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DESCRIPTION OF THE THERMOELASTIC/PLASTIC COMPUTER PROGRAM TEPCO

Memorandum Report RSI-0040

William G. Pariseau

September 15, 1975

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MEMORANDUM REPORT RSI-0040

DESCRIPTION OF THE THERMOELASTIC/PLASTIC COMPUTER PROGRAM TEPCO

Submitted To

Holifield National Laboratory
Oak Ridge, Tennessee

Operated By

Union Carbide Corporation
Nuclear Division
for the
Energy Research and Development Administration

by

William G. Pariseau

RE/SPEC INC.
P. O. BOX 725 - RAPID CITY, S. D. 57701 - 605/343-7868

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FOREWORD

The contents of this report have been reviewed by Dr. Paul F. Gnirk, Dr. Arlo F. Fossum, and Mr. Joe L. Ratigan of RE/SPEC Inc.

(RSI-0040)

RE/SPEC INC.

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September 15, 1975

MEMORANDUM REPORT RSI-0040

TO: Dr. William C. McClain
Holifield National Laboratory
P. O. Box Y
Oak Ridge, TN 37830

FROM: Dr. William G. Pariseau
RE/SPEC Inc.
P. O. Box 725
Rapid City, SD 57701

SUBJECT: Description of the Thermoelastic/Plastic Computer Program TEPCO (Union Carbide Corporation, Nuclear Division Subcontract NO. 4269, RSI/001000/FY76).

1. INTRODUCTION

The purpose of this report is to present a description of the two-dimensional (plane strain, axial symmetry) thermoelastic/plastic computer program TEPCO utilized by RE/SPEC Inc. in conjunction with an investigation of rock mechanics aspects of underground radioactive waste disposal. The program shares many features with other small scale finite element programs. Unusual features relate to mine-out capability and temperature dependent yielding of anisotropic (orthotropic) materials. The program is a modified and extended version of a previously developed basic isothermal code written expressly for rock mechanics analyses of surface and underground excavations. The basic code has also been modified for elastic/plastic analyses of rock mechanics problems involving time dependent material properties. The time and temperature dependent formulations are similar in many respects. Because of this fact, much of the contents of this report describing the temperature dependent formulation are taken verbatim from a section of a report describing the time dependent program.* There are, of course, essential differences between the time and temperature dependent programs.

*Pariseau, W. G. "Interpretation of Rock Mechanics Data: Single Entry System, Sunnyside Mine, Utah", Annual Report, H0220077, USMB/SMRC, June, 1973.

2. PROGRAM DESCRIPTION

2.1. Introductory Remarks

Most rocks and soils respond elastically to an initial application of load, but eventually undergo permanent deformation and fail. Permanent deformation of a material with a well defined yield point is plastic deformation. An appropriate mathematical model is the elastic-plastic idealization. Numerous mechanisms for permanent deformation of rock exist. Among them are micro-cracking and more generally cataclasis as well as dislocation mechanisms.

Plasticity theory for gravitating geologic media is nonlinear in even the simplest formulations. Analytical solution to problems of interest is a practical impossibility and resort to numerical techniques is required. Finite element methods are therefore essential to stability analyses of underground mine openings. Finite difference approaches are not generally competitive with finite element techniques.

Most small scale finite element programs have much in common. Real differences arise in the formulation of element response which in turn depends on the stress-strain relations assumed for the material. A clearly exhibited analytical statement of the stress strain law is therefore essential to proper computer code development. Once this statement is obtained, the element response can be determined and programming can proceed. Attempts to analyze complicated material behavior with finite element programs based on simplified material models should be viewed with skepticism.

The stress-strain relationship (or constitutive equation) is the heart of the theory. The key to computer code development is the element response. The latter depends on the former; both are discussed below. In addition, the organization of the program is described, and example problems are presented.

2.2. Plasticity Theory for Geologic Media

2.2.1. Governing Equations

The principal groups of equations describing the quasi-static behavior of elastic-plastic media are:

(a) stress equations of equilibrium;

(b) equations of deformation geometry;

(c) stress strain relations (constitutive equations);

(d) yield function.

Equilibrium and deformation geometry are independent of the material. The yield function is determined by experiment and testing. Strain increments are assumed small, so that the total strain increment is composed of elastic and plastic parts. The elastic contribution is computed from Hooke's law; the plastic contribution is computed from the yield function taken as a plastic potential according to Drucker's stability postulate(2). Yield functions and failure criteria play central roles in plasticity theory.

Two general types of yield functions are in common use: (1) those influenced by the intermediate principal stress, and (2) those that are not. The latter are the well known Mohr-Coulomb (or extended Tresca) type; the former may be referred to as the extended von Mises type. Mohr-Coulomb criteria may be the more appropriate physically, but von Mises types are mathematically more tractable. Finite element programs that employ rigorous treatment of Mohr-Coulomb yield are unknown to the writer. An extended von Mises type of yield condition appropriate to rock is used in the present work.

2.2.2. Stress Strain Relations

For material in the elastic domain, the strains e_{ij} are related to the stress σ_{ij} by Hooke's law in incremental form

$$de_{ij} = H^{-1}_{ijk\ell} d\sigma_{k\ell} \tag{2-1}$$

where $H^{-1}_{ijk\ell}$ are the inverse elastic coefficients. Subscript notation and summation convention are in force. In the elastic-plastic domain

$$de_{ij} = H^{-1}_{ijk\ell} d\sigma_{k\ell} + \lambda \frac{\partial Y}{\partial \sigma_{ij}} \tag{2-2}$$

where λ is an unknown scalar function and Y is the yield condition. Difficulties obviously rise if Y is not continuously differentiable. This is the case for all Mohr-Coulomb yield criteria. Such criteria lead to singular yield functions. In principle, these difficulties can be overcome.

