MIGRATION OF BRINE AND NITROGEN IN CREEPING SALT*

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ABSTRACT

Although the excavations in bedded salt at the Waste Isolation Pilot Plant (WIPP) are, for all practical purposes, dry, small amounts of brine have been observed to weep from exposed surfaces in the repository horizon and seep into drill holes in the underground excavations. As part of the Brine Sampling and Evaluation Program (BSEP) at the WIPP, this study has been made to formulate the complex problem of brine and nitrogen flow through deforming salt as completely as possible. The derived equations are coupled where appropriate in order to closely describe the natural phenomena. The main objective of this paper is to suggest a method by which the formulation might be solved in order to estimate the brine inflow rate into the excavated rooms at the WIPP repository level. The suggested solution method requires the modification and combination of two finite element codes which may necessitate a large amount of computer memory for data storage.

INTRODUCTION

The WIPP is a Department of Energy (DOE) research and development facility to demonstrate the safe disposal of radioactive wastes derived from the defense activities of the United States. The WIPP facility is located approximately 42 kilometers east of Carlsbad, New Mexico. The underground portion of the facility is located at a depth of approximately 655 meters in the bedded salt deposits of the Salado Formation, part of an evaporate sequence over 1,000 meters thick (Fig. 1). Although the excavations at the site are, for all practical purposes, dry, small amounts of brine have been observed to weep from exposed surfaces in the repository horizon and seep into drill holes in the underground excavations. These occurrences have been the focus of the BSEP at WIPP, and have been described previously (Deal and Case, 1987 (1); Deal, 1988 (2)) and in a companion paper in this symposium (Deal and Roggenthen, 1989 (3)). The assessment and understanding of the brine occurrences becomes important when considering what the long-term effects of brine seepage might be on the rates of resaturation and repressurization of the excavations after closure.

Excavations at the WIPP create openings at atmospheric pressure and the resulting pressure gradients induce fluids (contained in the salt) to flow toward the excavated rooms. The excavation also creates a stress differential between atmospheric pressure and the virgin rock stress in the intact salt. This stress differential causes salt to creep into the excavated rooms. Gasses (mostly nitrogen) dissolved in the brine, exsolve and also move toward the excavation, moving through both the salt and the brine. The result is that excavation-induced flow of three phases (represented by salt, brine, and nitrogen) occur simultaneously.

The processes of salt creep and fluid flow are intimately coupled. The creep of the salt will change the permeability and porosity of the salt itself, which in turn results in fluid pressure changes. Fluid pressure in rock pores then affects stresses in the rock and consequently changes the salt creep rate. Because detailed experimental data on these coupling effects are not available at present, the relative importance of each mechanism is difficult to assess.

Based on the current understanding, brine inflow is a complex process (Deal and Case, 1987 (1)). Factors in the process include: (1) nonuniform distribution of brine; (2) the surrounding salt is continuously deforming resulting in local changes in permeability; (3) a probable coupling of salt deformation and the flow of brine; (4) the presence of unsaturated flow conditions, especially in the proximity of excavations; (5) appearance of fractures around excavations; (6) dissolution of nitrogen from brine; and (7) stratigraphic variations within the salt sequence. The purpose of the BSEP is to investigate the origin, hydraulic characteristics, extent, and composition of the brine occurrences in the excavations for the WIPP repository. As part of BSEP, it is the intention of this study to formulate this complex problem as completely as possible and to suggest a method for solving the derived equations. This paper is an abbreviation of a more complete formulation that will be included in the 1988 BSEP Report (4) presently in preparation.

Occurrence of Brine and Nitrogen in Bedded Salt

The complex evaporite sequence exposed in and near the WIPP excavations was initially deposited in a part of the Permian Sea where normal marine waters were concentrated by evaporation. Rainfall, muddy runoff from nearby land, and influxes of normal marine water caused the salinity of the water to fluctuate, so that times of precipitation of halite alternated with periods of resolution. Although the Salado Formation is composed predominantly of halite, the resultant rock contains some clay and other evaporite minerals, such as polyhalite, anhydrite, and various potash minerals. Some residual sea water containing

