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# A Validation Test for Adagio through Replication of Big Hill and Bayou Choctaw JAS3D Models

Byoung Yoon Park

Prepared by
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**Abstract**

JAS3D, a three dimensional iterative solid mechanics code, has been used for structural analyses for the Strategic Petroleum Reserve system since the 1990s. JAS3D is no longer supported by Sandia National Laboratories, and has been replaced by Adagio. To validate the transition from JAS3D to Adagio, the existing JAS3D input decks and user subroutines for Bayou Choctaw and Big Hill models were converted for use with Adagio. The calculation results from the Adagio runs are compared to the JAS3D. Since the Adagio results are very similar to the JAS3D results, Adagio is judged to be performing satisfactorily.

# ACKNOWLEDGMENTS

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Dr. Courtney G. Herrick (SNL, Dept. 6211) provided a technical review and Dr. David J. Borns (SNL, Dept. 6912) and Dr. Moo Y. Lee (SNL, Dept. 6914) provided a management review. This report has been improved by these individuals.

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# NOMENCLATURE

| | |
|---|---|
| BC | Bayou Choctaw |
| BH | Big Hill |
| DOE | Department of Energy |
| D-P | Drucker-Prager |
| M-D | Multimechanism Deformation |
| MMB | Million Barrels |
| PLC | Power Law Creep |
| RF | Reduction Factor |
| SMF | Structural Multiplication Factor |
| SPR | Strategic Petroleum Reserve |
| SRN | Sandia Restricted Network |
| UTM | Universal Transverse Mercator |
| UTP | Union Texas Petroleum |
| WIPP | Waste Isolation Pilot Plant |

# 1. INTRODUCTION

JAS3D, a three-dimensional iterative solid mechanics code for analyzing the large deformation response of nonlinear materials subjected to a variety of loads, has been used for structural analyses for the Strategic Petroleum Reserve (SPR) system since the 1990s. JAS3D is no longer supported by Sandia, and has been replaced by Adagio. Adagio is written for parallel computing environments, and its solvers allow for scalable solutions of very large problems. The Adagio structure is different from JAS3D. Adagio uses the SIERRA Framework, which allows for coupling with other SIERRA mechanics codes. Extant JAS3D input decks and user subroutines for the SPR works have to be converted for use with Adagio. The calculation results from the Adagio run on the SIERRA Framework have to be verified. This test should take precedence over the others for the future work.

These tests are based on Sandia report SAND2006-7589 entitled “Three Dimensional Simulation for Bayou Choctaw (SPR)” [Park and Ehgartner, 2006], and Sandia report SAND2012-1206 entitled “Interface Modeling to Predict Well Casing Damage for Big Hill Strategic Petroleum Reserve” [Park and Ehgartner, 2012]. The computational procedures and data described in those reports were used in this test so a direct comparison between the results using JAS3D and Adagio can be made. Therefore, this set of tests includes a replicate of the storage loss due to salt creep, compressive stresses, and minimum safety factor for dilatant damage over a 46 year period following initial leach and five drawdown leaches for Bayou Choctaw (BC) model. It also includes a replicate of the storage loss and relative displacements in the interbed between salt dome top and caprock bottom over a 56 year period for Big Hill (BH) model. The data used in these tests, such as the stratigraphy, salt dome geometry, cavern geometry and layout, cavern internal pressure history and material properties, etc. are identical to those used in the BC and BH JAS3D models [Park and Ehgartner, 2006; Park and Ehgartner, 2012]. These tests represent complex geomechanics problems in which the creep response of SPR caverns is modeled.

## 1.1. Software Identifier

- Code name: Adagio
- Version: 4.25.10-modified (BC model), 4.27.3-modified (BH model)

## 1.2. Points of Contact

- Testers/Evaluators: Byoung Yoon Park, Org. 6914, bypark@sandia.gov, 505/284-2729
- Point of Contact for Adagio: Kendall Pierson, Org. 1542, khpiers@sandia.gov, 505/284-5894
- For help or general questions concerning Adagio: sierra-help@sandia.gov

# 2. BAYOU CHOCTAW MODEL

## 2.1. Model Description

Three dimensional finite element analyses were performed to evaluate the structural integrity of caverns located within the BC site, which is considered a candidate for expansion. Fifteen active and nine abandoned caverns exist at BC, with a total cavern volume of some 164 MMB. A 3D model allowing control of each cavern individually was constructed because the location and depth of caverns and the date of excavation are irregular. The total cavern volume has practical interest, as this void space affects total creep closure in the BC salt mass. Operations including both cavern workover, where wellhead pressures are temporarily reduced to atmospheric, and cavern enlargement due to leaching during oil drawdowns, which occurs when water is used to displace the oil from the caverns, were modeled to account for as many as the five future oil drawdowns in the six SPR caverns.

## 2.2. Geomechanical Model

### *2.2.1. Salt dome geometry*

The stratigraphy near the BC salt dome is shown in Figure 1. The top layer of overburden, which consists of sand, silts and clays, has an average thickness of 500 ft. The caprock, consisting of gypsum, anhydrite, and sand, is on average 150 ft thick. The bottom of the deepest cavern (Cavern 25) is at an elevation of 5,790 ft. For the vertical direction constraint at the bottom of the model, sufficient thickness between the lowest cavern bottom and the model bottom is necessary so as to not affect the structural reaction by the bottom boundary. Therefore, the depth of the salt dome is considered to 8,000 ft below the surface. All SPR caverns are located below 2,000 ft.

The horizontal section of the dome forms an ellipse as shown Figure 2. The major and minor radii are obtained using the 4,000 ft contour, which is half of the model depth, by hand measuring the distances in Figure 2. Cavern 20 is closest to the dome edge. The elevation of Cavern 20 is approximately 4,000 ft below the surface. Thus, the 4,000 ft contour was selected to get the radii of salt dome. The major and minor radii are measured to be 4,882 ft and 4,265 ft, respectively.

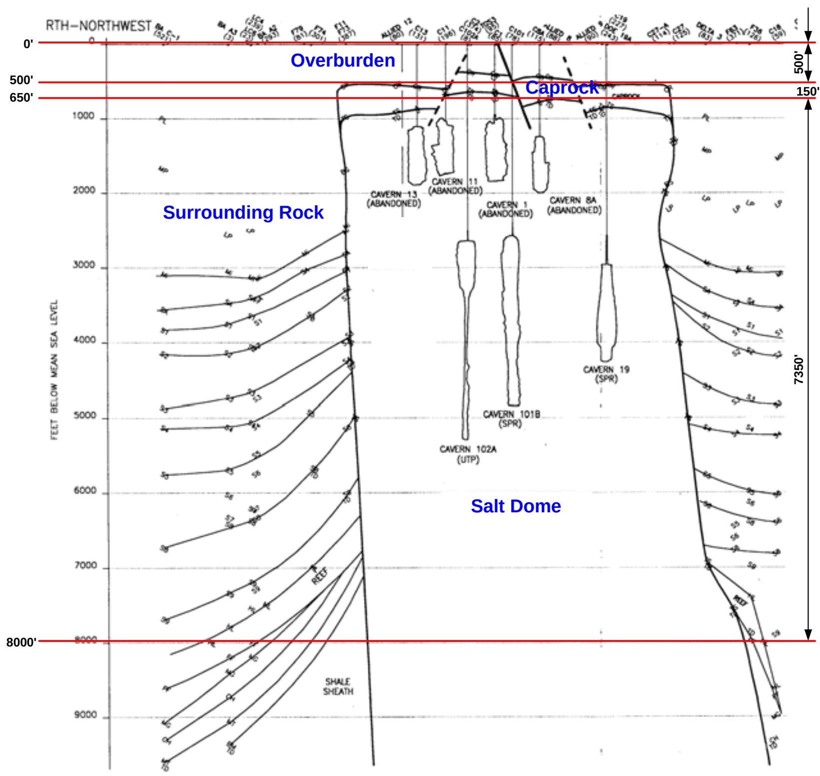



**Figure 1: Stratigraphy near the Bayou Choctaw salt dome [Neal et al., 1993] and the thickness of each layer used for modeling.**

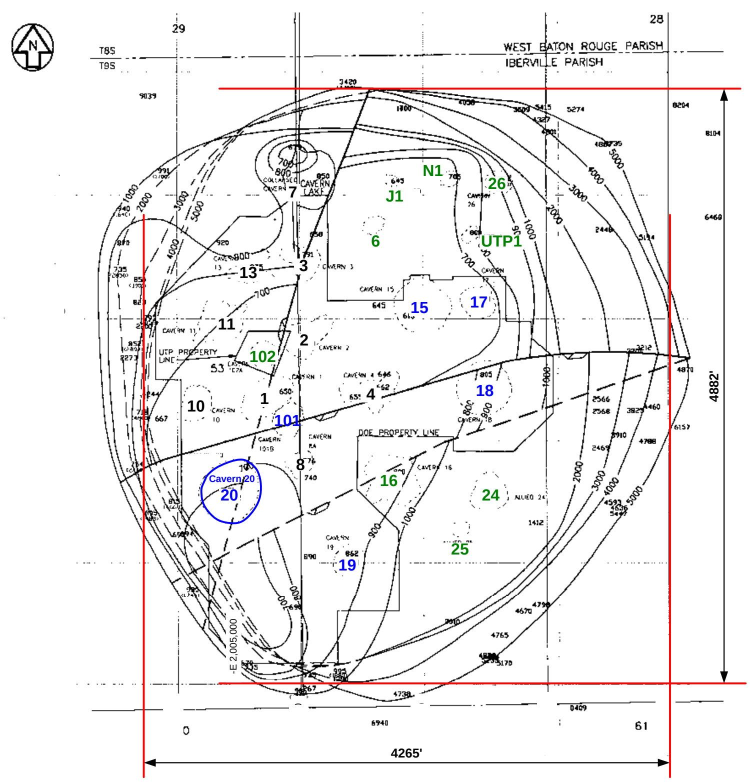



**Figure 2: Major diameter and minor diameter of BC salt dome used for modeling.**

### 2.2.2. Salt constitutive model

A power law creep model is used for the salt creep constitutive model, which considers only secondary or steady-state creep. The creep strain rate is determined from the following effective stress law:

$$\dot{\varepsilon} = A\left(\frac{\sigma}{\mu}\right)^n \exp\left(-\frac{Q}{RT}\right) \tag{1}$$

where, $\dot{\varepsilon} =$ creep strain rate,

$\sigma =$ effective or von Mises stress,

$\mu =$ shear modulus, E/2(1+ν), where E is Young's modulus and ν is Poisson's ratio

$T$ = absolute temperature,

$A$, $n$ = creep constants determined from fitting the model to creep data,

$Q$ = effective activation energy,

$R$ = universal gas constant.

The material properties, including calibrated values (bold font), in Table 1 are used as salt material data in the test.

**Table 1: Material parameters used for the Bayou Choctaw salt.**

| Parameter | Unit | Value | References |
|---|---|---|---|
| Young's modulus (E) | psi | $4.496\times10^{6}$ | Krieg, 1984 |
| Density (ρ) | lb/in$^3$ | 0.083 | Krieg, 1984 |
| Poisson's ratio (ν) | - | 0.25 | Krieg, 1984 |
| Elastic modulus reduction factor (RF) | - | 12.5 | Morgan and Krieg, 1988 |
| Bulk modulus (K) | psi | $2.397\times10^{5}$ | Calculated using E and ν |
| Shear modulus (μ) | psi | $1.439\times10^{5}$ | Calculated using E and ν |
| Creep constant (A) | Pa$^{-4.9}$/s | $5.79\times10^{-36}$ | Krieg, 1984 |
| Structure multiplication factor (SMF) | - | 0.12 | Park and Ehgartner, 2006 |
| Calibrated creep constant | Pa$^{-4.9}$/s | $0.695\times10^{-36}$ | Park and Ehgartner, 2006 |
| Stress exponent (n) | - | 4.9 | Krieg, 1984 |
| Thermal constant (Q) | cal/mol | 12000 | Krieg, 1984 |
| Universal gas constant (R) | cal/(mol·K) | 1.987 | |
| Input thermal constant (Q/R) | cal/mol | 6039 | |

### 2.2.3. Material properties of lithologies around the salt dome

The surface overburden layer, which is mostly comprised of sand, is expected to exhibit elastic material behavior. The sand layer is considered isotropic, and has no assumed failure criteria. The caprock layer, consisting of gypsum, anhydrite and sand, is also assumed to behave elastically. The sedimentary rock surrounding the salt dome is assumed to be an isotropic, homogeneous elastic sandstone. The mechanical properties used in the present analysis are listed in Table 2.

**Table 2: Material properties of the lithologies around the BC salt dome used in the analyses.**

| | Unit | Overburden | Caprock | Surrounding Rock |
|---|---|---|---|---|
| Young's modulus | psi | $1.450 \times 10^4$ | $2.277 \times 10^6$ | $5.076 \times 10^6$ |
| Density | $lb/in^3$ | 0.068 | 0.090 | 0.090 |
| Poisson's ratio | - | 0.33 | 0.29 | 0.33 |

## 2.3. Cavern Model

### *2.3.1. Cavern geometry and layout*

The cavern shapes and locations vary widely as shown in Figure 1 and Figure 2. Fifteen active and nine abandoned caverns exist at BC, producing a total cavern volume of some 164 million barrels (MMB). This includes 81 MMB in six SPR caverns, 31 MMB in nine Union Texas Petroleum (UTP) caverns, and about 52 MMB in abandoned caverns. Cavern 7 collapsed in 1954 and was filled with overburden material. The total cavern volume is important since the void space affects total creep closure (and consequent subsidence) in the BC salt mass.

Table 3 lists the geotechnical parameters for the twenty four caverns considered in the present simulation [Neal et al., 1993; Stein, 2005]. The origin of the coordinates system used in the modeling is the center coordinates of the dome. The shapes of caverns were simplified to the cylindrical shapes using the geometric parameters in Table 3. The faults shown in Figure 1 and Figure 2 are assumed not to affect the structural behavior of the SPR caverns in the analysis because they do not extend to the deep salt beyond the top of abandoned caverns.

### *2.3.2. Model history*

The last sonar dates to measure the shape of caverns were between 1977 and 1993, as listed in Table 3. For the purposes of the present simulation, it is assumed that all caverns were leached twenty-one years ago (i.e., 1985) to simplify the model history. This simulation start time was chosen because it is the average of the sonar measurement dates. The sonar measurement dates represent a time when the cavern geometry had been measured with surety and therefore give a baseline from which volume changes can be determined.

The analysis simulates caverns that were leached to full size over a one year period by means of gradually switching from salt to fresh water in the caverns. It was assumed that the SPR caverns were filled with petroleum and non-SPR caverns were filled with brine at year one, and then permitted to creep for twenty years to reach the preset twenty-one year age for the caverns to be simulated. Subsequently, every five (5) years after the twenty first year, the SPR caverns were instantaneously leached. Modeling of the leaching process of the caverns was accomplished by deleting elements along the walls of the caverns so that the volume increased by 15% with each leach. The good salt quality at BC should provide a leach of 15 percent. Leaching is assumed to occur uniformly along the entire height of the cavern. However, leaching is not permitted in the floor or roof of the caverns. The 5-year period between each drawdown allows the stress state in the salt to return to a steady-state condition, as will be evidenced in the predicted closure rates. The simulation was terminated right before sixth leach to investigate the structural behavior of the dome for 46 years, during which creep closure to occur in all caverns.

The pressure conditions applied to the caverns were based on average wellhead pressures listed in Table 4. Cavern 15 operates over a range of pressures from 815 to 990 psi under normal conditions. The pressure starts at 815 psi, then, due to creep and thermal expansion of fluids, the pressure gradually rises to 990 psi. At that time the brine is removed from the cavern to reduce the pressure down to 815 psi again. Thus, on average, a pressure of 903 psi is used for Cavern 15 wellhead pressure operating under normal conditions. In the same manner, the pressures of 903, 715, 925, 850, and 913 psi are used for the normal operating wellhead pressures of Cavern 17, 18, 19, 20, and 101, respectively.

**Table 3: Geometric parameters for 24 caverns considered in the simulation [Neal et al., 1993; Stein, 2005; Hogan, 1980; Ehgartner et al., 2003]**

| Cavern Number | X Coordinate of Center | Y Coordinate of Center | Gross Volume | Elevation of Cavern Top | Elevation of Cavern Bottom | Cavern Height | Diameter Average | Last Sonar Date |
|---|---|---|---|---|---|---|---|---|
| | ft | ft | MMB | ft | ft | ft | ft | mmm-yyyy |
| Cavern 1 | -1002 | -27 | 8.42 | -950 | -1810 | 860 | 250.0 | 1977 |
| Cavern 2 | -817 | 369 | 9.02 | -715 | -1590 | 875 | 260.0 | 1977 |
| Cavern 3 | -821 | 1082 | 5.01 | -890 | -1875 | 985 | 200.0 | 1977 |
| Cavern 4 | -212 | 12 | 5.98 | -620 | -1710 | 1090 | 280.0 | 1980 |
| Allied 6 | -192 | 1353 | 0.82 | -1195 | -1562 | 367 | 126.4 | Nov-1990 |
| Cavern 7 | -786 | 1679 | 4.01 | -440 | -1560 | 1120 | 160.0 | Unknown |
| Cavern 8 | -811 | -604 | 3.12 | -1235 | -1976 | 741 | 200.0 | 1980 |
| Cavern 10 | -1706 | -118 | 6.40 | -990 | -1902 | 912 | 200.0 | 1980 |
| Cavern 11 | -1458 | 521 | 9.50 | -1030 | -1800 | 770 | 280.0 | 1978 |
| Cavern 13 | -1241 | 969 | 4.31 | -1103 | -1880 | 777 | 240.0 | 1977 |
| Cavern 15 | 92 | 669 | 16.45 | -2605 | -3296 | 691 | 412.0 | Mar-1993 |
| Cavern 16 | -68 | -675 | 10.49 | -2612 | -3228 | 616 | 349.1 | Mar-1989 |
| Cavern 17 | 573 | 736 | 12.17 | -2600 | -4023 | 1423 | 238.0 | Mar-1993 |
| Cavern 18 | 609 | 43 | 17.44 | -2125 | -4219 | 2094 | 244.0 | Jun-1993 |
| Cavern 19 | -477 | -1362 | 12.67 | -2935 | -4228 | 1293 | 260.0 | Jun-1993 |
| Cavern 20 | -1561 | -936 | 9.17 | -3830 | -4225 | 395 | 514.0 | Mar-1993 |
| Allied 24 | 664 | -798 | 5.59 | -3100 | -4337 | 1237 | 179.1 | Apr-1992 |
| Allied 25 | 451 | -1167 | 7.08 | -3575 | -5790 | 2215 | 151.2 | Jun-1992 |
| Cavern 26 | 747 | 1669 | 0.71 | -3076 | -3470 | 394 | 113.2 | Sep-1991 |
| Cavern 101 | -951 | -325 | 13.06 | -2550 | -4830 | 2280 | 201.0 | Jun-1993 |
| Cavern 102 | -1169 | 270 | 4.20 | -2640 | -5339 | 2699 | 105.5 | Oct-1984 |
| Allied J1 | -92 | 1682 | 0.75 | -2854 | -3945 | 1091 | 69.9 | Jul-1989 |
| Allied N1 | 358 | 1686 | 0.49 | -2670 | -3590 | 920 | 61.9 | Jan-1987 |
| UTP 1 | 369 | 1223 | 1.41 | -2360 | -3502 | 1142 | 94.0 | Aug-1989 |

**Table 4: Range of operating pressures measured at the wellhead for SPR caverns at BC.**

| Cavern | Operating Pressure Range (psi) | | |
|---|---|---|---|
| | Low | High | Average Pressure |
| Cavern 15 | 815 | 990 | 903 |
| Cavern 17 | 815 | 990 | 903 |
| Cavern 18 | 690 | 740 | 715 |
| Cavern 19 | 900 | 950 | 925 |
| Cavern 20 | 825 | 875 | 850 |
| Cavern 101 | 825 | 1000 | 913 |

Workovers on the five SPR caverns were performed from 12/10/2000 to 7/25/2003. Caverns 15 and 17 are currently operated as a gallery, maintaining equal pressures at all times including during the workover periods. Thus Caverns 15 and 17 were workovered together and workovers on Caverns 19, 18, and 101B followed in order. Rather than complicating the analyses, the following assumptions were made based on the actual field conditions for the six SPR caverns:

- A constant pressure is applied for the majority of the time, with pressure drops periodically included.
- For workover conditions, zero wellhead pressure is used.
- The workovers on the Caverns 15 and 17 are performed one year after switching from brine to petroleum. Cavern 19 is workovered 3 months after the workover of Caverns 15 and 17 have been completed. The workover of Cavern 18 starts as soon as the workover of Cavern 19 has been completed. Then, Cavern 20 is workovered 2.5 years later. Finally, Cavern 101 is workovered as soon as the workover of Cavern 20 has been completed. This workover cycle is repeated every 5 years.
- Workover durations are 3 months for all caverns.
- For both normal and workover conditions, the caverns are assumed to be full of oil with a pressure gradient of 0.37 psi/ft of depth.

In the case of non-SPR caverns, except Cavern 7, the pressure due to brine head with a pressure gradient of 0.52 psi/ft is applied on the cavern walls. Cavern 7 was drilled in 1942 to a depth of 1,951 ft. It collapsed in 1954 and was filled with overburden material, which has an assumed density and Poisson’s ratio as listed in Table 2. Thus the pressure gradient of 0.4 psi/ft is applied on the wall and 0.812 psi/ft is applied on the floor and roof.

## 2.4. Thermal conditions

The finite element model includes a depth-dependent temperature gradient which starts at 84.02 °F (28.90 °C) at the surface and increases at the rate of 0.0138 °F/ft (0.0251 °C/m). The temperature profile is based on the average temperature data recorded in well logs from BC prior to leaching [Ballard and Ehgartner, 2000]. The temperature distribution is important because the creep response of the salt is temperature dependent. Radial temperature gradients due to cavern cooling effects of the cavern product are not considered in these calculations. Previous 2D cavern studies have shown the predicted cavern deformation to be insensitive to the developed radial thermal gradients [Hoffman, 1992].

## 2.5. Mesh

A three dimensional mesh, which allows each cavern to be configured individually, was constructed. Figure 3 shows the overview of the finite element mesh of the stratigraphy and cavern field at BC. The mesh has been separated to show the individual material blocks. The X-axis of model is in the EW (East-West) direction, Y-axis is in the NS (North-South) direction, and Z-axis is the vertical direction.

Four material blocks are used in the model for the overburden, caprock, salt dome, and surrounding rock. The surrounding rock block encloses the caprock and salt dome block. The salt dome block contains 24 caverns. The caprock contains the upper part of Cavern 7 because

Cavern 7 collapsed, becoming filled mainly with sand up to the caprock layer. The caprock is made of gypsum, anhydrite, and sand. The surrounding rock is sedimentary rock that consists of sandstone and shale. In order to simplifying the mesh, the surrounding rock is assumed to be made of entirely sandstone because the Young's moduli of sandstone and shale are similar [Carmichael, 1984].

An elliptical shape is applied to the section of the dome as an approximation for the actual shape. The major and minor diameters of the salt dome are 4,882 ft and 4,265 ft, respectively. The lower boundary of the salt dome is considered to extend 8,000 ft below the surface. Since the overburden is 500 ft thick and the caprock is 150 ft thick, the height of the salt dome is assumed to be 7,350 ft. Each SPR cavern is modeled as having five cylindrical layers to be removed to account for the drawdown activities. The diameter of the SPR caverns will be increased by 7.24% per drawdown by deleting elements in the cylindrical layers at 21 years, and subsequently every 5 year. The shapes of all caverns are simplified by cylindrical shapes using the geometrical parameters in Table 3. The caverns can be classified by two groups. One group consists of those caverns located above 2,000 ft depth and the other group consists of those caverns located below 2,000 ft depth (Figure 1). All the caverns in the upper group are abandoned except Cavern 6. The caverns in the lower group are operated by DOE and Union Texas Petroleum (UTP).

Figure 4 shows the assembled mesh and the boundary conditions used for the BC model. The salt dome is modeled as being subjected to a regional far-field stresses acting from an infinite distance away. The lengths of the confining boundaries are 24,410 ft in the NS direction and 21,325 ft in the EW direction. These lengths are about five times the major or minor diameter of the salt dome, respectively. This ratio (5) is far better than the generally accepted ratio (3 to 4) between the maximum dimensions/minimum excavation sizes. The model consists of 409,248 nodes and 398,090 elements.

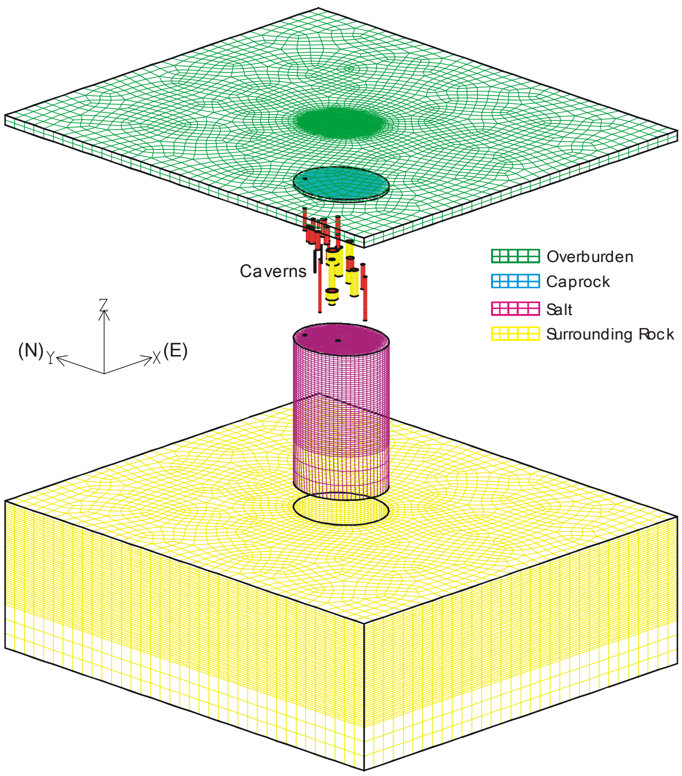



**Figure 3: Overview of the finite element mesh of the stratigraphy and cavern field at Bayou Choctaw.**

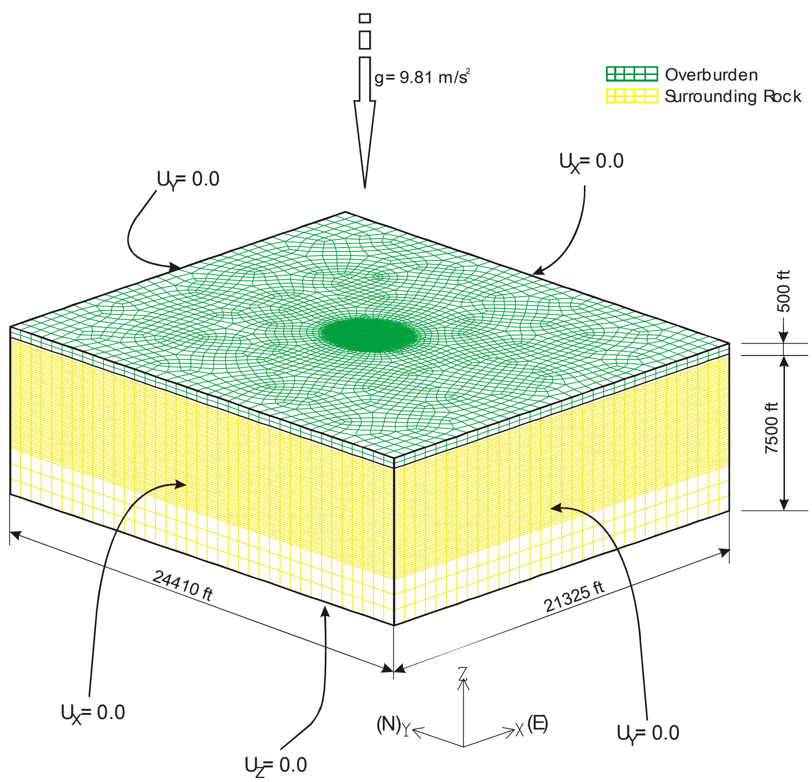



**Figure 4: Finite mesh discretization and boundary conditions at Bayou Choctaw.**

## 2.6. Test Objective

This test case will be used to specifically verify the following functional requirements:

- Computes the quasi-static, inelastic response of 3-dimensional solids using a nonlinear conjugate gradient solution algorithm.
- Use hexahedral element with hour glass control.
- Apply initial stress as the element variable.
- Apply no displacement kinematic boundary conditionss.
- Use a pressure boundary condition according to user defined subroutine.
- Models multilayer, multi-material stratigraphy of large physical extent.
- Individually control time intervals in the solution period.
- Use the Power Law Creep (PLC) model.
- Apply a gravity body force.

The following external interface requirements are also not specifically addressed but are verified implicitly:

- ASCII input
- GENESIS mesh file
- EXODUS output
- ASCII output

Adagio results will be compared to the results using previously qualified code JAS3D.

## 2.7. Input/Output

This test was run on Red Sky Unclassified Sandia Restricted Network (SRN) which is assembled in the space where legendary system ASCI Red once stood. Red Sky was open for limited user availability in January 2010. Red Sky on SRN has 2,816 nodes / 22,528 cores.

The common files used in JAS3D and Adagio input decks are provided in Appendix I. The input decks for JAS3D and Adagio are provided in Appendix II-A and B, respectively.

## 2.8. Evaluation of Results

The data from JAS3D version 2.2 was originally performed on a computer system named ELO, a Compaq Tru64 workstation, on which UNIX V.5.1.B is installed. The files and run control summary are described in Park et al. [2006].

Figure 5 shows a comparison of overall volumetric closure normalized to overall storage volume for the six SPR caverns immediately following each leach between JAS3D and Adagio, over the entire simulation period of 46 years. Adagio results lie on top the JAS3D results. Figures 6 through 11 show the comparisons of normalized volumetric closure of Caverns 15, 17, 18, 19, 20, and 101 over time between JAS3D and Adagio, respectively. The volumes were normalized by the volume of caverns immediately following each leach. In all cases the Adagio results are extremely close to the JAS3D.

Figure 12 shows a comparison of the calculated minimum compressive stress histories between JAS3D and Adagio over the entire simulation period of 46 years. The negative sign (-) indicates a compressive stress. Figure 13 shows a comparison of the minimum safety factor histories for dilatancy damage. The Adagio results are very similar to the JAS3D.

JAS3D was qualified for use in the SPR program before becoming unsupported. JAS3D has been validated through several programs (most notably for the Waste Isolation Pilot Project) for modeling the creep behavior of salt in mined operations such as radioactive waste storage, oil storage, and so on. Overall, since the Adagio results are extremely close to the JAS3D results, Adagio is judged to be performing satisfactorily.