Equation (2-2) must be inverted for finite element coding. Early attempts to avoid this task resulted in a number of special treatments of plasticity, some of which are now known to lead to numerical instabilities. Inversion of equation (2-2) depends on the nature of the yield function Y. The simplest case occurs for linear, non-hardening, isotropic materials with constant properties.

Inversion for this case and the more complicated hardening case are described by Marcal[2] and Zienkiewicz[3].

In the present work, the yield function is one proposed originally by Pariseau[4] and the anisotropic (orthotropic) geologic media:

$$Y = \{F(\sigma_{yy}-\sigma_{zz})^2 + G(\sigma_{zz}-\sigma_{xx})^2 + H(\sigma_{xx}-\sigma_{yy})^2$$

$$+ L\sigma_{yz}^2 + M\sigma_{zx}^2 + N\sigma_{xy}^2\}^{(n/2)}$$

$$+ (U\sigma_{xx} + V\sigma_{yy} + W\sigma_{zz}) - 1 \qquad (2\text{-}3)$$

where x,y,z are the principal axes of anisotropy and n = 1 or n = 2 in the present computer program. Other values of n are possible, of course.

In several recent reports[5], the yield function (2-3) is erroneously attributed to Hill[6]. Hill's formulation is intended for metal plasticity problems and therefore includes only deviatoric stresses. However, geologic media are characterized by confining pressure dependency. Anisotropic geologic media therefore require the appearance of the direct stresses in the yield condition. Inclusion of the direct stresses leads to a considerable increase in mathematical complexity[4]. Addition of the last three stress terms in equation (2-3) is by no means trivial.

The nine plastic moduli (F,G,H,L,M,N,U,V,W,) are expressable in terms of the more familiar unconfined tensile, compressive and shear strengths obtained by routine testing. Equation (2-3) reduces to the isotropic case for vanishing anisotropy and contains Hill's criteria for anisotropic metals as a special case.

If the plastic moduli are temperature dependent, then $F = F(T)$, $G = G(T)$, etc. If the material is also hardening, then $F = F(T, e_{ij}^p)$, etc. where e_{ij}^p are the plastic components of strain. Other factors such as temperature and moisture content may also influence yield. More generally, if the plastic moduli are denoted as α_{ij} and the N parameters of interest as β_n $(n = 1,2,\text{---}N)$, then $\alpha_{ij} = \alpha_{ij}(\beta_n, e_{k\ell}^p)$.

---

* The sign convention for the linear terms in stress depends on the algebraic sign designation for tension.

For plastically deforming elements $dY = 0$, thus

$$0 = (\partial Y/\partial \sigma_{ij}) d\sigma_{ij} + (\partial Y/\partial \alpha_{ij})(\partial \alpha_{ij}/\partial e^{P}_{k\ell}) de^{P}_{k\ell}$$

$$+ (\partial Y/\partial \alpha_{ij})(\partial \alpha_{ij}/\partial \beta_n) d\beta_n \qquad (2\text{-}4)$$

The required inversion of equation (2-2) is accomplished by using equations (2-3) and (2-4) in equation (2-2); λ is eliminated in the process. The result is:

$$d\sigma_{k\ell} = \left[H_{ijk\ell} - \frac{H_{mnkl}(\partial Y/\partial \sigma_{mn})(\partial Y/\partial \sigma_{pq}) H_{ijpq}}{D} \right]$$

$$\times \left[de_{ij} - \sigma_{k\ell} \, (\partial H^{-1}_{ijk\ell}/\partial \beta_n) d\beta_n \right]$$

$$- \left[\frac{H_{ijk\ell}(\partial Y/\partial \sigma_{ij})(\partial Y/\partial \alpha_{pq})(\partial \alpha_{pq}/\partial \beta_n) d\beta_n}{D} \right] \qquad (2\text{-}5\text{-}A)$$

where

$$D = (\partial Y/\partial \sigma_{k\ell}) \, H_{ijk\ell} \, (\partial Y/\partial \sigma_{ij})$$

$$-(\partial Y/\partial \alpha_{ij})(\partial \alpha_{ij}/\partial e^{P}_{k\ell})(\partial Y/\partial \sigma_{k\ell}) \qquad (2\text{-}5\text{-}B)$$

and dependency on stress and β_n of the elastic coefficients has been introduced. This formulation is an extension of the work of Hibbitt and Marcal in metal plasticity[9].

With $\beta_1 = T$ (temperature) and all other $\beta = 0$, equation (2-5) in matrix form is

$$\{\Delta\sigma\} = ([E] - [EP])(\{\Delta e\} - \{\overline{E}'\}) - \{\overline{Y}'\} \qquad (2\text{-}6)$$

Where { } denote 6x1 column matrices and [ ] are 6x6 square matrices. Terms of equations (2-5-A) and (2-6) correspond to the order in which they are written. The prime is used to signify temperature differentiation. If the elastic and plastic moduli do not vary with temperature, then the last two terms of equation (2-6) vanish.

2.2.3. Element Response

Element response can be developed from the virtual work identity[7] and equation (2-6). The virtual work identity for continuous fields is

$$\int_A S_i u_i dA + \int_V S_i u_i dV = \int_V \Sigma_{ij}\varepsilon_{ij} dV \qquad (2\text{-}7)$$

where the surface A bounds the volume V; S_i are surface tractions; u_i are displacements; X_i are body force components per unit volume; Σ_{ij} are the components of equilibrium stress, and ε_{ij} are the strain components derived from the u_i.

