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SANTOS COMPUTER CODE
IN WIPP PERFORMANCE ASSESSMENT

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EXECUTIVE SUMMARY

This report presents an evaluation of accuracy issues that have arisen regarding the U.S. Department of Energy's (DOE's) SANTOS computer code. The SANTOS code is used in Waste Isolation Pilot Plant (WIPP) performance assessment calculations to predict closure of a representative waste room by halite creep. Most of the issues associated with SANTOS appear to result in overestimating waste room porosity during room closure. Waste room porosity is potentially important to WIPP performance because it is used to calculate repository gas pressure, which drives spallings and direct brine releases. The objective of this report is to evaluate whether an over prediction of waste room porosity by SANTOS may have a significant effect on the radionuclide releases predicted in WIPP performance assessments.

This review determined that the SANTOS code tends to over estimate waste room porosity for three principal reasons related to the code's treatment of waste-halite interaction: (1) the mathematical formulation of the code appears to under predict the stresses on the waste when little gas is generated; (2) the numerical model appears to limit stresses on the waste due to nonphysical constraints on halite creep; and (3) the constitutive stress-strain properties of the waste are based on undegraded, surrogate waste materials and may over estimate the stiffness of the waste when it degrades. The over estimations were found to be greatest when little gas is generated in the repository and gas pressures are low. Under higher gas pressures, the decrease in effective stress on the waste reduces and may eliminate waste-halite interaction.

This review concluded that the WIPP repository performance is not sensitive to the over estimates of waste room porosity by the SANTOS code, based on the following principal lines of reasoning:

- Higher than expected values of waste room porosity are most significant at very low gas generation rates that do not result in sufficiently high gas pressures to drive significant releases.
- Very low gas generation rates and therefore unexpectedly high estimates of waste room porosity are rare in WIPP performance assessment because brine enters the waste room and gas is generated in every realization.
- The two most significant types of releases influenced by gas pressure, spallings and direct brine releases, are secondary or minor contributors to repository performance and small increases in releases by these mechanisms would have no significant effect on total releases.

- A DOE analysis that replaced SANTOS results with constant waste room porosities showed that the effects of the SANTOS porosity estimates were small and had no significant impact on releases.

The SANTOS model was found to be capable of reproducing the fundamental aspects of room closure including simulation of large-scale halite deformation and waste compaction. The accuracy issues with SANTOS are more a question of approximation rather than omission, and based on the foregoing, the SANTOS code was found to be adequate for use in WIPP performance assessment.

1.0 INTRODUCTION

The SANTOS code is used in WIPP performance assessment to predict the effects of creep closure of a representative waste room. Inputs to the code, such as the stresses generated by the overlying strata, the geomechanical properties of the Salado halite surrounding the WIPP repository, and the strength characteristics of the waste, are used to predict the creep movement of halite into the waste room, the stresses generated on the waste by contact with the halite, and the changes in waste room porosity as a function of those stresses and of the pressure of gas generated by degrading waste. The SANTOS results are used to prepare a lookup table called a "porosity surface" that is used in the BRAGFLO performance assessment code to determine the value of waste room porosity for a given repository gas pressure and time. DOE's position relative to this method is stated in the Appendix PA, Attachment PORSURF "The adequacy of the method is documented in Freeze (1996), who concludes that the approximation is valid so long as the rate of room pressurization in final calculations is bounded by the room pressurization history that was used to develop porosity surface".

Accuracy issues have arisen during WIPP recertification concerning the SANTOS code. These issues fall into three major categories, all tending to over predict waste room porosity during creep closure: (1) the mathematical formulation of the code appears to under predict the stresses on the waste when little gas is generated; (2) the numerical model appears to limit stresses on the waste due to nonphysical constraints on halite creep; and (3) the constitutive stress-strain properties of the waste are based on undegraded, surrogate waste materials that may over estimate the stiffness of the waste when it degrades.

The total porosity of the waste room is the total pore volume in the waste room divided by the total volume of the waste room. In most performance assessment scenarios, brine enters the waste room from the surrounding rock and the total pore volume consists of saturated pores containing brine and free pores containing gas. The total porosity is a function of time because the waste is compressed as the room is closed by halite creep. The free porosity is an important parameter in performance assessment because it affects the pressure of gas in the waste room that drives two of the four most significant types of radionuclide releases from the repository: spallings releases and direct brine releases.

Gas is generated by decomposition of the waste resulting from exposure to brine. A lower porosity limits the volume that can be occupied by both gas and brine. Limiting the gas volume because of a lower porosity would tend to increase gas pressure, but limiting the brine volume would tend to decrease gas production and therefore decrease gas pressure. The complex interrelationships between waste room porosity, brine availability, gas production, and gas pressure are determined by the BRAGFLO performance assessment code, which combines inputs from SANTOS and other codes to predict repository gas pressure over time.

The objective of this report is to evaluate whether an over prediction of waste room porosity by SANTOS may have a significant effect on radionuclide releases predicted for the WIPP in the U.S. Department of Energy (DOE) performance assessment.

2.0 SANTOS CONCEPTUAL MODEL

A conceptual model is a qualitative description of a physical process that forms the basis for preparing quantitative mathematical and numerical models. The DOE's conceptual model supporting the SANTOS code describes waste room closure by halite creep and the interactions of the creeping halite with the back stress provided by the waste and the pressure of pore gas in the room. The following description was taken from several sources, including Stone (1997a and 1997b), Butcher (1997), Butcher and Mendenhall (1993), and DOE (2004).

The waste room is assumed to be excavated in a massive bed of halite with occasional horizontal anhydrite interbeds. The waste rooms are long and narrow, with dimensions determined by the repository layout. Halite creep into the room is controlled by scaling or rock bolts during the operational period, so the room dimensions remain essentially unchanged during that period. Creep closure modeling begins immediately after the waste room is filled with waste.

During creep closure, the halite acts as a viscoelastic material that has both viscous and elastic properties. Halite therefore moves into the waste room through both elastic strain and viscous creep, but the large-scale deformation that ultimately results in encapsulating the waste is due to viscous creep. The anhydrite is a stiffer material subject to plastic deformation after the elastic yield stress is reached. Halite movement into the room is governed by the geomechanical properties of the materials involved, the shape of the room, and the stresses applied. Room closure due to viscous creep is expected to occur relatively quickly, within a few hundred years. The vertical lithostatic stress caused by the weight of the overlying rock is the primary driver in room closure.

Prior to room excavation, the rock is assumed to be in a state of isotropic, lithostatic equilibrium with no relic horizontal tectonic stress. Thus at a given depth the vertical and horizontal stresses are the same and equal to the overburden pressure. When disturbed by room excavation, equilibrium conditions no longer exist in the vicinity of the room and are replaced by stress fields determined by variations in the geomechanical properties of the halite and anhydrite, and by the geometry of the room. Vertical stresses increase in the room walls because the excavated halite no longer supports the overburden, while horizontal stresses are generally relieved by the excavation, which allows the halite to spread horizontally under the increased vertical wall compression.

The DOE's conceptual model for room closure under halite creep is described in Appendix PA of the WIPP Compliance Recertification Application (CRA) (DOE 2004, Appendix PA, Attachment PORSURF, Section PORSURF.3). As the halite moves into the room, it contacts the waste and encounters increasing back pressure as the waste is compressed. Although halite behaves as a brittle material under high strain rates when unconfined, its behavior becomes increasingly viscous as the confining stress increases. The SANTOS conceptual model does not incorporate the fracturing that accompanies brittle behavior. If the room were empty, rather than partially filled with waste, closure would proceed to the point where the void volume created by the excavation would be essentially eliminated and the surrounding halite would return to its undisturbed, uniform lithostatic stress state. In a room filled with waste, the former state of uniform lithostatic stress will ultimately be reestablished when the back pressure of the waste equals the lithostatic stress of the overlying rock. At that point, vertical stress will equal horizontal stress. Both stresses will equal the lithostatic stress and if no gas is generated, the stress will be the same in the halite and in the waste. With no gas generation, no gas is assumed to be present and the final porosity of the waste room will therefore approximate the porosity of the waste under a uniform lithostatic stress.

If significant gas is generated by waste decomposition, the back pressure of the waste on the creeping halite will be a function of the gas pressure as well as the waste stiffness. Depending on its magnitude, the gas pressure will take some of the pressure off the waste, thereby supporting a higher waste porosity for a given lithologic load and slowing room closure. Gas pressure can build in the waste room because the very low permeability of the halite and anhydrite and the high pressure of water in those rocks do not allow the gas to readily escape. As the gas pressure approaches lithostatic, it will begin to open existing fractures or create new fractures in the anhydrite that allow gas to escape the waste room. The escape of gas through fractures and the limited mass of gas that can be produced by waste degradation provide an ultimate upper limit on the gas pressure in the waste room. Although the conceptual model of a fracture mechanism to bleed off high gas pressures has been incorporated in the BRAGFLO model, SANTOS does not have such a mechanism. Instead the SANTOS conceptual model allows the waste room to expand if the gas pressure exceeds the lithostatic stress, increasing the waste room porosity above its former state. As a result, gas pressures in the SANTOS conceptual model can exceed the lithostatic stress.

3.0 SANTOS MATHEMATICAL MODEL

The SANTOS mathematical model was prepared within the context of the conceptual model and the processes to be characterized. The principal components of the mathematical model relevant to this report are the constitutive models for the halite, anhydrite, and waste, and the calculated porosity surface used to relate gas pressure and time to waste room porosity in WIPP performance assessment.

3.1 Halite and Anhydrite Constitutive Models

The halite constitutive model is described by Stone (1997a, p. 11-13; 1997b, Section 4.12). A combined transient-secondary creep constitutive model was used for the halite surrounding the waste room. The model has an elastic volumetric part and a deviatoric part defined by both elastic and viscous components. The elastic volumetric part of the model is a function of the constant elastic bulk modulus and is invariant with time. The viscous part of the model is a function of the deviatoric stress and temperature and allows for either transient or steady-state creep to occur depending on the steady-state creep strain rate and the transient strain limit (Stone 1997a, p. 11-13). This allows creep behavior to transition from the faster, transient creep observed in early time to the slower, steady-state creep observed in later times. The sources of model input parameters are described by Butcher (1997). The model was validated for short-term behavior by comparison with laboratory tests and in situ measurements of WIPP halite, but the predicted behavior over the 10,000-year regulatory time frame must be confirmed by comparison with the conceptual model and its underlying theoretical basis. Despite limitations in validating the model's long-term accuracy, the model's parametric data base has been accepted by other investigators for use in illustrating the geomechanical behavior of halite (see, for example, Bruno and Dusseault 2002, Table 2).