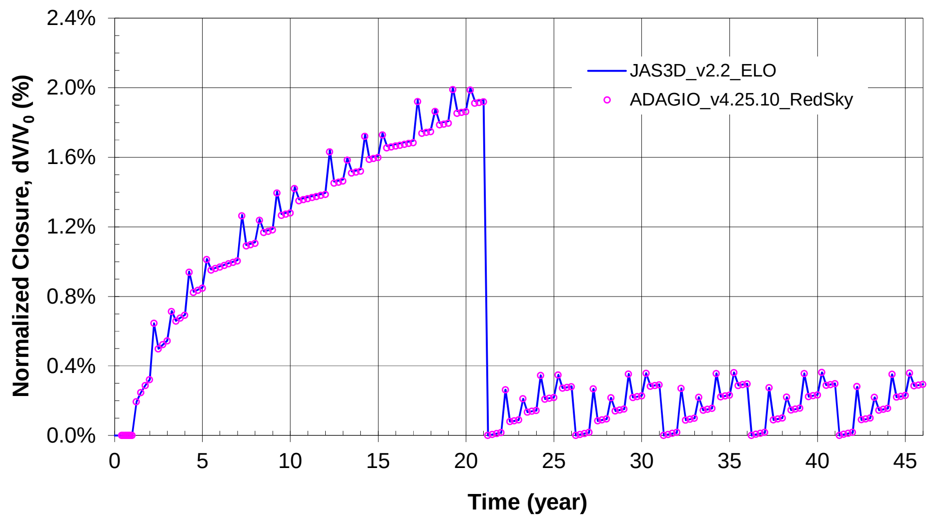



**Figure 5: Comparison of overall volumetric closure normalized to overall storage volume for the six SPR caverns immediately following each leach between JAS3D and Adagio. Adagio results are indicated by symbols.**

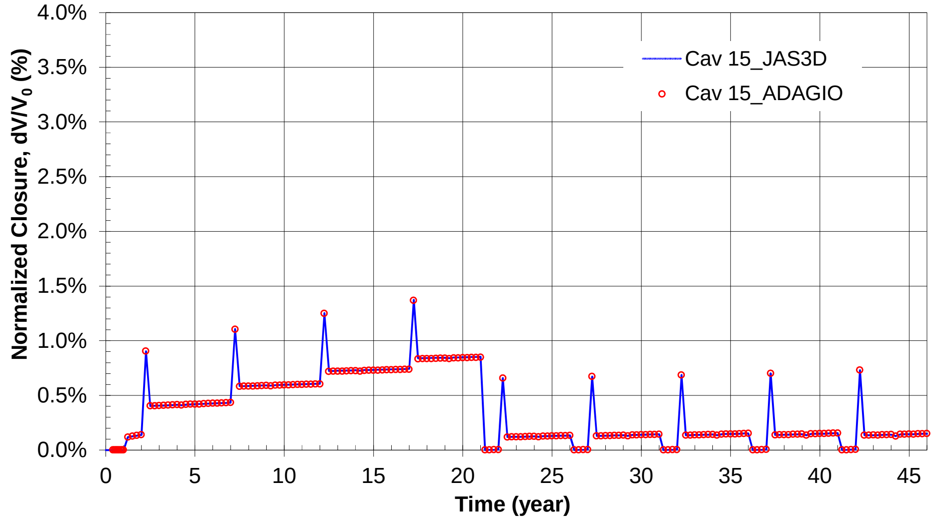



**Figure 6: Comparison of normalized volumetric closure of Cavern 15 over time between JAS3D and Adagio. The volume was normalized by the volume of Cavern 15 immediately following each leach.**

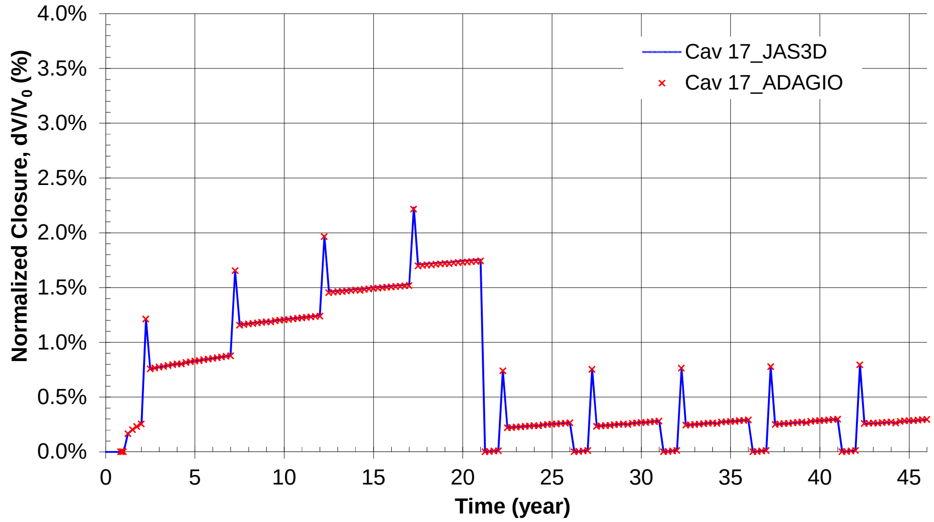



**Figure 7: Comparison of normalized volumetric closure of Cavern 17 over time between JAS3D and Adagio. The volume was normalized by the volume of Cavern 17 immediately following each leach.**

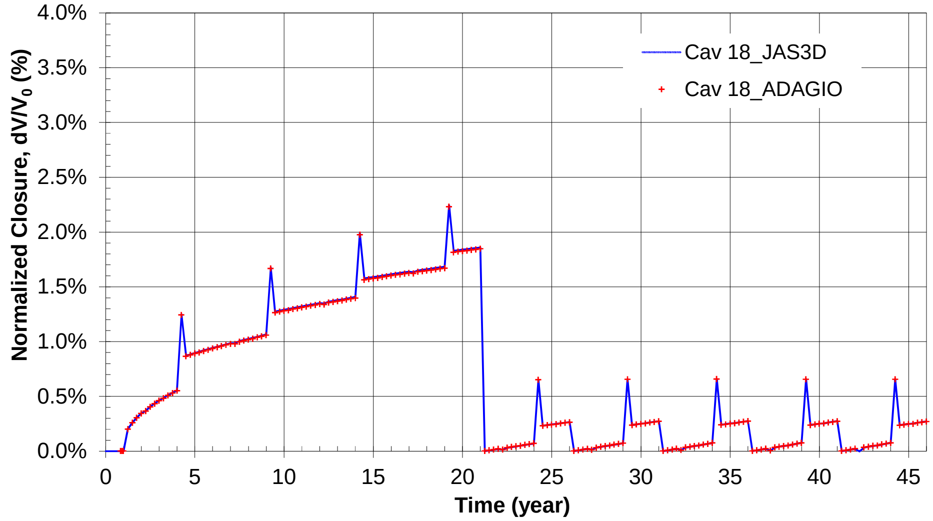



**Figure 8: Comparison of normalized volumetric closure of Cavern 18 over time between JAS3D and Adagio. The volume was normalized by the volume of Cavern 18 immediately following each leach.**

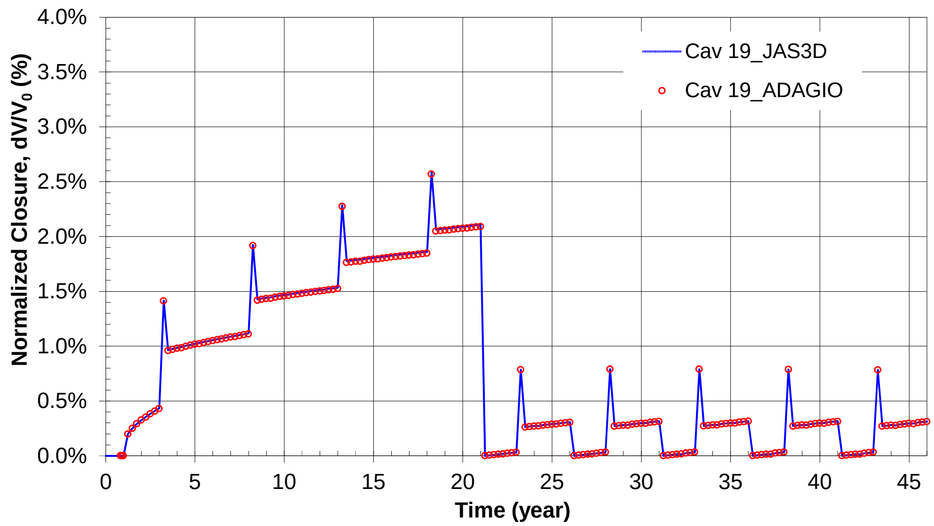



**Figure 9: Comparison of normalized volumetric closure of Cavern 19 over time between JAS3D and Adagio. The volume was normalized by the volume of Cavern 19 immediately following each leach.**

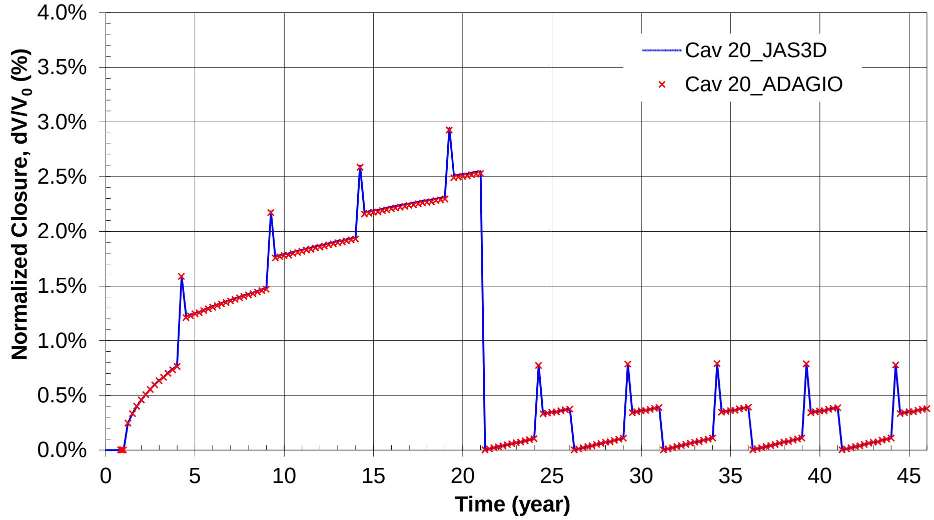



**Figure 10: Comparison of normalized volumetric closure of Cavern 20 over time between JAS3D and Adagio. The volume was normalized by the volume of Cavern 20 immediately following each leach.**

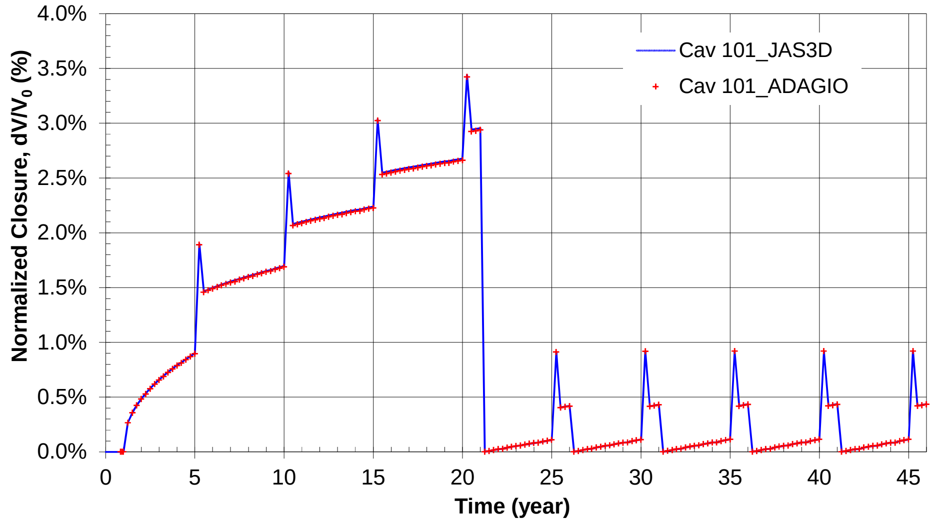



**Figure 11: Comparison of normalized volumetric closure of Cavern 101 over time between JAS3D and Adagio. The volume was normalized by the volume of Cavern 101 immediately following each leach.**

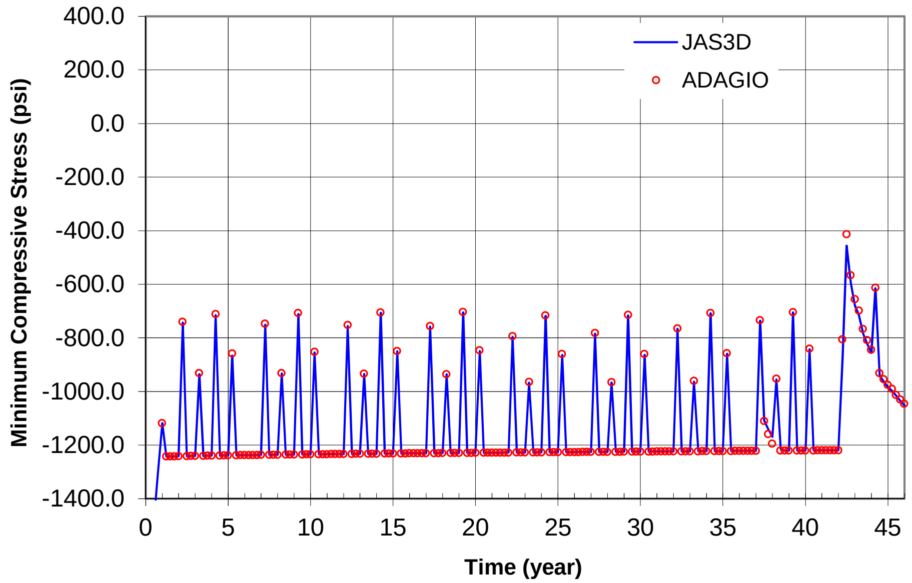



**Figure 12: Comparison of calculated minimum compressive stress histories between JAS3D and Adagio.**

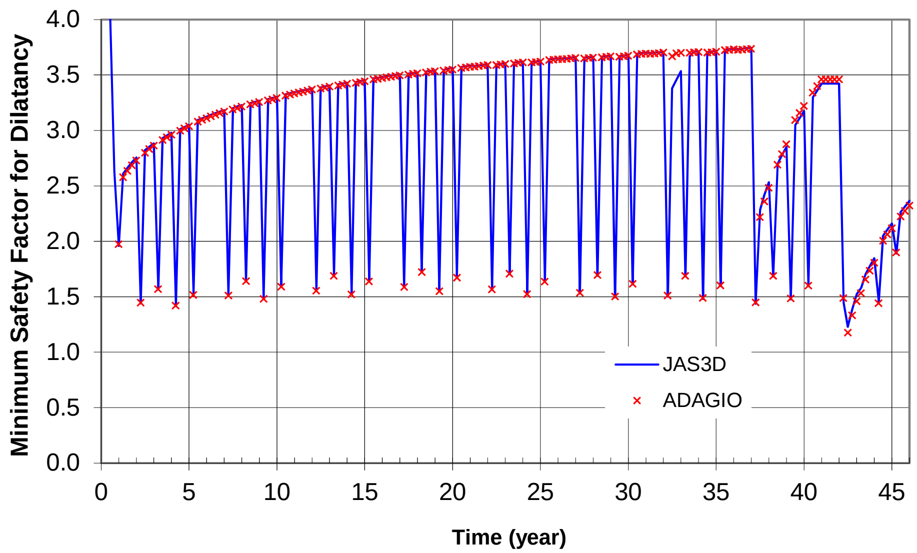



**Figure 13: Comparison of calculated minimum safety factor history for dilatant damage between JAS3D and Adagio.**

# 3. BIG HILL MODEL

## 3.1. Model Description

Oil leaks were found in well casings of Caverns 105 and 109 at the Big Hill Strategic Petroleum Reserve site. According to field observations, two instances of casing damage occurred at the depth of the interface between the caprock and top of salt. This damage could be caused by interface movement induced by cavern closure due to salt creep. A three dimensional finite element model, which allows each cavern to be configured individually, was constructed to investigate shear and vertical displacements across each interface. The model contains interfaces between each lithology and a shear zone to examine the interface behavior in a realistic manner. The advanced model in this test is a full 3-D rendering of the site and includes the lithologic interfaces and a fault, needed to simulate motion between the caprock and the salt dome. This model considers actual geometries and locations of the fourteen caverns. It also contains interfaces between the overburden and caprock; the two caprock lithologies; the caprock and salt dome; the dome and surrounding rock, and within a fault in the overburden and caprock layers. The shear displacement and vertical strain above the center of each cavern in the interface between caprock and salt dome will be calculated using Adagio and compared to the JAS3D results.

## 3.2. Geomechanical Model

### *3.2.1. Salt dome geometry*

Figure 14 shows a plan view of the BH site with contour lines defining the approximate location of the salt dome top. The locations of the 14 SPR caverns currently in-use (101-114) and five potential expansion caverns (X1-5) are indicated. The figure also specifies the undeveloped area north of the DOE property line (Sabine Pass Terminal). The horizontal shape of the dome is approximately elliptical. The major and minor ellipse axes are measured as 7000 ft and 5800 ft, respectively. The West-East cross-section #1 through the northern-most row of caverns (Cavern 101-105) provides a geologic representation near the middle of the dome (Figure 15). The site has a thin overburden layer consisting of sandy soil; and an exceptionally thick caprock sequence comprised of two layers. The upper caprock is comprised mainly of gypsum and limestone, whereas the lower caprock is mostly anhydrite. A major fault extends approximately North-South along the entire length of the caprock and for an unknown depth into the salt. This fault zone has a pronounced effect on the subsidence measured above the site and is a consideration for future cavern placement [Ehgartner and Bauer, 2004]. For analysis purposes, the top layer of overburden is modeled as having a thickness of 300 ft, the upper caprock 900 ft thick, and the lower caprock 430 ft thick. The salt thickness over the caverns is approximately 660 ft. The bottom boundary of the present analysis model is set at 6000 ft below the surface.

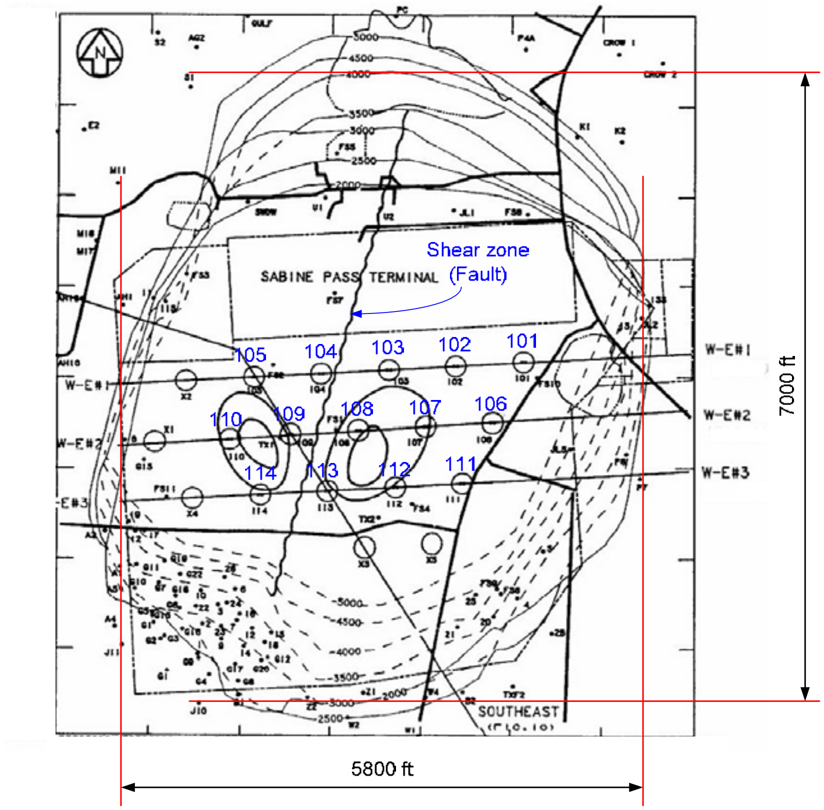



**Figure 14: Big Hill site plan view [Magorian and Neal, 1988]**

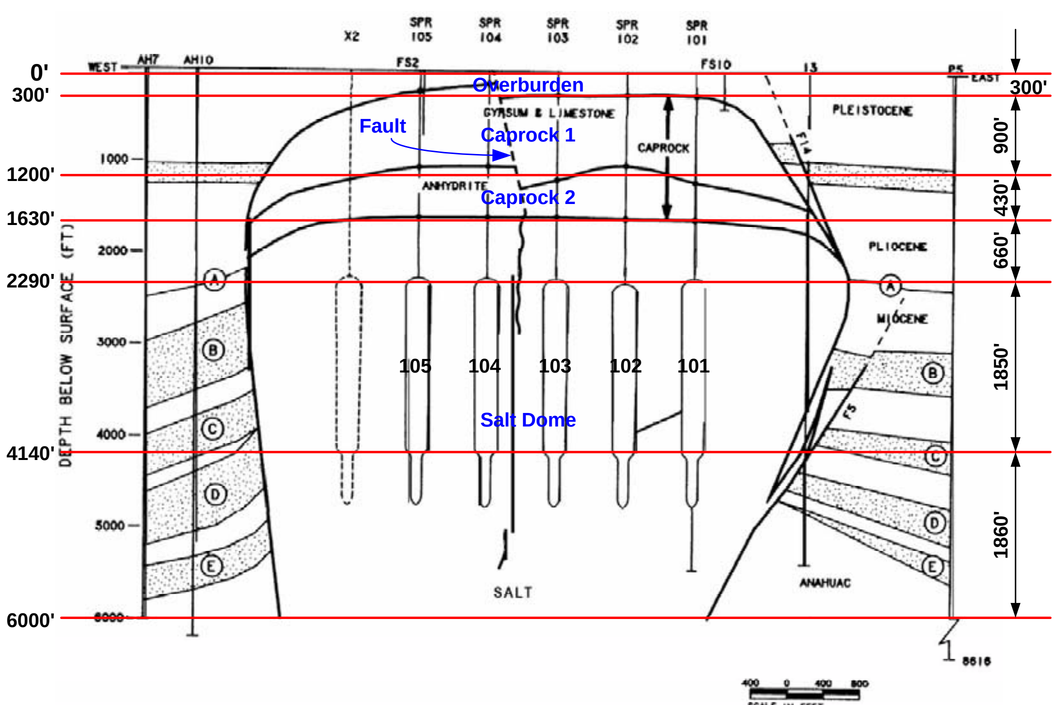



**Figure 15: Cross-section (W-E #1 in Figure 14) near middle of dome [Magorian and Neal, 1988] looking north.**

### *3.2.2. Salt Constitutive model and parameter values*

The salt constitutive model is the same as used in BC model (see Section 2.2.2). The creep constant, *A*, in Eq. (1) is adjusted by a structural multiplication factor (SMF) which is used to match the volumetric closure of caverns. Through a number of back-fitting analyses [Park et al., 2005], a calibrated power law creep constant was determined. The values used as input data in the test analyses are listed in Table 5.

**Table 5. Material properties of Big Hill salt used in the analysis.**

| Parameter | Unit | Value | Reference |
|---|---|---|---|
| Young's modulus (E) | GPa | 31 | Krieg, 1984 |
| Density (ρ) | $kg/m^3$ | 2300 | Krieg, 1984 |
| Poisson's ratio (v) | - | 0.25 | Krieg, 1984 |
| Elastic modulus reduction factor (RF) | - | 12.5 | Krieg, 1984 |
| Bulk modulus (K) | GPa | 20.67 | Using E, v |
| Shear modulus (μ) | GPa | 12.40 | Using E, v |
| Creep constant (A) | $Pa^{-4.9}/s$ | $5.79\times10^{-36}$ | Krieg, 1984 |
| Structural multiplication factor (SMF) | - | 1.5 | Park et al., 2005 |
| Calibrated creep constant | $Pa^{-4.9}/s$ | $8.69\times10^{-36}$ | Park et al., 2005 |
| Stress exponent (n) | - | 4.9 | Krieg, 1984 |
| Thermal constant (Q) | cal/mol | 12000 | Krieg, 1984 |
| Universal gas constant (R) | cal/(mol·K) | 1.987 | Mohr et al., 2011 |
| Input thermal constant (Q/R) | K | 6039 | Using Q and R |

### *3.2.3. Lithologies around the salt dome*

The surface overburden layer, which is mostly comprised of sandy soil, is modeled as exhibiting elastic material behavior. The sand layer is also considered isotropic and elastic, and has no assumed failure criteria. The upper caprock layer, consisting of gypsum and limestone, is also assumed to be elastic. The rock surrounding the salt dome is assumed to be isotropic, homogeneous elastic sandstone.

The anhydrite in the lower caprock layer is expected to experience inelastic material behavior. The anhydrite layer is considered isotropic and elastic until yield occurs [Butcher, 1997]. Once the yield stress is reached, plastic strain begins to accumulate. Yield is assumed to be governed by the Drucker-Prager (D-P) criterion:

$$\sqrt{J_2} = C - aI_1 \tag{2}$$

where $I_1 = \sigma_1 + \sigma_2 + \sigma_3 = 3\sigma_m$ is the first invariant of the stress tensor;

$\sqrt{J_2} = \sqrt{\dfrac{(\sigma_1 - \sigma_2)^2 + (\sigma_2 - \sigma_3)^2 + (\sigma_3 - \sigma_1)^2}{6}}$ is the square root of the second invariant of the deviatoric stress tensor;

$\sigma_1$, $\sigma_2$, and $\sigma_3$ are the maximum, intermediate, and minimum principal stresses, respectively;

$\sigma_m$ is the mean stress; and

$C$ and $a$ are D-P constants.

However, the material properties of the BH anhydrite are unknown. Therefore, the behavior of the BH anhydrite is assumed to be the same as the Waste Isolation Pilot Plant (WIPP) anhydrite. A non-associative flow rule is used to determine the plastic strain components. To use the soil and foams model for the lower caprock, JAS3D input parameters are derived from the elastic properties and the D-P constants, *C* and *a* [Park et al., 2005]. The material in Tables 5 and 6 are used as input data for Adagio.

**Table 6. Material properties of lithologies around salt dome used in the analyses.**

| | Unit | Overburden (Sandy soil) | Caprock 1 (Limestone and gypsum) | Caprock 2 (Anhydrite) | Surrounding Rock (Sandstone) |
|---|---|---|---|---|---|
| Young's modulus | GPa | 0.1 | 21 | 75.1 | 70 |
| Density | kg/m$^3$ | 1874 | 2500 | 2300 | 2500 |
| Poisson's ratio | 0.25 | 0.33 | 0.29 | 0.35 | 0.33 |
| Bulk modulus | GPa | N/A | N/A | 83.44 | N/A |
| Shear modulus | GPa | N/A | N/A | 27.82 | N/A |
| $A_0$ | MPa | N/A | N/A | 2338 | N/A |
| $A_1$ | | N/A | N/A | 2.338 | N/A |
| $A_2$ | | N/A | N/A | 0 | N/A |

### *3.2.4. Interfaces and Fault Model*

To investigate causes of well casing damage between the salt dome and the caprock, horizontal shear displacements and vertical strains at the interfaces need to be examined. Thus, interface blocks, special purpose analysis tools, are used to represent the interfaces between overburden and caprock 1; caprock 1 and caprock 2; caprock 2 and salt dome; surrounding rock and dome. The material behavior away from the interfaces is represented by material properties of caprock 1, caprock 2, and salt. The fault is considered in this model so as to better represent the large scale deformation.

There is no interface geometry and material property data obtained from the field. The interfaces and fault are assumed to behave mechanically like sandy soil, thus the overburden material properties (Table 6) are used in the analyses. In geology and related fields, a stratum is a layer of sedimentary rock or soil with internally consistent characteristics that distinguish it from other layers. A "stratum" is the fundamental unit in a stratigraphic column and forms the basis of the study of stratigraphy. Strata are typically seen as bands of different colored or differently structured material exposed in cliffs, road cuts, quarries, and river banks. Individual bands may vary in thickness from a few millimeters to a kilometer or more. In this study, the thicknesses of the interface materials are assumed to be a uniform 14 ft based on the measured largest thickness of the salt/caprock interface from a Weatherford multi-arm caliper survey data [Sattler and Ehgartner, 2011]. The thickness of fault varies from a millimeter to a hundred meters with fault displacement (Figure 16).

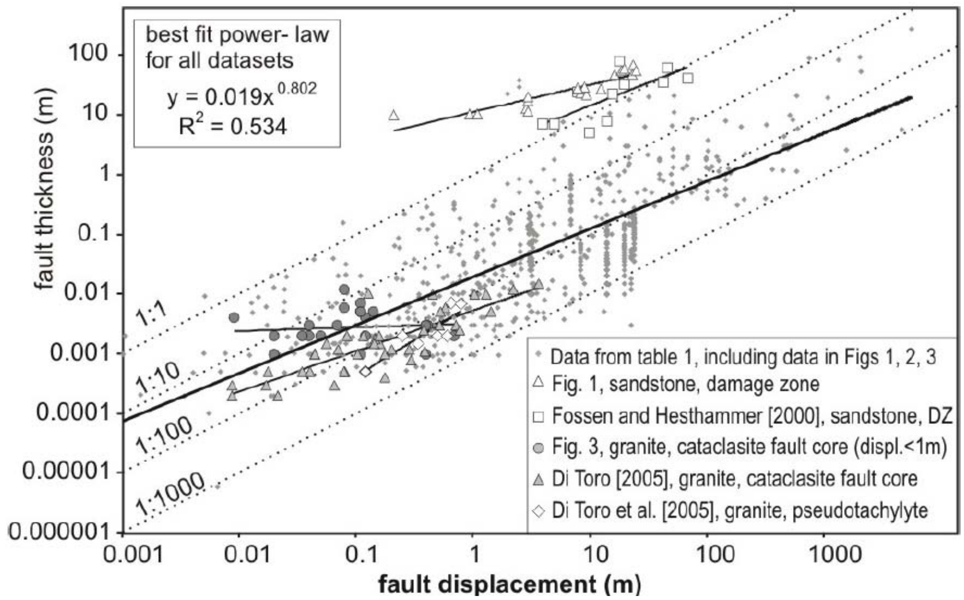



**Figure 16: Log-log plot of a compilation of 16 fault thickness datasets reported in the literature including the data used by Hull [1988], and the three datasets in Shipton, et al. [2006].**

## 3.3. Cavern Model

### *3.3.1. Cavern geometry and layout*

The cavern shapes are approximately cylindrical and the cavern array is regular as shown in Figure 17. The cavern dimensions used in the model are simplified and are listed in Table 7 based on sonar data. The completion date for the initial leach of each cavern is also listed. The X- and Y-coordinates for the center of each cavern were calculated by subtracting the Universal Transverse Mercator (UTM) coordinates of the center of the dome from UTM coordinates of each cavern. That is, the origin for the coordinate system of the model is the center of the dome.

