APPENDIX C

MATHEMATICAL SIMULATION OF UNDERGROUND IN SITU BEHAVIOR

CONTENTS

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C.1 INTRODUCTION

The methodology described in the following sections presents analytical techniques for simulating underground behavior in salt formations. Consideration is given to time-dependent non-linear material behavior and incorporation of in situ measurements to predict structural responses. The theoretical background and procedures presented by this methodology are explained.

C.2 MATERIAL BEHAVIOR OF HOST ROCKS

The most significant physical property of halite is that it creeps. Its creep behavior is dependent upon the variations of stress and temperature with respect to time. The creep phenomenon is also affected by the physical properties of the geologic strata adjacent to the halite and by discontinuities in the geologic layers. Therefore, non-halitic interbeds and clay seams should also be considered when modeling and simulating the structural behavior of salt formations. The following subsections summarize the material behavior of various host rocks (ref. C-1).

C.2.1 Halitic Materials

The constitutive equation for halitic materials can be expressed as:

$$\dot{\varepsilon}_{ij} = -\frac{\nu}{E}\dot{\sigma}_{kk}\,\delta_{ij} + \frac{1+\nu}{E}\,\dot{\sigma}_{ij} + \dot{\varepsilon}^{c}_{ij} \qquad \text{(C.2-1)}$$

where: $\dot{\varepsilon}_{ij}$ are the components of the strain tensor;

ν is Poisson's ratio;

E is Young's modulus;

δ_{ij} is the Kronecker delta;

$\dot{\sigma}_{ij}$ are the components of the stress tensor; and the creep strain rate, $\dot{\varepsilon}^{c}_{ij}$, is given by:

$$\dot{\varepsilon}^{c}_{ij} = |\dot{\varepsilon}^{c}_{kl}| \frac{\sigma'_{ij}}{|\sigma'_{mn}|} \qquad \text{(C.2-2)}$$

where: σ'_{ij} are the components of the deviatoric stress tensor.

The magnitude of the creep strain rate can be expressed in terms of the effective creep strain rate, ε, or the effective stress, σ. Thus,

$$|\dot{\varepsilon}^{c}_{ij}| = \sqrt{1.5}\,\dot{\bar{\varepsilon}} \qquad \text{(C.2-3)}$$

where the effective strain rate $\dot{\bar{\varepsilon}}$ is defined as:

$$\dot{\bar{\varepsilon}} = \left(\frac{2}{3}\, \dot{\varepsilon}^{c}_{ij}\, \dot{\varepsilon}^{c}_{ij} \right)^{1/2} \qquad \text{(C.2-4)}$$

which is the sum of the primary and secondary creep strain rates, namely

$$\dot{\bar{\varepsilon}} = \dot{\varepsilon}_p + \dot{\varepsilon}_s \qquad \text{(C.2-5)}$$

where the primary creep strain rate is defined as:

$$\dot{\varepsilon}_p = (A - B\,\varepsilon_p)\,\dot{\varepsilon}_s \qquad \text{for } \dot{\varepsilon}_s \geq \dot{\varepsilon}^*$$

and (C.2-6)

$$\dot{\varepsilon}_p = \left(A - B\,\frac{\dot{\varepsilon}^*}{\dot{\varepsilon}_s}\varepsilon_p\right)\dot{\varepsilon}_s \qquad \text{for } \dot{\varepsilon}_s < \dot{\varepsilon}^*$$

where $\dot{\varepsilon}_s$ can be defined by an exponential law

$$\dot{\varepsilon}_s = D\,\sigma^{-n}\,e^{-Q/R\Theta} \qquad \text{(C.2-7)}$$

and $\bar{\sigma} = \left(\frac{3}{2}\, \sigma'_{ij}\, \sigma'_{ij} \right)^{1/2}$ is the effective stress;

$\dot{\varepsilon}^*$, A and B are primary creep constants;

D and n are secondary creep constants;

Θ is temperature in Kelvin;

Q is the effective activation energy in cal/mole; and

R is the universal gas constant, 1.987 cal/mole-K.