Although long-term accuracy is difficult to validate, SANTOS has been shown to be consistent with the conceptual model of relatively rapid room closure. In a study of the closure rate of an empty waste room by D.E. Munson of Sandia National Laboratories (SNL), the SANCHO model (Stone et al. 1985) predicted nearly 100 percent closure within 200 years (Munson 1987, Figure 20). SANCHO is a forerunner of the SANTOS model that uses the same basic numerics and produces similar results. In another early study with the SANCHO model (Butcher 1989), the volume of an empty waste room was predicted to drop to 5 percent of its initial volume in 20 years and the porosity of a room filled with crushed salt was predicted to drop to 5 percent in 30 years. By comparison, the porosity of a room filled with waste and crushed salt (using a preliminary waste constitutive model) was predicted in that same study to drop to 5 percent in 90 years and to less than 1 percent after 130 years. The early modeling results assumed varying waste room conditions and parameter values, and produced slightly different results, but had in common a prediction of essentially complete closure of an empty waste room within several hundred years.

The anhydrite constitutive model is also described by Stone (1997b) and by Butcher (1997). The anhydrite is considered to be isotropic and elastic until yield occurs. Once the yield stress is reached, plastic strain begins to accumulate.

3.2 Waste Constitutive Model

The constitutive model for the waste describes the volumetric changes in the waste resulting from stresses applied by the creeping halite. An elastic-plastic "crushable foam" model is used in WIPP performance assessment for the waste, wherein the waste is given the combined properties of both an elastic and a plastic material (Stone 1997b, Section 4.6). Strength parameters for the waste were developed from one-dimensional, uniaxial laboratory tests on simulated waste materials that consisted of undegraded cellulosics, plastics, and metals. For purposes of developing volumetric strain data, it was assumed that a mean three-dimensional, triaxial compressive stress on the waste equal to one-third of the uniaxial compressive stress applied in the laboratory tests would produce the same volumetric strain and therefore the same waste porosity reduction as measured in the laboratory tests. This approach assumes that the waste does not expand laterally as it is compressed vertically, and therefore has a Poisson's ratio of zero. DOE anticipates that when a drum filled with loosely compacted waste is compressed axially, the drum will not undergo significant lateral expansion until most of the void space inside the drum has been eliminated (Stone 1997a, p. 14). This was observed to be the case for undegraded, supercompacted waste drums from the Advanced Mixed Waste Treatment Project (AMWTP) at the Idaho National Engineering and Environmental Laboratory (C.W. Hansen et al. 2003, Figure 1).

The uniaxial test results for the various simulated waste materials were combined according to the expected ratios of those materials in the WIPP waste to produce a single curve of waste volumetric strain versus mean triaxial compressive stress for use in the SANTOS calculations (Stone 1997a, Figure 6). This curve is shown in Figure 1 of this report. Because of the load limitations in the uniaxial tests, it was necessary to extrapolate the curve to a maximum mean triaxial compressive stress of 12 MPa and a corresponding maximum volumetric strain of about 1.1. The final mean triaxial stress of 12 MPa corresponds to an axial stress on a waste drum of 36 MPa (Stone 1997a, p. 14).

The assumption of plane strain was used in applying the two-dimensional SANTOS model to the waste room. The plane strain condition assumes that all deformation occurs in the plane of the room cross-section, and that there is no deformation in the out-of-plane direction along the length of the room. In plane strain calculations, the stresses in the third (longitudinal) dimension along the length of the room must therefore be adjusted to maintain the plane strain assumption for materials, such as the waste, that deform volumetrically in three dimensions. The plane strain assumption allows the use of a simpler, two-dimensional model for room closure, and is generally appropriate for structures such as tunnels and culverts that are much longer than they are wide or high, and are loaded by forces that are perpendicular to their length and do not vary along their length. The plane strain assumption is therefore most appropriately applied to the center of a waste room and does not apply at the ends of the room.

Deviatoric stress describes the non-hydrostatic components of a stress field. In a hydrostatic stress field, the stresses are equal in all directions but not necessarily equal to the overburden pressure, as in a lithostatic stress field. Deviatoric stresses vary in direction and are responsible for distorting the shape of a body. Under a hydrostatic state of stress, the deviatoric stress is zero. A deviatoric stress model can be used to predict stress on a body in one direction resulting from a load applied in another direction. The deviatoric stress model for the waste is based on elastic-perfectly plastic behavior, but because of a lack of data, the deviatoric stress parameters had to be assumed and were developed to be consistent with a Poisson's ratio of 0.2 (as calculated from the assumed bulk and shear modulus data in Stone 1997a, Table 5).

The elastic-plastic volumetric constitutive model for the waste is applied to the plane strain conditions in the waste room in several steps. First, the stresses in the waste at the end of the previous time step are used to calculate new nodal point locations for the next time step. These new locations are then used to calculate new trial stresses in the waste using the volumetric (elastic) part of the waste constitutive model. The volumetric part of the waste constitutive model is based on the mean stress and therefore on an equal compression of the waste in every direction, including the out-of-plane direction along the length of the drift. However, the plane strain assumption does not allow for volume changes due to strain in the out-of-plane direction, so the new trial stresses must correct for the out-of-plane compression by applying a tensile stress in that direction to pull the waste back to zero strain. The amount of tensile stress needed to return the waste to zero out-of-plane strain is determined using the elastic component of the waste constitutive model because plastic deformation in the crushable foam model is inelastic and non-recoverable. The resultant expansion in the out-of-plane direction is accompanied by contraction in the in-plane directions, determined by the aforementioned value of Poisson's ratio (0.2) used for the waste in the model. Because the model does not allow the waste to fail, the new trial stresses are checked against the elastic yield surface for the waste. If the trial stresses do not exceed the yield surface, they are accepted as an appropriate starting point for the next time step. If they exceed the yield surface, they are projected back to the yield surface using the deviatoric stress model. This process is described in Stone (1997b, Section 4.6).

DOE conducted investigation "to examine the influence of the TRU waste constitutive model and to gain an understanding of the generation of out-of-plane tensile stresses including their impact on room porosity" (RESPEC for Sandia National Laboratory, Topical Report RSI-1783,2004). In this study three different TRU waste constitutive models with noticeable differences in their representation of the TRU waste were studied. These included elastic - plastic crushable foam, nonlinear elastic and fluid constitutive models. The difference in the outcomes of these models was primarily due to the out-of-plane stress and its effects on mean stress without gas generation. The study conducted by RESPEC also pointed out that the uncertainty in the constitutive model for TRU waste was insignificant and "inconsequential" with the gas generation scenario. Gas generation reduced the rate of room closure, increased the room porosity value and also reduced the influence of the mechanical properties of the waste. It was also expected that with gas generation the difference in the results between the waste models would also be reduced.

3.3 The Porosity Surface

The SANTOS model is not directly used in performance assessment because of its computational intensity. Instead, the effects of room closure and gas generation on waste room porosity are determined using a reference surface, called a "porosity surface," generated by SANTOS. The porosity surface used in WIPP performance assessment is a three-dimensional plot that correlates the gas-filled waste room porosity with time and with the pressure of the gas produced by waste degradation. An illustration of a porosity surface is shown in Figure 2. The range of gas generation rates used in SANTOS to develop the porosity surface is intended to be broad enough to span the possible range of gas pressures predicted for the repository by the BRAGFLO code.

In SANTOS, the predicted gas pressure, p_g, in the waste room is computed from the ideal gas law by the following relationship:

$$p_g = NRT/V$$

where N is the mass of gas in moles at a given time t in the room, R is the universal gas constant, T is the absolute temperature (assumed to be constant at 300 K), and V is the current free volume in the room at time t calculated from the SANTOS results. The mass of gas in the room is a function of the gas generation rate at time t and the amount of gas-generating waste in the room, which is assumed to be constant.

In performance assessment, the mass of gas produced by waste degradation is independently calculated by the BRAGFLO code at each time step using a model that accounts for the inventory of gas-generating waste, the saturation of the waste material, and the parameters in the gas generation model. At each time step, the porosity surface is entered knowing the BRAGFLO-predicted gas pressure and porosity in the room from the previous time step, the current rate of gas production, and the time. Using these data, a new gas pressure is computed and the corresponding gas-filled waste room porosity is determined from the porosity surface.

In SANTOS, the porosities are calculated for a waste room with dimensions that decrease during creep closure. However, in BRAGFLO, the waste room dimensions are kept constant at the original excavated values. Therefore, in BRAGFLO the waste room porosity calculated by SANTOS is used to compute a fictitious BRAGFLO porosity that gives the correct total waste room pore volume. This is accomplished using the relationship:

$$\phi_S V_S = \phi_B V_B$$

E

where ϕ_S and ϕ_B are the porosities associated with SANTOS and BRAGFLO, and V_S and V_B are the total waste room volumes as represented in SANTOS and BRAGFLO. Note that while V_S changes with time, V_B does not.

4.0 SANTOS NUMERICAL MODEL

SANTOS is a two-dimensional finite element structural analysis code designed to compute the quasi-static, large deformation, inelastic response of two-dimensional planar or axisymmetric solids. SANTOS uses uniform strain, 4-node quadrilateral elements. SANTOS is supported by several peripheral subroutines that, for purposes of this report, are considered part of the SANTOS numerical model. These subroutines include the FPRES code for setting the gas generation parameter *f* that determines the rate of gas production and the NUMBERS code that provides input to the porosity surface by calculating the deformed waste room volume and porosity from the SANTOS finite element mesh. The SANTOS model was verified by its developer (Stone 1997b, Appendix E) and its proper functionality was recently reconfirmed by

SNL (WIPP PA 2003). SANTOS has also been shown in EPA-DOE Technical Exchange meetings to be successfully benchmarked against other codes including use of the PHENIX code to couple SANTOS with TOUGH2 (Larson 1994), JAS-3D (EPA 2004c, *Evaluation of SANTOS and Porosity Surfaces,* meeting handout by Bill Thompson, Golder Associates) and SPECTROM-32 (EPA 2004b, *Evaluation of the TRU Waste Constitutive Model,* meeting handout by Gary Callahan, RESPEC).