Introducing the matrix notation of Zienkiewicz[3], equation (2-7) in incremental form is

$$\{\Delta F_n\} + \{\Delta F_g\} + \{\Delta F_\sigma\} = \int_V [B]^T \{\Delta\sigma\} dV \qquad (2\text{-}8)$$

where:

$\{F_n\} = \int_A [N]^T \{S\} dA$ = nodal forces prescribed on A

$\{F_g\} = \int_V [N]^T \{X\} dV$ = nodal forces due to gravity

$\{F_\sigma\} = -\int_V [B]^T \{\sigma_o\} dV$ = nodal forces due to initial stress

$\Sigma_{ij} = \sigma_{ij} + \sigma^o_{ij}$ = equilibrium stress

$\varepsilon_{ij} = e_{ij} + e^o_{ij}$ = strains derived from displacements

$\{\varepsilon\} = [B]\{u_n\}$ = nodal displacements to element strain transformation

$\{u\} = [N]\{u_n\}$ = nodal displacement to element displacement transformation

$\{u_n\}$ = matrix of nodal displacements

Δ = increment

$[\ ]^T$ = transpose

σ^o_{ij} = initial stress

e^o_{ij} = initial strain

and σ_{ij} is stress associated with e_{ij}. Figure 1 illustrates the stress strain relations. Substitution of equation (2-6) into (2-8) results in:

$$\{\Delta F_n\} + \{\Delta F_g\} + \{\Delta F_\sigma\} + \{\Delta F_e\} + \{\Delta F_Y\} + \{\Delta F_E\} = [k]\{\Delta u_n\} \tag{2-9}$$

where

$\{F_e\} = \int_V [B]^T([E] - [EP])\ \{e_o\} dV$ = nodal forces due to initial strain

$\{\Delta F_E\} = \int_V [B]^T([E] - [EP])\{\bar{E}'\} dV$ = nodal force due to change in elastic coefficients

$\{\Delta F_Y\} = \int_V [B]^T\{\bar{Y}'\} dV$ = nodal force due to change in plastic coefficients

$[k] = \int_V [B]^T([E] - [EP])[B] dV$ = element stiffness matrix

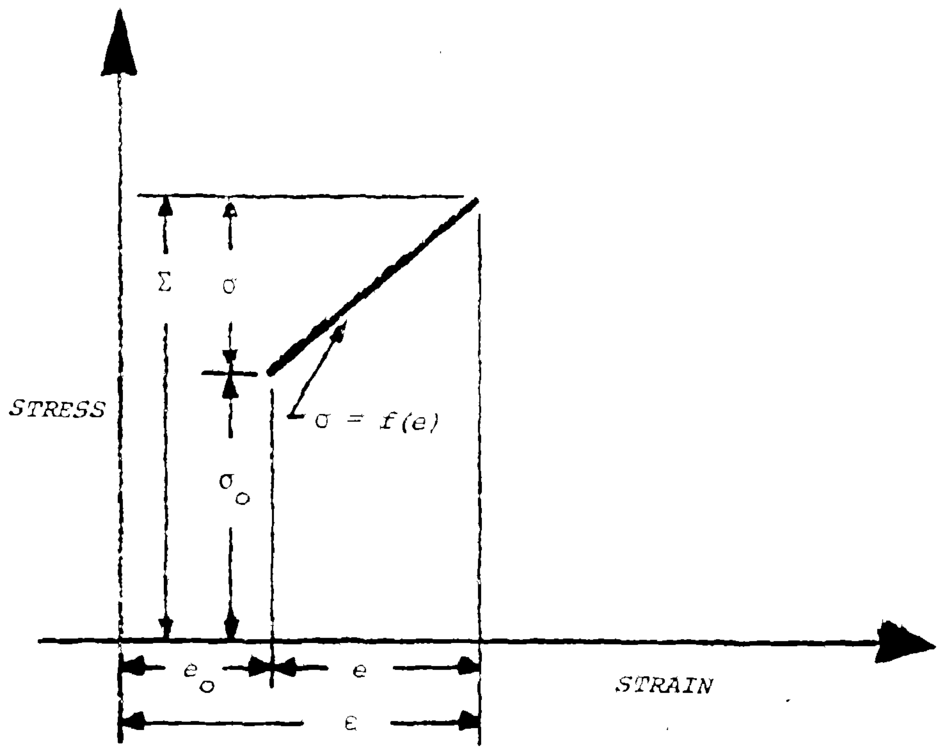

Figure 1. Stress Strain Relations

2.3. Program Organization

2.3.1. Basic Elements and Capabilities of the Program

The program is currently capable of handling two dimensional (plane strain, axial symmetry) problems involving temperature dependent, anisotropic, non-hardening, gravitating elastic-plastic materials that may be initially stressed. Arbitrary sequences of cuts and fills simulating mining operations are possible. Linear and nonlinear extended von Mises yield conditions for anistropic geologic materials are available. Nonlinearities in material properties can be approximated.

The program consists of a mainline and eight subroutines. Mainline logic acts as an executive routine calling subroutines for specialized tasks and performing other necessary calculations. Figure 2 illustrates the thought flow. The subroutine names are ELSTIF, ASSEM, SOLVE, WRITER, ELYELD, AXES, TMODUL, and TFORCE. The names suggest their purpose. ELSTIF formulates element stiffness matrices. ASSEM adds and subtracts element stiffness from the master stiffness matrix. SOLVE is the equation solver. WRITER prints the results of the analysis. ELYELD locates the intersection of load paths with the current yield surface. AXES accounts for boundary conditions specified in local rather than global coordinates. TMODUL reads data and calculates moduli as functions of temperature. TFORCE calculates temperature dependent loads. The program is similar in some ways to one written by Dahl[8], but differs considerably in the ELSTIF subroutine logic, in the temperature dependent capability, in handling transition elements, and in local coordinate boundary specifications.

2.3.2. Element Stiffness Matrix

The ELSTIF subroutine forms three important matrices; i.e., the material property matrices $[E]$ and $[EP]$, the matrix $[B]$ and the element stiffness matrix $[S]$. The latter need not always be formed.

