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THERMOELASTIC CAPABILITIES FOR THE SANDIA-BMINES PROGRAM

J. R. Tillerson and M. M. Madsen

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ABSTRACT

The capability for simulating the thermoelastic behavior of geologic media has been added to the SANDIA-BMINES finite element code. The equations governing the response of a continuum to a known temperature field are delineated in this report. In addition, the specifics of the implementation of the continuum equations into the existing finite element program are described. Finally, the results of validation studies performed to assess the accuracy of the modified program are presented along with recommendations concerning future research and development efforts in this field.

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INTRODUCTION

In direct support of the design of a pilot plant for the disposal of radioactive wastes in bedded salt formations, modifications have been made to the SANDIA-BMINES finite element analysis program to simulate the thermoelastic response of geologic materials to time-varying temperature fields. Simulation of the excavation of rooms in the applicable bedded salt horizon followed by the prediction of the elastic response of the salt due to the emplacement of the waste canisters will now be possible. In addition to the current project support applications of this modeling effort, there are other geophysical applications in which similar capabilities are needed. Other applications in the area of the disposal of radioactive wastes generated in the nuclear fuel cycle include investigating the potential for emplacing the high level wastes in geologic media other than bedded salt. For example, preliminary studies and experiments are now being made considering shale formations, domal salt deposits, granite formations, and undersea formations suitable for the disposal of wastes in the seabed. Additionally, structural problems associated with in situ retorting of oil shale can now be simulated. The increased use of large underground caverns for the cost effective storage of hot liquids and gases necessitates employment of similar capabilities in the design and construction stages of cavern development. Although the list of potential applications for thermoelastic modeling of geologic materials could readily be extended, the aforementioned examples should suffice to indicate the importance of this addition to the original BMINES code.

The BMINES finite element program was originally developed by Jeremy Isenberg and his associates at Agbabian Associates, El Segundo,

California, under the auspices of the personnel in the Bureau of Mines Office in Spokane, Washington. Since its installation on the computing system at Sandia Laboratories, the program has been substantially modified by the addition of thermal effects, the incorporation of a new creep law, the development of interface routines to allow use of post-processors to provide graphical display of output quantities, and by numerous other changes made to improve either the accuracy or efficiency of the program. This modified computer program will be referred to as the SANDIA-BMINES code to distinguish it from the original (1973) version of the program. The present report will emphasize the addition of thermoelastic effects to the code.

SANDIA-BMINES is a versatile, multipurpose code developed for application in analyses of rock mechanics problems. An incremental Lagrangian formulation, limited to small strains and displacements, is used. Mesh generation capabilities with automated grading of element sizes are available for cost effective preparation of computationally efficient grid patterns in both two and three dimensions. The extensive element library allows meaningful simulation of many important problems in the field of rock mechanics. The basic element in two-dimensional analyses is the four node, isoparametric, quadrilateral element which uses a bilinear displacement field assumption for plane strain, plane stress and axisymmetric analyses. In three-dimensional analyses a similar eight node, isoparametric, hexahedron element is the basic element. Additional elements which are available include bar, beam, thick shell and joint elements. The thermoelastic modifications are at present restricted to the basic two- and three-dimensional elements but can be extended to the special elements that are used to simulate the rock bolts, liners, etc. The versatility of the

computer code is perhaps most evident when considering the material properties package available for use. A comprehensive set of options exist for both linear and nonlinear models of isotropic and anisotropic behavior. A complete description of the capabilities of the original BMINES code is found in the manuals prepared by Isenberg [1].

In the remaining sections of this report, the discourse will be devoted primarily to detailing the applicable equations which were programmed, the restrictions associated with the expressions as implemented in the SANDIA-BMINES program, and to the validation studies that have been performed. A brief section containing conclusions and recommendations for the future upgrading of these thermal capabilities concludes the report.