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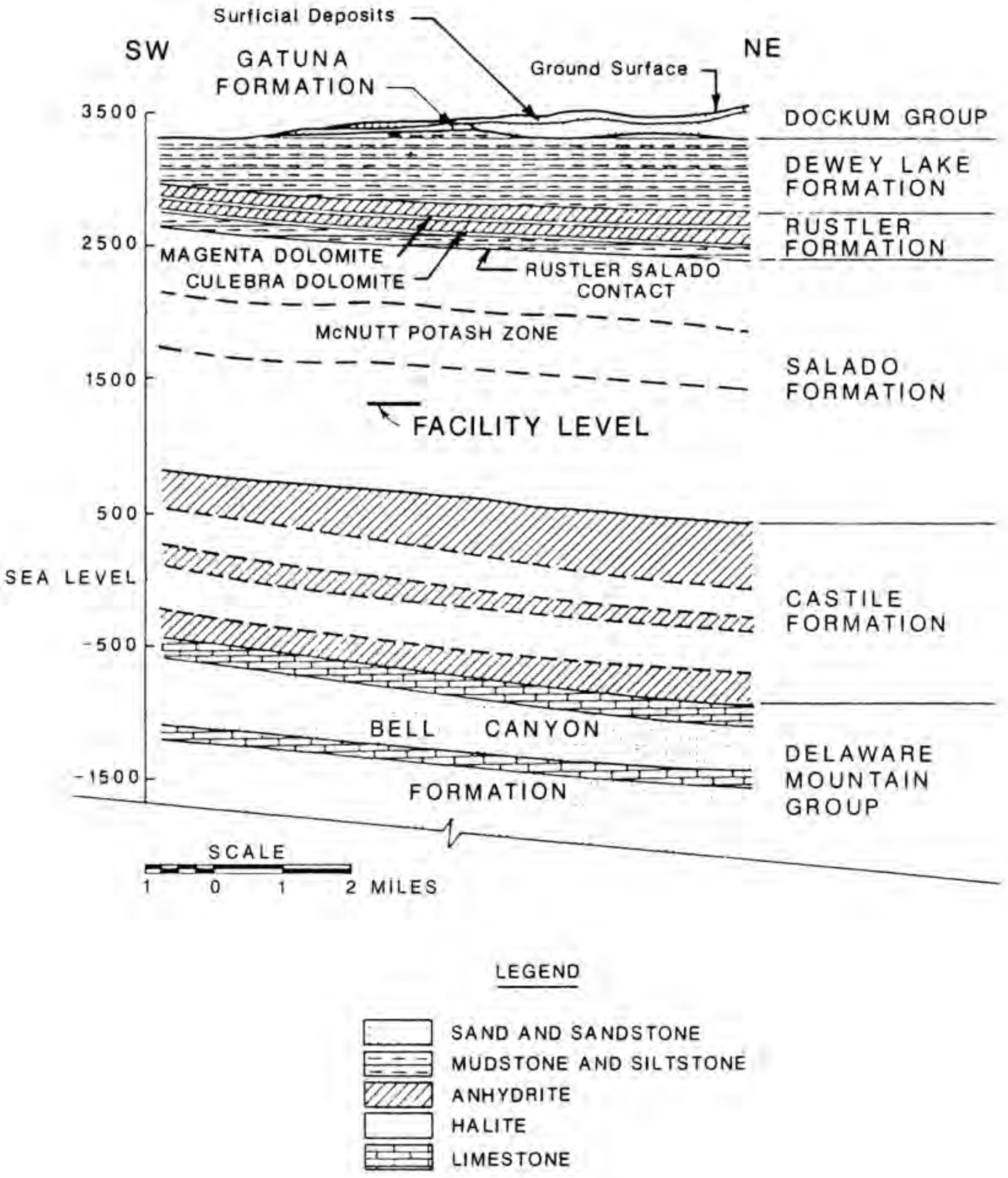

Fig. 1. Generalized Stratigraphic Cross Section (Modified from Fig. 1-2, Deal and Case, 1987).

gasses dissolved from the Permian atmosphere was trapped in the precipitating evaporites.

