SAND2022-11749C

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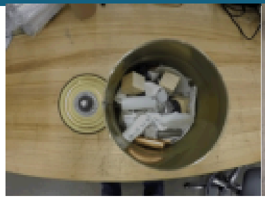
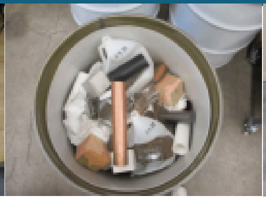
WIPP Disposal Room Porosity Calculations

12th US/German Salt Workshop on Salt Repository Research, Design, and Operation, Braunschweig, Germany, September 8, 2022

Presented by

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Major Contributors- Benjamin Reedlunn, Chet Vignes, Richard Jensen, and Courtney Herrick

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Outline

- Background/Motivation
- Geomechanical Model
- Gas Generation Model
- Simulated Waste Container Tests and Constitutive Model
- Disposal Room Porosity Model Results

Background and Motivation

- The disposal room porosity model simulates the evolution (deformation) of a disposal room containing waste containers.
- The production of gas, through a combination of anoxic corrosion, biodegradation and radiolysis, results in pressure being applied to the room surfaces.
- The waste containers and the gas pressure resist the inward creep of the salt.
- The room only stops evolving when the resistance from the containers and gas pressure are balanced with the stresses from the surrounding rock salt.
- The WIPP Performance Assessment Group model of brine and gas flow (BRAGFLO) uses the disposal room porosity results from mechanical simulations of room closure **as input** to account for the time dependent porosity changes in the waste disposal areas.

Background and Motivation

- To do these disposal room porosity simulations we need to have:
  - geomechanical model capable of reproducing closure measurements from past underground room scale tests
  - constitutive model for the waste containers
  - gas model

- The WIPP Performance Assessment (PA) group performs **1800** brine and gas flow simulations for each Compliance Recertification Application (CRA). These simulations account for parameter and model uncertainties and various scenarios (ex. borehole into the waste area).

Background and Motivation

- We do not currently have the capability to perform fully coupled flow and mechanical deformation simulations.
- As an alternative, we solve the mechanical deformation problem using the same geomechanical model setup while only varying the amount of gas generated.
- From this set of simulations, a response surface (look-up table) for the disposal room porosity as a function of time and amount of gas generated is produced.
- The flow simulator uses interpolation of the response surface porosity data to continuously adjust the disposal area porosity during each simulation.

Background and Motivation

- In this uncoupled approach for the disposal room porosity model, the disposal room is a closed system to fluid flow; there is no flow of brine and gas into or out of the room.
- The porosity we calculate for the look-up table is based on the volume of the room and the amount of solid material initially in the waste. There is no consideration of spatial variation of porosity within the room.
- A rapid change in pressure in the room could produce a instantaneous change in porosity during a flow simulation. We would expect that the porosity would change more gradually if a fully coupled approach were employed.

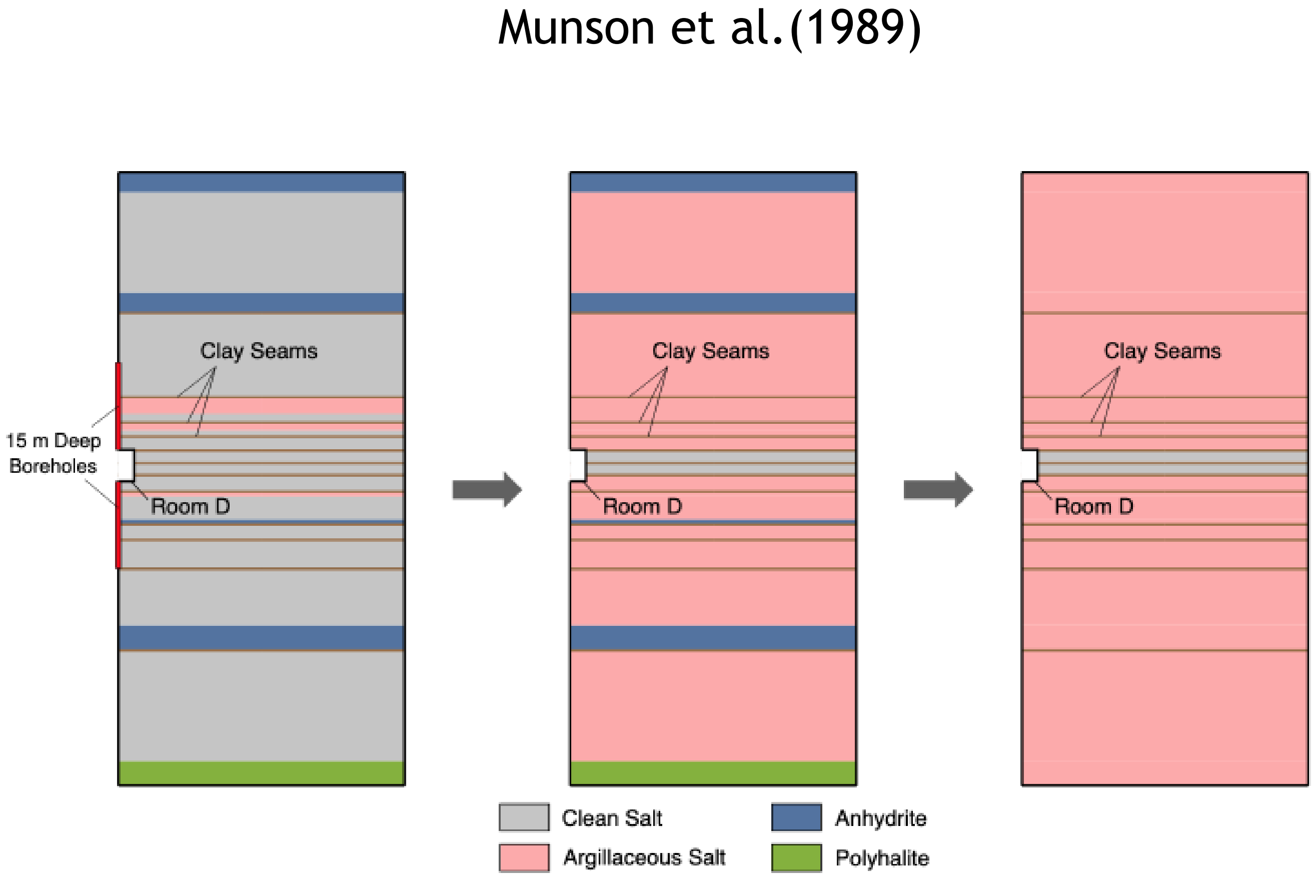
Geomechanical Model

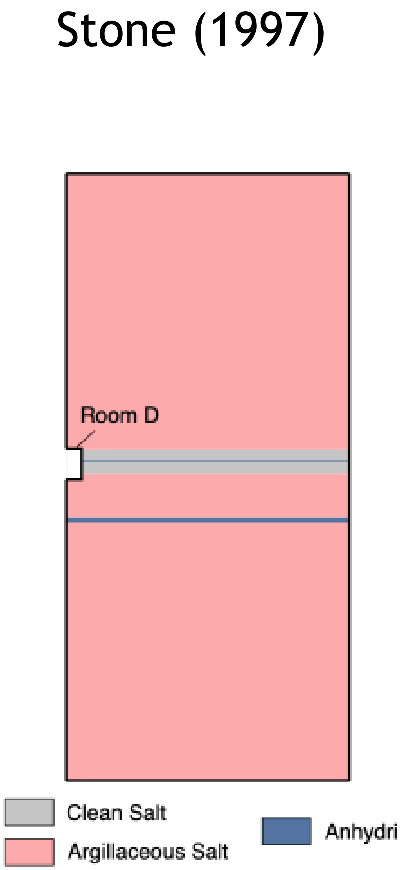
Geomechanical Model

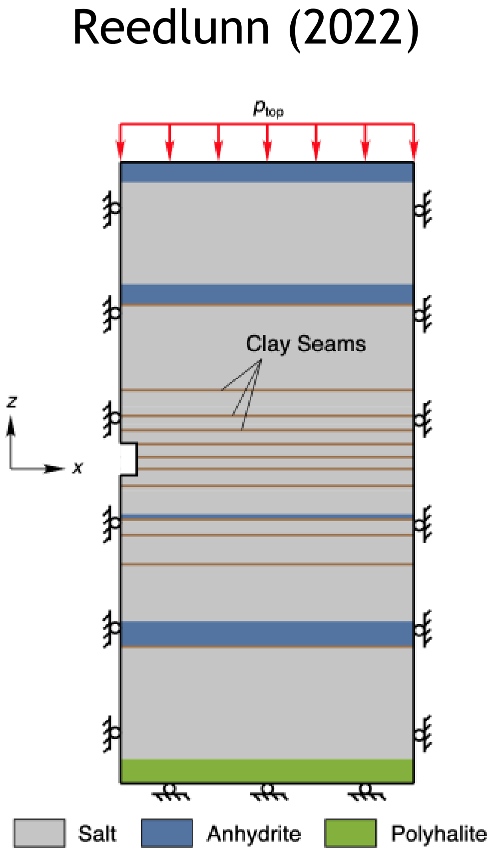
Reedlunn (2022) performed a detailed reinvestigation of experimental room closure measurements and modeling for Experimental Rooms B, D, G, and Q and found some areas that could make the geomechanical model more defensible and produce better agreement with the experimental room measurements.

- Ensured that numerical model solver tolerances, domain size, and mesh discretization provided converged results for horizontal and vertical room closure.
- Use the same stratigraphy as proposed in 1983 for all simulations. Reintroduced the anyhydrite layers, polyhalite, and clay seams to the model that were sometimes ignored.
- Used a single salt type, no distinction between clean and argillaceous salt.
- Introduced a low equivalent stress mechanism to account for pressure solution creep in the MD model.
- Calibrated the Munson-Dawson (MD) model using new laboratory data as much as possible. No parameter adjustment were made to calibrate against the experimental room tests

Geomechanical Model- Comparison of legacy and "new" stratigraphy



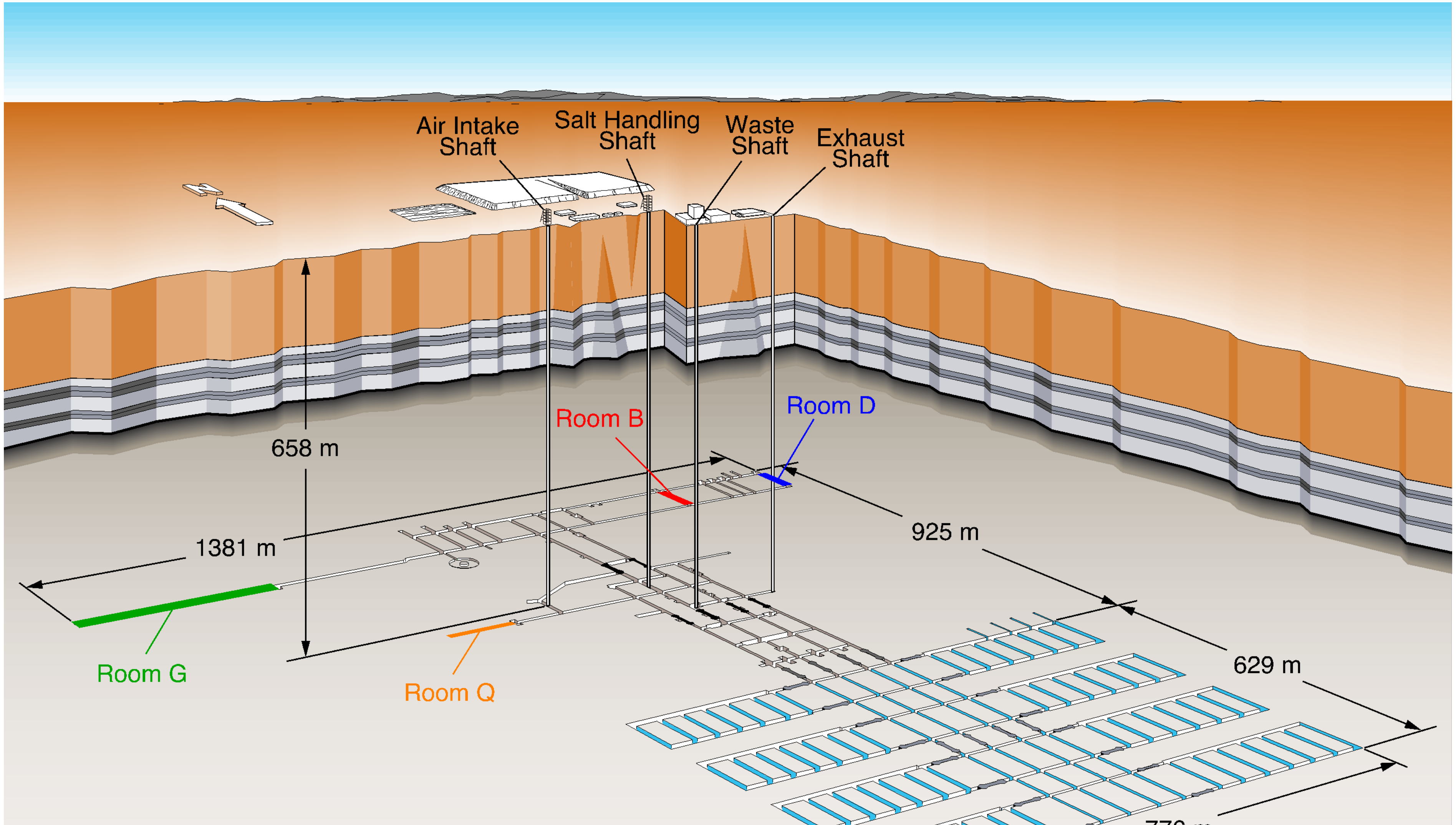




Stratigraphy shown in Stone (1997) was used in last disposal room porosity calculations

