SAND2007-6500P

Salado Flow Modeling in WIPP Performance Assessment

KHNP Training Program
Module 6: Assembly of a Safety Case

October 16, 2007

Martin B. Nemer
Sandia National Laboratories
Carlsbad Programs Group

SAND 2007-XXXP

Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company,
for the United States Department of Energy's National Nuclear Security Administration
under contract DE-AC04-94AL85000.

Outline

I. Introduction to Two-Phase Porous Media Flow

II. Description of Conceptual Model

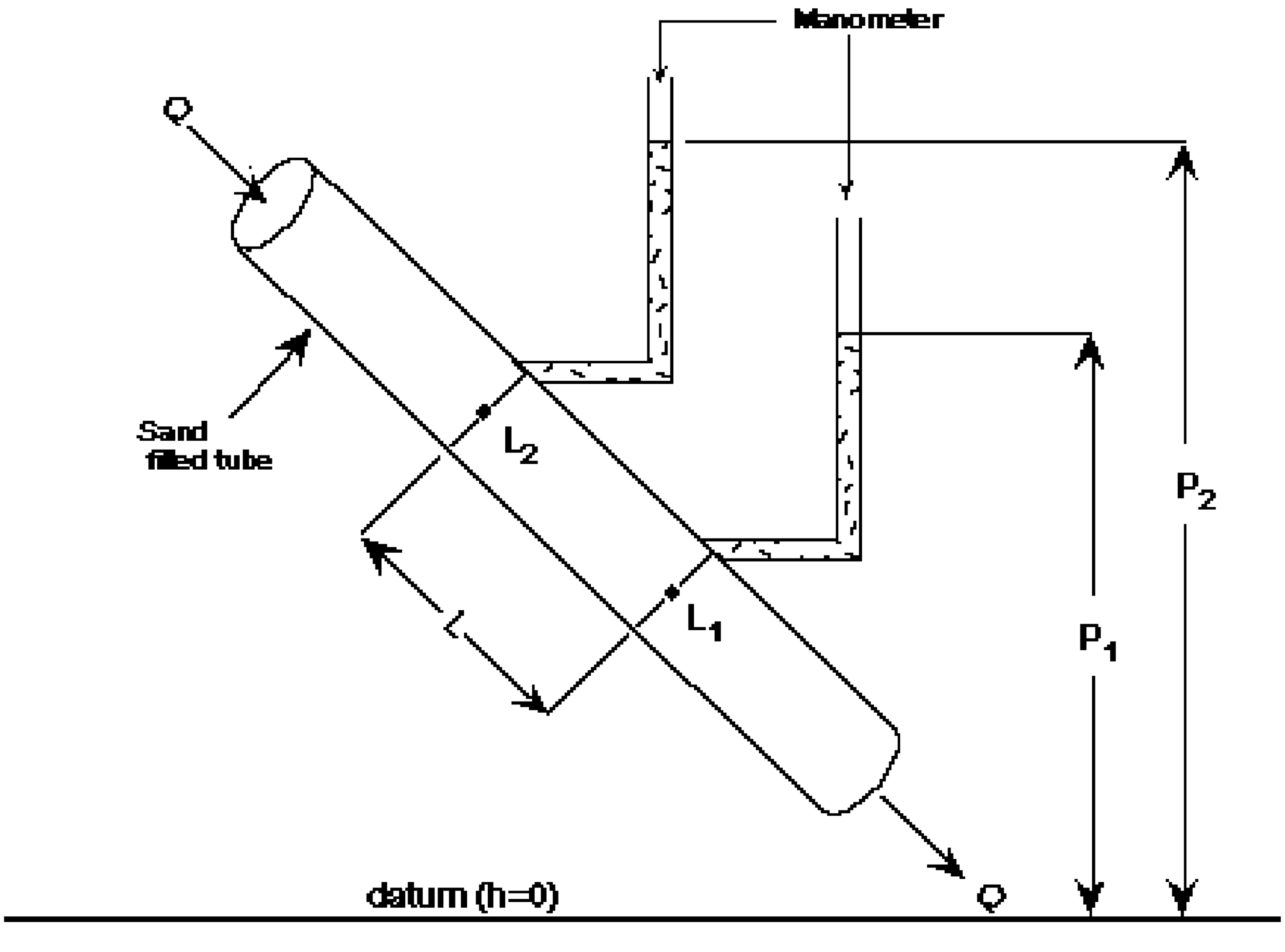
III. Numerical Implementation

IV. PABC Results

Sandia National Laboratories

Introduction to Two-Phase Porous Media Flow

Darcy’s Experiment



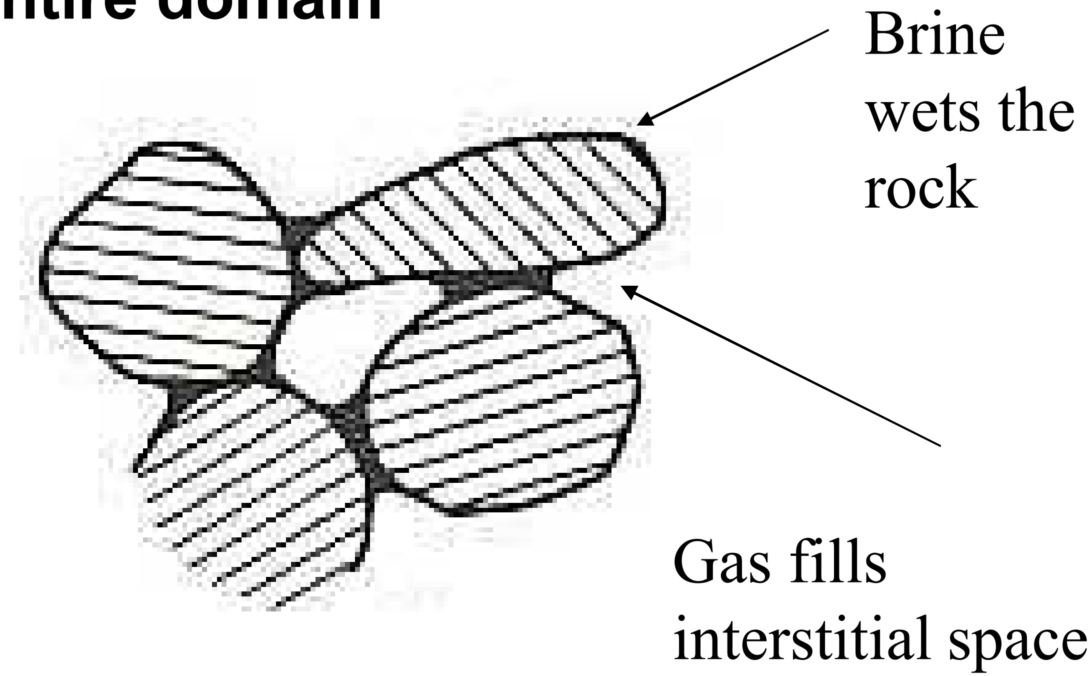
Darcy's Law

$$q = \frac{-k\rho}{\mu}\left(\nabla P + \rho g \nabla h\right)$$

- **q = mass flow rate per unit of crossectional area**
- ***k*** **= permeability**
- ***A*** **= cross-sectional area**
- ***μ*** **= viscosity**
- ***P*** **= pressure**
- **ρ = density**
- **g = gravitational acceleration**
- **h = height above reference point**

Two Phase Porous Media Flow

- **Assumption: two immiscible continuous phases occupy the entire domain**



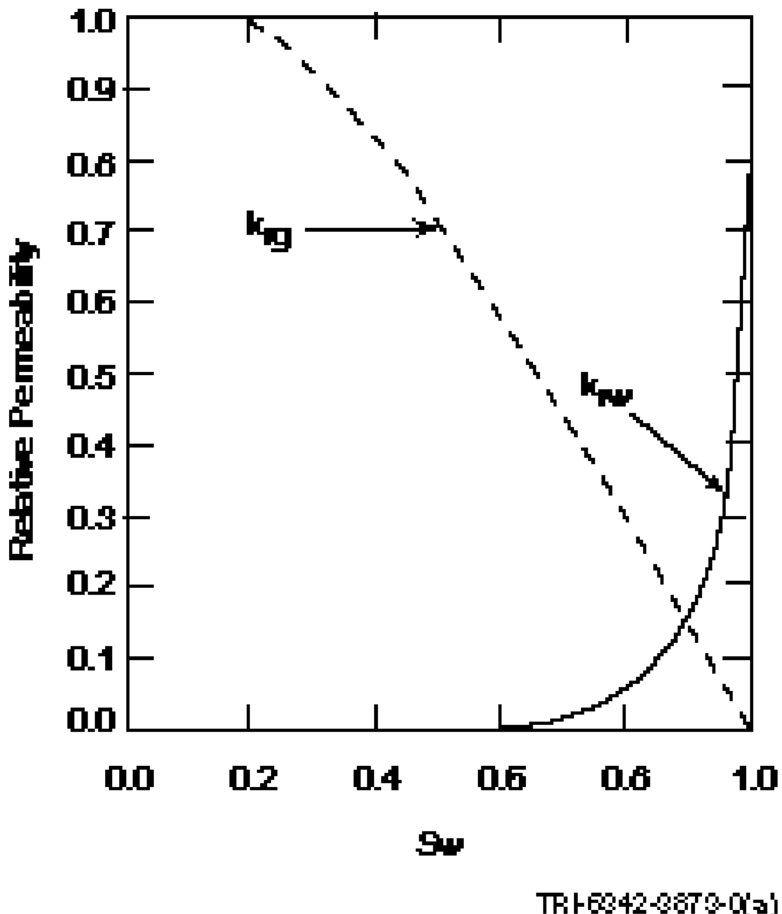
Two Phase Porous Media Flow

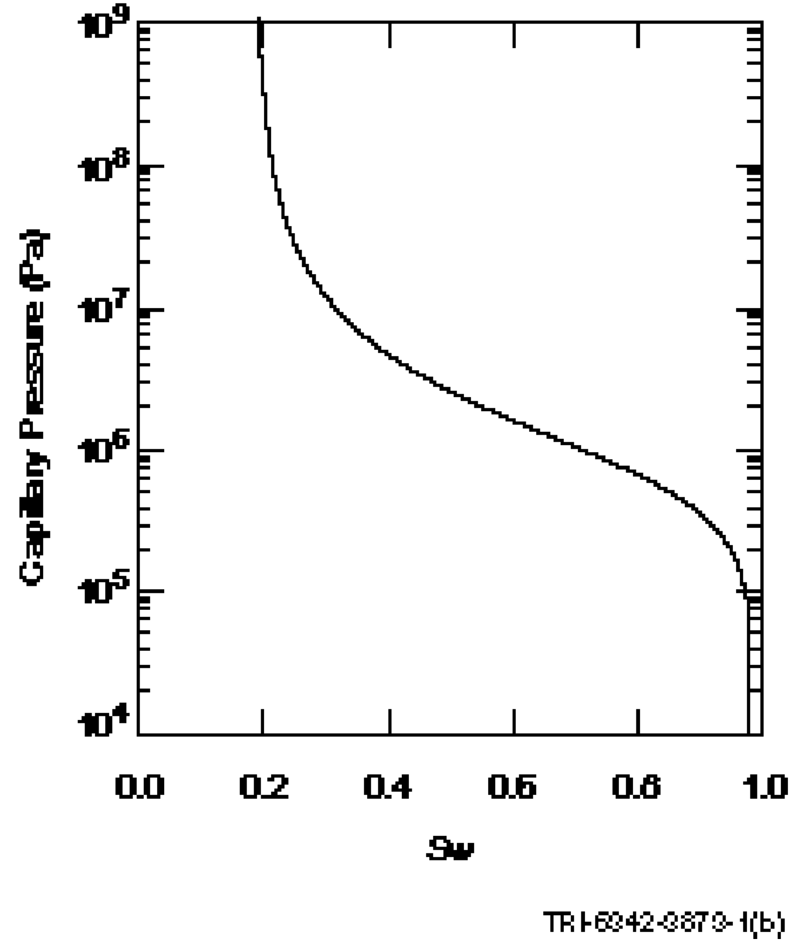
$$q_{brine} = -\frac{kk_b \rho_b}{\mu_b}\left(\nabla P_b + \rho_b g \nabla h\right).$$

$$q_{gas} = -\frac{kk_g \rho_g}{\mu_g}\left(\nabla P_g + \rho_g g \nabla h\right).$$

