**Interim Report on Development of a
Semi-Empirical Numerical Model for
Simulating the Deformational Behavior of a
High-Level Radioactive Waste Repository
in Bedded Salt**

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MASTER

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INTERIM REPORT ON
DEVELOPMENT OF A SEMI-EMPIRICAL NUMERICAL MODEL
FOR SIMULATING THE DEFORMATIONAL BEHAVIOR OF A
HIGH-LEVEL RADIOACTIVE WASTE REPOSITORY IN BEDDED SALT

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ABSTRACT

This report describes a computer model for simulating the deformational behavior of the rock surrounding a high-level radioactive waste repository in a bedded salt formation. The model assumes that the rock mass is isotropic and linearly elastic. It also assumes that all nonlinear, inelastic effects are confined to a single seam, or salt bed, where deformations are related to time, stress, and temperature. The seam thickness is assumed to be negligible in relation to the depth and lateral extent of the mined areas; the mining horizon is viewed as a single plane surface, with relative movements (i.e., closures) between the two sides of the plane used to specify the state of deformation and stress in the rock mass. Because of the assumed linear behavior of the rock, superposition is used to analyze the repository problem in terms of three interrelated phenomena: (1) elastic closure of the excavated areas with consequent elastic deformation of the rock mass; (2) time-, stress-, and temperature-dependent closure of the unmined portions of the seam; and (3) thermal stress and displacement changes throughout the rock mass, including the seam, where stress and temperature variations affect the creep behavior of the seam material.

The computer model is based on the displacement discontinuity method of analysis, in which the seam is treated as a number of individual displacement discontinuities (or dislocations) whose values are determined such that the appropriate boundary conditions are satisfied at the plane of the repository. The boundary conditions, in turn, are governed by the overburden stress, the thermal stress, and temperature changes caused by the decay of the radioactive wastes and the inelastic behavior of the salt in the seam. The radioactive waste is modeled as a series of heat sources with specified heat generation characteristics. The creep deformation of the seam is computed from a creep law whose form was derived from laboratory model pillar tests; the parameters for the creep law were established from full-scale field data obtained from the Project Salt Vault experiment.

The computer program that was written to analyze the repository problem is briefly described, and the modifications necessary to make it applicable to actual repository design studies are discussed. The current version of the Repository Program is based on a 50 by 50 grid of square elements (displacement discontinuities) representing the plane of the repository. The fundamental objective of the program is to find the closure occurring at each element as a function of time, because these values specify the state of deformation and stress in the surrounding rock mass. In order to permit the analysis of a full-scale repository, about 10,000 ft long by 5000 ft wide (and about 2000 ft deep), it is necessary to ignore the detailed room and pillar geometry and to treat the plane of the repository as a series of elements that are partially extracted, with some specified initial extraction ratio, and backfilled with crushed salt. As each element is "excavated," it is considered to act as a heat source with prescribed heat generation characteristics; these characteristics are determined by the density of the radioactive waste canister in the actual problem and are chosen such that the average heat generation per unit area is the same in the model as in reality.

A series of check-out runs was performed to confirm that the various portions of the Repository Program were functioning satisfactorily and to investigate the sensitivity of the model to variations of particular parameters over appropriate ranges to confirm that the computed results were reasonable. These runs were performed successfully, and it is concluded that the Repository Program should be put into a form that is convenient for actual design studies.

1. INTRODUCTION

The design of a high-level radioactive waste repository in bedded salt requires the analysis of two general rock mechanics problems: (1) investigation of the short-term stability of the various underground rooms, corridors, and access tunnels; and (2) prediction of the displacements and stresses in the surrounding rock mass (including the surface) over long periods of time. Although these problems overlap to some extent, they essentially are being treated on an independent basis. The first problem is being examined by finite element analysis and will not be discussed further in this report. The second problem is being examined by a specialized, semi-empirical numerical model. The purposes of this report are to describe this model and to document the present status of its development.

The objective of the work presented here is to develop a computer model for simulating the three-dimensional deformational behavior of a high-level radioactive waste repository in a bedded salt formation. In order to accomplish this goal, the model should incorporate the following characteristics and capabilities:

1. Simulation of a large (5000 by 10,000 ft in plan) underground repository area with sequential and time-phased emplacement of waste with a decaying heat generation rate.
2. Inclusion of the effects of the free (ground) surface in the calculations for repository workings at any specified depth.
3. Simulation of the effects of reconsolidation and recrystallization of the crushed salt used to backfill the waste disposal rooms.
4. Calculation, at any desired point in the rock mass and over total time periods of several hundred years, of the displacements and stresses resulting from both creep closure of the excavations and bulk thermal expansion of the rock.

The semi-empirical numerical model is based on the face-element, or displacement discontinuity, method of analysis and a pillar creep law derived from laboratory experiments. The original work, which was performed by A. M. Starfield, led to the development of a three-dimensional model for the analysis and interpretation of the in situ rock deformation measurements made during the Project Salt Vault experiment.¹ This model was correlated with field measurements in order to determine the values of the various model parameters. This step in the approach is the reason for entitling the model "semi-empirical;" that is, it incorporates parameter values obtained from empirical (but full-size) data. Starfield and McClain have discussed this aspect of the approach in detail.² The semi-empirical model is based on the form of a pillar creep law determined from laboratory pillar model experiments. However, the values of the parameters in the creep law are obtained by trial-and-error fitting of model predictions to deformations actually measured in a field

situation — the Project Salt Vault experiment in this case. In this way, the model is "calibrated" to prototype size, and the usual problems of scaling up laboratory data are avoided. Because of the importance of this correlation step, a brief summary is included here.

Two separate and independent correlations of this special "Experimental Area Model" with the Project Salt Vault room closure data were carried out; these are identified as runs Z-11 and Z-15. In Z-11, the thermal stress transference factors (EQ) of the array heaters and pillar heaters were restricted to approximately the same values; however, this restriction was lifted in Z-15. The values for the various rock property parameters used in these correlations are shown in Table 1. The general procedure was to compare the model-generated room closures with actual vertical "convergence" measurements from the experiment at eight points along the longitudinal centerline of the experimental area (Fig. 1). When an acceptable correlation was obtained at these points, it was confirmed by using data from the other convergence stations indicated in Fig. 1. The comparison of the room closures for the correlation runs Z-11 and Z-15 with the actual convergence data is given in Figs. 2-5.

Following the successful development of the model for simulating the behavior of the Project Salt Vault experimental area and its correlation with actual deformation results, work was begun aimed at modifying and expanding the model to simulate a full-scale waste repository area over long time periods. Although these efforts are not complete, a preliminary version of the model is described in this report. The analytical and numerical aspects of the model are presented in Sects. 2 and 3; the results of a series of check-out procedures are summarized in Sect. 4. Finally, the remaining work necessary to make the semi-empirical numerical model applicable to actual repository design is outlined in Sect. 5.

Table 1. Parameter values for PSV mode correlation and basic case of the repository model

	Parameter name (in program)	PSV model correlation		Repository program - basic ^a
		Run Z-11	Run Z-15	
Elastic modulus of roof and floor rock (psi)	E	10 ⁶	10 ⁶	10 ⁶
Poisson's ratio of roof and floor	V	0.4	0.4	0.4
Initial ambient temperature at mining horizon (°K)	TEMPR	300	300	300
Mean thermal diffusivity in disposal horizon (ft ² /hr)	DIFF	0.1	0.1	0.1
Premining vertical stress (psi)	P	1000	1000	1000
Elastic modulus of seam (psi)	ES	10 ⁶	10 ⁶	10 ⁶
Coefficients in creep equation $\epsilon(t) = A t^b T^c$				
A	ALF	0.65 X 10 ⁻³⁶	0.65 X 10 ⁻³⁶	0.65 X 10 ⁻³⁶
b	BET	0.4	0.4	0.4
c	PWR	9.5	9.5	9.5
	GAM	3.0	3.0	3.0
Creep effective stress parameter	FRAC	0.4	0.3	0.25
Mean depth of burial of heat sources (ft)	DPQ	9.0	9.0	9.0
Seam thickness (ft)	THICK	14.0	14.0	14.0
Length of time step (days)	DT	25	25	1825
Half-width of small grid elements (ft)	H	2.5	2.5	125
Thermal stress coefficient	THSTR	1.0	0.5	--
Heat source data-arrays				
Initial "ON" (°C·ft ³ /hr); (psi/°C)	Q;EQ	118;55	118;85	--
40% power boost (°C·ft ³ /hr); (psi/°C)	Q;EQ	45;45	45;55	--
Power "OFF" (°C·ft ³ /hr); (psi/°C)	Q;EQ	-163;8.7	-163;10	--
Heat source data-pillar heaters				
Initial "ON" (°C·ft ³ /hr); (psi/°C)	Q;EQ	101;60	101;100	--
Power "OFF" (°C·ft ³ /hr); (psi/°C)	Q;EQ	-101;10	-101;15	--
Depth of mining horizon below surface (ft)	DEPTH	--	--	1000
Mining extraction ratio	EXTO	--	--	0.33
Limit of room closure (ft)	CLOMX	--	--	3.75
Width-to-height ratio of pillars	WHR	--	--	4.0
Heat source data				
Constant portion of heat (kW/acre)	QCON	--	--	65.0
Exponential decay portion of heat (kW/acre)	QEXP	--	--	65.0
Heat rate decay constant (year)	ACON	--	--	0.0277
Coefficient of thermal expansion (°C ⁻¹)	ALPHA	--	--	40 X 10 ⁻⁶

^aSee Sect. 4.

Fig. 1. Project Salt Vault experimental area as modeled for correlation.

Fig. 2. Comparison of model with measured closure at Station 106.

Fig. 3. Comparison of model with measured closure at Station 118.

Fig. 4. Comparison of model with measured closure at Station 138.

Fig. 5. Comparison of model with measured closure at Station 159.

2. GOVERNING EQUATIONS FOR NUMERICAL METHOD

2.1 Introduction

The general approach adopted for the repository analysis is essentially the same as that used to analyze the experimental area of Project Salt Vault, which is described elsewhere.^{1,2} In this approach, the rock mass is assumed to be isotropic and linearly elastic, and all nonlinear, inelastic effects are confined to the "seam," where deformations are related to stress, time, and temperature. The thickness of the seam is assumed to be negligible in relation to the depth and the lateral extent of the mined areas; and the mining horizon is viewed as a single plane surface, with relative movements between the two sides of the plane being used to specify the state of deformation and stress in the rock mass. Because the rock mass is assumed to behave linearly, superposition may be used and the repository problem is analyzed in terms of three interrelated phenomena: (1) elastic closure of the excavated areas with consequent elastic deformation of the rock mass; (2) time-, stress-, and temperature-dependent closure of the unmined portions of the seam; and (3) thermal stress and displacement changes throughout the rock mass, including the seam, where stress and temperature variations affect the creep behavior of the seam material. Analytical aspects of these three parts of the problem are treated in this section; their use in the development of a general computer model is covered in Sect. 3.

2.2 Elastic Closure for Excavations at Finite Depth

2.2.1 Definition of the problem

Consider a rock mass containing a thin seam lying parallel to the surface of the earth and at some depth H beneath it (Fig. 6). Suppose that the thickness of the seam is h , but that relative to the depth and the lateral extent of excavations in the seam h is sufficiently small to allow the seam to be viewed as a single plane surface. The "bottom" of the surface, $z = H_+$, represents the footwall, while the "top," $z = H_-$, represents the hanging wall.

Fig. 6. Coordinate axes for a near-surface, flat-lying seam.

Let u_x , u_y , and u_z be the x-, y-, and z-components of displacement, and let σ_{xx} , σ_{yy} , σ_{zz} , σ_{xz} , σ_{yz} , and σ_{xy} be the stress changes* at any point in the rock mass caused by excavations in the seam. The displacements will be continuous everywhere in the mass except across the plane of the seam $z = H$, where they will generally be discontinuous. Physically, displacement discontinuities at the seam can be interpreted as relative movements between the footwall and the hanging wall, and the seam can be visualized as a dislocation in an otherwise continuous mass. The normal component of relative movement is called the closure and is defined as $S_z = u_z(x, y, H_+) - u_z(x, y, H_-)$, while the transverse movements are called the ride components and are defined as $S_x = u_x(x, y, H_+) - u_x(x, y, H_-)$ and $S_y = u_y(x, y, H_+) - u_y(x, y, H_-)$.

It may be shown that the induced stresses and displacements everywhere in the mass can be expressed as linear combinations of the closure and ride components at the seam. When the x-, y-, and z-axes are principal directions of the preexisting (or "primitive") stress field, and when H is large, the seam is a plane of symmetry and both the primitive and induced shear tractions at the seam are zero. In this case, it follows that the ride components S_x and S_y are zero, and that the displacements and stresses in the mass are specified by the closure distribution, $S_z(x, y)$. When the seam is close to the surface, it cannot be a plane of symmetry because its two sides will deform differently. Therefore, the ride components should, strictly speaking, be taken into account for the finite depth case. However, for a flat-lying seam, the ride components are second-order effects whose influence on the closure distribution decreases rapidly with depth; in most instances, it is possible to ignore them without introducing appreciable error. For example, Crouch³ has shown that, when the ride is neglected, the closure at the center of a long, slit-like excavation of width "a" is in error by only about 2% when $H/a = 0.5$. In the case of a radioactive waste repository, the seam is

*Compressive stresses are assumed to be positive in this report.

only partially extracted over a large area. If the excavations are contained within a region 5000 ft long x 10,000 ft wide x 2000 ft deep, H/a is 0.4 and the error caused by neglecting the ride components should be only a few percent.

