

SUPPORTING HYDRATION CALCULATIONS FOR SMALL- TO LARGE-SCALE SEAL TESTS IN UNSATURATED TUFF\*

JAN 21 1992

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ABSTRACT

The design of cementitious repository seals requires an understanding of cement hydration effects in developing a tight interface zone between the rock and the seal. For this paper, a computer code, SHAFT.SEAL, is used to model early-age cement hydration effects and performs thermal and thermomechanical analysis of cementitious seals. The model is described, and then used to analyze for the effects of seal size, rock temperature and placement temperature. The model results assist in selecting the instrumentation necessary for progressive evaluation of seal components and seal-system tests. Also, the results identify strategies for seal emplacement for a series of repository seal tests for the Yucca Mountain Site Characterization Project (YMP).

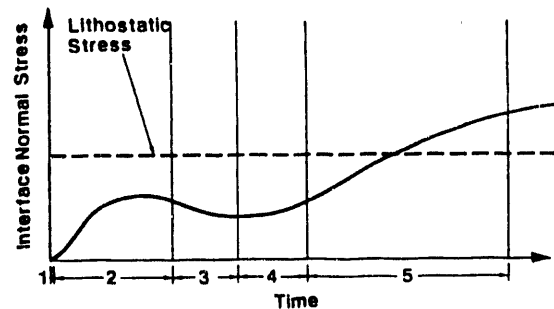
INTRODUCTION

Sandia National Laboratories (SNL), a participant in the YMP, currently is planning to perform a series of borehole- and shaft-seal tests comprised of cementitious materials in welded and nonwelded tuff. As shown in previous sealing studies<sup>1,2</sup>, the interface zone can be important in controlling flow for various seal sizes and under various emplacement and in situ conditions. Therefore, a tentative design goal in seal design is to develop a tight interface zone as well as an adequate seal itself. As the YMP obtains hydrologic information, the necessity for a low conductivity seal and a tight interface zone will be reassessed.

The purpose in performing the calculations summarized in this paper is to characterize the thermal and volumetric stress development at the interface zone between the seal and the rock as the cementitious seal hydrates. The calculations assume variable properties of, and various thermal conditions for, the rock and seal.

THERMAL AND THERMOMECHANICAL BEHAVIOR OF SEALS

Interface stress develops through various stages (Figure 1), including seal placement (Stage 1), seal curing (Stages 2 and 3), and response to loading (Stages 4 and 5). The following discussion identifies several important design considerations in the initial stages (1 to 3). This paper gives no consideration to seal response during backfilling operations (Stage 4), and repository heating during the postclosure period (Stage 5), although these factors also may affect interface-zone performance.



1. Initial mixing and placement
2. Volumetric and thermal expansion (cement hydration)
3. Thermal contraction during cooling
4. Backfill emplacement and subsequent deformational response of plug
5. Postclosure period

Figure 1. Stages in Plug Development

Stage 1: The design criteria for the cement mix include such factors as the water-to-cement ratio, aggregate size, and temperature and moisture environments at depth. The design mix partially attains workability through control of these factors. The geothermal conditions at depth control temperature of the surrounding

\*This work was performed under the auspices of the United States Department of Energy, Office of Civilian Radioactive Waste Management, Yucca Mountain Site Characterization Project, under Contract DE-AC04-76DP00789

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rock. The placement temperature controls the initial temperature of the mix, then exothermic chemical reactions during cement hydration elevate temperature. The water-to-cement ratio, humidity, and containment (or addition) of moisture during the curing process controls moisture content.

Stages 2 and 3: Residual compressive or tensile stresses can develop within the seal and could result in potential separation at the interface zone. The permanent effect, shown subsequently by modeling, depends on several factors. These include (1) the heat evolution resulting from hydration, (2) thermal diffusion to the surrounding welded or nonwelded tuff, (3) the thermal expansion of the seal, (4) the evolution of the thermomechanical properties of the seal during the curing process, and (5) volumetric expansion from formation of hydrous phases.