- k_{brine} = relative brine permeability
- k_{gas} = relative gas permeability

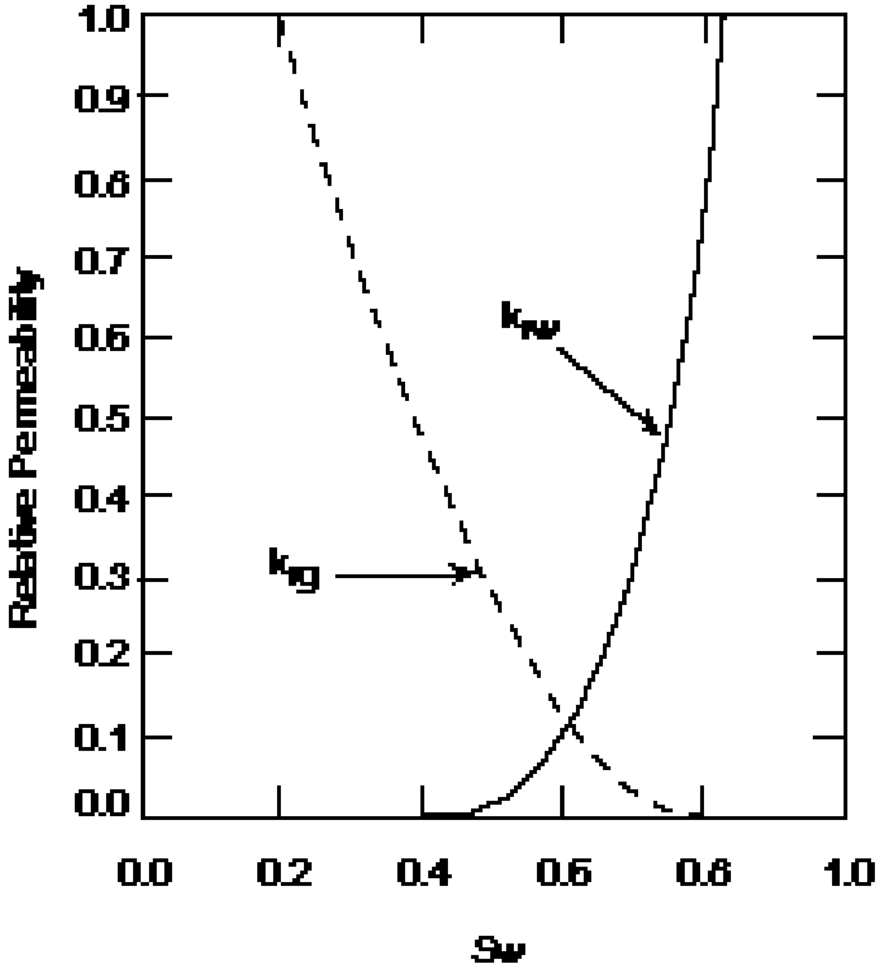
Capillary Pressure and Relative Permeabilities: van Genuchten-Parker Model



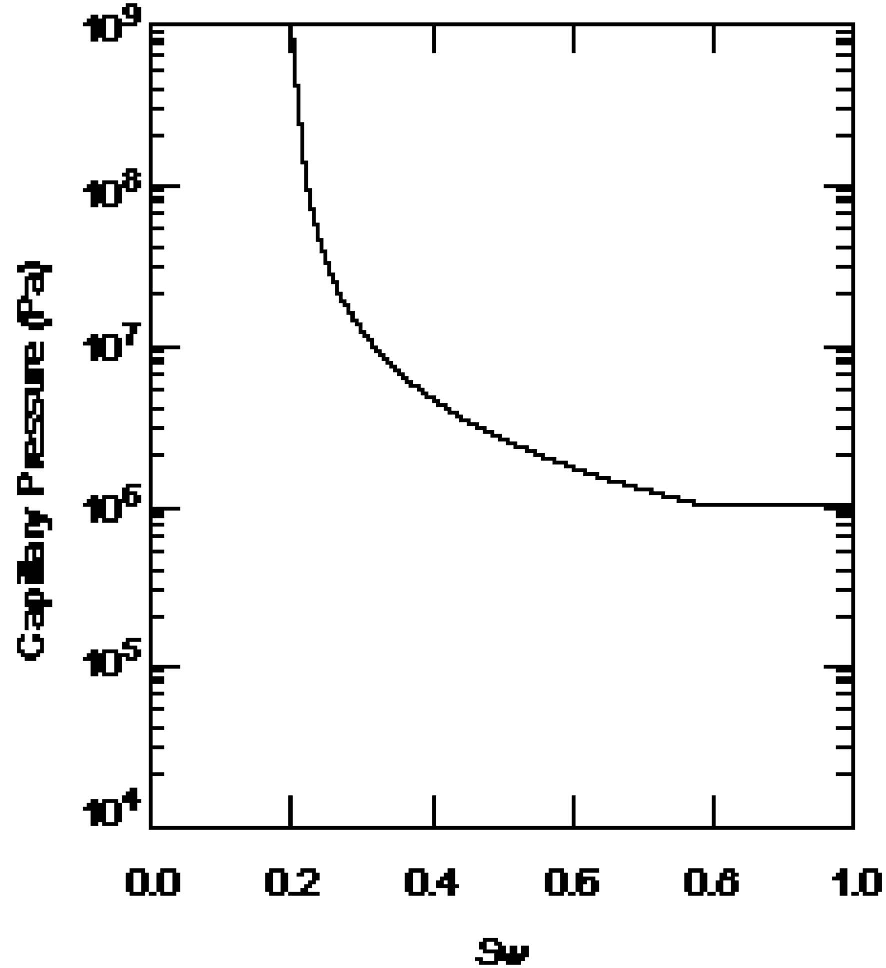


S_w = brine saturation

Brooks-Corey Model



TRI-6342-0870-0(a)



Sandia National Laboratories

Conservation of mass

$$\nabla \bullet q_{brine} + q_{sb} = \frac{\partial\left(\phi\rho_b S_b\right)}{\partial t}$$

$$\nabla \bullet q_{gas} + q_{sg} = \frac{\partial\left(\phi\rho_g S_g\right)}{\partial t}$$

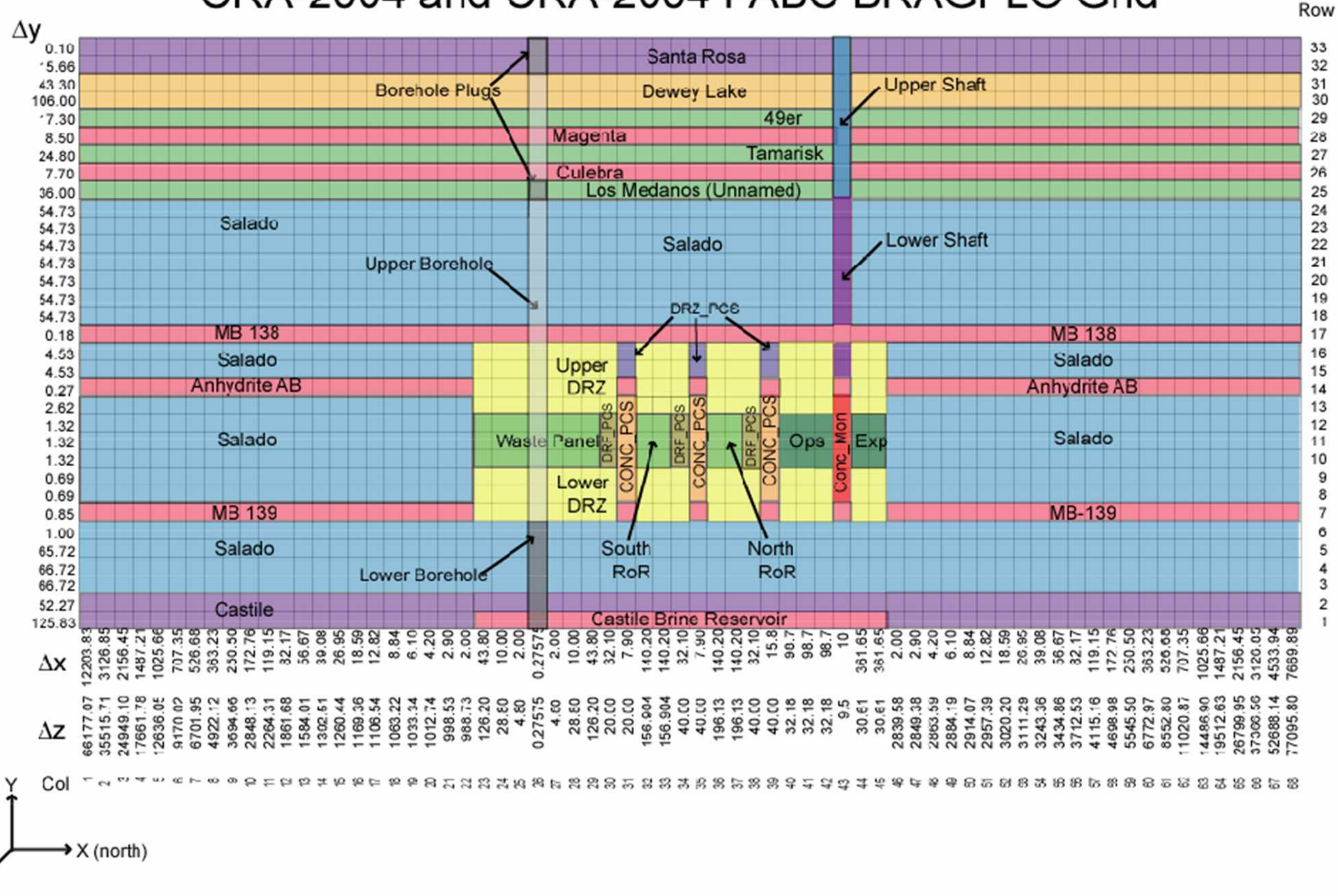
- q_{sb} = source (or sink) of brine
- q_{sg} = source (or sink) of gas
- φ = porosity
- S_b = brine saturation
- S_g = gas saturation = 1 - S_b

Description of Conceptual Model

BRAGFLO code

- Brine And Gas Flow (BRAGFLO)
  - Developed by oil and gas industry pre 1980
  - Brought to Sandia with Palmer Vaughn for WIPP project
  - Simple well documented finite-element code
  - Capable of 2-D or 3-D modeling, although 3-D has never been extensively used

CRA-2004 and CRA-2004 PABC BRAGFLO Grid



Key Geometric Assumptions

- Two Dimensional Grid with flaring adequately predicts flow
- Single (down-dip) panel models what would happen in any given panel
- Single borehole into a waste panel can be used to adequately model multiple intrusions
- Remainder of repository can be modeled as a two large areas

Conceptual Model

- Geology is defined by the: Santa Rosa, Dewey Lake, Rustler, Salado, Castile
- Culebra is the only unit of the Rustler that is allowed flow
- Anhydrite marker beds in the Salado above and below the repository: MB138, AB, MB139
- Disturbed Rock Zone (DRZ) remains permeable for 10,000 years
- Waste filled areas remain permeable for 10,000 years

Modeled Permeabilities

Unit	Permeability (m^2)
Santa Rosa	10^{-10}
Dewey Lake	10^{-16}
Culebra	10^{-13}
Anhydrite Marker Beds	10^{-19}
DRZ	10^{-17}
Intact Halite	10^{-23}
Waste Area	10^{-13}
Borehole (sand)	10^{-14}
Castile	10^{-12}

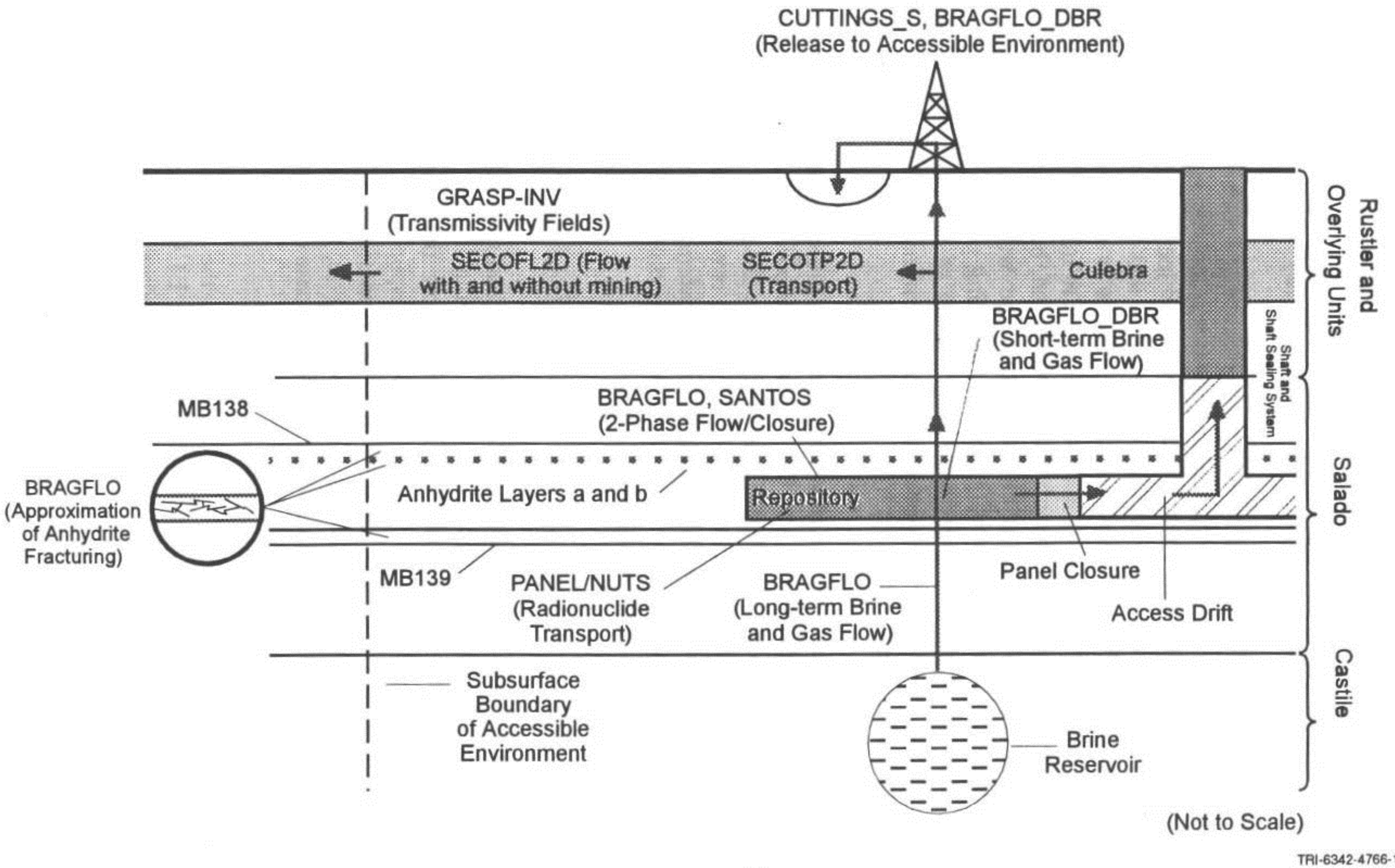
Sandia National Laboratories

Shaft Seals

- **Portion of the Shaft that resides in the Salado is assumed to undergo significant permeability decrease after 200 years due to salt healing**
- **SHFTL_T1** **$k = 10^{-18}$**
- **SHFTL_T2 (200 years after closure)** **$k = 10^{-20}$**

