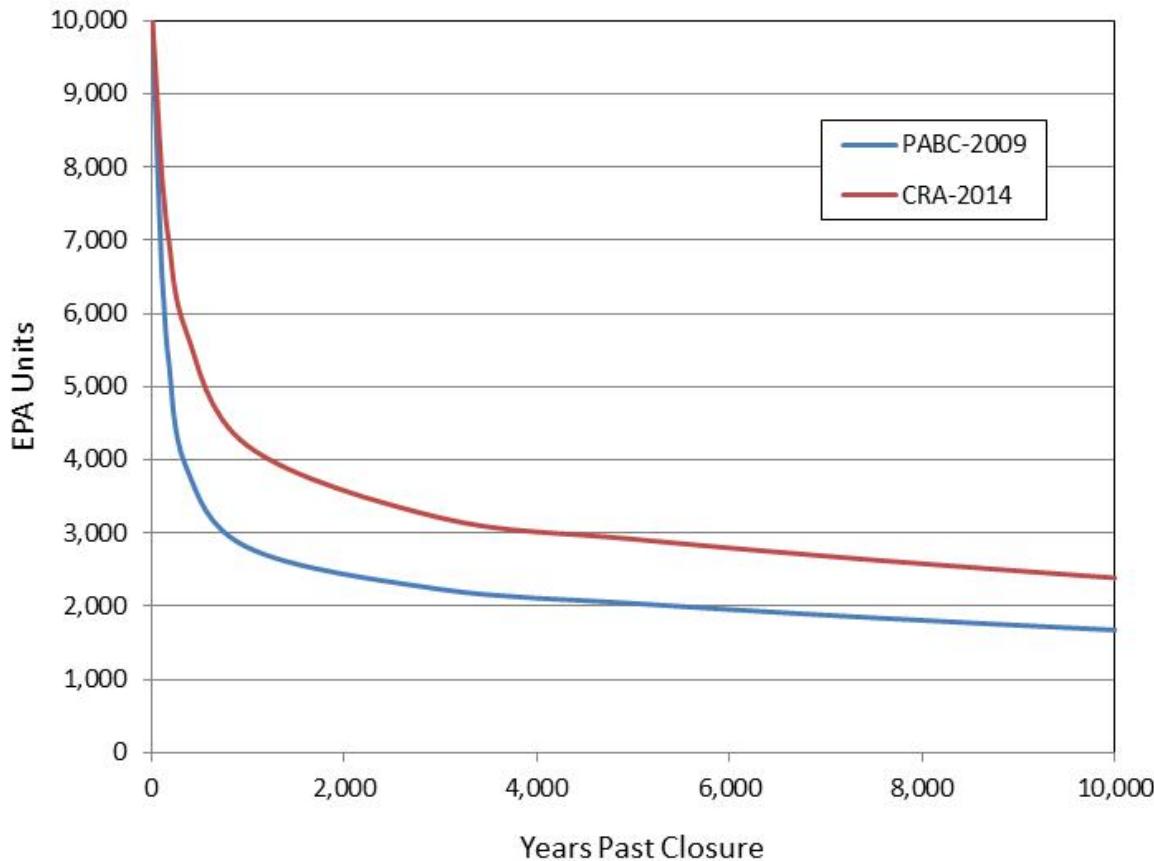
# Update: WIPP Panel Closures



- Function is to protect workers during the operational period of the repository.
- Included in PA because they are part of the disposal system, not because they inhibit releases. *The panel closure system was not designed or intended to support long-term repository performance.*
- Subject of a Planned Change Request submitted by DOE to the EPA to formally request a change to the approved design.
- Design was changed to a Run-of-Mine Panel Closure System (ROMPCS), with approval via a federal rulemaking process.

# Update: Waste Inventory

Inventory parameters in the CRA-2014 PA are updated to reflect information collected through December 31, 2011.



Difference primarily due to increased  $^{239}\text{Pu}$  in the CRA-2014 PA waste inventory

# Update: Waste Shear Strength

The waste shear strength is the ability of waste to resist erosion, and is one of the most important parameters in WIPP PA.



Cavings volumes are a function of waste shear strength.

SNL vertical flume experimental facility and the data obtained therein enabled a refinement to the waste shear strength parameter.

Surrogate degraded waste samples were used to determine lower value of shear strength uncertainty range

# CRA-2014 PA Approach

CRA-2014 PA changes are included sequentially so that compliance impacts can be reasonably isolated.  
(benefit for DOE and EPA)

The CRA-2014 PA is comprised of 4 cases:

## Case CRA14-BL

Includes:

- New Panel Closure
- Additional Excavation
- Updated Inventory
- Updated Solubilities (Single Brine Volume)
- Updated Drilling Parameters
- Revised Colloid Factors

## Case CRA14-TP

Includes CRA14-BL changes plus:

- Waste shear strength update
- Update to the probability of encountering pressurized brine during a hypothetical drilling intrusion

## Case CRA14-BV

Includes CRA14-TP changes plus:

- Variable Brine Volume

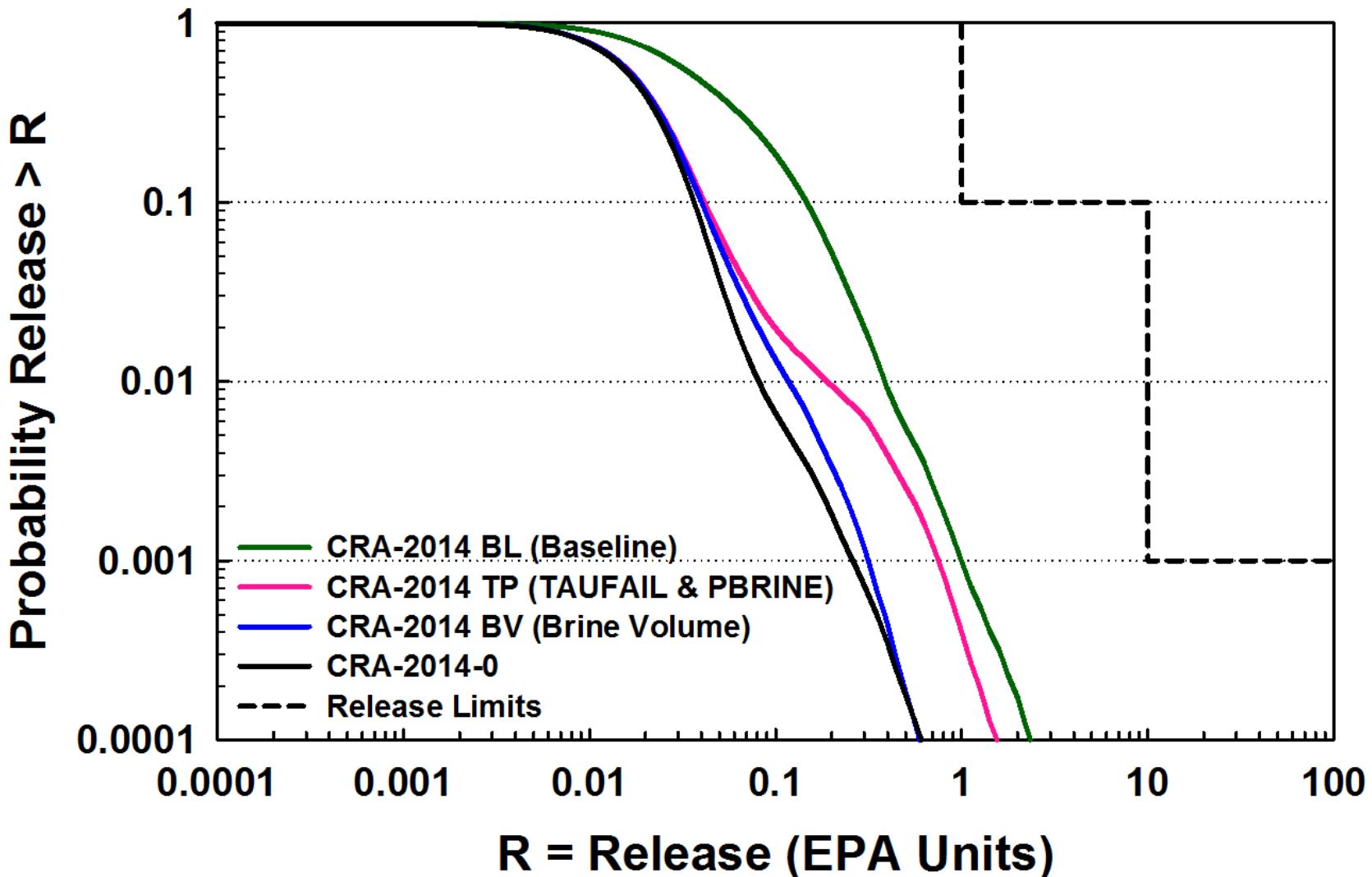
## Case CRA14-0

Includes CRA14-BV changes plus:

- Steel Corrosion Update
- Water Budget Refinement

Case CRA14-0 includes all changes in the CRA-2014 PA, and is the “formal” compliance calculation.