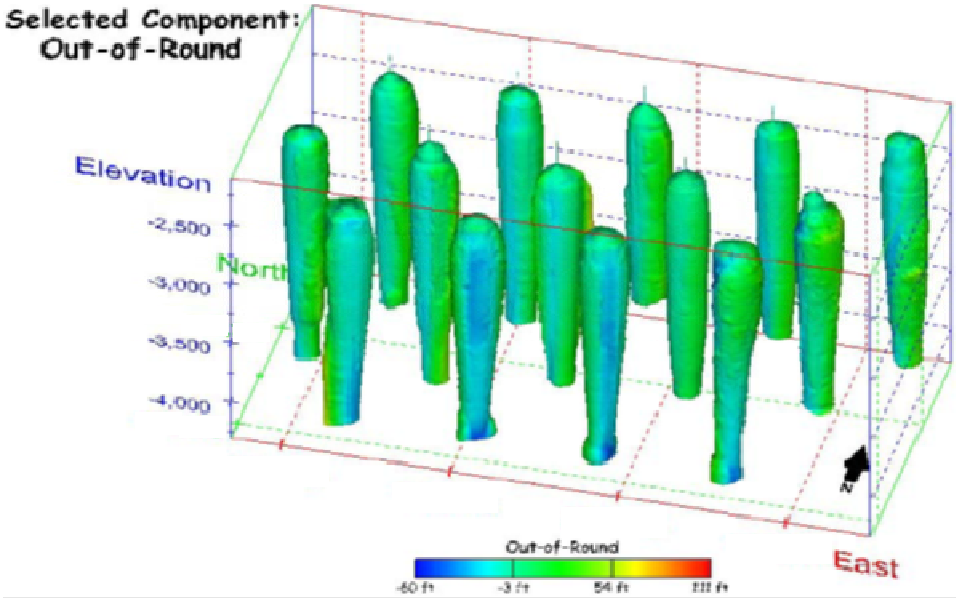



**Figure 17: Perspective view of the cavern field at the Big Hill SPR site from the southeast [Rautman and Lord, 2007]. Elevation unit is feet.**

**Table 7: Geometric parameters and initial leach completion dates for the fourteen extant caverns.**

| Cavern ID | X (East) | Y (North) | Z (Vertical Center) | Diameter | Radius | Cavern Top | Cavern Bottom | Cavern Height | Leach Done Date |
|---|---|---|---|---|---|---|---|---|---|
| | m | m | m | m | m | m | m | m | mm/dd/yyyy |
| **101** | 571.5 | -167.9 | -979.9 | 67.1 | 33.5 | -698 | -1262 | 563.9 | 9/18/1990 |
| **102** | 342.9 | -167.9 | -979.9 | 67.1 | 33.5 | -698 | -1262 | 563.9 | 10/21/1990 |
| **103** | 114.3 | -167.9 | -979.9 | 67.1 | 33.5 | -698 | -1262 | 563.9 | 11/28/1990 |
| **104** | -114.3 | -167.9 | -979.9 | 67.1 | 33.5 | -698 | -1262 | 563.9 | 10/21/1990 |
| **105** | -342.9 | -167.9 | -979.9 | 67.1 | 33.5 | -698 | -1262 | 563.9 | 11/11/1990 |
| **106** | 457.2 | -365.8 | -979.9 | 67.1 | 33.5 | -698 | -1262 | 563.9 | 10/16/1990 |
| **107** | 228.6 | -365.8 | -979.9 | 67.1 | 33.5 | -698 | -1262 | 563.9 | 4/24/1990 |
| **108** | 0.0 | -365.8 | -979.9 | 67.1 | 33.5 | -698 | -1262 | 563.9 | 6/14/1990 |
| **109** | -228.6 | -365.8 | -979.9 | 67.1 | 33.5 | -698 | -1262 | 563.9 | 7/24/1990 |
| **110** | -457.2 | -365.8 | -979.9 | 67.1 | 33.5 | -698 | -1262 | 563.9 | 4/19/1990 |
| **111** | 342.6 | -563.6 | -979.9 | 67.1 | 33.5 | -698 | -1262 | 563.9 | 7/15/1991 |
| **112** | 114.0 | -563.9 | -979.9 | 67.1 | 33.5 | -698 | -1262 | 563.9 | 6/19/1991 |
| **113** | -114.6 | -563.6 | -979.9 | 67.1 | 33.5 | -698 | -1262 | 563.9 | 5/1/1991 |
| **114** | -343.2 | -563.6 | -979.9 | 67.1 | 33.5 | -698 | -1262 | 563.9 | 8/29/1991 |

### *3.3.2. Model history*

The caverns were leached from April 1990 through August 1991 as listed in Table 7. To simplify the model history for the purposes of the present simulation, it is assumed that all existing caverns were initially leached in 1990, which is considered time $t$ = 1 year in the simulation. The analysis simulates caverns that were leached to full size over a one year period by means of gradually switching from salt to fresh water in the caverns. It was assumed that the SPR caverns were filled with petroleum one year after their initial leaches start. The caverns are simulated as creeping for thirty years. The simulation then performs oil drawdowns in the SPR caverns.

Every five years after the 31st year from the beginning of the simulation, every SPR cavern is modeled as being instantaneously leached. Modeling of the drawdown process of the caverns is performed by deleting elements along the walls of the caverns so that the volume is increased by 16% over the current volume. Leaching is assumed to occur uniformly along the entire height of the cavern. However, leaching is not permitted in the floor or roof of the caverns. The 5-year period between each drawdown allows the stress state in the salt to return to a steady-state condition, as will be evidenced in the predicted closure rates. The simulation continued until the 5th drawdown was completed to examine the evolution of the shear displacement and vertical strain in the interfaces for a total of 56 years. Creep closure is allowed to occur in all caverns during the simulation period.

To investigate the cause of oil leaks and evaluate the other casings at the site, the slick well casing above the caverns were recently inspected with Weatherford multi-arm caliper. The time frame for the multi-arm caliper (present day), to survey the oil leaks at the well casings of Caverns 105 and 109, corresponds to approximately 21 years of simulation time and the corresponding analysis results will be compared to the field inspection data. Figure 18 shows the time sequence for this study of the BH site, including the initial cavern leaching and the five drawdown leaches modeled in the simulation.

The pressure condition applied to each cavern is based on an average wellhead pressure of 905 psi which occurs when the wells are operated at normal or static conditions. An analysis of cavern pressures at BH between the years 1990 to 2010 indicates a cavern is pressurized within its normal operating range 74.3% of the time (1351 days during each five year period between drawdown leaches). Other operations, such as fluid transfers and workovers, require lower cavern pressures for 20.8% of the time (380 days during each five year period). Recently, operations have been improved to minimize low cavern pressures to assist in reducing volumetric losses due to creep [Ehgartner, 2010]. Therefore, pressure drops are periodically included to simulate times during workover conditions. For simulation purposes, the pressure drop to 0 psi within each cavern lasts for 3 months which is about 4.9% of the time (89 days) during each 5-year period. Rather than complicating the analyses, the following assumptions were made for the workover scenario. To better simulate actual field conditions, not all caverns are in workover mode at the same time.

**Workover scenario:**

- A constant pressure (905 psi) indicating a normal condition is applied for the majority of the time.
- For cavern workover, the wellhead pressure is dropped to zero.
- Workover of Cavern 101 begins one year after the initial leach is completed. After that, workovers are performed on Caverns 102 through 114 in numerical order. Workovers begin as soon as the workover of the prior cavern is completed.
- Workover durations are 3 month for all caverns.
- This workover cycle is repeated every 5 years.
- For both normal and workover conditions, the caverns are assumed to be full of oil having a pressure gradient of 0.37 psi/ft of depth.

- Pressure due to the oil head plus the wellhead is applied on the cavern boundary during the normal operation.

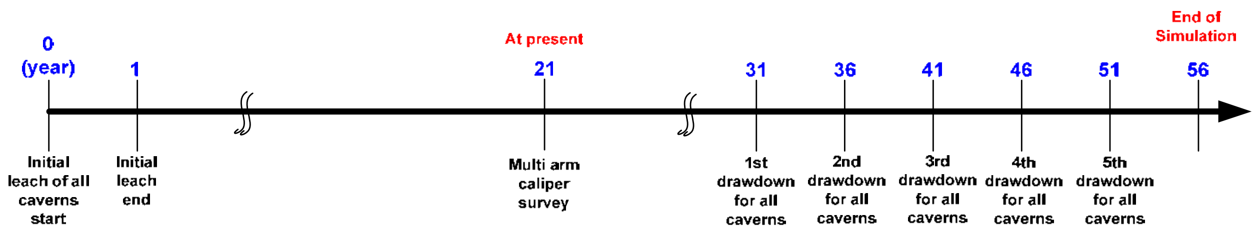



**Figure 18: Time sequence for the simulation.**

## 3.4. Thermal Conditions

The finite element model includes a depth-dependent temperature gradient which starts at 76.7 °F (24.84 °C) at the surface and increases at the rate of 1.41 °F/100ft (2.57 °C/100 m). The temperature profile is based on the average temperature data recorded in well logs from BH prior to leaching [Ballard and Ehgartner, 2000]. The temperature distribution is important because the creep response of the salt is temperature dependent. Radial temperature gradients due to cavern cooling effects from the cavern contents are not considered in these calculations. Previous 2D cavern studies have shown the predicted cavern deformation to be insensitive to the developed radial thermal gradients [Hoffman, 1992].

## 3.5. Mesh

A three dimensional mesh, which allows each cavern to be configured individually, was constructed to investigate shear displacements and vertical strains at the interfaces. Figure 19 shows the overview of the finite element mesh of the stratigraphy and cavern field at BH. The mesh has been separated to show the individual material blocks. The X-axis of model is in the East direction, Y-axis is along the North direction, and Z-axis is the vertical direction, up being positive. The mesh consists of nineteen material blocks. Five blocks used are Overburden, Caprock 1, Caprock 2, Salt Dome, and Surrounding Rock. Four blocks are used for the interfaces, and another four blocks are used for the fault. The other six blocks are used for the initial leach and five drawdown leaches for the fourteen caverns.

The Surrounding Rock block encircles Caprock 1, Caprock 2, and Salt Dome. The interface block under the Overburden block is split off from it. The thickness of every interface is 14 ft, thus the thickness of Overburden block becomes 286 ft (= 300 ft – 14 ft). In the same manner, the interface under Caprock 1 block is split off from it, thus the thickness of Caprock 1 block becomes 886 ft. The interface under Caprock 2 block is split off from it, thus the thickness of Caprock 2 block becomes 416 ft. The interface surrounding Caprock 1, Caprock 2, and Salt dome is split off from the inside of the Surrounding Rock block, thus the radii of Caprock1, Caprock 2, and Salt Dome are not changed but the inside radius of Surrounding Rock increases 14 ft.

The thickness of the fault (shear zone) is also assumed to be 14 ft. The strike direction and dip of the fault are 22º and 90º, respectively. The strike direction was approximated from Figure 14, and the dip was assumed to be vertical for the simplification. The fault runs between Caverns

103 and 104, Caverns 108 and 109, and Caverns 113 and 114. The fault is assumed to extend down to the top of Salt Dome from the surface.

The interior of the model consists of material blocks Salt Dome, Caprock 1, and Caprock 2. It is idealized as an elliptical cylinder with its 7000 ft major diameter in the N-S direction, 5800 ft minor diameter in the E-W direction, and being 5700 ft high (the salt dome is 4370 ft high). Fourteen cavern blocks exist inside the Salt Dome block. All caverns are idealized as cylinders 1850 ft high with 220 ft diameters. The cylinder blocks are surrounded by five onion ring blocks to idealize five drawdowns. The thickness of ring increases from inside to outside with 8.5, 9.1, 9.8, 10.6, and 11.4 ft to idealize 16% volume increments. The top of caverns is 660 ft down from the top of salt (2290 ft below the surface).

Figure 20 shows the assembled mesh and the boundary conditions. The salt dome is modeled as being subjected to a regional far-field stresses acting from an infinite distance away. The lengths of the confining boundaries are 14,000 ft (two times the dome's major diameter) in the N-S direction and 11,600 ft (two times the dome's minor diameter) in the E-W direction. The mesh consists of 554,540 nodes and 545,580 elements with 19 element blocks, 6 node sets, and 84 side sets. The mesh was created using CUBIT† version 13.0.

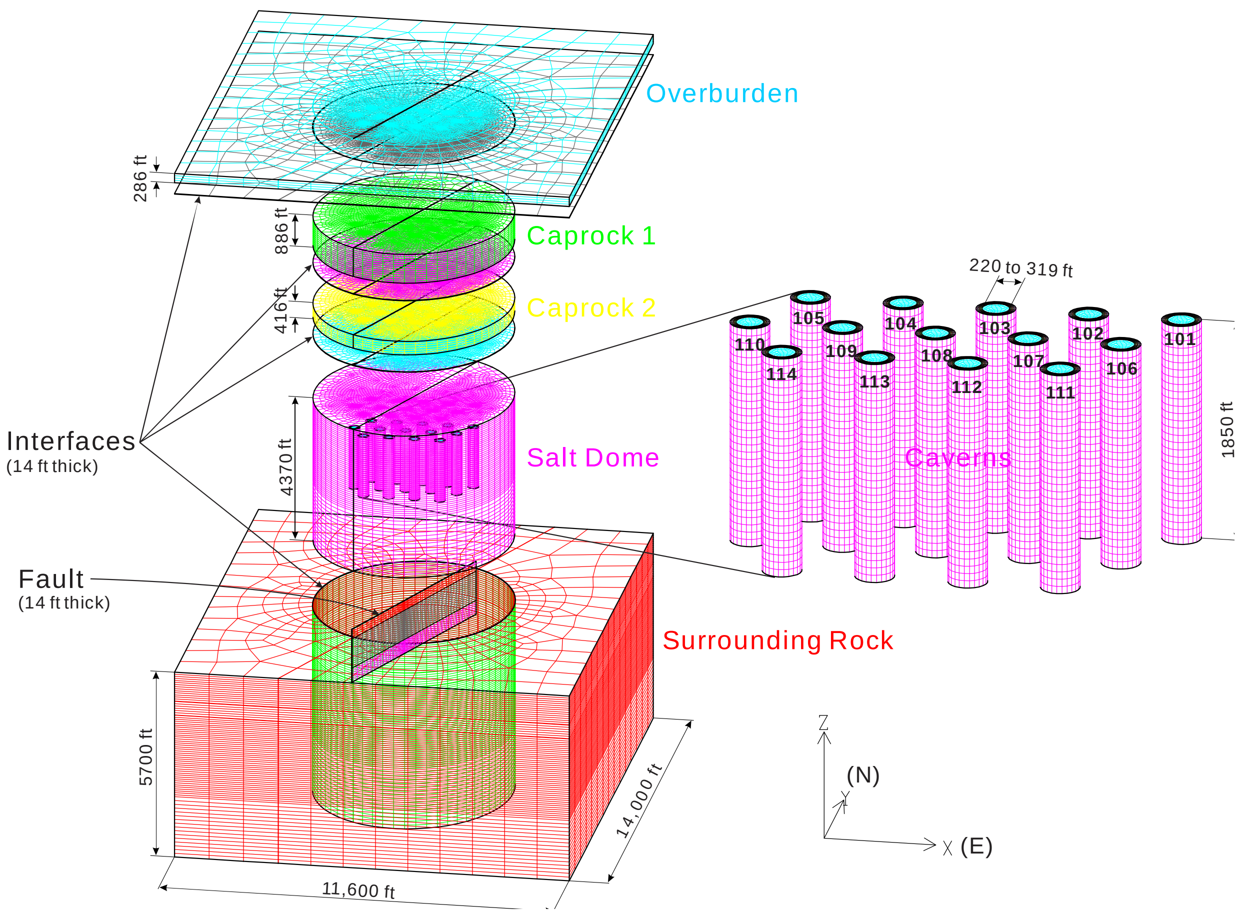



**Figure 19: Overview of the finite element mesh of the stratigraphy and cavern field at Big Hill.**

† A mesh generation software copyrighted by Sandia Corporation

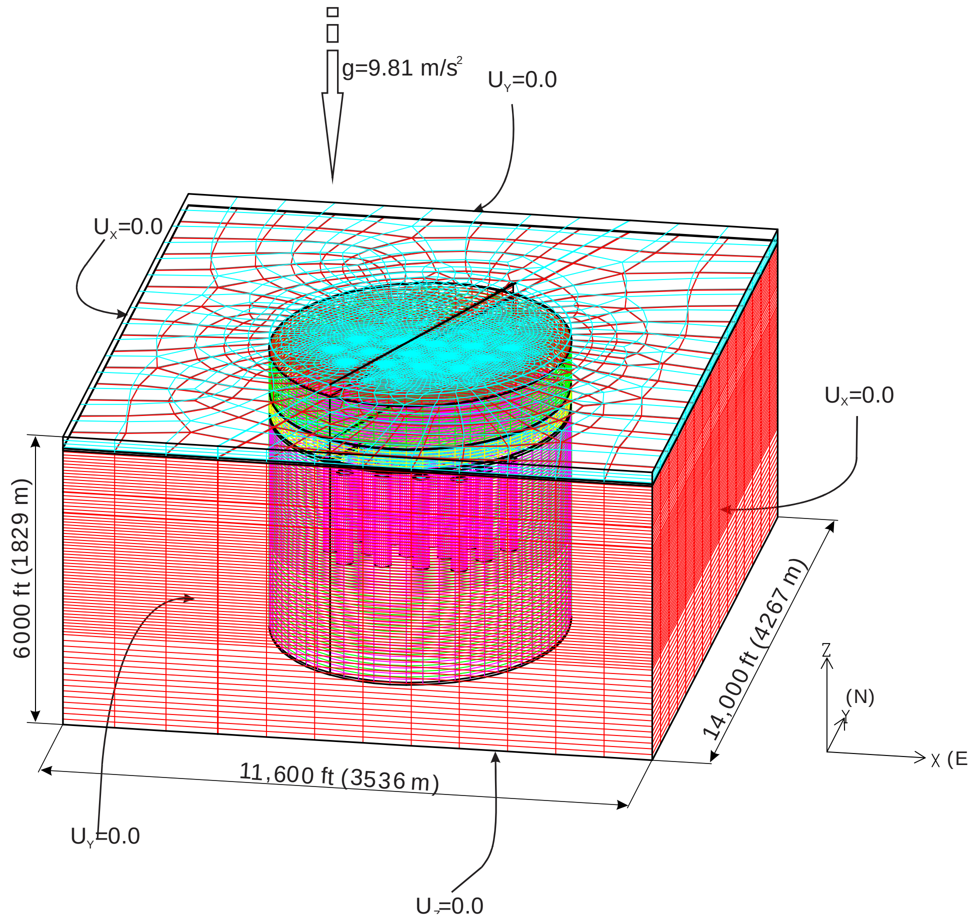



**Figure 20: Finite mesh discretization and boundary conditions at Big Hill.**

## 3.6. Test Objective

This test case will be used to specifically verify the following functional requirements:

- Computes the quasi-static, inelastic response of 3-dimensional solids using a nonlinear conjugate gradient solution algorithm.
- Use hexahedral element with hour glass control.
- Apply initial stress as the element variable.
- Apply no displacement kinematic boundary conditionss.
- Use a pressure boundary condition according to user defined subroutine.
- Models multilayer, multi-material stratigraphy of large physical extent.
- Individually control time intervals in the solution period.
- Use the Power Law Creep (PLC) model.
- Use the Soil and Foams model.
- Use the Drucker-Prager (D-P) yield criterion
- Apply a gravity body force.

The following external interface requirements are also not specifically addressed, but are verified implicitly:

- ASCII input
- GENESIS mesh file
- EXODUS output
- ASCII output

Adagio results will be compared to the results using previously qualified code JAS3D.

## 3.7. Input/Output

This test was run on RedSky Unclassified SRN which is assembled in the space where legendary system ASCI Red once stood. Red Sky was open for limited user availability in January 2010. RedSky on SRN has 2,816 nodes / 22,528 cores.

The input decks for JAS3D and Adagio are provided in Appendix III-A and B, respectively.

## 3.8. Evaluation of Results

The analysis using JAS3D version 2.4.C was originally performed on RedSky which Adagio is currently installed on. The detail descriptions of the analysis results are provided in Park and Ehgartner [2012].

Figure 21 shows a comparison of overall volumetric closure normalized to overall storage volume for the fourteen SPR caverns immediately following each leach between JAS3D and Adagio, over the entire simulation period of 56 years. The Adagio results are indicated by symbols. The Adagio results lie on top of the JAS3D results.

Figure 22 shows a comparison between the JAS3D and Adagio results for the volume change of each cavern due to salt creep during the first 11 years. The JAS3D results are indicated by symbols. The JAS3D results match the Adagio results.

Figure 23 shows a comparison between the JAS3D and Adagio results for the predicted relative displacements between Caprock2 and Salt Dome blocks right above the center of each cavern over time. The Adagio results are indicated by dashed lines. The Adagio results are in excellent agreement with the JAS3D results.

JAS3D was previously qualified for use in the SPR program. Overall, since the Adagio results lie match the JAS3D results very closely, Adagio is judged to be performing satisfactorily.

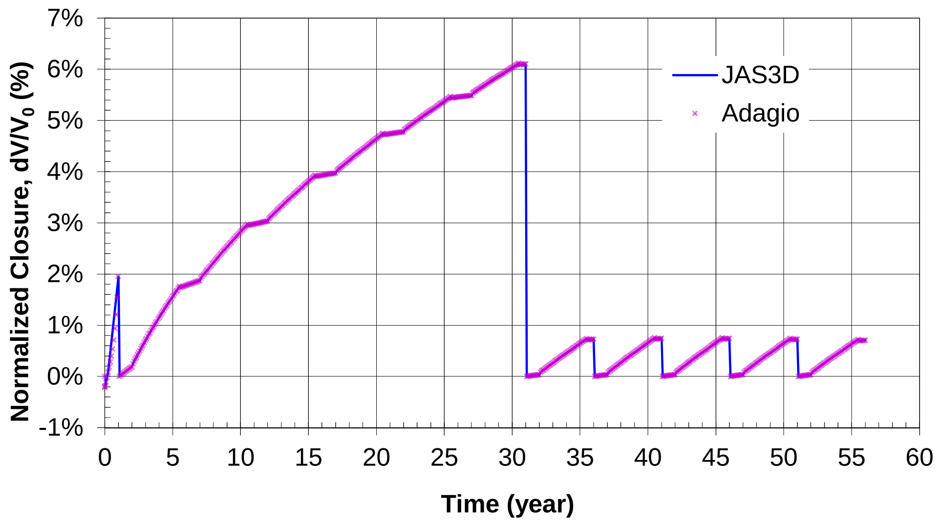
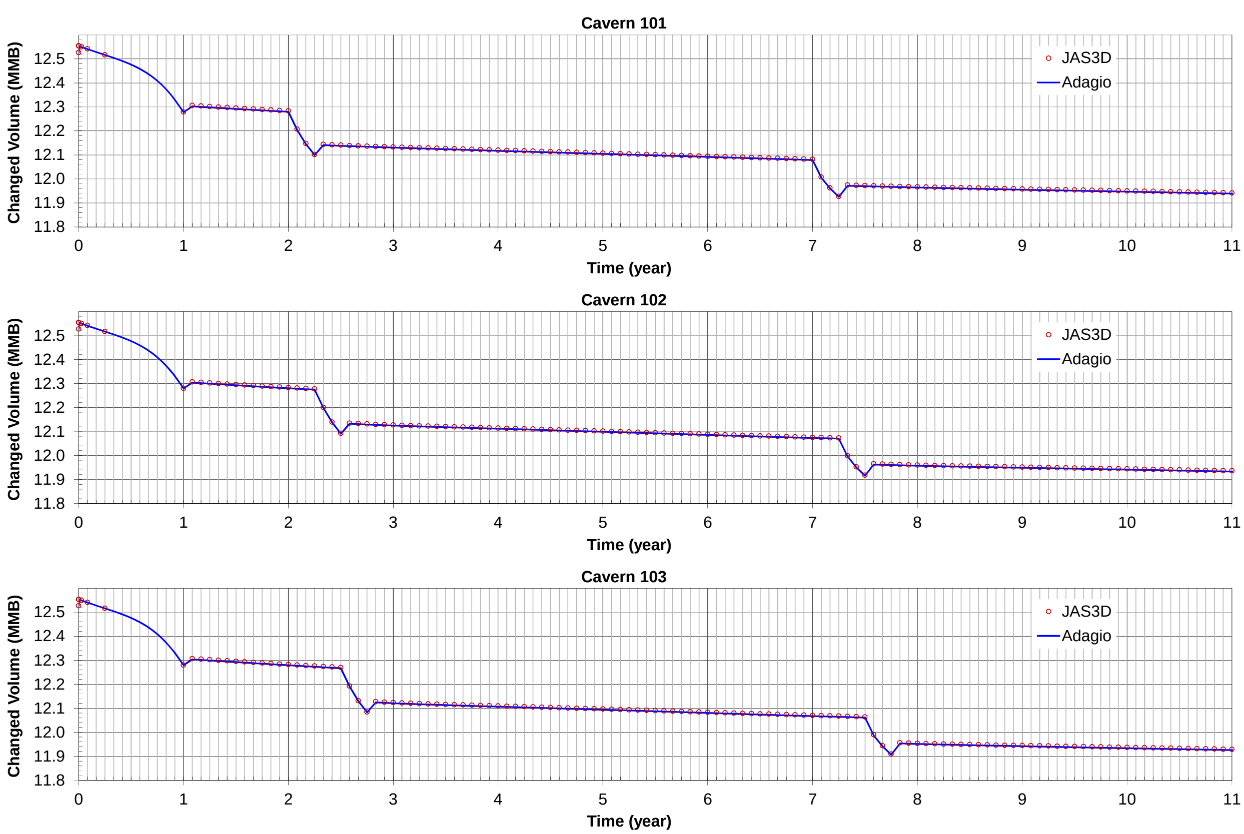
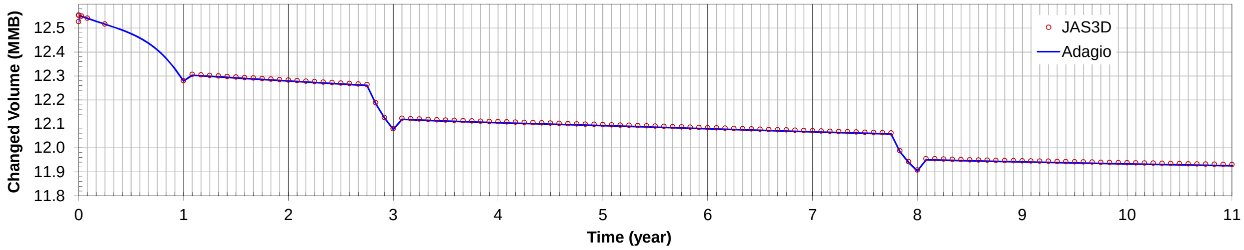


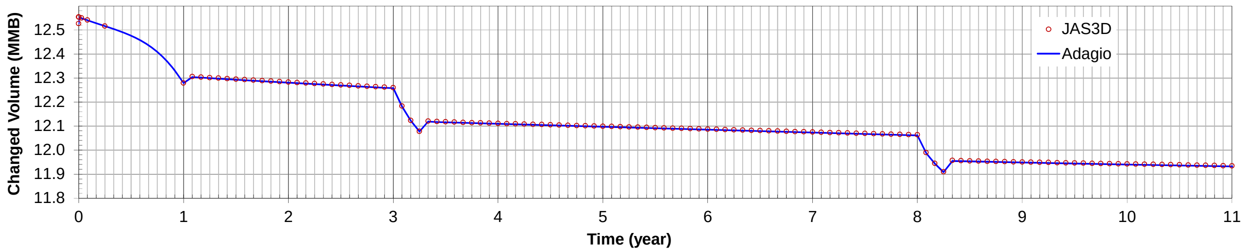

**Figure 21: Comparison of overall volumetric closure normalized to overall storage volume for the fourteen SPR caverns immediately following each leach between JAS4D and Adagio. Adagio results are indicated by symbols.**