"Analysis Report for Development of a Simplified Shaft Seal Model for the WIPP Performance Assessment," James (2003), ERMS 525203

Intrusion Scenarios

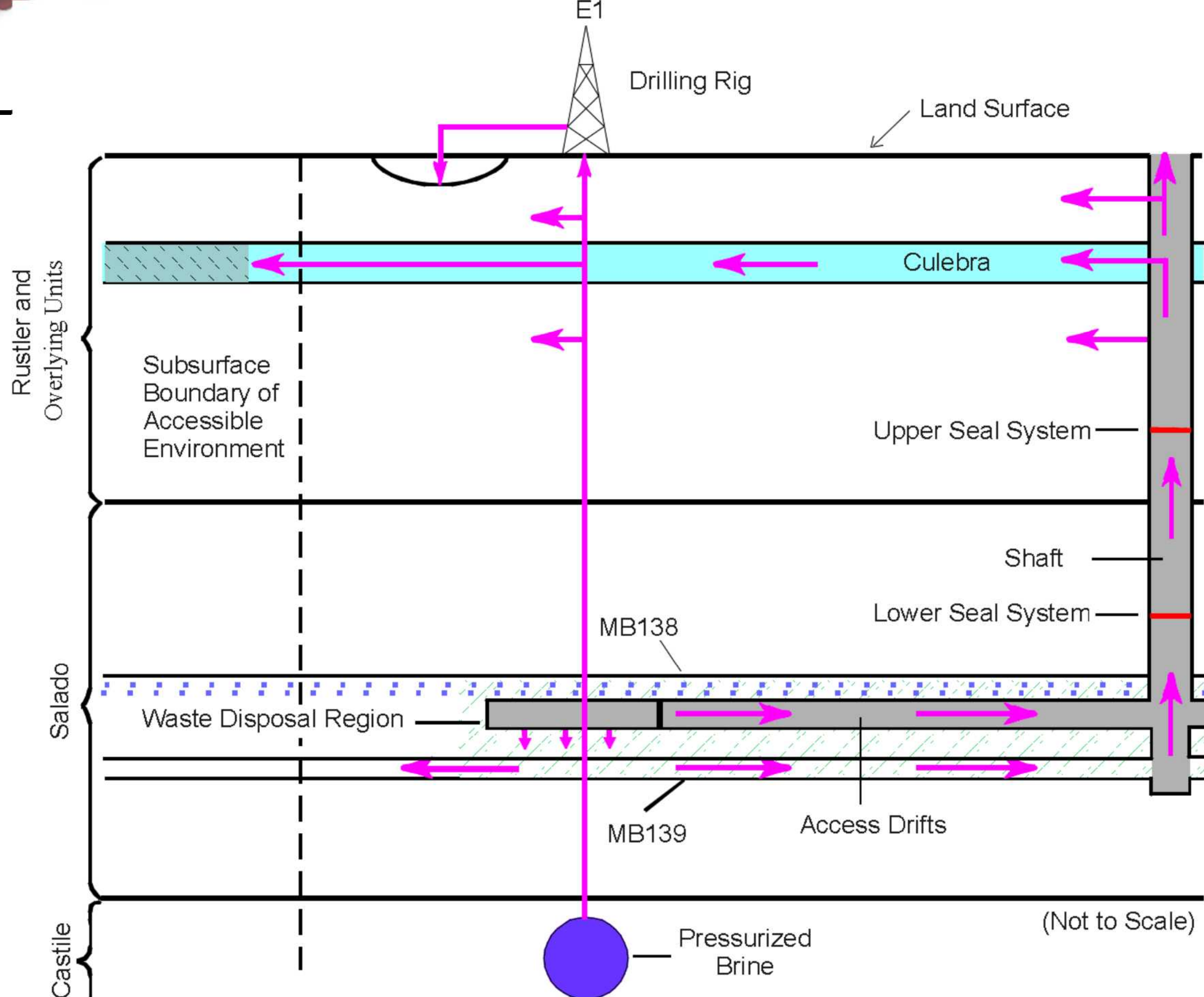


Sandia National Laboratories

Intrusion Scenarios

- **Undisturbed Scenario**
  - **No drilling events into the repository**
- **Disturbed Scenario**
  - **Predict consequences if someone were to drill through the repository looking for oil or gas**
    - **Hit a Castile brine reservoir (E1 intrusion)**
    - **Never hit brine capable of reaching the repository (E2 intrusion)**

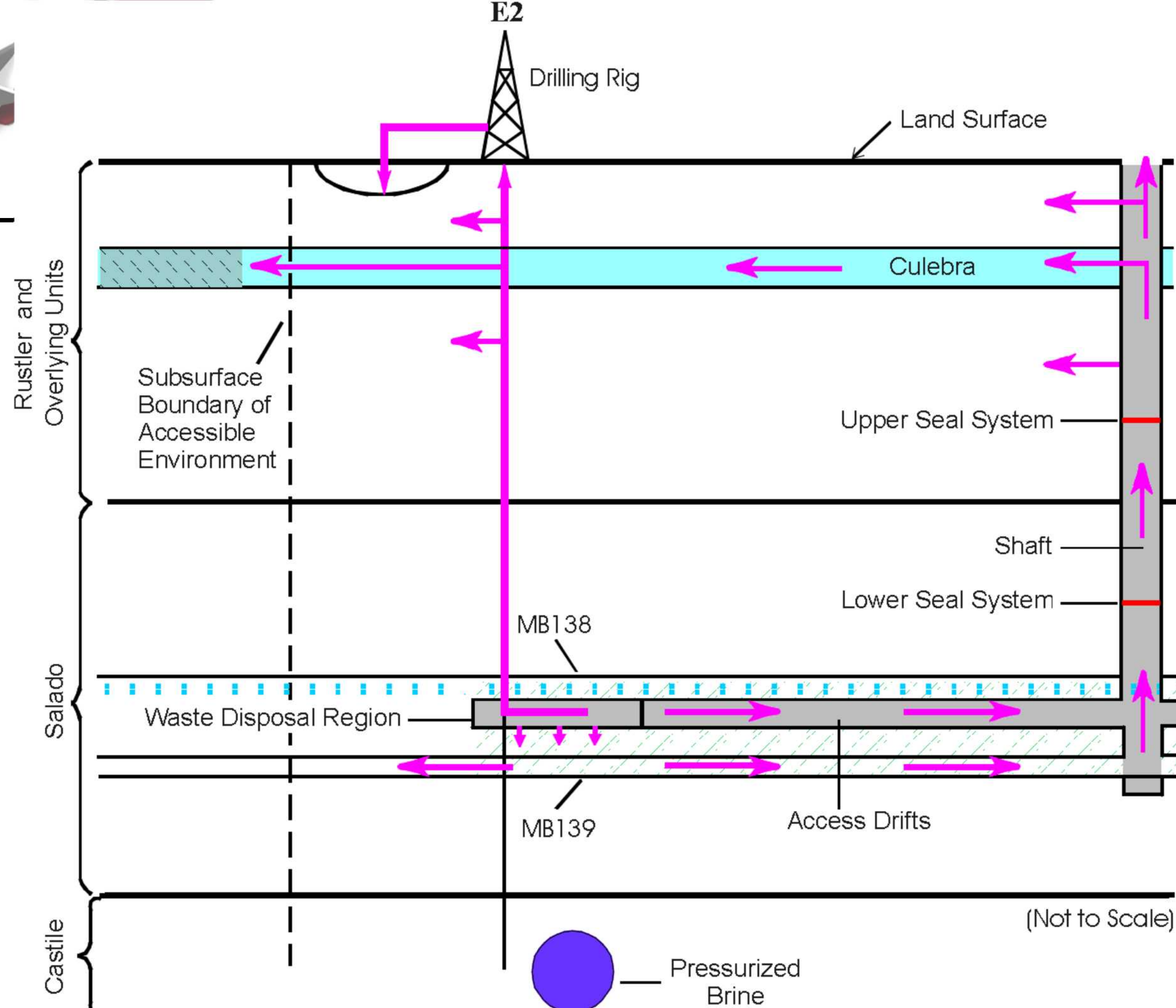
Disturbed Scenario Sequence: E1 Intrusion into Castile Brine Reservoir



Sandia National Laboratories

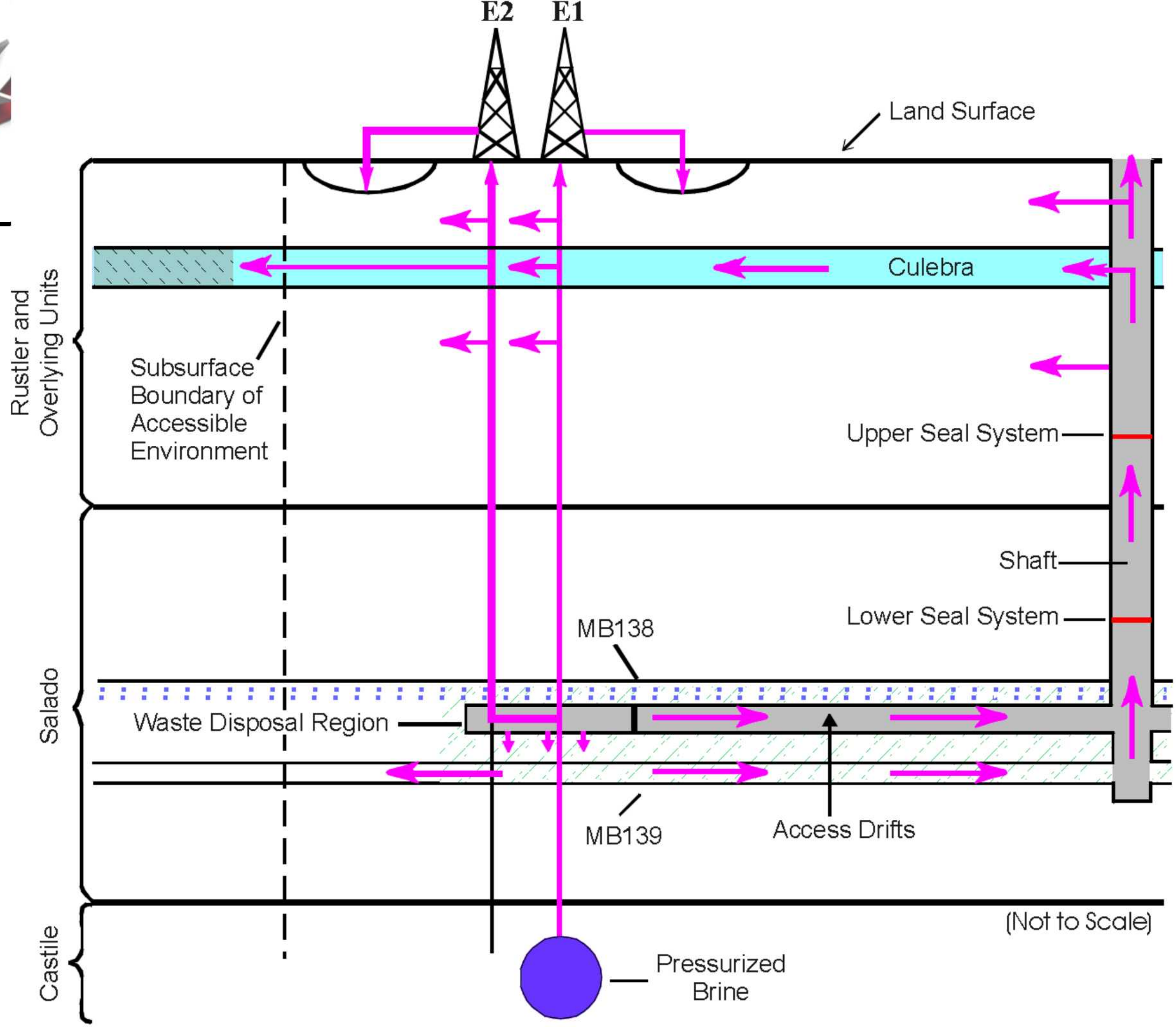
Disturbed Scenario Sequence: E1 Intrusion into Castile Brine Reservoir