The waste room is modeled as a rectangular opening that is initially 3.96 m high by 10.06 m wide. The 91.44 meter length of the room is sufficient to accommodate the aforementioned plane strain assumption and the use of a two-dimensional model. The waste is assumed to be stored in 7-pack units of standard waste drums with 6,804 drums per room. The initial porosity of the waste was calculated to be 0.681 and the initial solid waste volume was 551.2 m^3 (Stone 1997a, p. 3). This gives an initial porosity of the undeformed waste room of 0.849. Initial stresses before room excavation were assumed to be lithostatic, equal in all directions and equal to the overburden load (Stone 1997a, p. 7).

The objective of the SANTOS numerical model is to approximate the conceptual and mathematical models. Illustrations of the SANTOS mesh and its simplified stratigraphy before room closure begins are presented in Figures 3 and 4. Making use of symmetry, only half the room needed to be modeled. In the actual repository, the waste is placed as close as possible to the room walls. However, to preserve an accurate continuum representation of the waste and account for the large void volume between drums, the drums are assumed to be already pushed together horizontally at time zero. This assumption creates the initial gap between the waste and room wall shown in Figure 3. The DOE considers the presence of this gap to be acceptable because closure of this void volume is assumed to offer little to no resistance to lateral deformation of the waste room wall (Stone 1997a, p. 11). Contact surfaces were defined in the model between the waste and the floor, wall, and roof of the waste room. These surfaces allow the waste to slide as the room deforms and also allow the room to reopen under increasing gas pressure (Stone 1997a, p. 11).

SANTOS computes the stress on the enclosed but deforming volume of waste shown in Figure 3 and applies the resulting forces to nodes on the waste boundary. During each time step, the current total room volume is calculated based on the displaced positions of the nodes on the boundary of the room. The free room volume is then computed by subtracting the initial solid volume of the waste (551.2 m^3) from the total room volume. This approach assumes that only the pore volume of the waste compresses during room closure and no significant compression occurs in the solid volume of the waste. This approach also calculates total room porosity and assumes that all pores are available to be occupied by gas. It implicitly assumes that the reduction in free pore volume by brine-filled pores can be neglected. SANTOS predicts creep closure to proceed relatively rapidly until the halite contacts the waste and closure is slowed by increasing resistance from the waste and the gas-filled pores.

Figures 5a and 5b show the SANTOS-predicted, deformed waste room after 300 and 10,000 years for the case of no gas generation (*f* = 0; Stone 1997a, Figures 9 and 10). As shown in the illustrations, the free space around the waste closes relatively quickly. The waste is essentially fully contacted within 300 years and undergoes relatively little subsequent volume reduction. Figures 6a and 6b show the SANTOS-predicted, deformed waste room after 300 and 10,000 years for gas production at half the reference case rate (*f* = 0.5; Stone 1997a, Figures 11 and 12). Here the gas pressure becomes sufficiently high to allow essentially no further waste volume reduction after 300 years, and to reduce horizontal wall deformation to the point that no significant horizontal back pressure is provided by the waste for 10,000 years. This suggests that waste porosities can remain high and stresses on the waste can remain low when gas is produced in the repository.

The foregoing conclusion is supported by the results on Figures 7 and 8. For purposes of generating the porosity surface, gas production in SANTOS is assumed to cease after 1,050 years (Stone 1997a, p. 4). Figures 7 and 8 show that for *f* = 0.5, after about 1,000 years the waste room gas pressure remains relatively constant at about 16 MPa and the porosity remains approximately constant at about 0.6. This gas pressure is more than sufficient to support the lithostatic pressure of about 15 MPa (F.D. Hansen et al 2003, Section 4.5). Of greater interest is the predicted porosity, shown in Figure 8, of about 0.235 after 10,000 years with no gas production (*f* = 0). Considering the aforementioned initial waste porosity of 0.681, a reduction to 0.235 represents a volume strain of about 0.87. From Figure 1, this strain is equivalent to an average applied pressure of about 4 MPa, which is less than the lithostatic equilibrium pressure of about 15 MPa. This indicates that average stresses on the waste are predicted to remain well below lithostatic after 10,000 years, even with no gas pressure in the room. It is also noted that for the higher gas generation rates, generally for *f* > 0.5, the porosity history curves in Figure 8 show an increase in waste room porosity between about 500 and 1,000 years corresponding to room dilation.

Final equilibration of the halite with waste room pressure and a return to the initial lithostatic stress state are predicted by SANTOS to proceed slowly, as evidenced by the relatively slow decline of gas pressure and slow increase in room porosity for the higher values of *f* shown in Figures 7 and 8. Although room expansion occurs relatively quickly due to internal pressures rapidly increasing above lithostatic during the gas generation phase, the subsequent decline in gas pressure is slow. As Stone notes, for the highest values of *f* (1.6 and 2.0), the porosity still appears to be increasing and the gas pressure decreasing at 10,000 years as the internal gas pressure and overburden try to reach equilibrium (Stone 1997a, p. 17). From Figure 7, the gas pressures for the highest values of *f* are still 2 to 3 MPa higher than the lithostatic stress after about 9,000 years of no additional gas production. The SANTOS closure results at high gas pressures are independent of the waste constitutive model because the gas pressure is sufficiently high to reduce the effective stress on the waste to zero. They provide an indication of the deviation from lithostatic that SANTOS predicts to endure at 10,000 years due to the halite constitutive model alone.

5.0 ACCURACY ISSUES WITH SANTOS

EPA accepts the basic conceptual model for halite creep and room closure described in Section 2. The accuracy issues that have arisen primarily involve discrepancies between that conceptual model and the SANTOS modeling results. Most of these issues appear to result in overestimating the waste porosity.

5.1 Low Stress on Waste with No Gas Generation

EPA's principal accuracy issue with SANTOS is the relatively low mean stress exerted on the waste when no gas in generated, even after 10,000 years when halite creep should have caused the stress to more closely approach a lithostatic state. This low stress has resulted in higher porosities for the waste than would be expected. Several factors, discussed below, are believed to have caused this condition.

Volumetric Strain Model for the Waste. The final waste porosity for each time step is determined by SANTOS using a waste constitutive model based on the average of the three principal stresses acting on the waste. As described in Section 3.2, tensile stresses are predicted by SANTOS on the waste in the out-of-plane direction to preserve the plane strain assumption of the model. If tensile stresses are given a positive sign and compressive stresses a negative sign, then the positive tensile stresses will have a significant effect on reducing the average compressive stress on the waste and therefore reducing the predicted porosity of the waste. These tensile stresses are predicted by SANTOS to endure for 10,000 years. However, they are fictitious and cannot exist in the waste after it is contacted by the halite because all applied stresses, including the out-of-plane stresses, will be compressive.

Low Horizontal Stresses. Horizontal stresses acting on the waste during room closure with no gas production appear to be unrealistically low. After 10,000 years, when the stress state should be more closely approaching lithostatic, the horizontal stress in the wall on the midplane of the waste room, about 6 MPa, is considerably less than the lithostatic stress of about 15 MPa. The horizontal stress is also low when compared with the 12 MPa vertical stress at the midpoint of the waste room roof after 10,000 years (Park 2005). The SANTOS model appears to correctly predict rapid closure of empty space and an empty room with no gas generation, but does not appear to also predict the expected, more rapid buildup of stress on the waste.

The horizontal stress on the surface of the waste room wall is initially zero because the wall is an excavated, free surface. The horizontal stress increases with increasing depth into the wall because of the increasing confinement of the halite. However, the horizontal stress on the surface of the wall will remain zero until the wall creeps far enough to contact a resisting surface, such as the waste, and a back pressure is established. The halite creep rate due to viscous flow is a function of the deviatoric stress, which is greatest in the model elements forming the surface of the waste room wall because the average horizontal stresses are low and the vertical stresses are high. SANTOS therefore appropriately predicts more rapid halite creep in the wall elements than in the elements deeper into the wall. This same principle also applies to the roof and floor elements, which creep vertically into the room at the same time that the walls are creeping horizontally. Roof and floor creep rates would be expected to be greater than wall creep rates because of the greater span of the roof and floor. This effect becomes more pronounced at later times when the roof and floor elements contact the wall elements in the corners of the room, as illustrated in Figure 5. The resulting back pressure reduces the deviatoric stress and slows the creep rate in the contacting elements. The impact of this effect on overall creep rates is greater on the walls than on roof and floor because the walls are shorter than the roof and floor, and the fraction of elements in contact is greater for the walls than for the roof and floor. This effect reduces the free wall span more rapidly than the free roof and floor spans, and slows wall movement more rapidly than roof and floor movement. It delays contact between the walls and waste, and therefore delays buildup of horizontal stress in the walls and in the waste.

The foregoing considerations suggest that horizontal wall movement into the room would be less rapid than vertical roof and floor movement, even at early times. This expectation has been confirmed by convergence measurements in test drifts at WIPP, as illustrated by Figures 9 and 10 (EPA 2005, *SANTOS and Porosity Surfaces,* meeting handout by Bill Thompson, Golder Associates). The greater span of the roof and floor and the compounding effects of model element contact in the corners of the room provide an adequate qualitative explanation for the SANTOS model prediction of a lower horizontal stress in the walls, however the true magnitude of that stress and the accuracy of the related long-term, secondary halite creep rate after 10,000 years remain uncertain. Although the WIPP field measurements confirm the predicted short-term creep behavior of the halite, they do not address the accuracy of the very slow, long-term rate of return to a lithostatic stress state predicted by SANTOS. The conceptual model of a fairly rapid rate of return to lithostatic equilibrium conditions appears to have been based on recent and historic observations of room closure and halite encapsulation occurring within time frames of tens to hundreds of years and the assumption that the observed closure is accompanied by an equally rapid return to equilibrium stress conditions. However, the room closure observations have not been accompanied by in situ stress measurements and the rate of stress buildup accompanying room closure is therefore uncertain.