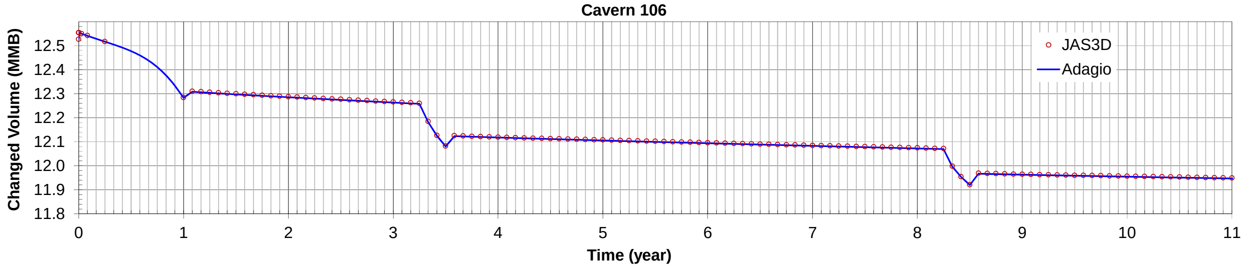
Cavern 104



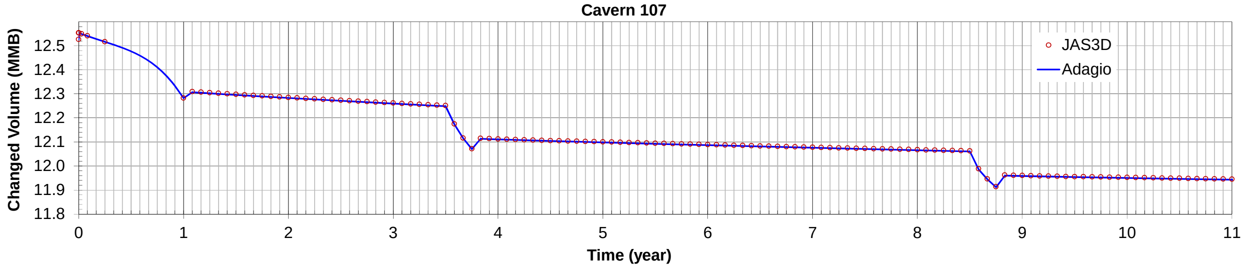

Cavern 105



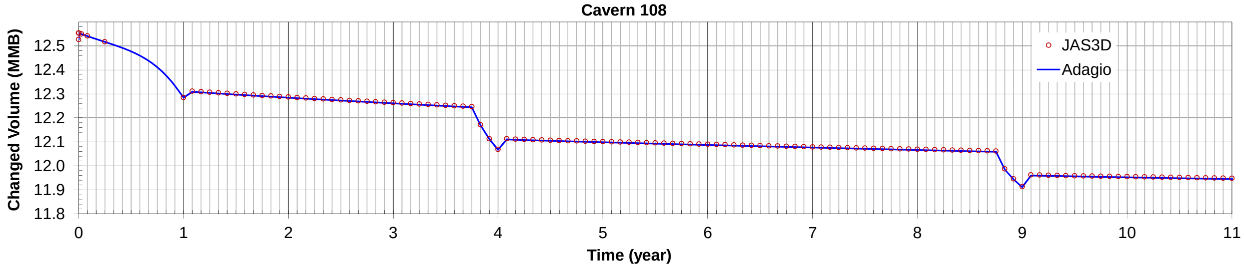

Cavern 106



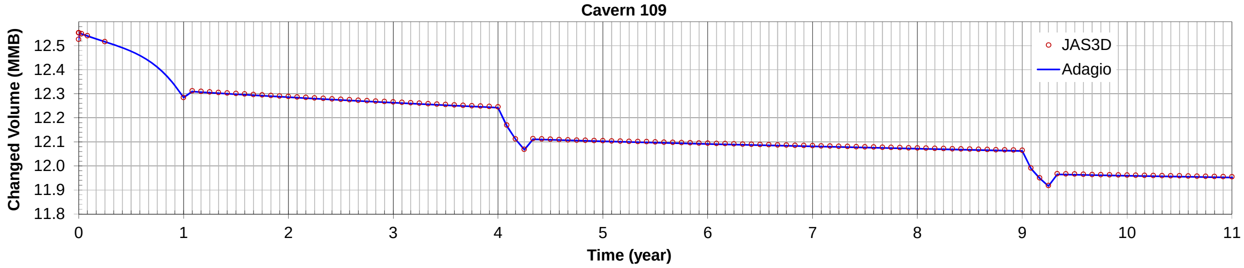

Cavern 107




Cavern 108




Cavern 109



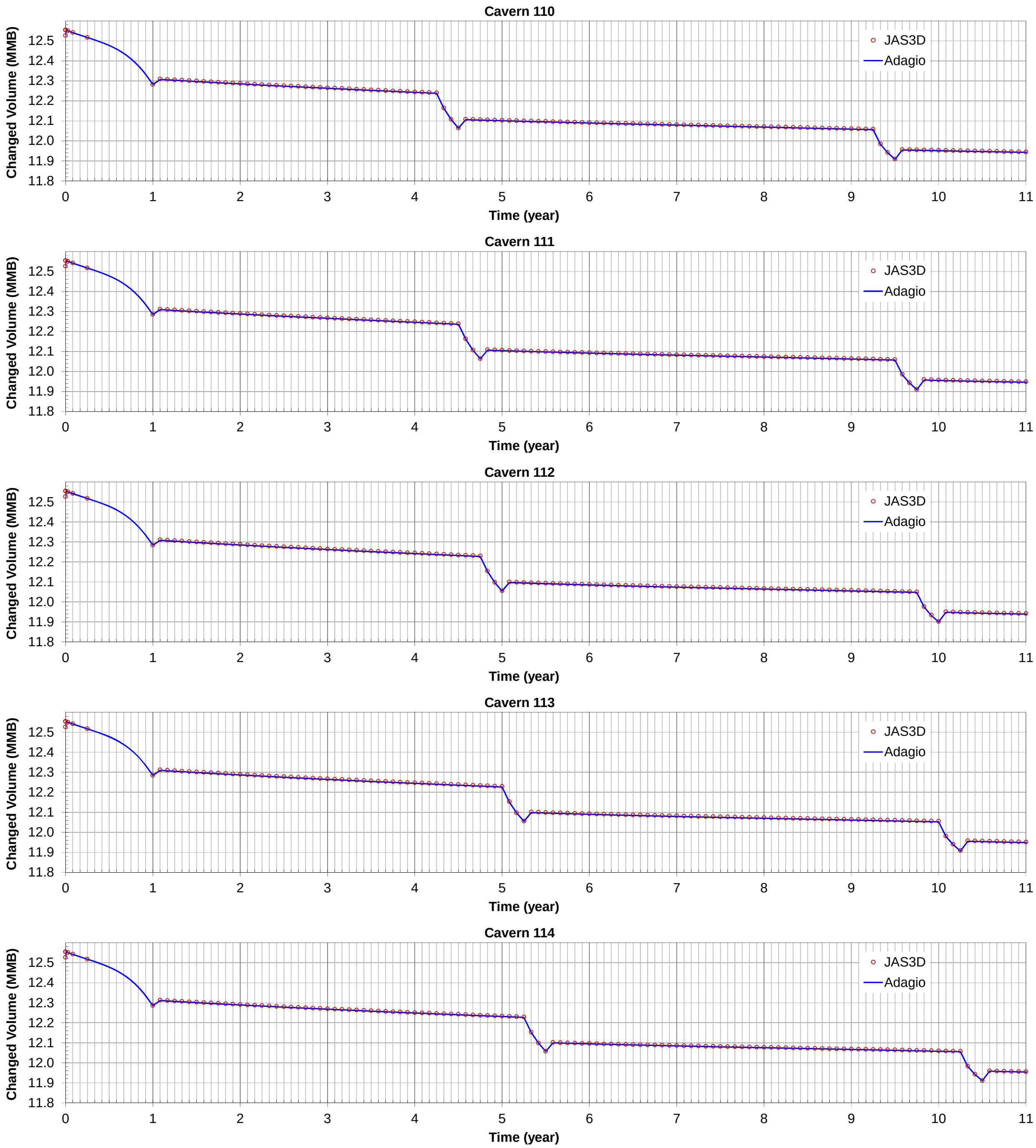
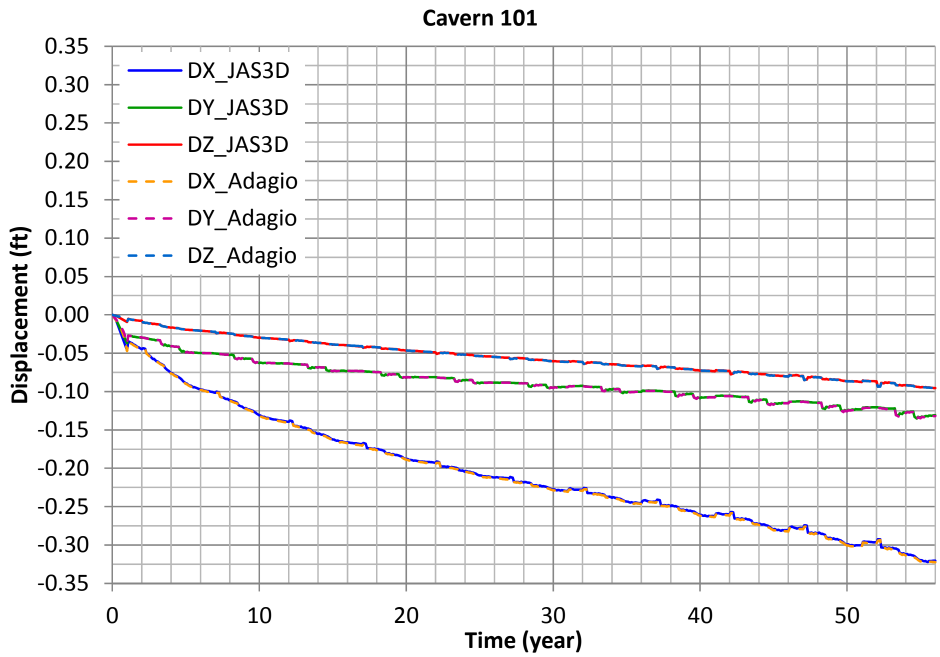
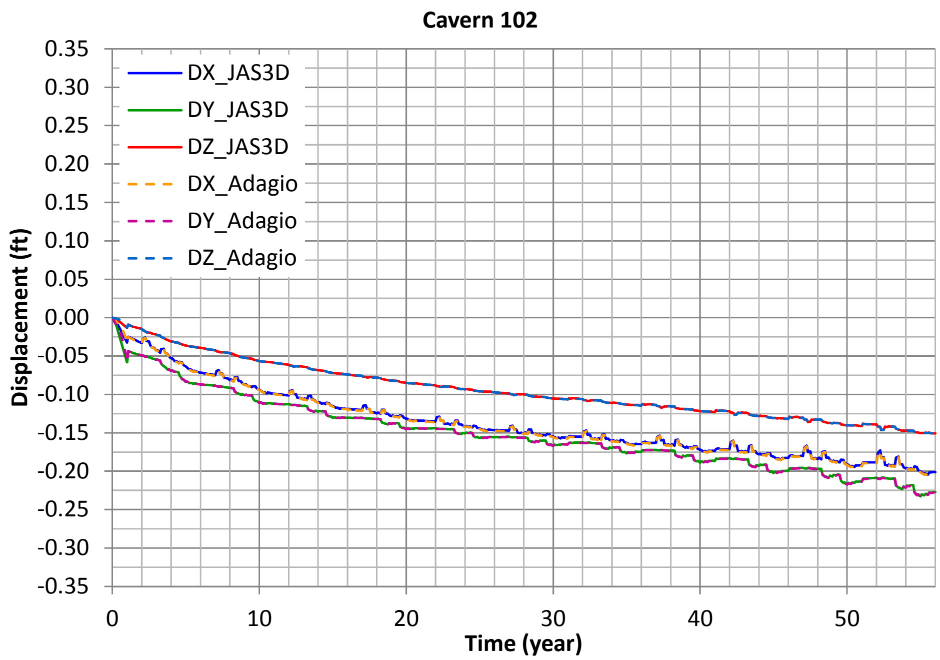


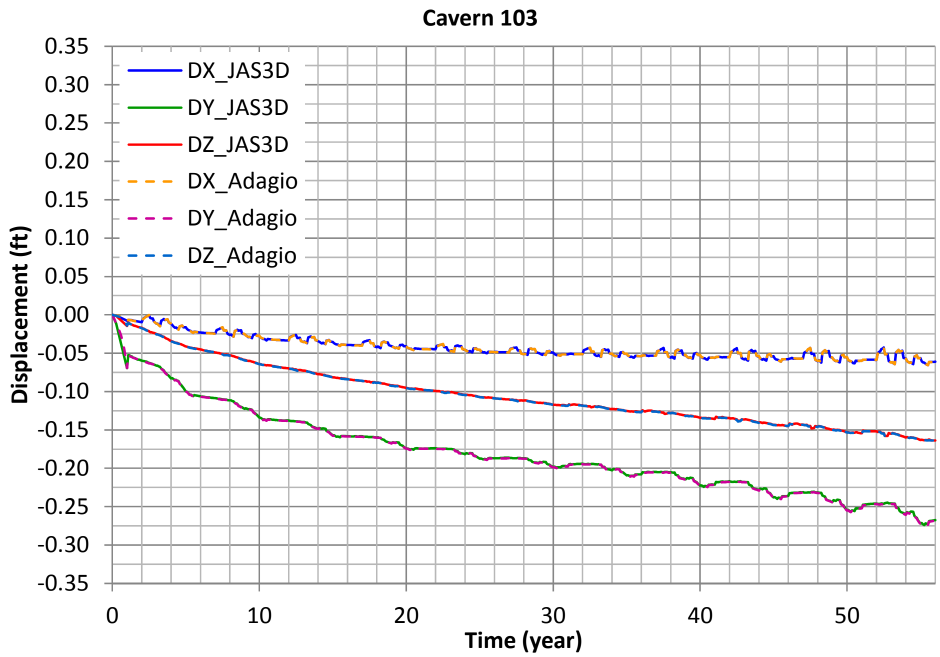

**Figure 22: Comparison between the JAS3D and Adagio results for the volume change of each cavern due to salt creep for first 11 years. JAS3D results are indicated by symbols.**

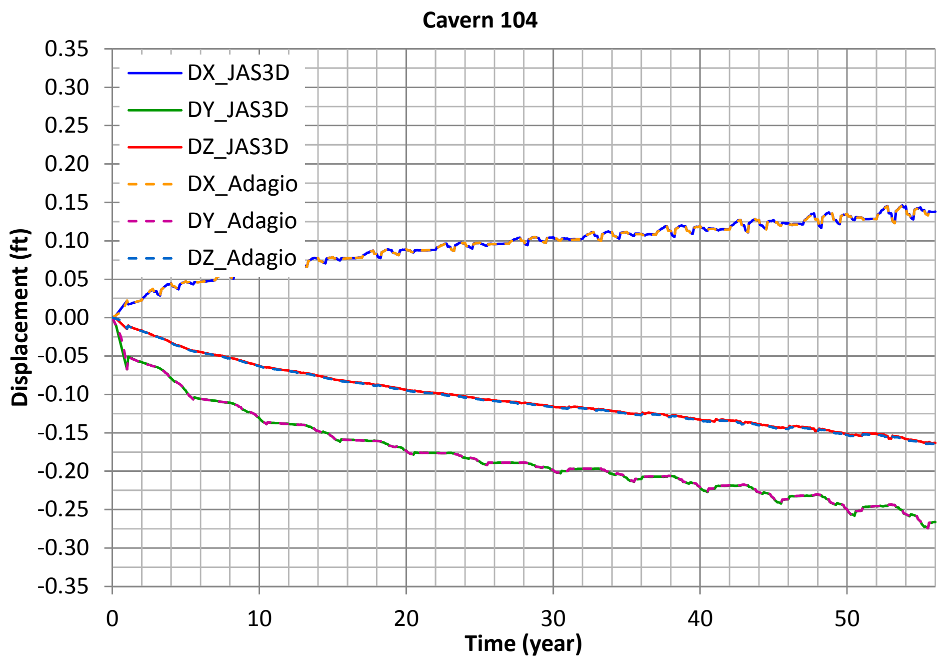


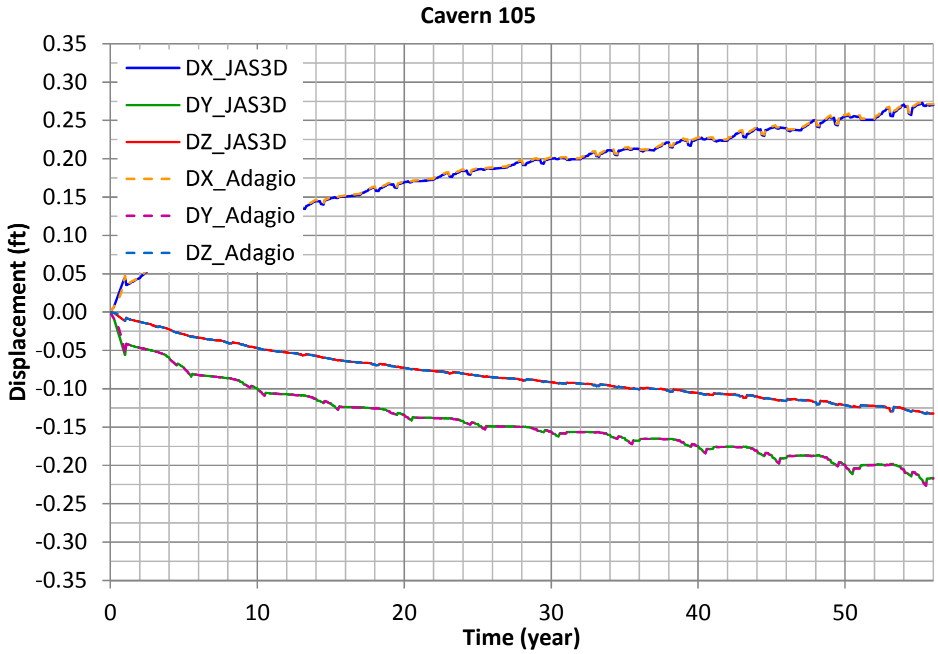
Cavern 101
Displacement (ft)
Time (year)
DX_JAS3D
DY_JAS3D
DZ_JAS3D
DX_Adagio
DY_Adagio
DZ_Adagio
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
-0.05
-0.10
-0.15
-0.20
-0.25
-0.30
-0.35
0
10
20
30
40
50

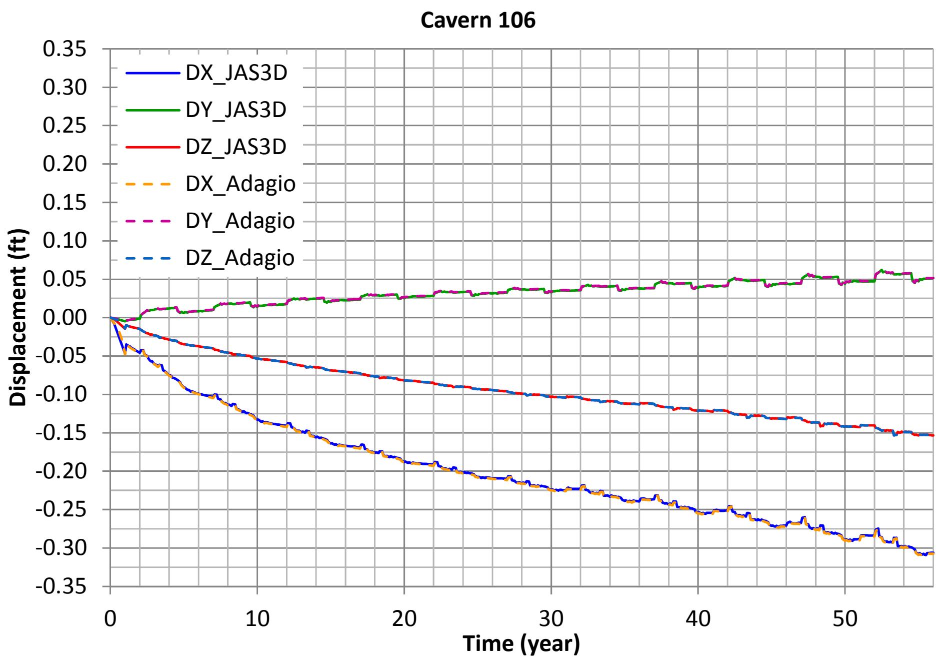



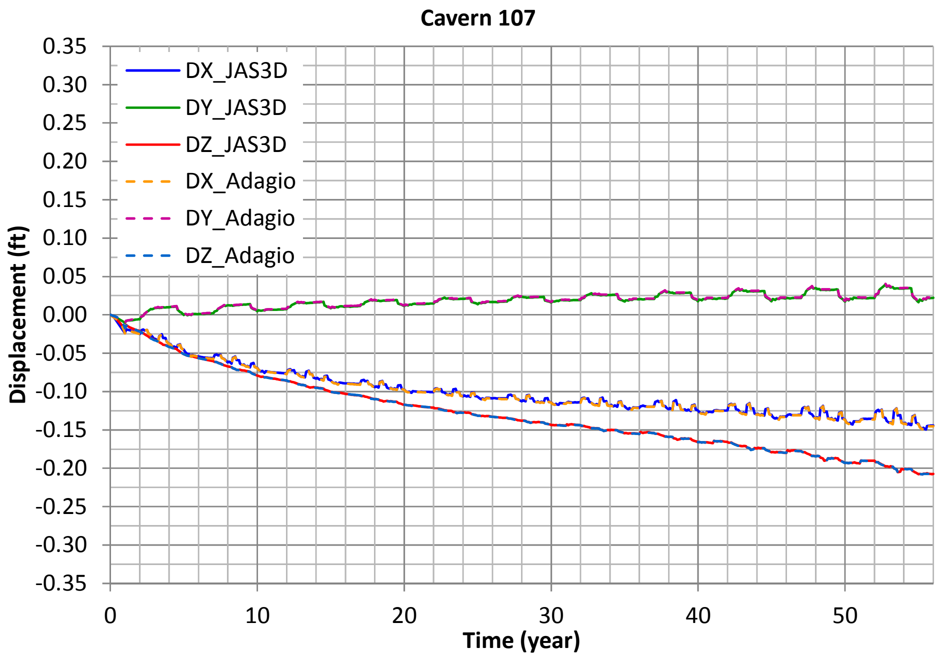
Cavern 102
Displacement (ft)
Time (year)
DX_JAS3D
DY_JAS3D
DZ_JAS3D
DX_Adagio
DY_Adagio
DZ_Adagio
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
-0.05
-0.10
-0.15
-0.20
-0.25
-0.30
-0.35
0
10
20
30
40
50

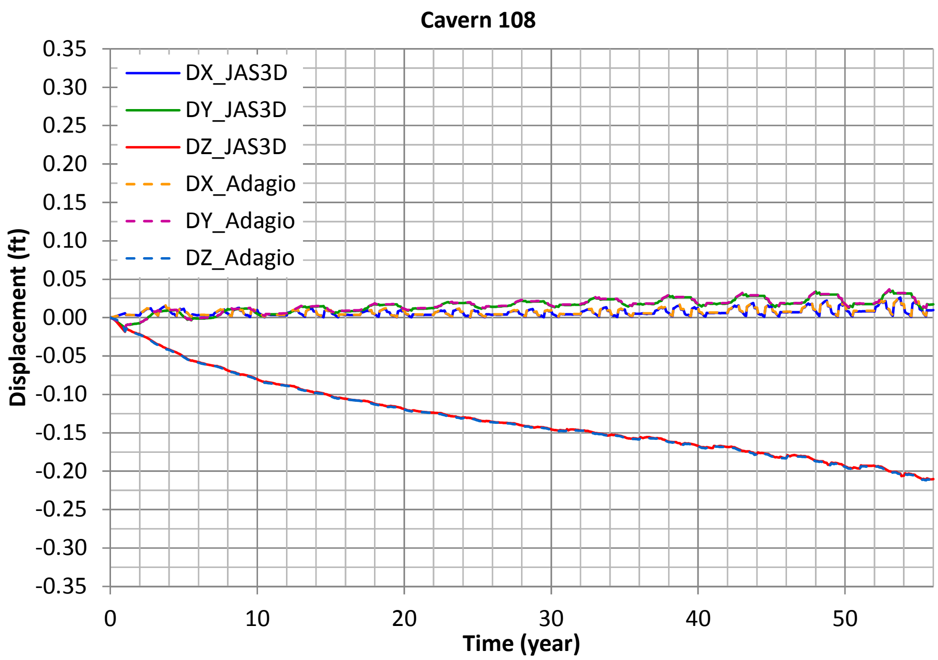

Cavern 103
DX_JAS3D
DY_JAS3D
DZ_JAS3D
DX_Adagio
DY_Adagio
DZ_Adagio
Displacement (ft)
Time (year)

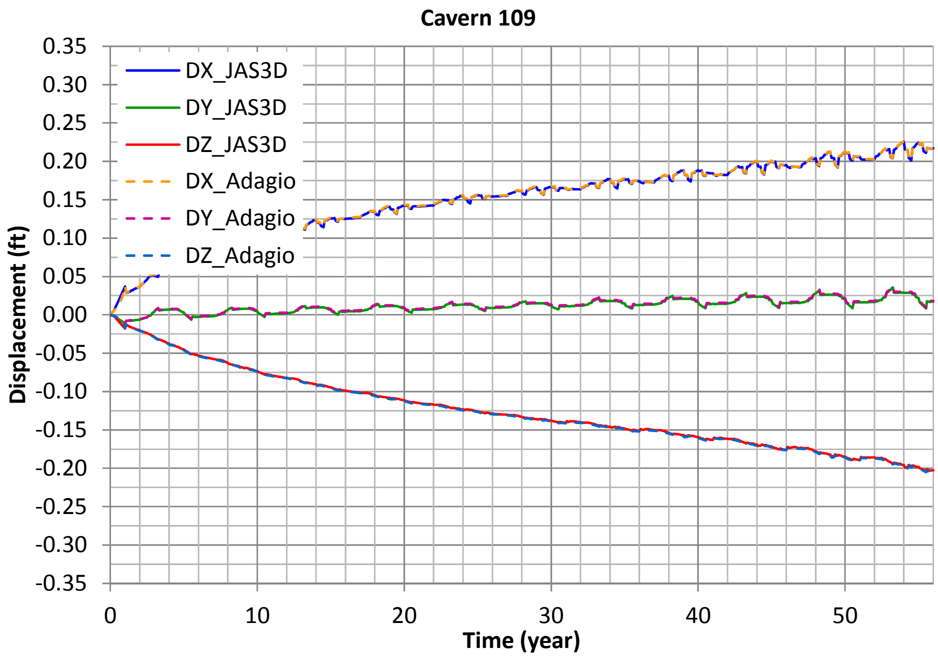

Cavern 104
DX_JAS3D
DY_JAS3D
DZ_JAS3D
DX_Adagio
DY_Adagio
DZ_Adagio
Displacement (ft)
Time (year)

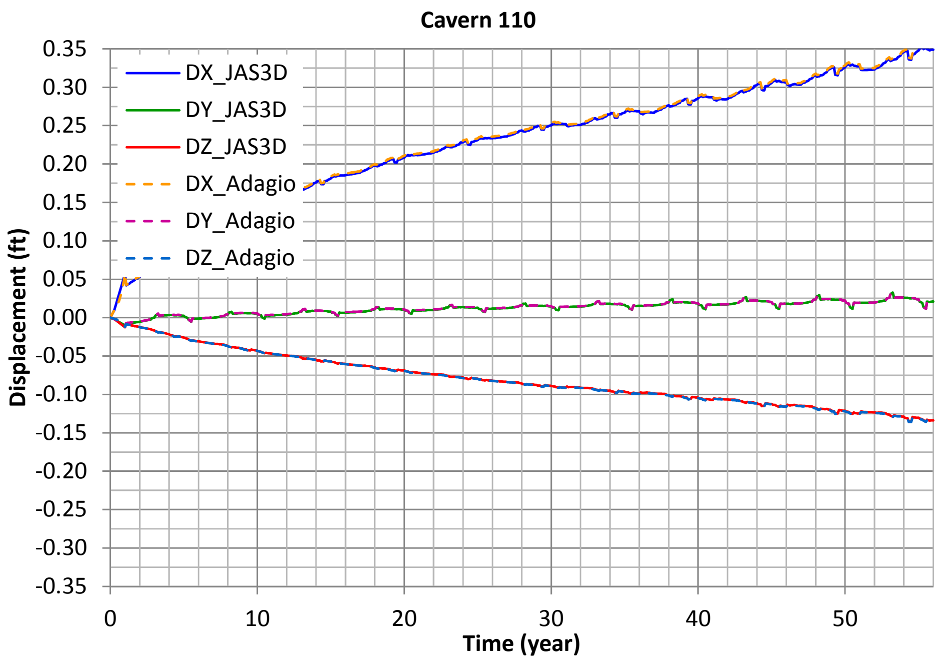

Cavern 105
Displacement (ft)
Time (year)
DX_JAS3D
DY_JAS3D
DZ_JAS3D
DX_Adagio
DY_Adagio
DZ_Adagio
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
-0.05
-0.10
-0.15
-0.20
-0.25
-0.30
-0.35
0
10
20
30
40
50

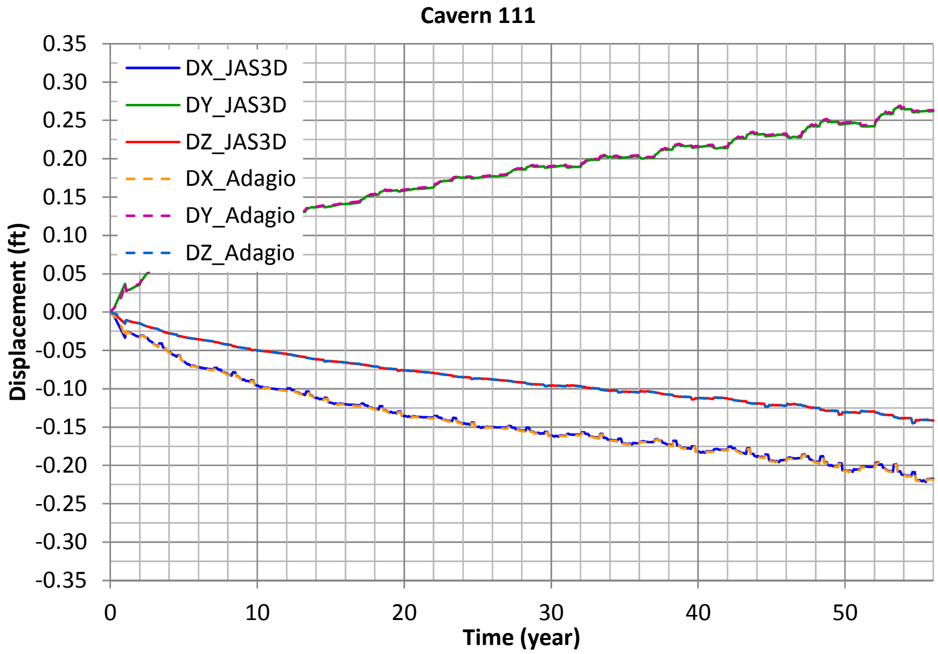

Cavern 106
Displacement (ft)
Time (year)
DX_JAS3D
DY_JAS3D
DZ_JAS3D
DX_Adagio
DY_Adagio
DZ_Adagio
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
-0.05
-0.10
-0.15
-0.20
-0.25
-0.30
-0.35
0
10
20
30
40
50


Cavern 107
DX_JAS3D
DY_JAS3D
DZ_JAS3D
DX_Adagio
DY_Adagio
DZ_Adagio
Displacement (ft)
Time (year)
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
-0.05
-0.10
-0.15
-0.20
-0.25
-0.30
-0.35
0
10
20
30
40
50

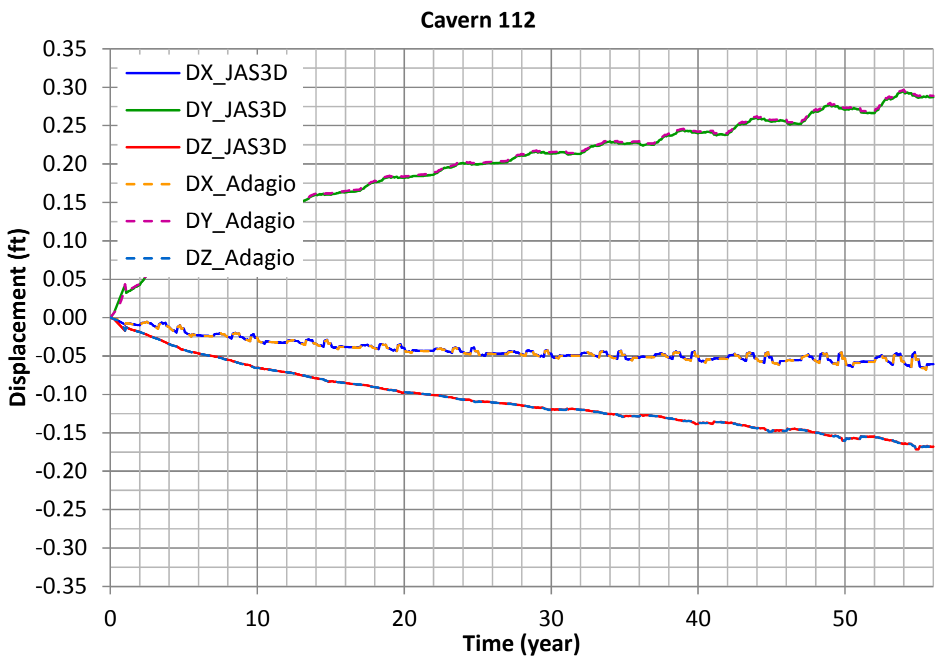

Cavern 108
DX_JAS3D
DY_JAS3D
DZ_JAS3D
DX_Adagio
DY_Adagio
DZ_Adagio
Displacement (ft)
Time (year)
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
-0.05
-0.10
-0.15
-0.20
-0.25
-0.30
-0.35
0
10
20
30
40
50


Cavern 109
DX_JAS3D
DY_JAS3D
DZ_JAS3D
DX_Adagio
DY_Adagio
DZ_Adagio
Displacement (ft)
Time (year)
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
-0.05
-0.10
-0.15
-0.20
-0.25
-0.30
-0.35
0
10
20
30
40
50

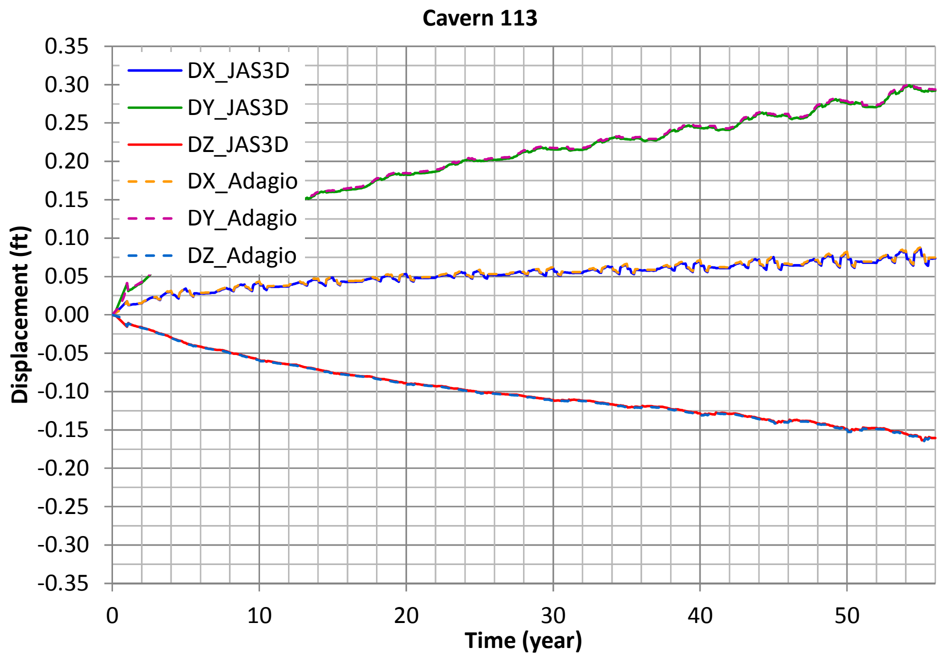

Cavern 110
DX_JAS3D
DY_JAS3D
DZ_JAS3D
DX_Adagio
DY_Adagio
DZ_Adagio
Displacement (ft)
Time (year)
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
-0.05
-0.10
-0.15
-0.20
-0.25
-0.30
-0.35
0
10
20
30
40
50



Cavern 111
DX_JAS3D
DY_JAS3D
DZ_JAS3D
DX_Adagio
DY_Adagio
DZ_Adagio
Displacement (ft)
Time (year)
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
-0.05
-0.10
-0.15
-0.20
-0.25
-0.30
-0.35
0
10
20
30
40
50

Cavern 112
DX_JAS3D
DY_JAS3D
DZ_JAS3D
DX_Adagio
DY_Adagio
DZ_Adagio
Displacement (ft)
Time (year)
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
-0.05
-0.10
-0.15
-0.20
-0.25
-0.30
-0.35
0
10
20
30
40
50



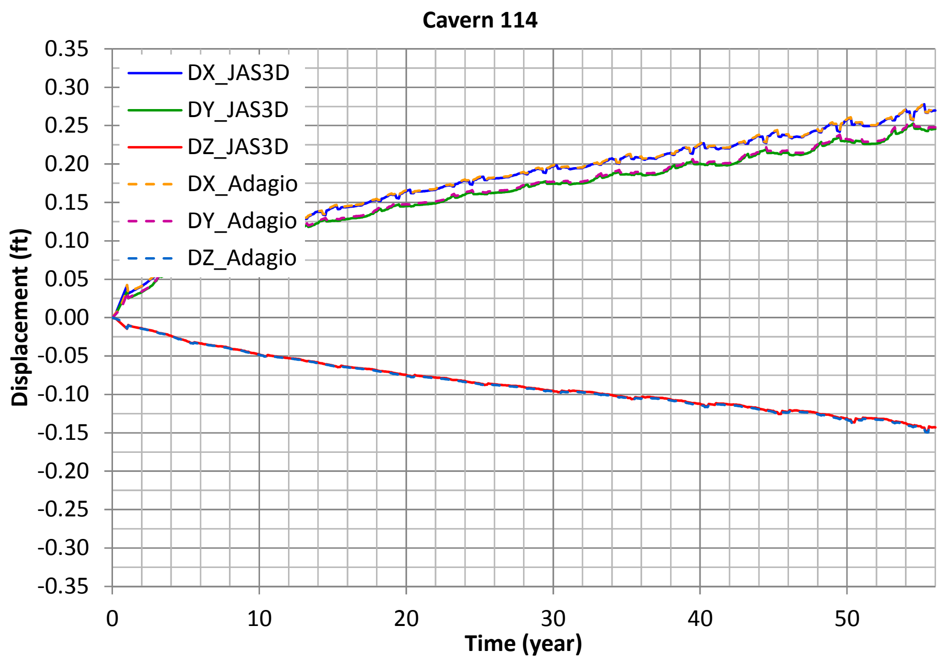




**Figure 23: Comparison between the JAS3D and Adagio results for the predicted relative displacements between Caprock2 and Salt Dome right above the center of each cavern over time. Adagio results are indicated by dashed lines.**

# 4. CONCLUSIONS AND RECOMMENDATIONS

To validate the transition from JAS3D to Adagio, the existing JAS3D input decks and user subroutines for Bayou Choctaw and Big Hill models were converted for use with Adagio. The calculation results from the Adagio runs are compared to the JAS3D. Since the Adagio results are very similar to the JAS3D results, Adagio is judged to be performing satisfactorily.