- **Borehole intrusion (E1) through the Waste Panel into a hypothetical pressurized brine reservoir in the underlying Castile Formation. Concrete borehole plugs are immediately emplaced in the borehole at the Culebra and at the surface.**
- **200 years later: Borehole plugs fail and the borehole (top to bottom) is assumed to have properties equivalent to sand (material: BH_SAND).**
- **1,000 years later: the permeability of the borehole between the repository and the Castile Formation decreases due to creep closure of the salt (material: BH_CREEP).**


E2
Drilling Rig
Land Surface
Culebra
Rustler and Overlying Units
Subsurface Boundary of Accessible Environment
Upper Seal System
Shaft
Lower Seal System
MB138
Salado
Waste Disposal Region
MB139
Access Drifts
(Not to Scale)
Castile
Pressurized Brine

Disturbed Scenario Sequence: E2 Intrusion without penetrating Castile Brine Reservoir

- **Borehole intrusion (E2) through a Waste Panel terminating at the base of the DRZ in the modeling grid (no connection to the underlying Castile Formation). Two plugs are present in the upper part of the borehole.**
- **200 years later: Borehole plugs fail and the borehole (top to bottom) is assumed to have properties equivalent to sand (material: BH_SAND).**

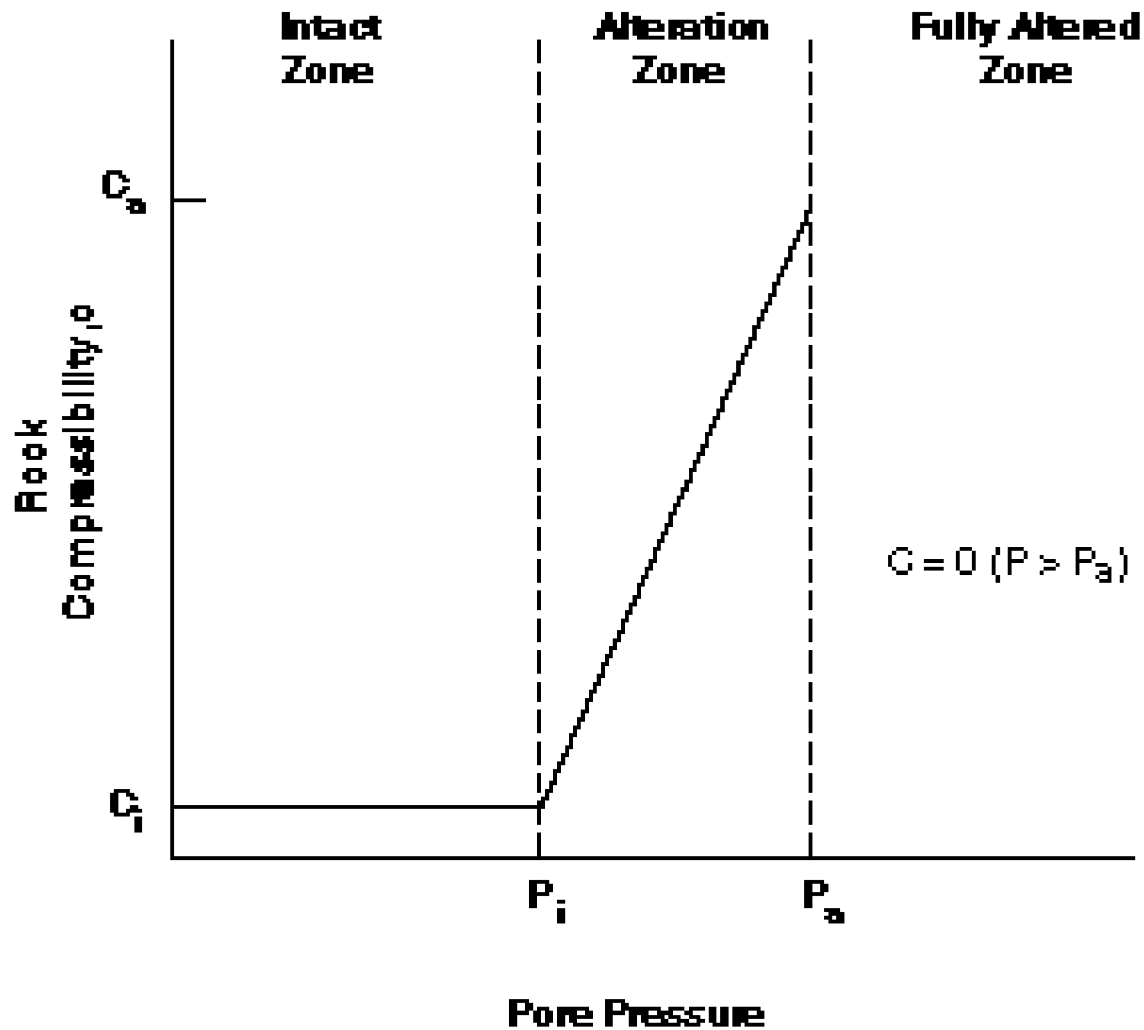

E2
E1
Land Surface
Culebra
Rustler and Overlying Units
Subsurface Boundary of Accessible Environment
Upper Seal System
Shaft
Lower Seal System
MB138
Salado
Waste Disposal Region
MB139
Access Drifts
(Not to Scale)
Castile
Pressurized Brine

Disturbed Scenario Sequence: E2E1 Two Intrusions

- Borehole intrusion (E2) through a Waste Panel terminating at the base of the DRZ in the modeling grid (no connection to the underlying Castile Formation) Borehole filled with sand.
- 1,000 years later: borehole intrusion (E1) through a Waste Panel into a hypothetical pressurized brine reservoir in the underlying Castile Formation
- 1,200 years later: Borehole plugs fail and the borehole (top to bottom) is assumed to have properties equivalent to sand (material: BH_SAND).
- 2,200 years later: the permeability of the borehole between the repository and the Castile Formation decreases due to creep closure of the salt (material: BH_CREEP).

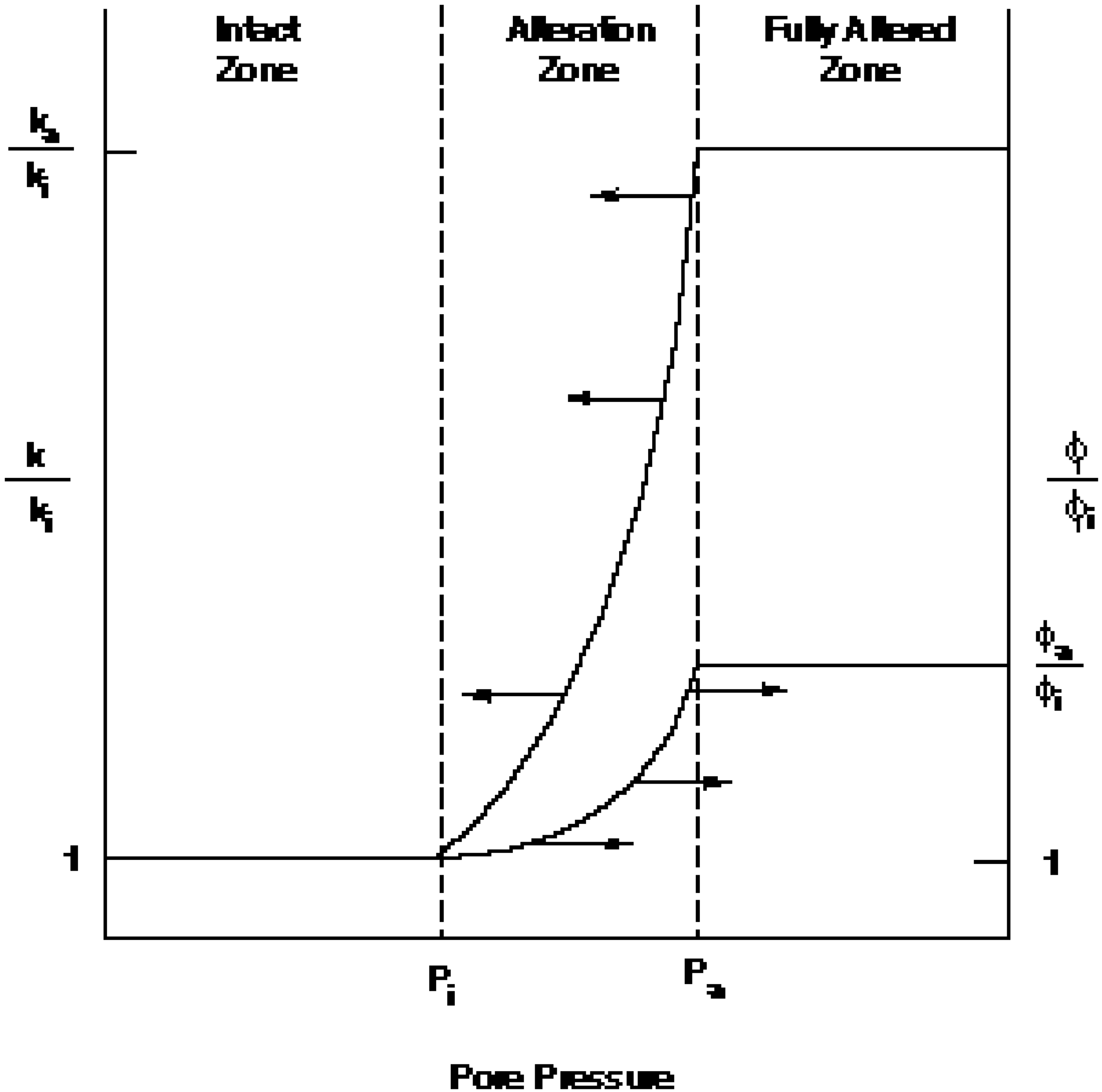
Fracturing

- **Rock is modeled as fractured if pressures are > lithostatic + fracture initiation pressure**