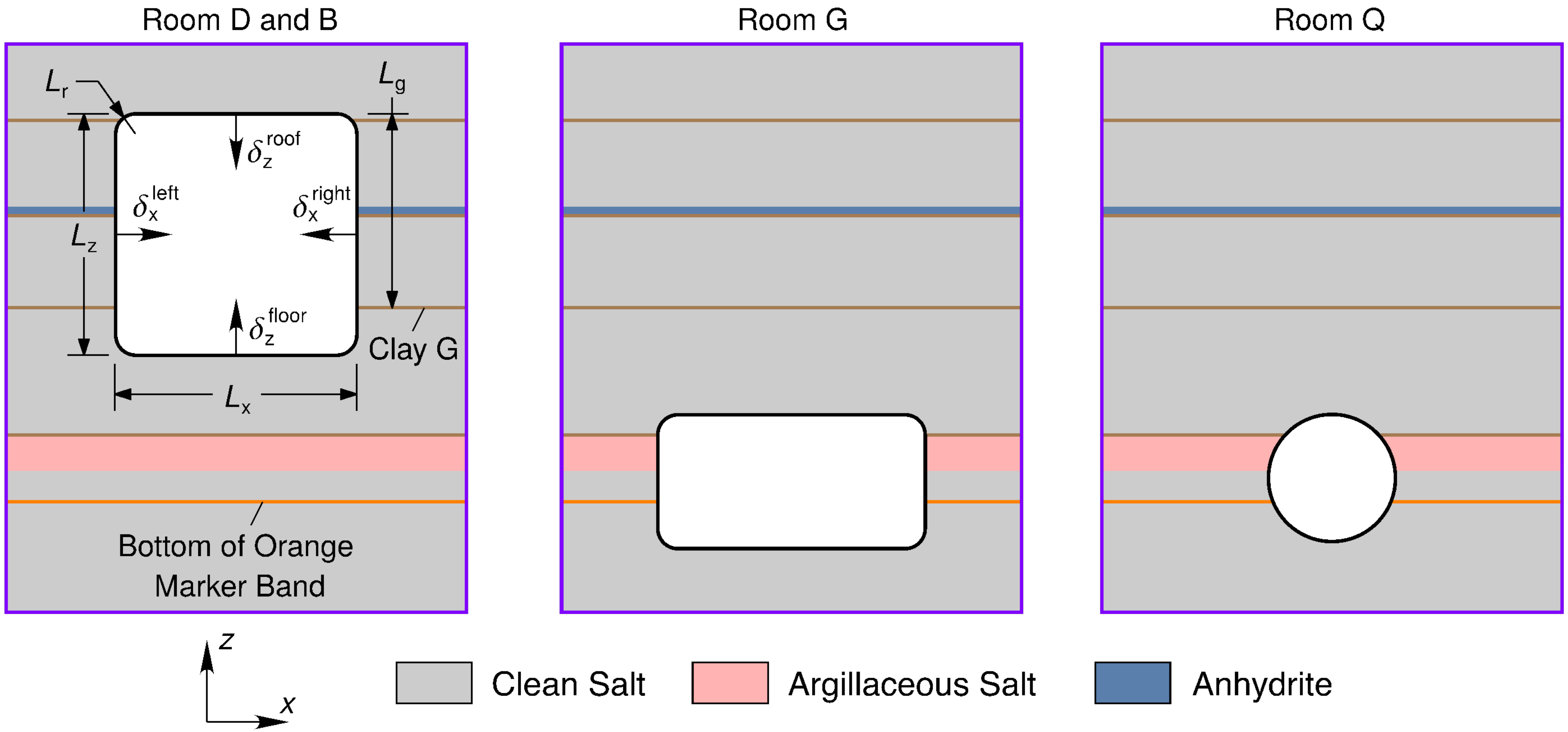
Geomechanical Model

Layout of WIPP and location of selected room closure experiments



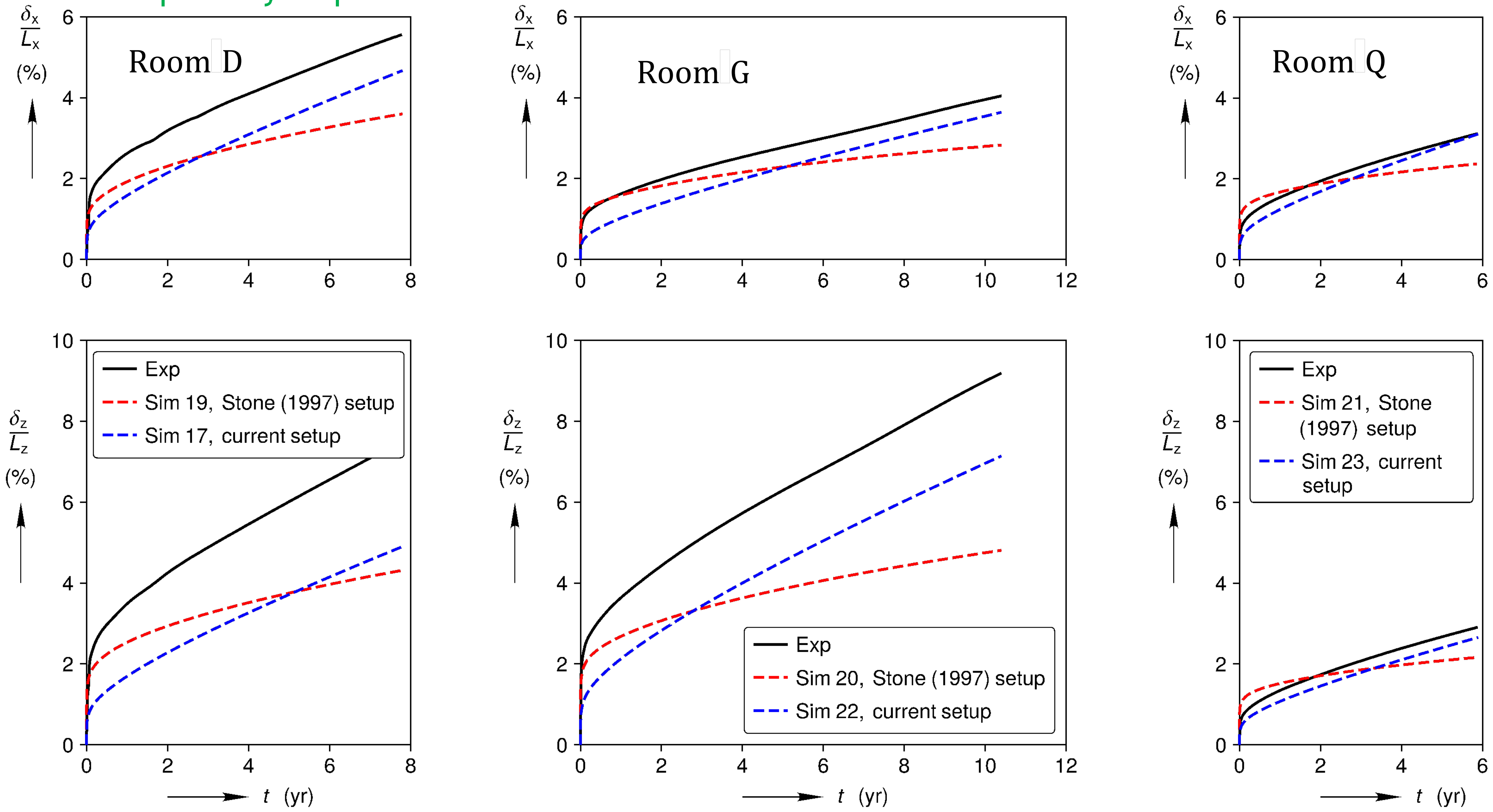
WIPP is approximately 650 m below the surface

Geomechanical Model - Room Closure Experiments



Room Closure Experiments

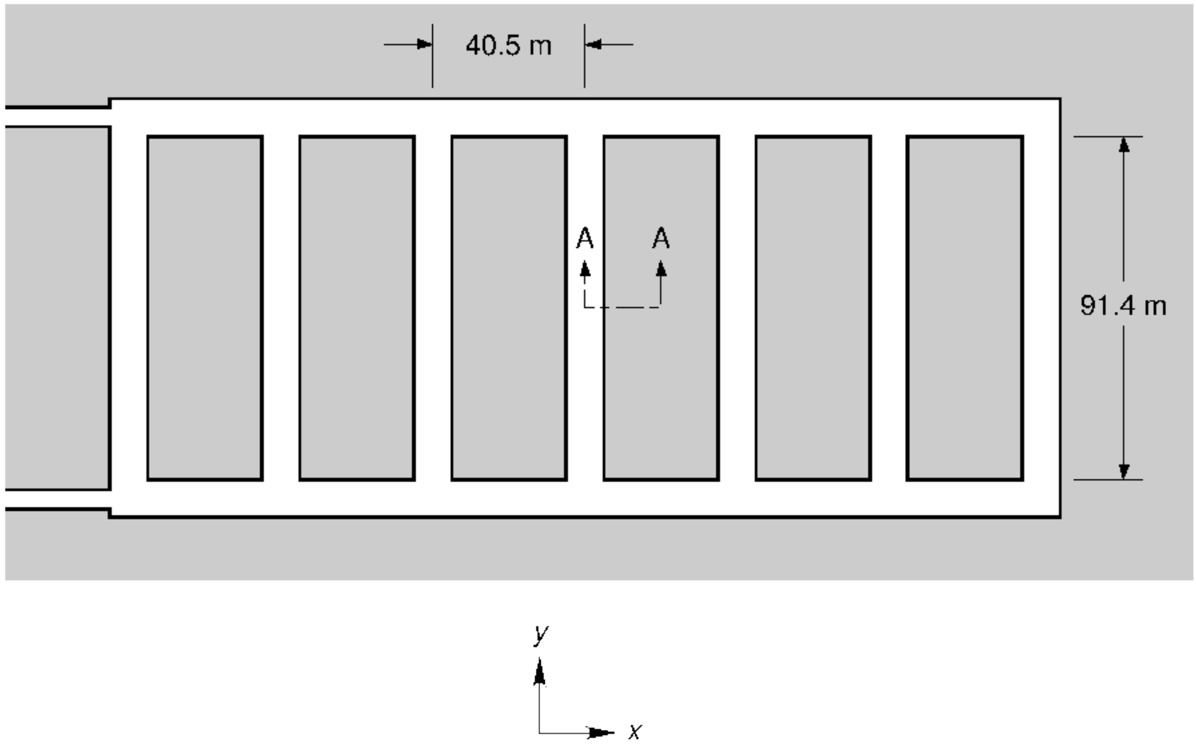
Predictions- Comparison of new geomechanical model results with model used in Stone's 1997 porosity response surface calculations



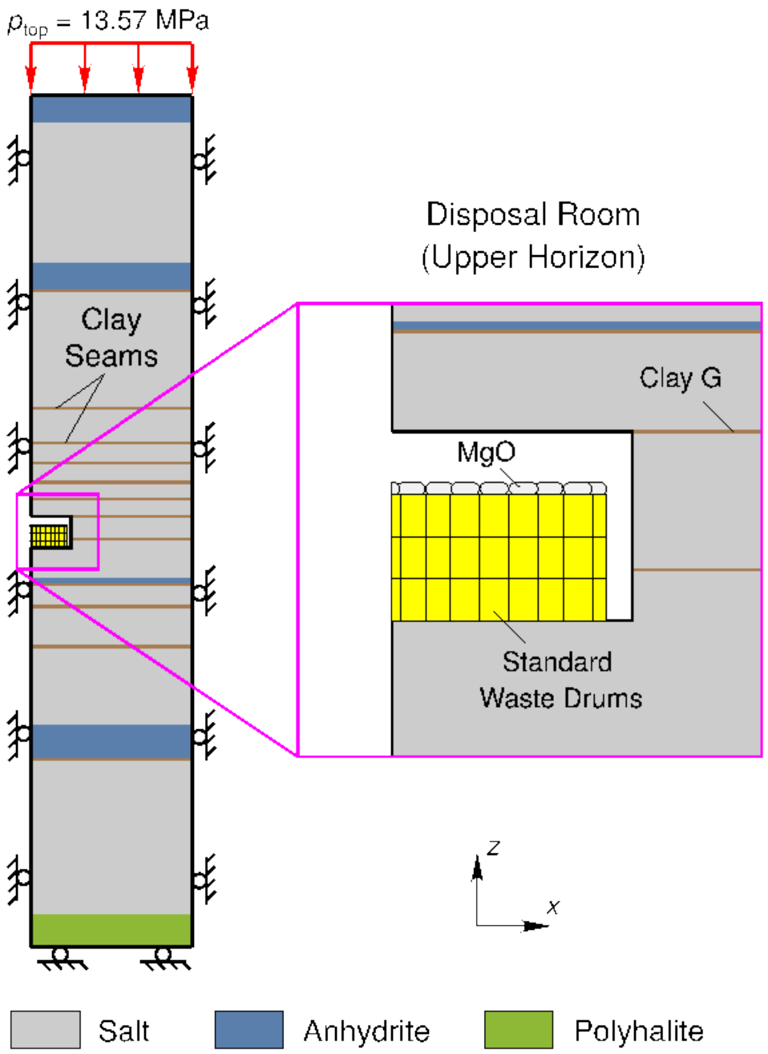
Geomechanical Model- Assumptions and Simplifications

Plane strain model of an infinite array of rooms filled with waste adequately represents the average drift porosity at WIPP.