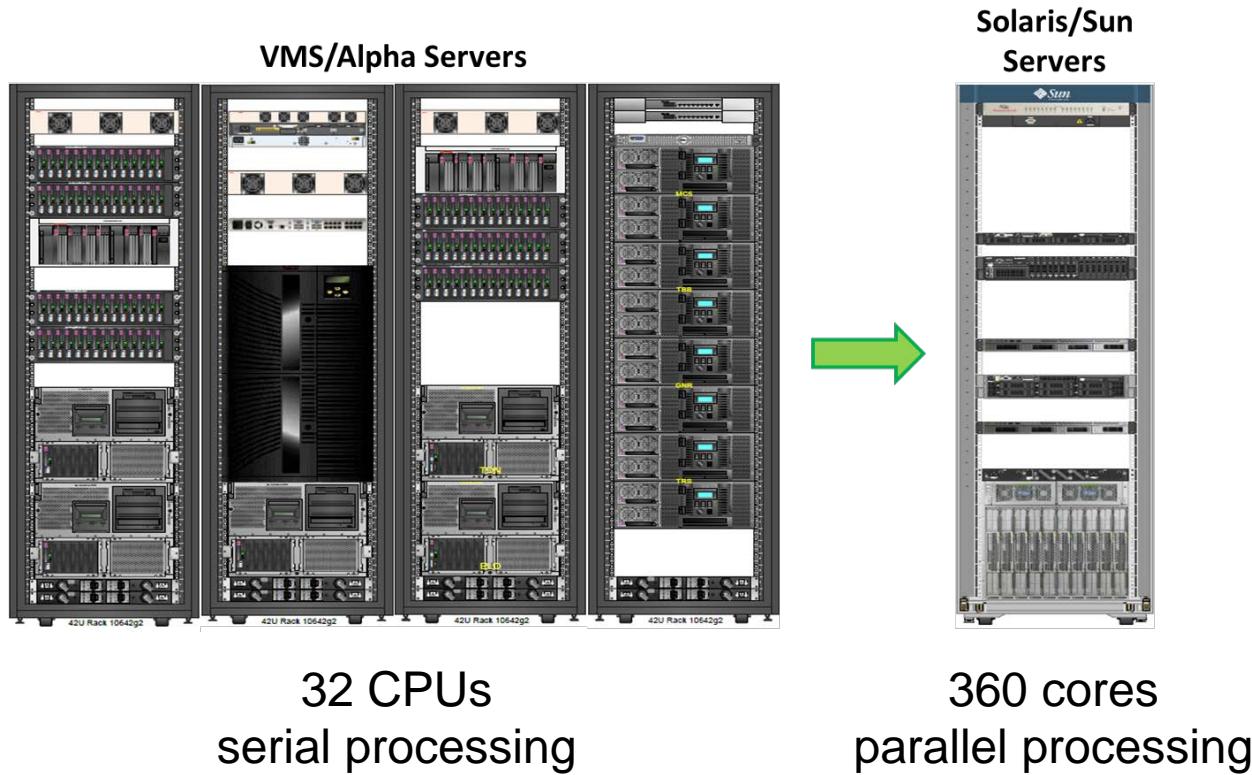
# CRA-2014 PA Results



# Outline

- WIPP Regulatory Requirements and PA
  - Release Mechanisms and Compliance Metric
- 2014 WIPP Compliance Recertification Application
  - Updates and Parameter Refinements
  - Approach and Results
- Future Changes to WIPP PA
  - PFLOTRAN as a Means to 3D modeling
- Summary

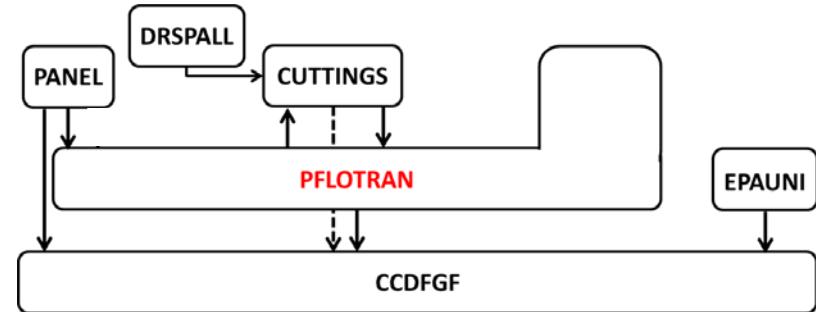
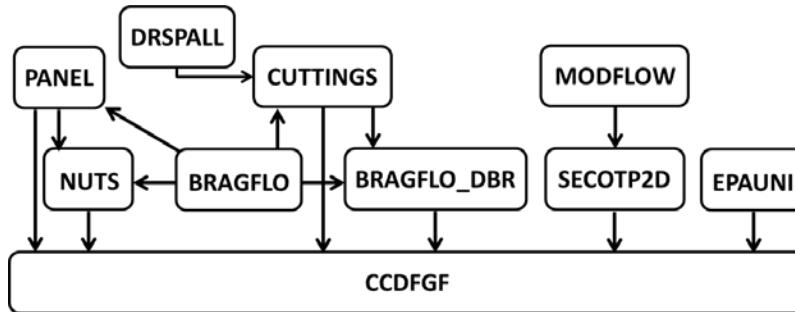
# Significant Hardware Update and Software Migration Effort



Migration of all PA codes from VMS to Solaris system

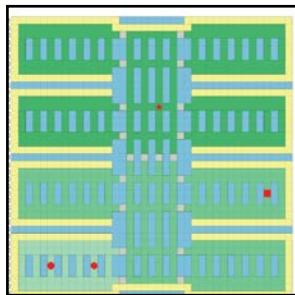
- QA code qualification
- Verification of results

# PA Code Map/Description

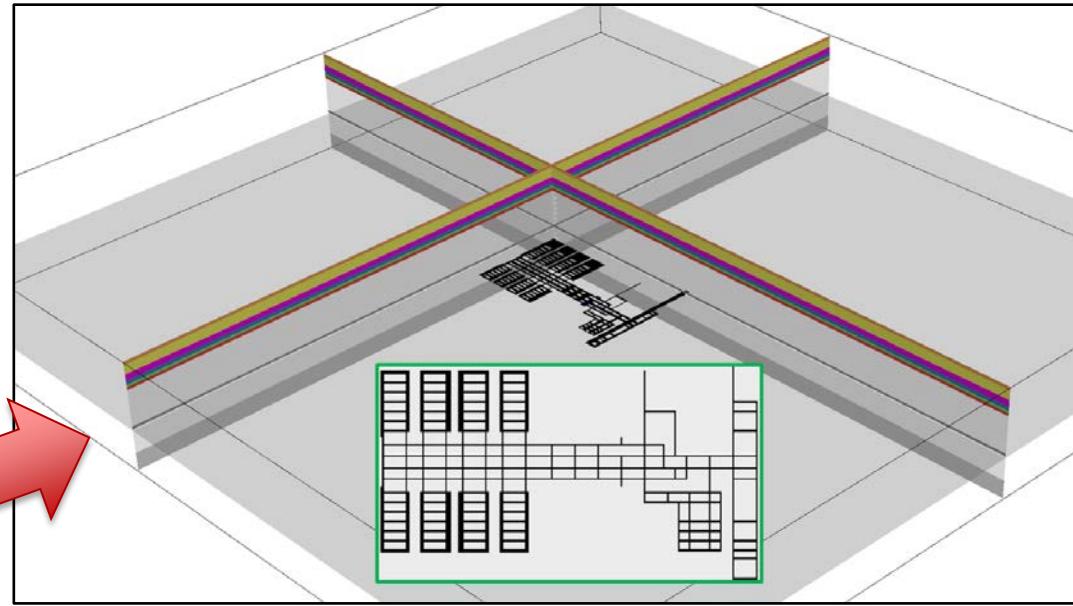


Codes	Description
BRAGFLO	Simulates porous media flow in and surrounding the repository over 10,000 years
NUTS	Calculates radionuclide transport in the Salado Formation including the repository
BRAGFLO-DBR	Predicts release from the repository to the environment via borehole intrusion
MODFLOW	Used to calculate flow field away from the repository in the Culebra member of the Rustler Formation
SECOTP2D	Computes radionuclide transport in fractured porous media (Culebra)
PFLOTRAN	Massively parallel reactive flow and transport model for describing surface and subsurface processes