C.2.2 Non-halitic Materials

In the underground facility horizon at the WIPP site, certain portions of the rock are non-halitic. The stress-strain relationship for non-halitic materials is assumed to follow the Prandtl-Reuss constitutive equation:

$$\dot{\varepsilon}_{ij} = -\frac{\nu}{E}\dot{\sigma}_{kk}\,\delta_{ij} + \frac{1+\nu}{E}\dot{\sigma}_{ij} + \dot{\varepsilon}^{P}_{ij} \qquad \text{(C.2-8)}$$

The plastic behavior is defined by the two-dimensional Mohr-Coulomb criterion:

$$\sigma_3 - \sigma_1 = 2\Theta_0\cos\beta - (\sigma_3 + \sigma_1)\sin\beta \qquad \text{(C.2-9)}$$

and the Drucker-Prager criterion, which is the generalized form of the Mohr-Coulomb criterion:

$$\sqrt{J_2'} = c - aJ_1 \qquad \text{(C.2-10)}$$

where: σ_3 and σ_1 are the two principal stresses, which are positive in tension;

Θ_0, β, c and a are the plastic constants;

$\sqrt{J_2'}$ is the second deviatoric stress invariant; and

J_1 is the first stress invariant.

The numerical modeling does not include failure criterion for the non-halitic materials. Anhydrite is assumed to be linearly elastic.

C.2.3 Clay Seams

Thin seams of clay are present between some of the rock layers. These clay seams can allow relative slippage and separation of the layers across the clay seams. The slippage of the clay seams follows a dry friction law:

$$\sigma_{12} = \mu \; |\sigma_{11}| \tag{C.2-11}$$

where: μ is the frictional coefficient; direction 1 of the stress is normal to the plan of the seam; and direction 2 of the stress is in the direction of motion or incipient motion.

C.3 FORMULATION OF GOVERNING EQUATIONS

The underground behavior of salt can be determined by solving the following governing equations:

(1) Equation of equilibrium:

$$\sigma_{ij,j} + X_i = 0 \tag{C.3-1}$$

where: σ_{ij} is the stress tensor; and
X_i is the body force vector.

(2) Strain-rate velocity relation:

$$2\dot{\varepsilon}_{ij} = \dot{u}_{i,j} + \dot{u}_{j,i} \tag{C.3-2}$$

where: $\dot{\varepsilon}_{ij}$ is the strain rate tensor;
$\dot{u}_i$ is the velocity vector; and
$(\dot{\ })$ represents the derivative of ( ) with respect to time t.

(3) Stress strain relations:
<u>halitic materials</u>

$$\dot{\varepsilon}_{ij} = -\frac{\nu}{E}\ \dot{\sigma}_{kk}\delta_{ij} + \frac{1+\nu}{E}\ \dot{\sigma}_{ij} + \dot{\varepsilon}^{c}_{ij} \tag{C.3-3}$$

where: $\dot{\varepsilon}^{c}$ is defined in subsection C.2.1.

<u>non-halitic materials</u>

$$\dot{\varepsilon}_{ij} = -\frac{\nu}{E}\ \dot{\sigma}_{kk}\ \delta_{ij} + \frac{1+\nu}{E}\ \dot{\sigma}_{ij} + \dot{\varepsilon}^{P}_{ij} \tag{C.3-4}$$

(4) Boundary conditions:

$$\dot{u}_i = \dot{U}_i \qquad \text{over } S_u \qquad \text{(C.3-5)}$$

$$\sigma_{ij} n_j = T_i \qquad \text{over } S_\sigma \qquad \text{(C.3-6)}$$

where: S_u is the surface on which $\dot{u}_i$ is specified as U_i and S_σ is the surface on which the traction vector $\sigma_{ij} n_j$ is specified as T_i where n_j is the component of the outward-pointing unit normal vector.

C.4 NORMALIZATION OF GOVERNING EQUATIONS

In order to determine the creep properties of halite, the governing equations in Section C.3 need to be solved before knowing the values of the creep constants. This can be achieved by normalizing the governing equations to the creep function and solving the normalized equations. The creep constants can then be determined by correlating the analytical results with in situ data.

Consider the creep behavior of halitic material follows a power law:

$$\dot{\varepsilon} = F \sigma^{-n} \tag{C.4-1}$$

where: F is a creep function.

The governing equations in Section C.2 can be normalized to F by transforming to a normalized time domain in terms of time t* such that:

$$dt^* = F\, dt \tag{C.4-2}$$

By substituting equation (C.4-2) into equations (C.3-1) through (C.3-6), a system of normalized equations can be formed:

(1) Equation of equilibrium:

$$\sigma_{ij,j} + X_i = 0 \tag{C.4-3}$$

(2) Strain-rate velocity relation:

$$2\dot{\varepsilon}^*_{ij} = \dot{u}^*_{i,j} + \dot{u}^*_{j,i} \tag{C.4-4}$$

where: $(\dot{\ }^*)$ represents the derivative of ( ) with respect to the normalized time t*.