With the assumption that the ride components S_x and S_y are zero, the boundary conditions for the problem are as follows:

- (1) All induced stresses and displacements must approach zero as x , y , and z approach infinity.
- (2) The induced tractions σ_{zz} , σ_{xz} , and σ_{yz} at the surface $z = 0$ must be zero.
- (3) In mined areas (on $z = H$) where the roof and floor do not make contact, the resultant force in the z -direction must be zero. That is, the induced stress σ_{zz} must balance the primitive stress P_{zz} :

$$\sigma_{zz} = -P_{zz}. \quad (1)$$

If, on the other hand, the roof and floor come into contact (in the present case due to the presence of crushed salt backfill), Eq. (1) must be modified to account for the amount of load taken up by the backfill. This modification is described in detail in Sect. 3.2.

- (4) Unmined areas (on $z = H$) will be subjected to increasing stresses as excavation proceeds, the effect of which will be to compress the material in the seam. Thus, the boundary condition for the unmined portions of the seam can be represented approximately as a general functional relationship between stress and closure, or

$$\sigma_{zz} = f(S_z), \quad (2)$$

in which function f has to be specified for particular locations in the seam and for different seam materials.

2.2.2 Mathematical analysis and numerical solution

The problem specified by the foregoing boundary conditions can be solved by superposition, using the classical method of images, in a manner similar to that described by Crouch³ for the two-dimensional case. This is accomplished by the following steps:

- (1) Determine the elastic solution for a normal displacement discontinuity, or dislocation, over a small square area on $z = H$ in an infinite mass, and superpose a number of such discontinuities to represent the seam in the area of interest.
- (2) Add "image" dislocations at $z = -H$ to make the plane $z = 0$ (the surface of the earth as in Fig. 1) free from shear stress.
- (3) Superpose a continuous distribution of normal stress on the plane $z = 0$ such that the surface of the semi-infinite mass $z \geq 0$ is traction-free.

Infinite mass. The displacements in an infinite, homogeneous, isotropic, linearly elastic mass containing a shear-free plane $z = H$ can be expressed in terms of a single harmonic function $\bar{\phi}$ as:

$$\bar{u}_x = - (1 - 2\nu) \frac{\partial \bar{\phi}}{\partial x} - (z - H) \frac{\partial^2 \bar{\phi}}{\partial x \partial z}, \quad (3)$$

$$\bar{u}_y = - (1 - 2\nu) \frac{\partial \bar{\phi}}{\partial y} - (z - H) \frac{\partial^2 \bar{\phi}}{\partial y \partial z},$$

$$\bar{u}_z = 2(1 - \nu) \frac{\partial \bar{\phi}}{\partial z} - (z - H) \frac{\partial^2 \bar{\phi}}{\partial z^2},$$

where ν is Poisson's ratio. The stresses corresponding to these displacements are:

$$\begin{aligned} \bar{\sigma}_{xx} &= 2G \left[\frac{\partial^2 \bar{\phi}}{\partial z^2} + (1 - 2\nu) \frac{\partial^2 \bar{\phi}}{\partial y^2} - (z - H) \frac{\partial^3 \bar{\phi}}{\partial x^2 \partial z} \right], \\ \bar{\sigma}_{yy} &= 2G \left[\frac{\partial^2 \bar{\phi}}{\partial z^2} + (1 - 2\nu) \frac{\partial^2 \bar{\phi}}{\partial x^2} - (z - H) \frac{\partial^3 \bar{\phi}}{\partial y^2 \partial z} \right], \end{aligned} \quad (4)$$

$$\bar{\sigma}_{zz} = 2G \left[\frac{\partial^2 \bar{\phi}}{\partial z^2} - (z - H) \frac{\partial^3 \bar{\phi}}{\partial z^3} \right],$$

$$\bar{\sigma}_{xz} = -2G(z - H) \frac{\partial^3 \bar{\phi}}{\partial x \partial z^2},$$

(4)

$$\bar{\sigma}_{yz} = -2G(z - H) \frac{\partial^3 \bar{\phi}}{\partial y \partial z^2},$$

$$\bar{\sigma}_{xy} = -2G \left[(1 - 2\nu) \frac{\partial^2 \bar{\phi}}{\partial x \partial y} + (z - H) \frac{\partial^3 \bar{\phi}}{\partial x \partial y \partial z} \right],$$

where G is the shear modulus. Because the shear stresses $\bar{\sigma}_{xz}$ and $\bar{\sigma}_{yz}$ vanish on $z = H$ (provided $\frac{\partial^3 \bar{\phi}}{\partial x^2 \partial z}$ and $\frac{\partial^3 \bar{\phi}}{\partial y^2 \partial z}$ are finite), specifying the function $\bar{\phi}$ is equivalent to specifying either $\bar{\sigma}_{zz}$ or $\bar{u}_z$ on $z = H$.

The harmonic function $\bar{\phi} = W/\bar{R}$, where W is a constant and $\bar{R} = [(x - \xi)^2 + (y - \eta)^2 + (z - H)^2]^{\frac{1}{2}}$, has the following properties on $z = H$:

$$\frac{1}{A} \iint_A S_z(x, y) dx dy = 0, \quad (\xi, \eta) \text{ not in } A$$

(5)

$$\frac{1}{A} \iint_A S_z(x, y) dx dy = \frac{8\pi W(1 - \nu)}{A}, \quad (\xi, \eta) \text{ in } A.$$

In other words, for this value of $\bar{\phi}$ the average closure over any area A containing the point $x = \xi$, $y = \eta$ is constant; otherwise, it is zero. Thus, $\bar{\phi} = W/\bar{R}$ corresponds to an integrated average normal displacement discontinuity, or dislocation, over the area A on $z = H$. This dislocation produces continuous stresses and displacements elsewhere in the mass, and it follows that any number of such linearly independent, constant displacement discontinuities can be distributed along $z = H$ to build up complicated

dislocation patterns. (The discontinuities can be distributed anywhere in the mass,⁴ but for the purposes of this discussion we will assume that they all lie in $z = H$. For arbitrary distributions in three-dimensional space, it is not generally permissible to ignore the ride components.)

The numerical procedure for the infinite mass problem is developed from the above results as follows:⁵ Divide the region of interest in the plane $z = H$ into a number of squares, each of side $2h_0$, and number the squares such that a typical one, say the $ijth$ one, is ith along the y -axis and jth along the x -axis. Let $(S_z)_{ij}$ and $(\bar{\sigma}_{zz})_{ij}$ be the (integrated) average values of closure and normal traction over the $ijth$ square, and consider the case for which the closure is zero everywhere except at the $klth$ square. The solution to this problem is given by the harmonic function

$$\bar{\phi} = h_0^2 (S_z)_{kl} / 2\pi(1 - \nu)\bar{R}, \quad (6)$$

where $\bar{R} = [(x - \xi)^2 + (y - \eta)^2 + (z - H)^2]^{\frac{1}{2}}$ as before, but (ξ, η) now represents the midpoint of the $klth$ square. For this case, $(\bar{\sigma}_{zz})_{ij}$ is found to be:

$$(\bar{\sigma}_{zz})_{ij} = a_{ijkz} (S_z)_{kl}, \quad (7)$$

where, if $m = i - k$ and $n = j - l$,

$$\begin{aligned} a_{ijkz} = & f(2m + 1, 2n - 1) + f(2m - 1, 2n + 1) \\ & - f(2m + 1, 2n + 1) - f(2m - 1, 2n - 1) \end{aligned} \quad (8)$$

with

$$f(m, n) = \frac{G}{4\pi(1 - \nu)h_0} (m^2 + n^2)^{\frac{1}{2}} / mn. \quad (9)$$

If closure occurs at all of the squares, then the stress at the ij^{th} square will be the sum of terms such as those in Eq. (7):

$$(\bar{\sigma}_{zz})_{ij} = \sum_{\text{all } k} \sum_{\text{all } l} a_{ijk l} (S_z)_{kl}. \quad (10)$$

Semi-infinite mass. The displacements and stresses in an infinite mass due to a normal displacement discontinuity that is the "image" (i.e., reflected in $z = 0$) of $(S_z)_{kl}$ are given by:

$$\begin{aligned} \bar{u}_x &= - (1 - 2\nu) \frac{\partial \bar{\Phi}}{\partial x} - (z + H) \frac{\partial^2 \bar{\Phi}}{\partial x \partial z} \\ \bar{u}_y &= - (1 - 2\nu) \frac{\partial \bar{\Phi}}{\partial y} - (z + H) \frac{\partial^2 \bar{\Phi}}{\partial y \partial z} \\ \bar{u}_z &= 2(1 - \nu) \frac{\partial \bar{\Phi}}{\partial z} - (z + H) \frac{\partial^2 \bar{\Phi}}{\partial z^2} \end{aligned} \quad (11)$$

and

$$\begin{aligned} \bar{\sigma}_{xx} &= 2G \left[\frac{\partial^2 \bar{\Phi}}{\partial z^2} + (1 - 2\nu) \frac{\partial^2 \bar{\Phi}}{\partial y^2} - (z + H) \frac{\partial^3 \bar{\Phi}}{\partial x^2 \partial z} \right] \\ \bar{\sigma}_{yy} &= 2G \left[\frac{\partial^2 \bar{\Phi}}{\partial z^2} + (1 - 2\nu) \frac{\partial^2 \bar{\Phi}}{\partial x^2} - (z + H) \frac{\partial^3 \bar{\Phi}}{\partial y^2 \partial z} \right] \\ \bar{\sigma}_{zz} &= 2G \left[\frac{\partial^2 \bar{\Phi}}{\partial z^2} - (z + H) \frac{\partial^3 \bar{\Phi}}{\partial z^3} \right] \\ \bar{\sigma}_{xz} &= -2G (z + H) \frac{\partial^3 \bar{\Phi}}{\partial x \partial z^2} \\ \bar{\sigma}_{yz} &= -2G (z + H) \frac{\partial^3 \bar{\Phi}}{\partial y \partial z^2} \\ \bar{\sigma}_{xy} &= -2G \left[(1 - 2\nu) \frac{\partial^2 \bar{\Phi}}{\partial x \partial y} + (z + H) \frac{\partial^3 \bar{\Phi}}{\partial x \partial y \partial z} \right]. \end{aligned}$$

The harmonic function for the image discontinuity is:

$$\bar{\bar{\phi}} = h_0^2 (S_z)_{kz} / 2\pi(1 - \nu) \bar{R}, \quad (13)$$

where $\bar{R} = [(x - \xi)^2 + (y - \eta)^2 + (z + H)^2]^{\frac{1}{2}}$ and (ξ, η) is the midpoint of the kz th square on the image plane $z = -H$. Function $\bar{\bar{\phi}}$ produces continuous displacements and stresses everywhere in the infinite mass except at the kz th square on $z = -H$, where the normal displacement $\bar{u}_z$ is discontinuous. In particular, the image dislocation does not contribute directly to the closure at the seam $z = H$. The average normal traction $(\bar{\bar{\sigma}}_{zz})_{ij}$ at the ij th square of the seam due to a number of image discontinuities on $z = -H$ could be computed at this stage, but it is convenient to defer this computation for the present.

It easily follows from Eqs. (4), (6), (12), and (13) that on the plane $z = 0$ the shear stresses $\bar{\sigma}_{xz}$ and $\bar{\bar{\sigma}}_{xz}$, $\bar{\sigma}_{yz}$ and $\bar{\bar{\sigma}}_{yz}$ are equal but of opposite sign, while the normal stresses $\bar{\sigma}_{zz}$ and $\bar{\bar{\sigma}}_{zz}$ are equal. Thus, superposition of the solutions for the seam dislocation and its image leaves the plane $z = 0$ free from shear stress but subject to a resultant normal traction of $2\bar{\sigma}_{zz}$ or $2\bar{\bar{\sigma}}_{zz}$. Therefore, the plane $z = 0$ can be cleared of tractions by superposing the single- and double-bar solutions and the solution of the following problem for the half-plane $z \geq 0$:

$$\sigma_{zz}^* = -2\bar{\bar{\sigma}}_{zz}, \quad \sigma_{xz}^* = \sigma_{yz}^* = 0 \text{ on } z = 0. \quad (14)$$

This problem is posed in terms of $\bar{\bar{\sigma}}_{zz}$ because function $\bar{\bar{\phi}}$ does not introduce additional displacement discontinuities in $z \geq 0$.