The Adagio is now the primary code for SPR geomechanical analyses. Several additional validation tests are recommended to be performed to complete the present code validation.

- Kayenta model – The Big Hill wellbore model is constructued to predict well casing damage. The Sandia Geomodel, which is a constitutive model in JAS3D that can be used to express cement behavior, is contained in the wellbore model. The Geomodel was not validated for parallel computing environments, and is no longer supported. The Kayenta model is the successor of the Geomodel in Adagio.
- Elastic-Plastic model – Elastic-plastic linear hardening models are used to model materials, typically metals, that undergoing plastic deformation at finite strains. Linear hardening generally refers to the shape of a uniaxial stress-strain curve where the stress increases linearly with the plastic, or permanent, strain. This model is contained in the wellbore model to express the steel casing behavior.
- Multimechanism Deformation (M-D) model – This constitutive model considers three fundamental features of a creeping material such as a steady-state creep rate, a transient strain limit, and both a work-hardening and recovery time rate of change [Sobolik, et al., 2010]. The M-D model will be used for future SPR analyses.
- Contact surface algorithm – This model is used to express the interbeds between lithologies, and the interfaces between the material blocks for future SPR analyses.

# 5. REFERENCES


Ballard, S. and B.L. Ehgartner, 2000, *CAVEMAN Version 3.0: System for SPR Cavern Pressure Analysis,* SAND2000-1751, Sandia National Laboratories, Albuquerque, NM 87185-0750.

Butcher, B.M. 1997. *A Summary of the Sources of Input Parameter Values for the WIPP Final Porosity Surface Calculations*, SAND97-0796, Albuquerque, NM: Sandia National Laboratories.

Carmichael, R. S., 1984, *CRC Handbook of Physical Properties of Rocks*, CRC (Chemical Rubber Company) Press, Inc. Boca Raton, Fl.

Ehgartner, B. L., S. Bauer, C. Rautman, T. Hinkebein, and S. Wallace, 2003, *Bayou Choctaw 20 Raw Water Drawdown*, Letter to Robert E. Myers, DOE SPR PMO FE-4421 dated April 23, 2003, Sandia National Laboratories, Albuquerque, NM.

Ehgartner, B.L. and S. Bauer, 2004, *Large Scale Salt Deformation: Comments on Subsidence Using Thermal, Creep and Dissolution Modeling to Assess Volumetric Strain*, SAND2004-0095C, Sandia National Laboratories, Albuquerque, NM 87185.

Ehgartner, B.L., 2010, *Ullage Losses*, Memorandum from B. Ehgartner to R.E. Myers, DOE SPR PMO dated October 27, 2010. Sandia National Laboratories, Albuquerque, New Mexico.

Hoffman, E.L., 1992, *Investigation of Analysis Assumptions for SPR Calculations,* memo to J. K. Linn dated February 7, 1992, Sandia National Laboratories, Albuquerque, New Mexico.

Hogan, R. G., 1980, *Strategic Petroleum Reserve (SPR) Geological Site Characterization Report Bayou Choctaw Salt Dome*, SAND80-7140, Sandia National Laboratories, Albuquerque, New Mexico.

Hull, J., 1988. *Thickness-displacement relationships for deformation zones,* J. Struct. Geol., 10, 431-435.

Krieg, R. D., 1984, *Reference Stratigraphy and Rock Properties for the Waste Isolation Pilot Plant (WIPP) Project*, SAND83-1908, Sandia National Laboratories, Albuquerque, NM 87185.

Magorian, T.R, and J.T. Neal, 1988. *Strategic Petroleum Reserve (SPR) Addition Geological Site Characterization Studies Big Hill Salt Dome, Texas*, SAND88-2267**,** Albuquerque, NM: Sandia National Laboratories.

Mohr, P.J., B.N. Taylor, and D.B. Newell, 2011, *The 2010 CODATA Recommended Values of the Fundamental Physical Constants (Web Version 6.0)*, Available at http://physics.nist.gov/constants, National Institute of Standards and Technology, Gaithersburg, MD 20899.

Neal, J. T., T. R Magorian, K. O. Byrne, and S. Denzler, 1993, *Strategic Petroleum Reserve (SPR) Additional Geologic Site Characterization Studies Bayou Choctaw Salt Dome, Louisiana*, SAND92-2284, Sandia National Laboratories, Albuquerque, New Mexico 87185, Livermore, California 94550.

Park, B.Y., B.L. Ehgartner, M.Y. Lee, and S.R. Sobolik, 2005. *Three Dimensional Simulation for Big Hill Strategic Petroleum Reserve (SPR)*, SAND2005-3216, Sandia National Laboratories, Albuquerque, NM.

Park, B.Y., B.L. Ehgartner, and M.Y. Lee, 2006. *Three Dimensional Simulation for Bayou Choctaw Strategic Petroleum Reserve (SPR)*, SAND2006-7589, Sandia National Laboratories, Albuquerque, NM.

Park, B.Y., B.L. Ehgartner, 2012, *Interface Modeling to Predict Well Casing Damage for Big Hill Strategic Petroleum Reserve*, SAND2012-1206, Sandia National Laboratories, Albuquerque, NM.

Rautman, C.A. and A.S. Lord, 2007. *Sonar Atlas of Caverns Comprising the U.S. Strategic Petroleum Reserve Volume 2: Big Hill Site, Texas*, SAND2007-6023, Sandia National Laboratories, Albuquerque, NM.

Sattler, A. and B. Ehgartner, 2011. *Big Hill Logging Results with the Weatherford Multi Arm Caliper Tasks 1.1.4 Activity a1 and Task 1.1.6 activity a1*, Letter report to Robert E. Myer, DOE Project Manager, dated June 7, 2011.

Shipton, Z.K., A.M. Soden, J.D. Kirkpatrick, A.M. Bright, and R.J. Lunn, 2006. *How thick is a fault? Fault displacement-thickness scaling revisited. In Abercrombie,* R. (Eds) Earthquakes: Radiated Energy and the Physics of Faulting, pages pp. 193-198, AGU.

Sobolik, S.R., J.E. Bean, and B.L. Ehgartner, 2010. *Application of the Multi-Mechanism Deformation Model for Three-Dimensional Simulations of Salt Behavior for the Strategic Petroleum Reserve*, the 44$^{th}$ US Rock Mechanics Symposium and 5$^{th}$ U.S.-Canada Rock Mechanics Symposium held in Salt Lake City, TU June 27-30, 2010.

Stein, J. S., 2005, *RE: Data of Bayou Choctaw*, E-mail to B.Y. Park, Sandia National Laboratories, Carlsbad, NM, dated July 11, 2005.

# APPENDIX I: COMMON FILES

## I-A. Units.txt

```
$Unit conversion (A_B = A to B):
$
$Angular:
$ rad  = {rad_deg  =180/3.1415926536} deg
$ deg  = {deg_rad  =1/rad_deg} rad
$
$Length:
$ mm   = {mm_m=0.001 } m
$ m    = {m_mm=1/mm_m} mm
$ cm   = {cm_mm=10 } mm
$ mm   = {mm_cm=1/cm_mm} cm
$ cm   = {cm_m=0.01  } m
$ m    = {m_cm=1/cm_m} cm
$ ft   = {ft_m=0.3048} m
$ m    = {m_ft=1/ft_m} ft
$ in   = {in_m=0.0254} m
$ m    = {m_in=1/in_m} in
$
$Pressure:
$ MPa  = {MPa_Pa  = 1E6} Pa
$ Pa   = {Pa_MPa  = 1/MPa_Pa} MPa
$ psi  = {psi_Pa=6894.757} Pa
$ Pa   = {Pa_psi=1/psi_Pa} psi
$ Pa   = {Pa_psf=0.0208854} psf
$ psf  = {psf_Pa=1/Pa_psf} Pa
$ MPa  = {MPa_psf=MPa_Pa*Pa_psf} psf
$ MPa  = {MPa_psi=MPa_Pa*Pa_psi} psi
$ psf  = {psf_psi=psf_Pa*Pa_psi} psi
$
$Time:
$ mus  = {mus_s   = 1e-6         } s
$ min  = {min_s   = 60           } s
$ h    = {h_min   = 60           } min
$ d    = {d_h     = 24           } h
$ mon  = {mon_d   = 30.4166666667} d
$ yr   = {yr_d    = 365          } d
$ dec  = {dec_yr  = 10           } yr
$ cen  = {cen_dec = 10           } dec
$ mil  = {mil_cen = 10           } cen
$ h    = {h_s     = h_min*min_s  } s
$ d    = {d_s     = d_h*h_s      } s
$ mon  = {mon_s   = mon_d*d_s    } s
$ yr   = {yr_s    = yr_d*d_s     } s
$ dec  = {dec_s   = dec_yr*yr_s  } s
$ cen  = {cen_s   = cen_dec*dec_s} s
$ mil  = {mil_s   = mil_cen*cen_s} s
$ s    = {s_mus   = 1/mus_s      } mus
$ s    = {s_min   = 1/min_s      } min
$ s    = {s_h     = 1/h_s        } h
$ s    = {s_mon   = 1/mon_s      } mon
$ s    = {s_yr    = 1/yr_s       } yr'
```

## I-B. BC_stratigraphy.txt

```
$ Thicknesses of each layer
$
$ thickness of overburden:    t_OB={t_OB=500*ft_m} m
$ thickness of caprock:       t_CR={t_CR=150*ft_m} m
$ height of salt dome:        h_SD={h_SD=7350*ft_m} m
$ thickness of surrounding rock:t_SR={t_SR=t_CR+h_SD} m
```

## I-C. BC_materials_PLC.txt

```
$=======================================================================
$Material Properties
$
$Common:
$ NAME______VALUE_______________________Description_(UNIT)___________
$ T         = {T=300}                $ Absolute temperature (K)
$ R         = {R=1.9858775}          $      Universal      gas      constant      (cal/(mol*K))
(previous:1.988071571)
$-Reference: "Gas constant" in Wikipedia
$
$Halite at Bayou Choctaw:
$ NAME______VALUE_______________________Description_(UNIT)___________
```

```
$ SMF       = {SMF    = 0.12    }    $ Structure Multiplication Factor from WIPP 25oC Hailite Baseline
$ RF_bch    = {RF_bch = 12.5    }    $ Salt redution factor
$ E_bch     = {E_bch  = 31.0E9}      $ Young's Modulus(Pa)
$ rho_bch   = {rho_bch= 2300.}       $ Density (kg/m^3)
$ nu_bch    = {nu_bch = 0.25}        $ Poisson's Ratio
$ K_bch     = {K_bch  = E_bch/(3.*(1.-2.*nu_bch))}  $ Bulk Modulus (Pa)
$ mu_bch    = {mu_bch = E_bch/(2.*(1.+nu_bch))}     $ Shear Modulus (Pa)
$ n2_bch    = {n2_bch = 4.9}         $ Stress exponent for undefined mechanism
$ A2_bch    = {A2_bch = 9.672E12}    $ Creep constant for undefined mechanism (1/s)
$ A_PLC     = {A_PLC  = 5.79E-36}    $ Creep constant used in power law creep model (Pa^-n/s)
$ Q2_bch    = {Q2_bch = 12000   }    $ Activation energy for undefined mechanism (cal/mol)
$-Temperatures are not applied to each node in the mesh
$-Reference: Kriet, 1984; Morgan and Krieg, 1988
$
$Caprock at Bayou Choctaw:
$ NAME______VALUE_______________________Description_(UNIT)___________
$ E_bcc     = {E_bcc  = 1.572E10}    $ Young's Modulus(Pa)
$ rho_bcc   = {rho_bcc= 2319.   }    $ Density (kg/m^3)
$ nu_bcc    = {nu_bcc = 0.288   }    $ Poisson's Ratio
$-Reference: Hogan,R.G.,1980(SAND80-7140)
$
$
$Overburden:
$ NAME______VALUE_______________________Description_(UNIT)___________
$ E_bco     = {E_bco  = 0.1E9  }     $ Young's Modulus(Pa)
$ rho_bco   = {rho_bco= 1874.  }     $ Density (kg/m^3)
$ nu_bco    = {nu_bco = 0.33   }     $ Poisson's Ratio
$-Reference: -Reference: Hoffman and Ehgartner, 1992 (SAND92-2183c)
$
$Surrounding Rock:
$ NAME______VALUE_______________________Description_(UNIT)___________
$ E_bcs     = {E_bcs  = 35.0e9 }     $ Young's Modulus(Pa) (Carmichael, 1984)
$ rho_bcs   = {rho_bcs= 2500.  }     $ Density (kg/m^3) (Lama and Vutukuri, 1978)
$ nu_bcs    = {nu_bcs = 0.33   }     $ Poisson's Ratio (Lama and Vutukuri, 1978)
$-Reference:
$==========================================================================
```

# I-D. BH_stratigraphy_sftele.txt

```
$ Thicknesses of each layer
$
$ Thickness of soft element {TSE=14.0*ft_m} m
$ thickness of overburden:        t_OB= {t_OB =300*ft_m-TSE} m
$ thickness of under_ob:            t_UOB={t_UOB=TSE} m
$ thickness of caprock (limestone): t_CRL={t_CRL=900*ft_m-TSE} m
$ thickness of under_c1:            t_UC1={t_UC1=TSE} m
$ thickness of caprock (anhydrite): t_CRN={t_CRN=430*ft_m-TSE} m
$ thickness of under_c2:            t_UC2={t_UC2=TSE} m
$ height of salt dome:            h_SD= {h_SD =4370*ft_m} m
$ height of model:                h_MDL={h_MDL=t_OB+t_UOB+t_CRL+t_UC1+t_CRN+t_UC2+h_SD} m
$ thickness of surrounding rock:    t_SR= {t_SR =h_MDL-t_OB-t_UOB} m
$ height of dome perimeter:         h_DP= {h_DP =h_MDL-t_OB} m
$ depth of fault:                 d_FLT={d_FLT=h_MDL} m
```

# I-E. BH_materials_PLC.txt

```
$==========================================================================
$Material Properties
$
$Common:
$ NAME______VALUE_______________________Description_(UNIT)___________
$ T         = {T=300}                $ Absolute temperature (K)
$ R         = {R=1.9858775}          $ Universal gas constant (cal/(mol*K)) (previous:1.988071571)
$-Reference: "Gas constant" in Wikipedia
$
$Halite at Big Hill:
$ NAME______VALUE_______________________Description_(UNIT)___________
$ SMF       = {SMF    = 1.5     }    $ Structure Multiplication Factor from WIPP 25oC Hailite Baseline
$ RF_bhh    = {RF_bhh = 12.5    }    $ Salt redution factor
$ E_bhh     = {E_bhh  = 31.0E9}      $ Young's Modulus(Pa)
$ rho_bhh   = {rho_bhh= 2300.}       $ Density (kg/m^3)
$ nu_bhh    = {nu_bhh = 0.25}        $ Poisson's Ratio
$ K_bhh     = {K_bhh  = E_bhh/(3.*(1.-2.*nu_bhh))}  $ Bulk Modulus (Pa)
$ mu_bhh    = {mu_bhh = E_bhh/(2.*(1.+nu_bhh))}     $ Shear Modulus (Pa)
$ n2_bhh    = {n2_bhh = 4.9}         $ Stress exponent for undefined mechanism
$ A2_bhh    = {A2_bhh = 9.672E12}    $ Creep constant for undefined mechanism (1/s)
$ A_PLC     = {A_PLC  = 5.79E-36}    $ Creep constant used in power law creep model (Pa^-n/s)
$ Q2_bhh    = {Q2_bhh = 12000   }    $ Activation energy for undefined mechanism (cal/mol)
```

```
$-Temperatures are not applied to each node in the mesh
$-Reference: Kriet, 1984; Morgan and Krieg, 1988
$
$Overburden:
$ NAME______VALUE_______________________Description_(UNIT)___________
$ E_bho     = {E_bho   = 0.1E9  }     $ Young's Modulus(Pa)
$ rho_bho   = {rho_bho = 1874.  }     $ Density (kg/m^3)
$ nu_bho    = {nu_bho  = 0.33   }     $ Poisson's Ratio
$--Reference: Hoffman and Ehgartner, 1992 (SAND92-2183c)
$
$Caprock 1 (Limestone) at Big Hill:
$ NAME______VALUE_______________________Description_(UNIT)___________
$ E_bhl     = {E_bhl   = 21e9   }     $ Young's Modulus(Pa)
$ rho_bhl   = {rho_bhl = 2500.  }     $ Density (kg/m^3)
$ nu_bhl    = {nu_bhl  = 0.29   }     $ Poisson's Ratio
$-Reference: Hoffman and Ehgartner, 1992 (SAND92-2183c)
$
$Caprock 2 (Anhydrite) at Big Hill:
$ NAME______VALUE_______________________Description_(UNIT)___________
$ E_bhn     = {E_bhn   = 75.1E9}      $ Young's Modulus(Pa)
$ rho_bhn   = {rho_bhn = 2300.}       $ Density (kg/m^3)
$ nu_bhn    = {nu_bhn  = 0.35}        $ Poisson's Ratio
$ K_bhn     = {K_bhn   = E_bhn/(3.*(1.-2.*nu_bhn))} $ Bulk Modulus (Pa)
$ mu_bhn    = {mu_bhn  = E_bhn/(2.*(1.+nu_bhn))} $ Shear Modulus (Pa)
$ C_bhn     = {C_bhn   = 1.35E6}      $ Elastic constant (Pa)
$ a_bhn     = {a_bhn   = 0.45}        $ Drucker-Prager constant
$ A0_bhn    = {A0_bhn  = sqrt(3)*C_bhn}      $ JAS3D input constant (Pa)
$ A1_bhn    = {A1_bhn  = 3*sqrt(3)*a_bhn}    $ JAS3D input constant
$ A2_bhn    = {A2_bhn  = 0.0}         $ JAS3D input constant
$-Reference: Butcher,1997 (SAND97-0796)
$
$Surrounding Rock:
$ NAME______VALUE_______________________Description_(UNIT)___________
$ E_bhs     = {E_bhs   = 70.0e9 }     $ Young's Modulus(Pa) (Carmichael, 1984)
$ rho_bhs   = {rho_bhs = 2500.  }     $ Density (kg/m^3) (Lama and Vutukuri, 1978)
$ nu_bhs    = {nu_bhs  = 0.33   }     $ Poisson's Ratio (Lama and Vutukuri, 1978)
$-Reference:
$=========================================================================
```

# APPENDIX II. FILES RELATED TO BAYOU CHOCTAW MODEL

## II-A. JAS3D Input Deck

```
title
SPR Bayou Choctaw, 24cav5l (BC salt,SMF={SMF=0.12},E4={E4=35e9},WHP=each)

$Material Properties
$
$Salt (Material 1):
$ Young's Modulus={E1=31.0E9}(Krieg, 1984)
$ Density={rho1=2300.},Poisson's Ratio={nu1=0.25}(Krieg, 1984)
$ Bulk Modulus={K1=E1/(3.*(1.-2.*nu1))},Shear Modulus={mu1=E1/(2.*(1.+nu1))}
$ Creep Constant={A=5.79e-36},Stress Exponent={n=4.9},Thermal Constant={Q=12.0E3}(Krieg, 1984)
$ Salt Reduction Factor={RF=12.5} (Morgan and Krieg, 1988)
$ Structure Factor Multiplication Factor={SMF}(Adjusted through back analysis)
$ Thermal Constant Multiplication Factor={TCMF=0.503}(Ehgartner and Sobolik, 2002)
$
$Caprock (Material 2):
$ Young's Modulus={E2=1.572E10}(Hogan,R.G., SAND80-7140)
$ Density={rho2=2319.},Poisson's Ratio={nu2=0.288}(Hogan,R.G., SAND80-7140)
$
$Overburden (Material 3):
$ Young's Modulus={E3=0.1E9}(Hoffman and Ehgartner, 1993)
$ Density={rho3=1874.},Poisson's Ratio={nu3=0.33}(Hoffman and Ehgartner, 1993)
$
$Surrounding Rock (Material 4):
$ Young's Modulus={E4}(Carmichael, 1984)
$ Density={rho4=2500.},Poisson's Ratio={nu4=0.33}(Lama and Vutukuri, 1978)

$ minute     = {minute=60.} s
$ hour       = {hour=60.*minute} s
$ day        = {day=24.*hour} s
$ week       = {week=7.*day} s
$ month      = {month=day*30.} s
$ year       = {year=day*365.} s
$ decade     = {decade=10.*year} s
$ century    = {century=10.*decade} s

start time 0.0
  ITERATION PRINT, 20
  MAXIMUM ITERATIONS, 40000
  TARGET TOLERANCE, .00005
  ACCEPTABLE TOLERANCE .00001
  predictor scale factor, 0.0,0.0
  time steps, 1
  PLOT every, 1
  print every, 1
  write restart frequency, 0
next time {1.*day}   $ 1 day - transition to freshwater in well
  time steps, 9
  PLOT every, 9
  print every, 9
  write restart frequency, 0
next time {10.*day}  $ 10 days
  time steps, 4
  PLOT every, 4
  print every, 1
  write restart frequency, 0
next time {month}    $ 1 month
  time steps, 12
  PLOT every, 12
  print every, 12
  write restart frequency, 0
next time {3.*month} $ 3 months
  time steps, 9      $ = (12-3) months
  PLOT every, 1
  print every, 9
next time {year}     $ 1 year - change to oil/brine/liquid in caverns
  time steps, 540    $ 540 months = 45 years
  write restart every, 0
  PLOT every, 1
  print every, 30
end time  {46.*year}     $ 46 years - all of this to setup up initial

$ Output
thermal stress external, tmpnod
```

```
plot state, EqCS, temp
plot nodal, displacement, tmpnod
plot element, sig, vonmis, eps, pressure

$ Node boundary
no displacement Z 2 $ Bottom of mesh
no displacement x 3 $ West side
no displacement x 4 $ East side
no displacement y 5 $ South side
no displacement y 6 $ North side

$ Pressures on side set are the initial cavern pressure
pressure   10 user 1. $ 1$ pressure in cavern   1
pressure   20 user 1. $ 2$ pressure in cavern   2
pressure   30 user 1. $ 3$ pressure in cavern   3
pressure   40 user 1. $ 4$ pressure in cavern   4
pressure   60 user 1. $ 5$ pressure in cavern   6
pressure   70 user 1. $ 6$ pressure in cavern   7 Wall
pressure   71 user 1. $ 6$ pressure in cavern   7 Floor and Roof
pressure   80 user 1. $ 7$ pressure in cavern   8A
pressure  100 user 1. $ 8$ pressure in cavern  10
pressure  110 user 1. $ 9$ pressure in cavern  11
pressure  130 user 1. $10$ pressure in cavern  13
pressure  150 user 1. $11$ pressure in cavern  15A
pressure  160 user 1. $12$ pressure in cavern  16
pressure  170 user 1. $13$ pressure in cavern  17
pressure  180 user 1. $14$ pressure in cavern  18
pressure  190 user 1. $15$ pressure in cavern  19A
pressure  200 user 1. $16$ pressure in cavern  20A
pressure  240 user 1. $17$ pressure in cavern  24
pressure  250 user 1. $18$ pressure in cavern  25
pressure  260 user 1. $19$ pressure in cavern  26
pressure 1010 user 1. $20$ pressure in cavern 101B
pressure 1020 user 1. $21$ pressure in cavern 102A
pressure 1030 user 1. $22$ pressure in cavern  J1
pressure 1040 user 1. $23$ pressure in cavern  N1
pressure 1050 user 1. $24$ pressure in cavern  UTP1

$ Pressures on side set are the pressures after the 1st leach
pressure  151 user 1. $ pressure in cavern  15A
pressure  171 user 1. $ pressure in cavern  17
pressure  181 user 1. $ pressure in cavern  18
pressure  191 user 1. $ pressure in cavern  19A
pressure  201 user 1. $ pressure in cavern  20A
pressure 1011 user 1. $ pressure in cavern 101B

$ Pressures on side set are the pressures after the 2nd leach
pressure  152 user 1. $ pressure in cavern  15A
pressure  172 user 1. $ pressure in cavern  17
pressure  182 user 1. $ pressure in cavern  18
pressure  192 user 1. $ pressure in cavern  19A
pressure  202 user 1. $ pressure in cavern  20A
pressure 1012 user 1. $ pressure in cavern 101B

$ Pressures on side set are the pressures after the 3rd leach
pressure  153 user 1. $ pressure in cavern  15A
pressure  173 user 1. $ pressure in cavern  17
pressure  183 user 1. $ pressure in cavern  18
pressure  193 user 1. $ pressure in cavern  19A
pressure  203 user 1. $ pressure in cavern  20A
pressure 1013 user 1. $ pressure in cavern 101B

$ Pressures on side set are the pressures after the 4th leach
pressure  154 user 1. $ pressure in cavern  15A
pressure  174 user 1. $ pressure in cavern  17
pressure  184 user 1. $ pressure in cavern  18
pressure  194 user 1. $ pressure in cavern  19A
pressure  204 user 1. $ pressure in cavern  20A
pressure 1014 user 1. $ pressure in cavern 101B

$ Pressures on side set are the pressures after the 5th leach
pressure  155 user 1. $ pressure in cavern  15A
pressure  175 user 1. $ pressure in cavern  17
pressure  185 user 1. $ pressure in cavern  18
pressure  195 user 1. $ pressure in cavern  19A
pressure  205 user 1. $ pressure in cavern  20A
pressure 1015 user 1. $ pressure in cavern 101B

gravity
  gravitational constant = 9.81
  direction 0. 0. -1.
```

```
end gravity

material 1, power law creep, {rho1}    $ Salt
 bulk modulus = {K1/RF}
 two mu = {2*mu1/RF}
 creep constant = {SMF*A}
 stress exponent = {n}
 thermal constant = {TCMF*Q}
END
$ {thick1=2240.28}

active limits, 10, 0.0,0.01   $ Initial leaching of cavern
material 10, power law creep, {rho1} $ Salt
 bulk modulus = {K1/RF}
 two mu = {2*mu1/RF}
 creep constant = {SMF*A}
 stress exponent = {n}
 thermal constant = {TCMF*Q}
END

active limits, 11, 0.0,{21.*year}    $ 1st leach at 21 years
material 11, power law creep, {rho1} $ Salt
 bulk modulus = {K1/RF}
 two mu = {2*mu1/RF}
 creep constant = {SMF*A}
 stress exponent = {n}
 thermal constant = {TCMF*Q}
END

active limits, 12, 0.0,{26.*year}    $ 2nd leach at 26 years
material 12, power law creep, {rho1} $ Salt
 bulk modulus = {K1/RF}
 two mu = {2*mu1/RF}
 creep constant = {SMF*A}
 stress exponent = {n}
 thermal constant = {TCMF*Q}
END

active limits, 13, 0.0,{31.*year}    $ 3rd leach at 31 years
material 13, power law creep, {rho1} $ Salt
 bulk modulus = {K1/RF}
 two mu = {2*mu1/RF}
 creep constant = {SMF*A}
 stress exponent = {n}
 thermal constant = {TCMF*Q}
END

active limits, 14, 0.0,{36.*year}    $ 4th leach at 36 years
material 14, power law creep, {rho1} $ Salt
 bulk modulus = {K1/RF}
 two mu = {2*mu1/RF}
 creep constant = {SMF*A}
 stress exponent = {n}
 thermal constant = {TCMF*Q}
END

active limits, 15, 0.0,{41.*year}    $ 5th leach at 41 years
material 15, power law creep, {rho1} $ Salt
 bulk modulus = {K1/RF}
 two mu = {2*mu1/RF}
 creep constant = {SMF*A}
 stress exponent = {n}
 thermal constant = {TCMF*Q}
END

material 2, elastic, {rho2}    $ Caprock (Gypsum and Limestone)
 youngs modulus = {E2}
 poissons ratio = {nu2}
end
$ {thick2=45.72}

material 3, elastic, {rho3}    $ Overburden (sand)
 youngs modulus = {E3}
 poissons ratio = {nu3}
end
$ {thick3=152.4}

material 4, elastic, {rho4}    $ Rock surrounding salt dome (sandstone)
 youngs modulus = {E4}
 poissons ratio = {nu4}
end
```

```
$ {thick4= 2286.}

initial value USIGZZ=Function Z 3, 1., material 3
initial value USIGXX=Function Z 3, {nu3/(1.-nu3)}, material 3
initial value USIGYY=Function Z 3, {nu3/(1.-nu3)}, material 3
initial value USIGZZ=Function Z 2, 1., material 2
initial value USIGXX=Function Z 2, {nu2/(1.-nu2)}, material 2
initial value USIGYY=Function Z 2, {nu2/(1.-nu2)}, material 2
initial value USIGZZ=Function Z 4, 1., material 4
initial value USIGXX=Function Z 4, {nu4/(1.-nu4)}, material 4
initial value USIGYY=Function Z 4, {nu4/(1.-nu4)}, material 4
initial value USIGZZ=Function Z 1, 1., material 1
initial value USIGXX=Function Z 1, 1., material 1
initial value USIGYY=Function Z 1, 1., material 1
initial value USIGZZ=Function Z 1, 1., material 10
initial value USIGXX=Function Z 1, 1., material 10
initial value USIGYY=Function Z 1, 1., material 10
initial value USIGZZ=Function Z 1, 1., material 11
initial value USIGXX=Function Z 1, 1., material 11
initial value USIGYY=Function Z 1, 1., material 11
initial value USIGZZ=Function Z 1, 1., material 12
initial value USIGXX=Function Z 1, 1., material 12
initial value USIGYY=Function Z 1, 1., material 12
initial value USIGZZ=Function Z 1, 1., material 13
initial value USIGXX=Function Z 1, 1., material 13
initial value USIGYY=Function Z 1, 1., material 13
initial value USIGZZ=Function Z 1, 1., material 14
initial value USIGXX=Function Z 1, 1., material 14
initial value USIGYY=Function Z 1, 1., material 14
initial value USIGZZ=Function Z 1, 1., material 15
initial value USIGXX=Function Z 1, 1., material 15
initial value USIGYY=Function Z 1, 1., material 15

function 3 polynomial $ initial stress function for overburden (mat. 3)
  {a0_3=0.} $ a0
  {a1_3=rho3*9.81} $a1
end

function 2 polynomial $ initial stress function for caprock (mat. 2)
  {a0_2=rho2*9.81*thick3-a1_3*thick3}         $a0
  {a1_2=rho2*9.81}    $a1
end

function 1 polynomial $ initial stress function for salt (mat. 1, 10~15)
  {a0_1=rho1*9.81*(thick2+thick3)-a1_2*thick2-a1_3*thick3} $a0
  {a1_1=rho1*9.81}    $a1
end

function 4 polynomial $ initial stress function for surrounding rock (mat. 4)
  {a0_4=rho4*9.81*thick3-a1_3*thick3}         $a0
  {a1_4=rho4*9.81}    $a1
end

exit
```