(3) Stress strain relations:

<u>halitic materials</u>

$$\dot{\varepsilon}^*_{ij} = -\frac{\nu}{E}\dot{\sigma}^*_{kk}\,\delta_{ij} + \frac{1+\nu}{E}\dot{\sigma}^*_{ij} + \dot{\varepsilon}^{*c}_{ij} \tag{C.4-5}$$

$$\text{where:}\quad \dot{\varepsilon}^*_s = \sigma^{-n} \tag{C.4-6}$$

<u>non-halitic materials</u>

$$\dot{\varepsilon}^*_{ij} = -\frac{\nu}{E}\dot{\sigma}^*_{kk}\,\delta_{ij} + \frac{1+\nu}{E}\dot{\sigma}^*_{ij} + \dot{\varepsilon}^{*P}_{ij} \tag{C.4-7}$$

(4) Boundary conditions:

$$\dot{u}^*_i = \dot{U}^*_i \qquad \text{over } S_u \tag{C.4-8}$$

where: $\dot{U}^*_i$ is computed as $\dot{U}^*_i = U_i/F$

$$\sigma_{ij}n_j = T_i \qquad \text{over } S_\sigma \tag{C.4-9}$$

The above normalized governing equations are similar to the governing equations before normalization, except that the time derivatives in the normalized equations are taken with respect to normalized time t*, and the creep function F has been eliminated. Since the normalized governing equations have the same form as the governing equations before normalization, a conventional method such as the finite element technique can be used to solve the normalized governing equations for the analytical results in terms of normalized time t*, without knowing the creep function F.

After obtaining the normalized analytical result, the creep function F can be determined for establishing the relationship between the real and the normalized time domains. From Equations (C.2-5) through (C.2-7), the function F can be expressed as:

$$F = [f(\varepsilon_p, \dot{\varepsilon}_s) + 1]C \qquad (C.4\text{-}10)$$

where: $C = D\ e^{-Q/R\Theta}$; A is defined in equation (C.2-6); D, Q, R and Θ are defined in equation (C.2-7); and $f(\varepsilon_p, \varepsilon_s)$ represents the portion inside the parentheses of equation (C.2-6), which is expressed as:

$$f(\varepsilon_p, \dot{\varepsilon}_s) = A - B\ \varepsilon_p \qquad \text{for } \dot{\varepsilon}_s \geq \dot{\varepsilon}^*$$

and (C.4-11)

$$f(\varepsilon_p, \dot{\varepsilon}_s) = A - B\ \frac{\dot{\varepsilon}^*}{\dot{\varepsilon}_s} \varepsilon_p \qquad \text{for } \dot{\varepsilon}_s < \dot{\varepsilon}^*$$

From equation (C.4-11), it can be found that at time $t = 0$, $\varepsilon_p = 0$, which provides an initial condition:

$$f(\varepsilon_p, \dot{\varepsilon}_s) = A \qquad \text{for } t = 0 \qquad (C.4\text{-}12)$$

When the time t approaches the steady state stage t_s, primary creep is no longer active. Therefore:

$$f(\varepsilon_p, \dot{\varepsilon}_s) \rightarrow 0 \qquad \text{for } t \rightarrow t_s \qquad (C.4\text{-}13)$$

since the primary creep decreases exponentially with time (ref. C-1). Based on the auxiliary conditions (C.4-12) and (C.4-13), the function f can be expressed as an exponential function:

$$f = A\ e^{-zt} \qquad (C.4\text{-}14)$$

By substituting equation (C.4-14) into equation (C.4-1), function F can be written as:

$$F = [A\ e^{-zt} + 1]C \qquad (C.4\text{-}15)$$

where: the constants C, A and z can be determined from in situ data.

The relationship between the real time domain and the normalized time domain can then be obtained by integrating equation (C.4-2):

$$t^* = \int_0^t F\ dt \qquad (C.4\text{-}16)$$

Substituting equation (C.4-15) into equation (C.4-16) and using the initial condition t* = 0, when t = 0, equation (C.4-16) becomes:

$$t^* = C\ [t + A/z\ (1 - e^{-zt})] \qquad (C.4\text{-}17)$$

After determining the creep constants, the analytical results can then be mapped from the normalized time domain to the real time domain using equation (C.4-17).