The SANTOS halite constitutive model incorporates two stages of creep, the first involving relatively rapid, short-term transient (or primary) creep followed by a slower, long-term steady state (or secondary) creep (Stone 1997a, p. 11-13). These two phases of creep are commonly seen in laboratory tests. As previously mentioned, the creep component of the model is a function of the deviatoric stresses and temperature, and is not a function of the confining pressure. The model therefore correctly predicts rapid room closure from primary, transient creep under the high deviatoric stresses that exist around an open room, but a very slow asymptotic return to lithostatic conditions under secondary creep following room closure as the deviatoric stresses are relaxed. EPA believes that the effect of higher confining pressures following room closure, which were not considered in the model, may accelerate creep rates beyond those related to deviatoric stresses alone. However, little is known about halite behavior over time frames of several thousand years, and the accuracy of SANTOS' predicted slow buildup of horizontal stress and return to lithostatic conditions is uncertain.

The effect of possibly under predicting the long-term horizontal stress affects the predicted waste porosity by reducing the mean stress on the waste. This functions in the same manner as the effect of the out-of-plane tensile stresses described above, but has a lower impact on waste porosity because the predicted horizontal stresses, although low, remain compressive.

Low Vertical Stresses. The vertical stress on the waste along the centerline of a waste room with no gas production was predicted by SANTOS to be about 12 MPa after 10,000 years (Park 2005). This is somewhat but not excessively less than the lithostatic stress of about 15 MPa. The less than lithostatic vertical stress is likely due in part to the same types of modeling constraints that reduce the predicted horizontal stress, but the impact is less because of the vertical direction of the lithologic load and the wider span of the roof. This allows the roof to contact the waste sooner and results in an earlier buildup of back pressure. As previously noted, final equilibration of the halite with waste room pressure is predicted by SANTOS to proceed slowly.

5.2 Waste Room Dilation with Gas Generation

The SANTOS model predicts that the waste room will inflate (expand in volume) when the internal gas pressure exceeds the lithostatic stress (Stone 1997a, p. 17). Although waste room dilation is not necessarily interpreted as equivalent to expansion of the waste because waste room porosity is calculated as the ratio of the free room volume to the total room volume, room dilation is accompanied by a calculated increase in room porosity. Waste room dilation is represented in the porosity surface and is carried into WIPP performance assessment through the BRAGFLO code. However, unlike SANTOS, maximum gas pressures in BRAGFLO are limited by escape of gas from the waste room by pressure-induced expansion of existing fractures or creation of new fractures in the anhydrite interbeds (DOE 2004, p. 6-103). As a result, gas pressures in BRAGFLO do not significantly exceed the lithostatic stress of 15 MPa.

An alternative conceptual model, preferred by EPA, would allow waste room closure to be slowed or stopped by increasing gas pressure, but would not allow the waste room to dilate or the waste room porosity to increase. This is because any significant dilation of the waste room could reduce stresses in the halite and anhydrite to the extent that fractures would open at discontinuities in the room walls, either induced by the pressurized gas or by the brittle nature of poorly confined halite and anhydrite. EPA therefore believes that waste room porosity will either decrease monotonically or remain constant during creep closure, and that gas pressures will be regulated by porosity increases outside the waste room due to fracture initiation and expansion in the halite and anhydrite.

Although BRAGFLO does consider porosity increases through opening fractures outside the waste room, the increase in porosity in SANTOS due to room dilation occurs quickly while the increase in porosity in BRAGFLO due to opening fractures is delayed. Removing waste room dilation from SANTOS and the porosity surfaces while retaining the existing fracture opening model in BRAGFLO may have the overall effect of delaying an increase in pore volume due to high gas pressure in WIPP performance assessment and result in increased repository pressures in realizations with moderate to high gas production.

5.3 Physical and Chemical Influences on Pore Volume

SANTOS calculates total room porosity assuming that all pores are open and free to contain gas. In BRAGFLO, however, brine is predicted to flow into the waste room and occupy some of the pores, making them unavailable for gas. The amount of brine saturation varies differently with time for each realization, depending on the rate of brine inflow into the repository and the rate of brine depletion through chemical reaction with the waste and flow out of the repository. The chemical reactions with the waste also decrease free pore volume below that predicted by SANTOS because the corrosion products occupy more volume than the undegraded waste. However, the assumption in SANTOS that only the pores compress and the waste material itself does not compress would tend to underestimate the porosity if a significant portion of the waste was compressible. Although some of these influences may be minor and offsetting, they have not been incorporated in SANTOS.

5.4 Waste Constitutive Model

The constitutive model for the waste was developed based on tests of undegraded, surrogate waste materials such as metals, plastic, rubber, cellulosics such as wood, sorbents, and sludges. Cellulosics comprise the largest volume fraction (30%) in the expected WIPP waste, followed by sludges (26%), metals (22%), rubbers and plastics (15%), and sorbents (7%) (Stone 1997a, Table 1). The metal fraction of the waste is expected to degrade over time due to anoxic corrosion and the organic fraction may degrade through microbial action. DOE expects waste stiffness to decrease over time due to such degradation (F.D. Hansen et al. 2003, Section 2), but this decrease was apparently not incorporated in developing the waste constitutive model for SANTOS. As a result, waste stiffness may be over estimated in SANTOS and the resulting waste porosities may be too high, particularly at later times after the waste has degraded.

It may be noted from the foregoing discussion that the assumption of Poisson's ratio for the waste is inconsistently used in SANTOS. In developing the waste constitutive model, a Poisson's ratio of zero was assumed, but in applying the model in SANTOS, a Poisson's ratio of 0.2 was assumed. This inconsistency may be related to the observed lack of lateral expansion during the uniaxial tests used to develop the constitutive model, supporting a ratio of zero, whereas a ratio greater than zero in SANTOS is more appropriate for degraded waste. Although the use of Poisson's ratio remains inconsistent, it is probably not significant to performance assessment.

5.5 Potential Impacts of SANTOS on other Performance Assessment Models

If the over estimate of waste room porosity in SANTOS results in significant increases in predicted repository gas pressures, the direct brine and spallings releases may be affected because those releases are gas pressure-driven. Direct brine releases (DBR) are triggered when there is brine in the repository and the gas pressure is sufficiently high (greater than 8 MPa) to eject the brine to the ground surface through an exploratory borehole intersecting the repository. Similarly, spallings releases are triggered when the gas pressure is sufficiently high to mobilize and eject degraded waste materials to the ground surface through an exploratory borehole. The greatest impact may occur if the frequency of reaching the threshold pressures for these releases in the repository is significantly increased.

A second issue is the discrepancy between the repository lithostatic stress (15 MPa) assumed in the spallings model (DRSPALL), and the lower stress state predicted by SANTOS. The stress assumed in DRSPALL is consistent with the conceptual model that essentially lithostatic conditions will be reestablished in the repository relatively soon (within a few hundred years) after the room is filled with waste and operational maintenance ceases. The SANTOS results are not consistent with that conceptual model and, as previously discussed, raise questions about the rate at which lithostatic conditions will be reestablished. In response to an EPA concern about this issue, the DOE noted that the gas pressure in the repository must exceed the 8 MPa wellbore pressure before a spall event could occur, and that a DRSPALL model run with an initial pore pressure and far field stress of about 10 MPa resulted in lower spallings releases than the maximum releases computed for the CRA, which occurred at about lithostatic pressure and stress (F.D. Hansen et al. 2004, Figure 2). In addition to this evidence that the current DRSPALL far field stress conditions are conservative, EPA believes that the long-term rates of stress buildup may be underestimated by SANTOS because the effect of confining pressure on halite creep is not considered. Based on these observations, EPA concludes that the far-field stress conditions assumed in the DRSPALL model are reasonable.

The Department has conducted analysis to determine the potential impact of uncertainty in the porosity surface on the repository performance (Appendix PA, Attachment MASS, Section 2.0). It was concluded that the uncertainty in the porosity surface did not have “significant effects on repository performance”. This analysis also indicated that uncertainty in the porosity surface can be due to the “heterogeneity in the rigidity of the waste packages and uncertain spatial arrangement of waste in the repository”.

5.6 Impacts of Accuracy Issues

Virtually all of the SANTOS accuracy issues raised in this report appear to result in overestimating waste room porosity during room closure. Most of these issues have been raised in technical exchange meetings between EPA and DOE, and several studies of the impacts of overestimating porosity have been performed at EPA’s request by Sandia National Laboratory and other DOE contractors. The results of these studies and EPA's evaluation of their significance are summarized below.

The problem of overestimating waste room porosity was found to be most significant at very low gas generation rates (EPA 2004b, *Evaluation of the TRU Waste Constitutive Model,* meeting handout by Gary Callahan, RESPEC). After successfully matching SPECTROM-32 model results with SANTOS results using the same crushable foam constitutive model for the waste, Dr. Callahan examined the influences of several alternative constitutive models including variations of the crushable foam model and a new, nonlinear elastic model. The alternative models did show less porosity at 10,000 years than SANTOS when no gas was generated, but in runs with gas generation at $f = 1$, the room porosity results were within a few percent. This is likely because at significant gas generation rates, generally when $f > 0.5$, the gas pressure in the room is predicted to exceed the lithostatic stress of 15 MPa (see Figure 7). With pore pressures of this magnitude, the effective stress on the waste drops to zero and the waste constitutive model plays no role in determining room porosity. Although EPA does not believe that the significant room dilation shown in the SANTOS model and carried over into Dr. Callahan's results would actually exist, EPA does believe that significant gas generation can stop waste room closure and maintain porosity at an elevated level as long as gas pressures remain high. EPA therefore agrees that the problem of overestimating waste room porosity is most significant at low gas generation rates and that high gas pressures can result in maintaining elevated room porosities.

RESPEC (Calahan,2005) based on their comparative analysis of all three TRU waste constitutive models concluded that the room closure was almost the same in the CF (crushable foam) and NE (nonlinear elastic material) models and the NE model predicts more realistic states of stress. However, the NE model has an important limitation. Butcher (1997) stated in the Waste Isolation Pilot Plant Disposal Room Model that " In order to maintain the condition of Zero total out-of-plane strain for the large strains that might be encountered during compaction the computed out-of-plane stress can become unrealistically large, and of different sign (compressive) than the stress predicted using volume plasticity model (Labreche et al.,1995)" the model will not work therefore, without an arbitrary an physically unreasonable fix, where as the volume plasticity model works very well". The deviatoric portion of the CF model can be used to project more realistic state of stress through parameter changes. However, the overall impact of these on the performance of the repository remains very low.