After burial beneath the sea floor, a chemically and physically complex set of diagenetic processes acted on the deposits, causing extensive recrystallization to occur. The composition of the residual brine and gasses in the salt was also changed during diagenesis, and is likely that whatever residual oxygen was present combined with other elements at that time. Ongoing work has shown that the WIPP brines are notable for the fact that they contain essentially no dissolved oxygen or carbon dioxide, and that the gas exsolving from the brine is mostly nitrogen, with traces of methane. The nitrogen today may either exist within the rock matrix as free gas or be dissolved in the brine. The amount of nitrogen dissolved in the brine depends upon the pressure and temperature of the undisturbed salt.

Salt is a plastic material. It compresses under normal stresses and creeps under deviatoric stresses. As a consequence, rock salt has a very low permeability and porosity. Fluid pressure in the salt is probably equivalent to the undisturbed normal stresses acting on the rock. When rock stresses are relieved by excavation, fluid pressure lowers, dissolved nitrogen is released from the brine and becomes free gas, partially offsetting the fluid pressure drop.

Fluid Flow Through Deformable Rocks

Observations in the WIPP excavations indicate that delicate features formed during deposition and diagenesis are very well preserved, and that the bedding is nearly horizontal and appears to be essentially undisturbed since Permian time. Only burial, uplift, and gently warping has occurred. This is evidence that local pressure gradients in the salt near the WIPP repository were probably insignificant and that little or no flow of salt or brine occurred for a long time prior to excavation.

Since salt deforms plastically, it is hard to conceive that pore pressures in the salt were anything other than lithostatic prior to excavation. The atmospheric pressure in the excavated rooms acts like a pressure sink for fluids and gasses stored in the salt. As brine and nitrogen flow toward the pressure sinks (rooms), the steepness of the pressure gradient decreases with time. Distribution of pore pressures may eventually reach steady state after some time. The presence of visible fractures around excavations indicates that unsaturated flow conditions exist, at least after atmospheric pressure is reached.

Derivation of the fluid flow equations start with the continuity equation. A typical set of two-phase flow equations can be found in Aziz and Settari (1979) (5):

$$(\lambda_w \Phi_{w,i})_{,j} = \frac{D}{Dt}\left(\phi \frac{S_w}{B_w}\right) + q_w \qquad \text{(Eq. 1)}$$

$$(\lambda_n \Phi_{n,i})_{,j} = \frac{D}{Dt}\left(\phi \frac{S_n}{B_n}\right) + q_n \qquad \text{(Eq. 2)}$$

$$P_c = P_n - P_w = f(S_w) \qquad \text{(Eq. 3)}$$

$$S_w + S_n = 1 \qquad \text{(Eq. 4)}$$

where subscript w denotes the wetting phase and n denotes the non-wetting phase, and

$\lambda_1 = \frac{K_{r1}}{\mu_1 B_1} K_{ij}$
k_{ij} = Permeability (absolute) of rock
K_{r1} = Relative permeability of phase 1, a function of S_1
S_1 = Saturation of phase 1 = V_1/V_v
μ = Viscosity

$$B_1 = \frac{V_1 \textit{ in reservoir}}{V_1 \textit{ at surface condition}} = \frac{\rho_1 \textit{ at surface condition}}{\rho_1 \textit{ in reservoir}}$$

z = Elevation
ϕ = Porosity = V_v/V_r
q = Fluid production (or injection)
P_c = Capillary pressure
Φ_1 = Fluid potential of phase 1. (= $P_1 + \rho_1 g z$)
V_1 = Volume of phas 1 in or fixed, volume rock element
V_v = Void volume of a rock element
V_r = Volume of a rock element
ρ_{gas} = 1.25 kg/m^3 at 15°C and 1 atm (or nitrogen)
ρ_{brine} = 1,200 kg/m3 at 15° and 1 atm.