C.5 DETERMINATION OF CREEP CONSTANTS

The computational method can also be considered as a two-phased process which allows structural responses to be determined for any time in question. The first phase is a transformation from the real to the normalized time domain by use of parametric equations containing creep constants. The second phase is relating a structural response to that the normalized time by performing a structural analysis. The fundamental relationship can be represented graphically as shown on Figure C-1. The upper curve indicates the expression relating the two time domains which depends on the creep constants C, A and z. The double vertical axes represent the relationship between the normalized time t* and response as indicated by the results of the structural analysis.

The terms A and z represent primary creep constants that can be viewed in a number of ways. By themselves, 'A' relates the ratio of initial to steady-state creep rates and 'z' corresponds to the primary creep decay constant. A simplified relationship can be used utilizing only the ratio of A to z when the term inside the parentheses in equation (C.4-15) approaches unity in the steady-state period. As Figure C-2 indicates, the value of A/z (also identified as t_0) represents a real time offset such that the following equation can be used:

$$t^* = C\ (t + A/z) \qquad \text{(C.5-1)}$$

A Salt Creep Constant Evaluation computer program (SCCE, Bechtel computer program CE 465) was developed for the purpose of evaluating the creep constants from in situ data.

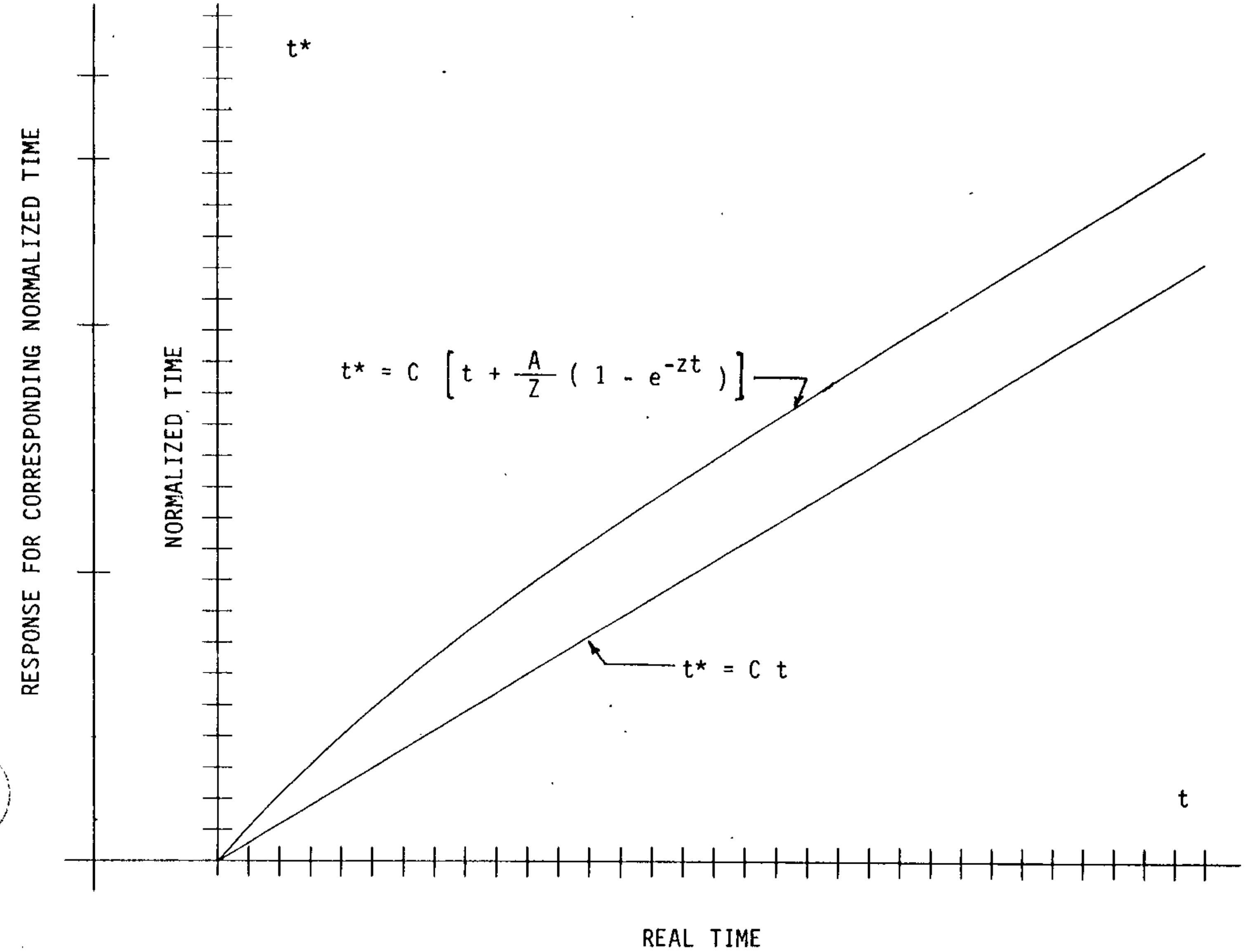

FIGURE C-1

TIME RESPONSE RELATIONSHIP OF THE NORMALIZED CREEP ANALYSIS METHOD

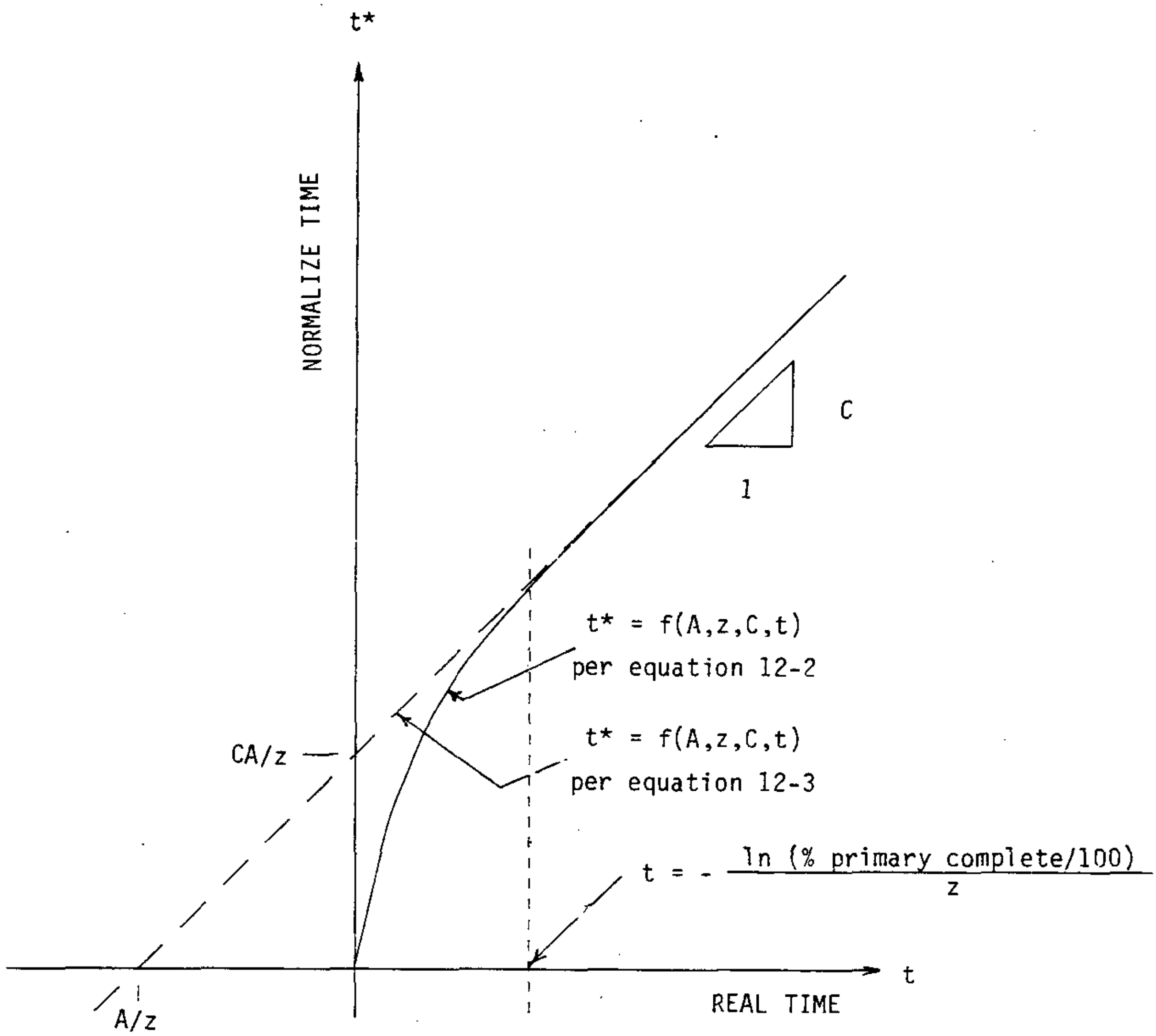

FIGURE C-2

GRAPHICAL REPRESENTATION OF

CREEP CONSTANTS RELATING TIME DOMAINS

The link between real time and response is completed by relating the normalized time to the response determined from the structural analysis. In brief, if the creep constants are known, the normalized time associated with any real time can be determined from equation (C.4-17) and the response corresponding to this time is found from the analysis results. Conversely, if in situ data which relates real time to response is available, this two-phased process can be worked backwards to evaluate the creep constants.