# 2D→3D Representation of Repository



Current 2-D Grids



Representative Future 3-D Grid

- additional detail
- asymmetry

# Current PA vs PFLOTRAN

Codes	Current PA	PFLOTRAN
BRAGFLO (porous media flow)	<ul style="list-style-type: none"> <li>- Immiscible (gas/liquid)</li> <li>- Isothermal</li> <li>- Two-phase flow</li> </ul>	<ul style="list-style-type: none"> <li>- <b>Miscible</b></li> <li>- <b>Anisothermal</b></li> <li>- Multiphase Flow</li> <li>- <b>Diffusion</b></li> </ul>
NUTS (radionuclide transport)	<ul style="list-style-type: none"> <li>- Multicomponent transport</li> <li>- Single porosity</li> <li>- Constant sorption</li> <li>- Single continuum model</li> </ul>	<ul style="list-style-type: none"> <li>- <b>Biogeochemical Transport</b></li> <li>- Dissolution/precipitation</li> <li>- <b>Multi-rate sorption</b></li> <li>- <b>Multi-continuum model</b></li> </ul>
General Comparison	<ul style="list-style-type: none"> <li>- <b>2D</b></li> <li>- Structured grid</li> <li>- <b>Parallel with single core simulations</b></li> <li>- Limitations on simulation size</li> <li>- Many I/O interfaces required</li> <li>- Network of coupled 2D simulations</li> <li>- <b>Simplified process models and coarse mesh</b> for quicker overall calculation time</li> </ul>	<ul style="list-style-type: none"> <li>- <b>3D</b></li> <li>- Unstructured/structured grid</li> <li>- <b>Massively parallel</b></li> <li>- Simulation size only depends on hardware capability</li> <li>- Need to develop WIPP-specific functionalities</li> <li>- <b>Detailed process models and high mesh resolution</b>, but overall PA calculation may be longer</li> </ul>

# Other Advantages of PFLOTRAN

- **Open source development**
  - A broad research community that leverages innovation in subsurface and computational sciences.
- In-house code development expertise
  - **Multiple Sandians are PFLOTRAN developers with authorization to commit changes to the code.**
- Managed under a modern support infrastructure
  - **Distributed source control management through Mercurial**
  - **Central, open source repository resides on Bitbucket**
  - Comprehensive regression and unit testing using Python
  - Automated building and testing through Buildbot
- PFLOTRAN HDF5 file formats
  - **Compatible with open source visualization tools** (i.e. VisIt and Paraview)

# Test Case: Two-Dimensional Infiltration

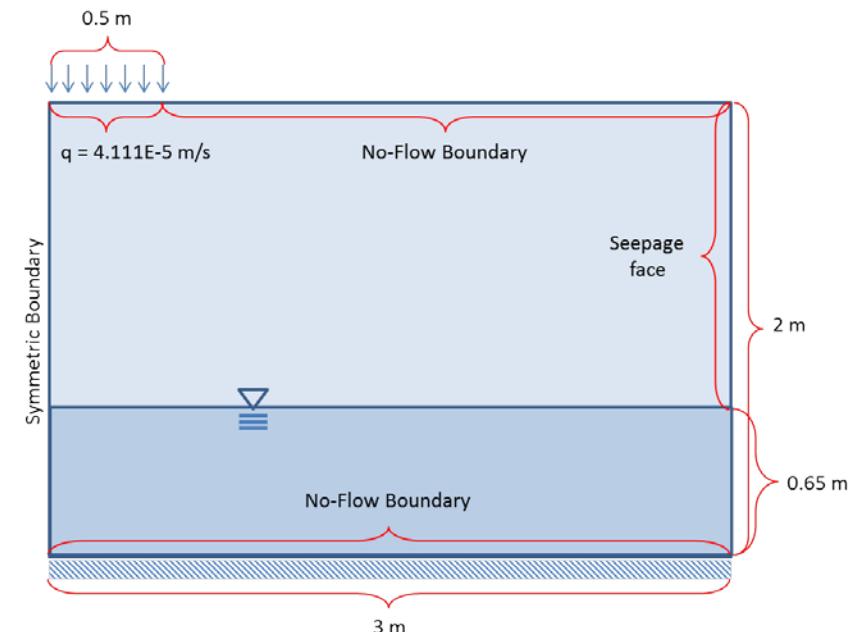
- The original experimental setup was done by Vauclin et al.
- Seepage face only allows outflow
- Capillary/Relative Permeability relations:

$$S_e = \frac{1 - S_w}{S_w}$$

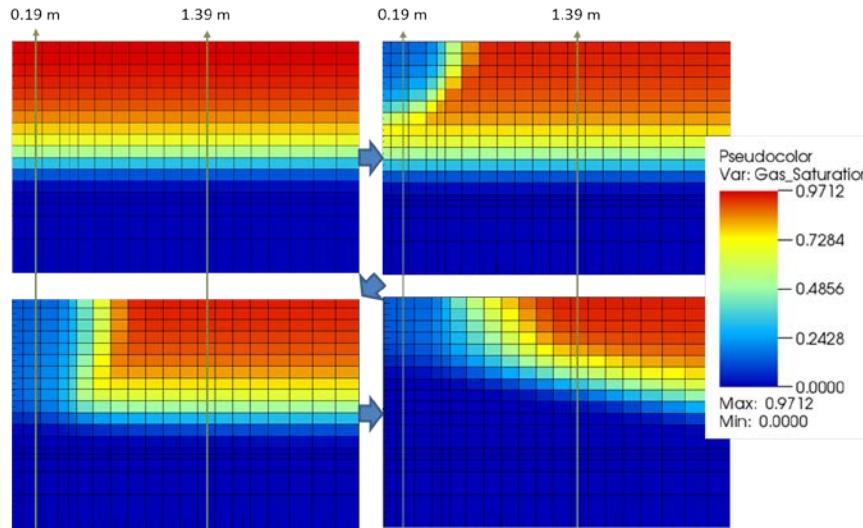
$$k_{rw} = \frac{1}{1 + 28.768353 S_e^{1/0.58}}$$