The heat of hydration for the selected seal material produces an increase in temperature and thermal gradients that can result in thermal stress. With completion of hydration, heat diffuses into the surrounding rock mass, reducing temperatures. (Note that in the initial stages, the temperature of the seal may be less than that of the surrounding rock. Yet, after hydration is complete, the temperature of the seal is always higher than the surrounding rock.) The rate of heat dissipation depends on the thermal diffusivity of the plug and that of the surrounding host rock. The seal expands during hydration, and subsequently contracts during cooling; the magnitude of these effects depend on the temperature and the thermal expansion coefficient for the plug. The formation of expansive-constituents that leads to the volumetric expansion of cement<sup>3</sup> can result in a higher compressive interface stress. Moisture and temperature environments affect the rate of exothermic reaction and therefore the rates of expansive-constituent formation and hardening.<sup>4</sup> Clearly, a reduction in water available for cement hydration reduces the rate and amount of expansive-constituent formation.

Analysis of the development of interface stress during curing requires knowledge of expansivity and stiffness as functions of time and restraint in representative environmental conditions. Volumetric expansion and stiffness properties both change with time during curing. The relationship between the seal-material stiffness and the volumetric expansivity can be characterized as early stiffening (i.e., the material stiffens before the main expansive phase), or late stiffening (i.e., the material stiffens after the main expansive phase). An early-stiffening material develops a higher interface stress. A late-stiffening material

would develop a lower interface stress because the volumetric expansion precedes hardening or stiffening of the material.

The degree of restraint offered by the surrounding rock mass and formwork also affects the development of interface stress. In principle, the seal will expand preferentially toward regions where lower restraining forces are acting. In tests on cement done by Ish-Shalom and Bentur<sup>5</sup>, uniaxial restraint developed a stress value of 0.4 MPa, whereas isotropic triaxial restraint developed values exceeding 9.8 MPa.

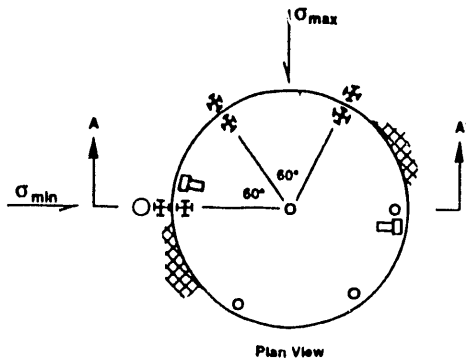
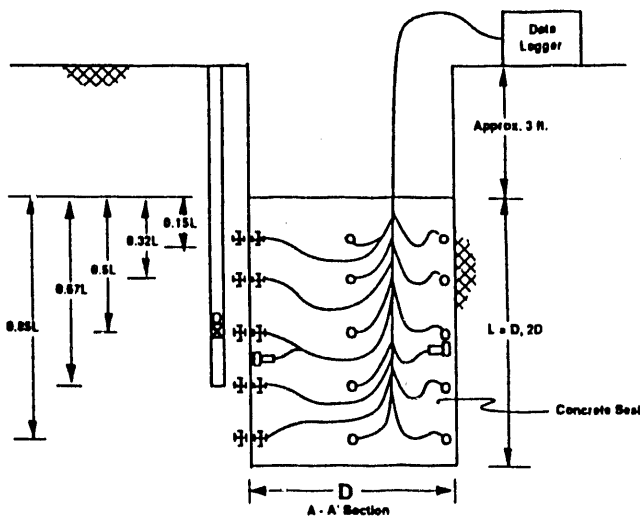
The supporting calculations presented in this paper evaluate seal properties and conditions favorable to developing a tight interface. Further, the supporting calculations provide predictions of temperature and interface stress used in finding the required range, sensitivity and accuracy for instrumentation for the seal tests. The model presented subsequently is preliminary, and will undergo refinement as additional information on seal properties and in situ seal performance information becomes available.