Because the response in both the in situ measurements and the structural analysis must be consistent, the displacements caused by creep are related.

In the analysis, the total response is an accumulation of elastic and creep responses,

$$R_t(t^*) = R_c(t^*) + R_e(t^*) \qquad \text{(C.5-2)}$$

where: R_t is the total response;
R_c is the creep response; and
R_e is the elastic response.

In as much as the total response at time $t^* = 0$ consists of elastic response only, and the elastic response $R_e(t^*)$ is always approximately equal to $R_t(0)$, the following equation can be used in lieu of equation (C.5-2):

$$R_c(t^*) = R_t(t^*) - R_t(0) \qquad \text{(C.5-3)}$$

The in situ readings represent the response relative to the time when the instrument was installed. In order for an actual creep response to be determined, the creep response which takes place between the time the excavation was made and the time when the instrument was installed must be found. Theoretically, if an instrument had been installed very shortly after excavation, this difference between measured and actual creep responses would be negligible. In reality, the excavation of all material contributing to the support of a specific location in an opening cannot be completed within a few days. As a result, the measured response from an instrument installed immediately after excavation would be a combination of initial creep and elastic responses. The term "instrument offset" is introduced to identify the difference between the actual creep response and the measured response starting at time t_1 when nearby excavations no longer introduce initial creep and elastic responses. This relationship is shown below:

$$R_I(t) = R_M(t) + R_I(t_1) \qquad \text{(C.5-4)}$$

where: R_I is the actual in situ response;
R_M is the measured response; and
$R_I(t_1)$ is the instrument offset.

Determination of the constant C, which represents the steady state creep rate, requires that the in situ readings are well into the steady state range. If this is the case, the relationship

$$dt^* = F\ dt \qquad \text{(C.5-5)}$$

can be used to determine the value of C since C equals F at very large values of t. The expression for C is:

$$C = (t^*_n - t^*_m) \ / \ (t_n - t_m) \qquad \text{(C.5-6)}$$

If t_m and t_n represent the times at which instrument readings are taken and $R_I(t_m)$ and $R_I(t_n)$ are the actual creep responses at these times, then the values of t^*_m and t^*_n can be found by relating these actual in situ creep responses with the analytical creep responses.

Assuming for the moment that the true value of instrument offset is known, equation (C.4-15) can be written for two time-response situations to produce two simultaneous equations which contain only the two remaining creep constants, A and z. By cancelling out the A term, the solution of the following equation provides the value of z.

$$\frac{1 - e^{-zt_n}}{1 - e^{-zt_m}} - \frac{t^*_n/C - t_n}{t^*_m/C - t_m} = 0 \qquad (C.5\text{-}7)$$

Once the value of z is found to satisfy the expression, A can be found from the following equation:

$$A = z\ (t_m^*/C - t_m)\ /\ (1 - e^{-zt}) \qquad (C.5\text{-}8)$$

Graphically this method determines constants which force the analytical curve to match the in situ data at the two time-response situations used in calculating the constants. Each different set of data points yields different values of A and z. Figure C-3 compares analytical and in situ responses for a few different sets of data points. Whereas creep behavior is history dependent, matching the last available data point is advantageous in predicting future responses. The determination of best values of A and z is done by minimizing the area between in situ and analytic response histories. The least area yields the best values. The SCCE program can be set up to search for this optimal condition.