Plan View of a Panel

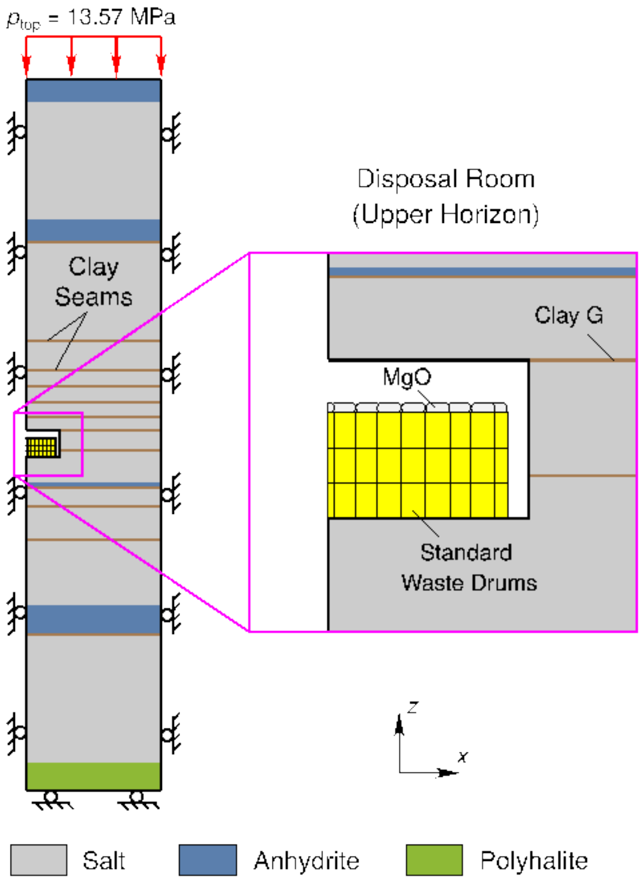


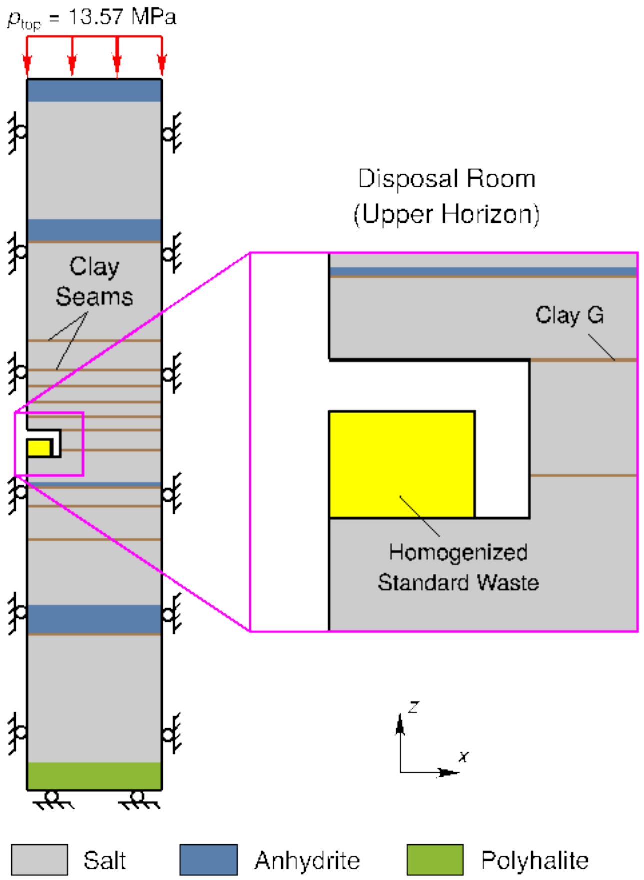
Section A-A



Geomechanical Model- Simplifications

- Rooms are filled with standard 55-gallon waste containers and treating them as a homogenous continuum adequately captures the behavior of discrete containers.
- MgO sacks have negligible effect on room porosity so they are not included.
- No fracture-damage or rock fall effects included in room porosity modeling.





Gas Generation Model

Gas Generation Model

- Gas generation in the repository is from anoxic corrosion of iron, biodegradation of cellulosics, plastics and rubbers, and radiolysis of brine.
- Compared to the legacy gas generation model (~1997), the new model (King, 2021) incorporates these changes-
  - Increased iron inventory
  - Increased iron corrosion rate
  - Decreased microbial gas generation rate
  - Radiolysis of brine
- The biggest change from legacy models is the inclusion of radiolysis. Gas generation as a result of radiolysis continues for the entire regulatory period of the repository (10,000 years) because the radionuclide inventory will not be exhausted and brine can flow into the repository from the surrounding rock.
- The maximum gas pressure is not limited in the disposal room porosity model. The gas pressure is calculated using the ideal gas law and depends on the number of moles of gas and the current room volume.

Gas generation models- Repository Panel Scale

- New gas generation model (**red**) vs. legacy gas generation model model (**blue**)
- New model: increased iron corrosion rate, increased iron inventory, decreased microbial gas generation rate and added brine radiolysis source (King, 2021, ERMS 575793)

Legacy Gas Generation

Bio- 0 - 550 yrs

Corrosion- 0 – 1050 yrs

Radiolysis- N/A

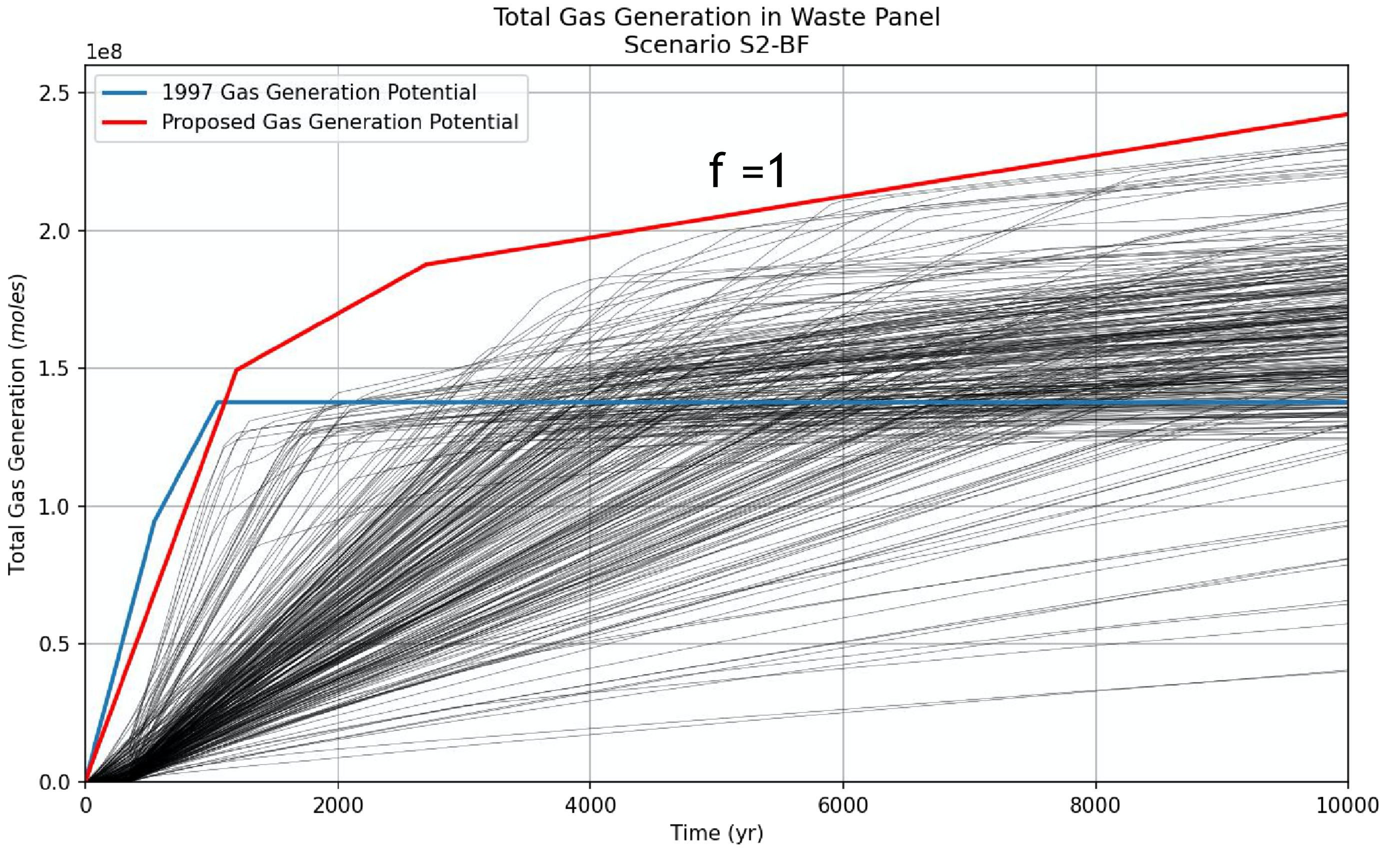
New Gas Generation

Corrosion- 0 - 1200 yrs

Bio- 0 - 2700 yrs

Radiolysis- 0 – 10K yrs

We run mechanical simulations with different values of f to account for the effect of gas generation uncertainty on room porosity

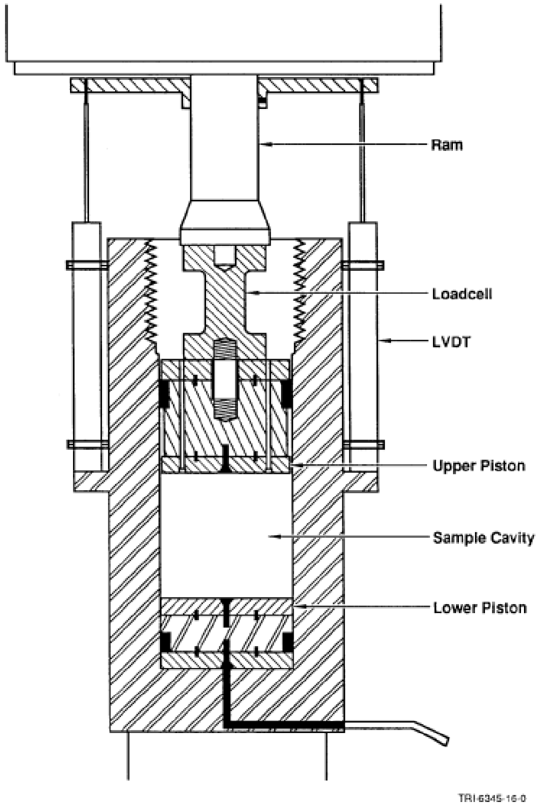


Waste Container Experiments and Model

Waste Container Experiments and Model

Original Container Tests (Butcher et al., 1991)

- Surrogate Non-degraded Waste – assumed waste containers were **nearly filled to capacity**
- Used mixture rule to determine the composite response of waste
- Two types of tests
  - Uniaxial strain loading on material constituents – performed in oedometer
  - Uniaxial stress tests on waste filled, 55-gallon drums
    - No lateral strain measurements – assumed to be minimal



From Butcher et al., 1991

Waste Container Experiments and Model

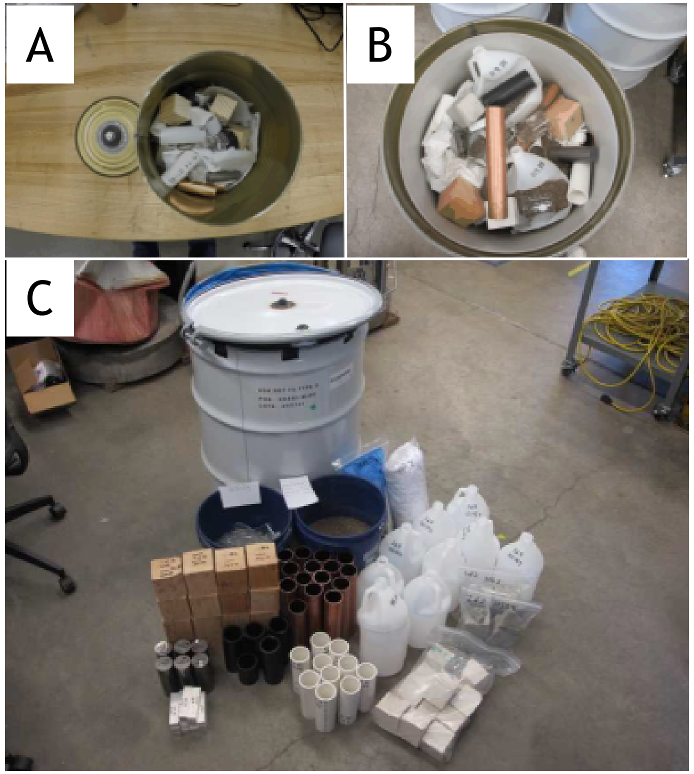
New Tests

An updated dataset is available from new container tests performed by Broome et al., 2016

- Based on CRA 2014 Inventory
- Surrogate Non-Degraded Waste – only filled to ~2/3 capacity (initial solid volume fraction = 0.175)
- Uniaxial (UC), Hydrostatic (HC), and Triaxial (TXC) Compression datasets
- Measured axial and volumetric strains so lateral strain can be computed
- Two sizes of waste containers
  - 55 gallon drum (uniaxial and hydrostatic compression tests only)
  - ¼ -scale drum (#12 food can)
- Loading axial strain rate of $1x10^{-4}$ s^{-1}