The solution of problem (14) is found by using Eqs. (3) and (4), modified such that the plane $z = 0$ (rather than $z = H$) is free from shear stress:

$$\begin{aligned} u_x^* &= - (1 - 2\nu) \frac{\partial \phi^*}{\partial x} - z \frac{\partial^2 \phi^*}{\partial x \partial z} \\ u_y^* &= - (1 - 2\nu) \frac{\partial \phi^*}{\partial y} - z \frac{\partial^2 \phi^*}{\partial y \partial z} \\ u_z^* &= 2(1 - \nu) \frac{\partial \phi^*}{\partial z} - z \frac{\partial^2 \phi^*}{\partial z^2} \end{aligned} \quad (15)$$

$$\begin{aligned}
\sigma_{xx}^* &= 2G \left[\frac{\partial^2 \phi^*}{\partial z^2} + (1 - 2\nu) \frac{\partial^2 \phi^*}{\partial y^2} - z \frac{\partial^3 \phi^*}{\partial x^2 \partial z} \right] \\
\sigma_{yy}^* &= 2G \left[\frac{\partial^2 \phi^*}{\partial z^2} + (1 - 2\nu) \frac{\partial^2 \phi^*}{\partial x^2} - z \frac{\partial^3 \phi^*}{\partial y^2 \partial z} \right] \\
\sigma_{zz}^* &= 2G \left[\frac{\partial^2 \phi^*}{\partial z^2} - z \frac{\partial^3 \phi^*}{\partial z^3} \right] \\
\sigma_{xz}^* &= -2G z \frac{\partial^3 \phi^*}{\partial x \partial z^2} \\
\sigma_{yz}^* &= -2G z \frac{\partial^3 \phi^*}{\partial y \partial z^2} \\
\sigma_{xy}^* &= -2G \left[(1 - 2\nu) \frac{\partial^2 \phi^*}{\partial x \partial y} + z \frac{\partial^3 \phi^*}{\partial x \partial y \partial z} \right].
\end{aligned} \tag{16}$$

From Eqs. (12), (14), and (16) the boundary value of ϕ^* is determined by

$$\frac{\partial^2 \phi^*}{\partial z^2} = -2 \frac{\partial^2 \bar{\bar{\phi}}}{\partial z^2} + 2H \frac{\partial^3 \bar{\bar{\phi}}}{\partial z^3} \quad \text{on } z = 0. \tag{17}$$

The right-hand side of this expression defines a function that is harmonic for all values of z , and it follows from the uniqueness theorem for the Dirichlet problem that this relation holds everywhere in $z \geq 0$, not only at the boundary.⁶

Thus, ϕ^* is given by

$$\phi^* = -2\bar{\bar{\phi}} + 2H \frac{\partial \bar{\bar{\phi}}}{\partial z}, \tag{18}$$

where the integration variables are taken as zero to ensure that all displacements and stresses vanish at infinity. Finally, Eq. (18) allows the "asterisk" and "double bar" displacements and stresses to be written in terms of the harmonic function $\bar{\bar{\phi}}$ for the image discontinuity (complete expressions are given in Appendix A). In particular,

$$\bar{\bar{\sigma}}_{zz} + \sigma_{zz}^* = -2G \left[\frac{\partial^2 \bar{\bar{\phi}}}{\partial z^2} - (z + H) \frac{\partial^3 \bar{\bar{\phi}}}{\partial z^3} + 2Hz \frac{\partial^4 \bar{\bar{\phi}}}{\partial z^4} \right],$$

which, at the seam level $z = H$, becomes

$$\bar{\sigma}_{zz} + \sigma_{zz}^* = -2G \left[\frac{\partial^2 \bar{\phi}}{\partial z^2} - 2H \frac{\partial^3 \bar{\phi}}{\partial z^3} + 2H^2 \frac{\partial^4 \bar{\phi}}{\partial z^4} \right] \text{ on } z = H. \quad (19)$$

The average value of $\bar{\sigma}_{zz} + \sigma_{zz}^*$ over the ij th square on $z = H$ is:

$$(\bar{\sigma}_{zz} + \sigma_{zz}^*)_{ij} = \sum_{\text{all } k} \sum_{\text{all } l} a'_{ijkl} (S_z)_{kl}, \quad (20)$$

where

$$\begin{aligned} a'_{ijkl} = & g(2m + 1, 2n - 1) + g(2m - 1, 2n + 1) \\ & - g(2m + 1, 2n + 1) - g(2m - 1, 2n - 1) \end{aligned} \quad (21)$$

In Eq. (21), for $m = i - k$, $n = j - k$, and $p = 2H/h$,

$$\begin{aligned} g(m, n) = & \frac{-G}{4\pi(1 - \nu)h} \frac{mn}{(m^2 + n^2 + p^2)^{\frac{1}{2}}} \left\{ \left[1 + \frac{1}{2} p^2 \frac{(m^2 + n^2 + 4p^2)}{(m^2 + n^2 + p^2)^2} \right] \right. \\ & \cdot \left[\frac{1}{m^2 + p^2} + \frac{1}{n^2 + p^2} \right] - p^2 \left[2 - \frac{(m^2 + n^2 - p^2)}{(m^2 + n^2 + p^2)} \right] \\ & \cdot \left. \left[\frac{1}{(m^2 + p^2)^2} + \frac{1}{(n^2 + p^2)^2} \right] - 4p^4 \left[\frac{1}{(m^2 + p^2)^3} + \frac{1}{(n^2 + p^2)^3} \right] \right\}. \end{aligned} \quad (22)$$

Equations (10) and (20) allow the total induced stress at the ij th square of the seam to be expressed in terms of the closure distribution as:

$$\begin{aligned} (\sigma_{zz})_{ij} = & (\bar{\sigma}_{zz})_{ij} + (\bar{\sigma}_{zz} + \sigma_{zz}^*)_{ij} \\ = & \sum_{\text{all } k} \sum_{\text{all } l} (a_{ijkl} + a'_{ijkl}) (S_z)_{kl}. \end{aligned} \quad (23)$$

In general, the closure distribution is unknown and must be found from Eq. (23) by ensuring that suitable boundary conditions — expressed either in terms of known stresses or by some prescribed relationship between

stress and closure — are satisfied. Excluding for the moment the possibility that "complete closure" occurs (with or without backfill), the ij th square will be either mined or unmined. If it is mined, boundary condition (1) yields:

$$(P_{zz})_{ij} = - \sum_{\text{all } k} \sum_{\text{all } z} (a_{ijkz} + a'_{ijkz})(S_z)_{kz}; \quad (24)$$

if it is unmined, boundary condition (2) yields:

$$f[(S_z)_{ij}] = \sum_{\text{all } k} \sum_{\text{all } z} (a_{ijkz} + a'_{ijkz})(S_z)_{kz}. \quad (25)$$

Equations (24) and (25) can be solved for $(S_z)_{ij}$ by iteration.⁵

2.3 Inelastic Deformation of the Seam Material

It is found from laboratory tests that the strain ϵ at time t in a model salt pillar under the conditions of constant temperature T_0 and constant uniaxial stress p_0 is given by a relation of the form⁷

$$\epsilon(t) = At^a T_0^b p_0^c, \quad (26)$$

where A , a , b , and c are constants. If it is assumed for the field-scale problem that all inelastic deformation is confined to the seam material, and that this material behaves qualitatively in the same fashion as a laboratory model pillar, then the simple one-dimensional constitutive equation given above can be adopted to describe approximately the behavior of a portion of a salt seam in the vicinity of an excavation. The following discussion is concerned with generalizing Eq. (26) to accommodate the time-varying stresses and temperatures that occur in the radioactive waste repository problem. The objective of this work is to develop a general procedure for modeling time-stress-temperature-dependent deformation of a salt seam; this procedure is to be used together with the numerical model outlined in the previous section, and will serve to specify function f in Eq. (25).

It should be noted at the outset that, in general, the $ijth$ element of the seam will not be subjected to a purely uniaxial stress; thus, it will be necessary to assume that Eq. (26) holds for "triaxial" stress conditions if p_0 is interpreted as a (principal) stress difference. In the field-scale problem, the stress difference varies from a maximum (nearly uniaxial loading) adjacent to an excavation to zero (hydrostatic loading) in the undisturbed portions of the salt seam. In other words, different portions of the seam will behave differently, depending upon their distance from an excavated area. Starfield and McClain² introduced the concept of a "creep effective stress" to describe this behavior; they defined this type of stress as:

$$\sigma_0 = \sigma' e^{-\lambda(d-1)}, \quad (27)$$

where σ' is the total stress acting across the seam at an element (i.e., the sum of the induced and primitive stresses), λ is a parameter, and d is the average distance (number of elements) from the nearest excavated area. The basic equation assumed to describe the deformation of a general element of the seam under the conditions of constant temperature T_0 and constant creep effective stress σ_0 is then found by replacing p_0 in Eq. (26) by σ_0 :

$$\epsilon(t) = At^a T_0^b \sigma_0^c. \quad (28)$$

This relation is generalized to include time-varying stress and temperature conditions by a procedure originally developed by Starfield,¹ which is reproduced (with minor revisions) below for completeness.

Suppose that the temperature is constant but that the creep effective stress is a function of time, $\sigma(t)$. Then the stress will be $\sigma(\tau)$ at time τ ; and if a small change in stress $d\sigma(\tau)$ occurs at that time, the change in strain $d\epsilon(t)$ at any subsequent time t will be, by analogy with Eq. (28),

$$d\epsilon(t) = cAT_0^b (t - \tau)^a \sigma(\tau)^{c-1} d\sigma(\tau). \quad (29)$$

If this expression is integrated for all stress increments between times 0 (when $\epsilon = \text{zero}$) and t , then the total strain is:

$$\epsilon(t) = cAT_0^b \int_0^t (t - \tau)^a \sigma(\tau)^{c-1} \frac{\partial \sigma(\tau)}{\partial \tau} d\tau, \quad (30)$$

which reduces to Eq. (28) if $\sigma(\tau) = \sigma_0$ for $\tau > 0$.

The effect of temperature changes is included in Eq. (30) by using an equivalence between time and temperature.⁸ It can be seen from Eq. (28) that the strain at time t_1 and temperature T_1 is the same as that at time t_0 and temperature T_0 if $t_0 = (T_1/T_0)^{b/a} t_1$; this implies that a change in temperature is equivalent to a change in time scale. Such an observation allows us to write Eq. (30) as follows for a time-varying temperature $T(t)$:

$$\epsilon(t) = cA \int_0^t \left[\int_0^t T(u)^{b/a} du - \int_0^\tau T(u)^{b/a} du \right]^a \sigma(\tau)^{c-1} \frac{\partial \sigma(\tau)}{\partial \tau} d\tau$$

or

$$\epsilon(t) = cA \int_0^t \left[\int_\tau^t T(u)^{b/a} du \right]^a \sigma(\tau)^{c-1} \frac{\partial \sigma(\tau)}{\partial \tau} d\tau. \quad (31)$$

This equation reduces to Eq. (28) if both T and σ are constant, that is, if $T = 0$, $\sigma = 0$ at $t = 0$ and $T = T_0$, $\sigma = \sigma_0$ for $t > 0$. Equation (31) thus expresses, in a general form, the relationship between the creep effective stress and the strain for an element of the seam at any time and under any temperature conditions.

For computational purposes, the integral with respect to τ in Eq. (31) is reduced to a sum. Thus, the strain ϵ_N after N time steps of size Δt (i.e., at time $t = N\Delta t$) is:

$$\epsilon_N = cA \sum_{n=1}^N \int_{(n-1)\Delta t}^{n\Delta t} \left[\int_\tau^{N\Delta t} T(u)^{b/a} du \right]^a \sigma(\tau)^{c-1} \frac{\partial \sigma}{\partial \tau} d\tau \quad (32)$$

or

$$\epsilon_N = cA \sum_{n=1}^N \int_{(n-1)\Delta t}^{n\Delta t} I(\tau) \sigma(\tau)^{c-1} \frac{\partial \sigma}{\partial \tau} d\tau. \quad (33)$$

Suppose now that Δt is small so that $I(\tau)$ can be taken to be constant over each of the intervals. Then, as an approximation,*

$$\epsilon_N = cA \sum_{n=1}^N I[(n-1)\Delta t] \int_{(n-1)\Delta t}^{n\Delta t} \sigma(\tau)^{c-1} \frac{\partial \sigma}{\partial \tau} d\tau \quad (34)$$

$$= A \sum_{n=1}^N I[(n-1)\Delta t] \left\{ \sigma(n\Delta t)^c - \sigma[(n-1)\Delta t]^c \right\}$$

$$= A \sum_{n=1}^N \left[\int_{(n-1)\Delta t}^{n\Delta t} T(u)^{b/a} du \right]^a \left\{ \sigma(n\Delta t)^c - \sigma[(n-1)\Delta t]^c \right\}.$$

Writing σ_n for $\sigma(n\Delta t)$ and $\psi_{N-(n-1)}$ or ψ_{N-n+1} for

$$\left[\int_{(n-1)\Delta t}^{n\Delta t} T(u)^{b/a} du \right]^a, \text{ Eq. (34) becomes:}$$

$$\epsilon_N = A \sum_{n=1}^N \psi_{N-n+1} (\sigma_n^c - \sigma_{n-1}^c).$$

*The analysis presented in ref. 1 takes the contribution of $I(\tau)$ over the n th interval to be $\{I(n\Delta t) + I[(n-1)\Delta t]\}/2$. It can be shown that this procedure leads to a final result that is dependent upon the absolute size of the time step, while the formulation given above does not.