2.3.3. Master Stiffness Matrix

Assembly of element stiffness matrices into the master stiffness is performed in the subroutine ASSEM. A call of ASSEM may also result in removal of an element stiffness matrix from the master stiffness matrix. This occurs during updating of the master stiffness matrix. Only elements in the plastic domain require updating.

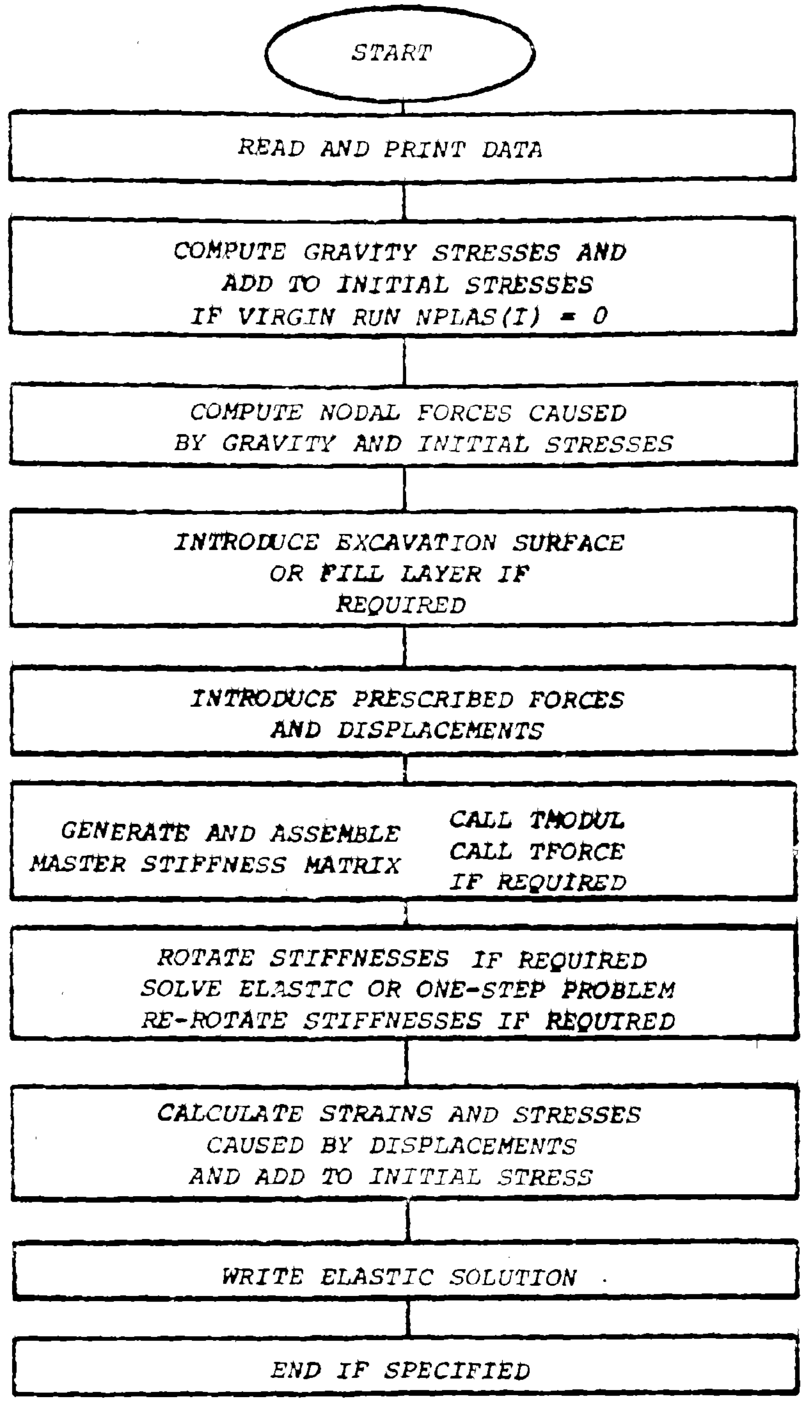

Figure 2. Program Thought Flow

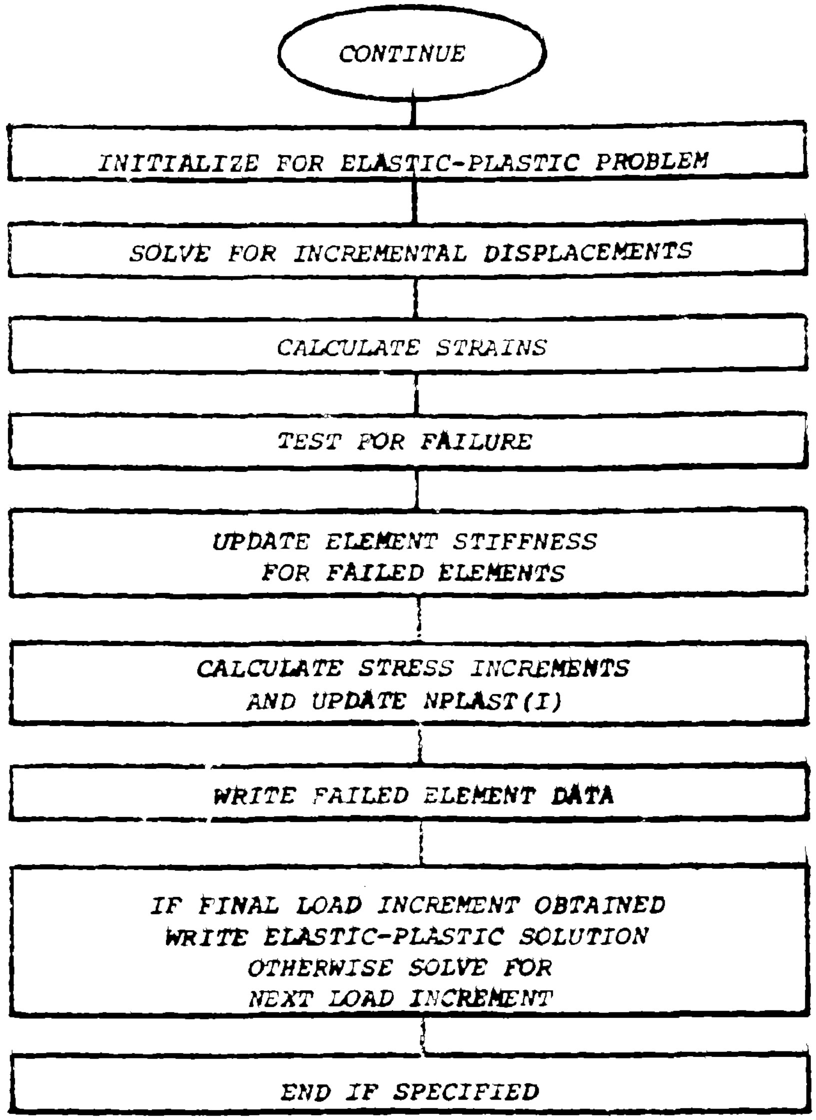

Figure 2, Cont'd. Program Thought Flow

2.3.4. Equation Solver

The assembled system of equations has the form $\{F\} = [K]\{U\}$, where $\{F\}$ and $\{U\}$ are the nodal point forces and displacement; $[K]$ is the master stiffness matrix. Gauss-Seidel line iteration is used to solve the system for the unknown displacements. Iterative methods are preferred over direct methods for solving large sparse systems of equations. They tend to be self-corrective in contrast to direct methods(10). If a nodal point displacement component is prescribed, the corresponding row equation is simply skipped during the iteration. No manipulation of the master stiffness matrix is required. This approach gives great flexibility in the prescription of boundary conditions. For example, maximum displacements as well as displacements can be specified.

The differential, nonlinear form of the stress-strain law indicates that final loads should be applied in increments. Iteration then occurs within each load step. Iteration, that is a call of the solver subroutine, can also be done between load steps. This procedure has several forms. The basic aim is to reduce the difference between the applied loads and deformation forces before proceding to the next load step, and thus to reduce possible error accumulation. If the residuals are used as a closeness of solution measure rather than displacements, then the procedure is of little value. Residuals are used in the SOLVE subroutine, and calls of SOLVE between load steps are not made.

A procedure that is sometimes helpful in reducing cumulative error consists of computing the difference $\{R\}_n$ between applied forces $\{F\}_n$ and internal forces $\{S\}_n$ at the end of the $n\underline{th}$ load step and adding the difference to the $n+1$ load increment $\{\Delta F\}_{n+1}$ before calling the solve subroutine. Physically this procedure uses nodal force imbalance as a force in its own right to move nodal points closer to equilibrium positions. Mathematically it amounts to replacing load increment $\{\Delta F\}_{n+1}$ by $\{F\}_{n+1} - \{S\}_n$, where $\{S\}_n = \int_V [B]^T \{\sigma\}_n dV$. The