TRI-6342-0498-3

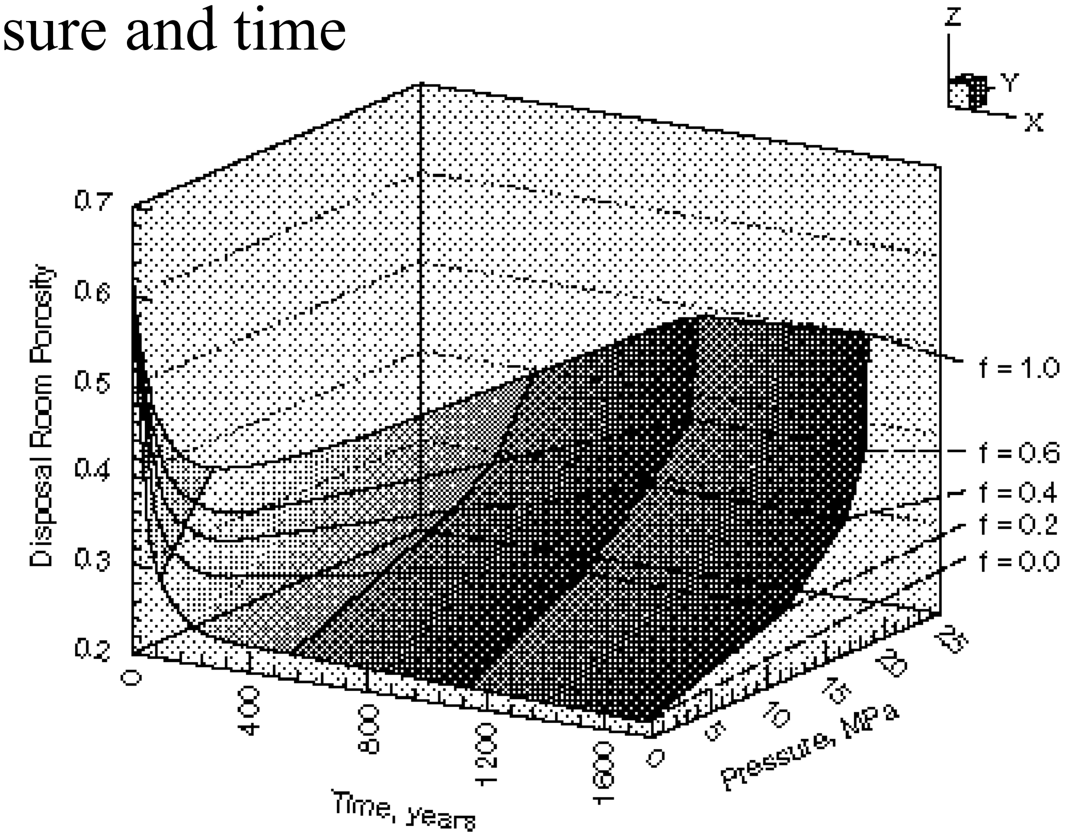
Fractured Rock Permeability



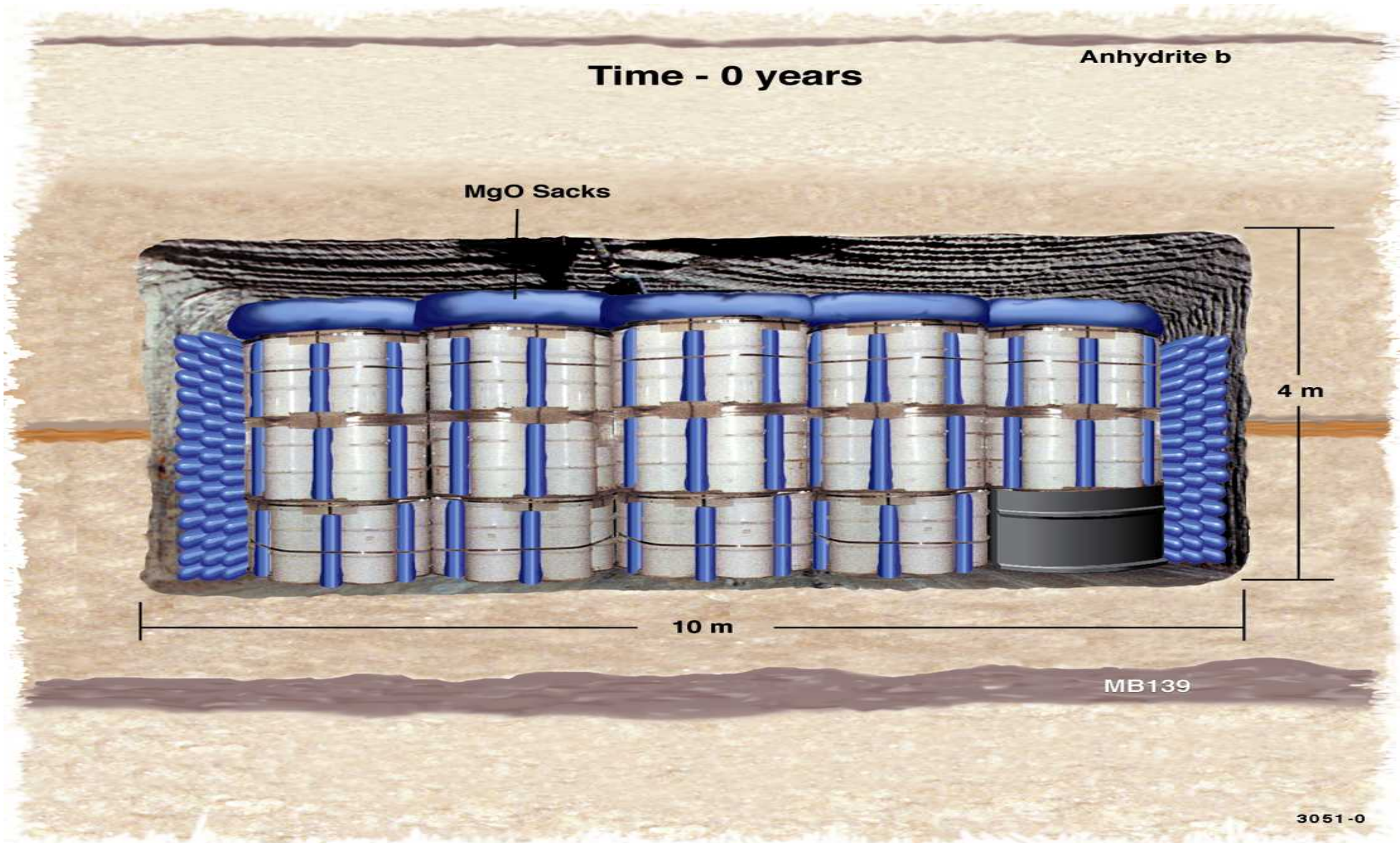
Sandia National Laboratories

Room closure Due to Salt Creep

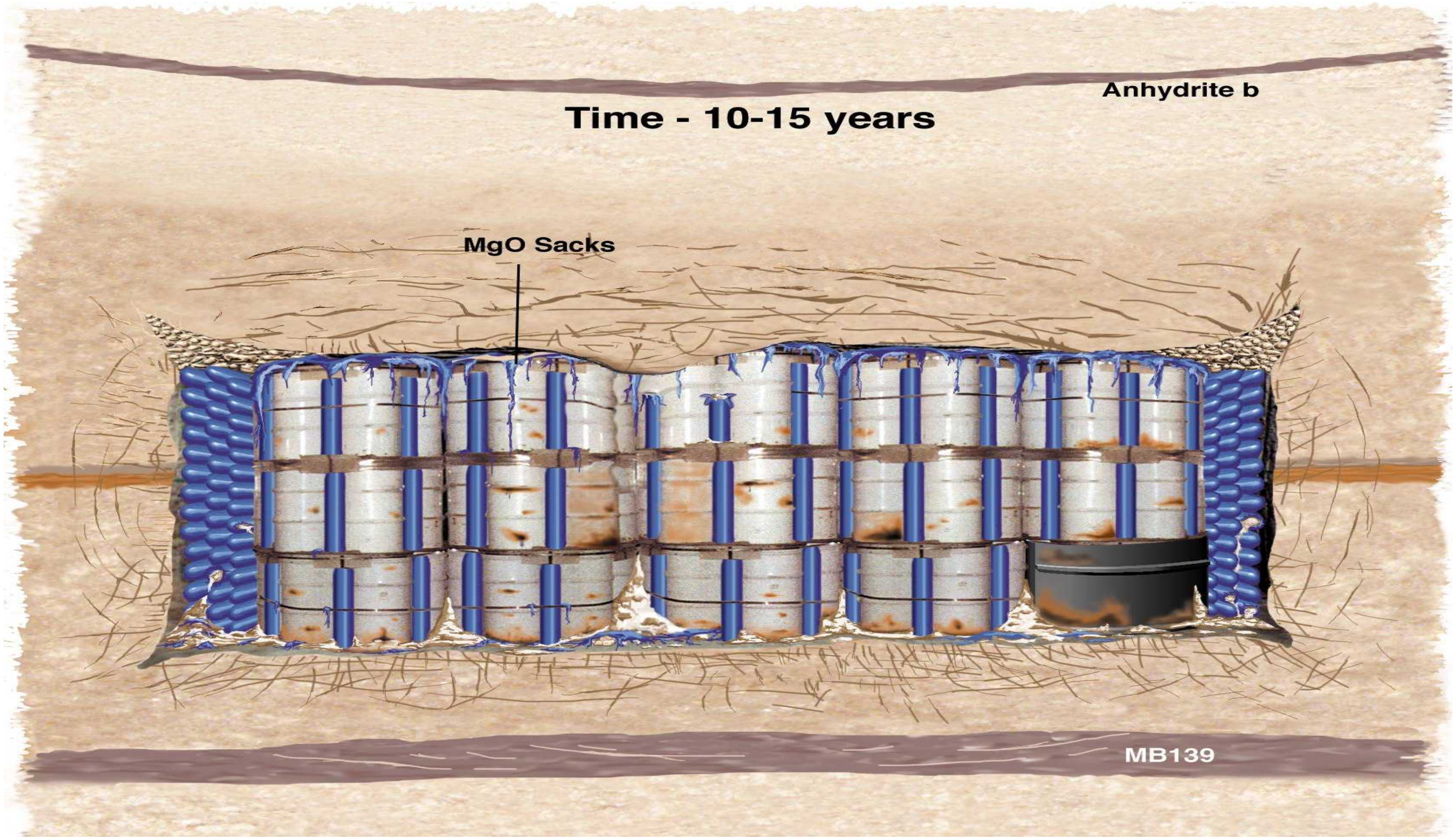
•SANTOS calculates Waste Area porosity as a function of pressure and time