FORMULATION

The modifications made to the SANDIA-BMINES code to simulate the thermoelastic response of geologic materials are currently restricted to isotropic elastic bodies with material properties that are independent of temperature. The formulation of the governing equations of motion is described on succeeding pages along with the limitations of applicability of the program.

Equations of Equilibrium

This computer program employs a total Lagrangian formulation of the equations of equilibrium written in incremental form. The small strain assumption employed in the development of these equations is further restricted by the assumption that the displacements will also be small. In light of these restrictions, the original (undeformed) coordinate system is employed at all stages in the calculations. The governing equilibrium equations in the finite element formulation may be written

$$[K]_n \{\Delta u\}_{n+1} = \{P\}_{n+1} - \{F\}_n \quad (1)$$

where

$[K]_n$ = the structural stiffness matrix evaluated at the nth time (or load) step

$\{\Delta u\}_{n+1}$ = increments in the nodal displacements occurring during the (n+1)th step

$\{P\}_{n+1}$ = the total load vector existing at the end of the (n+1)th step

$\{F\}_n$ = load vector corrections existing at the end of the nth step

The total displacements at the end of the (n+1)th step may be written in terms of the displacement increment occurring during the step and the displacements existing at the end of the previous step, i.e.,

$$\{u\}_{n+1} = \{u\}_n + \{\Delta u\}_{n+1} . \quad (2)$$

In the absence of nonlinear material behavior, the structural stiffness matrix remains constant except as it reflects the removal or addition of elements to simulate construction sequencing. The loads vector $\{P\}_{n+1}$ contains the effects of the applied external loads, the internal loads (gravity forces), and the effects of temperature fields. Representation of temperature effects through this force vector is deemed an initial strain approach in the finite element literature [2]. Other influences which are often treated as "initial strains" in finite element studies are creep, in situ loads, and even material or geometric nonlinearities when these nonlinear effects are small. In order to show more clearly the manner in which the loads vector is modified to reflect thermal effects we will separate the load vector into contributions due to thermal effects $\{P^T\}$ and contributions due to the other loads $\{P^L\}$, or

$$\{P\}_{n+1} = \{P^L\}_{n+1} + \{P^T\}_{n+1} . \quad (2)$$

It is the thermal contribution to the loads vector which we seek to define.

Strain Decomposition

In finite element studies it is often convenient to write the total strain vector $\{\epsilon\}$ as the sum of its component parts, i.e., its elastic, plastic, creep or thermal parts. If only the elastic and thermal contributions are considered, the total strain becomes

$$\{\epsilon\} = \{\epsilon^e\} + \{\epsilon^T\} . \quad (3)$$

Quite obviously, a similar expression holds for incremental additions to these component terms. The total strain components are computed from the displacement components by the use of the following relationship

$$\{\epsilon\} = [B]\{u\} \quad (4)$$

where the components of the matrix $[B]$ are obtained by combining the strain-displacement relations obtained in continuum theory with the displacement functions assumed for each type of finite element model available in a code. Since, as will be noted in the next section, the thermal strain components will be computed from the temperature field, the elastic strains existing in the body can be determined from the known quantities in Eq. 3 as

$$\{\epsilon^e\} = \{\epsilon\} - \{\epsilon^T\} \quad (5)$$

Thermal Strains

The thermal strain components at any point can be computed in the three-dimensional case as

$$\epsilon_x^T = \epsilon_y^T = \epsilon_z^T = \int_{T_0}^T \alpha(T) dT \quad (6)$$

where T is the temperature at a point in the body, T_0 is the reference or ambient temperature and $\alpha(T)$ is the coefficient of linear thermal expansion which may be a function of temperature. It has been assumed that the coefficient of thermal expansion is the same for each of the coordinate directions and that the presence of a temperature increment ($\Delta T = T - T_0$) in a body will only result in normal (volumetric) strains.