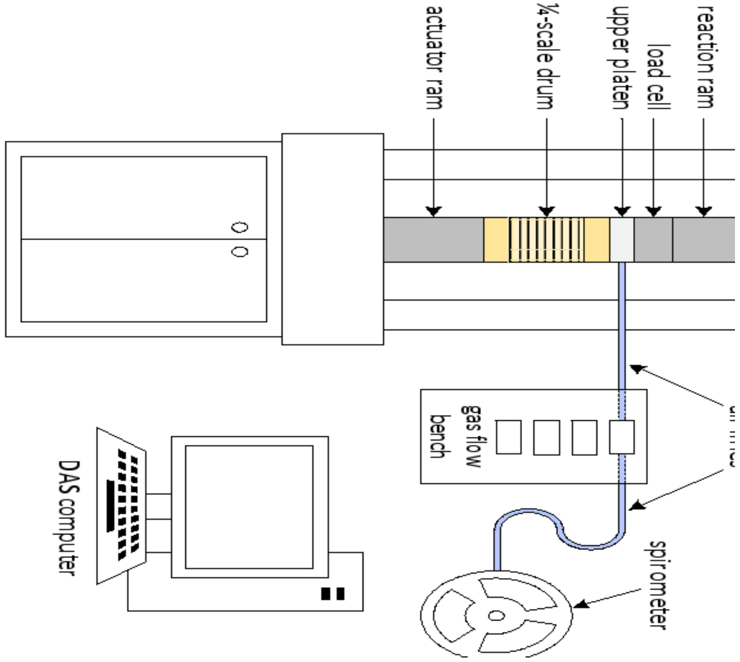
Additional uniaxial compression tests performed by Courtney Herrick and Michael Hileman in 2021-2022

- Three strain rates
  - $1.0x10^{-5}$ s^{-1}
  - $2.1x10^{-6}$ s^{-1}
  - $1.0x10^{-7}$ s^{-1}



A) ¼-scale (#12 food can), B) full-scale (55 gallon drum) Waste containers loaded with surrogate waste ready for lid installation. C) full-scale sample with surrogate waste. (Figure from Broom et al. 2016)

Pictorial Summary of Uniaxial Test



Schematic for Uniaxial Compression Test

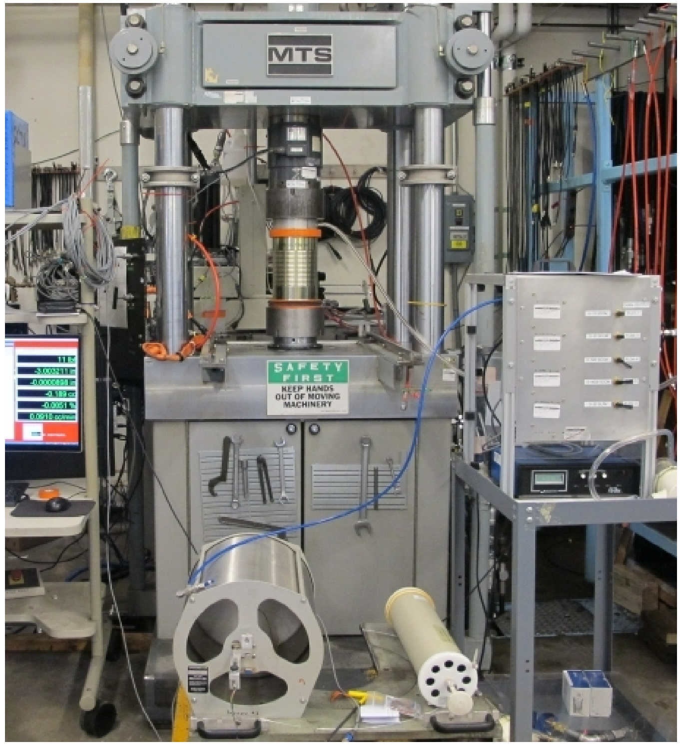
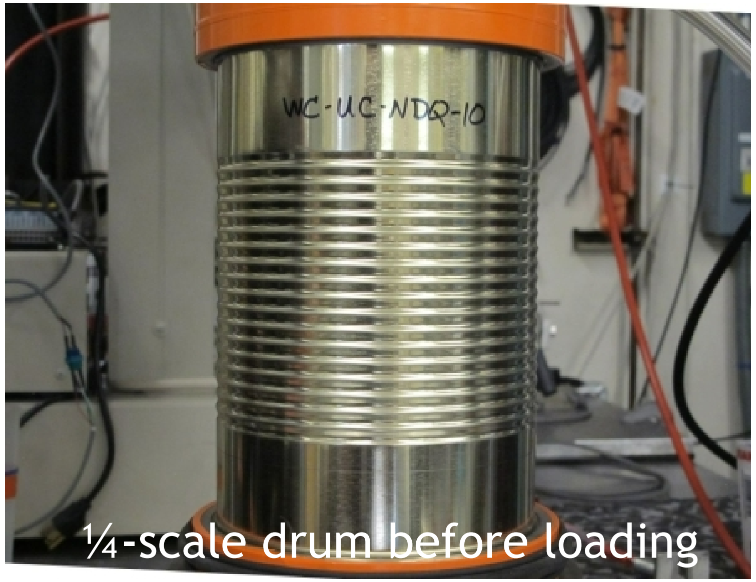
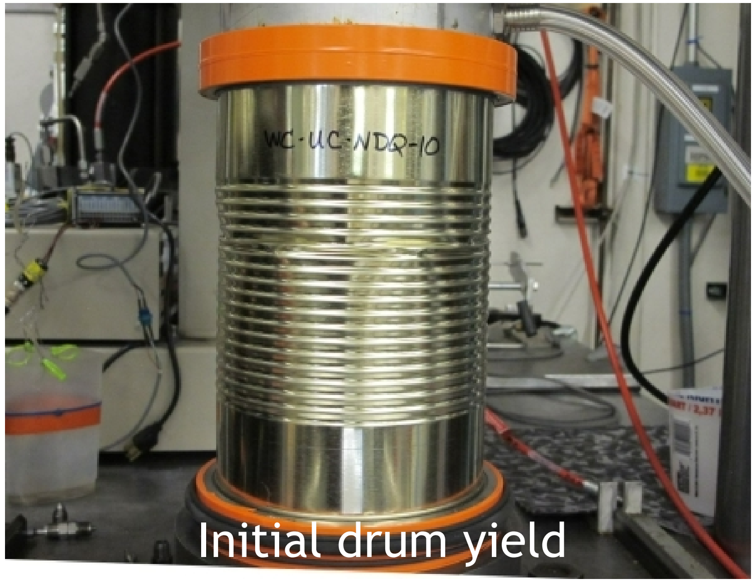


Image of Uniaxial Compression Test



¼-scale drum before loading



Initial drum yield

Equation used to convert measured volumetric and axial strains to lateral strains.

$$\sqrt{\frac{\epsilon_{vol}+1}{1+\epsilon_z}} - 1 = \epsilon_x$$

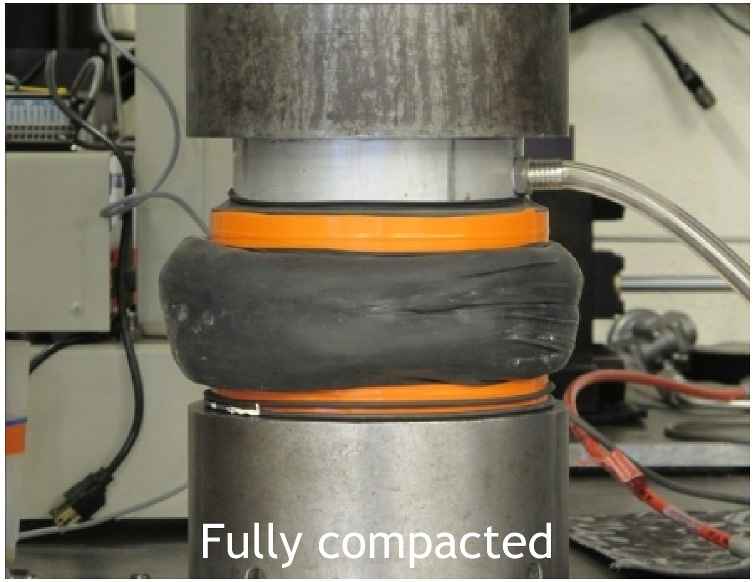
Pictorial Summary of Uniaxial Test (cont.)

About 40% crushed


Drum breech

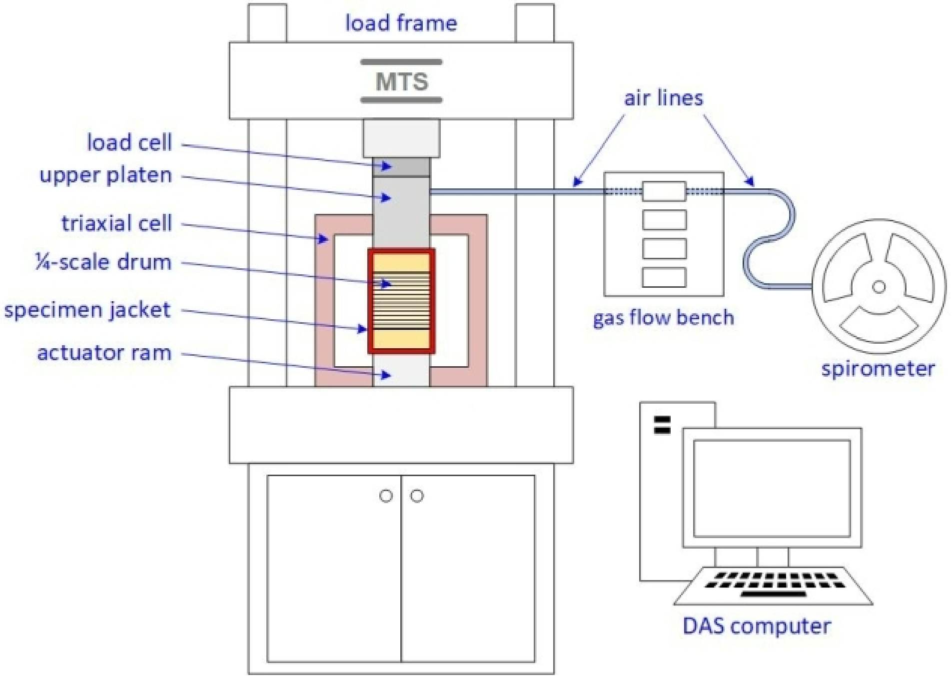

Wrapped in modeling clay


Secondary balloon seal

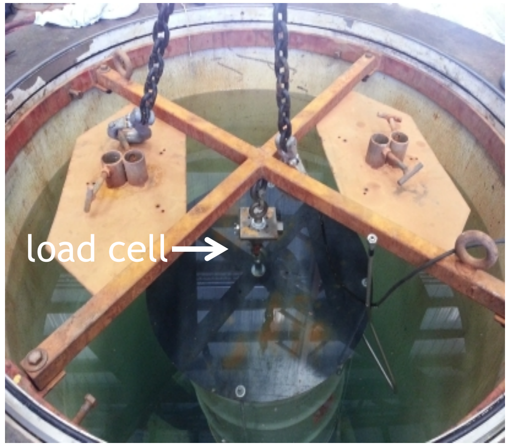

Fully compacted

Final state of drum

Hydrostatic and Triaxial Compression Tests



Schematic for hydrostatic and triaxial compression Test



Hydrostatic compression test for full-size waste drums

Pressure Vessel and Load-frame for ¼ scale waste drum hydrostatic and triaxial compression tests

Hydrostatic and Triaxial Compression Test Results

Hydrostatic compression test results --
¼-scale waste container

Hydrostatic compression test results –
Full-size waste drum

Triaxial compression test results -- ¼
-scale waste container

Waste Container Experiments and Model

Soil and Foam Model (SAF) was used in previous disposal room porosity simulations

- Elastic behavior - Isotropic (constant bulk and shear moduli)
- Inelastic (plastic) behavior defined by "uncoupled" 2 surface model :
  - Non-hardening shear surface defined in terms of 2 stress invariants (Drucker-Prager)
  - Strain hardening "cap" behavior defined using a table of pressure- volume strain data

- Assumed that the data from the drum/waste testing are representative of uniaxial stress conditions

- **Calibrated as if the stress in the lateral directions was zero in uniaxial strain tests which allowed the conversion of axial stress-axial strain to pressure-volume strain.**

SAF Issues

- The model behaves according to theoretical formulation but produces

Waste Container Experiments and Model

Foam Damage Model (or Unified Creep Plasticity Damage Model)

- Developed at SNL by Mike Nielsen and others (Nielsen et al., 2015)
- Describes the mechanical response of foams to large deformation
- Significant increase to load resistance as porosity decreases
- Lateral expansion can be made to vary with porosity
- Can incorporate strain rate dependence