To account for the fact that the flow media are continuously deforming, the total derivative with respect to time is used at the right-hand side of the partial differential equations. Introducing the gas equation of state and Darcy's law into Eqs. (1) and (2), the following equations are

$$\frac{K_{rb}}{\mu_b}\{[P_{b,j}(1 + gz\rho_b C_f) + \rho_b g z_{,j}] (C_b k_{ij} P_{b,i} + k_{ij,i}) + k_{ij}[P_{b,ji} + g\rho_b C_b (P_{b,j} z_{,i} + P_{b,i} z_{,j})]]\}$$
$$= \frac{1}{1200\ V_r}\left[V_b C_b \frac{\partial P_b}{\partial t} + \frac{\partial V_b}{\partial t} - \frac{V_b}{V_r}\frac{\partial V_r}{\partial t} + v_i\left(V_b C_b P_{b,i} + V_{b,i} - \frac{V_b}{V_r} V_{r,i}\right)\right] \qquad \text{(Eq. 5)}$$

$$\frac{k_{ra}}{\mu_a}\left(\frac{k_{ij}}{P_a} P_{a,j} + k_{ij,j} P_{a,i} + k_{ij} P_{a,ji}\right)$$

$$= \frac{1}{1.25\ V_r}\left[\left(\frac{V_a}{P_a}\frac{\partial P_a}{\partial t} + \frac{\partial V_a}{\partial t} - \frac{V_a}{V_r}\frac{\partial V_r}{\partial t}\right)\right.$$

(Eq. 6)

$$\left. + v_i\left(\frac{V_a}{P_a}P_{a,i} + V_{a,i} - \frac{V_a}{V_r}V_{r,i}\right)\right] + \frac{q_a}{\rho_a}$$

Terms in the continuity equation are expanded based on several proposed constitutive relationships, such as fluid density versus pore pressure and porosity versus effective stress. Equations (3), (4), (5), and (6) are the governing equations for the two-phase fluid flow through deformable porous media.

The assumptions involved in this derivation are: (1) rocks can be modeled as continuous and porous media, (2) permeability and porosity of rock salt are affected by salt creep and brine migration, (3) Darcy's law applies, (4) linear relationships are applied whenever possible, (5) compressibility of brine is constant over the applicable range of pressure, and (6) isothermal conditions prevail.

The salt initially dilates in response to a decreased confining stress, with a resultant increase in both intercrystalline and intracrystalline porosity. Intercrystalline permeability also increases. Fracturing of rocks close to excavated rooms is also part of the salt deformation process. Fluid transport properties of the fractured rocks are altered from virgin rocks depending on the aperture, length, width, and orientation of each fracture and how fractures intersect each other. In general, permeability of the salt close to the excavations is dominated by the fracture permeability. To model brine transport phenomenon through fracturing and deforming rocks, one may take either a fractured media approach or an equivalent porous media approach. Both approaches lack field measurement data. Without detailed information about fracture geometries and orientations, however, the more complicated and time-consuming fractured media approach may not be any better than the porous media approach. The porous media approach is applicable prior to the development of open fractures. Thus throughout this paper, the flow media are assumed to be porous and continuous.

Time-Dependent Deformation of Rock Salt Around Excavation Rooms

Rock salt is known to be a rheologic material. Deformation of rock salt around underground excavations is dependent on time, stress and temperature. Part of the roof-floor convergence of the excavations at WIPP can be attributed to fracture development. Induced fractures in the vicinity of excavated rooms complicate the stress-deformation analysis. Deformation of fractured salt is attributed to the propagation of fractures as well as the plastic flow of salt grains. Unfortunately, it is essentially impossible to predict the initiation and propagation of fractures in the field. As a simplification, salt is analyzed as a continuum which follows the stress equilibrium states and displacement continuity conditions. This approach tends to underestimate the induced porosity of salt in the fractured zone and overestimate the same porosity away from the fractured zone.

To describe the deformation process, we need three sets of equations: the equations of equilibrium, the displacement compatibility equations, and the stress-strain constitutive equations. The effects of moisture and time on salt deformation are considered and incorporated when the stress-strain equations are derived.

The equation of equilibrium states that in the absence of external forces, the change in stress over space is either zero or equal to the body force. For time-dependent deformations, equilibrium may never exist and the equilibrium equation may not apply. However, creep of salt around excavations is generally within the order of 10^{-9} meters/second, which is very slow. The force caused by movements of salt is thus negligible and the equilibrium equation may be assumed valid.