With regard to underestimating porosity at lower gas generation rates, there will always be some gas pressure in the room. For example, when compressed to the SANTOS-calculated minimum porosity of 23.5 percent, the pressure of the ambient air trapped in the waste room would, under isothermal conditions, increase from near atmospheric (about 0.1 MPa) to about 0.3 MPa. In addition, SNL pointed out and EPA concurs that some brine enters the repository and some gas is generated through waste degradation in every performance assessment realization (Stein 2005). Because the underestimation of porosity is most extreme for SANTOS runs where no gas is generated, this most extreme situation will not occur in WIPP performance assessment.

Further, spallings and DBR are the only significant releases influenced by gas pressure, and due to the weight of the drilling mud column in an intersecting borehole, these releases can only occur when the gas pressure is high enough (greater than about 8 MPa) to eject the drilling mud from the borehole. Because of the requirement of a relatively high gas pressure for these types of releases to occur, and because the accuracy of SANTOS' porosity calculations increases with increasing gas pressure, any influence of the porosity calculations on the occurrence and magnitude of these releases would be reduced. EPA also notes that spallings and DBR releases are relatively minor compared with cuttings and cavings releases. Spallings releases are typically half an order of magnitude lower than cuttings and cavings releases, and DBR releases are 0.5 to 3 orders of magnitude lower (C.W. Hansen et al. 2004, Figure 21). Because of the relatively minor contribution of spallings and DBR releases to total releases and because of the increased accuracy of SANTOS when these types of releases occur, EPA concludes that any influence of SANTOS' over estimates of waste room porosity on WIPP performance will be minor.

The remaining issue is whether a reduced waste room porosity would actually result in a significant increase in predicted gas pressure in the WIPP repository. If gas generation were independent of porosity, then for a given mass of gas produced, a lower porosity would provide a lower volume for the gas to occupy and a higher gas pressure would necessarily result. However, as noted earlier, gas generation is not necessarily independent of porosity. Brine is needed for gas-generating waste degradation to occur. The availability of brine to enter the repository is not continuous but episodic (such as when a Castile brine pocket is intersected by an exploratory borehole that also penetrates the repository), and a more limited pore volume would more severely restrict the volume of brine that could enter the repository and be available for gas generation. A more limited pore volume could also increase the rate of pressure buildup when gas is generated, which would act to more quickly slow brine inflow. Also, because DBR releases are a function of brine availability as well as gas pressure, having less brine in the repository would reduce the magnitude of DBR releases.

To test the effects of a reduced porosity on performance, EPA requested DOE to determine waste room porosity by sampling from a range of possible values rather than using the SANTOS results. In this approach, the waste room porosity was not varied as a function of gas pressure in BRAGFLO but rather was constant in a given realization with uncertainty expressed through sampling from a range of possible values. The results of this approach were documented by C.W. Hansen et al. (2004) and were independent of the porosity surface and the SANTOS model. The uncertain range of porosity values was determined assuming the entire waste panel was filled with supercompacted waste from the AMWTP. EPA's focus in this analysis is on the results of DOE's calculations where the constant porosity was not correlated with gas generation (called the PORU runs).

The porosity values were sampled from a uniform distribution of BRAGFLO porosities ranging from 9.1 to 23 percent. This is equivalent to waste room porosities ranging from 30.9 to 52.9 percent (C.W. Hansen et al. 2004, p. 9-10). The low end of this range is equivalent to the SANTOS-predicted porosity for standard waste at 10,000 years, for the low gas generation rate of *f* = 0.025. Because this rate is exceeded in almost every realization, this porosity provides a lower bound consistent with the lower bound expected from the BRAGFLO standard waste results. The high end of this range is less than the maximum porosity surface porosity of about 85 percent for the highest gas generation rate of *f* = 2.0, but as previously noted, this rate was selected to exceed the possible range of results obtained for standard waste in performance assessment. The SANTOS correlations between *f* values and porosity for standard waste are shown in Figure 8. Because both the lower and upper ends of the range of gas generation rates incorporated into the porosity surface for standard waste are rarely predicted by BRAGFLO, after the first 1,000 years the constant porosity range used in DOE's analysis for the undisturbed (S1) scenario is similar to the porosity range developed in the CRA using SANTOS results. This similarity is illustrated by comparing Figures 3a and 3d in C.W. Hansen et al. (2004). However, the constant porosities in DOE's analysis are generally smaller than those predicted for AMWTP waste, as illustrated by comparing Figures 3b and 3d in C.W. Hansen et al. (2004). For purposes of determining the effects of lower porosities, comparisons with the PORU results are therefore focused on both the CRA and AMWTP results.

The constant porosity BRAGFLO results for three output variables that are significant to repository performance (repository pressure; brine saturation in the waste, and brine flow out of the repository) were compared by DOE with CRA and AMWTP BRAGFLO results in which SANTOS porosity surfaces were used. These comparisons showed that assuming constant porosities resulted in a repository performance similar to both the CRA and AMWTP results, which had earlier been shown to be similar to each other (C.W. Hansen et al. 2003). The similarities in brine saturations for the undisturbed scenario are illustrated by comparing the mean, 10th, and 90th percentile curves in C.W. Hansen et al.'s (2004) Figure 6. For the disturbed (S2) scenario, brine saturations are generally lower in the constant porosity runs, as illustrated in C.W. Hansen et al.'s (2004) Figures 8 and 10, due to reduced brine inflow from the Castile. Lower brine saturations would generally result in reduced DBR releases. The total mass of gas produced in the PORU and AMWTP calculations was similar for both the undisturbed and disturbed scenarios, as illustrated in C.W. Hansen et al's (2004) Figures 12 and 13. Gas pressure in the waste room tended to be 0.5 to 1.5 MPa higher for the PORU calculations than for the AMWTP calculations in the undisturbed scenario, as shown in C.W. Hansen et al.'s (2004) Figure 15. This is likely due to a similar mass of gas occupying a smaller pore volume. In the disturbed scenario, gas pressures in the PORU runs tended to extend over a wider range, about 0.5 to 1 MPa higher on the high end and 1.5 to 2.5 MPa lower on the low end, than in the CRA and AMWTP runs. This is shown in C.W. Hansen et al.'s (2004) Figure 17. This is likely due to the correlation between gas generation and porosity in the CRA and AMWTP porosity surfaces, which combine high gas generation with high porosity and low gas generation with low porosity. The dampening effect this correlation has is lacking in the PORU results.

Releases in the undisturbed scenario only occur when repository brine passes through the anhydrite interbeds and crosses the land withdrawal boundary. The generally higher pressures in the undisturbed scenario do result in greater brine flow across the boundary, as illustrated in a comparison of C.W. Hansen et al.'s (2004) Figures 20b and 20d, but a calculation using the

NUTS performance assessment code showed that radionuclide transport remained below the threshold amount of $1x10^{-7}$ kg in all vectors (C.W. Hansen et al. 2004, p. 32). The changes in releases due to the pressure increases observed in the undisturbed scenario were therefore insignificant.

Releases in the disturbed scenario can occur through boreholes to the Culebra Formation and from spallings and DBR. Releases to the Culebra are essentially identical for the PORU and AMWTP models, as shown in C.W. Hansen et al.'s (2004) Figures 19b and 19d, and are not considered further. As previously mentioned, direct releases from the repository are dominated by cuttings and cavings. Spallings releases are of secondary importance (the mean is typically about half an order of magnitude lower than cuttings and cavings at the regulatory limits) and DBR is generally of little significance (mean releases range from 0.5 to 3 orders of magnitude lower than cuttings and cavings at the regulatory limits) (C.W. Hansen et al. 2004, Figure 21). SNL did not calculate cumulative complementary distribution functions (CCDFs) for the constant porosity BRAGFLO runs; however, DOE argued that the mean CCDFs for CRA and AMWTP releases are similar to each other, that the BRAGFLO results of the constant porosity PORU calculations are similar to those observed in the CRA or AMWTP calculations or both, and therefore the CCDFs for the constant porosity models would also be similar (C.W. Hansen et al. 2004, p. 33). Although DOE's argument is weakened by the similarity between the ranges of porosity in the constant porosity study and in the CRA analysis, the relatively small differences between the mean CCDFs for the CRA and AMWTP releases, where the porosities were markedly different, support DOE's conclusion that the observed changes in waste room porosity do not significantly affect releases. EPA accepts this conclusion based on the logic presented by DOE, EPA's experience that CCDFs are not particularly sensitive to these types of changes in performance assessment methodology (EPA 2004a), and the insensitivity of total releases to even relatively large changes in spallings and DBR releases due to the dominating influence of cuttings and cavings releases.

The result of DOE's constant porosity studies is consistent with EPA's earlier conclusion that the influence of SANTOS' over estimates of waste room porosity on WIPP performance will be minor. A sensitivity analysis conducted by C.W. Hansen et al. (2004) showed that the uncertainty in porosity did not contribute to uncertainty in repository pressure. Rather, uncertainty in repository pressure was largely determined by uncertainty in the parameters governing gas generation within the repository, such as the occurrence of biodegradation, and gas flow from the repository through, for example, leaking borehole plugs. Similar ranges of repository gas pressure were observed for both the constant porosity results and the AMWTP results.

DOE has performed series of structural calculations (Park and Holland, 2003) to determine the effect of raising the immediate roof of the disposal room to clay seam G. The distance was 2.43 meters. SANTOS was used in these calculations. The model used the same geomechanical response of the Salado stratigraphy, waste and gas generation as was in the CCA. The grid configuration was adjusted to accommodate the change due to raising of the roof. Difference between the two porosity surfaces (CCA and the raised roof up to clay seam G) was less than 5%. This difference can probably be attributed to the raising of the roof. This provides proof of consistency in the results of SANTOS.

6.0 CONCLUSIONS

Based on a number of lines of reasoning, EPA concludes that WIPP repository performance is not sensitive to the over estimation of waste room porosity by the SANTOS code.

