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subject: Calculations Performed in Support of Reconsolidation of Crushed Salt in Panel Closures

The calculations performed using JAS3D to answer the EPA's questions dated December 22, 2011 made use of the volumetric creep model to model the ROM salt used in the panel closure. The volumetric creep model is based on the work of Sjaardema and Krieg (1987). They developed their model based on the hydrostatic consolidation tests of crushed salt by Holcomb and Shields (1987). The following descriptions of the models are based on those found in Stone (1997) who describes how the models were implemented into various Sandia structural mechanics codes.

Model Description

The total strain rate is decomposed into volumetric and deviatoric parts. Because intact salt creeps deviatorically when subjected to a deviatoric stress condition, crushed salt should logically be expected to also creep deviatorically. This expectation becomes more reasonable as the density increases and the crushed salt approaches an intact condition. The deviatoric salt creep model used in the volumetric creep model is based on the power-law secondary creep model. The volumetric creep model is formulated such that the material response of the consolidated crushed salt becomes identical to that of the intact material as the density of the crushed salt approaches that of intact salt. The FLAC/FLAC3D crushed salt model used by RockSol differs from the Sandia model in that it appears to include primary creep as well as secondary creep in its implementation (Itasca, 2003). The solution technique is also quite different.

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The bulk, K, and shear, G, elastic moduli were found from Holcomb and Shields tests to depend on the density, ρ, of the material through relationships of the form

$$K = K_0 \exp\left(K_1 \rho\right) \tag{1}$$

$$G = G_0 \exp\left(G_1 \rho\right) \tag{2}$$

where K_0, K_1, G_0, and G_1 are material constants.

The power-law creep model is cast as a conventional power-law secondary creep model of the form

$$\dot{\varepsilon} = A\bar{\sigma}^m \exp\left(\frac{-Q}{R\Theta}\right) \tag{3}$$

where $\bar{\sigma}$ is the effective deviatoric stress, A and m are material constants, Θ is the absolute temperature, R is the universal gas constant, and Q is the activation energy. Using forward Euler integration and a creep strain rate for von Mises flow, the expression for the deviatoric stress rate is given by:

$$\dot{S}_{ij}^n = 2G\left(\dot{\varepsilon}_{ij} - \frac{3}{2}\exp\left(\frac{-Q}{R\Theta}\right)\bar{\sigma}^{m-1}S_{ij}^n\right) \tag{4}$$

The volumetric creep model is developed by extension of a one dimensional problem into three dimensions. A uniaxially compressed porous crushed salt sample is envisioned as being composed of cylinders of salt, each of which has intact salt secondary creep behavior separated by areas of open space. The local stress acting on the salt cylinders is stated in terms of the average stress on the porous sample. The cross-sectional area of the porous sample is expressed in terms of the net cross-sectional area of the salt cylinders. The final resulting continuum model for the rate of the deviatoric stress of the crushed salt is given as:

$$\dot{S}_{ij}^n = 2G(\rho)\left(\dot{\varepsilon}_{ij} - \frac{3}{2}A\left(\frac{\rho_\infty}{\rho}\right)^m \exp\left(\frac{-Q}{R\Theta}\right)\bar{\sigma}^{m-1}S_{ij}^n\right) \tag{5}$$

where the constants A, Q, m, and ρ_∞ refer to values for the intact salt, ρ is the density.

The volumetric part of the model is divided into elastic and inelastic parts as

$$d_{kk} = \frac{\dot{p}}{K(\rho)} + d_{kk}^c \tag{6}$$

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where d_{kk} is the volumetric strain rate, $\dot{p} = \frac{\dot{\sigma}_{kk}}{3}$ is the rate of change of the pressure, d_{kk}^{c} is the volumetric creep strain rate, and $K(\rho)$ is the density-dependent bulk modulus.

Laboratory consolidation tests have shown that the crushed salt volumetric creep rate can be fit by an expression of the form

$$d_{kk}^{c} = \frac{1}{\rho} B_0 \left[e^{B_1 p} - 1 \right] e^{A\rho} \tag{7}$$

where B_0, B_1, and A are material constants. The density is computed from the relationship

$$\rho = \rho_0 \exp\left(\int_{t_0}^{t} d_{kk} dt \right) \tag{8}$$

where ρ_0 is the density at time t_0.

Equation (6) is solved for $\dot{p}$ and combined with the definition of the volumetric creep strain rate, Eq. (7), to yield

$$\dot{p} = K(\rho) \left[d_{kk} - \frac{1}{\rho} B_0 \left(e^{B_1 p} - 1 \right) e^{A\rho} \right] \tag{9}$$

which is the expression that is integrated.