subscript n denotes quantities at the end of the $n\underline{th}$ load increment. The procedure is reminiscent of the Newton-Raphson technique(3) applied incrementally for one cycle. The stresses $\{\sigma\}$ are computed from displacements and do not include initial stresses. If initial stresses are present, as in the analysis of underground mine openings, the procedure requires modification.

Plasticity problems are highly nonlinear and consequently so is the resulting system of algebraic equations. Error is inevitable and always unknown unless a closed form solution is available. None are known to the writer, although some rigid-plastic (in contrast to elastic-plastic) stress distributions are available. The only real way of controlling error is by reducing the size of the load step. The incremental nature of the process then more closely approximates the differential nature of the stress-strain relations. Ten load steps appear adequate for most problems. If a very large plastic zone develops, as many as 20 load steps may be desirable.

2.3.5. Transition Elements

Elements that undergo transition from the elastic to the elastic-plastic domain during an increment of load require special treatment. Since all quantities remain constant during a load step, transition elements have stress points that move beyond the yield surface along an elastic load line as illustrated in Figure 3. In fact, only a fraction of the load line should be traversed elastically. The portion of the load applied after the stress point contacts the yield surface should cause elastic-plastic deformation. If the load path fraction is known, the stresses can be calculated correctly.

During the load step

$$\{\Delta\sigma\}=[E]\{\Delta\varepsilon\},$$
$$Y(\{\sigma_o\}+(f)\{\Delta\sigma\})=0. \qquad (2\text{-}10)$$

Equation (2-10) is a quadratic that can be solved for load fraction f. The subroutine ELYELD calculates f. The correct stress is then

$$\{\Delta\sigma\}=(f[E]+(1-f)([E]-[EP]))\{\Delta\varepsilon\}$$

An alternative method that appears to work satisfactorily is to estimate f by substituting $(1/n)\{\sigma\}$ for $\{\sigma_o\}+f\{\Delta\sigma\}$, so that $Y((1/n)\{\sigma\}) = 1$ which can be solved for n. The stress at the yield surface is $\{\sigma\}/n$, and the increment of stress that occurs thereafter to completion of the load step is $\{\Delta\sigma\} = ([E]-[EP])\ \{\Delta e^P\}$ with $\{\Delta e^P\} = (1-\frac{1}{n})\{\varepsilon\}$. If initial strains or strains corresponding to initial stresses are present, these must be added to $\{\varepsilon\}$. Considerable error may result otherwise.