- The problem of overestimating waste room porosity is most significant at very low gas generation rates that do not result in sufficiently high gas pressures to drive significant releases.
- Very low gas generation rates and therefore unexpectedly high estimates of waste room porosity are rare in WIPP performance assessment because brine enters the waste room and gas is generated in every realization.
- At higher gas generation rates, EPA questions the accuracy of the waste room dilation model in SANTOS but accepts that high porosities could be retained over long periods of time due to high gas pressures slowing or stopping waste room closure.
- Releases to the Culebra, releases through anhydrite interbeds, spallings releases, and direct brine releases through intruding boreholes are influenced by gas pressure. These are all secondary or minor contributors to repository performance and small increases in releases by these mechanisms would have no significant effect on total releases.
- An EPA-requested analysis that replaced SANTOS results with constant waste room porosities showed that the effects of the SANTOS results were small and had no significant impact on releases.

EPA concludes that although the accuracy of the SANTOS calculations may be limited, the SANTOS model is capable of reproducing the fundamental aspects of the conceptual model including simulation of the large-scale halite deformation and waste compaction accompanying room closure. The accuracy issues with SANTOS are more a question of approximation rather than omission, and based on the foregoing, EPA believes that the approximations of room closure and waste compaction developed by the SANTOS model are adequate for use in WIPP performance assessment.

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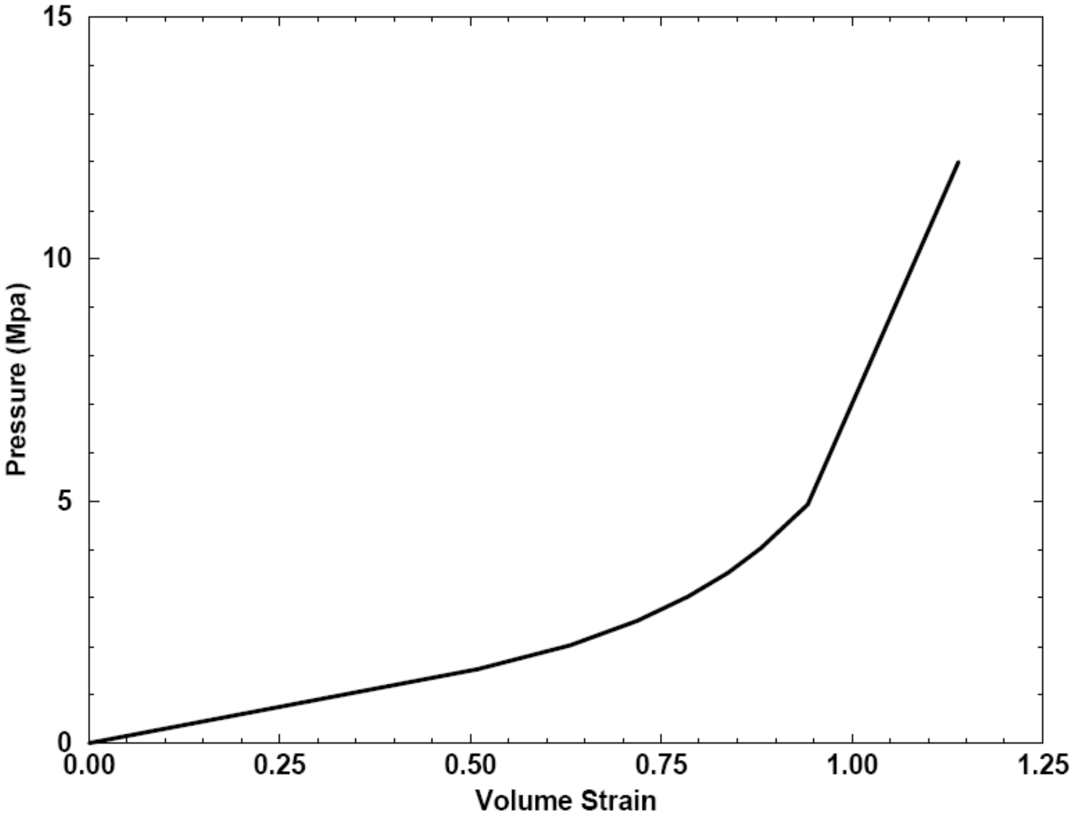


Figure 1. Pressure-volumetric strain curve for waste constitutive model
(from Stone 1997a, Figure 6).

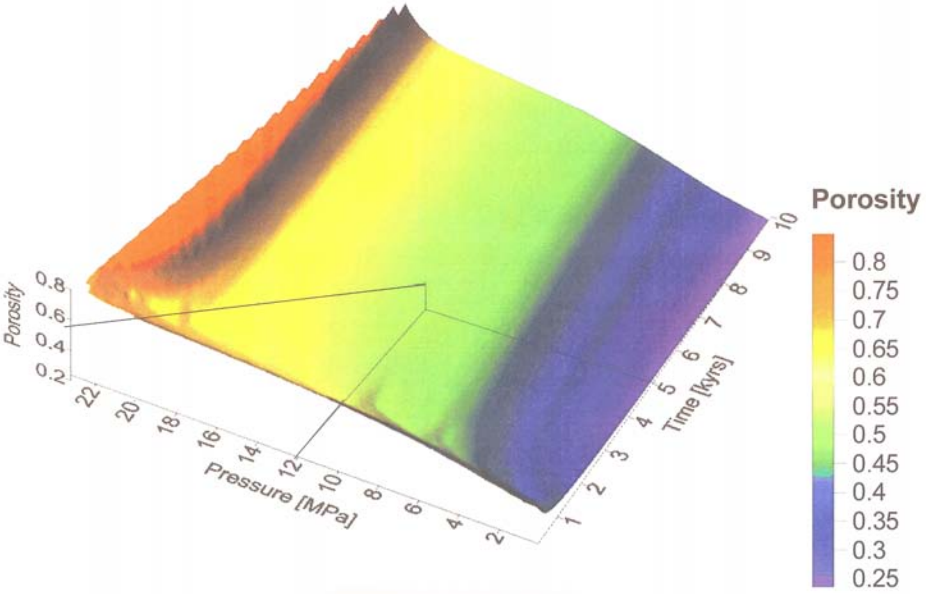

Porosity
0.8
0.6
0.4
0.2
22
20
18
16
14
12
10
8
6
4
2
Pressure [MPa]
1
2
3
4
5
6
7
8
9
10
Time [kyrs]
Porosity
0.8
0.75
0.7
0.65
0.6
0.55
0.5
0.45
0.4
0.35
0.3
0.25

Figure 2. Example porosity surface.
(from EPA 2005; *SANTOS and Porosity Surfaces*, meeting handout by Bill Thompson, Golder Associates)

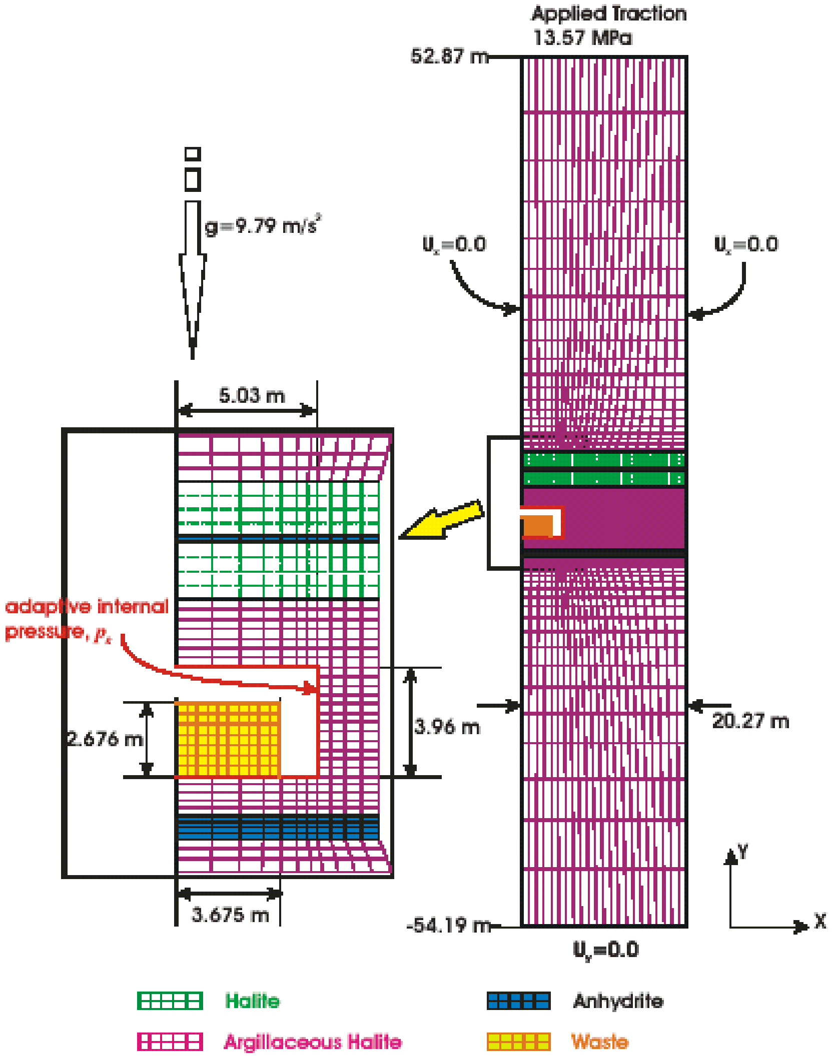


Figure 3. SANTOS mesh discretization and boundary conditions at time = 0
(from DOE 2004, Appendix PA, Attachment PORSURF, Figure PORSURF-2).