$$k_{rmw} = 1 - k_{rw}$$

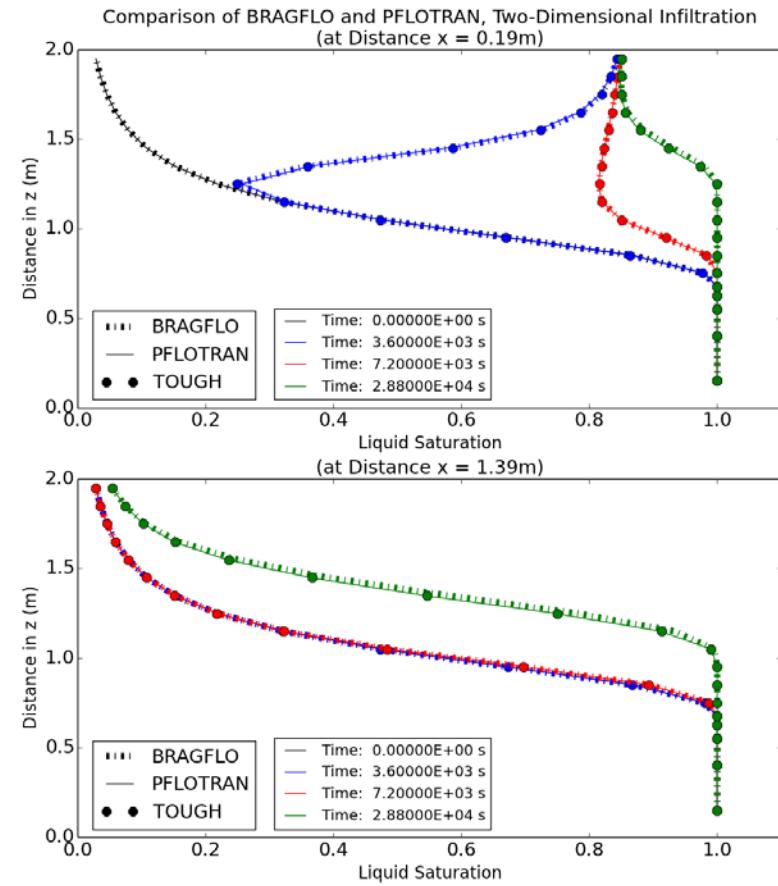
$$P_c = 3783 .0145 S_e^{(1/2.9)}$$



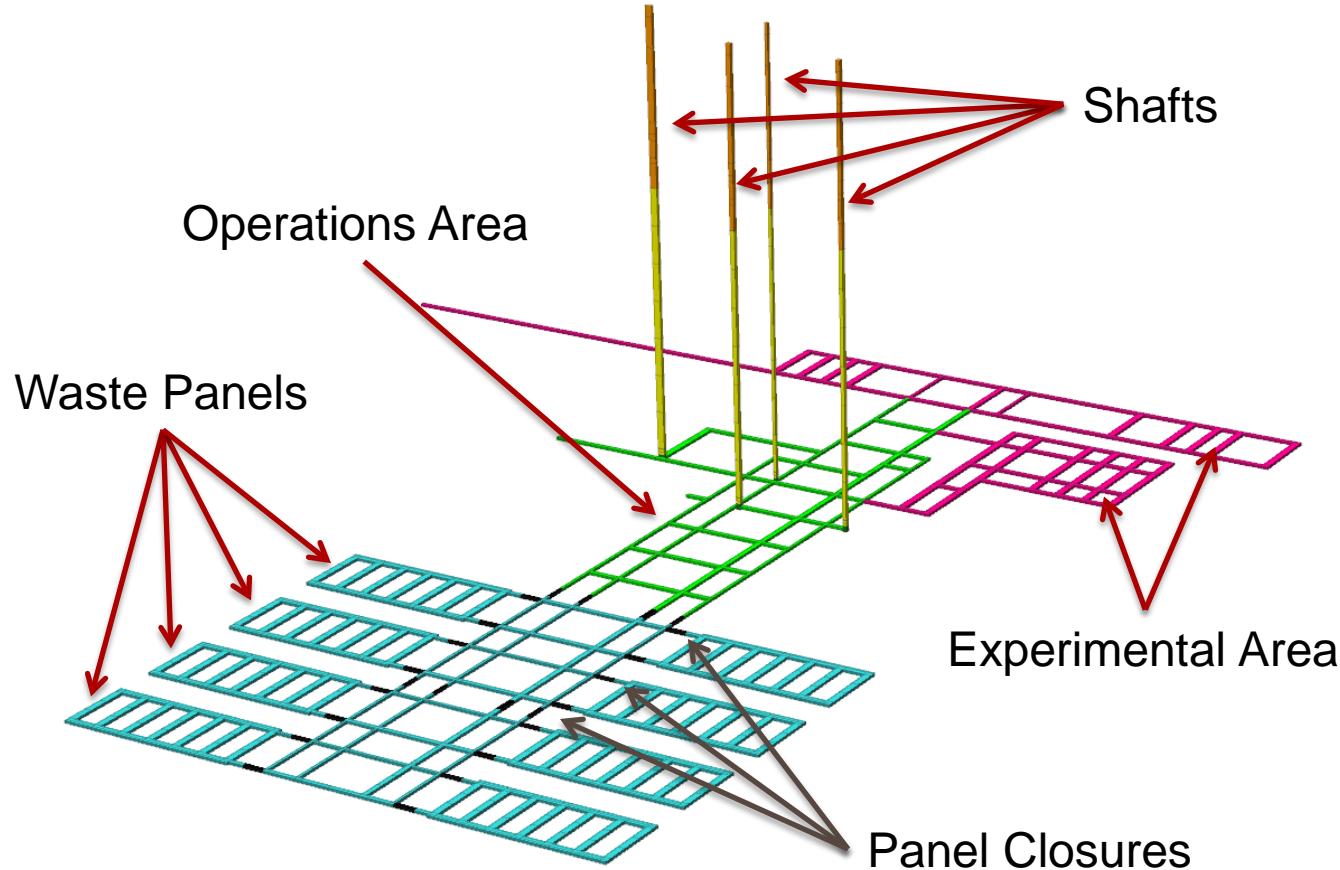
# Two-Dimensional Infiltration



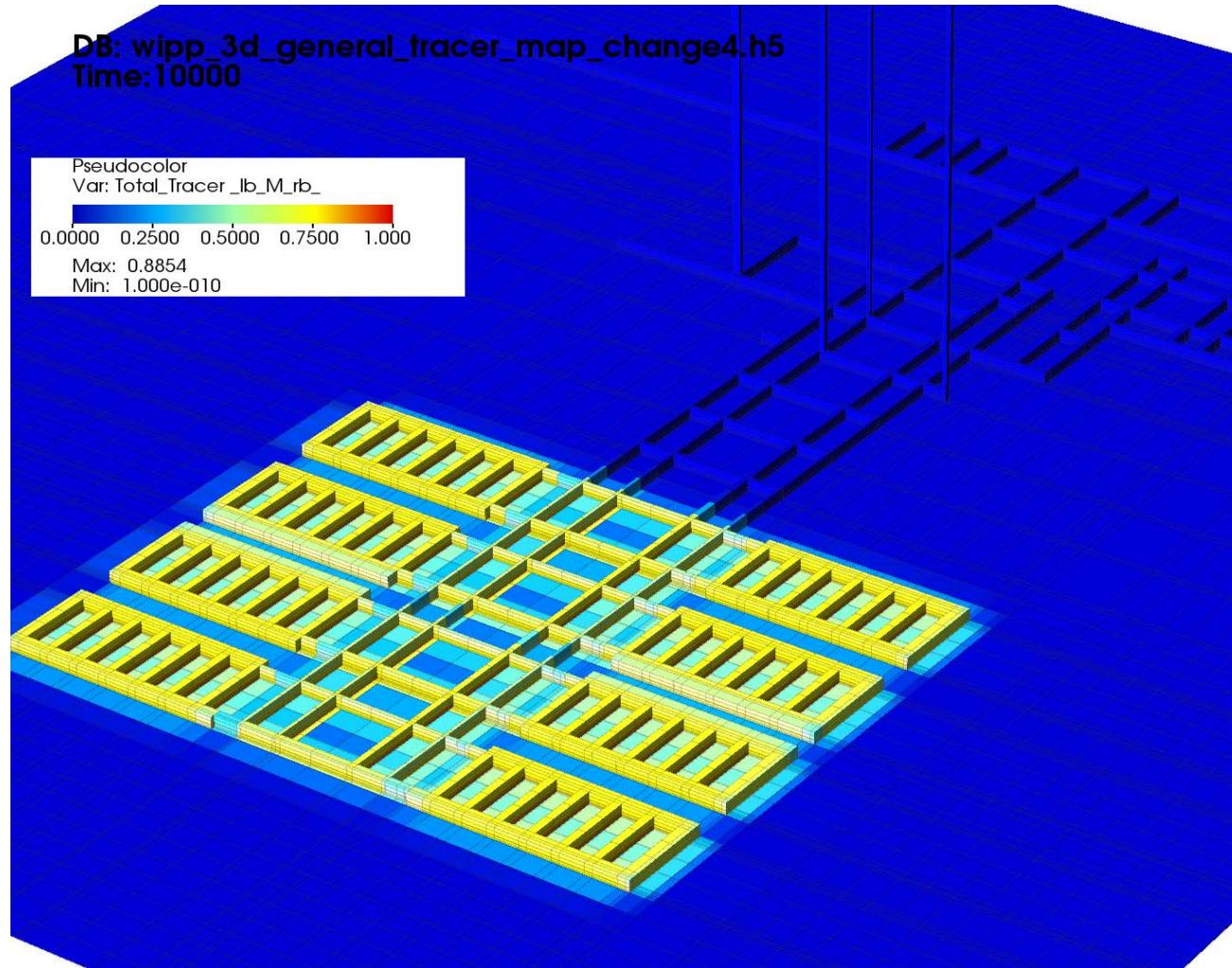
Water is being injected into the four left most cells in the top row. Gas saturation of the domain at 0 hour, 1 hour, 2 hours, and 8 hours from simulations of PFLOTRAN