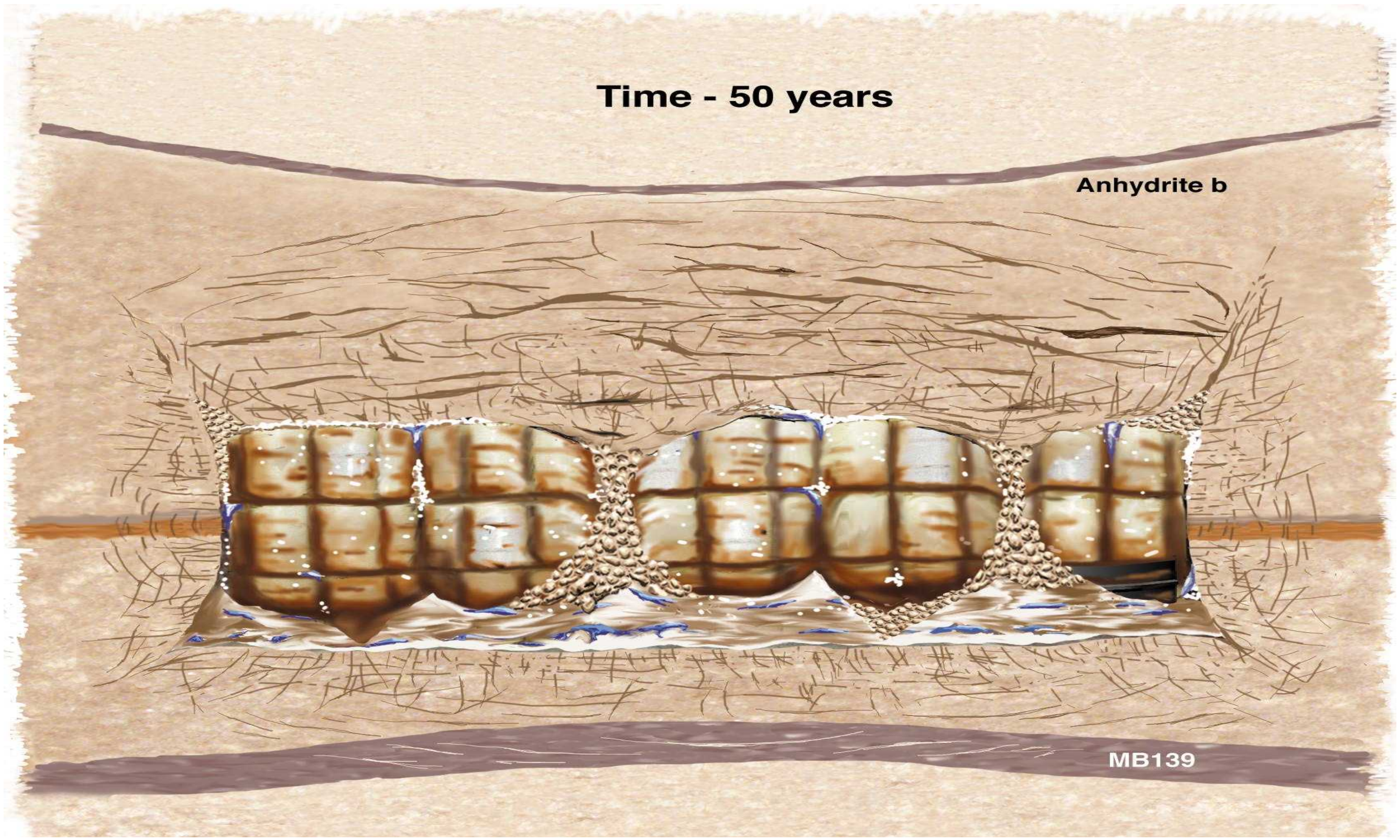
Room closure Due to Salt Creep: t = 0 y



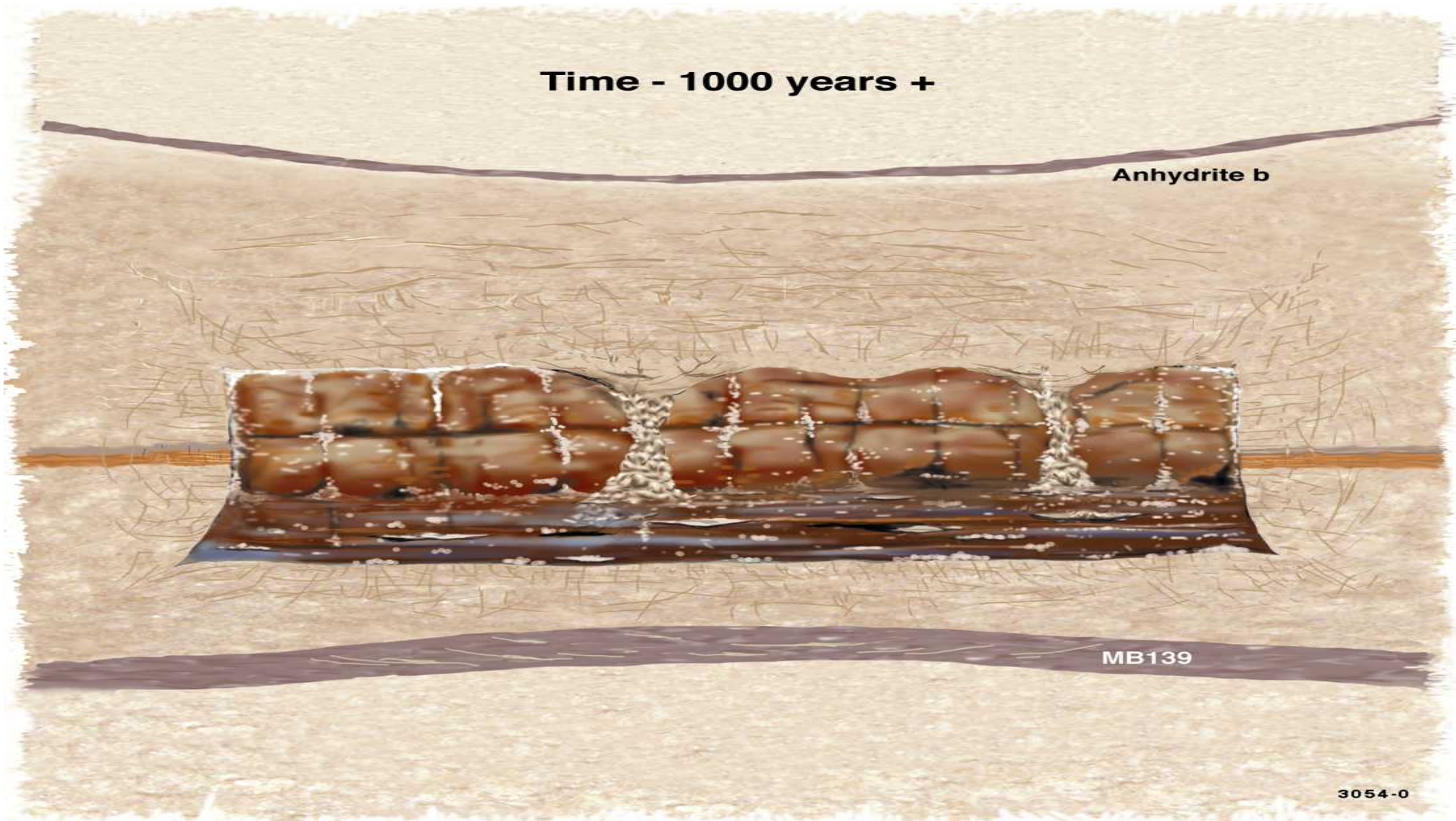
Room closure Due to Salt Creep: t = 15 y



Room closure Due to Salt Creep: t = 50 y



Room closure Due to Salt Creep: t = 1000+ y



Gas Generation

Corrosion of Fe- and Al-base metals

- Will produce H_2, consume H_2O

Possible microbial consumption of cellulosic, plastic, and rubber (CPR) materials

- Could produce CH_4, CO_2, H_2S, N_2

Alpha radiolysis of H_2O in brine, and of CPR materials

- Will produce H_2, O_2, other gases; and consume H_2O

Corrosion $\cong$ microbial activity >> radiolysis

Gas Generation (cont.)

Effects of gas generation on Salado Flow

- Brine inflow and outflow
- Room closure
  - Porosity and permeability of materials in the repository, DRZ, and marker beds
  - Resistance of waste to erosion and spalling in the event of human intrusion
- Gas drives spallings releases

Anoxic Corrosion

Relative importance of different types of corrosion:

- **Anoxic corrosion >> oxic corrosion**

Experimentally observed anoxic corrosion reactions

- $Fe + (x + 2)H_2O \rightleftharpoons Fe(OH)_2 \cdot xH_2O + H_2$
- $Fe + H_2O + CO_2 \rightleftharpoons FeCO_3 + H_2$
- $Fe + H_2S \rightleftharpoons FeS + H_2$

Other possible anoxic corrosion reactions

- $3Fe + 4H_2O \rightleftharpoons Fe_3O_4 + 4H_2$
- $Fe + 2H_2S \rightleftharpoons FeS_2 + 2H_2$

Microbial Activity

Significant microbial activity possible, but by no means certain

Implementation in the CCA PA, the PAVT, and the CRA-2004 PA

- Microbial consumption of all cellulosic materials possible:
  - Probability = 0.25 (included in ~25% of the PA vectors)
- Microbial consumption of all CPR materials possible:
  - Probability = 0.25 (included in ~25% of the vectors)
- No microbial activity:
  - Probability = 0.50 (included in the other~50% of the vectors)

Sandia National Laboratories

Microbial Activity

Implementation in the CRA-2004 PABC

- For the PABC, the EPA stipulated that microbial activity can occur in ALL vectors
- However, the EPA allowed the use of lower microbial gas-generation rates based on long-term results from the laboratory study of microbial gas generation at BNL
- Furthermore, the EPA established an arbitrary factor, which can vary from 0 to 1, used to multiply the sampled value of the microbial gas generation rate
- Microbial consumption of all cellulosic materials possible:
  - Probability – 0.75 (included in ~ 75% of the PA vectors
- Microbial consumption of all CPR materials possible:
  - Probability ~ 02.5 (included in the other ~25% of the vectors)

Sandia National Laboratories

Microbial Activity (cont.)

Potentially significant microbial respiratory pathways

- Denitrification
  - $C_6H_{10}O_5 + 4.8H^+ + 4.8NO_3^- \rightarrow 7.4H_2O + 6CO_2 + 2.4N_2$
- SO_4^{2-} reduction
  - $C_6H_{10}O_5 + 6H^+ + 3SO_4^{2-} \rightarrow 5H_2O + 6CO_2 + 3H_2S$
- Fermentation and methanogenesis
  - $C_6H_{10}O_5 + H_2O \rightarrow 3CH_4 + 3CO_2$

Implementation in PA

- Sequential use of electron acceptors
- However, the EPA has disallowed the use of methanogenesis
- Given the current inventory, denitrification will consume 4% and SO_4^{2-} reduction will consume 96& of the CPR materials in the repository <u>if</u> all CPR materials are consumed

Role of MgO

Functions as an engineered barrier by consuming CO_2 from possible microbial activity, thereby decreasing actinide solubilities

- Will react with CO_2 and H_2O in brine and water vapor to form hydrous and, eventually, anhydrous Mg carbonates
- Will consume essentially all CO_2 and remove CO_3^{2-} from brine
- Will buffer pH at ~9

Consumption of significant quantities of H_2O could also affect long-term performance

The DOE is emplacing sufficient MgO to consume all CO_2 that could be produced by microbial consumption of all cellulosic, plastic, and rubber (CPR) materials

Role of MgO (cont.)

DOE asserted in the 1996 Compliance Certification Application (CCA) that borehole plugs, MgO, panel closures, and shaft seals would help satisfy the EPA's assurance requirement for multiple natural and engineered barriers

- Barriers defined as "any material or structure that prevents or substantially delays movement of water or radionuclides toward the accessible environment." Barriers can be "… a geologic structure, a canister, a waste form, or a material placed over and around waste provided that material or structure substantially delays movement of water or radionuclides"

MgO recognized as the only engineered barrier in the WIPP disposal system in the EPA's 1998 certification of the WIPP

Role of MgO (cont.)

Hydration of periclase to form brucite:

- $MgO + H_2O = Mg(OH)_2$

Carbonation of brucite to form hydromagnesite or magnesite

- $5Mg(OH)_2 + 4CO_2 \rightleftharpoons Mg_5(CO_3)_4(OH)_2 \cdot 4H_2O$
  - Reaction assumed to control f_{CO_2} for the actinide-solubility calculations
- $Mg(OH)_2 + CO_2 \rightleftharpoons MgCO_3 + H_2O$
  - Likely long-term carbonation reaction

Reaction that will buffer pH:

- $Mg(OH)_2 \rightleftharpoons Mg^{2+} + 2OH^-$

Gas Generation in BRAGFLO

$$\text{C} + \text{unknown} \rightarrow y\,\text{H}_{2(g)} + \text{unknown}$$

$$\frac{dM_{CPR}}{dt} = k_{CPR,I} S_B + k_{CPR,H} (1 - S_B)$$

- $k_{CPR,I}$ = Inundated CPR consumption rate
- $k_{CPR,H}$ = Humid CPR consumption rate
- S_B = Brine saturation

Gas Generation in BRAGFLO contd.

$$Fe + (x + 2)\, H_2O \rightleftharpoons Fe(OH)_2.xH_2O + H_2$$

$$\frac{dM_{Fe}}{dt} = k_{Fe,I} S_B$$

$k_{Fe,I}$ = Inundated CPR consumption rate
S_B = Brine saturation

Gas Generation: Wicking

- **Waste is assumed to wick water by capillarity**

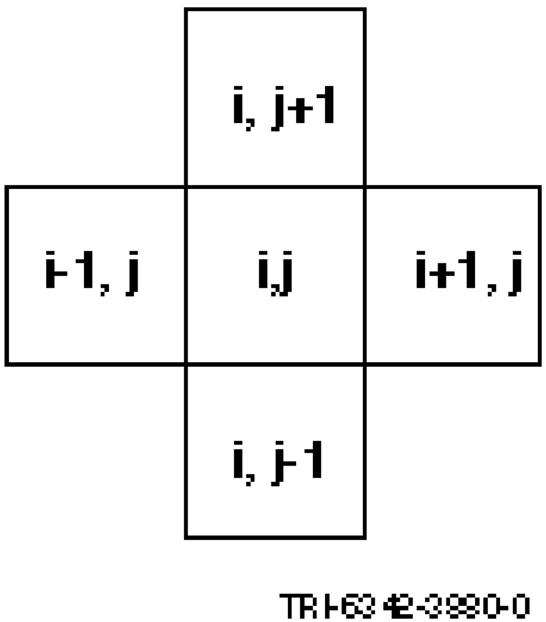
$$S_{eff} = S_b + S_{wick}\left(1 - e^{\alpha S_b}\right)$$

• Gas-generating reactions use a humid and inundated rate. However with wicking, most reactions use only the inundated rate

- **S_{eff} = wicked saturated in the waste**
- **S_{wick} = Sampled parameter [0 – 1]**
- **α = smoothing parameter [= -1000]**

Numerical Implementation

Finite Difference code



- Blocks
- Nodes
- Block interfaces

$$f_1(x_1, x_2) = f_1\left(x_1^k, x_2^k\right) + \frac{\partial f_1}{\partial x_1}\left(x_1^k, x_2^k\right)\left(x_1 - x_1^k\right) + \frac{\partial f_1}{\partial x_2}\left(x_1^k, x_2^k\right)\left(x_2 - x_2^k\right)$$

Upstream Weighting

$S_g > S_{gr}$	$S_g \leq S_{gr}$
$P_{g,i}$	$P_{g,i+1}$

x_i interface x_{i+1}

$$k_{\text{interface}} = \begin{cases} k_{i+1}, & P_i < P_{i+1} \\ k_i, & \text{otherwise.} \end{cases}$$

Implicit Time Stepping

$$\frac{\partial \hat{x}}{\partial t} = g(\hat{x})$$

$$\frac{\Delta \hat{x}}{\Delta t} = g(\hat{x}_{t+\Delta t}) \approx g(\hat{x}_t) + \frac{\partial g}{\partial \hat{x}} \Delta x$$