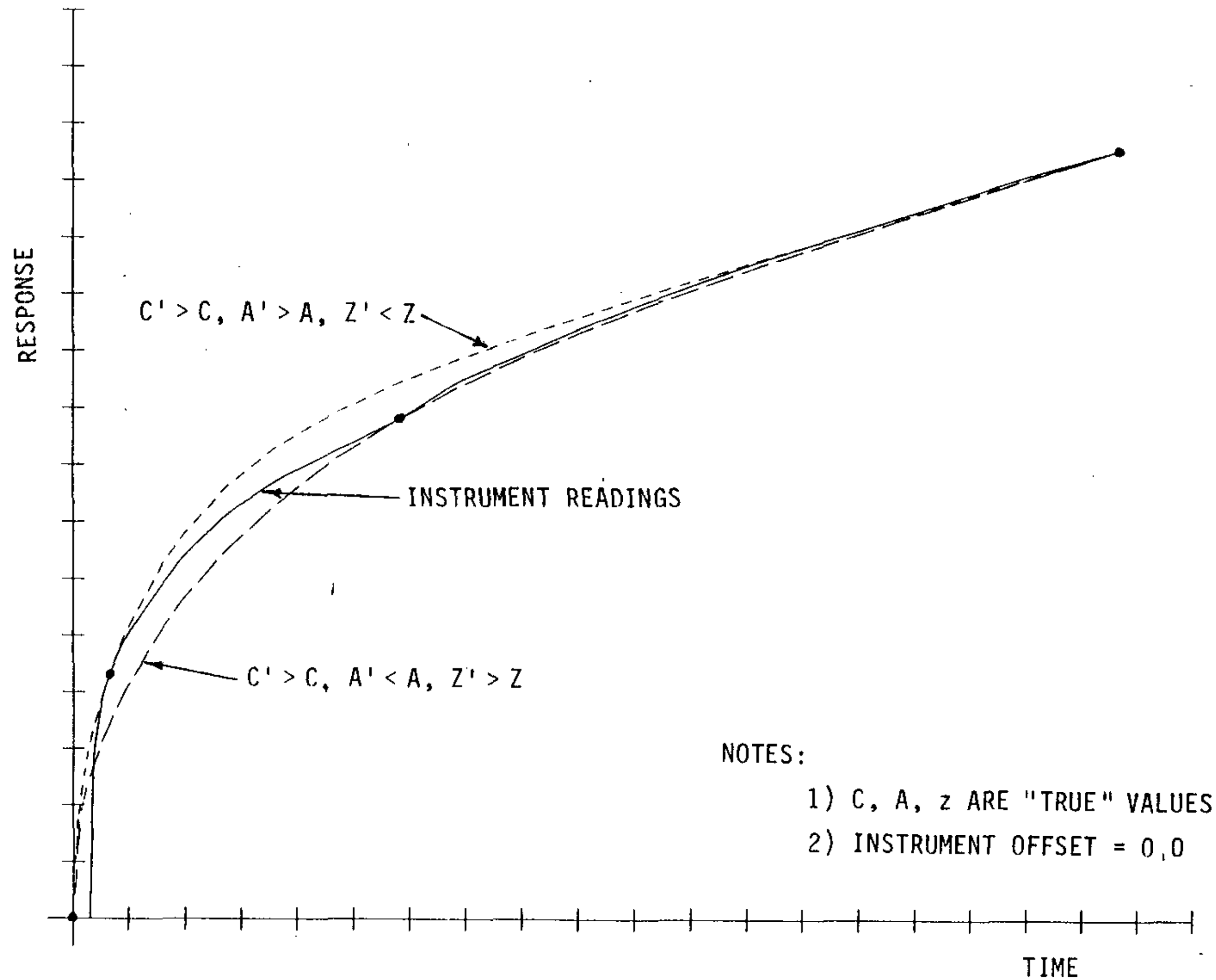

FIGURE C-3

COMPARISON OF ANALYTICAL RESULTS AND IN-SITU RESPONSES FOR VARIOUS DATA POINT SETS

The point which must be kept in perspective is that the determination of the constants A and z are dependent on both the instrument offset and the steady-state creep constant C. The effects of uncertainty in C can be minimized by assuring that no extraneous data are used in the solution of equation (C.5-6). The appropriate value of the instrument offset can only be found from minimizing the response deviation as was described in the previous paragraph. Figure C-4 shows how analytical and in situ responses compare for a few different values of the instrument offset. The curves in Figures C-3 and C-4 were generated through use of the SCCE program.

The SCCE computer program provides an effective means of determining salt creep properties by being able to process the large volume of in situ data and analytical results for design validation.

C.6 PREDICTION OF STRUCTURAL BEHAVIOR

After the creep constants C, A and z are determined, the structural response history can then be mapped from the normalized time domain into the real time domain using equation (C.4-15). Utilizing the in situ creep constants, additional mathematical models can also be used to predict the future structural responses for various facilities.