This equation can be written as

$$\epsilon_N = C_0 \sigma_N^C + B_N, \quad (35)$$

where

$$C_0 = A\psi_1 \quad (36)$$

$$B_N = A \sum_{n=1}^{N-1} (\psi_{N-n+1} - \psi_{N-n}) \sigma_n^C.$$

Equation (35) gives an instantaneous relationship between strain and the creep effective stress for a portion of a salt seam at the N th time step; this relationship, by virtue of Eq. (36), includes temperature and stress variations at all previous time steps.

2.4 Thermal Effects; Heat Sources at Finite Depth

2.4.1 Introduction

A quantity of radioactive waste generates heat as it decays. The effect of this heat in the repository will be to raise the temperature of the rock mass and to induce thermal stresses and displacements.

The following discussion is concerned with calculating the thermal effects due to an arbitrary distribution of time-varying heat sources along a single plane (just below "seam level") in a semi-infinite rock mass. The coupling of these effects with those already described for the elastic deformation of the rock mass (Sect. 2.2) and inelastic deformation of the seam material (Sect. 2.3) to model a full-scale radioactive waste repository is considered in Sect. 3.

2.4.2 Instantaneous heat source in an infinite body

The solution for an arbitrary distribution of time-varying heat sources along a single plane surface is developed by superposition from the solution for a single source with a given heat generation rate. This

basic solution, in turn, is found by integration from the well-known solution for a single, instantaneous heat source in an infinite, linearly elastic body. An instantaneous heat source is one that liberates a finite quantity of heat in a single "pulse." The strength Q of the source is the temperature to which this quantity of heat would raise a unit volume of material with fixed thermal properties.

The temperature field produced by an instantaneous heat source at point $(x,y,z) = (0,0,0)$ in an infinite body is:⁹

$$T(R,t) = \frac{Q}{(\pi\beta)^{3/2}} \exp\left(\frac{-R^2}{\beta}\right), \quad (37)$$

where $\beta = 4\kappa t$, in which κ is the thermal diffusivity, and R is the distance from the source to an arbitrary point in the body, $R^2 = x^2 + y^2 + z^2 = r^2 + z^2$. This temperature field represents a change, which, of course, must be added to the initial value T_0 to find the total temperature. The displacements and stresses (positive for compression) due to the point source are found from the thermoelastic potential⁹

$$\Phi(R,t) = \frac{mQ}{4\pi R} \operatorname{erf}\left(\frac{R}{\sqrt{\beta}}\right), \quad (38)$$

where $\operatorname{erf}(z) = \frac{2}{\sqrt{\pi}} \int_0^z e^{-\eta^2} d\eta$ is the error function and $m = \alpha(1 + \nu)/$

$(1 - \nu)$, in which α is the coefficient of thermal expansion of the body. The displacements and stresses in the body are given by the formulas⁹

$$u_i = \Phi_{,i} \quad (39)$$

$$\sigma_{ij} = 2G \left[\Phi_{,ij} - \delta_{ij} \Phi_{,kk} \right],$$

where, in the usual notation, for $i = x, y$, or z a comma indicates differentiation with respect to the index or indices following it, repeated indices imply summation, and δ_{ij} is the Kronecker delta symbol ($\delta_{ij} = 1$ for $i = j$; $\delta_{ij} = 0$ for $i \neq j$). It can easily be verified that $\Phi(R,t)$ satisfies the

Poisson equation

$$\nabla^2 \Phi = \Phi_{,kk} = -mT, \quad (40)$$

where $T = T(R, t)$ is the temperature field given by Eq. (37).

For numerical simulation of the waste disposal problem, it is necessary to obtain the solution for a time-varying heat source in the semi-infinite body $z \geq 0$. The following two sections are concerned with developing these results. The half-space solution for an instantaneous heat source is obtained in the next section, after which the results are generalized to include sources with both constant and exponentially decaying heat generation rates. The half-space solution is found by the method of images (cf. Sect. 2.2.2), while the effects of time-dependent heat sources $Q(\tau)$ are computed effectively by replacing Eqs. (37) and (38) with:

$$T(R, t) = \frac{1}{(4\pi\kappa)^{3/2}} \int_0^t Q(\tau) (t - \tau)^{-3/2} \exp\left[\frac{R^2}{4\kappa(t - \tau)}\right] d\tau, \quad (41)$$

$$\Phi(R, t) = \frac{m}{4\pi R} \int_0^t Q(\tau) \operatorname{erf}\left[\frac{R}{\sqrt{4\kappa(t - \tau)}}\right] d\tau.$$

2.4.3 Instantaneous heat source in a semi-infinite body

The solution to the problem of an instantaneous heat source at the point (ϵ, η, H) in the semi-infinite region $z \geq 0$ is given by Nowacki.⁹ The boundary conditions for the problem are:

$$\sigma_{zz} = 0, \sigma_{rz} = 0, T = 0 \quad \text{on } z = 0. \quad (42)$$

The first and last of these conditions are satisfied by placing a positive instantaneous heat source at the point (ϵ, η, H) in the infinite mass and a negative source of the same type at $(\epsilon, \eta, -H)$. The temperature field and the thermoelastic potential for this system of sources, then, are given by

[cf. Eqs. (37) and (38)]:

$$T(r, z, t) = \frac{Q}{(\pi\beta)^{3/2}} \left[\exp\left(\frac{-\bar{R}^2}{\beta}\right) - \exp\left(\frac{-\bar{\bar{R}}^2}{\beta}\right) \right], \quad (43)$$

$$\Phi(r, z, t) = \frac{Qm}{4\pi} \left[\frac{1}{R_1} \operatorname{erf}\left(\frac{\bar{R}}{\sqrt{\beta}}\right) - \frac{1}{R_2} \operatorname{erf}\left(\frac{\bar{\bar{R}}}{\sqrt{\beta}}\right) \right], \quad (44)$$

where $\bar{R} = [(x - \epsilon)^2 + (y - n)^2 + (z - H)^2]^{1/2} = [r^2 + (z - H)^2]^{1/2}$ and $\bar{\bar{R}} = [r^2 + (z + H)^2]^{1/2}$. The displacements and stresses in $z \geq 0$ are computed directly from Eqs. (39) and (44); complete expressions are given in Appendix B. The traction components on planes $z = \text{constant}$ are of particular interest for present purposes. Using a notation similar to that introduced in Sect. 2.2.2, these are:⁹

$$\begin{aligned} \bar{\sigma}_{zz} + \bar{\bar{\sigma}}_{zz} = & \frac{QmG}{2\pi\bar{R}^3} \left[\left(2 - \frac{3r^2}{\bar{R}^2} \right) \operatorname{erf}\left(\frac{\bar{R}}{\sqrt{\beta}}\right) \right. \\ & - \frac{2\bar{R}}{\sqrt{\pi\beta}} \exp\left(\frac{-\bar{R}^2}{\beta}\right) \left\{ 2 - \frac{3r^2}{\bar{R}^2} \left(1 + \frac{2\bar{R}^2}{3\beta} \right) \right\} \Bigg] \\ & - \frac{QmG}{2\pi\bar{\bar{R}}^3} \left[\left(2 - \frac{3r^2}{\bar{\bar{R}}^2} \right) \operatorname{erf}\left(\frac{\bar{\bar{R}}}{\sqrt{\beta}}\right) \right. \\ & \left. - \frac{2\bar{\bar{R}}}{\sqrt{\pi\beta}} \exp\left(\frac{-\bar{\bar{R}}^2}{\beta}\right) \left\{ 2 - \frac{3r^2}{\bar{\bar{R}}^2} \left(1 + \frac{2\bar{\bar{R}}^2}{3\beta} \right) \right\} \right], \end{aligned} \quad (45)$$

$$\begin{aligned}
\bar{\sigma}_{rz} + \bar{\bar{\sigma}}_{rz} = & \frac{3QmGr(z-H)}{2\pi\bar{R}^5} \left[\operatorname{erf}\left(\frac{\bar{R}}{\sqrt{\beta}}\right) \right. \\
& \left. - \frac{2\bar{R}}{\sqrt{\pi\beta}} \left(1 + \frac{2\bar{R}^2}{3\beta}\right) \exp\left(\frac{-\bar{R}^2}{\beta}\right) \right] \\
& - \frac{3QmGr(z+H)}{2\pi\bar{R}^5} \left[\operatorname{erf}\left(\frac{\bar{R}}{\sqrt{\beta}}\right) \right. \\
& \left. - \frac{2\bar{R}}{\sqrt{\pi\beta}} \left(1 + \frac{2\bar{R}^2}{3\beta}\right) \exp\left(\frac{-\bar{R}^2}{\beta}\right) \right].
\end{aligned} \tag{46}$$

Shearing stress components in Cartesian coordinates are computed from Eq. (46) by the relations

$$\begin{aligned}
\bar{\sigma}_{xz} + \bar{\bar{\sigma}}_{xz} &= \frac{(x-\xi)}{r} (\bar{\sigma}_{rz} + \bar{\bar{\sigma}}_{rz}) \\
&= \cos \theta (\bar{\sigma}_{rz} + \bar{\bar{\sigma}}_{rz}) \\
\bar{\sigma}_{yz} + \bar{\bar{\sigma}}_{yz} &= \frac{(y-\eta)}{r} (\bar{\sigma}_{rz} + \bar{\bar{\sigma}}_{rz}) \\
&= \sin \theta (\bar{\sigma}_{rz} + \bar{\bar{\sigma}}_{rz}).
\end{aligned} \tag{47}$$

It may be seen from Eq. (45) that $\bar{\sigma}_{zz} + \bar{\bar{\sigma}}_{zz} \equiv 0$ on $z = 0$, as asserted earlier. The shear stresses, on the other hand, do not vanish on the surface of the half-space and, similar to Sect. 2.2.2, must be removed by superposing the solution to the following boundary value problem for the half-space $z \geq 0$:

$$\sigma_{rz}^* = -(\bar{\sigma}_{rz} + \bar{\bar{\sigma}}_{rz}), \quad \sigma_{zz}^* = 0 \quad \text{on } z = 0. \tag{48}$$

Nowacki⁹ gives the solution of problem (48) obtained by integral transform methods, in the form of improper integrals involving Bessel functions. This solution is not convenient for computational purposes

and will not be presented here. An alternative form of the solution has not been found, owing to the essential difficulty that the thermoelastic potential $\Phi(r,z,t)$ is not harmonic. [If Φ were harmonic, problem (48) could be solved easily by methods similar to those used in Sect. 2.2.2.]

It will be assumed for the purposes of the analysis in this report that the surface components of shearing stress can be removed by applying, in pointwise fashion, Boussinesq's solution for concentrated shear forces on the surface of a half-space. The magnitudes and directions of the forces simply have to be chosen to negate, at each point of the surface and at each time of the analysis, the values of $\bar{\sigma}_{xz} + \bar{\bar{\sigma}}_{xz}$ and $\bar{\sigma}_{yz} + \bar{\bar{\sigma}}_{yz}$. The stress σ_{zz}^* at $z = H$ is of particular interest here; it is given by

$$\sigma_{zz}^* = \frac{3H^2}{2\pi[(x - \xi)^2 + (y - \eta)^2 + H^2]^{5/2}} \left[(x - \xi)T_x + (y - \eta)T_y \right]. \quad (49)$$