Stress Components

The stress components are determined from the components of the elastic strain using the Hooke's Law relation

$$\{\sigma\} = [C]\{\epsilon^e\} \quad (7)$$

where $[C]$ is generally referred to as the elasticity matrix. For isotropic three-dimensional elasticity studies, the terms in the symmetric matrix $[C]$ are defined as follows in terms of the modulus of elasticity, E , and the Poisson's ratio, ν ,

$$[C] = \frac{E}{(1+\nu)(1-2\nu)} \begin{bmatrix} 1-\nu & \nu & \nu & 0 & 0 & 0 \\ & 1-\nu & \nu & 0 & 0 & 0 \\ & & 1-\nu & 0 & 0 & 0 \\ & & & \frac{1-2\nu}{2} & 0 & 0 \\ \text{SYMMETRIC} & & & & \frac{1-2\nu}{2} & 0 \\ & & & & & \frac{1-2\nu}{2} \end{bmatrix} \quad (8)$$

In rock mechanics analyses it is often more convenient to write the elasticity matrix in terms of the bulk modulus, K , and shear modulus, G , of the material:

$$[C] = \begin{bmatrix} K + \frac{4}{3}G & K - \frac{2}{3}G & K - \frac{2}{3}G & 0 & 0 & 0 \\ & K + \frac{4}{3}G & K - \frac{2}{3}G & 0 & 0 & 0 \\ & & K + \frac{4}{3}G & 0 & 0 & 0 \\ \text{SYMMETRIC} & & & G & 0 & 0 \\ & & & & G & 0 \\ & & & & & G \end{bmatrix} \quad (9)$$

When Eq. 5 is substituted into Eq. 7 written with $[C]$ defined as in Eq. 8, the contribution of the thermally induced strains may readily be seen as

$$\{\sigma\} = [C]\{\epsilon\} - \frac{E}{1-2\nu} \begin{pmatrix} T \\ \epsilon_x \\ T \\ \epsilon_y \\ T \\ \epsilon_z \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \quad (10)$$

In terms of the bulk modulus we note that

$$\frac{E}{1-2\nu} = 3K \quad (11)$$

Looking at Eq. 10, the contribution of temperature effects to the stress vector may be seen to be

$$\sigma_x^T = \sigma_y^T = \sigma_z^T = - \frac{E}{1-2\nu} \epsilon_x^T \quad (12)$$

These stress components σ^T will be used to compute the contribution which the temperature terms make to the force vector.

Thermal Loads Vector

The contribution of the temperature field to the load vectors of each element may be written as

$$\{P_e^T\}_{n+1} = \int_V [B]^t [C] \{\epsilon^T\} dV \quad (13)$$

or

$$\{P_e^T\}_{n+1} = \int_V [B]^t \{\sigma^T\} dV \quad (14)$$

where the volume integration is performed over the undeformed shape of the element and $[B]^t$ is the transpose of the matrix shown in Eq. 4. The loads for each individual element are then summed with due regard to the element connectivity to give the total thermal loads vector mentioned in Eq. 2.

Readers interested in the straightforward summation process should consult Ref. [2], [3] or any other reference text describing the finite element displacement method.

COMPUTER PROGRAM MODIFICATIONS

The previously described formulation for simulation of thermoelastic effects in geologic media has been implemented into the BMINES program. The code modifications made to allow this simulation capability affect all three major portions of the SANDIA-BMINES program: the input (pre-processor), output (postprocessor), and execution sections. The major portion of the modifications appear in the execution phase of the code. The options regarding the input of temperature effects data to the program, the manner in which the computations are performed, and the limitations of applicability of the formulation as implemented in the code are described on succeeding pages. The changes in the internal data handling and the additional output data which is available are also discussed. The changes in the formats for specifying input data in the SANDIA-BMINES code are provided in the appendices included in this report. The appendices also document the tape formats used for input and output of the thermal quantities and the formats used in the plot files.