C.7 CONCLUSIONS

By normalizing the time in the governing equations to the creep function, the structural responses can be computed as functions of normalized time. This computation is performed without knowing the creep constants. After correlating the response history obtained from the analysis to the corresponding one measured from the site, the creep constants can be determined. Consequently, the relationship between the normalized and real time can be established, and the analytical responses can be mapped from the normalized time domain to the real time domain. Predicted results can therefore be provided for validating the adequacy of the underground behavior in the salt formation.

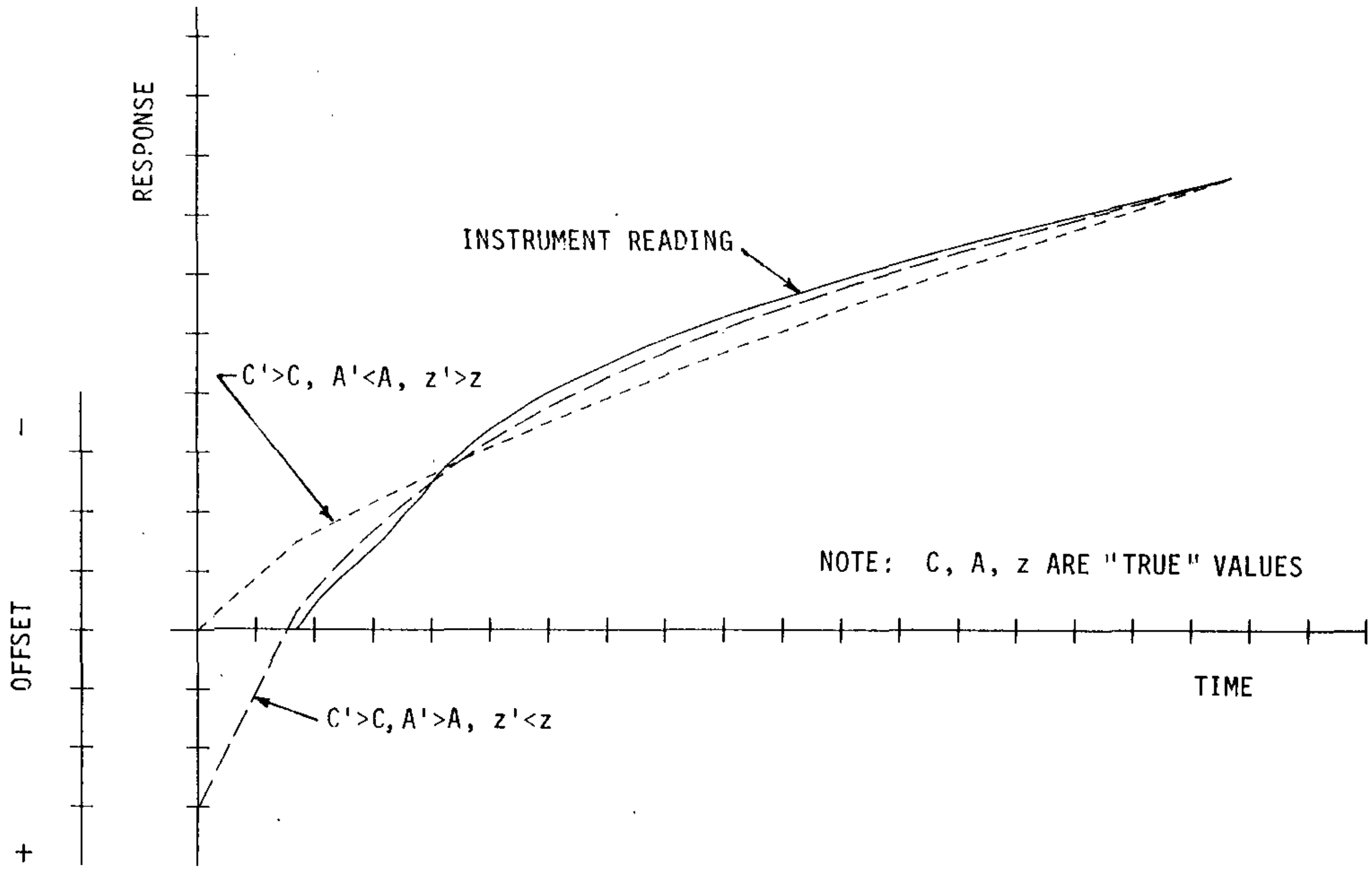

FIGURE C-4

COMPARISON OF ANALYTICAL RESULTS AND IN-SITU RESPONSE FOR VARIOUS INSTRUMENT OFFSET VALUES

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