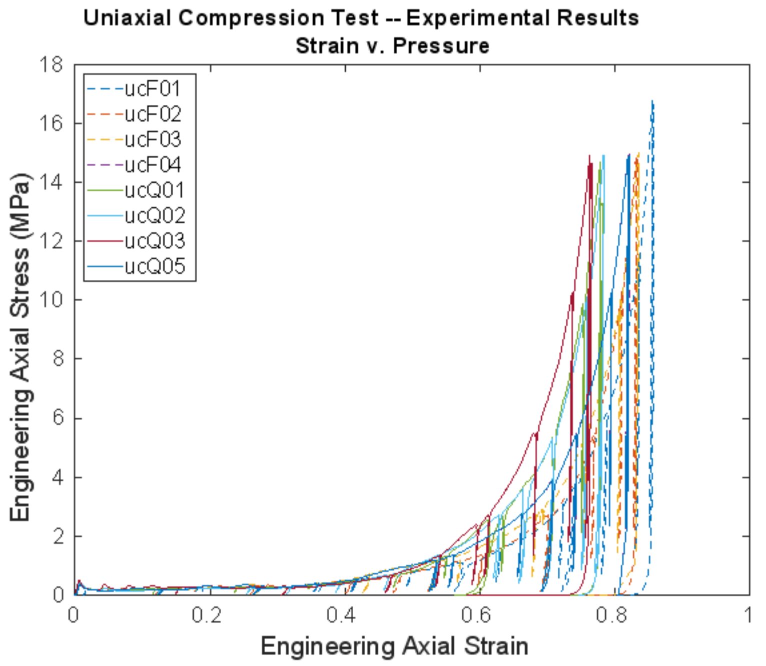
Waste Container Experiments and Model

Foam Damage model

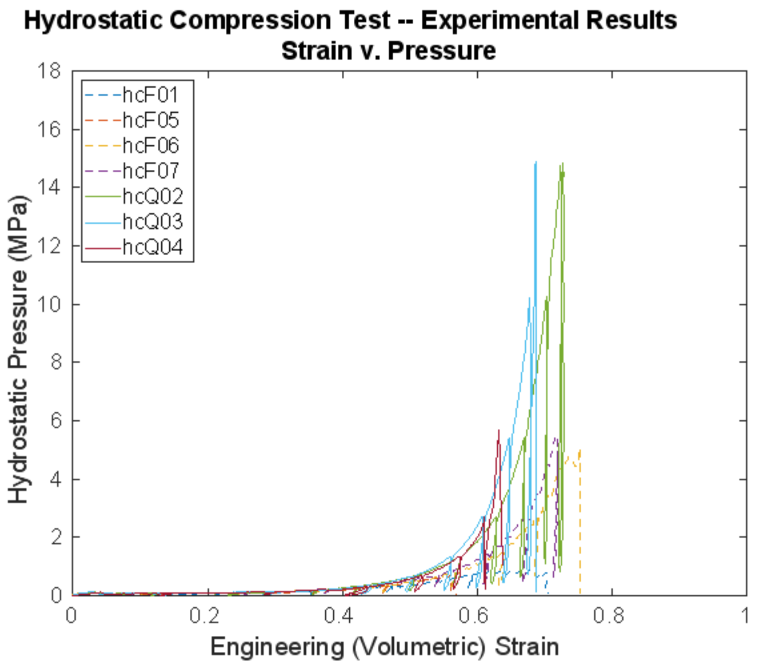
- Elastic response is assumed to be linear and isotropic
- Yield surface is ellipsoidal and centered about the hydrostat defined by
  - $\varphi = \frac{\bar{\sigma}^2}{a^2} + \frac{p^2}{b^2} - 1.0 = 0$
  - a, b are deviatoric and volumetric strengths and are functions of the porosity (or solid volume fraction)
  - $\bar{\sigma}$ is von Mises effective stress
  - p is pressure or mean stress
- Uses Perzyna-type formulation for rate dependence
  - $\dot{\boldsymbol{\varepsilon}}^{in} = \begin{cases} \lambda \mathbf{g} = \boldsymbol{e}^h \left\langle \frac{\boldsymbol{\sigma}^*}{\boldsymbol{a}} - \mathbf{1} \right\rangle^{\boldsymbol{n}} \mathbf{g} & when \frac{\boldsymbol{\sigma}^*}{\boldsymbol{a}} - 1 > 0 \\ \mathbf{0} & when \frac{\boldsymbol{\sigma}^*}{\boldsymbol{a}} - 1 \leq 0 \end{cases}$
- For associated flow, **g**, which defines the inelastic flow direction, is normal to the yield surface
- Overstress model because inelastic strain is power-law function of the overstress

Waste Container Experiments and Model

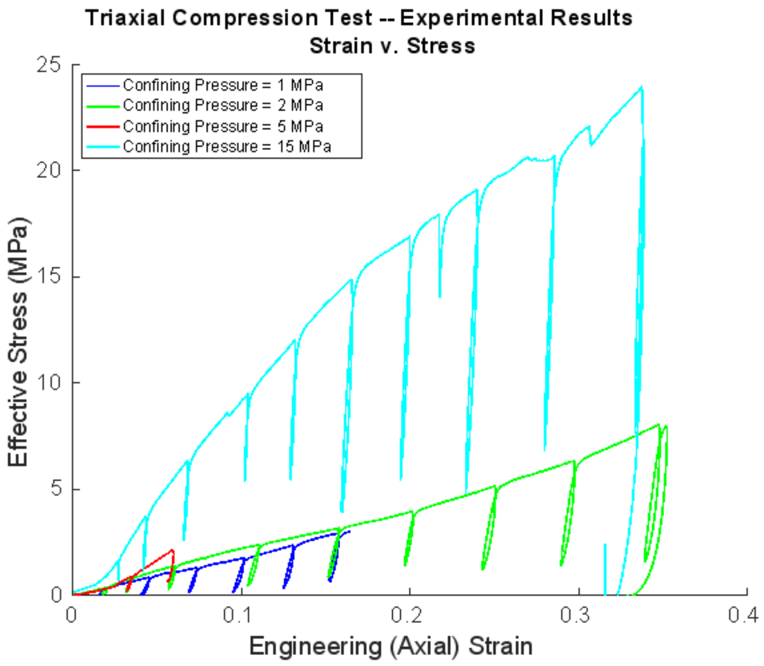
Experimental results from uniaxial compression, hydrostatic compression, and triaxial compression tests



Uniaxial stress tests



Hydrostatic compression tests



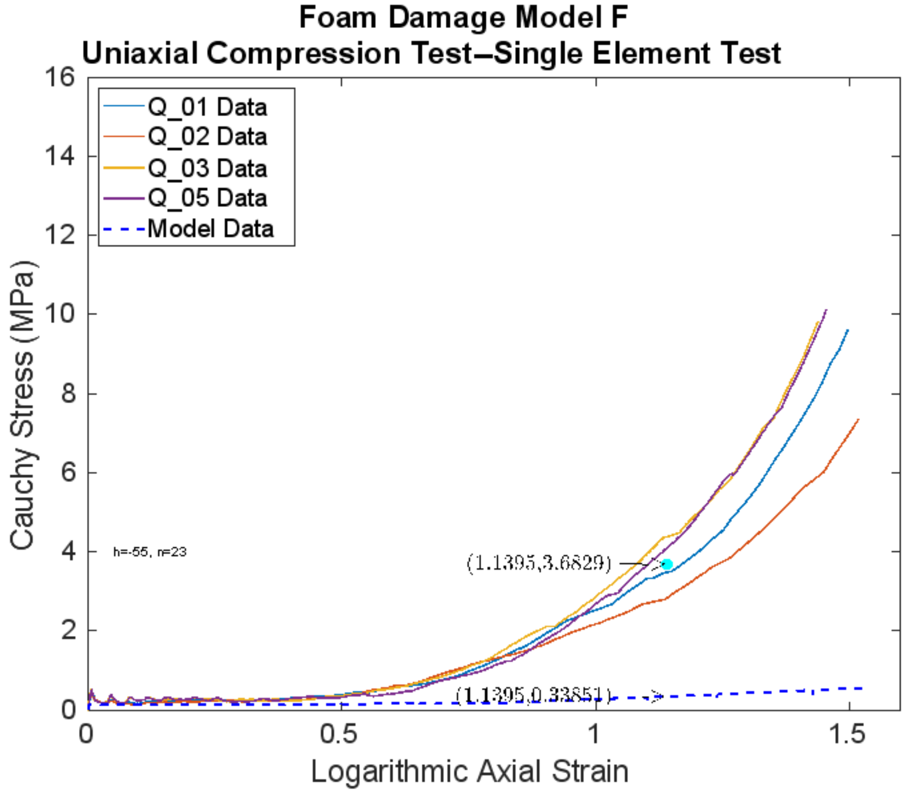
Triaxial compression tests

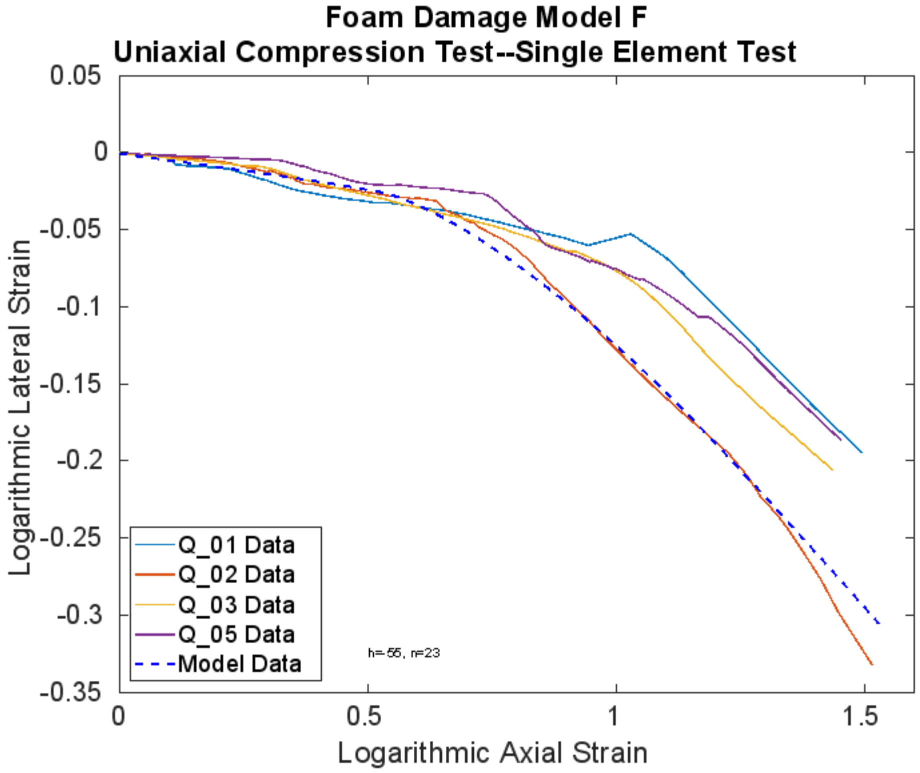
(from Broome et al., 2016)

(Triaxial compression tests were only performed using quarter-scale waste containers.)

Waste Container Experiments and Model

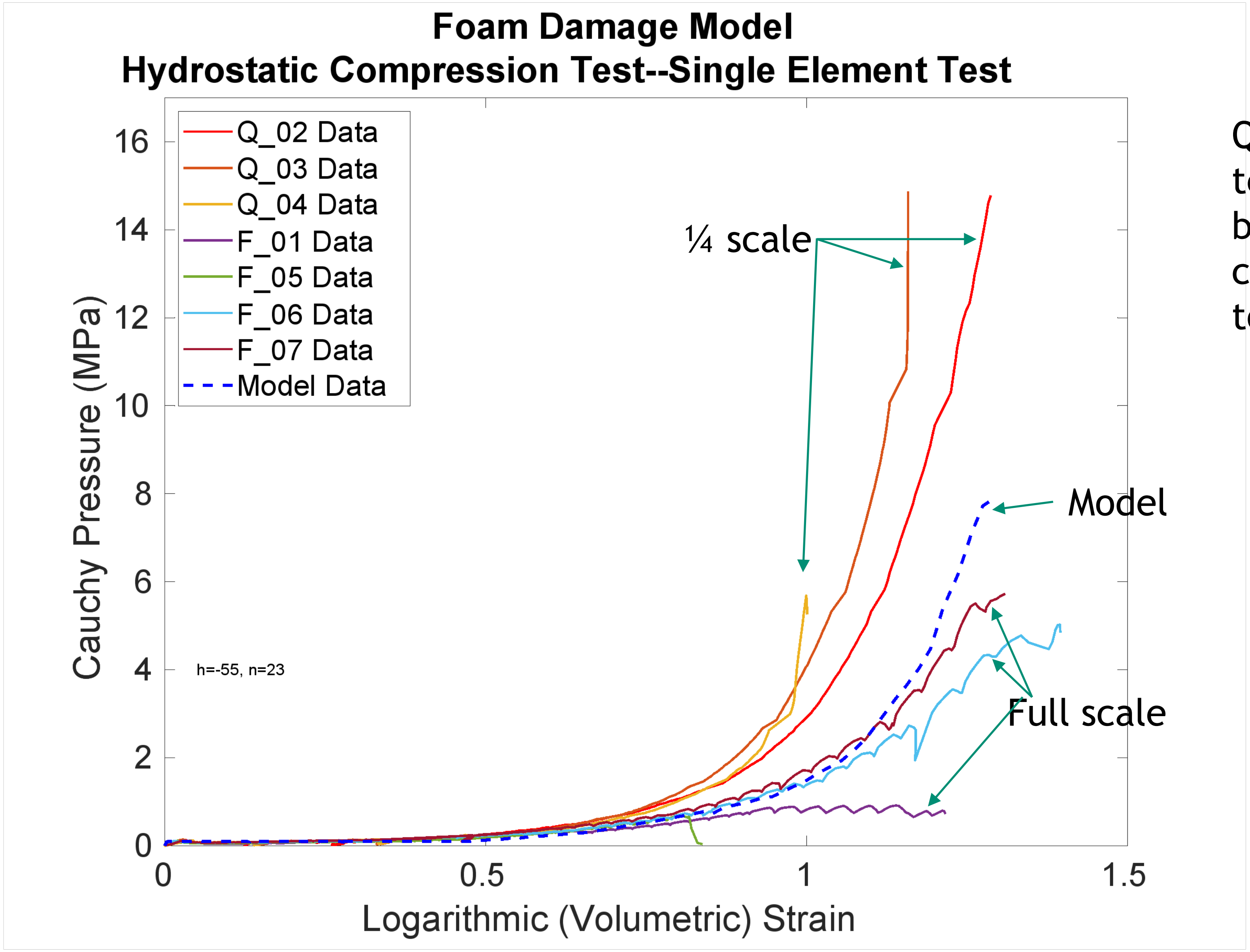
Uniaxial Compression Test





- Poor fit to uniaxial stress test data. In disposal room simulations uniaxial stress takes place early in room closure model; therefore; comparison to unconfined compression results less important