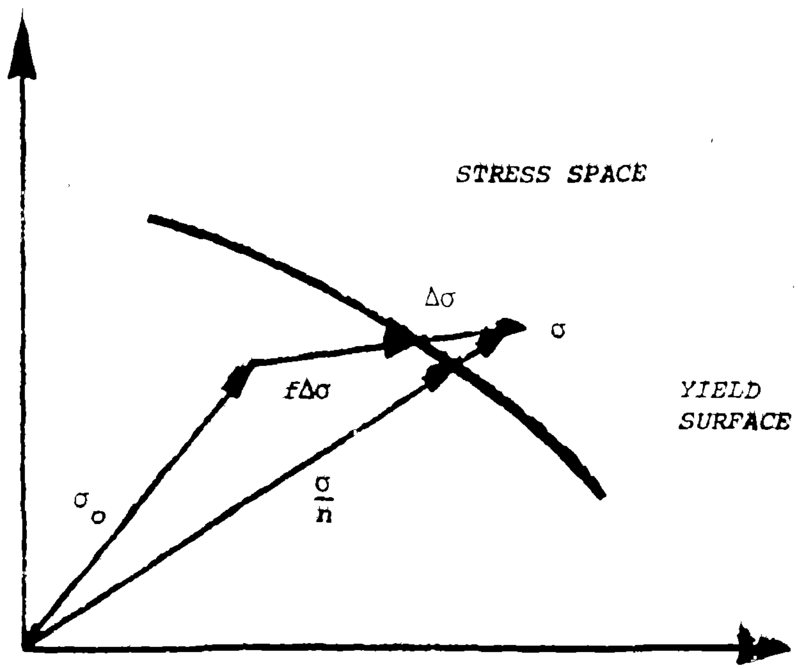

Figure 3. Transition Element Stress Changes

Elements are free to unload and return to the elastic domain from the elastic-plastic domain. All elements are tested for yield, and the stiffness matrices of all transition elements are updated after each step.

2.3.6. Boundary Conditions in Local Coordinates

The subroutine AXES transforms the master stiffness matrix, forces, and displacements to nodal point or local coordinates and back to global coordinates as required before entering and after exiting the solve subroutine. The transformation is a simple rotation. If local coordinates are the primed system and global the unprimed system and α is the angle between them, then

$$\{F_i'\}=[A_i]\{F_i\} \; ; \; \{U_i'\}=[A_i]\{U_i\} \; ; \; [A_i]= \begin{bmatrix} \cos(\alpha_i) & \sin(\alpha_i) \\ -\sin(\alpha_i) & \cos(\alpha_i) \end{bmatrix}$$

Expression of the forces and displacements at the ith node in local coordinates requires pre-multiplication of the ith 2x2 row and post-multiplication of the ith 2x2 column of the master stiffness matrix $[K]$ by $[A_i]$ and $[A_i^{-1}]$, respectively. These operations are performed by subroutine AXES.

2.3.7. Temperature Dependent Moduli

The subroutine TMODUL calculates present values of all material properties from specified functions of temperature. Derivatives of material properties with respect to temperature are also calculated in TMODUL. Let the temperature dependent material properties be $\alpha_{ij}=\alpha_{ij}(T)$. As material properties, the functions α_{ij} are assumed known from experiment and to be adequately represented by polynomials in the form:

$$\alpha_{ij}(T)=\alpha_{ij}^{o}+\sum_{k=1}^{n} a_k T^k \qquad \text{(n is some convenient number)}$$

where α_{ij}^{o} is the value of α_{ij} at the reference temperature T_o, and T is the temperature change from the reference temperature. In practical terms, α_{ij}^{o} is the value of α_{ij} just before mining and T is the temperature change since mining. The premining state is the reference state. Temperature dependent properties result in temperature dependent deformations.

3. EXAMPLE PROBLEMS

3.1. General Problem Definition

Two example problems involving a heated hollow cylinder are presented in abbreviated graphical form. These examples are almost trivial finite element calculations, but have been made for comparison purposes with available analytical solutions. The two problems are: (1) the hollow cylinder differentially heated under plane strain conditions, and (2) the hollow cylinder heated uniformly to plastic failure, also under plane strain conditions. Agreement between the finite-element and analytical results is excellent. Additional details and more complicated example problems illustrating TEPCO code capability and useage may be found in the Summary Progress Report RSI-0005 "Analysis and Evaluation of the Rock Mechanics Aspects of the Proposed Salt Mine Repository" of September 1973 [11].

3.2. Thermoelastic Hollow Cylinder Problem

Consider a hollow steel cylinder that is subjected to a steady differential temperature of 500°F between the inner and outer walls, with the maximum (constant) surface temperature applied at the outer wall. The deformation parallel to the axis of the cylinder is restricted to zero, i.e. a prescribed condition of plane strain. The cylinder is free of any surface tractions on body forces. The elastic stress and displacement fields are strictly induced by the steady differential temperature distribution across the wall of the hollow cylinder. The temperature distribution in the cylinder wall, as calculated by the computer code TRANCO [12], and the corresponding thermoelastic stress distributions, as calculated by the computer code TEPCO, are presented in Figures 4 and 5, respectively. In both instances, the comparison between the analytical and finite-element results is excellent.

3.3. Thermoelastic/Plastic Hollow Cylinder Problem

Consider a hollow cylinder that is uniformly heated to a temperature of 500°F. The deformation parallel to the axis of the cylinder is restricted to zero, i.e. a condition of plane strain. The cylinder is free of any surface tractions or body forces. As a consequence of the uniform temperature increase, the wall of the cylinder becomes uniformly plastic at a temperature of 308°F. The comparison between the theoretical and finite-element stress distributions at a uniform temperature of 500°F, illustrated in Figure 6, is exceptionally good.