#### CURRENT TEST PLANS

Fernandez et al.<sup>6</sup> describe the current test plans in more detail. Current test plans call for placement of seals in welded and nonwelded tuff. Figure 2 presents the layout for a small-scale in situ test. Seal length would be varied to assess end effects. The planned instrumentation for these tests includes thermocouples, radial and circumferential strain gages in the seal and host rock, stress meters in the seal, and multiple-position borehole extensometers. The instrumentation will measure the thermal and thermomechanical response of the seal at various points along the periphery of the seal at different orientations with respect to the principal stress field. The instrumentation also will measure differences in thermal and thermomechanical response between the center and the ends of the seal.

#### METHODS OF ANALYSIS

A one-dimensional radial numerical and analytical model, SHAFT.SEAL, solves for temperatures and stresses as a function of radial position, either in the seal or the surrounding host rock (Figure 3). The model analyzes the initial temperature rise and subsequent fall following completion of the hydration by the implicit finite-difference method.<sup>7</sup> The model assumes conductive heat transfer and does thermal and volumetric stress analysis using closed-form solutions that account for thermal or initial volumetric strains.



**Legend**

- Thermocouple
- ⊕ Strain Gage  
Radial and Circumferential
- Concrete Stress Meter
- ⊗ Rock Displacement Gage

Figure 2. Small-Scale In Situ Test

The thermal subprogram assumes that the length of the concrete seal is large in comparison to its diameter and that heat transfer is by one dimensional (radial) conduction to a surrounding rock mass of large extent. The governing equation for radial heat-transfer analysis is given by:

$$K_r \left[ \frac{1}{r} \frac{\partial T}{\partial r} + \frac{\partial^2 T}{\partial r^2} \right] + q = \rho C_p \frac{\partial T}{\partial t}$$

where

T = Temperature,

$K_r$  = Thermal conductivity in the radial direction for either the seal or the rock,

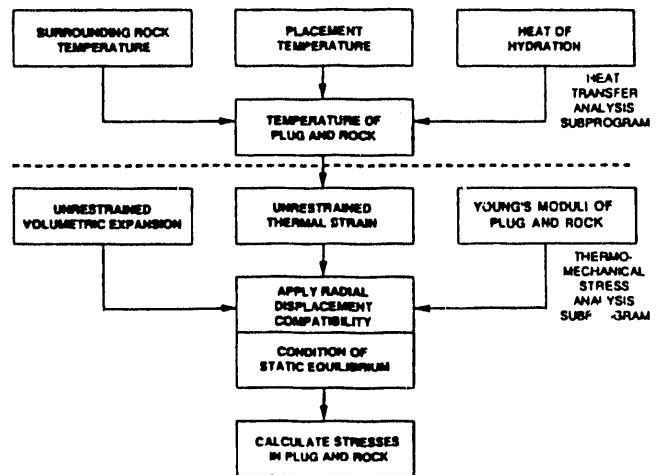


Figure 3. One-Dimensional Modeling and Analysis Using SHAFT SEAL

- $\rho$  = Density for either the seal or the rock,
- $C_p$  = Specific heat for either the seal or the rock,
- $q$  = Internal heat generation rate due to hydration for the seal,
- $r$  = Radius, and
- $t$  = Time.

The structural model uses the theory of linear elasticity for calculating thermal and volumetric stresses. Relations have been developed for a seal under axial restraint (plane-strain solution) and an unrestrained seal (zero axial force). The solutions are derived from the condition that the interface stress at the boundary of the seal must be equal in the rock and the seal, and that there is radial displacement compatibility at the interface. The basic relations for the plane-strain case are presented below:

$$\Delta \sigma_r = A_p + \Delta P - A_p^*$$

$$\Delta \sigma_\theta = -A_p + \Delta P - A_p^* - B_p$$

$$\Delta \sigma_z = -B_p + 2\nu_p(\Delta P - A_p^*) + E_p \delta_p$$

where

$\Delta \sigma_r$  = Incremental radial stress in the seal at radius  $r$ ,

$\Delta \sigma_\theta$  = Incremental tangential stress in the plug at radius  $r$ ,