2.4.4 Evaluation of integrals for constant and exponentially decaying heat sources

The expressions in the previous section and in Appendix B can be extended, by integration of the form noted in Eqs. (41), to the case of continuous heat sources. It may be seen that all of the results are expressible in terms of the following three integrals:

$$I_1(R,t) = \int_0^t Q(\tau) \operatorname{erf} \left(\frac{R}{\sqrt{\beta}} \right) d\tau \quad (50)$$

$$I_2(R,t) = \int_0^t Q(\tau) \beta^{-\frac{1}{2}} \exp \left(\frac{-R^2}{\beta} \right) d\tau \quad (51)$$

$$I_3(R,t) = \int_0^t Q(\tau) \beta^{-3/2} \exp \left(\frac{-R^2}{\beta} \right) d\tau, \quad (52)$$

where $\beta = 4\kappa(t - \tau)$ and R is $\bar{R}$ or $\bar{\bar{R}}$, defined as for Eqs. (43) and (44). For example, the temperature field for a continuously variable heat source in a semi-infinite body is, according to Eq. (43),

$$T(r, z, t) = \pi^{-3/2} \left[I_3(\bar{R}, t) - I_3(\bar{\bar{R}}, t) \right], \quad (53)$$

while the stress components in Eqs. (45) and (46) become:

$$\begin{aligned} \bar{\sigma}_{zz} + \bar{\bar{\sigma}}_{zz} = & \frac{mG}{2\pi\bar{R}^3} \left[\left(2 - \frac{3r^2}{R^2} \right) I_1(\bar{R}, t) \right. \\ & - \frac{2\bar{R}}{\sqrt{\pi}} \left(2 - \frac{3r^2}{R^2} \right) I_2(\bar{R}, t) + \frac{4\bar{R}r^2}{\sqrt{\pi}} I_3(\bar{R}, t) \Big] \\ & - \frac{mG}{2\pi\bar{\bar{R}}^3} \left[\left(2 - \frac{3r^2}{\bar{R}^2} \right) I_1(\bar{\bar{R}}, t) \right. \\ & - \frac{2\bar{\bar{R}}}{\sqrt{\pi}} \left(2 - \frac{3r^2}{\bar{R}^2} \right) I_2(\bar{\bar{R}}, t) + \frac{4\bar{\bar{R}}r^2}{\sqrt{\pi}} I_3(\bar{\bar{R}}, t) \Big], \end{aligned} \quad (54)$$

$$\begin{aligned} \bar{\sigma}_{rz} + \bar{\bar{\sigma}}_{rz} = & \frac{3mGr(z - H)}{2\pi\bar{R}^5} \left[I_1(\bar{R}, t) \right. \\ & - \frac{2\bar{R}}{\sqrt{\pi}} I_2(\bar{R}, t) - \frac{4\bar{R}^3}{3\sqrt{\pi}} I_3(\bar{R}, t) \Big] \\ & - \frac{3mGr(z + H)}{2\pi\bar{\bar{R}}^5} \left[I_1(\bar{\bar{R}}, t) \right. \\ & - \frac{2\bar{\bar{R}}}{\sqrt{\pi}} I_2(\bar{\bar{R}}, t) - \frac{4\bar{\bar{R}}^3}{3\sqrt{\pi}} I_3(\bar{\bar{R}}, t) \Big]. \end{aligned} \quad (55)$$

The integrals defined in Eqs. (50) - (52) have been evaluated for two cases: a constant heat source, $Q(\tau) = Q_c$, and an exponentially decaying heat source, $Q(\tau) = Q_e \exp(-A\tau)$. The results, which are tabulated below, were obtained by making use of some integrals given by Gautschi.¹⁰

Constant heat source, $Q(\tau) = Q_c$

$$I_1(R, t) = Q_c t \operatorname{erf} \frac{R}{\sqrt{4\kappa t}} - Q_c \frac{R^2}{2\kappa} \operatorname{erfc} \frac{R}{\sqrt{4\kappa t}} + Q_c \sqrt{\frac{t}{\pi\kappa}} R \exp\left(\frac{-R^2}{4\kappa t}\right). \quad (56)$$

$$I_2(R, t) = Q_c \sqrt{\frac{t}{\kappa}} \exp\left(\frac{-R^2}{4\kappa t}\right) - Q_c \frac{\sqrt{\pi}}{2\kappa} \operatorname{erfc}\left(\frac{R}{\sqrt{4\kappa t}}\right) \quad (57)$$

$$I_3(R, t) = \frac{\sqrt{\pi}}{4\kappa} \frac{R_c}{R} \operatorname{erfc}\left(\frac{R}{\sqrt{4\kappa t}}\right). \quad (58)$$

In these equations, $\operatorname{erfc}(z) = 1 - \operatorname{erf}(z)$ is the complementary error function.

Exponentially decaying heat source, $Q(\tau) = Q_e \exp(-A\tau)$

$$I_1(R, t) = -\frac{Q_e}{A} \exp(-At) + \frac{Q_e}{A} \left[\operatorname{erf}\left(\frac{R}{\sqrt{4\kappa t}}\right) + \exp\left(\frac{-R^2}{4\kappa t}\right) \operatorname{Re}\left\{ w\left(\sqrt{At} + i\frac{R}{\sqrt{4\kappa t}}\right) \right\} \right] \quad (59)$$

$$I_2(R, t) = \frac{Q_e \sqrt{\pi}}{\sqrt{4\kappa A}} \exp\left(\frac{-R^2}{4\kappa t}\right) \operatorname{Im}\left\{ w\left(\sqrt{At} + i\frac{R}{\sqrt{4\kappa t}}\right) \right\} \quad (60)$$

$$I_3(R, t) = \frac{Q_e \sqrt{\pi}}{4\kappa R} \exp\left(\frac{-R^2}{4\kappa t}\right) \operatorname{Re}\left\{ w\left(\sqrt{At} + i\frac{R}{\sqrt{4\kappa t}}\right) \right\}. \quad (61)$$

In these equations, $w(z)$ is the complex error function defined by

$$w(z) = \frac{2iz}{\pi} \int_0^\infty \frac{e^{-t^2}}{z^2 - t^2} dt, \quad \operatorname{Im}\{z\} > 0,$$

and $\operatorname{Re}\{z\}$ and $\operatorname{Im}\{z\}$ denote the "real part of z " and the "imaginary part of z " respectively.

3. COMPUTER SIMULATION OF A RADIOACTIVE WASTE REPOSITORY IN BEDDED SALT

3.1 Introduction

Currently, the reference design of a high-level radioactive waste repository envisages a series of long, parallel rooms about 18 ft wide and 17 ft high separated by pillars about 60 ft wide. The excavations will be in a bedded salt deposit about 2000 ft below the surface and will extend over a region roughly 5000 by 10,000 ft. Canisters of high-level radioactive waste (each with an initial heat generation not exceeding 5 kW) will be placed in 18-ft deep holes drilled 22 ft apart in the floors of the rooms along the center lines. Placement of the canisters will proceed in an orderly fashion, starting from the extremities of the repository and working back toward a central corridor. As the canisters are placed in the holes, the rooms will be backfilled as completely as possible with crushed salt.

From a rock mechanics point of view, this arrangement must be analyzed to determine what sort of displacements and stresses it will induce in the surrounding rock as a function of time. Physically, it may be reasoned that the repository rooms will close up and compress the crushed salt backfill, principally because the pillars will creep, shortening in one direction and expanding in the other. Eventually, the result of these deformations will be to recompact, or "recrystallize" the crushed salt in the rooms. At this stage, it appears that subsequent settling of the overlying rock will be comparatively small. However, the rock surrounding the repository will also be subjected to thermal stresses and displacements, both of which will continue long after complete closure of the rooms has occurred. Again, it may be reasoned that these thermal effects will tend to cause uplift of the overlying rock, essentially in opposition to the settlement due to room closure. Because of the time-dependent nature of both the room closure and the thermal expansion effects, the surrounding rock (particularly the overlying rock) may be subjected to cyclic deformations. For example, the ground surface above the repository may first settle, then bulge upward, and gradually settle again as the radioactive waste decays and loses its capacity to generate

heat. The objective of the analysis described in this report is to predict the history of such deformations and stresses in the rock.

The scale involved in an actual radioactive waste repository of the sort described above prohibits making a detailed analysis of the entire problem. For example, if one attempted to model the repository problem by the same approach used by Starfield and McClain,² who accounted for each individual room, pillar, and waste canister, a grid of more than 500 by 1000 elements would be needed just to model the active portion of the repository. Since this would involve a system of algebraic equations with more than 500,000 unknowns, it is apparent that an alternative approach must be sought to reduce the problem to manageable proportions.

The approach used in this report is to ignore the detailed room and pillar geometry and to treat the plane of the repository as a series of elements that are partially excavated, each with an initial extraction ratio e_0 . As each element is "excavated," it is considered to act as a heat source with prescribed heat generation characteristics; these characteristics are determined by the canister density in the actual problem and are chosen such that the average heat generation per unit area is the same in the model as in reality. With these approximations, it is possible to analyze the repository problem in a manner similar to that described by Starfield and McClain² for the experimental area of Project Salt Vault. The analysis, which makes use of the results given in Sect. 2 of this report, is described in the following portions of Sect. 3.

3.2 Description of Computer Model

The Repository Program essentially couples the effects of elastic room closure, inelastic pillar deformations, and the thermal effects due to the radioactive wastes. As presently structured, it is set up to compute only the closure over the plane of the repository; however, thermal effects are included in these computations because they alter the stresses and the temperatures over the plane of the repository, and these enter the boundary conditions for the system of equations used to find the

closure distribution. At any point in the surrounding rock, stresses and displacements will be induced by both the closure over the plane of the repository and the thermal effects due to heat generated by the radioactive wastes. These "off seam" stresses and displacements are found by a subsidiary computation, which is described in Sect. 5.

The Repository Program is based on a 50 by 50 grid of square elements representing the plane of the repository. The fundamental objective of the program is to find the closure occurring at each element as a function of time, that is, to find $(S_z)_{ij}$ for $i, j = 1$ to 50 at any time $t = N\Delta t$. The elements inside the repository may be mined at any time step and in any order, and each mined element is taken to act as a heat source. In this context, a "mined" element refers to one that has been excavated with initial extraction e_0 , loaded with radioactive waste, and backfilled with crushed salt, all in a single operation. For the overall problem, this of course means that the effects of the individual operations will not be separated.

As outlined above, the Repository Program does not distinguish between excavated (and backfilled) elements and elements containing heat sources. However, in computing the closure of each element (and, later, the stresses and displacements in the surrounding rock), it is necessary to examine separately the thermal effects and the effects of elastic deformation of the rock caused by inelastic deformation of the pillars and the backfill in the excavated areas.

3.2.1 Handling of heat sources

The closure distribution across the plane of the repository depends on the heat sources in two ways: through an increase in the temperatures of the pillars and the backfill, and through an increase in the normal stress acting across the seam. [The heat sources also induce shear stresses across the seam, but we assume here that the ride components (cf. Sect. 2.2.1) may be neglected; hence these stresses are not used in the computations.] The normal stress due to the heat sources acts essentially to alter the primitive stress at the seam; the nature of this alteration is computed from the results of Sect. 2.4.

Within the program, the heat source for each element is considered to be a plane source acting over the whole element and located at depth d beneath it. This is illustrated in Fig. 7, where element ij represents a heat source. The solution for the thermal stresses and the temperatures in the rock due to this plane heat source is obtained by numerically integrating the solution for a point heat source over the element. The integration is accomplished by considering the element as 15 by 15 (total 225) subelements, each containing a point heat source of strength $Q/225$, where Q is the total strength of the plane heat source. A similar integration is performed for the grid elements surrounding element ij . Because of symmetry, this integration only needs to be done explicitly for the elements shown in Fig. 8; the thermal stress and the temperature at element kz due to a plane heat source at element ij depend on the distances $|i-k|$ and $|j-z|$, with the same results obviously applying for other elements located the same distances from element ij . Similarly, if more than one element contains a heat source, the solution described above is applicable and complete results for all the elements are obtained by superposition.

Computations relative to the image heat source (cf. Sect. 2.4.3), including the removal of shear stress from the surface, are handled in an analogous fashion, except that an integration process is not used. Each image heat source is considered to act at a single point, directly above its corresponding grid element on the plane of the repository at a distance $2H$ from it. The effects of each such image sources on the temperatures and the stresses at all of the grid elements are then added to the effects already computed for the sources on the plane of the repository. Acting together, the heat sources on the plane of the repository and their images produce a certain distribution of shear stress at the ground surface. This distribution is computed by superposing results for the two sets of heat sources and is negated by applying, pointwise, a series of concentrated shear forces on the surface, as outlined in Sect. 2.4.3. Each such shear force necessarily produces displacements and stresses in the rock mass; in particular, it alters the normal stress acting across the plane of the repository.

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Fig. 7. Parameter description for grid and heat sources in repository model.

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Fig. 8. Grid elements requiring explicit calculation of thermal stresses.

For numerical purposes, the above procedure gives the solution to the problem of an arbitrary distribution of heat sources at $z = H$ (the plane of the repository) in an isotropic, homogeneous, linearly elastic half-space $z \geq 0$, the surface of which is free from tractions. It is necessary, of course, to employ this procedure for each time step of the analysis. Thus, at any time $t = n\Delta t$, each grid element (e.g., element ij) will have associated with it a temperature, T_{ij} , and an "effective primitive stress," $(P_{zz})_{ij}$. These quantities will depend on both the distribution and the nature (constant or decaying exponentially with time) of heat sources on the plane of the repository.

The Repository Program is set up to compute the values of T_{ij} and $(P_{zz})_{ij}$ for both, or some prescribed combination of, constant and exponentially decaying heat sources. The temperature and the effective primitive stresses are, at time $t = n\Delta t$:

$$\begin{aligned} T_{ij} &= T_{ij}^{\text{initial}} + T_{ij}^{\text{heat sources}}, \\ (P_{zz})_{ij} &= (P_{zz})_{ij}^{\text{initial}} + (\sigma_{zz})_{ij}^{\text{heat sources}}, \end{aligned} \tag{62}$$

where the initial values of T_{ij} and $(P_{zz})_{ij}$ are constants.

3.2.2 Handling of excavated areas

An element on the plane of the repository will be either excavated (and assumed to contain heat sources as explained above) or unexcavated. In either case, we must compute the closure between its "roof" and its "floor." This is done by using, in effect, Eqs. (23), (35), (36), and (62) in conjunction with an appropriate set of boundary conditions. The boundary conditions for the problem at hand must be deduced from Eq. (2); Eq. (1) cannot be used directly because an excavated (mined) element really is only partially excavated, with extraction e_0 . Hence, an "excavated" element is capable of transmitting the load between the roof and the floor.