## II-B. Adagio Input Deck

```
{include("/home/bypark/common/units.txt")}
{include("/home/bypark/common/BC_stratigraphy.txt")}
{include("/home/bypark/common/BC_materials_PLC.txt")}

$ Time at the initial leaches begin
$     bgn_s  = {bgn_s=0.} s
$ Times at the leaches for all SPR caverns start
$     D1st_s = {D1st_s=bgn_s + 21.*yr_s} s $ {D1st_s/yr_s} years
$     D2nd_s = {D2nd_s=D1st_s + 5.*yr_s} s $ {D2nd_s/yr_s} years
$     D3rd_s = {D3rd_s=D2nd_s + 5.*yr_s} s $ {D3rd_s/yr_s} years
$     D4th_s = {D4th_s=D3rd_s + 5.*yr_s} s $ {D4th_s/yr_s} years
$     D5th_s = {D5th_s=D4th_s + 5.*yr_s} s $ {D5th_s/yr_s} years
$Time at the simulaton completes
$     end_s  = {end_s =D5th_s + 5.*yr_s} s $ {end_s/yr_s} years

$ number of nodes = {nnod = 409248.}
# number of degree of freedom = {ndof = 6*nnod }
# MAXIMUM ITERATIONS = {nmax=10000}
#
# In-sute stress with stratigraphy
#
```

```
# Gravity, gr={gr=9.81} (m/s^2)
#
# {sigv_OB = -rho_bco*gr*t_OB           } Pa # Vertical stress at bottom of overburden (top of
caprock)
# {sigv_CR = sigv_OB-rho_bcc*gr*t_CR  } Pa # Vertical stress at bottom of caprock (top of salt
dome)
# {sigv_SD = sigv_CR-rho_bch*gr*h_SD  } Pa # Vertical stress at bottom of salt dome
# {sigv_SR = sigv_OB-rho_bcs*gr*t_SR  } Pa # Vertical stress at bottom of surrounding rock

#==================================================================
begin sierra  SPR Bayou Choctaw 24cav5d_scn2 BC salt SMF 0.12 E4 3.5e+10 WHP each

  title SPR Bayou Choctaw, 24cav5d_scn2, BC salt,SMF={SMF},E_bcs={E_bcs},WHP=each

# Define the file name containing the Fortran 77 user subroutine
  user subroutine file = usrpbc_bc24cav5d.F

  define direction y with vector 0.0 1.0 0.0
  define direction x with vector 1.0 0.0 0.0
  define direction z with vector 0.0 0.0 1.0
  define direction negative_z with vector 0.0 0.0 -1.0
  define point origin with coordinates 0.0 0.0 0.0

  #---------- Functions ---------

  # ASCENDING ORDER IS REQUIRED FOR DEFINING FUNCTION
  begin definition for function function_1  # Gravity
    type is piecewise linear
    begin values
     0.0     1.0
     {end_s} 1.0
    end values
  end definition for function function_1

  #---------- Materials ----------

  begin property specification for material mat_1 # Salt dome (salt)
    density = {rho_bch}
    begin parameters for model power_law_creep
      shear modulus    = {mu_bch/RF_bch } # (Pa)
      bulk modulus     = {K_bch/RF_bch }  # (Pa)
      creep constant   = {A_PLC*SMF  }         # (Pa^-n/s)
      creep exponent   = {n2_bch    }
      thermal constant = {Q2_bch/R }      # (K)
    end parameters for model power_law_creep
  end property specification for material mat_1

  begin solid section solid_1
    strain incrementation = midpoint_increment
    hourglass rotation = scaled
  end solid section solid_1

  begin property specification for material mat_2 # Caprock (gysum and limestone)
    density = {rho_bcc}
    begin parameters for model elastic
      youngs modulus = {E_bcc     }   # (Pa)
      poissons ratio = {nu_bcc    }
    end parameters for model elastic
  end property specification for material mat_2

  begin solid section solid_2
    strain incrementation = midpoint_increment
    hourglass rotation = scaled
  end solid section solid_2

  begin property specification for material mat_3 # Overburden (sand)
    density = {rho_bco}
    begin parameters for model elastic
      youngs modulus = {E_bco     }   # (Pa)
      poissons ratio = {nu_bco    }
    end parameters for model elastic
  end property specification for material mat_3

  begin solid section solid_3
    strain incrementation = midpoint_increment
    hourglass rotation = scaled
  end solid section solid_3

  begin property specification for material mat_4 # Farfield (sandstone)
    density = {rho_bcs}
    begin parameters for model elastic
```

```
      youngs modulus = {E_bcs    }   # (Pa)
      poissons ratio = {nu_bcs}
    end parameters for model elastic
  end property specification for material mat_4

  begin solid section solid_4
    strain incrementation = midpoint_increment
    hourglass rotation = scaled
  end solid section solid_4

  #---------- Finite Element Model -----------

$------------------------------------------------------------------------
$$ Defined blocks in CUBIT
$ Block 1  = salt dome except caverns
$       2  = caprock
$       3  = overburden
$       4  = surrounding rock (farfield)
$       10 = initial leach
$       11 = 1st drawdown leach
$       12 = 2nd drawdown leach
$       13 = 3rd drawdown leach
$       14 = 4th drawdown leach
$       15 = 5th drawdown leach
$------------------------------------------------------------------------

  begin finite element model bc_24cav5d_scn2

    Database name = 24cav5d_coar.g
    Database type = exodusII

    begin parameters for block block_1 # Salt dome
      material mat_1
      solid mechanics use model power_law_creep
      section = solid_1
    end parameters for block block_1

    begin parameters for block block_10 # initial leach
      material mat_1
      solid mechanics use model power_law_creep
      section = solid_1
    end parameters for block block_10

    begin parameters for block block_11 # 1st drawdown leach
      material mat_1
      solid mechanics use model power_law_creep
      section = solid_1
    end parameters for block block_11

    begin parameters for block block_12 # 2nd drawdown leach
      material mat_1
      solid mechanics use model power_law_creep
      section = solid_1
    end parameters for block block_12

    begin parameters for block block_13 # 3rd drawdown leach
      material mat_1
      solid mechanics use model power_law_creep
      section = solid_1
    end parameters for block block_13

    begin parameters for block block_14 # 4th drawdown leach
      material mat_1
      solid mechanics use model power_law_creep
      section = solid_1
    end parameters for block block_14

    begin parameters for block block_15 # 5th drawdown leach
      material mat_1
      solid mechanics use model power_law_creep
      section = solid_1
    end parameters for block block_15

    begin parameters for block block_2 # Caprock
      material mat_2
      solid mechanics use model elastic
      section = solid_2
    end parameters for block block_2

    begin parameters for block block_3 # Overburden
      material mat_3
```

```
    solid mechanics use model elastic
    section = solid_3
  end parameters for block block_3

  begin parameters for block block_4 # Surrounding rock
    material mat_4
    solid mechanics use model elastic
    section = solid_4
  end parameters for block block_4

end finite element model bc_24cav5d_scn2

begin adagio procedure procedure_1

  #---------- Time Step Control ----------

  begin time control
    begin time stepping block p0
      start time = 0.0
      begin parameters for adagio region region_1
        number of time steps = 1
      end parameters for adagio region region_1
    end time stepping block p0

    begin time stepping block p1
      start time = 0.01  # 0.01 sec
      begin parameters for adagio region region_1
        number of time steps = 99
      end parameters for adagio region region_1
    end time stepping block p1

    begin time stepping block p2
      start time = 1.0  # 1 sec
      begin parameters for adagio region region_1
        number of time steps = 59
      end parameters for adagio region region_1
    end time stepping block p2

    begin time stepping block p3
      start time = 60.0  # 60 sec = 1 min
      begin parameters for adagio region region_1
        number of time steps = 59
      end parameters for adagio region region_1
    end time stepping block p3

    begin time stepping block p4
      start time = {h_s}  # 3600 sec = 60 min = 1 hr
      begin parameters for adagio region region_1
        number of time steps = 23
      end parameters for adagio region region_1
    end time stepping block p4

    begin time stepping block p5
      start time = {d_s}  #  1 day
      begin parameters for adagio region region_1
        number of time steps = 9
      end parameters for adagio region region_1
    end time stepping block p5

    begin time stepping block p6
      start time = {10.*d_s}  #  10 day
      begin parameters for adagio region region_1
        number of time steps = 20 #1 step={(mon_s-10.*d_s)/20/d_s} days
      end parameters for adagio region region_1
    end time stepping block p6

    begin time stepping block p7
      start time = {mon_s}  #  1 month
      begin parameters for adagio region region_1
        number of time steps = 60  #1 step={(3*mon_s-mon_s)/60/d_s} days
      end parameters for adagio region region_1
    end time stepping block p7

    begin time stepping block p8
      start time = {3.*mon_s}  #  3 months
      begin parameters for adagio region region_1
        number of time steps = 270  #1 step={(yr_s-3*mon_s)/270/d_s} days
      end parameters for adagio region region_1
    end time stepping block p8

    begin time stepping block p9
```

```
      start time = {yr_s} # Change to oil/brine/liquid in caverns: 1 years
      begin parameters for adagio region region_1
        number of time steps = 240 # 1 step={(3.*yr_s-yr_s)/240/mon_s} month
      end parameters for adagio region region_1
    end time stepping block p9

    begin time stepping block p10
      start time = {3.*yr_s} # 3 years
      begin parameters for adagio region region_1
        number of time steps = 2160 # 1 step={(D1st_s-3.*yr_s)/2160/mon_s} month
      end parameters for adagio region region_1
    end time stepping block p10

    begin time stepping block p11
      start time = {D1st_s} $ 1st drawdown leach: {D1st_s/yr_s} years
      begin parameters for adagio region region_1
        number of time steps = 600 # 1 step={(D2nd_s-D1st_s)/600/mon_s} month
      end parameters for adagio region region_1
    end time stepping block p11

    begin time stepping block p12
      start time = {D2nd_s} $ 2nd drawdown leach: {D2nd_s/yr_s} years
      begin parameters for adagio region region_1
        number of time steps = 600 # 1 step={(D3rd_s-D2nd_s)/600/mon_s} month
      end parameters for adagio region region_1
    end time stepping block p12

    begin time stepping block p13
      start time = {D3rd_s} $ 3rd drawdown leach: {D3rd_s/yr_s} years
      begin parameters for adagio region region_1
        number of time steps = 600 # 1 step={(D4th_s-D3rd_s)/600/mon_s} month
      end parameters for adagio region region_1
    end time stepping block p13

    begin time stepping block p14
      start time = {D4th_s} $ 4th drawdown leach: {D4th_s/yr_s} years
      begin parameters for adagio region region_1
        number of time steps = 600 # 1 step={(D5th_s-D4th_s)/600/mon_s} month
      end parameters for adagio region region_1
    end time stepping block p14

    begin time stepping block p15
      start time = {D5th_s} $ 5th drawdown leach: {D5th_s/yr_s} years
      begin parameters for adagio region region_1
        number of time steps = 600 # 1 step={(end_s-D5th_s)/600/mon_s} month
      end parameters for adagio region region_1
    end time stepping block p15

    termination time = {end_s} # {(end_s-bgn_s)/yr_s} years since simulation starts

  end time control

  begin adagio region region_1

    use finite element model bc_24cav5d_scn2

    #--------- Restart ---------

#      begin restart data restart_1
#        database type = exodusII
#        output database Name = bc_24cav5d_scn2.rsout
#      end restart data restart_1

    #--------- Boundary Conditions ---------

    begin gravity
      include all blocks
      gravitational constant = {gr}
      direction = negative_z
      function = function_1
    end gravity

    begin prescribed temperature
      include all blocks
      read variable = tmpnod
    end prescribed temperature

    begin fixed displacement # Bottom of mesh
      node set = nodelist_2
      components = z
    end fixed displacement
```

```
      begin fixed displacement # West side
        node set = nodelist_3
        components = x
      end fixed displacement

      begin fixed displacement # East side
        node set = nodelist_4
        components = x
      end fixed displacement

      begin fixed displacement # South side
        node set = nodelist_5
        components = y
      end fixed displacement

      begin fixed displacement # North side
        node set = nodelist_6
        components = y
      end fixed displacement

#================================================================
#     The following sets of "begin pressure blocks" define the
#     surfaces and time periods associated with the sequential
#     leachings. Note that "cavity_pressure" is the subroutine
#     name not the file name. The file name is usrpbc_bc_24cav5d.F
#     which was specified earlier in this input file.
#================================================================

###
#     Pressures on side set after the initial leach (Non SPR caverns)
#     Time period from 0.01 seconds to {end_s/yr_s} years
###

      begin pressure
        surface = surface_10   surface_20   surface_30   surface_40   surface_60  \#
                  surface_80   surface_100  surface_110 \#
                  surface_130  surface_160  surface_240  surface_250  surface_260 \#
                  surface_1020 surface_1030 surface_1040 surface_1050
        surface subroutine = cavity_pressure_10
        active periods = p1 p2 p3 p4 p5 p6 p7 p8 p9 p10 p11 p12 p13 p14 p15
      end pressure

###
#     Pressures on side set after the initial leach (SPR caverns)
#     Time period from 0.01 seconds to {D1st_s/yr_s} years
###

      begin pressure # pressure in cavern 7 wall
        surface = surface_70
        surface subroutine = cavity_pressure_70
        active periods = p1 p2 p3 p4 p5 p6 p7 p8 p9 p10
      end pressure

      begin pressure # pressure in cavern 7 floor and ceiling
        surface = surface_71
        surface subroutine = cavity_pressure_71
        active periods = p1 p2 p3 p4 p5 p6 p7 p8 p9 p10
      end pressure

      begin pressure # pressure in cavern 15 and 17
        surface = surface_150 surface_170
        surface subroutine = cavity_pressure_1517
        active periods = p1 p2 p3 p4 p5 p6 p7 p8 p9 p10
      end pressure

      begin pressure # pressure in cavern 18
        surface = surface_180
        surface subroutine = cavity_pressure_18
        active periods = p1 p2 p3 p4 p5 p6 p7 p8 p9 p10
      end pressure

      begin pressure # pressure in cavern 19
        surface = surface_190
        surface subroutine = cavity_pressure_19
        active periods = p1 p2 p3 p4 p5 p6 p7 p8 p9 p10
      end pressure

      begin pressure # pressure in cavern 20
        surface = surface_200
        surface subroutine = cavity_pressure_20
```

```
      active periods = p1 p2 p3 p4 p5 p6 p7 p8 p9 p10
    end pressure

    begin pressure # pressure in cavern 101
      surface = surface_1010
      surface subroutine = cavity_pressure_101
      active periods = p1 p2 p3 p4 p5 p6 p7 p8 p9 p10
    end pressure

###
#     Pressures on side set after the 1st drawdown leach
#     Time period from {D1st_s/yr_s} years to {D2nd_s/yr_s} years
###

    begin pressure # pressure in cavern 15 and 17
      surface = surface_151 surface_171
      surface subroutine = cavity_pressure_1517
      active periods = p11
    end pressure

    begin pressure # pressure in cavern 18
      surface = surface_181
      surface subroutine = cavity_pressure_18
      active periods = p11
    end pressure

    begin pressure # pressure in cavern 19
      surface = surface_191
      surface subroutine = cavity_pressure_19
      active periods = p11
    end pressure

    begin pressure # pressure in cavern 20
      surface = surface_201
      surface subroutine = cavity_pressure_20
      active periods = p11
    end pressure

    begin pressure # pressure in cavern 101
      surface = surface_1011
      surface subroutine = cavity_pressure_101
      active periods = p11
    end pressure

###
#     Pressures on side set after the 2nd drawdown leach
#     Time period from {D2nd_s/yr_s} years to {D3rd_s/yr_s} years
###

    begin pressure # pressure in cavern 15 and 17
      surface = surface_152 surface_172
      surface subroutine = cavity_pressure_1517
      active periods = p12
    end pressure

    begin pressure # pressure in cavern 18
      surface = surface_182
      surface subroutine = cavity_pressure_18
      active periods = p12
    end pressure

    begin pressure # pressure in cavern 19
      surface = surface_192
      surface subroutine = cavity_pressure_19
      active periods = p12
    end pressure

    begin pressure # pressure in cavern 20
      surface = surface_202
      surface subroutine = cavity_pressure_20
      active periods = p12
    end pressure

    begin pressure # pressure in cavern 101
      surface = surface_1012
      surface subroutine = cavity_pressure_101
      active periods = p12
    end pressure

###
#     Pressures on side set after the 3rd drawdown leach
```

```
#     Time period from {D3rd_s/yr_s} years to {D4th_s/yr_s} years
###

      begin pressure # pressure in cavern 15 and 17
        surface = surface_153 surface_173
        surface subroutine = cavity_pressure_1517
        active periods = p13
      end pressure

      begin pressure # pressure in cavern 18
        surface = surface_183
        surface subroutine = cavity_pressure_18
        active periods = p13
      end pressure

      begin pressure # pressure in cavern 19
        surface = surface_193
        surface subroutine = cavity_pressure_19
        active periods = p13
      end pressure

      begin pressure # pressure in cavern 20
        surface = surface_203
        surface subroutine = cavity_pressure_20
        active periods = p13
      end pressure

      begin pressure # pressure in cavern 101
        surface = surface_1013
        surface subroutine = cavity_pressure_101
        active periods = p13
      end pressure

###
#     Pressures on side set after the 4th drawdown leach
#     Time period from {D4th_s/yr_s} years to {D5th_s/yr_s} years
###

      begin pressure # pressure in cavern 15 and 17
        surface = surface_154 surface_174
        surface subroutine = cavity_pressure_1517
        active periods = p14
      end pressure

      begin pressure # pressure in cavern 18
        surface = surface_184
        surface subroutine = cavity_pressure_18
        active periods = p14
      end pressure

      begin pressure # pressure in cavern 19
        surface = surface_194
        surface subroutine = cavity_pressure_19
        active periods = p14
      end pressure

      begin pressure # pressure in cavern 20
        surface = surface_204
        surface subroutine = cavity_pressure_20
        active periods = p14
      end pressure

      begin pressure # pressure in cavern 101
        surface = surface_1014
        surface subroutine = cavity_pressure_101
        active periods = p14
      end pressure

###
#     Pressures on side set after the 5th drawdown leach
#     Time period from {D5th_s/yr_s} years to {end_s/yr_s} years
###

      begin pressure # pressure in cavern 15 and 17
        surface = surface_155 surface_175
        surface subroutine = cavity_pressure_1517
        active periods = p15
      end pressure

      begin pressure # pressure in cavern 18
        surface = surface_185
```

```
    surface subroutine = cavity_pressure_18
    active periods = p15
  end pressure

  begin pressure # pressure in cavern 19
    surface = surface_195
    surface subroutine = cavity_pressure_19
    active periods = p15
  end pressure

  begin pressure # pressure in cavern 20
    surface = surface_205
    surface subroutine = cavity_pressure_20
    active periods = p15
  end pressure

  begin pressure # pressure in cavern 101
    surface = surface_1015
    surface subroutine = cavity_pressure_101
    active periods = p15
  end pressure

  #--------- Element Death --------------
###
#      Use element death option to simulate leachings
###

  begin element death leach_0  # Initial leach
    block = block_10
    criterion is always true
    death start time = 0.01
  end element death leach_0

  begin element death leach_1  # 1st drawdown leach
    block = block_11
    criterion is always true
    death start time = {D1st_s+d_s}
  end element death leach_1

  begin element death leach_2  # 2nd drawdown leach
    block = block_12
    criterion is always true
    death start time = {D2nd_s+d_s}
  end element death leach_2

  begin element death leach_3 # 3rd drawdown leach
    block = block_13
    criterion is always true
    death start time = {D3rd_s+d_s}
  end element death leach_3

  begin element death leach_4  # 4th drawdown leach
    block = block_14
    criterion is always true
    death start time = {D4th_s+d_s}
  end element death leach_4

  begin element death leach_5  # 5th drawdown leach
    block = block_15
    criterion is always true
    death start time = {D5th_s+d_s}
  end element death leach_5

  #--------- Initial Conditions ---------

  begin initial condition # Overburden (sand)
    block = block_3
    initialize variable name = unrotated_stress
    variable type = element
    subroutine real parameter: top = 0.0       # (m) surface
    subroutine real parameter: bot = {-t_OB}   # (m) overburden bottom
    subroutine real parameter: p1  = 0.0       # (Pa) vertical stress at surface
    subroutine real parameter: po  = {sigv_OB} # (Pa) vertical stress at overburden bottom
    subroutine real parameter: kvert_xx = {nu_bco/(1.-nu_bco)}
    subroutine real parameter: kvert_yy = {nu_bco/(1.-nu_bco)}
    subroutine real parameter: kvert_zz = 1.0
    subroutine real parameter: kvert_xy = 0.0
    subroutine real parameter: kvert_yz = 0.0
    subroutine real parameter: kvert_zx = 0.0
    subroutine string parameter: dir = Z
    element block subroutine = geo_is
```

```
end initial condition

begin initial condition # Caprock (gypsum and limestone)
  block = block_2
  initialize variable name = unrotated_stress
  variable type = element
  subroutine real parameter: top = {     -t_OB} # (m) caprock top
  subroutine real parameter: bot = {-t_CR-t_OB} # (m) caprock bottom
  subroutine real parameter: p1  = {sigv_OB   } # (Pa) vertical stress at caprock top
  subroutine real parameter: po  = {sigv_CR   } # (Pa) Vertical stress at caprock bottom
  subroutine real parameter: kvert_xx = {nu_bcc/(1.-nu_bcc)}
  subroutine real parameter: kvert_yy = {nu_bcc/(1.-nu_bcc)}
  subroutine real parameter: kvert_zz = 1.0
  subroutine real parameter: kvert_xy = 0.0
  subroutine real parameter: kvert_yz = 0.0
  subroutine real parameter: kvert_zx = 0.0
  subroutine string parameter: dir = Z
  element block subroutine = geo_is
end initial condition

begin initial condition # Salt dome
  block = block_1 block_10 block_11 block_12 block_13 block_14 block_15
  initialize variable name = unrotated_stress
  variable type = element
  subroutine real parameter: top = {     -t_CR-t_OB} # (m) Top of salt dome
  subroutine real parameter: bot = {-h_SD-t_CR-t_OB} # (m) Bottom of salt dome
  subroutine real parameter: p1  = {sigv_CR} # (Pa) vertical stress at salt dome top
  subroutine real parameter: po  = {sigv_SD} # (Pa) vertical stress at salt dome bottom
  subroutine real parameter: kvert_xx = 1.0
  subroutine real parameter: kvert_yy = 1.0
  subroutine real parameter: kvert_zz = 1.0
  subroutine real parameter: kvert_xy = 0.0
  subroutine real parameter: kvert_yz = 0.0
  subroutine real parameter: kvert_zx = 0.0
  subroutine string parameter: dir = Z
  element block subroutine = geo_is
end initial condition

begin initial condition # Surrounding rock (sandstone)
  block = block_4
  initialize variable name = unrotated_stress
  variable type = element
  subroutine real parameter: top = {          -t_OB} # (m) Top of caprock
  subroutine real parameter: bot = {-h_SD-t_CR-t_OB} # (m) Bottom of surrounding rock
  subroutine real parameter: p1  = {sigv_OB} # (Pa) vertical stress at caprock top
  subroutine real parameter: po  = {sigv_SR} # (Pa) vertical stress at surrounding rock
bottom
  subroutine real parameter: kvert_xx = {nu_bcs/(1.-nu_bcs)}
  subroutine real parameter: kvert_yy = {nu_bcs/(1.-nu_bcs)}
  subroutine real parameter: kvert_zz = 1.0
  subroutine real parameter: kvert_xy = 0.0
  subroutine real parameter: kvert_yz = 0.0
  subroutine real parameter: kvert_zx = 0.0
  subroutine string parameter: dir = Z
  element block subroutine = geo_is
end initial condition

#--------- Results Output ---------

begin results output output_1
  database name = bc_24cav5d.e
  database type = exodusII
  at time 0           increment = 0.01
  at time 0.01        increment = 0.99
  at time 1           increment = 59
  at time {min_s}     increment = {h_s-min_s}
  at time {h_s}       increment = {d_s-h_s}
  at time {d_s}       increment = {mon_s-d_s}  # At 1 day use 29 day increment
  at time {mon_s}     increment = {yr_s-mon_s} # At 1 month use 11 month increment
  at time {yr_s}      increment = {3.*mon_s}   # At 1 year use 3 month increment

  nodal variables   = displacement as displ
  nodal variables   = temperature as temp
  nodal variables   = force_external as fext

  element variables = temperature as tempe
  element variables = stress as sig
  element variables = von_mises as vonmis
  element variables = unrotated_stress as stress
  element variables = log_strain as eps
  element variables = ecreep as eqcs
```

```
        global variables = total_iter as itotal
      end results output output_1

      #--------- Solver ---------

      begin solver
        begin loadstep predictor
          type = scale_factor
          scale factor = 1.0 0.0
        end loadstep predictor

        begin cg
          target relative residual = 1.e-7 during p0 p1 p2 p3 p4 p5 p6 p7 p8 # 0~1 year
          target relative residual = 1.e-7 during p9 # 1~3 years
          target relative residual = 1.e-7 during p10 p11 p12 p13 p14 p15
          acceptable relative residual = 1.e-5 during p9 # Default is 10 times target relative
residual
          acceptable relative residual = 2.e-5 during p10 p11 p12 p13 p14 p15
          maximum iterations = {nmax}
          reset limits 10000000 500000000 1000 0.5
          iteration print = 20
          line search tangent
          preconditioner = diagonal
        end cg
      end solver
    end adagio region region_1

  end adagio procedure procedure_1

end sierra SPR Bayou Choctaw 24cav5d_scn2 BC salt SMF 0.12 E4 3.5e+10 WHP each
```