$\Delta \sigma_z$  = Incremental vertical stress in the seal at radius  $r$ ,

$\Delta P$  = Incremental interface stress at seal radius  $a$ ,

$$\Delta P = \frac{2A_p^* E_r (1-\nu_p^2) + E_r E_p (1+\nu_p) \delta_p}{E_p (1+\nu_r) + E_r (1+\nu_p) (1-2\nu_p)}$$

$$A_p = \frac{\alpha_p E_p}{(1-\nu_p)} \frac{1}{r^2} \int_0^r \Delta T r dr$$

$$B_p = \frac{-\alpha_p E_p \Delta T}{(1-\nu_p)}$$

$$A_p^* = \frac{\alpha_p E_p}{1-\nu_p} \frac{1}{a^2} \int_0^a \Delta T r dr$$

$\alpha_p$  - Thermal expansion coefficient of the plug,

$E_p$  - Young's modulus of the plug at time t,

$\nu_p$  - Poisson's ratio of the plug,

$\alpha_r$  - Thermal expansion coefficient of the rock,

$E_r$  - Young's modulus of the rock,

$\nu_r$  - Poisson's ratio of the rock,

$\delta_p$  - Incremental linear unrestrained expansion of the plug at time t, which is equal to  $(1 + \delta V_p)^{1/3} - 1$  where  $\delta V_p$  = incremental volumetric expansion, and

$\Delta T$  - Incremental difference in temperature between the present and previous time step as a function of radius.

#### INPUT PROPERTIES

The analyses used thermal and thermomechanical rock properties for welded tuff identified in the Reference Information Base.<sup>8</sup> Other thermal and thermomechanical properties for cementitious seals were taken from previous work.<sup>1</sup> Table 1 summarizes the thermal and thermomechanical input properties. Figure 4 summarizes the heat of hydration and Young's Modulus as a function of time.

In addition to the material properties, the analyses that were performed considered other variables that could affect the interface stress development. These variables included elevated rock-mass temperatures, placement temperatures of

Table 1. Summary of Thermal and Thermomechanical Input Properties for the Seal and Host Rock

Parameter	Units	Boreholes	Shafts
Seal Size	m	0.3 and 0.61	1.52 and 3.05
Seal Ultimate Young's Modulus	MPa	6,890	6,890 - 27,800
Seal Poisson's Ratio	-	0.2	0.2
Seal Thermal Expansion	C <sup>-1</sup>	12.6 X 10 <sup>-6</sup>	12.6 X 10 <sup>-6</sup>
Seal Density	kg/m <sup>3</sup>	2,080	2,290
Seal Thermal Conductivity	J/(m Day °C)	259,200	259,200
Specific Heat	J/kg °C	962.8	962.8
Ultimate Volumetric Expansion	%	0.03	0.03
Rock Young's Modulus	MPa	7,800	7,800
Rock Poisson's Ratio	-	0.16	0.16
Rock Thermal Expansion	C <sup>-1</sup>	6.4 X 10 <sup>-6</sup>	6.4 X 10 <sup>-6</sup>
Rock Thermal Conductivity	J/(m Day °C)	113,443	113,443
Thermal Capacitance	J/(m <sup>3</sup> °C)	1.97 X 10 <sup>6</sup>	1.97 X 10 <sup>6</sup>
Rock Temperature	°C	22-42	22-42
Horizontal In Situ Stress	MPa	2.4	2.4