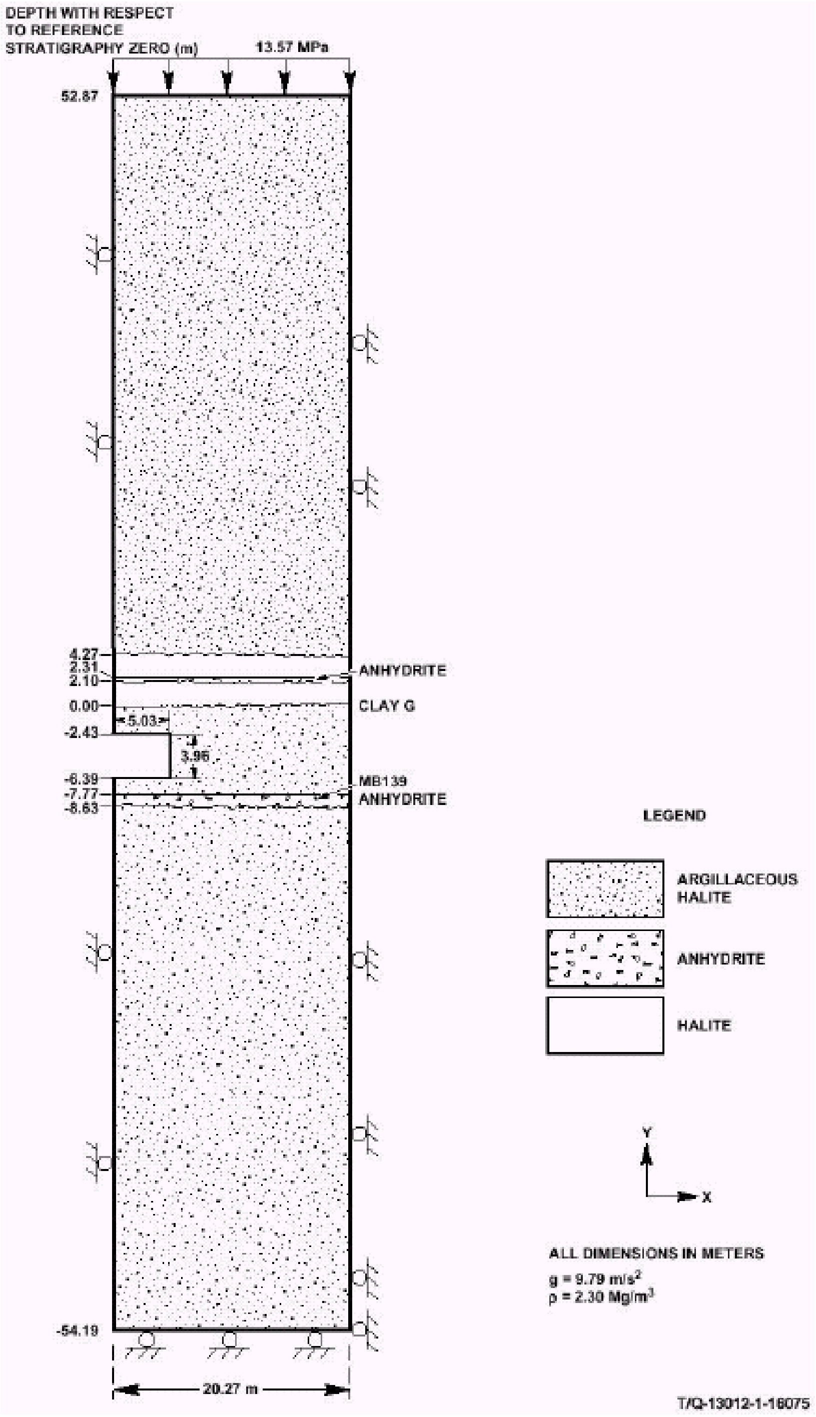


Figure 4. Simplified stratigraphic model used in SANTOS.
(from DOE 2004, Appendix PA, Attachment PORSURF, Figure PORSURF-1).

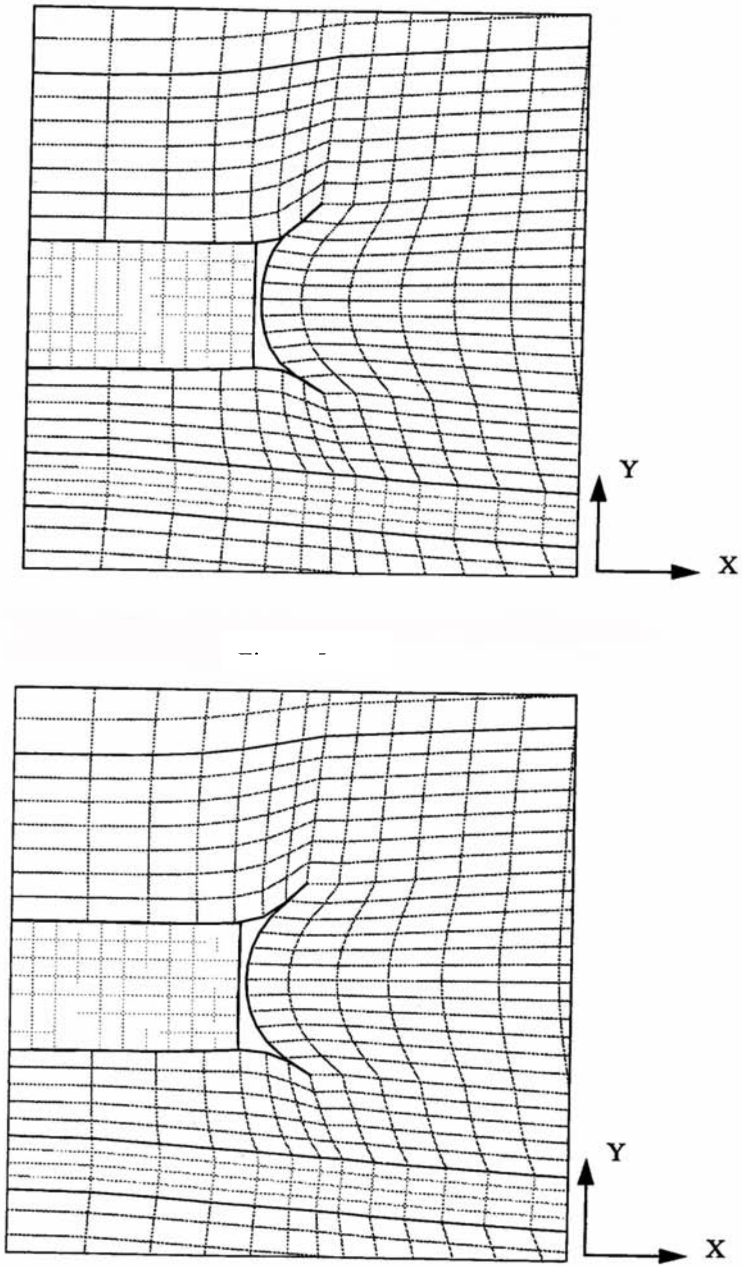
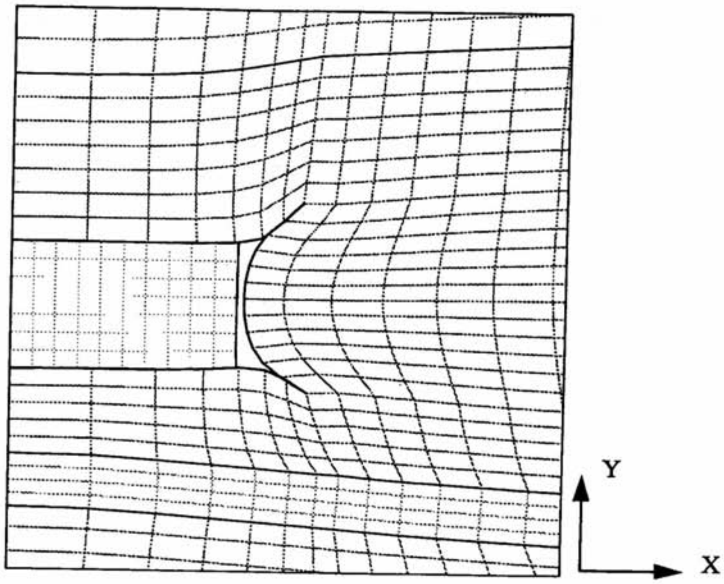
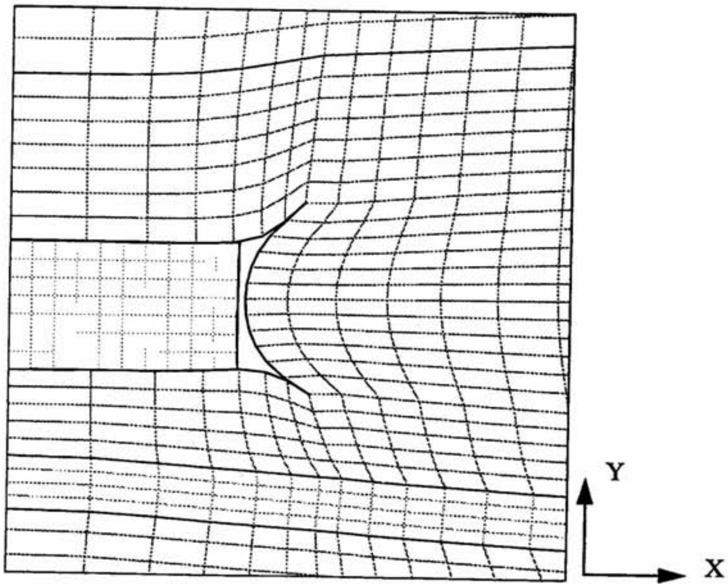


Figure 5. Detail of the deformed disposal room with waste for *f* = 0:
at 300 years (Figure 5a) and at 10,000 years (Figure 5b)
(from Stone 1997a, Figures 9 and 10).





at 500 years (Figure 6a) and at 10,000 years (Figure 6b)
(from Stone 1997a, Figures 11 and 12).

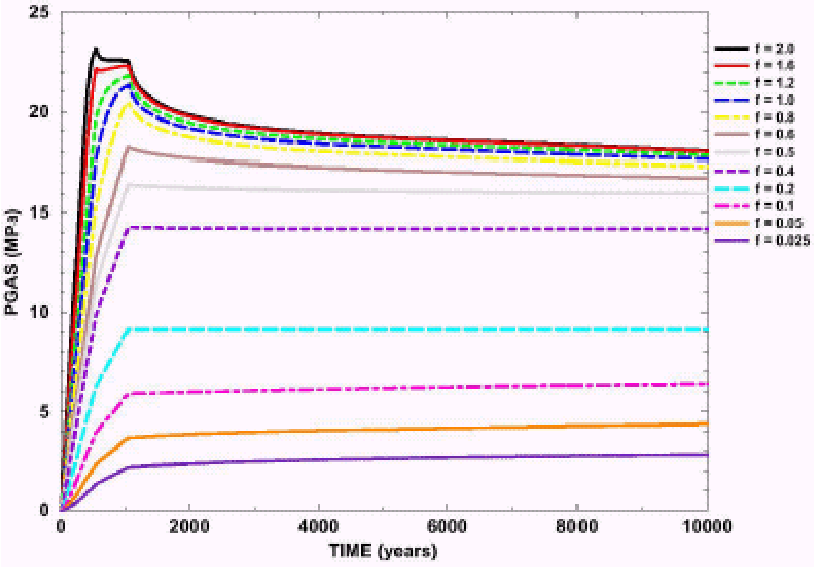


Figure 7. Pressure histories for various values of the gas generation parameter *f*
(from DOE 2004, Appendix PA, Attachment PORSURF, Figure PORSURF-3).