Waste Container Experiments and Model

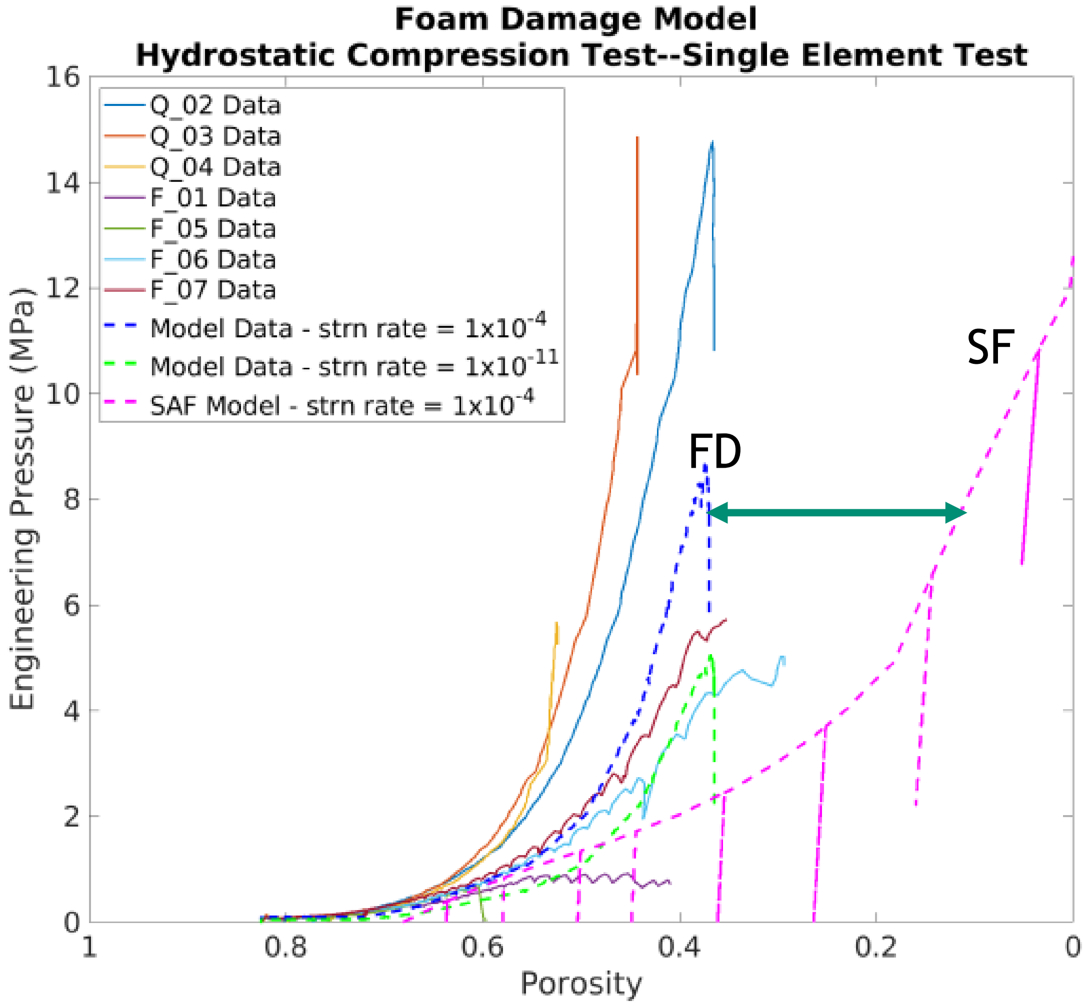


Quarter scale drum tests show stiffer behavior in hydrostatic compression compared to full size drum tests

Waste Container Experiments and Model

Comparison of Foam Damage Model to Soil and Foam Model in **hydrostatic** compression

The Foam Damage model becomes very stiff at a porosity of ~0.40 and further reduction in porosity is small with increasing pressure. The soil and foam model continues to undergo porosity reduction as the pressure increases.



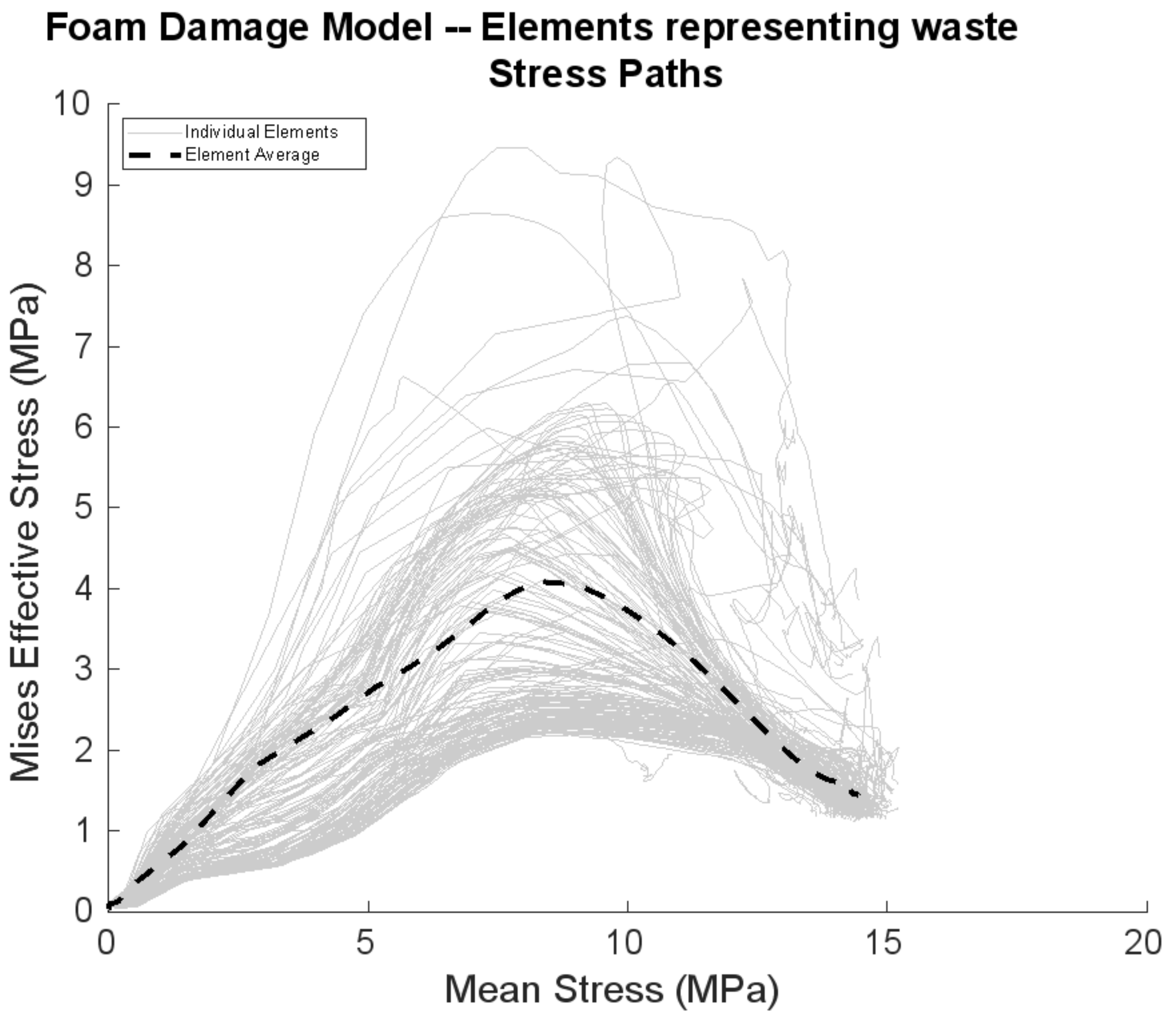
Waste Container Experiments and Model

- Uniaxial stress loading in disposal room simulations takes place early in process, therefore the simulation comparison to experimental results of the uniaxial compression tests is of lesser importance

- The disposal room simulations seem to indicate that the behavior of the waste canisters tend to evolve to a more hydrostatic condition.

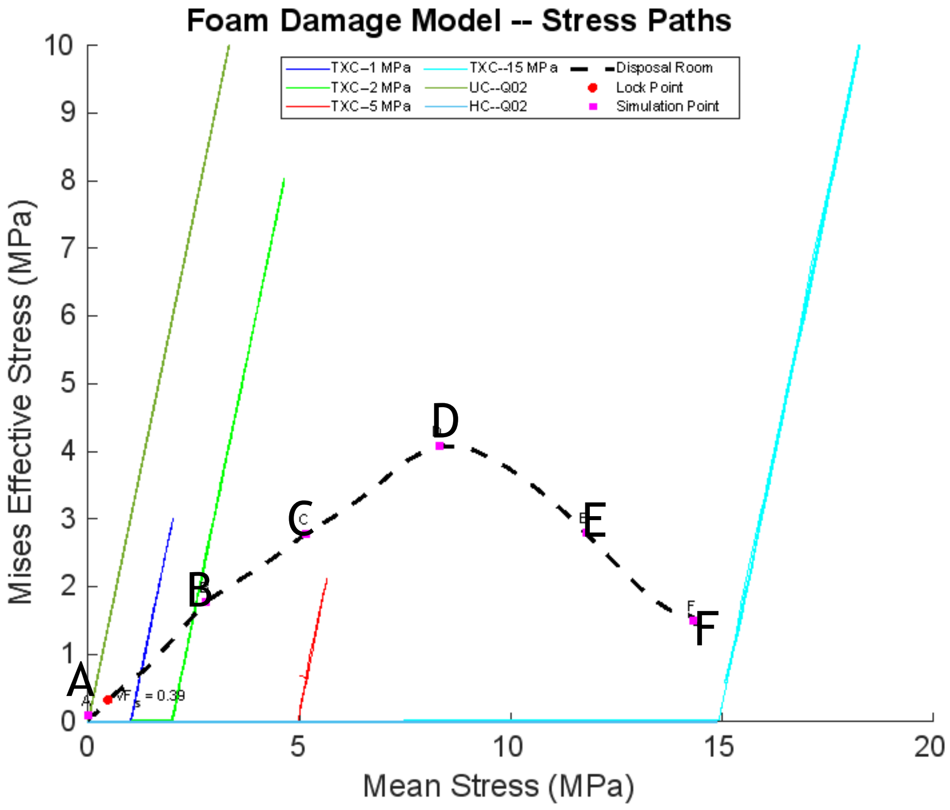
- Stress path from disposal room calculation is computed as an average of all the elements in the waste container block.