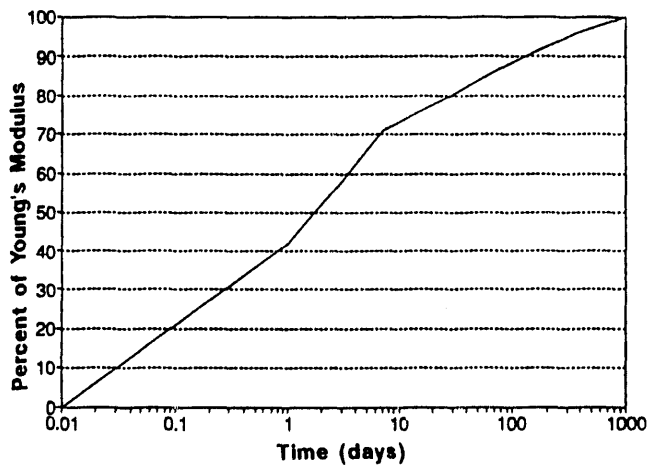
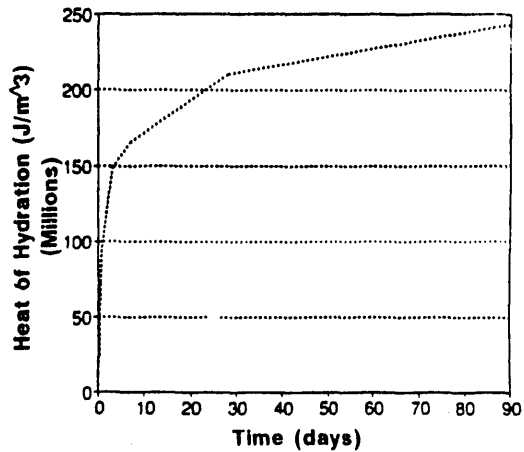


Figure 4. Evolution of Cementitious Material Properties (a) Heat of Hydration (Type II 82-22 Cement), and (b) Young's Modulus

the mix, injection pressure on the seal during curing, and seal size. The analyses used rock-mass temperatures ranging from ambient geothermal temperature (22°C) to elevated temperatures resulting from repository heating (42°C). The placement temperatures ranged from 4°C to the ambient geothermal temperature at depth. The lower temperature would be done by cooling the aggregate or circulating water through the seal. The injection pressures ranged from 0 to 50 percent of minimum horizontal stress at different sealing locations in welded and nonwelded tuff. The analyses also considered variation in seal diameters ranging from 0.3 and 0.61 m for borehole seals to 1.52 and 3.05 m for shaft

seals. The intent was to assess the effect of seal diameter on temperature and interface stress development.

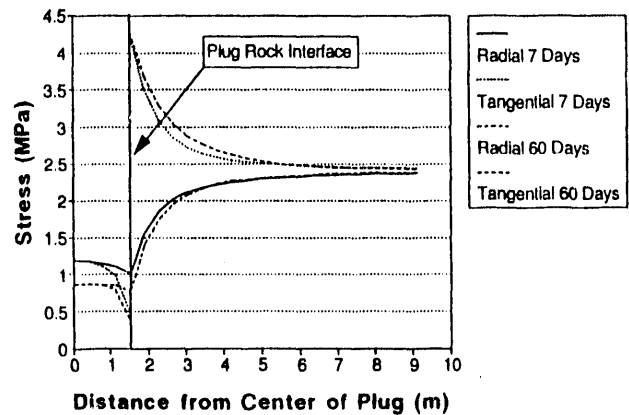
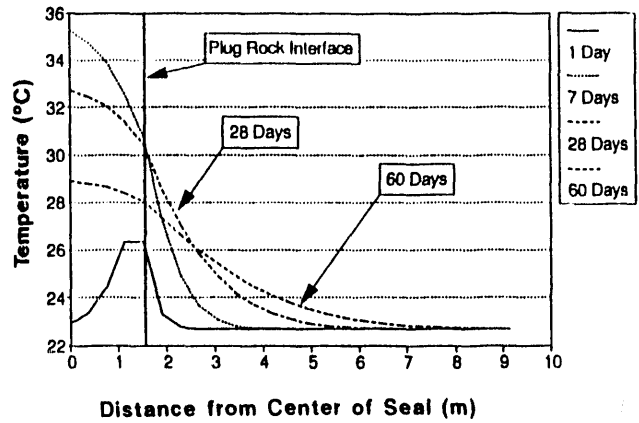