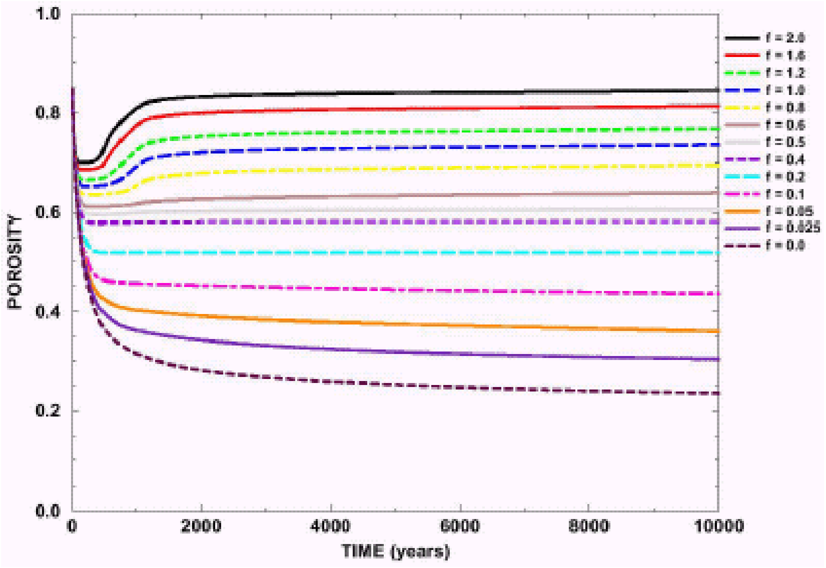


Figure 8. Porosity histories for various values of the gas generation parameter *f*
(from DOE 2004, Appendix PA, Attachment PORSURF, Figure PORSURF-4).

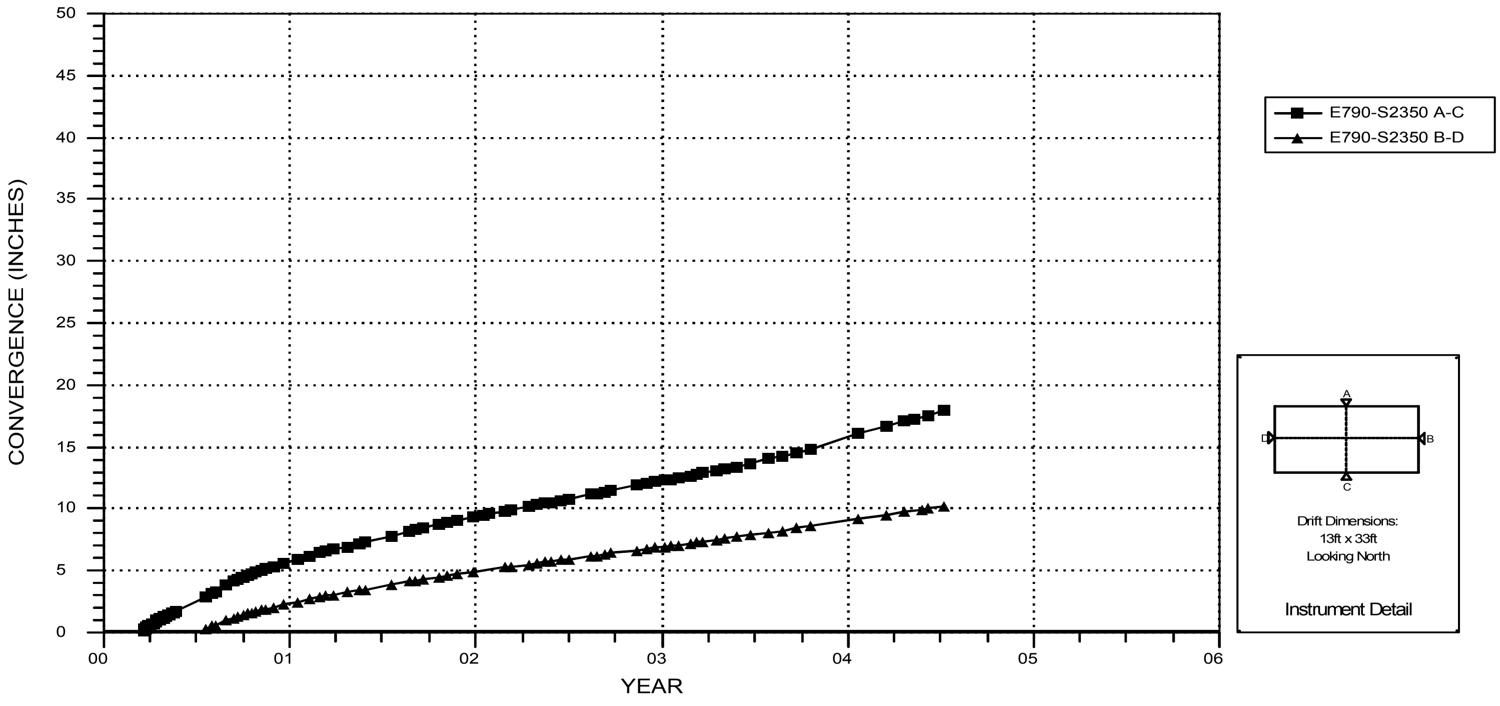


Figure 9. WIPP convergence plots for E790 Drift-S2350, Room 3, Panel 2
(from TEA 2005; *SANTOS and Porosity Surfaces*, meeting handout by Bill Thompson, Golder Associates)

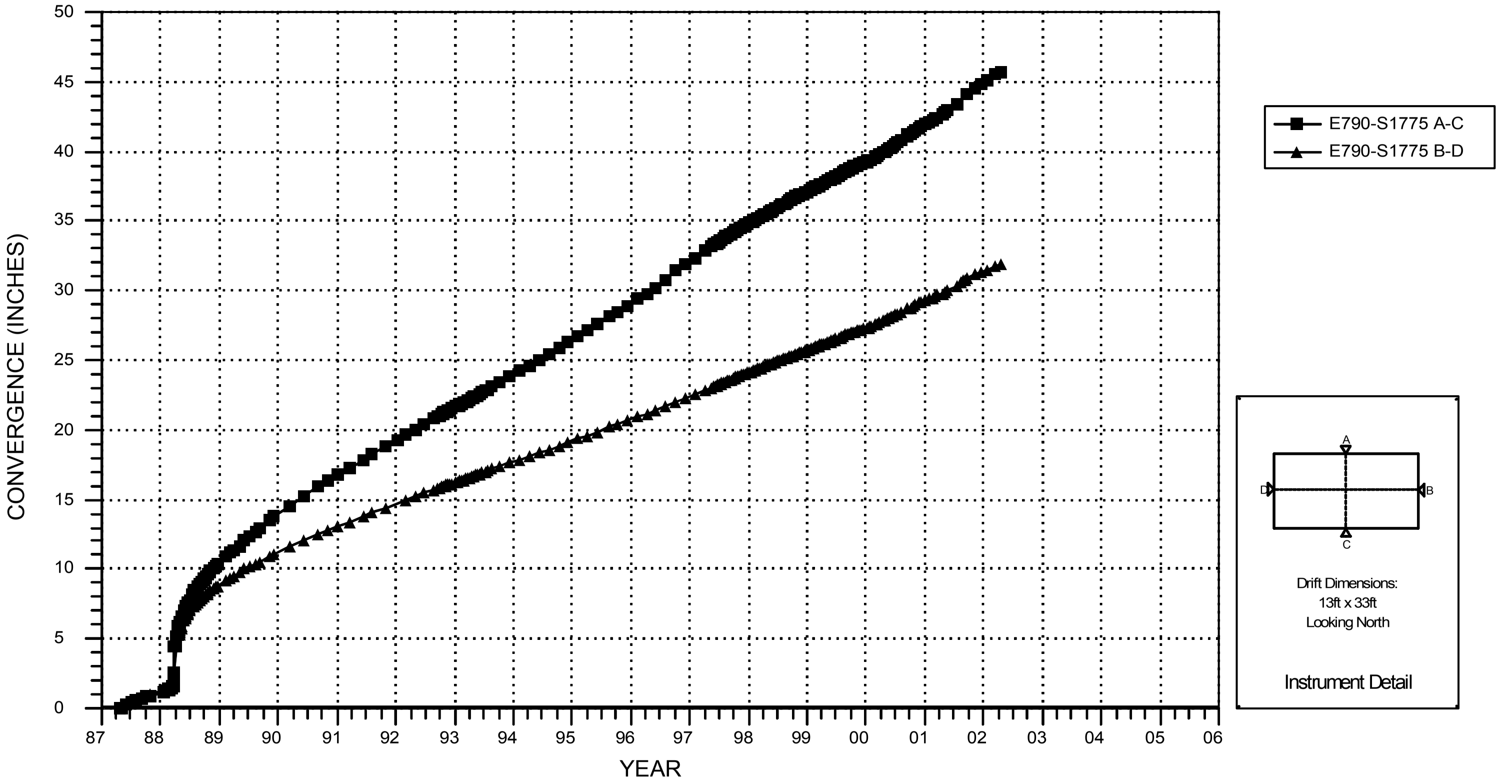


Figure 10. WIPP convergence plots for E790 Drift-S1775, Room 3, Panel 1-Center
(from TEA 2005; *SANTOS and Porosity Surfaces*, meeting handout by Bill Thompson, Golder Associates)