For convenience in writing, the following notations will be adopted:

- (1) The closure $(S_z)_{ij}$ at the ij th element will be denoted simply by S_{ij} .
- (2) The effective primitive stress $(P_{zz})_{ij}$ will be designated as P_{ij} .
- (3) The induced stress $(\sigma_{zz})_{ij}$ will be denoted by σ_{ij} .

The effective primitive stress is determined by Eq. (62), and the relation between the induced stress and the closure by Eq. (23).

The boundary conditions used in the Repository Program are as follows:

For ij th element unmined,

$$\frac{1}{E_s}(\sigma_{ij} + P_{ij}) = \frac{S_{ij}}{h}. \quad (63)$$

This states that the total stress and the closure are linearly related by a one-dimensional Hooke's law, with E_s being the modulus of elasticity of the seam. By Eq. (23), the following equation then obtains at the ij th element:

$$S_{ij} = \frac{h}{E_s} \left[\sum_{\text{all } k} \sum_{\text{all } z} (a_{ijkz} + a'_{ijkz}) S_{kz} + P_{ij} \right]. \quad (64)$$

This equation may be solved for S_{ij} by iteration.

For ij th element excavated with initial extraction e_0 ,

$$\frac{1}{E_s} \sigma'_{ij} + C_0 (k \sigma'_{ij})^C + B_N = \frac{S_{ij}}{h} \quad (65)$$

at time $t = N\Delta t$. This equation states that the (uniaxial) strain at the ij th element consists of an elastic component, σ'_{ij}/E_s , and an inelastic component, $C_0 (k \sigma'_{ij})^C + B_N$, cf. Eqs. (35) and (36). The stress σ'_{ij} in each case is given by:

$$\sigma'_{ij} = \frac{\sigma_{ij} + P_{ij}}{1 - e_{ij}}, \quad (66)$$

where e_{ij} is the current value of the extraction at the ij^{th} element, which, as will be described later, is a function of the closure: $e_{ij} = e_{ij}(S_{ij})$. The factor $1/(1 - e_{ij})$ in this expression is needed to reflect the fact that stress is transmitted partially through the pillars and partially through the backfill. Stress transmission through the backfill is modeled by allowing the extraction to be a function of the closure. For no closure (i.e., for $e_{ij} = e_0$), all of the stress is carried by the pillars, while for complete closure (i.e., for $e_{ij} = 0$), the stress on the pillars and on the backfill will be equal. Function $e_{ij} = e_{ij}(S_{ij})$ is referred to as the "recrystallization function" and will be described later.

The factor k in Eq. (65) characterizes the width-to-height ratio of the pillars in the excavated area. This factor, which is somewhat similar to the creep effective stress coefficient used by Starfield and McClain² (cf. Sect. 2.3), is needed to account for the observation that pillars with different width-to-height ratios creep at different rates. The factor k in this case is defined as:

$$k = e^{-\lambda(\frac{W}{h} - 1)}, \quad (67)$$

where λ is a parameter and W/h is the pillar width-to-height ratio.

Equation (65) may be written as:

$$S_{ij} = \frac{h}{E_s(1 - e_{ij})} \left[\sum_{\text{all } k} \sum_{\text{all } z} (a_{ijkz} + a'_{ijkz}) S_{kz} + P_{ij} \right] + C_0 h \left[\frac{k}{1 - e_{ij}} \sum_{\text{all } k} \sum_{\text{all } z} (a_{ijkz} + a'_{ijkz}) S_{kz} + P_{ij} \right]^c + B_N h, \quad (68)$$

which may be solved for S_{ij} by Newton-Raphson iteration.

Condition for "complete closure"; behavior of backfill. Complete closure of an excavated area is assumed to occur when the average closure over an element is sufficient to recompact, or recrystallize, the crushed salt backfill in the rooms. The amount of closure required to accomplish this will depend upon the bulk porosity of the backfill and the room

dimensions. Neglecting the lateral deformation of the pillars and denoting the maximum allowable room closure by S^* , the volume change per original volume in a room of unit length, height h , and width w is:

$$\frac{\Delta V}{V} = \frac{wh - w(h - S^*)}{wh} = \frac{S^*}{h} . \quad (69)$$

If the crushed salt backfill has an initial bulk porosity η , maximum closure will correspond to the condition $\Delta V/V = \eta$; that is,

$$S^* = h\eta \quad (70)$$

is the closure necessary to recrystallize the crushed salt. For example, if the seam thickness (room height) h is 15 ft and the bulk porosity η is 0.25, recrystallization of the crushed salt backfill will occur when the room closure S^* is 3.75 ft.

As closure over an element proceeds, the backfill will be subjected to stress. As mentioned earlier, compression of the backfill is modeled indirectly in the Repository Program by letting the extraction e_{ij} of the ij th element be a function of the closure. The "recrystallization function" assumed in this report is:

$$e_{ij} = e_0 \frac{\left[\exp (1 - S_{ij}/S^*) - 1 \right]}{\exp (1) - 1} , \quad (71)$$

that is, an exponential type of function. The recrystallization function is plotted in Fig. 9. When $S_{ij} = 0$, the extraction e_{ij} is the initial value, e_0 ; when $S_{ij} = S^*$, $e_{ij} = 0$. When $e_{ij} = e_0$, the backfill is unstressed and the pillars carry stress σ'_{ij} in Eq. (66); when $e_{ij} = 0$, the backfill and the pillars are subjected to the same stress, $\sigma_{ij} + P_{ij}$ [see Eq. (66)].

Fig. 9. Recrystallization function for crushed salt used to backfill rooms.

When the ij th element closes completely (i.e., when $S_{ij} = S^*$), the element no longer creeps and Eq. (65) must be replaced by the following condition:

ij th element completely closed ($S_{ij} \geq S^*$),

$$\frac{1}{E_s}(\sigma_{ij} + P_{ij}) = \frac{(S_{ij} - S^*)}{(h - S^*)}. \quad (72)$$

Equation (72) states that closure in excess of the maximum amount S^* required to recrystallize the crushed salt will occur according to a one-dimensional Hooke's law similar to that used in Eq. (63) to describe the behavior of unmined elements. Equation (72) may be written as:

$$S_{ij} = S^* + \frac{(h - S^*)}{E_s} \left[\sum_{\text{all } k} \sum_{\text{all } l} (a_{ijkl} + a'_{ijkl}) S_{kl} + P_{ij} \right], \quad (73)$$

which may be solved for S_{ij} by iteration.

3.3 Program Structure

The Repository Program is based on a 50 by 50 grid of square elements representing the plane of the repository. Within the program, this grid is actually treated as a "double grid," consisting of 10 by 10 large squares, each containing 5 by 5 small squares. This double grid is used for convenience in solving the equations [either Eqs. (64), (68), or (72)] by iteration; at each small square element ij , the closure is computed by accounting explicitly for the effects of all of the elements in the large squares immediately surrounding the large square containing element ij , while effects from all of the remaining elements are lumped together, large square by large square. This approach is possible because the influence coefficients a_{ijkl} and a'_{ijkl} [see Eqs. (8), (9), (21), and (22)] decay rapidly with distances $|i - k|$ and $|j - l|$.

The sequence of operations within the program is as follows:

- (1) Read and print input data. The input data for the program consist of elastic constants for the rock mass and the seam, coefficients in the creep equation, Eq. (35), thermal properties

of the rock, specification of heat source strength and decay rate, size of time step and total number of time steps, and various constants describing, for example, the size of the elements, the depth of the seam, the initial extraction ratio, and the width-to-height ratio of the pillars.

- (2) Compute the influence coefficients a_{ijkz} and a'_{ijkz} , and initialize arrays denoting the closures, primitive and induced stresses, temperatures, and mining pattern. The mining pattern at time $t = 0$ is assumed to be such that all elements of the grid are unmined and, therefore, elastic.
- (3) Compute the basic solution for a single plane heat source, plus its image, for all times to be considered during a single program run. This computation, which is done in Subroutine HEAT, gives a set of influence functions from which to compute, at a later stage in the program, the temperature and thermal stress distributions due to an arbitrary distribution of heat source elements (i.e., excavated elements) on the plane of the repository.
- (4) Read the mining pattern for the first time step. This consists simply of assigning the value "1" to the appropriate locations in the array used to designate the status of each of the grid elements.
- (5) Determine the total number of elements that have been mined, and therefore act as heat sources and are allowed to creep. This is accomplished in Subroutine ALTER, which is also arranged to check, for subsequent time steps, for simple errors in input data such as, for example, would result if an attempt were made to mine the same element twice.
- (6) Print the current mining pattern (Subroutine MINPAT). This consists of printing a "0" or a "1" in a 50 by 50 table representing the grid of elements on the plane of the repository, depending on whether the elements are unmined or mined.
- (7) Increment time by one time step.
- (8) Compute the temperature and thermal stresses due to the current pattern of heat sources (mined elements). This is done in

Subroutine THERMS, which uses the influence functions for the appropriate time as computed in Subroutine HEAT [see (3) above], and which is arranged to compute the surface shear stresses and then to remove them as described in Sect. 3.2.1. When this step is completed, the temperatures and effective primitive stresses at all of the grid elements are known for the time step in question.

- (9) Compute current creep variables [i.e., compute C_0 and B_N in Eq. (36)]. As outlined in Sect. 2.3, these quantities account for stress and temperature variations at all previous time steps.
- (10) Solve equations by iteration; that is, solve Eqs. (64), (68), or (73) according to whether element ij is unmined, mined but not completely closed, or mined and completely closed. In this process, Subroutine BURDEN is used to lump together the effects of closure at all outlying large squares, while another subroutine, Subroutine HELP, is used to account explicitly for the effects of closure at all small elements in the large squares immediately adjacent to the large square containing element ij . The total stress acting at each element is calculated during the course of iteration.
- (11) Print results at selected large squares for current time, if desired. This is accomplished in Subroutine OUTPUT, which prints, at selected time step intervals, the following information: (a) the location of the element, by large square--small square position; (b) the "status" of the element, that is, a "1" for a mined element, a number from "1" to "n" (where n is the total number of elements that have been allowed to creep), or a "-1" for a mined element that has closed completely; (c) the amount of closure; (d) the total stress; (e) the temperature; (f) the effective primitive stress; and (g) the xz and yz components of the surface shear stress due to the heat sources.

- (12) Read in changes in the mining pattern for the next time step by assigning a "1" to the mined elements.
- (13) Repeat steps (5) through (12) until the specified number of time steps have been simulated.

4. RESULTS OF PRELIMINARY PROGRAM CHECK-OUT

4.1 Introduction

As explained in the previous sections, the Repository Program (REPOS) is an outgrowth of a similar computer program originally devised to interpret the results of the Project Salt Vault experiment.¹ Substantial modifications had to be made to the original Experimental Area Program during the development of the preliminary version of REPOS, and considerable effort was expended in making runs to check out and validate the performance of the model in this version. The results obtained in these runs are discussed in this section.

The objectives of the check-out procedure were to confirm that the various modified portions of the program were functioning properly and to investigate the sensitivity of the model to variations of particular parameters over appropriate ranges to confirm that the computed results were "reasonable." The first series of results constitutes a set of internal, program reliability checks, while the second serves to demonstrate the influence of the model parameters and provides a basis for selecting values of the parameters for later repository design studies.

The basic repository excavation geometry chosen for these check-out runs was a single, square excavated area, 1250 ft on a side (one large square element, or 25 small square elements) at a depth of 1000 ft. Excavation of the entire square was assumed to be accomplished instantaneously with heat sources installed throughout the entire area at the same time. The other physical property and geometric parameters used for the basic case are given in Table 1 for ease in comparing with the Project Salt Vault correlation values. In the following results, any departures from this basic case will be noted.

All of the results are presented by plots of closure as a function of time, usually for the center of the large, square excavated area. This is largely a matter of convenience and custom. Closure is easily measured in the field; consequently, extensive previous experience with this quantity is applicable to the interpretation of the results. The associated

stress distributions for these runs were examined; however, since they are more difficult to interpret and do not increase our understanding and general appreciation of the results, they will not be given.

4.2 Internal Checks

4.2.1 Time step

The first internal check of the Repository Program was to confirm that the closures did not depend on the length of the time step. For this confirmation, two runs were made using identical setups except for the length of the time step; two years were used for one run and five years for the other. The results are presented in Fig. 10, where it is seen that the closures for both runs are essentially identical. Because of this close correlation, further runs at different time step lengths were deemed unnecessary and the check of this point was considered acceptable.