Figure 5. Radial Distribution in Seal and Adjacent Rock (a) Temperature and (b) Interface Stress (Size = 3.0 m, Placement Temperature = 4°C, and No Injection Pressure)

#### ANALYSIS RESULTS

The results from SHAFT.SEAL include temperature and stress histories in the seal and surrounding rock. Figure 5 presents typical results as radial temperature and stress distributions from one to 60 days. The thermal analysis shows that temperatures initially rise uniformly because of cement hydration, inducing a high radial thermal gradient near the interface zone. Subsequently, thermal gradients decrease with increasing time as hydration nears completion, and heat diffuses to the surrounding rock mass. After seven days, the temperature rises to 35°C maintaining a sharp thermal gradient at the interface zone. After this time, the temperatures fall and, though elevated, approach the in

situ rock temperature after 60 days. The temperatures in the seal and surrounding rock mass suggest that the transient heating pulse is of short duration compared to the time for heat to diffuse away from the seal.

Figure 5 also illustrates the radial and tangential stress distributions after 7 and 60 days for the seal and the surrounding rock. For the seal, the stresses result both from thermal and from volumetric effects after 7 days. After 60 days, the seal radial and tangential stresses fall as hydration nears completion. (Note that temperatures are still somewhat elevated for the massive plug as heat has not fully diffused into the surrounding rock mass.) In the surrounding rock, the tangential stress is higher, reflecting the in situ state of the stress. Comparisons of stress distributions within the rock after 60 days to the initial stress distributions (0 days) show that the rock radial stresses rise, while tangential stresses fall, because of the developing interface stress. In time, as temperatures approach the in situ placement temperature, the radial and tangential stress distributions reflect the in situ far-field and the residual radial interface stresses. This is because thermal stresses develop only where thermal gradients are present, and thermal gradients are absent over the long term.

The parametric studies examined the effects of seal size, injection pressure, rock temperature, and seal-placement temperature on temperature and stress. Figures 6 through 8 present temperature and stress histories as affected by seal size, rock temperature, and seal-placement temperature.

The preliminary analyses showed that the peak temperatures for seals placed at ambient rock temperature (22°C) ranged from 22°C to 38°C with radial interface stresses ranging from -0.4 to 0.8 MPa. For larger seals, hydration effects are more significant due to the mass of seal material (Figure 6). The temperatures rise to higher levels in comparison to smaller seals. This is because the volume-to-surface-area ratio is larger in larger seals, and heat dissipates more slowly into the surrounding rock mass. Because the stiffness of the seal is increasing with time, the larger seal is stiffer when temperatures fall, and the model predicts the development of residual radial tensile stresses at the interface zone after some period. The results suggest potential difficulty in obtaining a tight interface in a larger seal (assuming no injection pressure), and that contact grouting of this zone may be necessary.

These analyses showed that the development of a tight interface (high interface stress) also depends on the contrast in initial temperature between the seal and the rock, as illustrated in Figures 7b and 8b. A contrast in temperature

leads to the development of residual compressive stress. Compressive interface stress can be controlled in the planned tests by decreasing the placement temperature in relation to the surrounding rock temperature (Figure 8) and by emplacing the seal under a slight injection pressure (Figure 9b).

## CONCLUSIONS

SNL plans to do a series of sealing tests progressing from small-scale tests (borehole seal tests) to large-scale tests (shaft-seal tests). The SHAFT.SEAL results presented in this paper help in developing an understanding of the stress, strain and thermal response of a cementitious seal as it hydrates.

The SHAFT.SEAL results suggest the importance of emplacing a seal under a slight injection pressure (Figure 9b). Further, the results suggest emplacement of the seal with a temperature cooler than the surrounding host-rock formation (Figures 7b and 8b). The temperature contrast could be developed by reducing the emplacement temperature of the cement seal.