# APPENDIX III. FILES RELATED TO BIG HILL MODEL

## III-A. JAS3D Input Deck

```
{include("/home/bypark/common/units.txt")}
{include("/home/bypark/common/BH_stratigraphy_sftele.txt")}
{include("/home/bypark/common/BH_materials_PLC.txt")}

$ Time at the initial leaches begin
$     bgn_s  = {bgn_s=0.} s
$ Times at the drawdown leaches for all SPR caverns start
$     D1st_s = {D1st_s=bgn_s + 31.*yr_s} s $ {D1st_s/yr_s} years
$     D2nd_s = {D2nd_s=D1st_s + 5.*yr_s} s $ {D2nd_s/yr_s} years
$     D3rd_s = {D3rd_s=D2nd_s + 5.*yr_s} s $ {D3rd_s/yr_s} years
$     D4th_s = {D4th_s=D3rd_s + 5.*yr_s} s $ {D4th_s/yr_s} years
$     D5th_s = {D5th_s=D4th_s + 5.*yr_s} s $ {D5th_s/yr_s} years
$Time at the simulaton completes
$     end_s  = {end_s =D5th_s + 5.*yr_s} s $ {end_s/yr_s} years

$ number of nodes = {nnod = 554540}
$ number of degree of freedom = {ndof = 6*nnod }
$====================================================================
title
bh_full_5d, PLC, step=plot=1 mon, OB mat. for inter and fault in OB, C1 and C2

$Read Restart Continue  $ No restart
start time 0.0
  ITERATION PRINT, 20
  MAXIMUM ITERATIONS, {ndof} LEVEL 0        $ was {ndof}
  MAXIMUM ITERATIONS, {int(sqrt(ndof))} LEVEL 1  $ sqrt(nnod)/1 (level)
$ Acceptable tolerance is set larger than (or equal to) the target tolerance
  TARGET TOLERANCE, 5.e-5 LEVEL 0    $ was 5.e-5
  TARGET TOLERANCE, 5.e-4 LEVEL 1    $
  ACCEPTABLE TOLERANCE 1.e-4 LEVEL 0 $ was 1.e-5
  ACCEPTABLE TOLERANCE 1.e-3 LEVEL 1 $
$  predictor scale factor, 0.0,0.0
  time steps, {h_s/10}  $1 step={h_s/(h_s/10)} sec
  PLOT every, {h_s/10}
  print every, {h_s/10}
  write restart frequency, 0
next time {h_s}    $ 1 hour
  time steps, 230   $1 step={(d_s-h_s)/230/min_s} mins
  PLOT every, 230
  print every, 230
  write restart frequency, 0
next time {1.*d_s}  $ 1 days
  time steps, 90   $1 step={(10.*d_s-1.*d_s)/90/h_s} hours
  PLOT every, 90
  print every, 90
  write restart frequency, 0
next time {10.*d_s}  $ 10 days
  time steps, 40   $1 step={(mon_s-10.*d_s)/40/d_s} days
  PLOT every, 40
  print every, 10
  write restart frequency, 0
next time {mon_s}    $ 1 month
  time steps, {ITS=12}  $1 step={(3.*mon_s-mon_s)/ITS/d_s} days
  PLOT every, {ITS}
  print every, {ITS}
  write restart frequency, 0
next time {3.*mon_s} $ 3 months
  time steps, 9      $1 step={(bgn_s+yr_s-3.*mon_s)/9/d_s} days
  PLOT every, 9
  print every, 9
$----
next time {bgn_s+yr_s} $ Change to oil/brine/liquid in caverns: {(bgn_s+yr_s)/yr_s} years
  time  steps,  {(end_s/yr_s-1)*ITS}  $  1  step={(end_s-(bgn_s+yr_s))/((end_s/yr_s-1)*ITS)/mon_s}
months
  write restart every, 0
  PLOT every, 1
  print every, {ITS}
end time  {end_s} $ {(end_s-bgn_s)/yr_s} years since simulation starts
$----------------------------------------------------------------------
$$ Defined blocks in CUBIT
$ Block 1=salt dome except caverns
$       2=overburden
```

```
$       3=caprock1
$       4=caprock2
$       5=surrounding rock
$       6=interface between overburden and caprock1
$       7=interface between caprock1 and caprock2
$       8=interface between caprock2 and salt dome
$       9=interface between dome and surrounding rock
$       11=fault in salt dome
$       12=fault in overburden; and interface between overburden and caprock1
$       13=fault in caprock1; and interface between caprock1 and caprock2
$       14=fault in caprock2; and interface between caprock2 and salt dome
$       100=initial reach
$       101=1st drawdown leach
$       102=2nd drawdown leach
$       103=3rd drawdown leach
$       104=4th drawdown leach
$       105=5th drawdown leach
$-----------------------------------------------------------------------
$ Define Functions
$
$ In-sute stress with stratigraphy
$
$ Gravity, gr={gr=9.81} (m/s^2)
$
$ {sigv_OB = -rho_bho*gr*t_OB} Pa              $ Vertical stress at bottom of overburden (top of UOB)
$ {sigv_UOB= sigv_OB -rho_bho*gr*t_UOB} Pa      $ Vertical stress at bottom of UOB (top of caprock1)
$ {sigv_CRL= sigv_UOB-rho_bhl*gr*t_CRL} Pa      $ Vertical stress at bottom of caprock1 (top of UC1)
$ {sigv_UC1= sigv_CRL-rho_bho*gr*t_UC1} Pa      $ Vertical stress at bottom of UC1 (top of caprock2)
$ {sigv_CRN= sigv_UC1-rho_bhn*gr*t_CRN} Pa      $ Vertical stress at bottom of caprock2 (top of UC2)
$ {sigv_UC2= sigv_CRN-rho_bho*gr*t_UC2} Pa      $ Vertical stress at bottom of UC2 (top of salt dome)
$ {sigv_SD = sigv_UC2-rho_bhh*gr*h_SD}  Pa     $ Vertical stress at bottom of salt dome
$ {sigv_SR = sigv_UOB-rho_bhs*gr*t_SR}  Pa     $ Vertical stress at bottom of surrounding rock
$ {sigv_DP = sigv_OB -rho_bho*gr*h_DP}  Pa     $ Vertical stress at bottom of dome perimeter
$ {sigv_FOB= -rho_bho*gr*(t_OB+t_UOB)} Pa             $ Vertical stress at bottom of fault in overburden (top of caprock1)
$ {sigv_FC1= sigv_FOB-rho_bho*gr*(t_CRL+t_UC1)} Pa $ Vertical stress at bottom of fault in caprock1 (top of caprock2)
$ {sigv_FC2= sigv_FC1-rho_bho*gr*(t_CRN+t_UC2)} Pa $ Vertical stress at bottom of fault in caprock2 (top of salt dome)
$ {sigv_FSD= sigv_FC2-rho_bhh*gr*h_SD} Pa          $ Vertical stress at bottom of fault in salt dome
$ ASCENDING ORDER IS REQUIRED FOR DEFINING FUNCTION
function 1 linear $ initial stress function for salt dome area
  {-h_SD-t_UC2-t_CRN-t_UC1-t_CRL-t_UOB-t_OB} {sigv_SD}  $ Bottom of salt dome
  {     -t_UC2-t_CRN-t_UC1-t_CRL-t_UOB-t_OB} {sigv_UC2} $ Bottom of UC2 (top of salt dome)
  {           -t_CRN-t_UC1-t_CRL-t_UOB-t_OB} {sigv_CRN} $ Bottom of caprock2 (top of UC2)
  {                 -t_UC1-t_CRL-t_UOB-t_OB} {sigv_UC1} $ Bottom of UC1 (top of caprock2)
  {                       -t_CRL-t_UOB-t_OB} {sigv_CRL} $ Bottom of caprock1 (top of UC1)
  {                             -t_UOB-t_OB} {sigv_UOB} $ Bottom of UOB (top of caprock1)
  {                                   -t_OB} {sigv_OB } $ Bottom of overburden (top of UOB)
  0.0                                        0.0        $ Top of overburden
end function 1

function 2 linear $ initial stress function for surrounding rock area
  {-h_SD-t_UC2-t_CRN-t_UC1-t_CRL-t_UOB-t_OB} {sigv_SR}  $ Bottom of surrounding rock
  {                             -t_UOB-t_OB} {sigv_UOB} $ Bottom of UOB (top of caprock1)
  {                                   -t_OB} {sigv_OB } $ Bottom of overburden (top of UOB)
  0.0                                        0.0        $ Top of overburden
end function 2

function 3 linear $ initial stress function for dome perimeter area
  {-h_SD-t_UC2-t_CRN-t_UC1-t_CRL-t_UOB-t_OB} {sigv_DP}  $ Bottom of dome perimeter
  {                                   -t_OB} {sigv_OB } $ Bottom of overburden (top of UOB)
  0.0                                        0.0        $ Top of overburden
end function 3

function 4 linear $ initial stress function for fault area
  {-h_SD-t_UC2-t_CRN-t_UC1-t_CRL-t_UOB-t_OB} {sigv_FSD} $ Bottom of salt dome
  {     -t_UC2-t_CRN-t_UC1-t_CRL-t_UOB-t_OB} {sigv_FC2} $ Bottom of UC2 (top of salt dome)
  {                 -t_UC1-t_CRL-t_UOB-t_OB} {sigv_FC1} $ Bottom of UC1 (top of caprock2)
  {                             -t_UOB-t_OB} {sigv_FOB} $ Bottom of UOB (top of caprock1)
  0.0                                        0.0        $ Top of overburden
end function 4

function 11  $ Gravity and normal displacement function
```

```
 0.0     1.0
 {end_s} 1.0
end function 11

$-----------------------------------------------------------------------
$ Initial Condition
$
$$ Salt dome and each drawdown leach
$             cmpt            dir ftn scl          matid
initial value USIGZZ=Function Z   1,  1., material 1
initial value USIGXX=Function Z   1,  1., material 1
initial value USIGYY=Function Z   1,  1., material 1
initial value USIGZZ=Function Z   1,  1., material 100
initial value USIGXX=Function Z   1,  1., material 100
initial value USIGYY=Function Z   1,  1., material 100
initial value USIGZZ=Function Z   1,  1., material 101
initial value USIGXX=Function Z   1,  1., material 101
initial value USIGYY=Function Z   1,  1., material 101
initial value USIGZZ=Function Z   1,  1., material 102
initial value USIGXX=Function Z   1,  1., material 102
initial value USIGYY=Function Z   1,  1., material 102
initial value USIGZZ=Function Z   1,  1., material 103
initial value USIGXX=Function Z   1,  1., material 103
initial value USIGYY=Function Z   1,  1., material 103
initial value USIGZZ=Function Z   1,  1., material 104
initial value USIGXX=Function Z   1,  1., material 104
initial value USIGYY=Function Z   1,  1., material 104
initial value USIGZZ=Function Z   1,  1., material 105
initial value USIGXX=Function Z   1,  1., material 105
initial value USIGYY=Function Z   1,  1., material 105
$$ Overburden
initial value USIGZZ=Function Z   1,  1., material 2
initial value USIGXX=Function Z   1,  {nu_bho/(1.-nu_bho)}, material 2
initial value USIGYY=Function Z   1,  {nu_bho/(1.-nu_bho)}, material 2
$$ Interface between overburden and caprock1
initial value USIGZZ=Function Z   1,  1., material 6
initial value USIGXX=Function Z   1,  {nu_bho/(1.-nu_bho)}, material 6
initial value USIGYY=Function Z   1,  {nu_bho/(1.-nu_bho)}, material 6
$$ Caprock1
initial value USIGZZ=Function Z   1,  1., material 3
initial value USIGXX=Function Z   1,  {nu_bhl/(1.-nu_bhl)}, material 3
initial value USIGYY=Function Z   1,  {nu_bhl/(1.-nu_bhl)}, material 3
$$ Interface between caprock1 and caprock2
initial value USIGZZ=Function Z   1,  1., material 7
initial value USIGXX=Function Z   1,  {nu_bho/(1.-nu_bho)}, material 7
initial value USIGYY=Function Z   1,  {nu_bho/(1.-nu_bho)}, material 7
$$ Caprock2
initial value USIGZZ=Function Z   1,  1., material 4
initial value USIGXX=Function Z   1,  {nu_bhn/(1.-nu_bhn)}, material 4
initial value USIGYY=Function Z   1,  {nu_bhn/(1.-nu_bhn)}, material 4
$$ Interface between caprock2 and salt dome
initial value USIGZZ=Function Z   1,  1., material 8
initial value USIGXX=Function Z   1,  {nu_bho/(1.-nu_bho)}, material 8
initial value USIGYY=Function Z   1,  {nu_bho/(1.-nu_bho)}, material 8
$$ Surrounding rock
initial value USIGZZ=Function Z   2,  1., material 5
initial value USIGXX=Function Z   2,  {nu_bhs/(1.-nu_bhs)}, material 5
initial value USIGYY=Function Z   2,  {nu_bhs/(1.-nu_bhs)}, material 5
$$ Dome perimeter
initial value USIGZZ=Function Z   3,  1., material 9
initial value USIGXX=Function Z   3,  {nu_bho/(1.-nu_bho)}, material 9
initial value USIGYY=Function Z   3,  {nu_bho/(1.-nu_bho)}, material 9
$$ Fault in salt dome
initial value USIGZZ=Function Z   4,  1., material 11
initial value USIGXX=Function Z   4,  1., material 11
initial value USIGYY=Function Z   4,  1., material 11
$$ Fault in overburden; and interface between overburden and caprock1
initial value USIGZZ=Function Z   4,  1., material 2
initial value USIGXX=Function Z   4,  {nu_bho/(1.-nu_bho)}, material 12
initial value USIGYY=Function Z   4,  {nu_bho/(1.-nu_bho)}, material 12
$$ Fault in caprock1; and interface between caprock1 and caprock2
initial value USIGZZ=Function Z   4,  1., material 13
initial value USIGXX=Function Z   4,  {nu_bho/(1.-nu_bho)}, material 13
initial value USIGYY=Function Z   4,  {nu_bho/(1.-nu_bho)}, material 13
$$ Fault in caprock2; and interface between caprock2 and salt dome
initial value USIGZZ=Function Z   4,  1., material 14
initial value USIGXX=Function Z   4,  {nu_bho/(1.-nu_bho)}, material 14
initial value USIGYY=Function Z   4,  {nu_bho/(1.-nu_bho)}, material 14

$               dir  nset
no displacement Z    2    $ Bottom of mesh
```

```
no displacement x    3    $ West side
no displacement x    4    $ East side
no displacement y    5    $ South side
no displacement y    6    $ North side

Gravity
  Gravitational Constant {gr}
  Magnitude 1.0
  Use Function 11
  Direction 0. 0. -1
End Gravity
$-----------------------------------------------------------------------
$ Pressure Boundaries
$
$ Pressures on side set after the initial leach
$        sset ftn  scl
pressure 1010 user 1. $ pressure in cavern 1
pressure 1020 user 1. $ pressure in cavern 2
pressure 1030 user 1. $ pressure in cavern 3
pressure 1040 user 1. $ pressure in cavern 4
pressure 1050 user 1. $ pressure in cavern 5
pressure 1060 user 1. $ pressure in cavern 6
pressure 1070 user 1. $ pressure in cavern 7
pressure 1080 user 1. $ pressure in cavern 8
pressure 1090 user 1. $ pressure in cavern 9
pressure 1100 user 1. $ pressure in cavern 10
pressure 1110 user 1. $ pressure in cavern 11
pressure 1120 user 1. $ pressure in cavern 12
pressure 1130 user 1. $ pressure in cavern 13
pressure 1140 user 1. $ pressure in cavern 14

$ Pressures on side set after the 1st drawdown leach
pressure 1011 user 1. $ pressure in cavern 1
pressure 1021 user 1. $ pressure in cavern 2
pressure 1031 user 1. $ pressure in cavern 3
pressure 1041 user 1. $ pressure in cavern 4
pressure 1051 user 1. $ pressure in cavern 5
pressure 1061 user 1. $ pressure in cavern 6
pressure 1071 user 1. $ pressure in cavern 7
pressure 1081 user 1. $ pressure in cavern 8
pressure 1091 user 1. $ pressure in cavern 9
pressure 1101 user 1. $ pressure in cavern 10
pressure 1111 user 1. $ pressure in cavern 11
pressure 1121 user 1. $ pressure in cavern 12
pressure 1131 user 1. $ pressure in cavern 13
pressure 1141 user 1. $ pressure in cavern 14

$ Pressures on side set after the 2nd drawdown leach
pressure 1012 user 1. $ pressure in cavern 1
pressure 1022 user 1. $ pressure in cavern 2
pressure 1032 user 1. $ pressure in cavern 3
pressure 1042 user 1. $ pressure in cavern 4
pressure 1052 user 1. $ pressure in cavern 5
pressure 1062 user 1. $ pressure in cavern 6
pressure 1072 user 1. $ pressure in cavern 7
pressure 1082 user 1. $ pressure in cavern 8
pressure 1092 user 1. $ pressure in cavern 9
pressure 1102 user 1. $ pressure in cavern 10
pressure 1112 user 1. $ pressure in cavern 11
pressure 1122 user 1. $ pressure in cavern 12
pressure 1132 user 1. $ pressure in cavern 13
pressure 1142 user 1. $ pressure in cavern 14

$ Pressures on side set after the 3rd drawdown leach
pressure 1013 user 1. $ pressure in cavern 1
pressure 1023 user 1. $ pressure in cavern 2
pressure 1033 user 1. $ pressure in cavern 3
pressure 1043 user 1. $ pressure in cavern 4
pressure 1053 user 1. $ pressure in cavern 5
pressure 1063 user 1. $ pressure in cavern 6
pressure 1073 user 1. $ pressure in cavern 7
pressure 1083 user 1. $ pressure in cavern 8
pressure 1093 user 1. $ pressure in cavern 9
pressure 1103 user 1. $ pressure in cavern 10
pressure 1113 user 1. $ pressure in cavern 11
pressure 1123 user 1. $ pressure in cavern 12
pressure 1133 user 1. $ pressure in cavern 13
pressure 1143 user 1. $ pressure in cavern 14

$ Pressures on side set after the 4th drawdown leach
pressure 1014 user 1. $ pressure in cavern 1
```

```
pressure 1024 user 1. $ pressure in cavern 2
pressure 1034 user 1. $ pressure in cavern 3
pressure 1044 user 1. $ pressure in cavern 4
pressure 1054 user 1. $ pressure in cavern 5
pressure 1064 user 1. $ pressure in cavern 6
pressure 1074 user 1. $ pressure in cavern 7
pressure 1084 user 1. $ pressure in cavern 8
pressure 1094 user 1. $ pressure in cavern 9
pressure 1104 user 1. $ pressure in cavern 10
pressure 1114 user 1. $ pressure in cavern 11
pressure 1124 user 1. $ pressure in cavern 12
pressure 1134 user 1. $ pressure in cavern 13
pressure 1144 user 1. $ pressure in cavern 14

$ Pressures on side set after the 5th drawdown leach
pressure 1015 user 1. $ pressure in cavern 1
pressure 1025 user 1. $ pressure in cavern 2
pressure 1035 user 1. $ pressure in cavern 3
pressure 1045 user 1. $ pressure in cavern 4
pressure 1055 user 1. $ pressure in cavern 5
pressure 1065 user 1. $ pressure in cavern 6
pressure 1075 user 1. $ pressure in cavern 7
pressure 1085 user 1. $ pressure in cavern 8
pressure 1095 user 1. $ pressure in cavern 9
pressure 1105 user 1. $ pressure in cavern 10
pressure 1115 user 1. $ pressure in cavern 11
pressure 1125 user 1. $ pressure in cavern 12
pressure 1135 user 1. $ pressure in cavern 13
pressure 1145 user 1. $ pressure in cavern 14
$------------------------------------------------------------------------
$ Output
$
thermal stress external, tmpnod
plot state, EqCS, temp
plot nodal, displacement, tmpnod
plot element, sig, vonmis, eps, pressure
$------------------------------------------------------------------------
$  Define Material Properties
$
material 1, Power Law Creep, {rho_bhh}       $ Salt
 TWO MU               = {2*mu_bhh/RF_bhh } $ (Pa)
 BULK MODULUS         = {K_bhh/RF_bhh }    $ (Pa)
 CREEP CONSTANT               = {A_PLC*SMF  }            $ (Pa^-n/s)
 STRESS EXPONENT      = {n2_bhh   }
 THERMAL CONSTANT     = {Q2_bhh/R }       $ (K)
END material 1
$ Salt dome height={h_SD} m

active limits, 100, 0.0,0.01 $ Initial leaching of caverns
material 100, Power Law Creep, {rho_bhh}     $ Salt
 TWO MU               = {2*mu_bhh/RF_bhh } $ (Pa)
 BULK MODULUS         = {K_bhh/RF_bhh }    $ (Pa)
 CREEP CONSTANT               = {A_PLC*SMF  }            $ (Pa^-n/s)
 STRESS EXPONENT      = {n2_bhh   }
 THERMAL CONSTANT     = {Q2_bhh/R }       $ (K)
END material 100

active limits, 101, 0.0,{D1st_s} $ 1st leach at {D1st_s/yr_s} years
material 101, Power Law Creep, {rho_bhh}     $ Salt
 TWO MU               = {2*mu_bhh/RF_bhh } $ (Pa)
 BULK MODULUS         = {K_bhh/RF_bhh }    $ (Pa)
 CREEP CONSTANT               = {A_PLC*SMF  }            $ (Pa^-n/s)
 STRESS EXPONENT      = {n2_bhh   }
 THERMAL CONSTANT     = {Q2_bhh/R }       $ (K)
END material 101

active limits, 102, 0.0,{D2nd_s} $ 2nd leach at {D2nd_s/yr_s} years
material 102, Power Law Creep, {rho_bhh}     $ Salt
 TWO MU               = {2*mu_bhh/RF_bhh } $ (Pa)
 BULK MODULUS         = {K_bhh/RF_bhh }    $ (Pa)
 CREEP CONSTANT               = {A_PLC*SMF  }            $ (Pa^-n/s)
 STRESS EXPONENT      = {n2_bhh   }
 THERMAL CONSTANT     = {Q2_bhh/R }       $ (K)
END material 102

active limits, 103, 0.0,{D3rd_s} $ 3rd leach at {D3rd_s/yr_s} years
material 103, Power Law Creep, {rho_bhh}     $ Salt
 TWO MU               = {2*mu_bhh/RF_bhh } $ (Pa)
 BULK MODULUS         = {K_bhh/RF_bhh }    $ (Pa)
 CREEP CONSTANT               = {A_PLC*SMF  }            $ (Pa^-n/s)
 STRESS EXPONENT      = {n2_bhh   }
```

```
 THERMAL CONSTANT      = {Q2_bhh/R }       $ (K)
END material 103

active limits, 104, 0.0,{D4th_s} $ 4th leach at {D4th_s/yr_s} years
material 104, Power Law Creep, {rho_bhh}     $ Salt
 TWO MU                = {2*mu_bhh/RF_bhh } $ (Pa)
 BULK MODULUS          = {K_bhh/RF_bhh }    $ (Pa)
 CREEP CONSTANT               = {A_PLC*SMF  }            $ (Pa^-n/s)
 STRESS EXPONENT       = {n2_bhh    }
 THERMAL CONSTANT      = {Q2_bhh/R }       $ (K)
END material 104

active limits, 105, 0.0,{D5th_s} $ 5th leach at {D5th_s/yr_s} years
material 105, Power Law Creep, {rho_bhh}     $ Salt
 TWO MU                = {2*mu_bhh/RF_bhh } $ (Pa)
 BULK MODULUS          = {K_bhh/RF_bhh }    $ (Pa)
 CREEP CONSTANT               = {A_PLC*SMF  }            $ (Pa^-n/s)
 STRESS EXPONENT       = {n2_bhh    }
 THERMAL CONSTANT      = {Q2_bhh/R }       $ (K)
END material 105

material 2, elastic, {rho_bho}  $ Overburden (sand)
 YOUNGS MODULUS = {E_bho    } $ (Pa)
 POISSONS RATIO = {nu_bho   }
END material 2
$ Overburden thickness={t_OB} m

material 3, elastic, {rho_bhl}  $ Caprock 1 (Gypsum and Limestone)
 YOUNGS MODULUS = {E_bhl    } $ (Pa)
 POISSONS RATIO = {nu_bhl   }
END material 3
$ Caprock1 thickness={t_CRL} m

material 4, SOIL N FOAMS, {rho_bhn} $ Caprock 2 (Anhydrite)
 TWO MU = {2.*mu_bhn}
 BULK MODULUS = {K_bhn}
 A0 = {A0_bhn}
 A1 = {A1_bhn}
 A2 = {A2_bhn}
 PRESSURE CUTOFF = 0.0
 FUNCTION ID = 0
end material 4
$ Caprock2 thickness={t_CRN} m

material 5, elastic, {rho_bhs}  $ Farfield (sandstone)
 YOUNGS MODULUS = {E_bhs    } $ (Pa)
 POISSONS RATIO = {nu_bhs   }
END material 5
$ Surrounding rock thickness={t_SR} m

material 6, elastic, {rho_bho}  $ Interface between overburden and caprock1(sand)
 YOUNGS MODULUS = {E_bho    } $ (Pa)
 POISSONS RATIO = {nu_bho   }
END material 6
$ under_ob thickness={t_UOB} m

material 7, elastic, {rho_bho}  $ Interface between caprock1 and caprock2 (sand)
 YOUNGS MODULUS = {E_bho    } $ (Pa)
 POISSONS RATIO = {nu_bho   }
END material 7
$ under_c1 thickness={t_UC1} m

material 8, elastic, {rho_bho}  $ Interface between caprock2 and salt dome (sand)
 YOUNGS MODULUS = {E_bho    } $ (Pa)
 POISSONS RATIO = {nu_bho   }
END material 8
$ under_c2 thickness={t_UC2} m

material 9, elastic, {rho_bho}  $ Interface between dome and surrounding rock (sand)
 YOUNGS MODULUS = {E_bho    } $ (Pa)
 POISSONS RATIO = {nu_bho   }
END material 9
$ hight of dome perimeter={h_DP} m

material 11, Power Law Creep, {rho_bhh} $ Fault in salt dome
 TWO MU                = {2*mu_bhh/RF_bhh } $ (Pa)
 BULK MODULUS          = {K_bhh/RF_bhh }    $ (Pa)
 CREEP CONSTANT               = {A_PLC*SMF  }            $ (Pa^-n/s)
 STRESS EXPONENT       = {n2_bhh    }
 THERMAL CONSTANT      = {Q2_bhh/R }       $ (K)
END material 11
```

```
$ height of fault in salt dome={h_SD} m

material 12, elastic, {rho_bho} $ Fault in overburden and under_ob (sand)
 YOUNGS MODULUS = {E_bho    } $ (Pa)
 POISSONS RATIO = {nu_bho   }
END material 12
$ height of fault in Overburden={t_OB+t_UOB} m

material 13, elastic, {rho_bho} $ Fault in Caprock 1 and under_c1 (sand)
 YOUNGS MODULUS = {E_bho    } $ (Pa)
 POISSONS RATIO = {nu_bho   }
END material 13
$ height of fault in Caprock1={t_CRL+t_UC1} m

material 14, elastic, {rho_bho} $ Fault in Caprock 2 and under_c2 (sand)
 YOUNGS MODULUS = {E_bho    } $ (Pa)
 POISSONS RATIO = {nu_bho}
end material 14
$ height of fault in Caprock2={t_CRN+t_UC2} m

exit
```