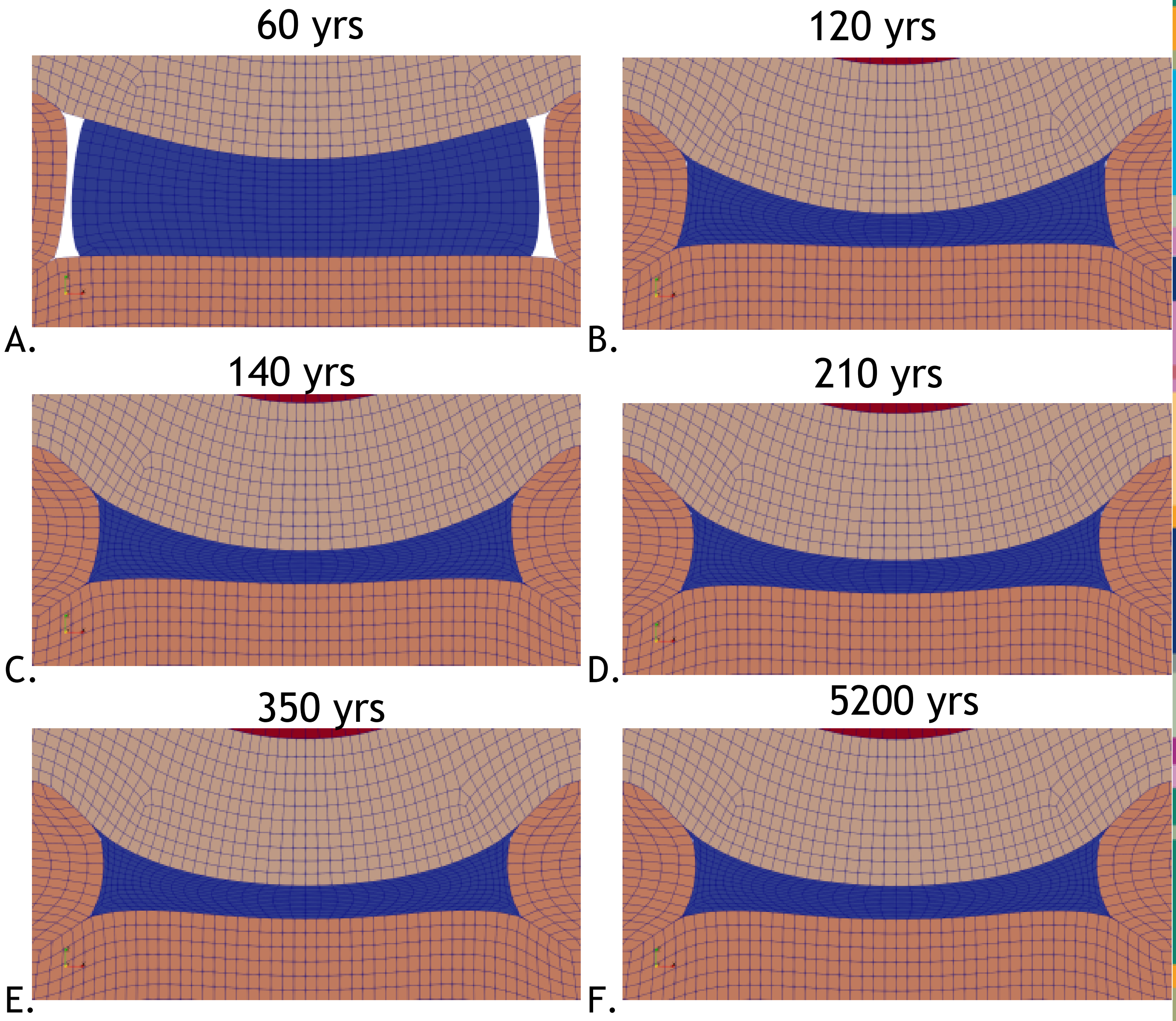
Disposal Room Stress Paths



Room Disposal Simulation Stress Paths

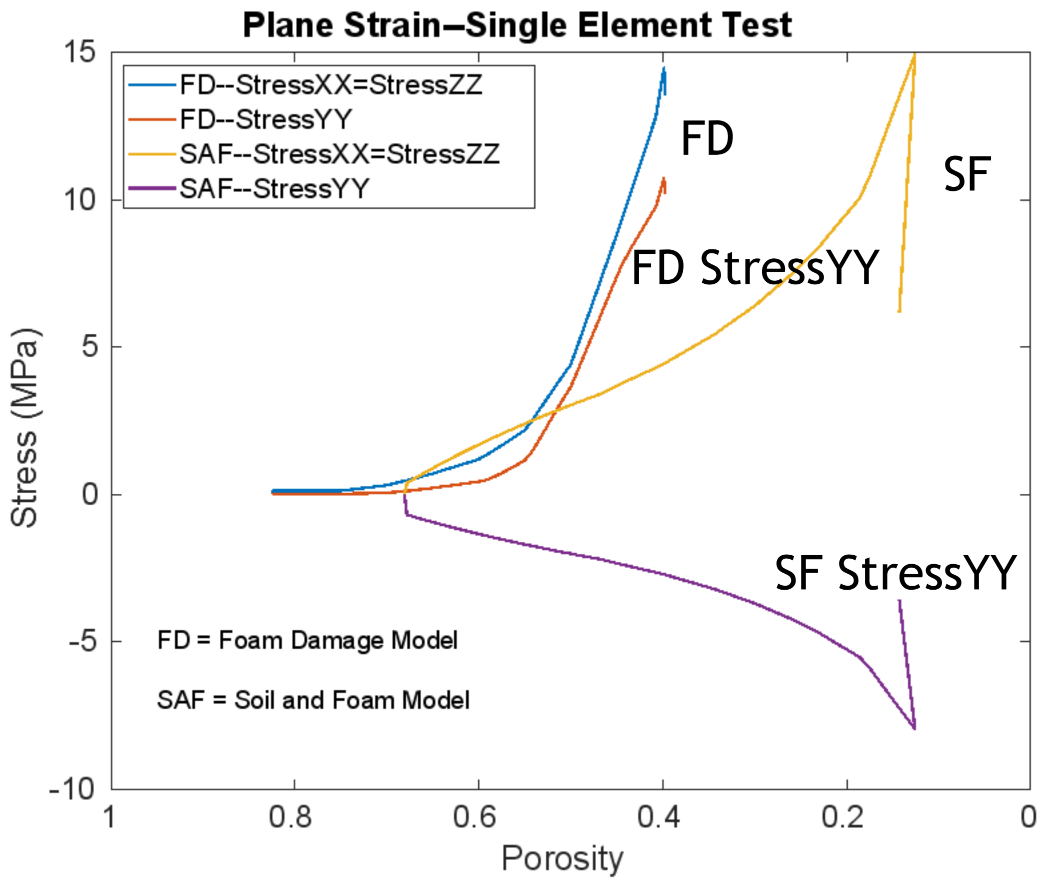
As indicated by the disposal room simulations, the behavior of the waste canisters tend to evolve to a more hydrostatic condition.





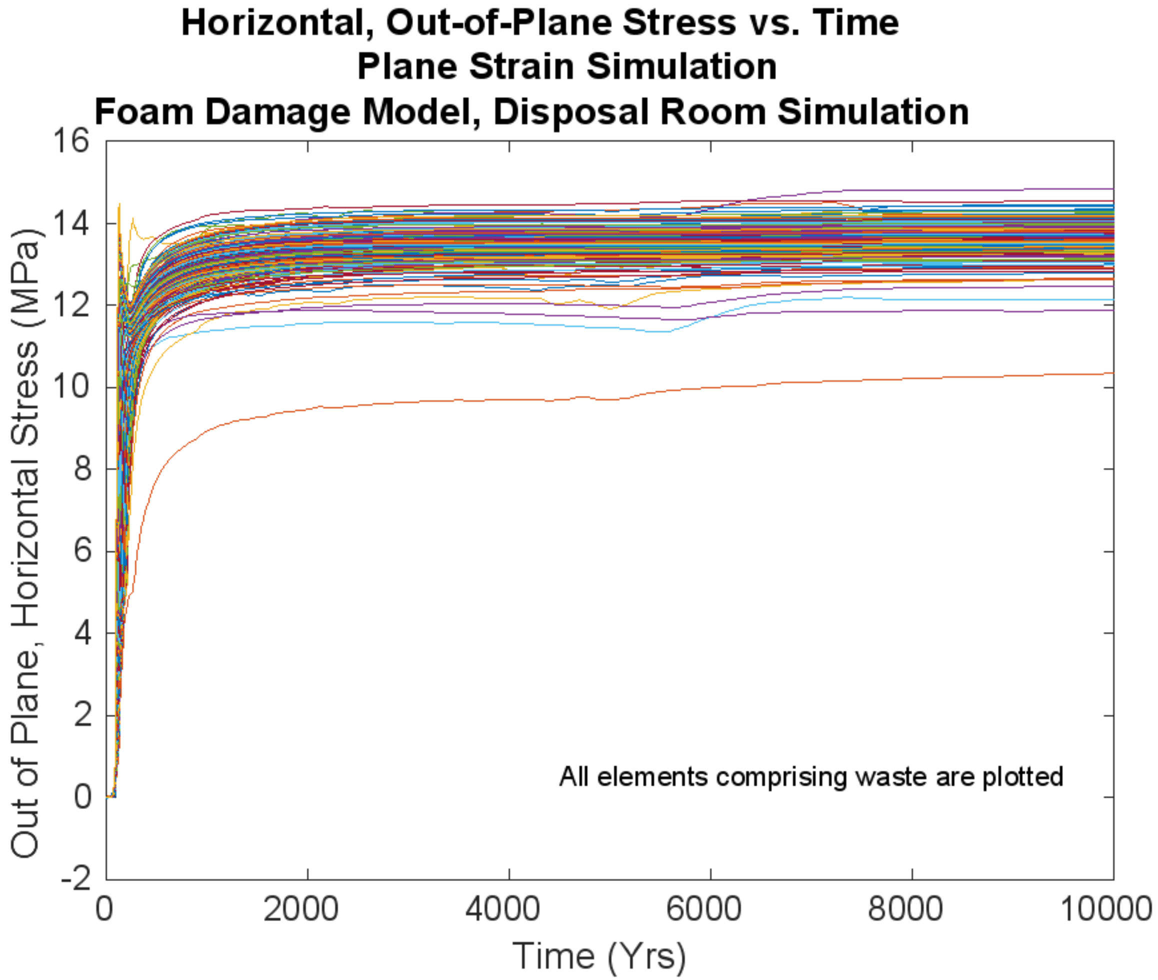
Waste Container Experiments and Model Plane Simulations

Foam Damage Model Single Element Plane Strain Test Results



StressYY is out of plane component- tension for soil and foam (SF)

Foam Damage Model Disposal Room Simulation -- Plane Strain Test Results



The StressYY (out-of-plane) remains compressive (positive) for all of the elements in the waste block.

Disposal Room Porosity Model Results

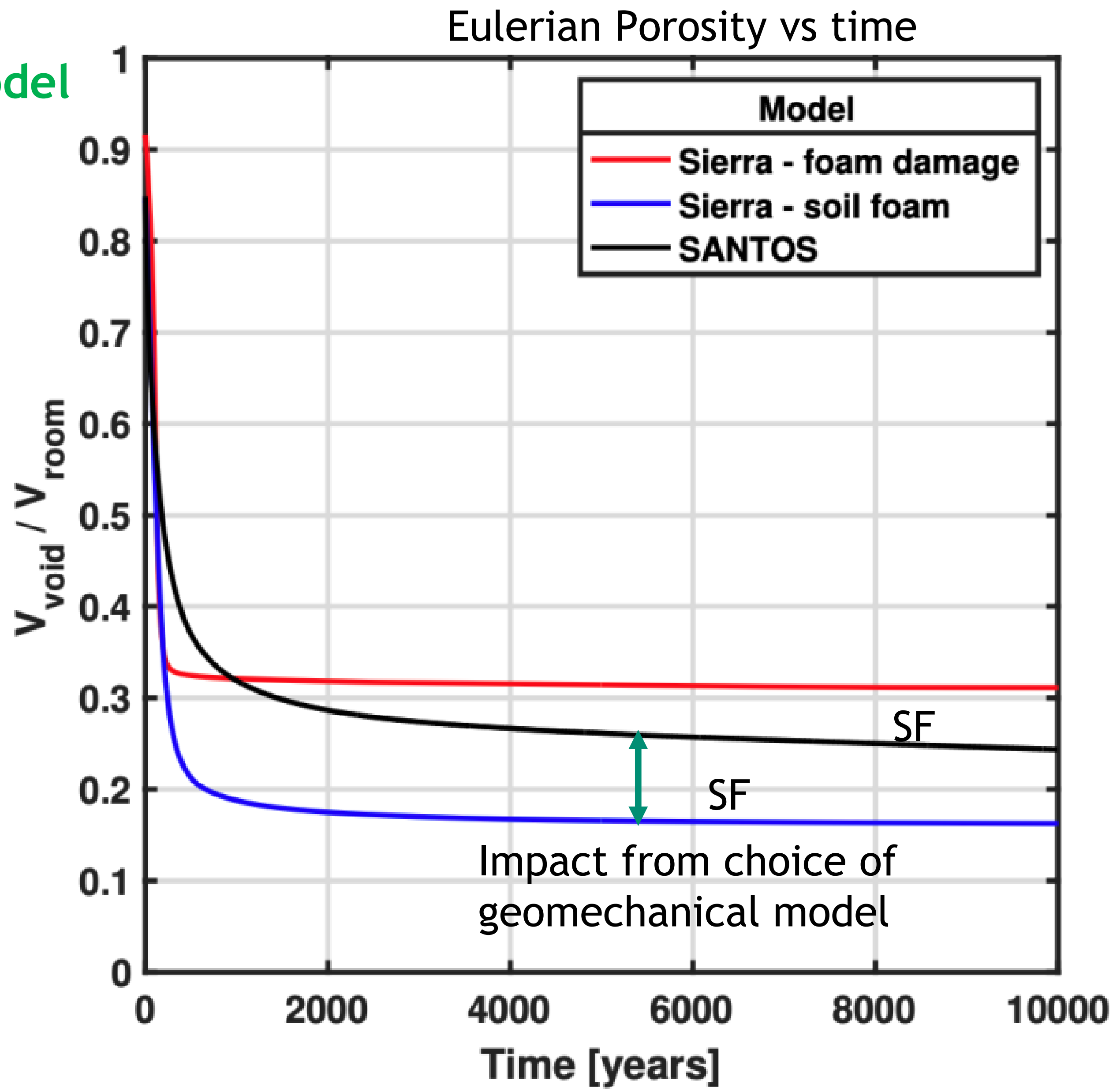
Disposal Room Porosity Model Results

Examine the impact of the geomechanical model while using legacy waste model (no gas generation: f=0)

3 Cases:

- New Geomechanical Model
  - Foam damage model
  - Legacy soil and foam model
- Legacy geomechanical model (SANTOS)
  - Soil and foam

The difference in porosity history due solely to the geomechanical model changes can be seen by comparing the blue and black curves. The porosity at 10K years in the new model is 0.16 while the legacy model is 0.24. This is primarily due to the addition of the low stress creep mechanism.