BRAGFLO calculates the Jacobian numerically

$$J(\hat{x}) = \frac{\partial g}{\partial \hat{x}}$$

Netwon's Method

$$F = \left\{ \nabla \bullet q_{brine} + q_{sb} = \frac{\partial \left(\phi \rho_b S_b \right)}{\partial \, t}, \nabla \bullet q_{gas} + q_{sg} = \frac{\partial \left(\phi \rho_g S_g \right)}{\partial \, t} \right\}$$

$$F(\hat{x}^k) = 0$$

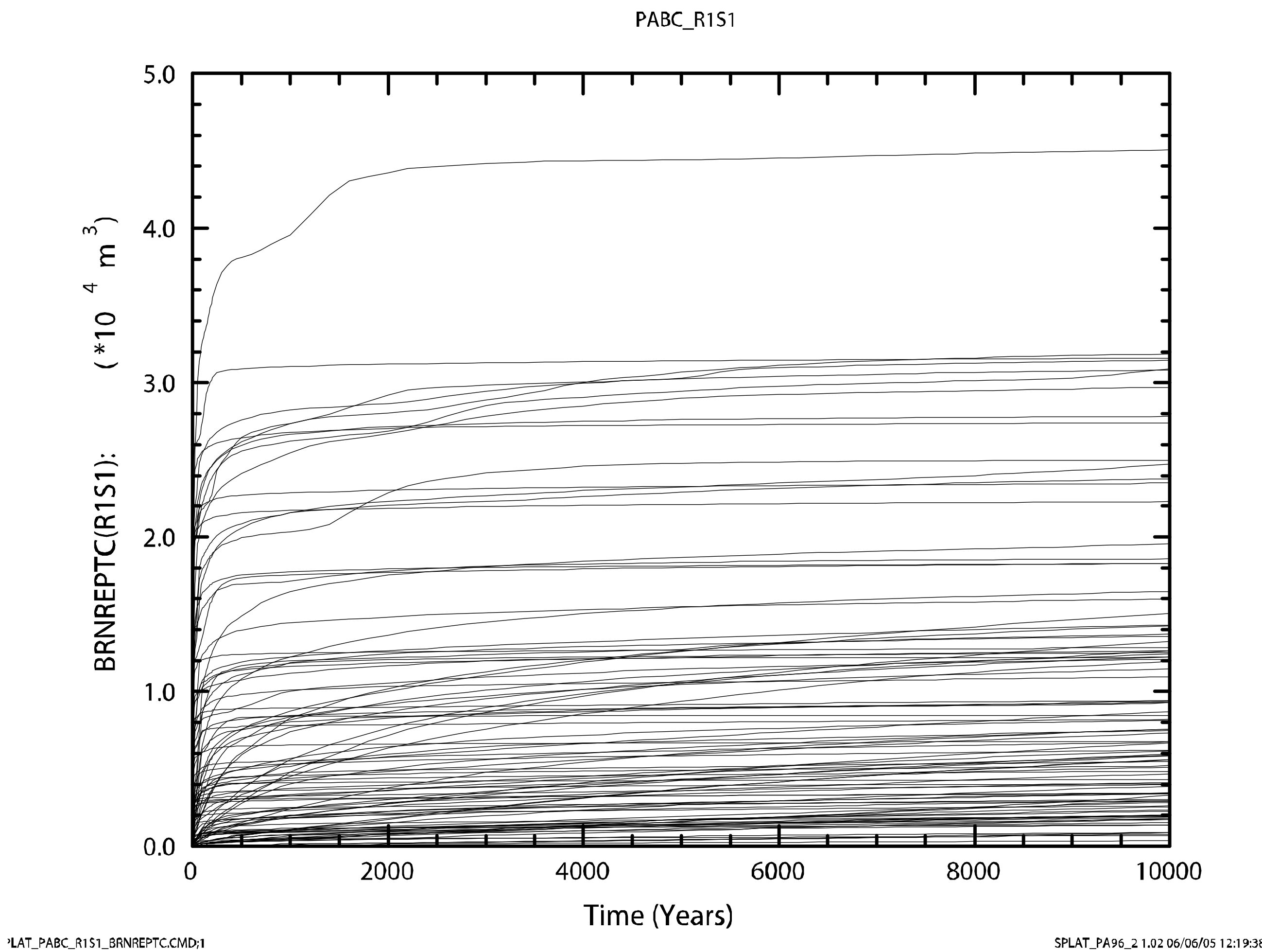
$$\hat{x} = \{P_b, S_g\}$$

$$\hat{\mathbf{x}}^{\mathrm{k}+1} = \hat{\mathbf{x}}^{\mathrm{k}} + \delta\, \hat{\mathbf{x}}.$$

$$\delta\hat{\mathbf{x}} = -\mathbf{J}^{-1}(\hat{\mathbf{x}}^{\mathrm{k}})\mathbf{F}(\hat{\mathbf{x}}^{\mathrm{k}})$$