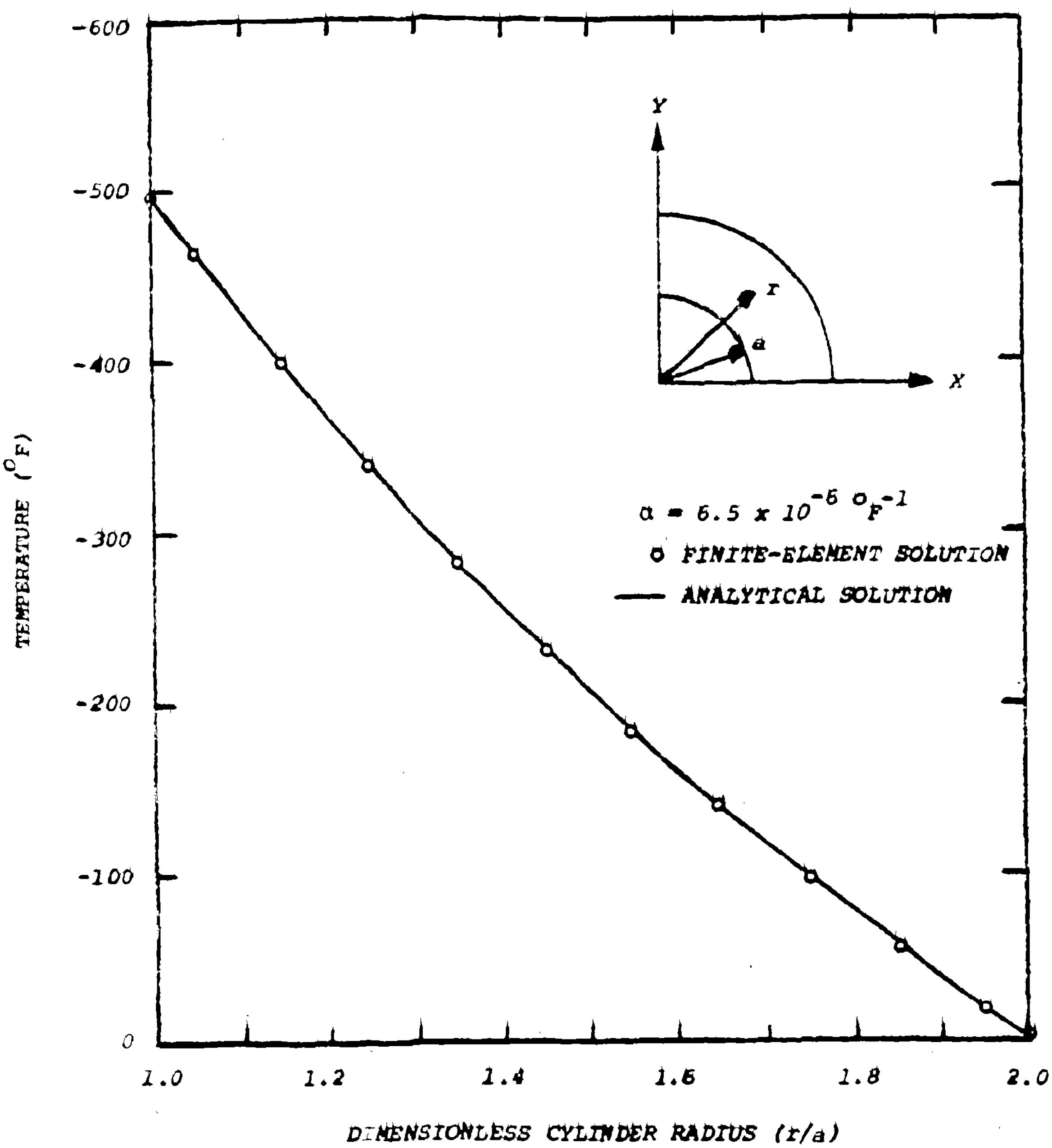

Figure 4. Comparison of the finite-element and analytical solutions for the steady, radial temperature distribution in a differentially-heated hollow cylinder (as used for the problem illustrated in Figure 5).