# Preliminary 3D WIPP Model



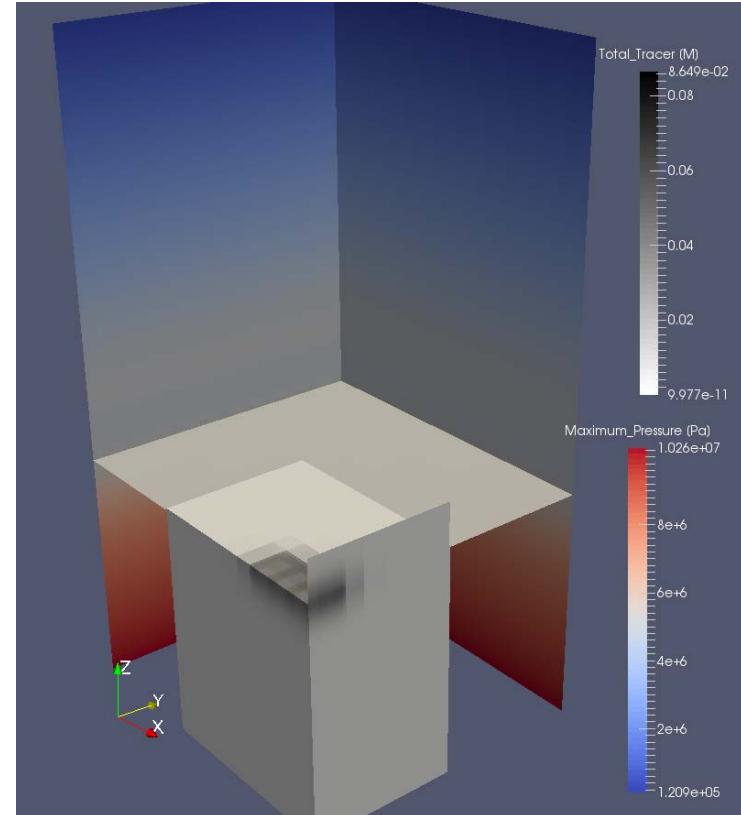
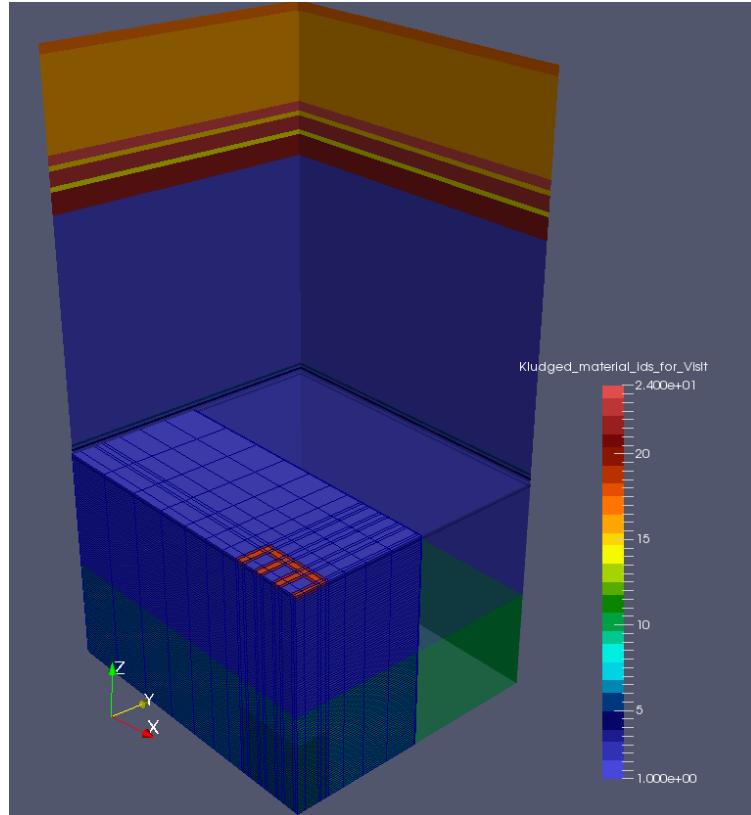
# Tracer Migration via Diffusion