4.2.2 Size effect

The "size effect check" involved comparison of the results obtained when the 1250 ft of excavated area was divided into 100 small grid elements ($H = 62.5$ ft)* rather than 25 small elements ($H = 125$ ft); all other parameters were unchanged. The results, given in Fig. 11, show that the difference in closure between the two runs is approximately 10% for a halving of the grid element size, with the larger elements giving more closure than the smaller ones. It may be reasoned from a similar set of results given by Crouch⁴ that the model, which is based on the displacement discontinuity method, will give an overestimate of the closure distribution across the excavated area. Crouch⁴ found that the two-dimensional numerical solution for the closure at the center of a crack in a uniaxial stress field is in error by about 5% when the crack is approximated by ten displacement discontinuities; although the numerical solution approaches the

*In this section, "H" refers to the FORTRAN code symbol used to identify the grid element half-width (Table 1) and not to the depth of the repository, which here is called "DEPTH."

Fig. 10. Effect of length of the time step on closure.

Fig. 11. Effect of size of small square elements on closure.

exact result as the grid spacing is made progressively finer, the closure is always overestimated. On this basis, a further subdivision of the 1250-ft-square repository into, say, 20 x 20 (or 400) elements, would produce another curve that would lie just below the lower curve in Fig. 11. Since it is anticipated that all future problem runs will be made at a constant grid element size, the results given in Fig. 11 were considered to be acceptable. It also must be kept in mind that, because of the scale of the problem, a finer subdivision would be impractical; it then would be necessary to account for detailed room and pillar geometry in the repository, and modeling the entire problem would not be feasible.

4.2.3 Effect of depth

A series of runs was made to check the performance of modifications made to the model to incorporate the effect of the stress-free ground surface. These runs simply compared the differences in closure for various depths, assuming that all other parameters remained the same (including pre-mining stress). The results, shown in Fig. 12, were interpreted as meaning that the modifications were performed correctly. The closure of the excavated area is greatest for the shallowest depths, as expected, and the differences decrease with increasing depth (i.e., as the free surface correction terms become small).

4.2.4 Heat source characteristics

As explained in Sect. 3.2.1, the heat generated by the radioactive waste is considered to act uniformly over each grid element. Each heat source may be treated as constant or exponentially decaying, or some combination of the two. In actuality, the heat generation rate will decrease exponentially with time. The capability of modeling a constant heat generation rate was developed partially to isolate the effect of the heat generation characteristics on the predicted closures and closure rates, and partially because it was found during the analysis of the Project Salt Vault experiment that a decreasing heat generation rate must be treated differently than an increasing one.^{1,2} These considerations led to a

Fig. 12. Effect of depth of the mining horizon on closure.

division of the mechanical effects of the heat generation rate of the radioactive waste between a constant component (QCON) and an exponentially decaying component (QEXP). (Regardless of the division between these mechanical effects, the temperature in and around the disposal area is calculated as though the total heating rate decays exponentially.) Therefore, the purpose of this series of runs was to examine the effects of different proportions of the two types of heating.

The results (see Fig. 13) indicate that the largest closure is obtained when all of the heat generation rate is considered constant, while the smallest closure occurs when all of the heat generation rate decays exponentially. This is as would be expected because the model "sees" a larger total quantity of heat in the former than in the latter. The data from one run with no heating are also shown in Fig. 13 for comparison. These data indicated that the handling of the heat source characteristics was satisfactory.

4.2.5 Width-to-height ratio and creep effective stress parameter

Another set of runs was made to check the performance of the creep effective stress coefficient, k , introduced in Eq. (67). This factor depends on both the width-to-height ratio (WHR) of the pillars and the creep effective stress parameter (FRAC). Because of the interrelationship between these two parameters, it was not possible to investigate them independently. The results of a series of runs made to examine the closure of the excavated area for different combinations of width-to-height ratios of the pillars and the creep effective stress parameter are given in Fig. 14. For this series of runs, it was considered advantageous to remove the portion of the program defining the load-deformation properties of the crushed salt backfill in the rooms. As expected, these results indicate that the closure rate decreases when both the height-to-width ratio and the creep effective stress parameter are increased. Since the anticipated mine geometry involves pillars with height-to-width ratios near 4.0, these results also served to identify an appropriate companion value of 0.25 for the creep effective stress parameter.

Fig. 13. Effects of different methods for handling heat generation on closure.

Fig. 14. Effects of pillar width-to-height ratios and creep effective stress parameter on closure.

4.2.6 Extraction ratio

Finally, the increase in scale required to enlarge the Experimental Area Program so as to be applicable to a repository size area meant that the modeling of the behavior of individual pillars was no longer possible. Instead, a single small grid element was used to describe the average deformation of several rooms and pillars. The basic parameter required to accomplish the averaging is the extraction ratio (see Sect. 3.2.2). Consequently, two series of runs were performed to check the performance of this portion of the model.

The results of the first series are shown in Fig. 15, where the closure at the center of the excavated area is plotted as a function of time for extraction ratios of 0.2, 0.33, and 0.5, both with and without heating. In this series of runs, the recrystallization of the backfill was omitted once again. As expected, the higher extraction ratios result in more rapid closure rates. In these results, the closure appears to be relatively insensitive to extraction ratio because of the geometry used.

In the second series of runs (Fig. 16), the exponential load-deformation function [see Eq. (71)] for the consolidation of the crushed salt backfill was inserted. In this case, the closure of the excavated area is even less sensitive to the extraction ratio because the backfill material carries an increasing portion of the pillar load as the deformation increases.

4.3 Influence of Fundamental Parameters

Following the completion of the internal check-out described above, which served primarily to confirm that the program was functioning properly, an additional series of runs was performed to develop an appreciation and understanding of the influence of the individual parameters.

4.3.1 Heating rate

Although the results given in Fig. 13 provided confirmation that the constant and exponentially decaying portions of the heat source characteristics were performing satisfactorily, it did not shed much light on the

Fig. 15. Effect of extraction ratio on closure: recrystallization of room backfill omitted.

Fig. 16. Effect of extraction ratio on closure: recrystallization of room backfill included.

sensitivity of the model or the closure rate to variations in the total heating rate. Consequently, a series of runs was made in which the total initial heating rate was varied from twice to one-fourth of the basic case of 130 kW/acre. In all runs, the total initial heat generation rate was equally divided between constant and exponentially decaying; again, the recrystallization and load-bearing capacity of the room backfill was omitted. The results of these runs are shown in Fig. 17.

4.3.2 Seam thickness

Another variable that had not been previously investigated was the seam thickness (or mining height) itself. The results of two runs made for this purpose are presented in Fig. 18, where it is seen that the higher mining height results in a larger closure of the rooms but that almost all of the difference occurs initially as a consequence of the elastic deformation acting over a longer "gauge length." The creep deformation closure rates are essentially identical.

4.3.3 Overall size

All of the check-out runs to this point had been made using a mine geometry consisting of a 1250-ft-square excavation. However, since the program is capable of handling much larger areas (and will do so in the analysis of actual repository geometries), a series of runs was executed with both larger and smaller overall excavated areas, all at a depth of 1000 ft. The size of the small grid elements was the same ($H = 125$ ft) in each case; thus, the size effect problem mentioned in Sect. 4.2.2 does not apply. The results (Fig. 19) indicate that the closure rate of a 750-ft-square excavation decreases with time. This is a consequence of the load on the "pillars" decreasing with increasing closure, since the overlying strata are able to "bridge across" the excavation span and transfer their weight to the abutments. Above a certain excavation span known as the "critical width," one would expect that the strata would be unable to develop this bridging action and that the pillar loads would be essentially independent of the closure. It follows that the closure rate should be constant for an excavation span greater than the critical width. As

Fig. 17. Effect of various heat generation rates on closure.

Fig. 18. Effect of various seam thicknesses on closure.

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Fig. 19. Effect of various overall excavation sizes on closure.

shown in Fig. 19, the closure rate at the center of a 2500-ft-square excavation is significantly greater than that for a 1250-ft-square excavation. Since 1250 ft is thought to be approximately critical size, these closures should not be as different as indicated. This result will be investigated further.

4.3.4 Sequential mining

All previous runs had been made with the instantaneous excavation and heat source installation over the entire area. However, since the program provides for sequential steps of excavation, it was of interest to examine the consequences of operation in this manner. Therefore, a run was made whereby an area 2500 ft square was excavated in four equal portions (1250 ft square) separated by five-year intervals. For each portion, heating was initiated simultaneously with excavation. Figure 20 illustrates the closure at the center (or what will eventually become the center) of this area and compares it with the same point for instantaneous excavation of the entire area. Except for the wrinkles noted early in the period as a result of subsequent adjacent excavation, the net effect was to delay closure by five years.

4.4 Summary

The various check-out runs served to confirm that (1) the present version of the model is functioning satisfactorily in all respects, (2) the closures and closure rates are within the ranges expected for the cases examined and, furthermore, (3) the influence of all of the various parameters is in the proper direction and of the correct magnitude. Perhaps the most important conclusion to be drawn from the various test runs is that the model behavior is not highly sensitive to variations in any single parameter.

Fig. 20. Effect of sequential excavation on closure.

5. PROGRAM EXPANSION AND FUTURE STUDIES

5.1 Introduction

The purpose of the semi-empirical numerical model described in this report is to examine the long-term deformational behavior of a high-level radioactive waste repository. One of the most important objectives of this effort is to study the displacements and stresses in the overlying rock for different overall repository designs, that is, for different repository geometries, waste emplacement densities, and mining and waste emplacement sequences and schedules. It is considered that the basic developmental work for the model has been completed, and that the Repository Program can now be put into a form that is convenient for actual design studies. This concluding section describes the contemplated revised structure of the Repository Program and briefly describes some of the general uses of the model.

5.2 Revised Program Setup and Structure

The basic structure of the revised Repository Program will be essentially the same as that of the current version, as outlined in Sect. 3.3. However, the following changes and additions will be made:

- (1) Grid size. The current program is based on a 50 by 50 grid of square elements representing the plane of the repository. In the revised version, the grid will be enlarged to 60 by 80 elements. This will enable, for example, a 5000- by 10,000-ft repository to be represented by the central 20 by 40 portion of the grid if the elements are 250 ft wide.
- (2) Separate "mining" and "heating". The current program assumes that each element is excavated, loaded with radioactive waste, and backfilled in a single operation. In the revised program, an option will be included to separate these operations. This option will make it possible for an element to be mined with initial extraction e_0 , but not to be backfilled and/or to act as a heat source. The program will allow the mined elements to be loaded with radioactive waste and backfilled at any specified time after they have been excavated.

- (3) Off-seam displacements and stresses. The displacements and stresses in the rock mass that occur because of the closure distribution across the seam and because of the heat sources may be calculated from the results given in Sect. 3 and Appendixes A and B. As an illustration, the displacement component u_z at an arbitrary point in the rock mass is determined as follows: The net value of u_z may be considered as the sum of two major contributions: one due to closure, the rate of which is, of course, influenced by elevated temperatures; and the other due directly to heat, by the bulk thermal expansion of a large mass above and below the seam; that is,

$$u_z = u_z^{\text{closure}} + u_z^{\text{heat}}. \quad (74)$$

The contribution from closure consists of essentially two parts: $\bar{u}_z$ due to the seam discontinuities [see the last one of Eq. (3)] and $\bar{\bar{u}}_z + u_z^*$ due to the supplemental solution required to introduce the surface $z = 0$ as a stress-free plane [see Eq. (A-3)]; that is,

$$u_z^{\text{closure}} = \bar{u}_z^{\text{closure}} + (\bar{\bar{u}}_z + u_z^*)^{\text{closure}}. \quad (75)$$

Displacements $\bar{u}_z$ and $\bar{\bar{u}}_z + u_z^*$ at a single point depend on the closures at all of the grid elements. The nature of this dependence is specified by Eq. (3) with 6 elements, and Eq. (A-3) with 13.

The contribution to the net value of u_z resulting from heat consists of two parts: $\bar{u}_z + \bar{\bar{u}}_z$ due to the seam heat source and its image [see Eq. (B-3)], and u_z^* due to the concentrated shear forces used to clear shear tractions from the surface $z = 0$; that is,

$$u_z^{\text{heat}} = (\bar{u}_z + \bar{\bar{u}}_z)^{\text{heat}} + u_z^{*\text{heat}}. \quad (76)$$

Again, displacements $\bar{u}_z + \bar{\bar{u}}_z$ at a single point depend on the heat sources at all of the grid elements, and u_z^* depends upon the individual shear forces applied at all points of the surface.

A large number of separate (but straightforward) computations must be made to evaluate the individual displacement and stress components at any point in the rock mass. No estimate has yet been made concerning the amount of time that will be needed to make these computations. It is evident, however, that the number of points to be examined will have to be kept to the bare minimum necessary in order to define the overall displacement and stress fields. Presently, it is anticipated that the calculations will be made so that the displacements and stresses at off-seam locations may be displayed by means of computer-drawn contour plots. The program will be structured in such a manner that these plots can be made for any specified time. The plots will be produced by generating displacement and stress values at points of a regularly spaced grid for the particular level in question. For most levels, it should be sufficient to consider the grid to lie directly above the "large squares" of the grid on the plane of the repository; that is, on each level the grid will consist of 12 by 16 squares, each five times as wide as the small squares on the repository grid.