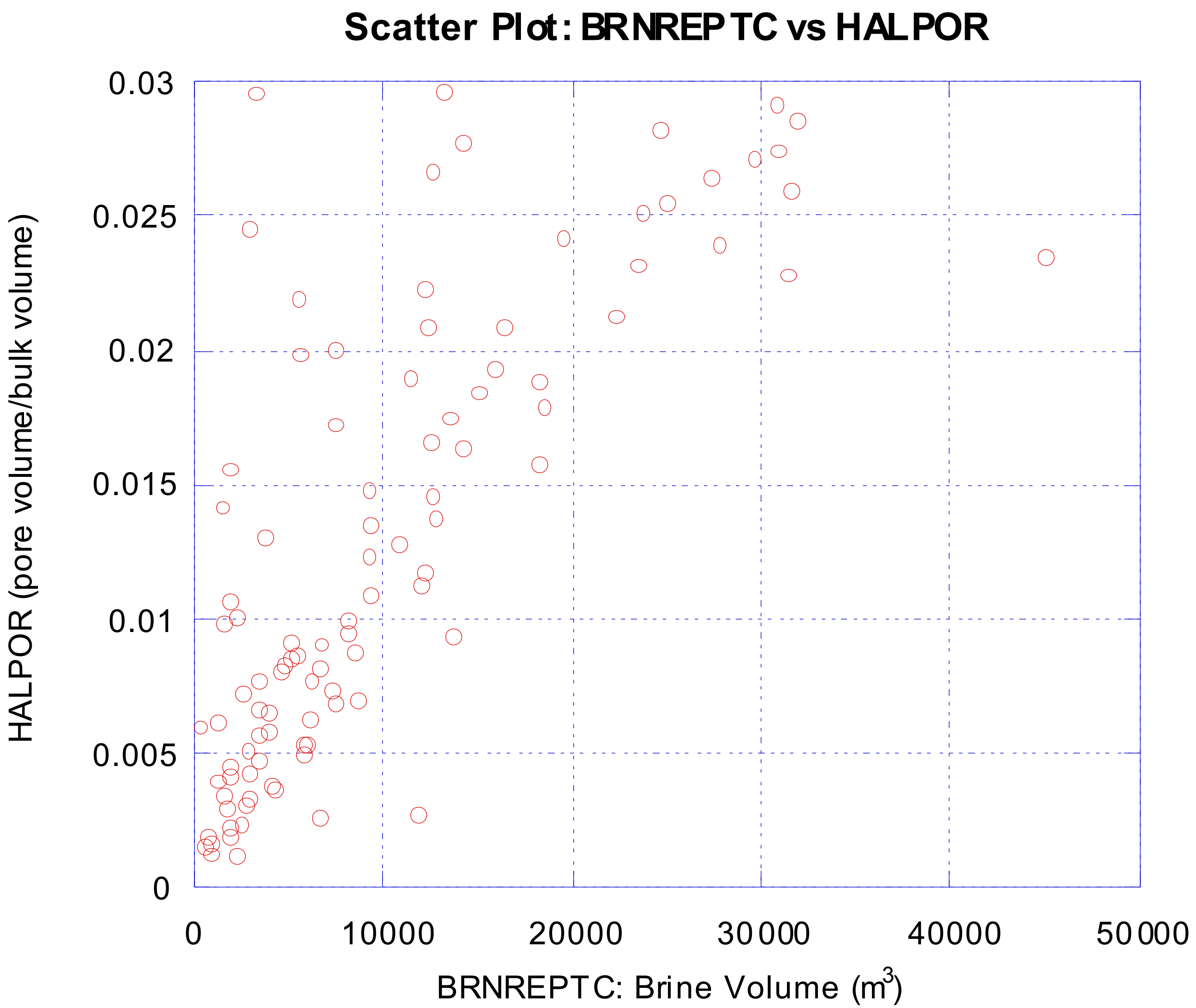
PABC Results

Undisturbed: Brine flow into Repository

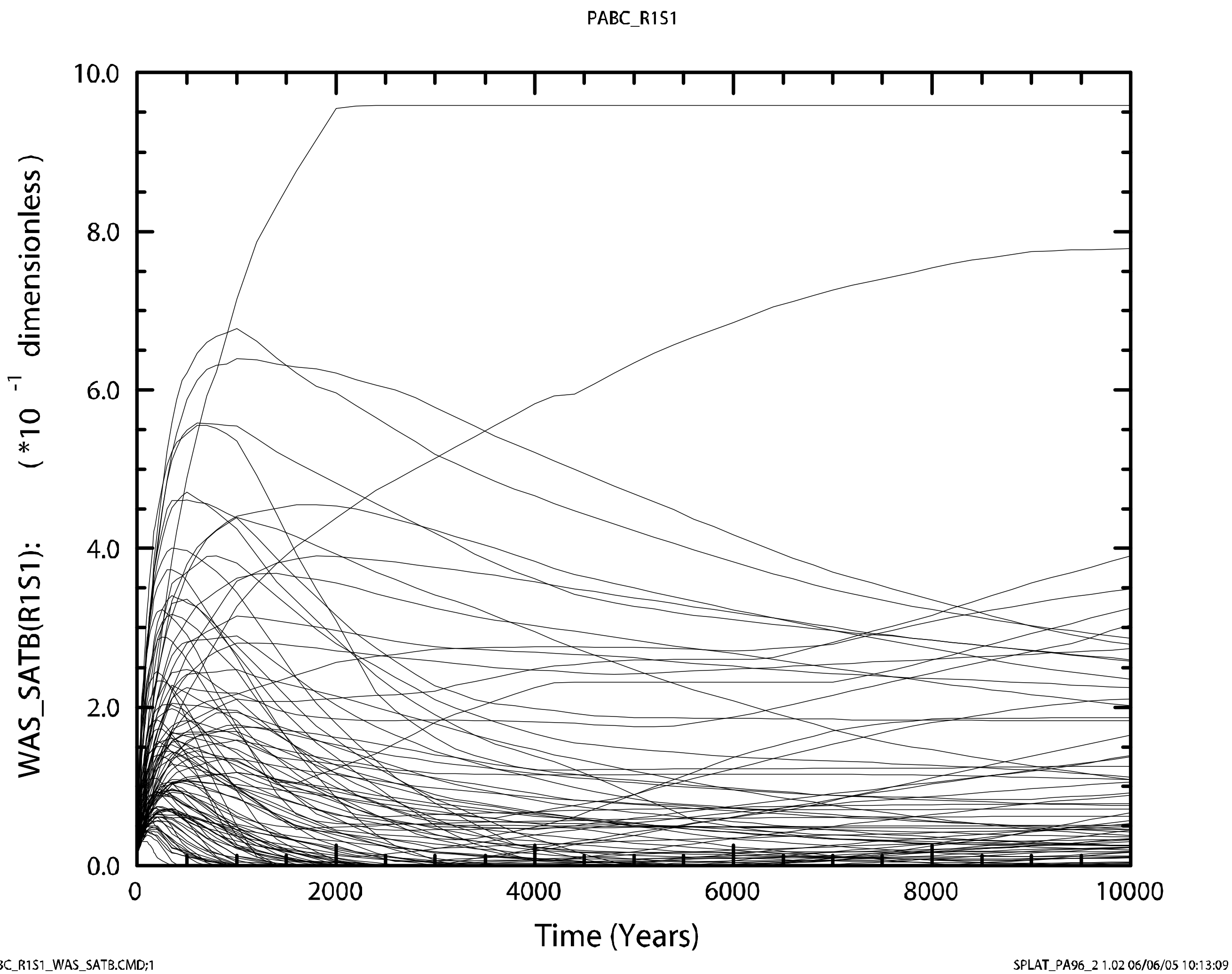


a) PABC

Undisturbed: Brine is coming from the DRZ

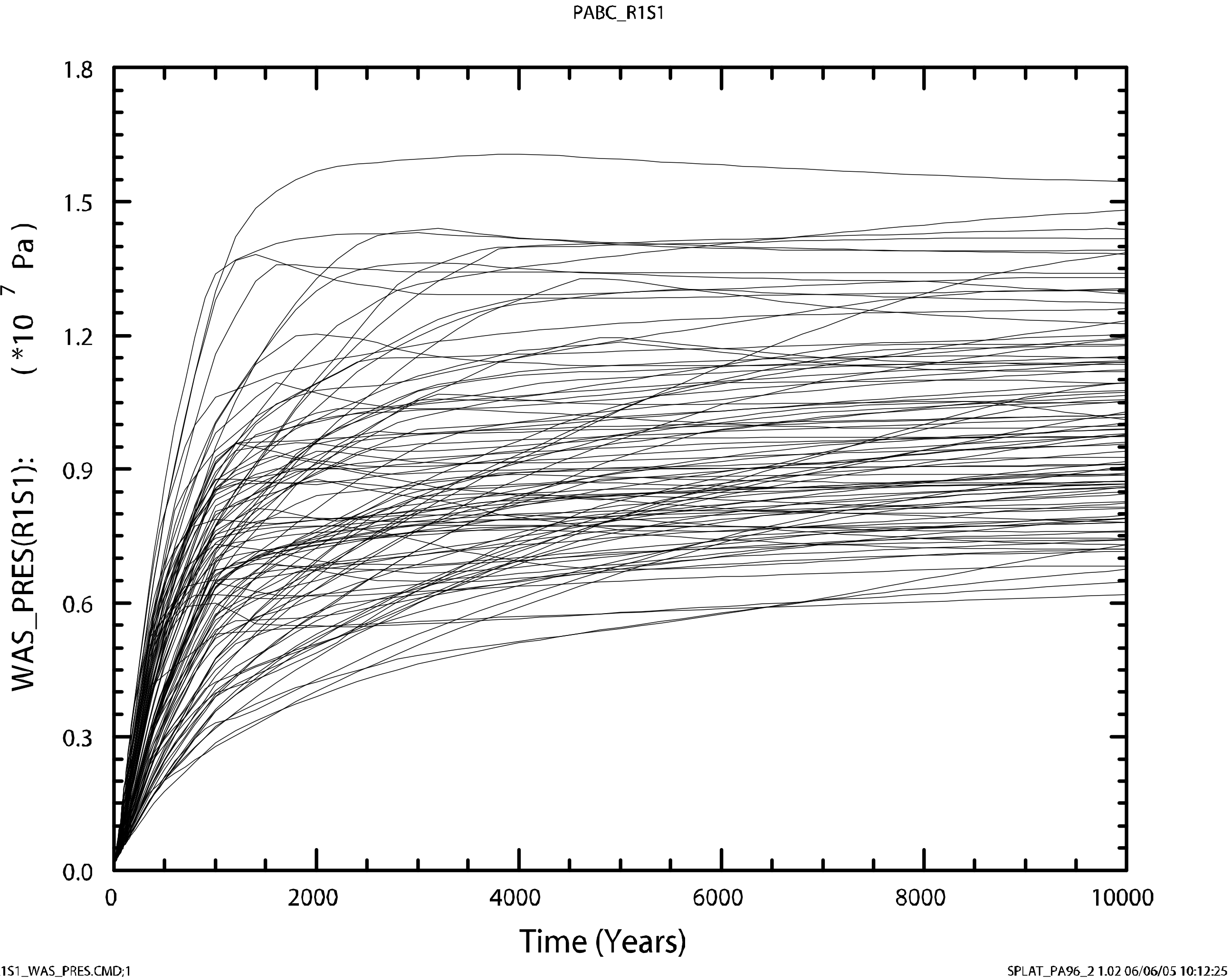


Undisturbed: Brine Saturation



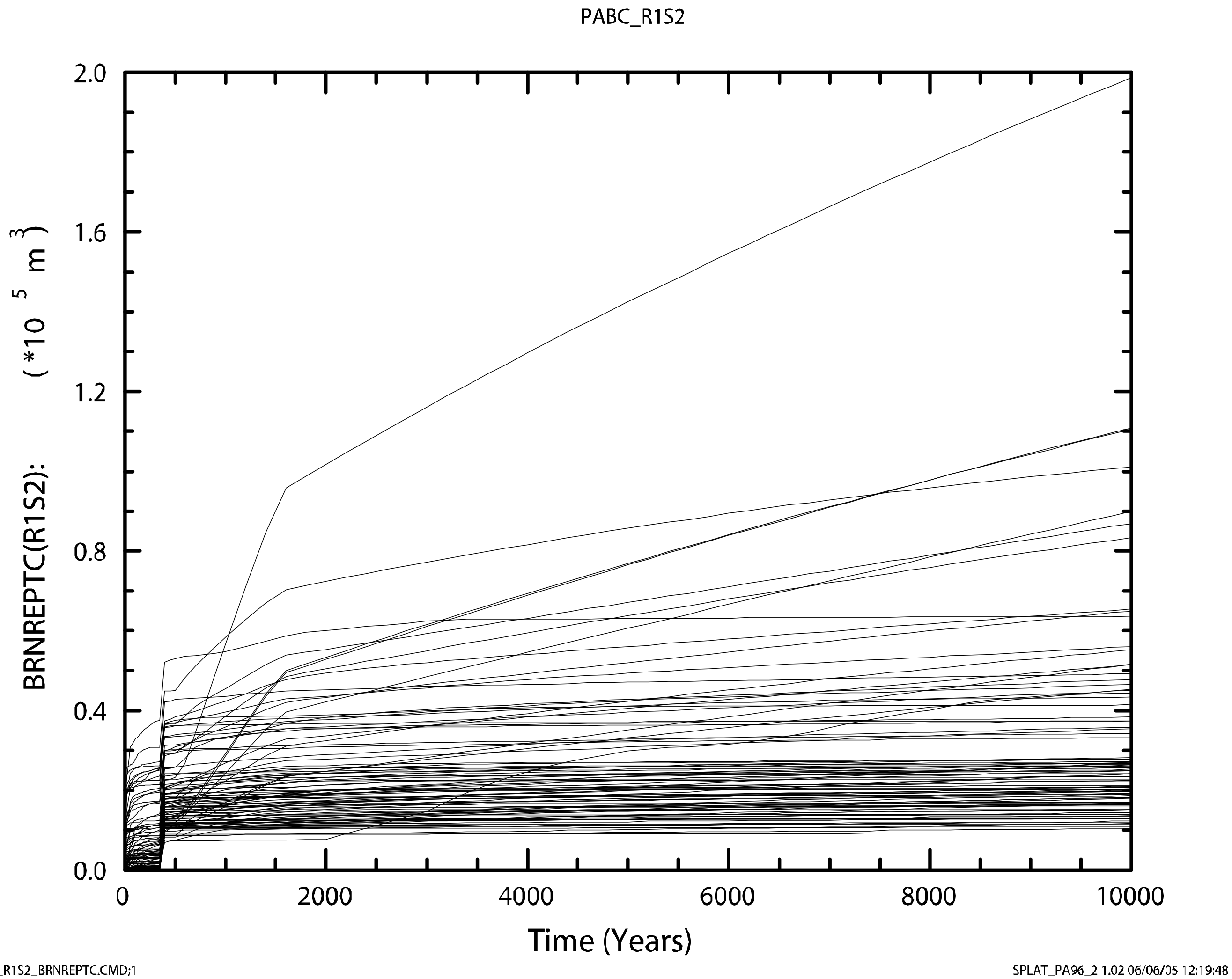
a) PABC

Undisturbed: Pressure



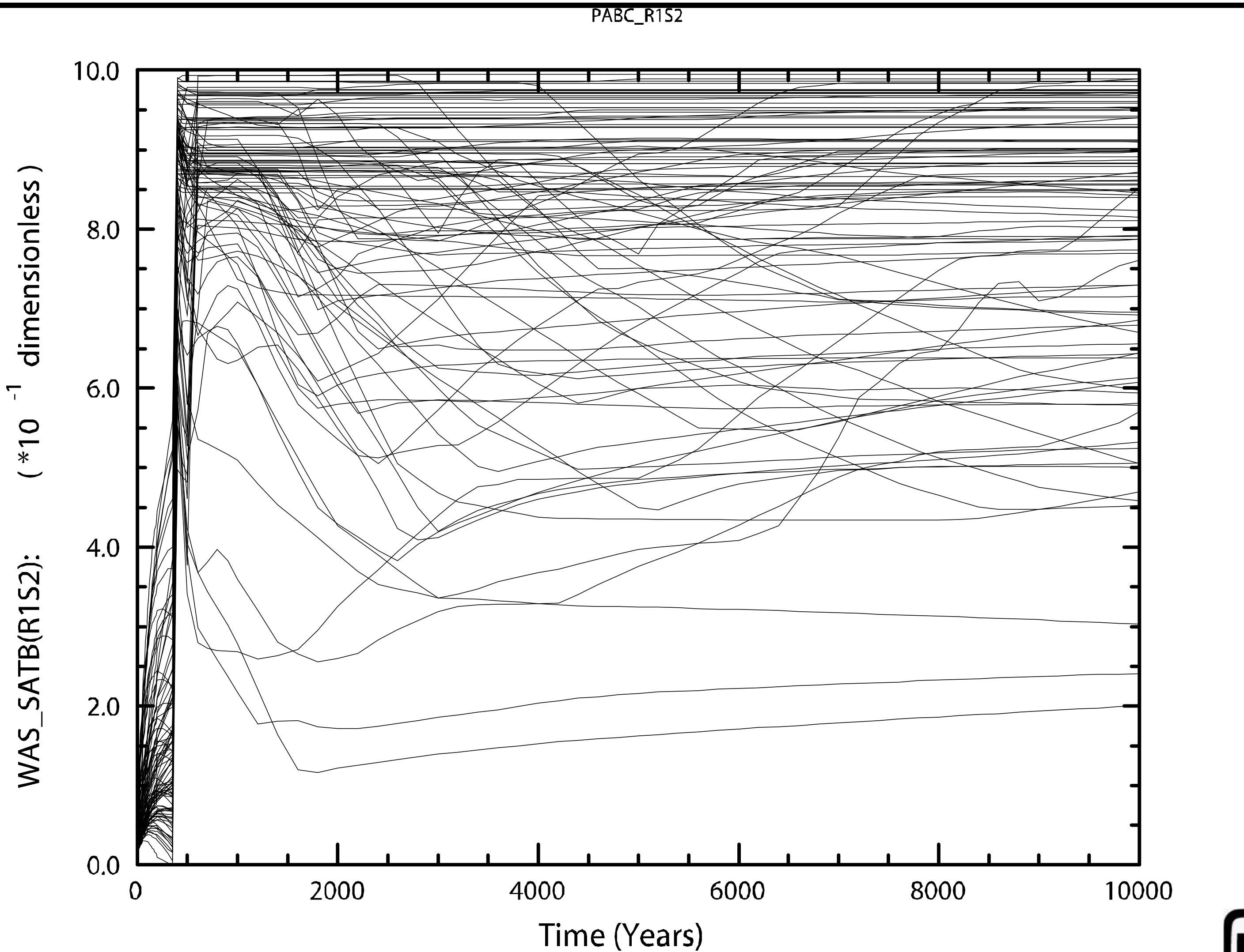
a) PABC

Disturbed E1: Brine Inflow into Repository



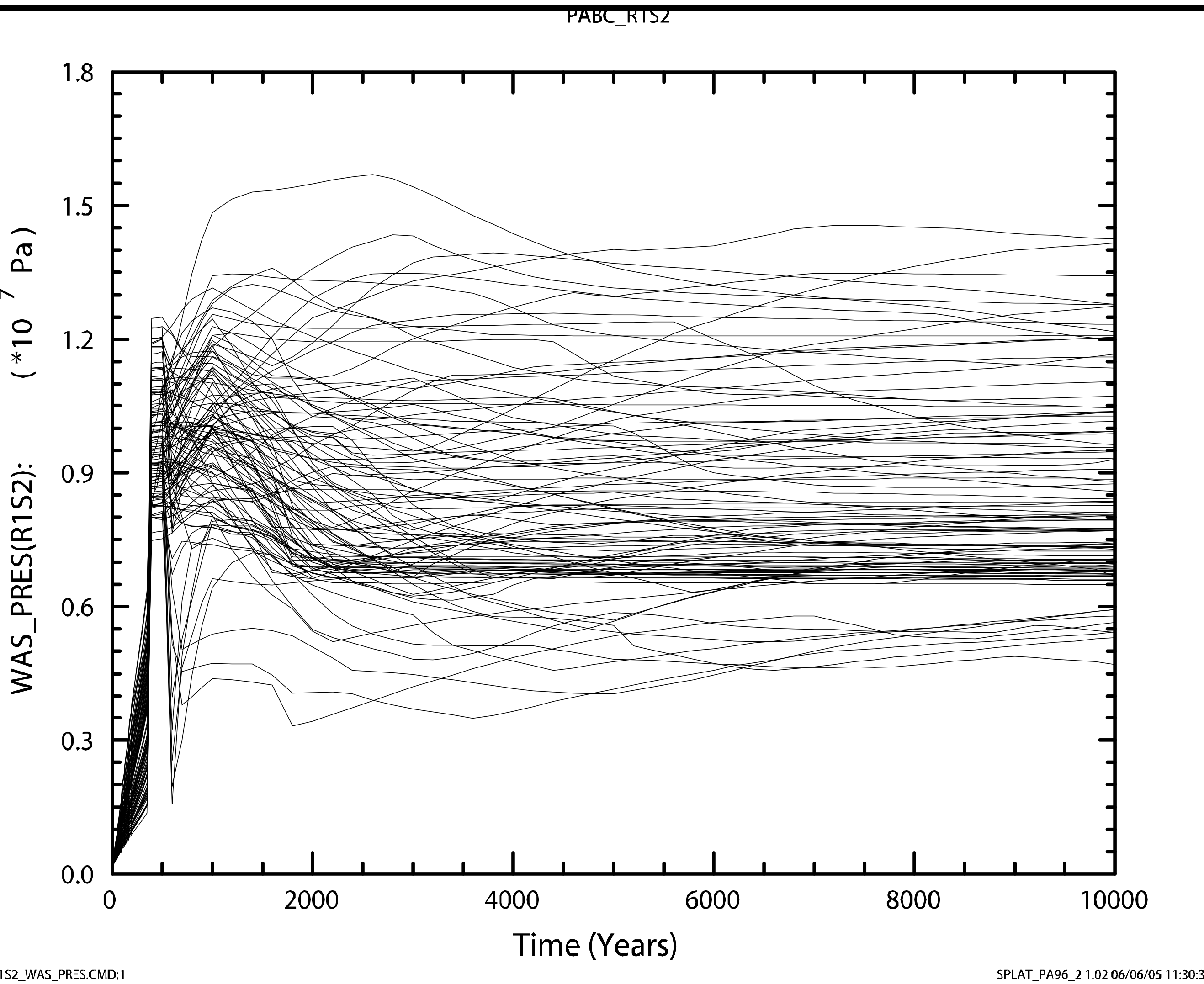
a) PABC

Disturbed E1: Brine Saturation



a) PABC

Disturbed E1: Pressure



a) PABC