The volumetric creep model requires the following material parameter inputs (Table 1):

Table 1. Input parameters used for the volumetric creep model.

Parameter	Value	Units	Source
$2G_0$	2.12E+04	Pa	Sjaardema and Krieg (1987), p. 59
K_0	1.76E+04	Pa	Sjaardema and Krieg (1987), p. 59
D	5.79E-36	$1/(Pa^n \cdot s)$	Krieg (1984), p. 18
n	4.9	—	Krieg (1984), p. 18
Q/RT	20.1422	—	Krieg (1984), p. 18
G_1	6.53E-03	m^3/kg	Sjaardema and Krieg (1987), p. 59
K_1	6.53E-03	m^3/kg	Sjaardema and Krieg (1987), p. 59
B_0	1.30E+08	$kg/(m^3 \cdot s)$	Sjaardema and Krieg (1987), pp. 14-15
B_1	8.20E-07	1/Pa	Sjaardema and Krieg (1987), pp. 14-15
A	-1.73E-02	m^3/kg	Sjaardema and Krieg (1987), p. 14
ρ_∞	2160	kg/m^3	Krieg (1984), p. 14; Brodsky (1994), p. 2
ρ_0	1440 *	kg/m^3	67% of intact

* Value is for an initial fractional density of 67% intact, which corresponds to a porosity of 33%. Initial density values at time t=0 vary depending on the predetermined porosity value being analyzed.

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Run Control

The JAS3D (version 2.4.C-WIPP) and its associated utilities (Algebra2 (version 1.28), Aprepro (version 2.06), BlotII2_cps (version 1.59A), FASTQ_cps (version 3.18), and GEN3DII (version 1.37a)) were run on March 17 and 29, 2012 on seals.sandia.gov using the Python run control script PC3R.py and the Python module rc.py. The Postscript files generated by BlotII2 (version 1.59A) were converted to PDF files using the UNIX utility ps2pdf. All input files for the runs were exported from the CVS repository $CVSLIB/Analyses/PC3R, modules Jas3d/Input/Trap and Jas3d/Input/Underground.

The run control scripts and an associated C shell script, RunJas3d.csh were exported from the RunControl module of the same repository. JAS3D and associated utility codes and scripts were exported from code-specific CVS repositories (Table 2). The output files from JAS3D, Algebra, BlotII2, and ps2pdf were stored in the Output module of the repository $CVSLIB/Analyses/PC3R. Additional Excel files produced by BlotII2 were added to the Jas3d/Output module of the repository after the PC3R.py script completed. The log file PC3R.log and an RTF version of that file, PC3R.rtf, are stored in the module RunControl/Log. All files were tagged with the CVS tag PC3R.

Table 2. Run control code-specific CVS repositories.

File	Repository	Comment
Builds/Linux64/algebra2 (Ver:1.28)	/nfs/data/CVSLIB/ACCESS_WIPP/ALGEBRA2	Manipulates EXODUS finite element output data by evaluating expressions
Builds/Linux64/aprepro (Ver:2.06)	/nfs/data/CVSLIB/ACCESS_WIPP/APREPRO	An algebraic preprocessing program
Builds/Linux64/blotII2_cps (Ver:1.59A)	/nfs/data/CVSLIB/ACCESS_WIPP/BLOTII2	Postscript driver for blot
Builds/Linux64/fastq_cps (Ver:3.18)	/nfs/data/CVSLIB/ACCESS_WIPP/FASTQ	Finite element 2-dimensional mesh generation program
Builds/Linux64/gen3d2 (Ver:1.37a)	/nfs/data/CVSLIB/ACCESS_WIPP/GEN3DII	Transforms a 2-dimensional GENESIS database into a 3-dimensional GENESIS database
Builds/Linux64/jas3d (Ver:2.4.C-WIPP)	/nfs/data/CVSLIB/ACCESS_WIPP/JAS3D	Finite element code for 3-dimensional analyses
RunControl/algebra2.sh	/nfs/data/CVSLIB/ACCESS_WIPP/ALGEBRA2	Script for manipulating EXODUS finite element output data by evaluating expressions
RunControl/blotII2.sh	/nfs/data/CVSLIB/ACCESS_WIPP/BLOTII2	Script for running graphics code for examining meshes
RunControl/fastq.sh	/nfs/data/CVSLIB/ACCESS_WIPP/FASTQ	Script for running finite element 2-dimensional mesh generation program
RunControl/gen3dII.sh	/nfs/data/CVSLIB/ACCESS_WIPP/GEN3DII	Script to transform a 2-dimensional GENESIS database into a 3-dimensional GENESIS database
RunControl/jas3d.sh	/nfs/data/CVSLIB/ACCESS_WIPP/JAS3D	Script for running jas3d.exe

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