The results presented here also show the following

- The required instrumentation should measure temperatures from 20°C to 50°C and stresses of up to 1.4 MPa.
- The temperature transient lasts from 10 days to more than 500 days, depending on seal size (Figure 6a).
- There are greater temperature effects in large-scale seals with a greater potential for developing residual tensile stress (Figure 6b).

The results suggest the need for progressive component evaluation in interpreting the results of smaller-scale tests, and then using these results to develop strategies for performing the larger-scale tests. After performing the small-scale tests, interpreting the results, and refining the thermal/structural model, the large-scale tests can be performed. These tests will support a better understanding of structural hydration effects as a function of different materials, rock temperature, seal-placement temperature, and seal size.

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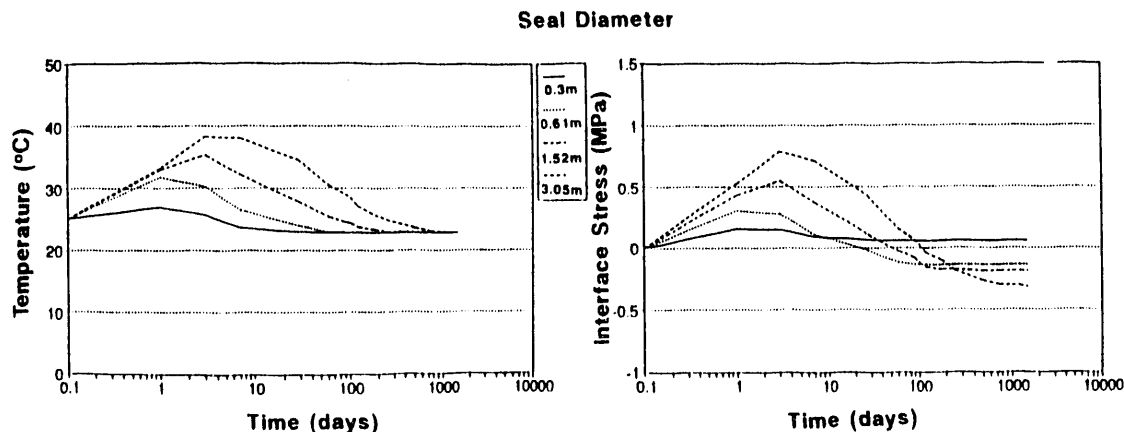


Figure 6. Influence of Seal Size on (a) Temperature and (b) Radial Interface Stress (Injection Pressure = 0, Seal Placement and Rock Temperature = 22°C)

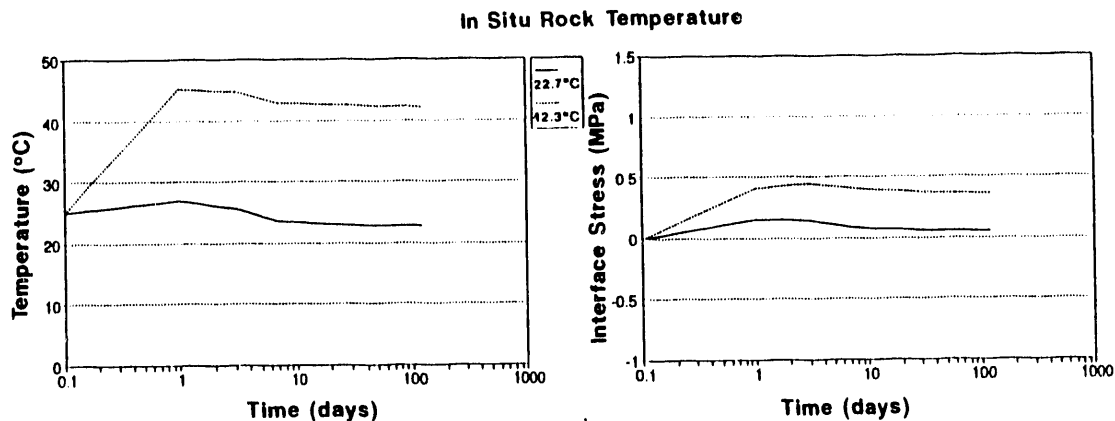


Figure 7. Influence of Rock Temperature on (a) Temperature and (b) Radial Interface Stress (Size = 0.3 m, Injection Pressure = 0, Placement Temperature = 22°C)