Figure 2 illustrates typical room convergence curves found at the WIPP repository site (6). In this figure, the room first shows a relatively rapid initial displacement. It is then followed by transient movements where displacement rates are decreasing until the rates become constant. It is thus assumed that:

total elastic viscoelastic viscoplastic
strain = strain + strain + strain

and

total viscoelastic viscoplastic
strain rate = strain rate + strain rate

The viscoplastic strain is used here to approximate the steady state creep of salt and the viscoelastic strain is to model the transient creep. A graphic representation of this model is shown in Fig. 3 (7). The authors acknowledge that there are many constitutive relationships proposed for modeling the creep of salt, yet this model is chosen for its simplicity and reasonable accuracy. Modification of this model is left open for better suggestions.

Moisture is known to have a weakening effect on rock salt (Spiers, et al., 1986 (8)). Moisture-salt interactions may fall into the following categories: (1) interaction between brine and fracture surfaces, (2) intracrystalline effects, and (3) interaction between brine and grain boundaries. It is proposed in this work that the following relationship describes these weakening effects:

$$\dot{\varepsilon} = (aS_b + b)\ \dot{\varepsilon}_{wet} \qquad \text{(Eq. 7)}$$

where a and b are constants and Sb is the saturation of brine in salt. The derived stress-strain constitutive equations are:

$$\varepsilon_i = (aS_b + b)\ \sigma_i\ \left(\frac{1}{E_1}\right.$$

(Eq. 8)

$$\left. + \frac{1}{E_2}\ \{1 - \exp[-(\frac{E_2}{C_4 T}\ t)]\}\right) - \alpha(T)\Delta T$$

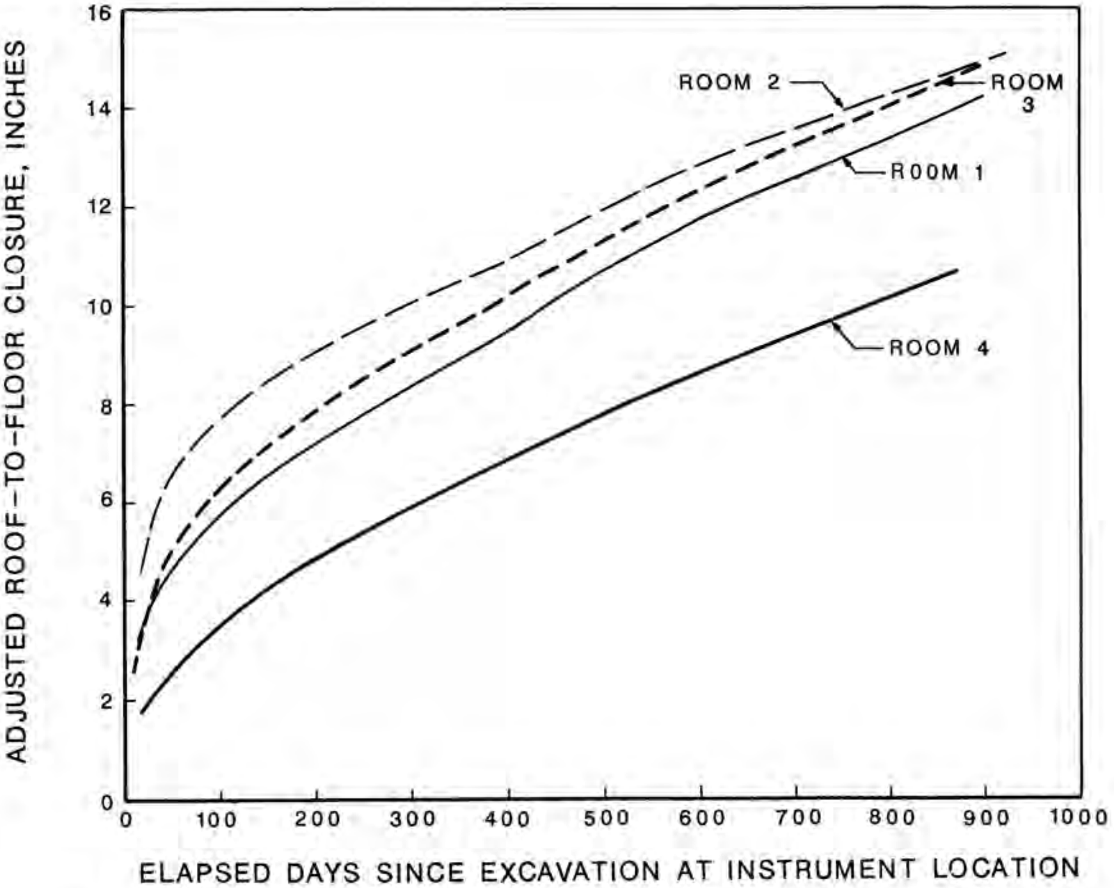

Fig. 2. Typical Room Closure Measured Rates (Modified from Bechtel National, Inc. 1986).