5.3 Applications

The revised Repository Program will provide the capability for predicting the displacements and stresses at any point in the rock mass surrounding a model of an entire radioactive waste repository area, including simulation of mining and waste emplacement sequences. Because of this overall large scale, the model will be a powerful tool in the development of a repository design, primarily by comparative examination of alternative designs. Part of such a comparison will be the identification of high stress zones or other anomalies requiring a more-detailed evaluation by other techniques such as finite element analysis. Another important application of the semi-empirical model will be in the detailed analysis of the repository design that is finally selected. Such an analysis will predict the overall deformations induced in the surrounding rocks, integrated for the various mechanisms involved, over a long period of time (several centuries). This history is required for an evaluation of the geologic and hydrologic processes that could influence the long-term isolation of the waste.

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7. APPENDIXES

7.1 Appendix A: "Supplemental" Displacements
and Stresses for a Normal Displacement
Discontinuity at Finite Depth

Complete expressions for the "asterisk" and "double bar" displacements and stresses from Eqs. (11), (15), (12), and (16) are given in this Appendix. These expressions are written in terms of a single harmonic function $\bar{\bar{\phi}}$ by virtue of Eq. (18).

$$\bar{u}_x + u_x^* = (1 - 2\nu) \frac{\partial \bar{\bar{\phi}}}{\partial x} + \left[(z - H) - 2(1 - 2\nu)H \right] \frac{\partial^2 \bar{\bar{\phi}}}{\partial x \partial z} - 2zH \frac{\partial^3 \bar{\bar{\phi}}}{\partial x \partial z^2} \quad (A-1)$$

$$\bar{u}_y + u_y^* = (1 - 2\nu) \frac{\partial \bar{\bar{\phi}}}{\partial y} + \left[(z - H) - 2(1 - 2\nu)H \right] \frac{\partial^2 \bar{\bar{\phi}}}{\partial y \partial z} - 2zH \frac{\partial^3 \bar{\bar{\phi}}}{\partial y \partial z^2} \quad (A-2)$$

$$\bar{u}_z + u_z^* = -2(1 - \nu) \frac{\partial \bar{\bar{\phi}}}{\partial z} + \left[(z - H) + 4(1 - \nu)H \right] \frac{\partial^2 \bar{\bar{\phi}}}{\partial z^2} - 2zH \frac{\partial^3 \bar{\bar{\phi}}}{\partial z^3} \quad (A-3)$$

$$\begin{aligned} \bar{\sigma}_{xx} + \sigma_{xx}^* = 2G \left[- \frac{\partial^2 \bar{\bar{\phi}}}{\partial z^2} - (1 - 2\nu) \frac{\partial^2 \bar{\bar{\phi}}}{\partial y^2} + \left\{ (z - H) - 2(1 - 2\nu)H \right\} \frac{\partial^3 \bar{\bar{\phi}}}{\partial x^2 \partial z} \right. \\ \left. + 4\nu H \frac{\partial^3 \bar{\bar{\phi}}}{\partial z^3} - 2zH \frac{\partial^4 \bar{\bar{\phi}}}{\partial x^2 \partial z^2} \right] \end{aligned} \quad (A-4)$$

$$\begin{aligned} \bar{\sigma}_{yy} + \sigma_{yy}^* = 2G \left[- \frac{\partial^2 \bar{\bar{\phi}}}{\partial z^2} - (1 - 2\nu) \frac{\partial^2 \bar{\bar{\phi}}}{\partial x^2} + \left\{ (z - H) - 2(1 - 2\nu)H \right\} \frac{\partial^3 \bar{\bar{\phi}}}{\partial y^2 \partial z} \right. \\ \left. + 4\nu H \frac{\partial^3 \bar{\bar{\phi}}}{\partial z^3} - 2zH \frac{\partial^4 \bar{\bar{\phi}}}{\partial y^2 \partial z^2} \right] \end{aligned} \quad (A-5)$$

$$\bar{\sigma}_{zz} + \sigma_{zz}^* = 2G \left[- \frac{\partial^2 \bar{\bar{\phi}}}{\partial z^2} + (z + H) \frac{\partial^3 \bar{\bar{\phi}}}{\partial z^3} - 2zH \frac{\partial^4 \bar{\bar{\phi}}}{\partial z^4} \right] \quad (A-6)$$

$$\begin{aligned} \bar{\sigma}_{xy} + \sigma_{xy}^* = 2G \left[(1 - 2\nu) \frac{\partial^2 \bar{\bar{\phi}}}{\partial x \partial y} + \left\{ (z - H) - 2(1 - 2\nu)H \right\} \frac{\partial^3 \bar{\bar{\phi}}}{\partial x \partial y \partial z} \right. \\ \left. - 2zH \frac{\partial^4 \bar{\bar{\phi}}}{\partial x \partial y \partial z^2} \right] \end{aligned} \quad (A-7)$$

$$\bar{\sigma}_{xz} + \sigma_{xz}^* = 2G \left[(z - H) \frac{\partial^3 \bar{\phi}}{\partial x \partial z^2} - 2zH \frac{\partial^4 \bar{\phi}}{\partial x \partial z^3} \right] \quad (A-8)$$

$$\bar{\sigma}_{yz} + \sigma_{yz}^* = 2G \left[(z - H) \frac{\partial^3 \bar{\phi}}{\partial y \partial z^2} - 2zH \frac{\partial^4 \bar{\phi}}{\partial x \partial z^3} \right] \quad (A-9)$$

7.2 Appendix B: Displacements and Stresses due
to an Instantaneous Heat Source
in a Semi-Infinite Body

The following results are computed from Eq. (44), according to formulas (39):

$$\begin{aligned} \bar{u}_x + \bar{u}_x = \frac{\partial \Phi}{\partial x} = \frac{Qm(x - \xi)}{2\pi\bar{R}^2} \left[\frac{1}{\sqrt{\pi\beta}} \exp\left(\frac{-\bar{R}^2}{\beta}\right) - \frac{1}{2\bar{R}} \operatorname{erf}\left(\frac{\bar{R}}{\sqrt{\beta}}\right) \right] \\ - \frac{Qm(x - \xi)}{2\pi\bar{R}^2} \left[\frac{1}{\sqrt{\pi\beta}} \exp\left(\frac{-\bar{R}^2}{\beta}\right) - \frac{1}{2\bar{R}} \operatorname{erf}\left(\frac{\bar{R}}{\sqrt{\beta}}\right) \right] \end{aligned} \quad (B-1)$$

$$\begin{aligned} \bar{u}_y + \bar{u}_y = \frac{\partial \Phi}{\partial y} = \frac{Qm(y - \eta)}{2\pi\bar{R}^2} \left[\frac{1}{\sqrt{\pi\beta}} \exp\left(\frac{-\bar{R}^2}{\beta}\right) - \frac{1}{2\bar{R}} \operatorname{erf}\left(\frac{\bar{R}}{\sqrt{\beta}}\right) \right] \\ - \frac{Qm(y - \eta)}{2\pi\bar{R}^2} \left[\frac{1}{\sqrt{\pi\beta}} \exp\left(\frac{-\bar{R}^2}{\beta}\right) - \frac{1}{2\bar{R}} \operatorname{erf}\left(\frac{\bar{R}}{\sqrt{\beta}}\right) \right] \end{aligned} \quad (B-2)$$

$$\begin{aligned} \bar{u}_z + \bar{u}_z = \frac{\partial \Phi}{\partial z} = \frac{Qm(z - H)}{2\pi\bar{R}^2} \left[\frac{1}{\sqrt{\pi\beta}} \exp\left(\frac{-\bar{R}^2}{\beta}\right) - \frac{1}{2\bar{R}} \operatorname{erf}\left(\frac{\bar{R}}{\sqrt{\beta}}\right) \right] \\ - \frac{Qm(z + H)}{2\pi\bar{R}^2} \left[\frac{1}{\sqrt{\pi\beta}} \exp\left(\frac{-\bar{R}^2}{\beta}\right) - \frac{1}{2\bar{R}} \operatorname{erf}\left(\frac{\bar{R}}{\sqrt{\beta}}\right) \right] \end{aligned} \quad (B-3)$$

$$\begin{aligned} \bar{\sigma}_{xx} + \bar{\sigma}_{xx} = 2G \left[\frac{\partial^2 \Phi}{\partial x^2} + mT \right] = \frac{QmG}{2\pi\bar{R}^3} \left[- \left\{ 1 - 3\frac{(x - \xi)^2}{\bar{R}^2} \right\} \operatorname{erf}\left(\frac{\bar{R}}{\sqrt{\beta}}\right) \right. \\ \left. + \frac{2\bar{R}}{\sqrt{\pi\beta}} \exp\left(\frac{-\bar{R}^2}{\beta}\right) \left\{ 1 - 3\frac{(x - \xi)^2}{\bar{R}^2} - 2\frac{[\bar{R}^2 - (x - \xi)^2]}{\beta} \right\} \right] \\ - \frac{QmG}{2\pi\bar{R}^3} \left[- \left\{ 1 - 3\frac{(x - \xi)^2}{\bar{R}^2} \right\} \operatorname{erf}\left(\frac{\bar{R}}{\sqrt{\beta}}\right) \right. \\ \left. + \frac{2\bar{R}}{\sqrt{\pi\beta}} \exp\left(\frac{-\bar{R}^2}{\beta}\right) \left\{ 1 - 3\frac{(x - \xi)^2}{\bar{R}^2} - 2\frac{[\bar{R}^2 - (x - \xi)^2]}{\beta} \right\} \right] \end{aligned} \quad (B-4)$$

$$\begin{aligned}
\bar{\sigma}_{yy} + \bar{\bar{\sigma}}_{yy} &= 2G \left[\frac{\partial^2 \Phi}{\partial y^2} + mT \right] = \frac{QmG}{2\pi\bar{R}^3} \left[- \left\{ 1 - 3\frac{(y-\eta)^2}{\bar{R}^2} \right\} \operatorname{erf}\left(\frac{\bar{R}}{\sqrt{\beta}}\right) \right. \\
&\quad \left. + \frac{2\bar{R}}{\sqrt{\pi\beta}} \exp\left(\frac{-\bar{R}^2}{\beta}\right) \left\{ 1 - 3\frac{(y-\eta)^2}{\bar{R}^2} - 2\frac{[\bar{R}^2 - (y-\eta)^2]}{\beta} \right\} \right] \\
&\quad - \frac{QmG}{2\pi\bar{R}^3} \left[- \left\{ 1 - 3\frac{(y-\eta)^2}{\bar{R}^2} \right\} \operatorname{erf}\left(\frac{\bar{\bar{R}}}{\sqrt{\beta}}\right) \right. \\
&\quad \left. + \frac{2\bar{\bar{R}}}{\sqrt{\pi\beta}} \exp\left(\frac{-\bar{\bar{R}}^2}{\beta}\right) \left\{ 1 - 3\frac{(y-\eta)^2}{\bar{\bar{R}}^2} - 2\frac{[\bar{\bar{R}}^2 - (y-\eta)^2]}{\beta} \right\} \right]
\end{aligned} \tag{B-5}$$

$$\bar{\sigma}_{zz} + \bar{\bar{\sigma}}_{zz} = 2G \left[\frac{\partial^2 \Phi}{\partial z^2} + mT \right] \tag{B-6}$$

[see Eq. (45)]

$$\begin{aligned}
\bar{\sigma}_{xy} + \bar{\bar{\sigma}}_{xy} &= 2G \frac{\partial^2 \Phi}{\partial x \partial y} = \frac{3QmG}{2\pi\bar{R}^5} (x - \xi) (y - \eta) \left[\operatorname{erf}\left(\frac{\bar{R}}{\sqrt{\beta}}\right) \right. \\
&\quad \left. - \frac{2\bar{R}}{\sqrt{\pi\beta}} \left(1 + \frac{2}{3} \frac{\bar{R}^2}{\beta} \right) \exp\left(\frac{-\bar{R}^2}{\beta}\right) \right] \\
&\quad - \frac{3QmG}{2\pi\bar{R}^5} (x - \xi) (y - \eta) \left[\operatorname{erf}\left(\frac{\bar{\bar{R}}}{\sqrt{\beta}}\right) \right. \\
&\quad \left. - \frac{2\bar{\bar{R}}}{\sqrt{\pi\beta}} \left(1 + \frac{2}{3} \frac{\bar{\bar{R}}^2}{\beta} \right) \exp\left(\frac{-\bar{\bar{R}}^2}{\beta}\right) \right]
\end{aligned} \tag{B-7}$$

$$\bar{\sigma}_{xz} + \bar{\bar{\sigma}}_{xz} = 2G \frac{\partial^2 \Phi}{\partial x \partial z} = \frac{(x - \xi)}{r} (\bar{\sigma}_{rz} + \bar{\bar{\sigma}}_{rz}) \tag{B-8}$$

[see Eq. (45)]

$$\bar{\sigma}_{yz} + \bar{\bar{\sigma}}_{yz} = 2G \frac{\partial^2 \Phi}{\partial y \partial z} = \frac{(y - \eta)}{r} (\bar{\sigma}_{rz} + \bar{\bar{\sigma}}_{rz}) \tag{B-9}$$

[see Eq. (45)]

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