# 3-D One Panel Model

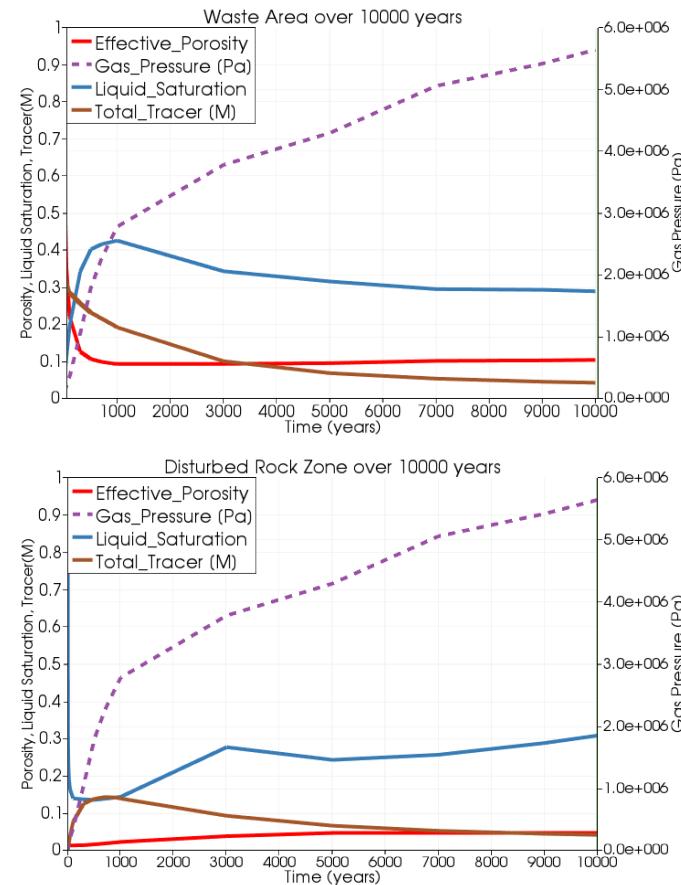
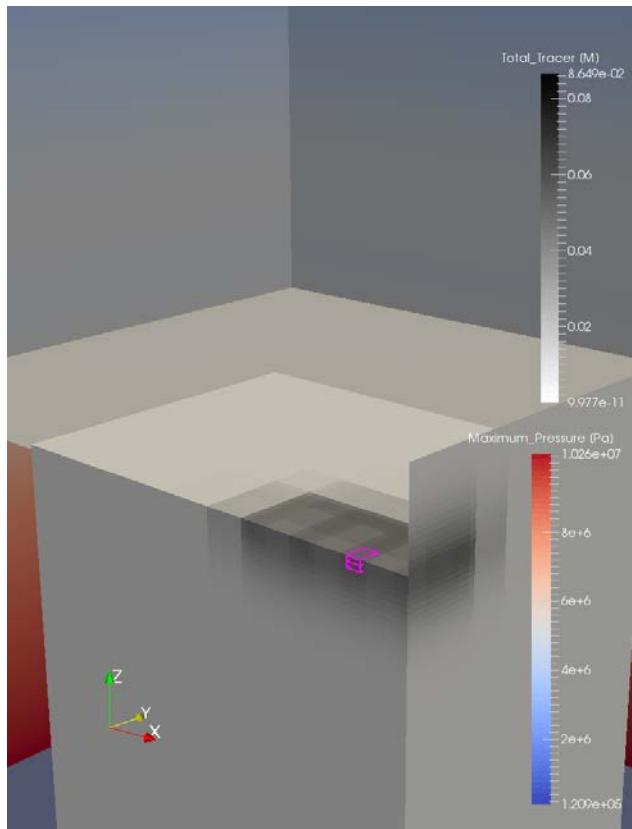
- Features
  - Uses two-phase general mode (hydrogen, brine)
  - Unsaturated excavated waste panel
  - Remainder of domain (including disturbed rock zone) is saturated
  - Gas generation from wastes
  - Creep closure, fractures, RKS equation of state for gas, Klinkenberg
  - Material property changes at specified times
- Issues
  - This model is discretized uniformly in z-direction in an effort to reduce convergence issues
  - 1.0E-3 scaled residual tolerance (relatively large)
  - Quarter symmetry

# 3-D One Panel Model



Material properties of each region is shown on the left. Total tracer spread of radioactive material near the panel with max(liquid, gas) pressures at 10,000 years.

# 3-D One Panel Model



The solid lines' axis are on the left and the dashed line's axis on the right. Gas generation causes gas pressure and gas density to increase, creep closure affect is shown by effective porosity, decrease of tracer in the waste area is seen due to diffusion and dispersion, and increase of liquid saturation over time occurs as brine flows into the excavated area.

# Outline

- WIPP Regulatory Requirements and PA
  - Release Mechanisms and Compliance Metric
- 2014 WIPP Compliance Recertification Application
  - Updates and Parameter Refinements
  - Approach and Results
- Future Changes to WIPP PA
  - PFLOTRAN as a Means to 3D modeling
- Summary

# Summary

- WIPP PA calculations are performed by SNL and used by DOE to demonstrate long-term repository performance.
- The CRA-2014 PA has been submitted to the EPA
  - Includes planned repository changes and numerous refinements/updates.
  - Predicted total normalized releases obtained in the CRA-2014 PA are less than those found in the PABC-2009.
  - The WIPP remains in compliance with long-term federal containment requirements.
- 3-D modeling capability is being developed for WIPP PA
- Thanks to WIPP PA team

WIPP PA is a coordinated effort by many dedicated people.

# Acknowledgements



Ross Kirkes

FEPS  
Analysis



Brad Day

Probabilistic  
Modeling



HeeHo Park

Repository  
Flow



Chris Camphouse

PA Manager



Todd Zeitzer

Repository  
Flow



Jennifer Long

Run Control



Steve Wagner

Compliance  
Monitoring



Je-Hun Jang

Geochemistry



Paul Domski

Geochemistry  
Modeling



Jonathan Icenhower

Geochemistry



Dwayne Kicker

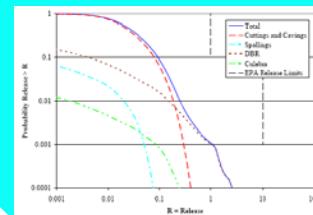
Rock  
Mechanics



Ayman Alzraiee

Repository  
Flow

WIPP PA



Courtney Herrick

Rock  
Mechanics



Yongliang Xiong

Geochemistry



Amy Gilkey

Build  
Consultant



Charlotte Sisk

Geochemistry