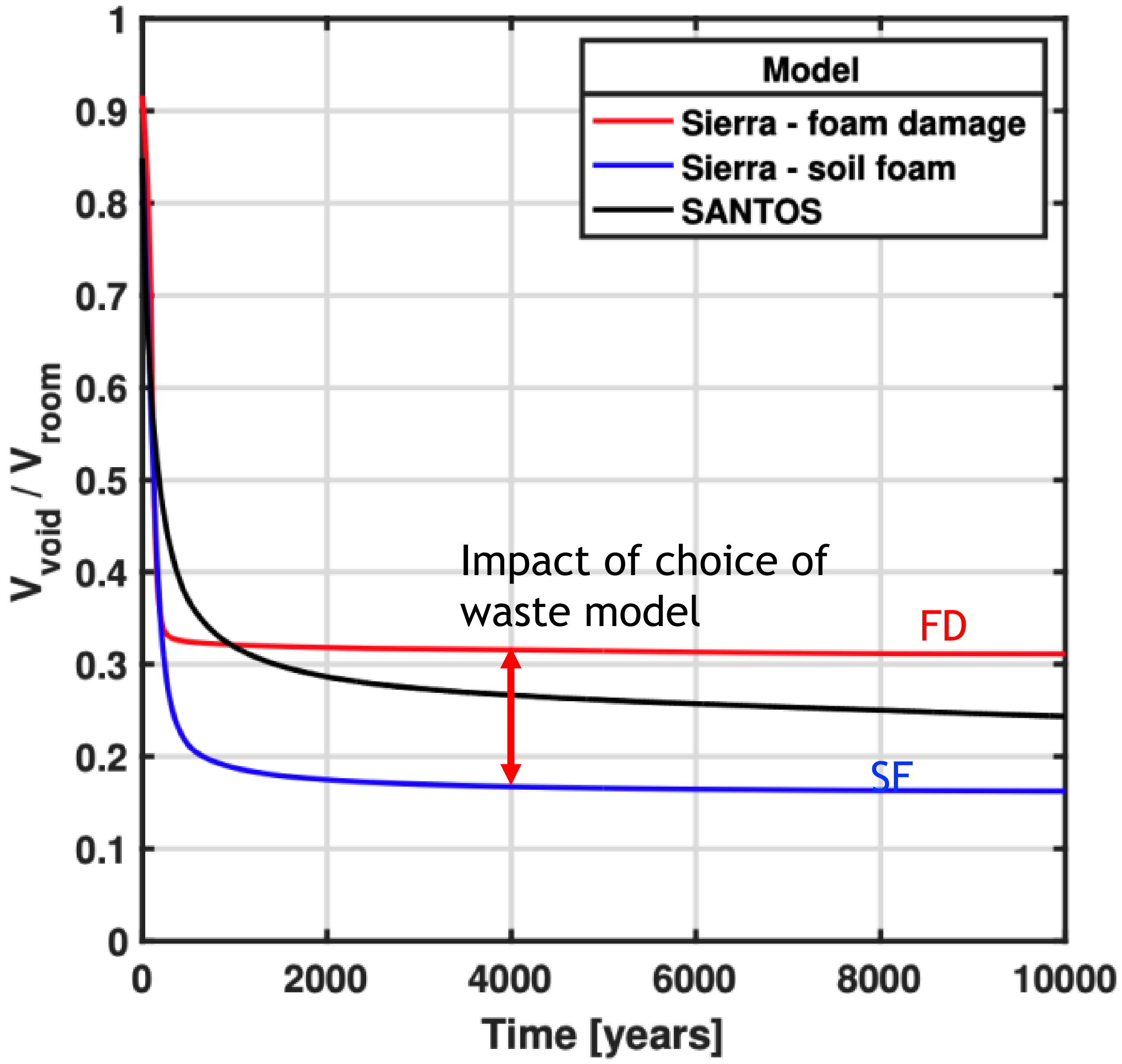


Disposal Room Porosity Model Results

Examine the impact of choice of waste model while using the same (new) geomechanical model (no gas generation: f=0)

The new waste model stiffens up much sooner that the legacy soil and foam model hence the ultimate porosity for the no gas generation case is higher with the foam damage model

Eulerian Porosity vs time



Disposal Room Porosity Model Results

Sensitivity of room closure to choice of clay seam friction coefficient

- No data available from WIPP site clay seams
- Experimental tests (Sobolik) as part of WEIMOS project:
  - Direct shear tests were performed
    - Samples with diffuse clay from a nearby potash mine
      - shear strength similar to that of intact salt- Coulomb friction = 0.42
    - Artificial clay seams
      - shear strength more like highly consolidated saturated clay- Coulomb friction = 0.0279

Disposal Room Porosity Model Results

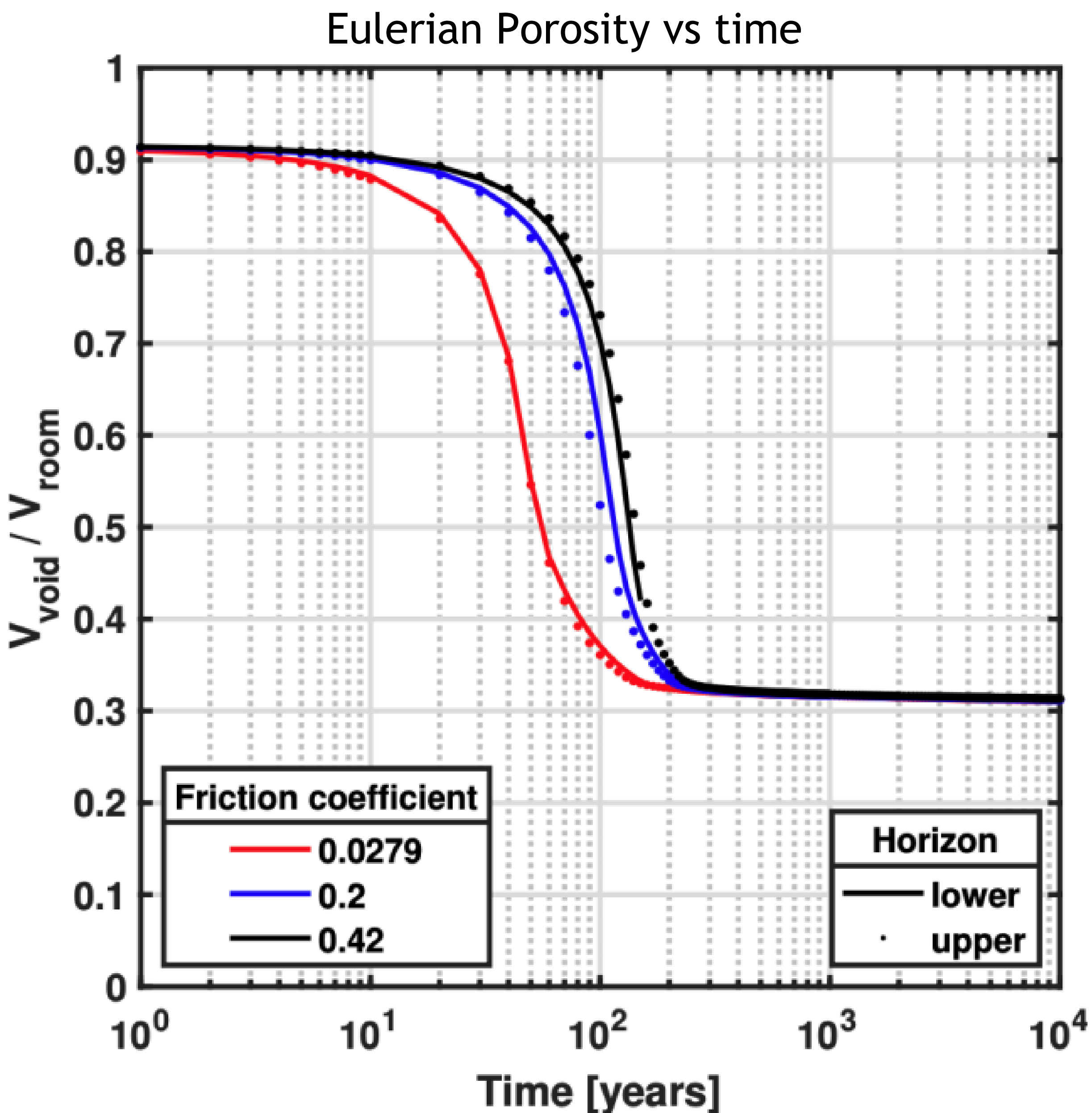
No gas generation case (f=0)

Clay Seam F is fixed at 0.42, and simulations were performed with other clay seams fixed at the lower bound, 0.2 and the upper bound of 0.42.

For times less than 300 years there is a sensitivity to clay seam friction coefficient.

As expected, the room closes faster with low friction.

The upper horizon (dots) closes faster than the lower horizon (solid line).



Disposal Room Porosity Model Results

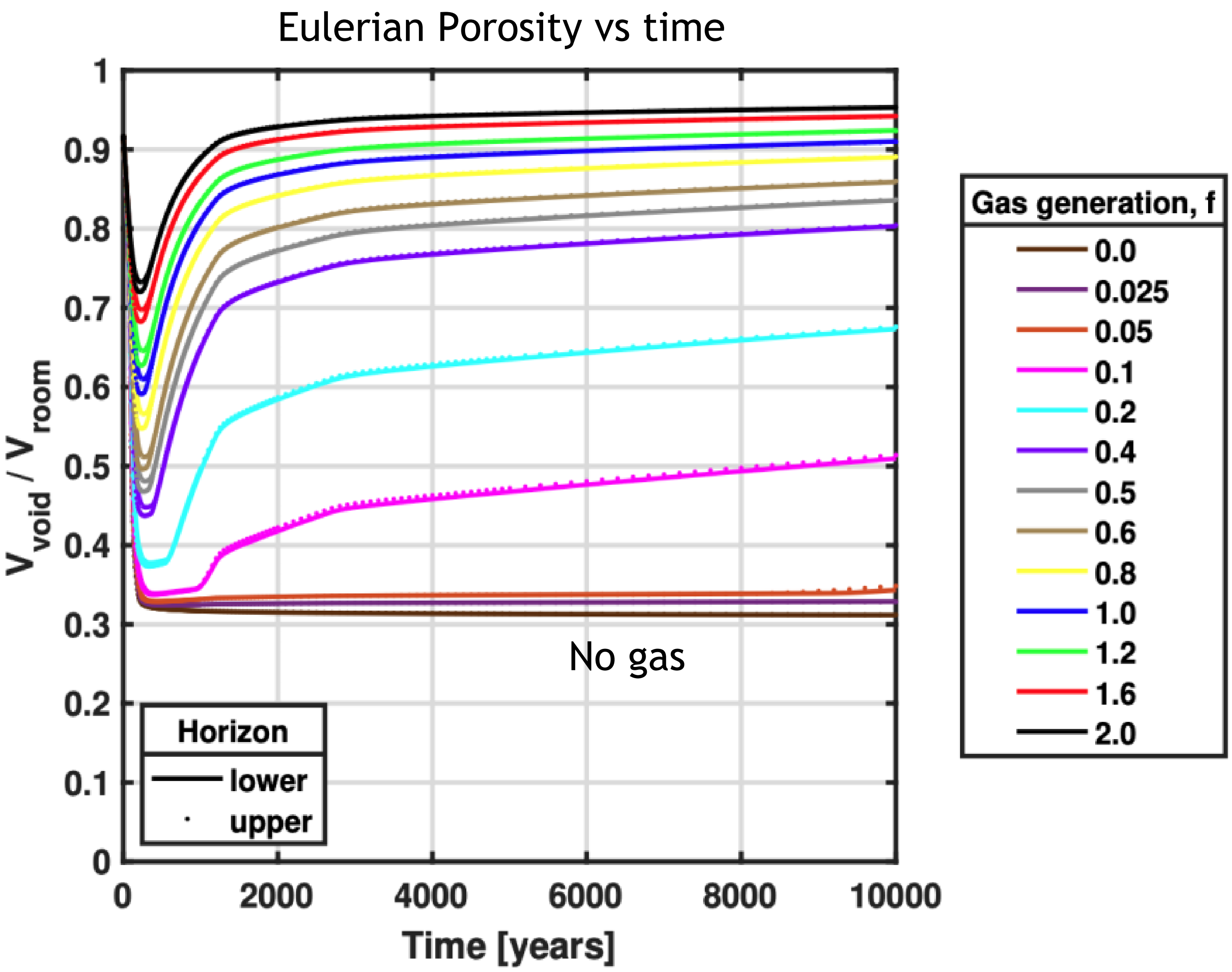
Upper and lower horizon disposal room porosity results

Gas Generation Cases- f scales the curve shown earlier

The upper horizon disposal room is mined 2.43m higher relative to the lower horizon disposal room. The roof is at the level of Clay Seam G and Clay Seam F intersects the wall of the room.

Porosity initially decreases until the gas pressure becomes large enough to overcome the inward movement due to creep.

Some slight differences between the lower and upper disposal room porosity during the first 400 years for most gas generation cases.



Summary and Conclusions

- We have presented the new models for the geomechanics, waste constitutive behavior, and gas generation with some select results from preliminary modeling.
- The addition of the low stress creep component increases the rate of disposal room closure.
- The Foam Damage model corrects the problem of tensile stresses in the out of plane direction seen when using the Soil and Foam model.
- The Foam Damage model becomes stiffer at a higher value of porosity and for low gas generation cases would have a higher final porosity compared to that calculated with the Soil and Foam model.
- For the maximum gas generation, f=1, the room porosity at 10K years is almost as large as the initial porosity (0.917); the room has returned to its initial volume due to the high gas pressure in the room.
- The impact of these changes to the disposal room porosity model on WIPP performance has not yet been determined.