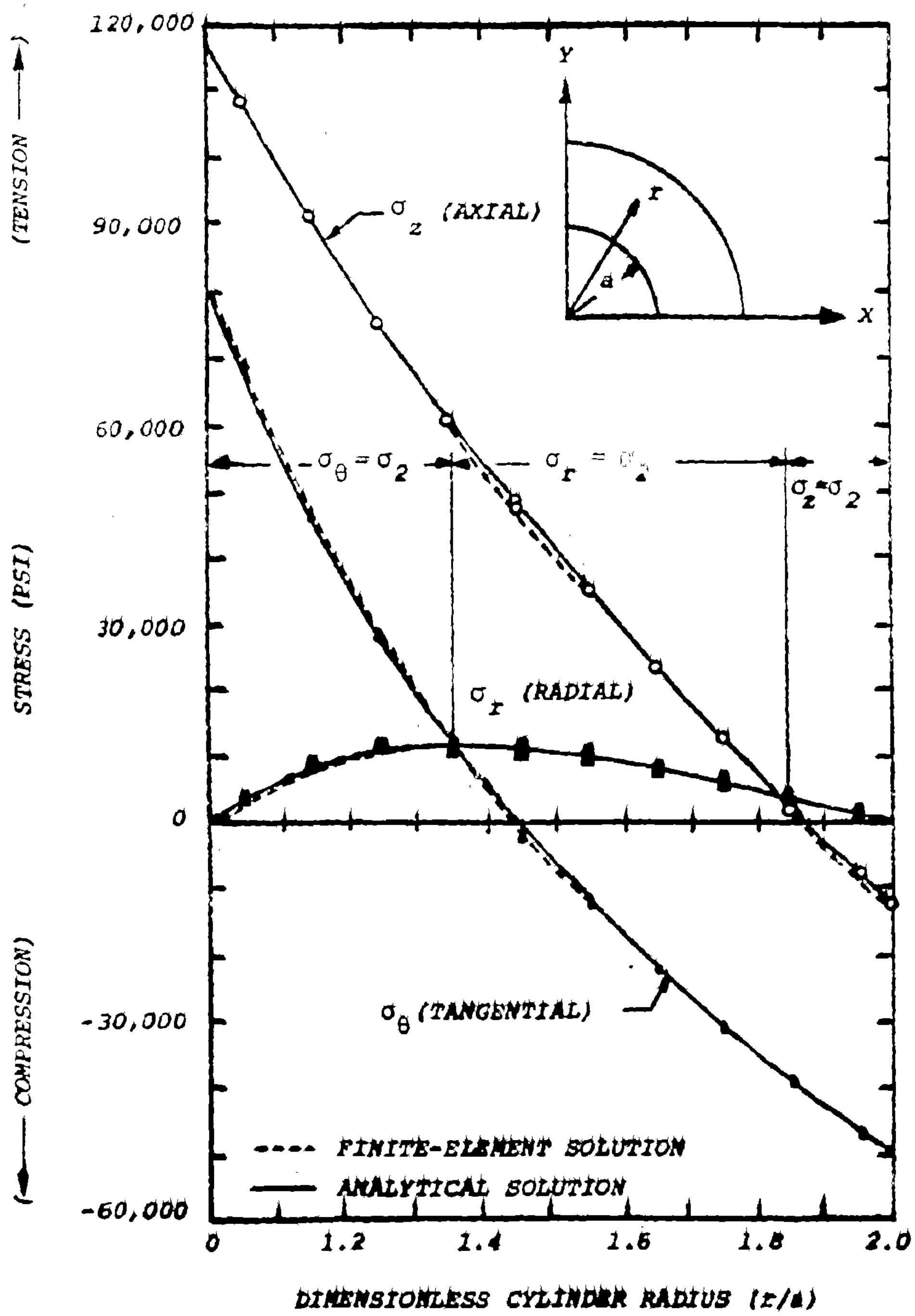

Figure 5. Thermoelastic analysis of a differentially-heated hollow cylinder; outer wall temperature is 500 °F higher than inner wall.

MATERIAL PROPERTIES

$E = 30 \times 10^6$ PSI

$\nu = 0.25$

$\alpha = 6.5 \times 10^{-6}\ {}^\circ F^{-1}$

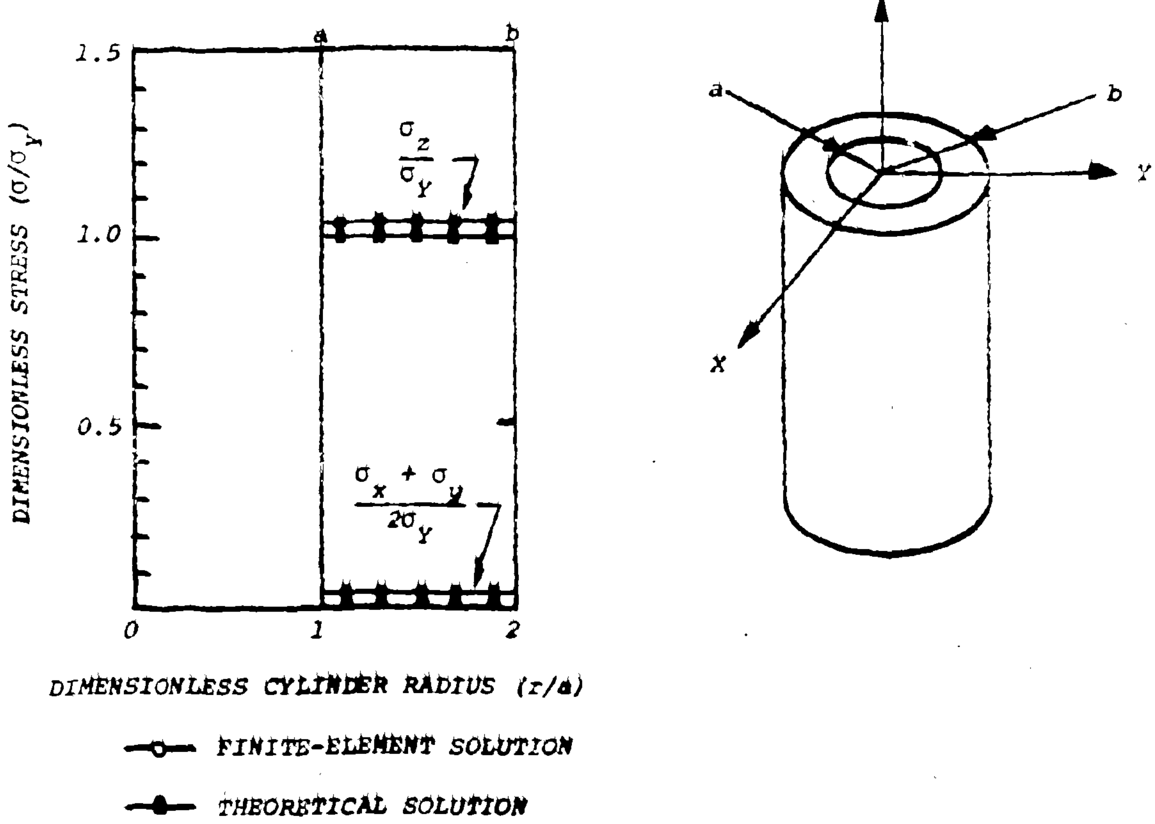

Figure 6. Thermoelastic/plastic analysis of a hollow cylinder uniformly heated to 500 °F; Zero strain in the z-direction with yielding first occurring at 308 °F.

4. CONCLUSION

A description of the computer program TEPCO, written by the author of this report and utilized by RE/SPEC Inc. for thermoelastic/plastic analyses of rock mechanics problems associated with the proposed salt mine repository concept, has been presented. Copies of the program reside with RE/SPEC Inc. in Rapid City, SD and with the author in Salt Lake City, UT. Its usage is familiar to a number of RE/SPEC Inc. personnel. The capability that TEPCO represents is therefore present at both locations. This redundancy assures availability of TEPCO for future analysis as may be desired.

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