and

$$\gamma_{ij} = (aS_b + b)\ \left(\frac{\tau_{ij}}{G_1} + \frac{\tau_{ij}}{G_2}\ \{1 - \exp\left[-\left(\frac{G_2}{C_4 T}\ t\right)\right]\}\ + A\ \left(\frac{\tau_{ij}}{\tau_c}\right)^n \exp\left(-\frac{Q_p}{RT}\right) t\ H\ (\tau_s)\right) \qquad \text{(Eq. 9)}$$

where A, and C_4 are constants, E is the elastic modulus, G is the shear modulus, and:

τ_c = A constant for normalizing shear stress
n = Stress exponent
Q_p = Activation energy
R = Universal gas constant
T = Temperature
vp = Viscoplastic
ε_i = Dilatational strain
γ_{ij} = Shear strain
V_p = Viscous factor of viscoplasticity
t = time

$H(\tau_s)$ = Step function = 0 when $\tau_o \leq \tau_s$
= 1 when $\tau_o > \tau_s$
τ_o = Octahedral shear stress.

When fluid pressure in the rock pores varies, it effects stresses in the rock structure. Jaeger and Cook (1976) (9) suggest that the effective stress be defined in the following way.

$$\bar{\sigma}_{ij} = \chi\sigma_{ij} - (1 - \chi)P\delta_{ij} \qquad \text{(Eq. 10)}$$

where

χ = A constant between 0 and 1
δ_{ij} = Kronecker delta.

This concept of effective stress should be applied to all stresses discussed in this paper.

A Coupled Two-Phase Flow and Rock Creep Approach

The main objective of this study is to formulate the mechanism of brine inflow and to suggest a method of solution in order to estimate the brine inflow rate into the excavated rooms at the WIPP repository level. Equations (5) and (6) are the main equations which describe fluid motions in the salt. These equations relate variations in permeability, fluid properties, and rock porosity to changes in pressure as a function of space and time. Equation (3) defines capillary pressure (Pc) as the difference between gas and brine pressures. The capillary pressure is a function of saturation of the wetting fluid (brine). Equation (4) states that rock pores are filled with mixtures of gas and brine. By using Eqs. (3) and (4), the governing equations of brine and gas flow can then be coupled together.

Because salt is highly deformable, elements of salt are moving with time and the porosity of salt also varies with time. To evaluate displacement rates and porosities of salt elements, Eqs. (8) and (9) are adopted.

With the strain tensor calculated through Eqs. (8) and (9), it is desired to convert strain components into volumetric changes and to recalculate the porosity of the salt. Letting the volume of solids in a rock element be constant, we have:

$$\phi = \frac{V_v}{V} = \frac{V_o \phi_o + \Delta V}{V_o + \Delta V} \qquad \text{(Eq. 11)}$$

where

V : Volume of a rock element

V_v : Volume of pores in the same rock element when strains are very small.

To relate porosity with permeability for rock salt, the following equation is suggested, which is obtained through laboratory tests (Lai, 1971 (10)):

$$\frac{\phi^3}{(1-\phi)^2} = \frac{K^a}{b} \qquad \text{(Eq. 12)}$$

Equation (12) does not completely describe the relationship between porosity and permeability found in the vicinity of a repository excavation. However, although it lacks field testing confirmation, this equation is used for the time being, until better relationships between rock deformation and permeability are available.

Suggestions on Solution Method

Generally, it is preferred to solve diffusion type equations such as Eqs. (3) and (4) by finite difference method and solve Laplace equations by the finite element method. When both types of equations are present in the same problem, and in this case, when the modeling area deforms continuously, it may be more straight forward to apply the finite element method.