# III-B. Adagio Input Deck

```
{include("/home/bypark/common/units.txt")}
{include("/home/bypark/common/BH_stratigraphy_sftele.txt")}
{include("/home/bypark/common/BH_materials_PLC.txt")}

$ Time at the initial leaches begin
$     bgn_s  = {bgn_s=0.} s
$ Times at the drawdown leaches for all SPR caverns start
$     D1st_s = {D1st_s=bgn_s + 31.*yr_s} s $ {D1st_s/yr_s} years
$     D2nd_s = {D2nd_s=D1st_s + 5.*yr_s} s $ {D2nd_s/yr_s} years
$     D3rd_s = {D3rd_s=D2nd_s + 5.*yr_s} s $ {D3rd_s/yr_s} years
$     D4th_s = {D4th_s=D3rd_s + 5.*yr_s} s $ {D4th_s/yr_s} years
$     D5th_s = {D5th_s=D4th_s + 5.*yr_s} s $ {D5th_s/yr_s} years
$Time at the simulaton completes
$     end_s  = {end_s =D5th_s + 5.*yr_s} s $ {end_s/yr_s} years

$ number of nodes = {nnod = 554540}
$ number of degree of freedom = {ndof = 6*nnod }
# MAXIMUM ITERATIONS = {nmax=10000}
#
# In-sute stress with stratigraphy
#
# Gravity, gr={gr=9.81} (m/s^2)
#
$ {sigv_OB = -rho_bho*gr*t_OB} Pa              $ Vertical stress at bottom of overburden (top of
UOB)
$ {sigv_UOB= sigv_OB -rho_bho*gr*t_UOB} Pa      $ Vertical stress at bottom of UOB (top of
caprock1)
$ {sigv_CRL= sigv_UOB-rho_bhl*gr*t_CRL} Pa      $ Vertical stress at bottom of caprock1 (top of
UC1)
$ {sigv_UC1= sigv_CRL-rho_bho*gr*t_UC1} Pa      $ Vertical stress at bottom of UC1 (top of
caprock2)
$ {sigv_CRN= sigv_UC1-rho_bhn*gr*t_CRN} Pa      $ Vertical stress at bottom of caprock2 (top of
UC2)
$ {sigv_UC2= sigv_CRN-rho_bho*gr*t_UC2} Pa      $ Vertical stress at bottom of UC2 (top of salt
dome)
$ {sigv_SD = sigv_UC2-rho_bhh*gr*h_SD}  Pa     $ Vertical stress at bottom of salt dome
$ {sigv_SR = sigv_UOB-rho_bhs*gr*t_SR}  Pa     $ Vertical stress at bottom of surrounding rock
$ {sigv_DP = sigv_OB -rho_bho*gr*h_DP}  Pa     $ Vertical stress at bottom of dome perimeter
$ {sigv_FOB= -rho_bho*gr*(t_OB+t_UOB)} Pa           $ Vertical stress at bottom of fault in
overburden (top of caprock1)
$ {sigv_FC1= sigv_FOB-rho_bho*gr*(t_CRL+t_UC1)} Pa $ Vertical stress at bottom of fault in
caprock1 (top of caprock2)
$ {sigv_FC2= sigv_FC1-rho_bho*gr*(t_CRN+t_UC2)} Pa $ Vertical stress at bottom of fault in
caprock2 (top of salt dome)
$ {sigv_FSD= sigv_FC2-rho_bhh*gr*h_SD} Pa          $ Vertical stress at bottom of fault in salt
dome

$===================================================================
begin sierra  bh_full_5d

  title  bh_full_5d PLC step plot 1 mon OB mat. for inter and fault in OB C1 and C2
```

```
# Define the file name containing the Fortran 77 user subroutine
  user subroutine file = usrpbc_bh_full_5d.F

  define direction y with vector 0.0 1.0 0.0
  define direction x with vector 1.0 0.0 0.0
  define direction z with vector 0.0 0.0 1.0
  define direction negative_z with vector 0.0 0.0 -1.0
  define point origin with coordinates 0.0 0.0 0.0

  #---------- Functions ---------

  # ASCENDING ORDER IS REQUIRED FOR DEFINING FUNCTION
  begin definition for function function_1  # Gravity
    type is piecewise linear
    begin values
     0.0     1.0
     {end_s} 1.0
    end values
  end definition for function function_1

  begin definition for function function_2
    type is piecewise linear
    begin values
     -10.  0.0
      0.0  0.0
      10.  8.344444444e+11
    end values
  end definition for function function_2

  #---------- Materials ----------

  begin property specification for material mat_1 # Salt
    density = {rho_bhh}
    begin parameters for model power_law_creep
      shear modulus    = {mu_bhh/RF_bhh } # (Pa)
      bulk modulus     = {K_bhh/RF_bhh }  # (Pa)
      creep constant   = {A_PLC*SMF  }         # (Pa^-n/s)
      creep exponent   = {n2_bhh   }
      thermal constant = {Q2_bhh/R }      # (K)
    end parameters for model power_law_creep
  end property specification for material mat_1

  begin solid section solid_1
    strain incrementation = midpoint_increment
    hourglass rotation = scaled
  end solid section solid_1

  begin property specification for material mat_2 # Overburden (sand)
    density = {rho_bho}
    begin parameters for model elastic
      youngs modulus = {E_bho    }   # (Pa)
      poissons ratio = {nu_bho   }
    end parameters for model elastic
  end property specification for material mat_2

  begin solid section solid_2
    strain incrementation = midpoint_increment
    hourglass rotation = scaled
  end solid section solid_2

  begin property specification for material mat_3 # Caprock 1 (Gypsum and Limestone)
    density = {rho_bhl}
    begin parameters for model elastic
      youngs modulus = {E_bhl    }   # (Pa)
      poissons ratio = {nu_bhl   }
    end parameters for model elastic
  end property specification for material mat_3

  begin solid section solid_3
    strain incrementation = midpoint_increment
    hourglass rotation = scaled
  end solid section solid_3

  begin property specification for material mat_4 # Caprock 2 (Anhydrite)
    density = 2300
    begin parameters for model soil_foam
      shear modulus     = {mu_bhn}  # (Pa)
      bulk modulus      = {K_bhn}   # (Pa)
      a0                = {A0_bhn}
      a1                = {A1_bhn}
      a2                = {A2_bhn}
```

```
      pressure cutoff   = 0.0
      pressure function = function_2
    end parameters for model soil_foam
  end property specification for material mat_4

  begin solid section solid_4
    strain incrementation = midpoint_increment
    hourglass rotation = scaled
  end solid section solid_4

  begin property specification for material mat_5 # Farfield (Sandstone)
    density = {rho_bhs}
    begin parameters for model elastic
      youngs modulus = {E_bhs    }   # (Pa)
      poissons ratio = {nu_bhs}
    end parameters for model elastic
  end property specification for material mat_5

  begin solid section solid_5
    strain incrementation = midpoint_increment
    hourglass rotation = scaled
  end solid section solid_5

#================= Finite Element Model ==================================

$-----------------------------------------------------------------------
$$ Defined blocks in CUBIT
$ Block 1=salt dome except caverns
$       2=overburden
$       3=caprock1
$       4=caprock2
$       5=surrounding rock
$       6=interface between overburden and caprock1
$       7=interface between caprock1 and caprock2
$       8=interface between caprock2 and salt dome
$       9=interface between dome and surrounding rock
$       11=fault in salt dome
$       12=fault in overburden; and interface between overburden and caprock1
$       13=fault in caprock1; and interface between caprock1 and caprock2
$       14=fault in caprock2; and interface between caprock2 and salt dome
$       100=initial reach
$       101=1st drawdown leach
$       102=2nd drawdown leach
$       103=3rd drawdown leach
$       104=4th drawdown leach
$       105=5th drawdown leach
$-----------------------------------------------------------------------

  begin finite element model bh_full_5d

    Database name = /gscratch2/bypark/bh_cs/mesh/sftele/bh_full_5d.g
    Database type = exodusII

    begin parameters for block block_1 # Salt dome
      material mat_1
      solid mechanics use model power_law_creep
      section = solid_1
    end parameters for block block_1

    begin parameters for block block_100 # initial leach
      material mat_1
      solid mechanics use model power_law_creep
      section = solid_1
    end parameters for block block_100

    begin parameters for block block_101 # 1st drawdown leach
      material mat_1
      solid mechanics use model power_law_creep
      section = solid_1
    end parameters for block block_101

    begin parameters for block block_102 # 2nd drawdown leach
      material mat_1
      solid mechanics use model power_law_creep
      section = solid_1
    end parameters for block block_102

    begin parameters for block block_103 # 3rd drawdown leach
      material mat_1
      solid mechanics use model power_law_creep
      section = solid_1
```

```
    end parameters for block block_103

    begin parameters for block block_104 # 4th drawdown leach
      material mat_1
      solid mechanics use model power_law_creep
      section = solid_1
    end parameters for block block_104

    begin parameters for block block_105 # 5th drawdown leach
      material mat_1
      solid mechanics use model power_law_creep
      section = solid_1
    end parameters for block block_105

    begin parameters for block block_2 # Overburden
      material mat_2
      solid mechanics use model elastic
      section = solid_2
    end parameters for block block_2

    begin parameters for block block_3 # Caprock 1
      material mat_3
      solid mechanics use model elastic
      section = solid_3
    end parameters for block block_3

    begin parameters for block block_4 # Caprock 2
      material mat_4
      solid mechanics use model soil_foam
      section = solid_4
    end parameters for block block_4

    begin parameters for block block_5 # Surrounding rock
      material mat_5
      solid mechanics use model elastic
      section = solid_5
    end parameters for block block_5

    begin parameters for block block_6 # Interface between overburden and caprock1
      material mat_2
      solid mechanics use model elastic
      section = solid_2
    end parameters for block block_6

    begin parameters for block block_7 # Interface between caprock1 and caprock2
      material mat_2
      solid mechanics use model elastic
      section = solid_2
    end parameters for block block_7

    begin parameters for block block_8 # Interface between caprock2 and salt dome
      material mat_2
      solid mechanics use model elastic
      section = solid_2
    end parameters for block block_8

    begin parameters for block block_9 # Interface between dome and surrounding rock
      material mat_2
      solid mechanics use model elastic
      section = solid_2
    end parameters for block block_9

    begin parameters for block block_11 # Fault in salt dome
      material mat_1
      solid mechanics use model power_law_creep
      section = solid_1
    end parameters for block block_11

    begin parameters for block block_12 # fault in overburden; and interface between overburden
and caprock1
      material mat_2
      solid mechanics use model elastic
      section = solid_2
    end parameters for block block_12

    begin parameters for block block_13 # fault in caprock1; and interface between caprock1 and
caprock2
      material mat_2
      solid mechanics use model elastic
      section = solid_2
    end parameters for block block_13
```

```
    begin parameters for block block_14 # fault in caprock2; and interface between caprock2 and
salt dome
      material mat_2
      solid mechanics use model elastic
      section = solid_2
    end parameters for block block_14

  end finite element model bh_full_5d

#================= Adagio PROCEDURE =====================================================
  begin adagio procedure procedure_1

    #---------- Time Step Control ----------

    begin time control
      begin time stepping block p0
        start time = 0.0
        begin parameters for adagio region region_1
          number of time steps = {h_s/10}  $1 step={h_s/(h_s/10)} sec
        end parameters for adagio region region_1
      end time stepping block p0

      begin time stepping block p1
        start time = {h_s}    $ 1 hour
        begin parameters for adagio region region_1
          number of time steps = 230   $1 step={(d_s-h_s)/230/min_s} mins
        end parameters for adagio region region_1
      end time stepping block p1

      begin time stepping block p2
        start time = {1.*d_s}  $ 1 day
        begin parameters for adagio region region_1
          number of time steps = 90   $1 step={(10.*d_s-1.*d_s)/90/h_s} hours
        end parameters for adagio region region_1
      end time stepping block p2

      begin time stepping block p3
        start time = {10.*d_s}  $ 10 days
        begin parameters for adagio region region_1
          number of time steps = 40   $1 step={(mon_s-10.*d_s)/40/d_s} days
        end parameters for adagio region region_1
      end time stepping block p3

      begin time stepping block p4
        start time = {mon_s}    $ 1 month
        begin parameters for adagio region region_1
          number of time steps = {ITS=12}  $1 step={(3.*mon_s-mon_s)/ITS/d_s} days
        end parameters for adagio region region_1
      end time stepping block p4

      begin time stepping block p5
        start time = {3.*mon_s} $ 3 months
        begin parameters for adagio region region_1
          number of time steps = 9      $1 step={(bgn_s+yr_s-3.*mon_s)/9/d_s} days
        end parameters for adagio region region_1
      end time stepping block p5

      begin time stepping block p6
        start time = {bgn_s+yr_s} $ Change to oil/brine/liquid in caverns: {(bgn_s+yr_s)/yr_s}
years
        begin parameters for adagio region region_1
          number of time steps = {(D1st_s-(bgn_s+yr_s))/yr_s*ITS} $ 1 step={(D1st_s-yr_s)/360} s
        end parameters for adagio region region_1
      end time stepping block p6

      begin time stepping block p7
        start time = {D1st_s} # {D1st_s/yr_s} years
        begin parameters for adagio region region_1
          number of time steps = {(D2nd_s-D1st_s)/yr_s*ITS} # 1 step={(D2nd_s-D1st_s)/60} s
        end parameters for adagio region region_1
      end time stepping block p7

      begin time stepping block p8
        start time = {D2nd_s} $ 1st drawdown leach: {D1st_s/yr_s} years
        begin parameters for adagio region region_1
          number of time steps = {(D3rd_s-D2nd_s)/yr_s*ITS} # 1 step={(D3rd_s-D2nd_s)/60} s
        end parameters for adagio region region_1
      end time stepping block p8

      begin time stepping block p9
```

```
      start time = {D3rd_s} $ 3rd drawdown leach: {D3rd_s/yr_s} years
      begin parameters for adagio region region_1
        number of time steps = {(D4th_s-D3rd_s)/yr_s*ITS} # 1 step={(D4th_s-D3rd_s)/60} s
      end parameters for adagio region region_1
    end time stepping block p9

    begin time stepping block p10
      start time = {D4th_s} $ 4th drawdown leach: {D4th_s/yr_s} years
      begin parameters for adagio region region_1
        number of time steps = {(D5th_s-D4th_s)/yr_s*ITS} # 1 step={(D5th_s-D4th_s)/60} s
      end parameters for adagio region region_1
    end time stepping block p10

    begin time stepping block p11
      start time = {D5th_s} $ 5th drawdown leach: {D5th_s/yr_s} years
      begin parameters for adagio region region_1
        number of time steps = {(end_s-D5th_s)/yr_s*ITS} # 1 step={((end_s-D5th_s))/60} s
      end parameters for adagio region region_1
    end time stepping block p11

    termination time = {end_s} # {(end_s-bgn_s)/yr_s} years since simulation starts

  end time control

  begin adagio region region_1

    use finite element model bh_full_5d

    #--------- Restart ---------

#      begin restart data restart_1
#        database type = exodusII
#        output database Name = bh_full_5d.rsout
#      end restart data restart_1

    #--------- Boundary Conditions ---------

    begin gravity
      include all blocks
      gravitational constant = {gr}
      direction = negative_z
      function = function_1
    end gravity

    begin prescribed temperature
      include all blocks
      read variable = tmpnod
    end prescribed temperature

    begin fixed displacement # Bottom of mesh
      node set = nodelist_2
      components = z
    end fixed displacement

    begin fixed displacement # West side
      node set = nodelist_3
      components = x
    end fixed displacement

    begin fixed displacement # East side
      node set = nodelist_4
      components = x
    end fixed displacement

    begin fixed displacement # South side
      node set = nodelist_5
      components = y
    end fixed displacement

    begin fixed displacement # North side
      node set = nodelist_6
      components = y
    end fixed displacement

#-----------------------------------------------------------------
#     The following sets of "begin pressure blocks" define the
#     surfaces and time periods associated with the sequential
#     leachings. Note that "cavity_pressure" is the subroutine
#     name not the file name. The file name is usrpbc_bh_full_5d.F
#     which was specified earlier in this input file.
#-----------------------------------------------------------------
```

```
###
#     Pressures on side set after the initial leach (SPR caverns)
#     Time period from 0.01 seconds to {D1st_s/yr_s} years
#     To reduce the impact of the death volume, apply the surface
#     pressure 1 period earlier, i.e. p4 rather than p5 (1 d_s).
###

      begin pressure # pressure in cavern 101
        surface = surface_1010
        surface subroutine = cavity_pressure_101
        active periods = p0 p1 p2 p3 p4 p5 p6
      end pressure

      begin pressure # pressure in cavern 102
        surface = surface_1020
        surface subroutine = cavity_pressure_102
        active periods = p0 p1 p2 p3 p4 p5 p6
      end pressure

      begin pressure # pressure in cavern 103
        surface = surface_1030
        surface subroutine = cavity_pressure_103
        active periods = p0 p1 p2 p3 p4 p5 p6
      end pressure

      begin pressure # pressure in cavern 104
        surface = surface_1040
        surface subroutine = cavity_pressure_104
        active periods = p0 p1 p2 p3 p4 p5 p6
      end pressure

      begin pressure # pressure in cavern 105
        surface = surface_1050
        surface subroutine = cavity_pressure_105
        active periods = p0 p1 p2 p3 p4 p5 p6
      end pressure

      begin pressure # pressure in cavern 106
        surface = surface_1060
        surface subroutine = cavity_pressure_106
        active periods = p0 p1 p2 p3 p4 p5 p6
      end pressure

      begin pressure # pressure in cavern 107
        surface = surface_1070
        surface subroutine = cavity_pressure_107
        active periods = p0 p1 p2 p3 p4 p5 p6
      end pressure

      begin pressure # pressure in cavern 108
        surface = surface_1080
        surface subroutine = cavity_pressure_108
        active periods = p0 p1 p2 p3 p4 p5 p6
      end pressure

      begin pressure # pressure in cavern 109
        surface = surface_1090
        surface subroutine = cavity_pressure_109
        active periods = p0 p1 p2 p3 p4 p5 p6
      end pressure

      begin pressure # pressure in cavern 110
        surface = surface_1100
        surface subroutine = cavity_pressure_110
        active periods = p0 p1 p2 p3 p4 p5 p6
      end pressure

      begin pressure # pressure in cavern 111
        surface = surface_1110
        surface subroutine = cavity_pressure_111
        active periods = p0 p1 p2 p3 p4 p5 p6
      end pressure

      begin pressure # pressure in cavern 112
        surface = surface_1120
        surface subroutine = cavity_pressure_112
        active periods = p0 p1 p2 p3 p4 p5 p6
      end pressure

      begin pressure # pressure in cavern 113
```

```
    surface = surface_1130
    surface subroutine = cavity_pressure_113
    active periods = p0 p1 p2 p3 p4 p5 p6
  end pressure

  begin pressure # pressure in cavern 114
    surface = surface_1140
    surface subroutine = cavity_pressure_114
    active periods = p0 p1 p2 p3 p4 p5 p6
  end pressure

###
#     Pressures on side set after the 1st drawdown leach
#     Time period from {D1st_s/yr_s} years to {D2nd_s/yr_s} years
###

  begin pressure # pressure in cavern 101
    surface = surface_1011
    surface subroutine = cavity_pressure_101
    active periods =  p7
  end pressure

  begin pressure # pressure in cavern 102
    surface = surface_1021
    surface subroutine = cavity_pressure_102
    active periods =  p7
  end pressure

  begin pressure # pressure in cavern 103
    surface = surface_1031
    surface subroutine = cavity_pressure_103
    active periods =  p7
  end pressure

  begin pressure # pressure in cavern 104
    surface = surface_1041
    surface subroutine = cavity_pressure_104
    active periods =  p7
  end pressure

  begin pressure # pressure in cavern 105
    surface = surface_1051
    surface subroutine = cavity_pressure_105
    active periods =  p7
  end pressure

  begin pressure # pressure in cavern 106
    surface = surface_1061
    surface subroutine = cavity_pressure_106
    active periods =  p7
  end pressure

  begin pressure # pressure in cavern 107
    surface = surface_1071
    surface subroutine = cavity_pressure_107
    active periods =  p7
  end pressure

  begin pressure # pressure in cavern 108
    surface = surface_1081
    surface subroutine = cavity_pressure_108
    active periods =  p7
  end pressure

  begin pressure # pressure in cavern 109
    surface = surface_1091
    surface subroutine = cavity_pressure_109
    active periods =  p7
  end pressure

  begin pressure # pressure in cavern 110
    surface = surface_1101
    surface subroutine = cavity_pressure_110
    active periods =  p7
  end pressure

  begin pressure # pressure in cavern 111
    surface = surface_1111
    surface subroutine = cavity_pressure_111
    active periods =  p7
  end pressure
```

```
      begin pressure # pressure in cavern 112
        surface = surface_1121
        surface subroutine = cavity_pressure_112
        active periods =  p7
      end pressure

      begin pressure # pressure in cavern 113
        surface = surface_1131
        surface subroutine = cavity_pressure_113
        active periods =  p7
      end pressure

      begin pressure # pressure in cavern 114
        surface = surface_1141
        surface subroutine = cavity_pressure_114
        active periods =  p7
      end pressure

###
#     Pressures on side set after the 2nd drawdown leach
#     Time period from {D2nd_s/yr_s} years to {D3rd_s/yr_s} years
###

      begin pressure # pressure in cavern 101
        surface = surface_1012
        surface subroutine = cavity_pressure_101
        active periods =  p8
      end pressure

      begin pressure # pressure in cavern 102
        surface = surface_1022
        surface subroutine = cavity_pressure_102
        active periods =  p8
      end pressure

      begin pressure # pressure in cavern 103
        surface = surface_1032
        surface subroutine = cavity_pressure_103
        active periods =  p8
      end pressure

      begin pressure # pressure in cavern 104
        surface = surface_1042
        surface subroutine = cavity_pressure_104
        active periods =  p8
      end pressure

      begin pressure # pressure in cavern 105
        surface = surface_1052
        surface subroutine = cavity_pressure_105
        active periods =  p8
      end pressure

      begin pressure # pressure in cavern 106
        surface = surface_1062
        surface subroutine = cavity_pressure_106
        active periods =  p8
      end pressure

      begin pressure # pressure in cavern 107
        surface = surface_1072
        surface subroutine = cavity_pressure_107
        active periods =  p8
      end pressure

      begin pressure # pressure in cavern 108
        surface = surface_1082
        surface subroutine = cavity_pressure_108
        active periods =  p8
      end pressure

      begin pressure # pressure in cavern 109
        surface = surface_1092
        surface subroutine = cavity_pressure_109
        active periods =  p8
      end pressure

      begin pressure # pressure in cavern 110
        surface = surface_1102
        surface subroutine = cavity_pressure_110
```

```
    active periods =  p8
  end pressure

  begin pressure # pressure in cavern 111
    surface = surface_1112
    surface subroutine = cavity_pressure_111
    active periods =  p8
  end pressure

  begin pressure # pressure in cavern 112
    surface = surface_1122
    surface subroutine = cavity_pressure_112
    active periods =  p8
  end pressure

  begin pressure # pressure in cavern 113
    surface = surface_1132
    surface subroutine = cavity_pressure_113
    active periods =  p8
  end pressure

  begin pressure # pressure in cavern 114
    surface = surface_1142
    surface subroutine = cavity_pressure_114
    active periods =  p8
  end pressure

###
#     Pressures on side set after the 3rd drawdown leach
#     Time period from {D3rd_s/yr_s} years to {D4th_s/yr_s} years
###

  begin pressure # pressure in cavern 101
    surface = surface_1013
    surface subroutine = cavity_pressure_101
    active periods =  p9
  end pressure

  begin pressure # pressure in cavern 102
    surface = surface_1023
    surface subroutine = cavity_pressure_102
    active periods =  p9
  end pressure

  begin pressure # pressure in cavern 103
    surface = surface_1033
    surface subroutine = cavity_pressure_103
    active periods =  p9
  end pressure

  begin pressure # pressure in cavern 104
    surface = surface_1043
    surface subroutine = cavity_pressure_104
    active periods =  p9
  end pressure

  begin pressure # pressure in cavern 105
    surface = surface_1053
    surface subroutine = cavity_pressure_105
    active periods =  p9
  end pressure

  begin pressure # pressure in cavern 106
    surface = surface_1063
    surface subroutine = cavity_pressure_106
    active periods =  p9
  end pressure

  begin pressure # pressure in cavern 107
    surface = surface_1073
    surface subroutine = cavity_pressure_107
    active periods =  p9
  end pressure

  begin pressure # pressure in cavern 108
    surface = surface_1083
    surface subroutine = cavity_pressure_108
    active periods =  p9
  end pressure

  begin pressure # pressure in cavern 109
```

```
    surface = surface_1093
    surface subroutine = cavity_pressure_109
    active periods =  p9
  end pressure

  begin pressure # pressure in cavern 110
    surface = surface_1103
    surface subroutine = cavity_pressure_110
    active periods =  p9
  end pressure

  begin pressure # pressure in cavern 111
    surface = surface_1113
    surface subroutine = cavity_pressure_111
    active periods =  p9
  end pressure

  begin pressure # pressure in cavern 112
    surface = surface_1123
    surface subroutine = cavity_pressure_112
    active periods =  p9
  end pressure

  begin pressure # pressure in cavern 113
    surface = surface_1133
    surface subroutine = cavity_pressure_113
    active periods =  p9
  end pressure

  begin pressure # pressure in cavern 114
    surface = surface_1143
    surface subroutine = cavity_pressure_114
    active periods =  p9
  end pressure

###
#     Pressures on side set after the 4th drawdown leach
#     Time period from {D4th_s/yr_s} years to {D5th_s/yr_s} years
###

  begin pressure # pressure in cavern 101
    surface = surface_1014
    surface subroutine = cavity_pressure_101
    active periods =  p10
  end pressure

  begin pressure # pressure in cavern 102
    surface = surface_1024
    surface subroutine = cavity_pressure_102
    active periods =  p10
  end pressure

  begin pressure # pressure in cavern 103
    surface = surface_1034
    surface subroutine = cavity_pressure_103
    active periods =  p10
  end pressure

  begin pressure # pressure in cavern 104
    surface = surface_1044
    surface subroutine = cavity_pressure_104
    active periods =  p10
  end pressure

  begin pressure # pressure in cavern 105
    surface = surface_1054
    surface subroutine = cavity_pressure_105
    active periods =  p10
  end pressure

  begin pressure # pressure in cavern 106
    surface = surface_1064
    surface subroutine = cavity_pressure_106
    active periods =  p10
  end pressure

  begin pressure # pressure in cavern 107
    surface = surface_1074
    surface subroutine = cavity_pressure_107
    active periods =  p10
  end pressure
```

```
      begin pressure # pressure in cavern 108
        surface = surface_1084
        surface subroutine = cavity_pressure_108
        active periods =  p10
      end pressure

      begin pressure # pressure in cavern 109
        surface = surface_1094
        surface subroutine = cavity_pressure_109
        active periods =  p10
      end pressure

      begin pressure # pressure in cavern 110
        surface = surface_1104
        surface subroutine = cavity_pressure_110
        active periods =  p10
      end pressure

      begin pressure # pressure in cavern 111
        surface = surface_1114
        surface subroutine = cavity_pressure_111
        active periods =  p10
      end pressure

      begin pressure # pressure in cavern 112
        surface = surface_1124
        surface subroutine = cavity_pressure_112
        active periods =  p10
      end pressure

      begin pressure # pressure in cavern 113
        surface = surface_1134
        surface subroutine = cavity_pressure_113
        active periods =  p10
      end pressure

      begin pressure # pressure in cavern 114
        surface = surface_1144
        surface subroutine = cavity_pressure_114
        active periods =  p10
      end pressure

###
#     Pressures on side set after the 5th drawdown leach
#     Time period from {D5th_s/yr_s} years to {end_s/yr_s} years
###

      begin pressure # pressure in cavern 101
        surface = surface_1015
        surface subroutine = cavity_pressure_101
        active periods =  p11
      end pressure

      begin pressure # pressure in cavern 102
        surface = surface_1025
        surface subroutine = cavity_pressure_102
        active periods =  p11
      end pressure

      begin pressure # pressure in cavern 103
        surface = surface_1035
        surface subroutine = cavity_pressure_103
        active periods =  p11
      end pressure

      begin pressure # pressure in cavern 104
        surface = surface_1045
        surface subroutine = cavity_pressure_104
        active periods =  p11
      end pressure

      begin pressure # pressure in cavern 105
        surface = surface_1055
        surface subroutine = cavity_pressure_105
        active periods =  p11
      end pressure

      begin pressure # pressure in cavern 106
        surface = surface_1065
        surface subroutine = cavity_pressure_106
```

```
    active periods =  p11
  end pressure

  begin pressure # pressure in cavern 107
    surface = surface_1075
    surface subroutine = cavity_pressure_107
    active periods =  p11
  end pressure

  begin pressure # pressure in cavern 108
    surface = surface_1085
    surface subroutine = cavity_pressure_108
    active periods =  p11
  end pressure

  begin pressure # pressure in cavern 109
    surface = surface_1095
    surface subroutine = cavity_pressure_109
    active periods =  p11
  end pressure

  begin pressure # pressure in cavern 110
    surface = surface_1105
    surface subroutine = cavity_pressure_110
    active periods =  p11
  end pressure

  begin pressure # pressure in cavern 111
    surface = surface_1115
    surface subroutine = cavity_pressure_111
    active periods =  p11
  end pressure

  begin pressure # pressure in cavern 112
    surface = surface_1125
    surface subroutine = cavity_pressure_112
    active periods =  p11
  end pressure

  begin pressure # pressure in cavern 113
    surface = surface_1135
    surface subroutine = cavity_pressure_113
    active periods =  p11
  end pressure

  begin pressure # pressure in cavern 114
    surface = surface_1145
    surface subroutine = cavity_pressure_114
    active periods =  p11
  end pressure

  #--------- Element Death --------------
###
#     Use element death option to simulate leachings
###

  begin element death leach_0  # Initial leach
    block = block_100
    criterion is always true
    death start time = 0.01
  end element death leach_0

  begin element death leach_1  # 1st drawdown leach
    block = block_101
    criterion is always true
    death start time = {D1st_s+1.0}
  end element death leach_1

  begin element death leach_2  # 2nd drawdown leach
    block = block_102
    criterion is always true
    death start time = {D2nd_s+1.0}
  end element death leach_2

  begin element death leach_3 # 3rd drawdown leach
    block = block_103
    criterion is always true
    death start time = {D3rd_s+1.0}
  end element death leach_3

  begin element death leach_4  # 4th drawdown leach
```

```
    block = block_104
    criterion is always true
    death start time = {D4th_s+1.0}
  end element death leach_4

  begin element death leach_5  # 5th drawdown leach
    block = block_105
    criterion is always true
    death start time = {D5th_s+1.0}
  end element death leach_5

  #--------- Initial Conditions ---------

  begin initial condition # Overburden (sand)
    block = block_2 block_6 block_12
    initialize variable name = unrotated_stress
    variable type = element
    subroutine real parameter: top = 0.0           # (m)  surface
    subroutine real parameter: bot = {-t_UOB-t_OB} # (m)  overburden bottom
    subroutine real parameter: p1  = 0.0           # (Pa) vertical stress at surface
    subroutine real parameter: po  = {sigv_UOB}     # (Pa) vertical stress at overburden
bottom
    subroutine real parameter: kvert_xx = {nu_bho/(1.-nu_bho)}
    subroutine real parameter: kvert_yy = {nu_bho/(1.-nu_bho)}
    subroutine real parameter: kvert_zz = 1.0
    subroutine real parameter: kvert_xy = 0.0
    subroutine real parameter: kvert_yz = 0.0
    subroutine real parameter: kvert_zx = 0.0
    subroutine string parameter: dir = Z
    element block subroutine = geo_is
  end initial condition

  begin initial condition # Caprock 1 (gypsum and limestone)
    block = block_3
    initialize variable name = unrotated_stress
    variable type = element
    subroutine real parameter: top = {      -t_UOB-t_OB} # (m) caprock 1 top
    subroutine real parameter: bot = {-t_CRL-t_UOB-t_OB} # (m) Bottom of caprock 1 (top of
UCL)
    subroutine real parameter: p1  = {sigv_UOB} # (Pa) vertical stress at overburden bottom
    subroutine real parameter: po  = {sigv_CRL} # (Pa) Vertical stress at bottom of caprock 1
(top of UCL)
    subroutine real parameter: kvert_xx = {nu_bhl/(1.-nu_bhl)}
    subroutine real parameter: kvert_yy = {nu_bhl/(1.-nu_bhl)}
    subroutine real parameter: kvert_zz = 1.0
    subroutine real parameter: kvert_xy = 0.0
    subroutine real parameter: kvert_yz = 0.0
    subroutine real parameter: kvert_zx = 0.0
    subroutine string parameter: dir = Z
    element block subroutine = geo_is
  end initial condition

  begin initial condition # Interface between caprocks 1 and 2
    block = block_7
    initialize variable name = unrotated_stress
    variable type = element
    subroutine real parameter: top = {      -t_CRL-t_UOB-t_OB} # (m) Bottom of caprock 1 (top
of UC1)
    subroutine real parameter: bot = {-t_UC1-t_CRL-t_UOB-t_OB} # (m) Bottom of UCL (top of
caprock 2)
    subroutine real parameter: p1  = {sigv_CRL} # (Pa) Vertical stress at bottom of caprock 1
(top of UC1)
    subroutine real parameter: po  = {sigv_UC1} # (Pa) vertical stress at bottom of UC1 (top
of caprock 2)
    subroutine real parameter: kvert_xx = {nu_bho/(1.-nu_bho)}
    subroutine real parameter: kvert_yy = {nu_bho/(1.-nu_bho)}
    subroutine real parameter: kvert_zz = 1.0
    subroutine real parameter: kvert_xy = 0.0
    subroutine real parameter: kvert_yz = 0.0
    subroutine real parameter: kvert_zx = 0.0
    subroutine string parameter: dir = Z
    element block subroutine = geo_is
  end initial condition

  begin initial condition # Caprock 2 (anhydrite)
    block = block_4
    initialize variable name = unrotated_stress
    variable type = element
    subroutine real parameter: top = {      -t_UC1-t_CRL-t_UOB-t_OB} # (m) Bottom of UC1 (top
of caprock 2)
```

```
        subroutine real parameter: bot = {-t_CRN-t_UC1-t_CRL-t_UOB-t_OB} # (m) Bottom of caprock anhydrite (top of UC2)
        subroutine real parameter: p1  = {sigv_UC1} # (Pa) vertical stress at bottom of UCL (top of caprock 2)
        subroutine real parameter: po  = {sigv_CRN} # (Pa) vertical stress at bottom of caprock anhydrite (top of UC2)
        subroutine real parameter: kvert_xx = {nu_bhn/(1.-nu_bhn)}
        subroutine real parameter: kvert_yy = {nu_bhn/(1.-nu_bhn)}
        subroutine real parameter: kvert_zz = 1.0
        subroutine real parameter: kvert_xy = 0.0
        subroutine real parameter: kvert_yz = 0.0
        subroutine real parameter: kvert_zx = 0.0
        subroutine string parameter: dir = Z
        element block subroutine = geo_is
      end initial condition

      begin initial condition # Interface between caprock 2 and salt dome
        block = block_8
        initialize variable name = unrotated_stress
        variable type = element
        subroutine real parameter: top = {       -t_CRN-t_UC1-t_CRL-t_UOB-t_OB} # (m) Bottom of caprock 2 (top of UC2)
        subroutine real parameter: bot = {-t_UC2-t_CRN-t_UC1-t_CRL-t_UOB-t_OB} # (m) Bottom of UC2 (top of salt dome)
        subroutine real parameter: p1  = {sigv_CRN} # (Pa) vertical stress at bottom of caprock anhydrite (top of UC2)
        subroutine real parameter: po  = {sigv_UC2} # (Pa) vertical stress at bottom of UC2 (top of salt dome)
        subroutine real parameter: kvert_xx = {nu_bho/(1.-nu_bho)}
        subroutine real parameter: kvert_yy = {nu_bho/(1.-nu_bho)}
        subroutine real parameter: kvert_zz = 1.0
        subroutine real parameter: kvert_xy = 0.0
        subroutine real parameter: kvert_yz = 0.0
        subroutine real parameter: kvert_zx = 0.0
        subroutine string parameter: dir = Z
        element block subroutine = geo_is
      end initial condition

      begin initial condition # Surrounding rock
        block = block_5
        initialize variable name = unrotated_stress
        variable type = element
        subroutine real parameter: top = {                               -t_UOB-t_OB} # (m) Bottom of UOB (top of caprock 1)
        subroutine real parameter: bot = {-h_SD-t_UC2-t_CRN-t_UC1-t_CRL-t_UOB-t_OB} # (m) Bottom of surrounding rock
        subroutine real parameter: p1  = {sigv_UOB} # (Pa) vertical stress at bottom of UOB (top of caprock 1)
        subroutine real parameter: po  = {sigv_SR}  # (Pa) vertical stress at bottom of surrounding rock
        subroutine real parameter: kvert_xx = {nu_bhs/(1.-nu_bhs)}
        subroutine real parameter: kvert_yy = {nu_bhs/(1.-nu_bhs)}
        subroutine real parameter: kvert_zz = 1.0
        subroutine real parameter: kvert_xy = 0.0
        subroutine real parameter: kvert_yz = 0.0
        subroutine real parameter: kvert_zx = 0.0
        subroutine string parameter: dir = Z
        element block subroutine = geo_is
      end initial condition

      begin initial condition # interface between dome and surrounding rock
        block = block_9
        initialize variable name = unrotated_stress
        variable type = element
        subroutine real parameter: top = {                               -t_UOB-t_OB} # (m) Bottom of UOB (top of caprock 1)
        subroutine real parameter: bot = {-h_SD-t_UC2-t_CRN-t_UC1-t_CRL-t_UOB-t_OB} # (m) Bottom of dome perimeter
        subroutine real parameter: p1  = {sigv_UOB} # (Pa) vertical stress at bottom of UOB (top of caprock 1)
        subroutine real parameter: po  = {sigv_DP}  # (Pa) vertical stress at bottom of dome perimeter
        subroutine real parameter: kvert_xx = {nu_bho/(1.-nu_bho)}
        subroutine real parameter: kvert_yy = {nu_bho/(1.-nu_bho)}
        subroutine real parameter: kvert_zz = 1.0
        subroutine real parameter: kvert_xy = 0.0
        subroutine real parameter: kvert_yz = 0.0
        subroutine real parameter: kvert_zx = 0.0
        subroutine string parameter: dir = Z
        element block subroutine = geo_is
      end initial condition
```

```
      begin initial condition # fault in caprock
        block = block_13 block_14
        initialize variable name = unrotated_stress
        variable type = element
        subroutine real parameter: top = {                          -t_UOB-t_OB} # (m) Bottom of
UOB (top of caprock 1)
        subroutine real parameter: bot = {-t_UC2-t_CRN-t_UC1-t_CRL-t_UOB-t_OB} # (m) Bottom of
UC2 (top of salt dome)
        subroutine real parameter: p1  = {sigv_FOB} # (Pa) vertical stress at bottom of UOB (top
of caprock 1)
        subroutine real parameter: po  = {sigv_FC2} # (Pa) vertical stress at bottom of UCN (top
of salt dome)
        subroutine real parameter: kvert_xx = {nu_bho/(1.-nu_bho)}
        subroutine real parameter: kvert_yy = {nu_bho/(1.-nu_bho)}
        subroutine real parameter: kvert_zz = 1.0
        subroutine real parameter: kvert_xy = 0.0
        subroutine real parameter: kvert_yz = 0.0
        subroutine real parameter: kvert_zx = 0.0
        subroutine string parameter: dir = Z
        element block subroutine = geo_is
      end initial condition

      begin initial condition # Salt dome and fault in the salt dome
        block = block_1 block_11 block_100 block_101 block_102 block_103 block_104 block_105
        initialize variable name = unrotated_stress
        variable type = element
        subroutine real parameter: top = {     -t_UC2-t_CRN-t_UC1-t_CRL-t_UOB-t_OB} # (m) Bottom
of UC2 (top of salt dome)
        subroutine real parameter: bot = {-h_SD-t_UC2-t_CRN-t_UC1-t_CRL-t_UOB-t_OB} # (m) Bottom
of salt dome
        subroutine real parameter: p1  = {sigv_UC2} # (Pa) vertical stress at bottom of UC2 (top
of salt dome)
        subroutine real parameter: po  = {sigv_SD}  # (Pa) vertical stress at bottom of salt dome
        subroutine real parameter: kvert_xx = 1.0
        subroutine real parameter: kvert_yy = 1.0
        subroutine real parameter: kvert_zz = 1.0
        subroutine real parameter: kvert_xy = 0.0
        subroutine real parameter: kvert_yz = 0.0
        subroutine real parameter: kvert_zx = 0.0
        subroutine string parameter: dir = Z
        element block subroutine = geo_is
      end initial condition

      #--------- Results Output ---------

      begin results output output_1
        database name = bh_full_5d.e
        database type = exodusII
        at time 0.0          increment = {h_s}
        at time {h_s}        increment = {d_s-h_s}
        at time {d_s}        increment = {9.*d_s}
        at time {10.*d_s}    increment = {mon_s-10.*d_s}
        at time {mon_s}      increment = {mon_s}
        at time {3.*mon_s}   increment = {mon_s}
        at time {bgn_s+yr_s} increment = {mon_s}

        nodal variables   = displacement as displ
        nodal variables   = temperature as tempn
        nodal variables   = force_external as fext

        element variables = temperature as tempe
        element variables = stress as sig
        element variables = von_mises as vonmis
        element variables = unrotated_stress as stress
        element variables = log_strain as eps         # log strain tensor
        element variables = ecreep as eqcs            # equivalent creep strain
        element variables = DEATH_STATUS as death_var # An element with 0.0 for DEATH_STATUS is a
dead element
        element variables = max_principal_stress as sig1            # Largest eigenvalue of the
stress tensor
        element variables = intermediate_principal_stress as sig2 # Middle eigenvalue of the
stress tensor
        element variables = min_principal_stress as sig3           # Smallest eigenvalue of the
stress tensor
        element variables = stress_invariant_1 as I1  # Trace of the stress tensor, Positive for
tension
                                                      # I1 = sig1 + sig2 + sig3
        element variables = stress_invariant_2 as I2  # Second invariant of the stress tensor
                                                      # I2 = sig1*sig2 + sig2*sig3 + sig3*sig1
        global variables = total_iter as itotal
```

```
      end results output output_1

      #--------- Solver ---------

      begin solver
        begin loadstep predictor
          type = scale_factor
          scale factor = 1.0 0.0
        end loadstep predictor

        begin cg
          target relative residual = 1.e-7 during p0 p1 p2 p3 p4 p5 # 0~1 year
          target relative residual = 1.e-7 during p6 p7 p8 p9 p10 p11
          acceptable relative residual = 1.e-5 during p6 # Default is 10 times target relative
residual
          acceptable relative residual = 2.e-5 during p7 p8 p9 p10 p11
          maximum iterations = {nmax}
          reset limits 10000000 500000000 1000 0.5
          iteration print = 20
          line search tangent
          preconditioner = diagonal
        end cg

      end solver

    end adagio region region_1

  end adagio procedure procedure_1

end sierra  bh_full_5d
```

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