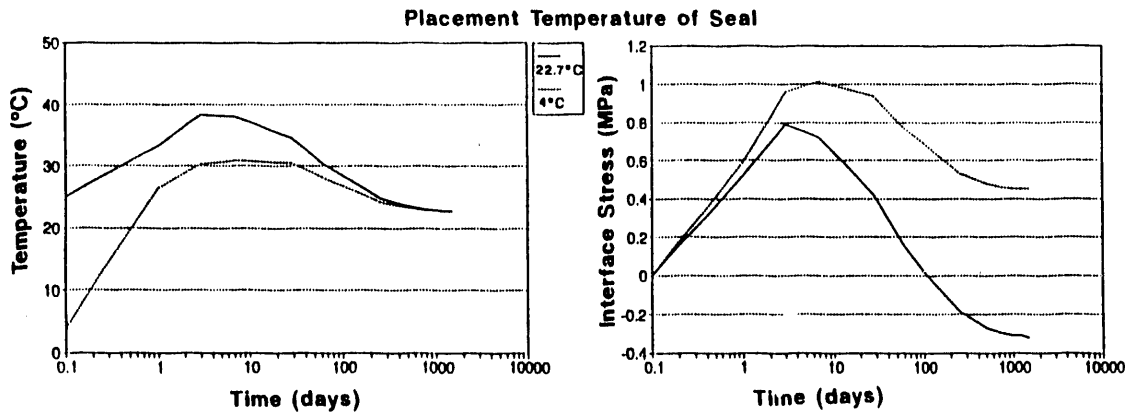


Figure 8. Influence of Placement Temperature on (a) Temperature and (b) Radial Interface Stress (Size = 3.05 m, Injection Pressure = 0, and Rock Temperature = 22°C)

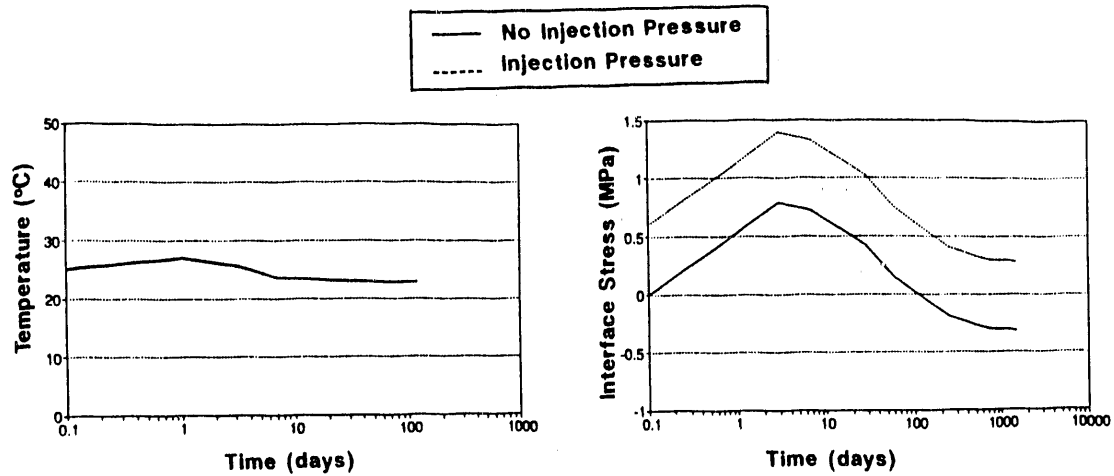


Figure 9. Influence of Injection Pressure on (a) Temperature and (b) Radial Interface Stress (Size = 0.3 m, Seal Placement and Rock Temperature = 22°C)

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