Two finite element codes are required, one for the flow process and one for the mechanical process. These programs should be modified according to the derived equations and then merged together as a complete package. The connection between these two programs should be put on rock porosity and fluid pressure. Iteration schemes are required to assure convergence and balance between the two parts.

The brine inflow rate and the cumulative brine inflow volume should be calculated and recorded at all time steps. Volume of exsolved gas is estimated explicitly through the use of gas solubility data and is a function of fluid pore pressure. The exsolved gas can be considered as gas injection or production depending on whether fluid pore pressure is dropping or rising.

Strains and strain rates of rock element movement are estimated by solving Eqs. 8 and 9. Porosity and permeability of rocks are then evaluated explicitly. Once the updated porosity and permeability are applied into flow equations (Eqs. (3) through (6)), the pressure distribution in the salt will be altered. The altered pressure distribution then changes rock effective stresses and consequently effects rock porosity. It is then desired to set up an iteration scheme for the balance among parameters such as fluid pressure, rock stress, permeability, and porosity.

CONCLUSION

We conclude by suggesting that a useful approximation of the solution to this problem can be made by modifying and combining two existing finite element codes, one describing the rock mechanics and the other the hydrology, in the manner suggested in this paper. This could require a large amount of computer memory for data storage. As additional in situ data become available from WIPP, especially on the way in which pore pressure and permeability vary in time and space away from the excavations, the equations can be modified to reach more accurate solutions.

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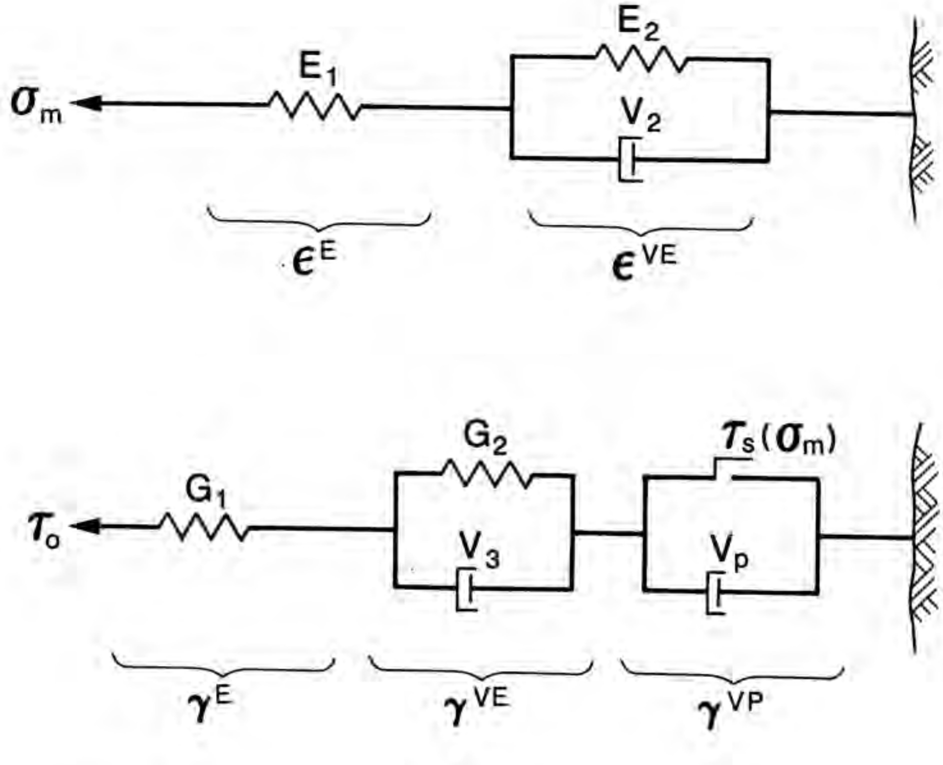

where

E = Young's modulus
G = Shear modulus
V = Viscous factor
τ_s = Shear strength of rock = $C_1\sigma_m + C_2$
σ_i = Normal stresses
τ = Shear stresses
σ_m = Mean stress = $1/3\ (\sigma_x + \sigma_y + \sigma_z)$

Fig. 3. Proposed Constitutive Models for Deformation of Rock Salt (Modified from Serata, et. al., 1985).