Preprocessor Modifications

Only minor modifications were made in the preprocessor portion of the program. The element temperatures are not read in this section; this information is read as needed during execution. In the original version of the code, all input data was read in the initial phase of the computations. This deviation from the procedure employed in the original version of the program was made in order to be able to change the temperature field without having to rerun the entire problem. This time-saving feature will be particularly important in parametric studies of waste emplacement following excavation of rooms in underground formations. For these problems

only the emplacement portion of the runs will have to be repeated to vary waste cannister input parameters.

Changes which were made in the preprocessor section include those to change the array containing logical unit numbers employed for the I/O devices thereby reflecting the use of 4 additional units to store thermal information. Two new control flags were added to the input data which must be specified. The first one (variable ITHPLT) is used to indicate whether or not element data (nodal coordinates, element connectivity, etc.) will be written to an output file for eventual use in heat transfer calculations or graphical display of the model. The time varying temperature fields which are generated by the heat transfer code can then serve as input data for the stress analysis computations. This will be discussed further in the "execution" section where the ways of specifying the element temperatures are described. Another change in this section of the code was the addition of a control parameter indicating whether or not thermal effects are to be simulated in a given problem. Finally, the input to the material properties package was changed to allow input of thermal expansion parameters; the parameters will be explained in the discussion of modifications made to the execution section of the code.

Execution Section Modifications

The most extensive modifications required for thermoelastic simulation were made in the execution module of the program. In order to "set the stage" for a discussion of the details of these additions to the program, let us refer to the two flow charts provided as Figures 1 and 2. The first chart is an executive view of the order in which the computations are performed in the execution section of the code. Program BMCAIC controls the code

FIG. 1. BASIC FUNCTIONS OF EXECUTIVE PROGRAM BMCALC

FIG. 2. CALCULATION STEPS FOR THERMOELASTIC ANALYSES - SUBROUTINE TDRIVR

execution by initializing variables, calling subroutine KFORM to set up the equilibrium equations and finally by calling various routines (problem dependent) to solve these equations for each load step. In addition, the preparation of restart file information is controlled by program BMCAIC.

Since the presence of a temperature field affects the equilibrium equations, the modifications and additions made to the BMINES program are concentrated in subroutine KFORM and the routines controlled by it. Subroutine KFORM oversees the computations which must be performed on an element level and then combined to yield structural equations of motion. The strain and stress vectors for each element are computed in the element loop of KFORM. Modifications to the element stiffness matrices resulting from nonlinear material behavior are also made in this loop. The contributions of the element stress field to the force unbalance vector are summed to yield the total force unbalance existing in the equations of motion. The mechanical loads are updated in routines called from KFORM. The modifications made to the code to simulate thermoelastic effects do not change the element stiffness matrices but, as previously noted, do contribute to changes in the loads vector and in the stress field.

The calculation steps leading to the modification of the loads vector for thermoelastic effects are shown in Fig. 2. This drawing delineates the major subroutines written to simulate thermal effects. A driver subroutine, appropriately named TDRIVR, is called by KFORM to control the flow of the thermal computations. If element temperatures are needed, either subroutine TINITL or TEMPS is called from TDRIVR to determine the element temperature and temperature increment.

Temperatures for a problem may be input in any one of three ways (see Appendix A). The element temperatures may be specified on data cards at

arbitrarily selected points in time in two different ways. For each of these two ways a set of cards is used to completely define the temperature field at the selected points in time. END OF FILE cards separate the data sets for each point in time. When the stress and displacement fields are computed at times intermediate between those at which the temperature field is specified, linear interpolation of the temperature fields is allowed.

The first method of card input is very straightforward as it uses 8 temperatures per card until all element temperatures have been specified. The second method of specifying the temperature field is extremely useful in minimizing the effort required to prepare the input data when large numbers of elements have the same temperature. With this approach each input card contains the temperature for a consecutively numbered group of elements, i.e., element A through element B are at a temperature T.

The third method of specifying time varying temperature fields is via input from permanent file. At each point in time, element temperatures are read in blocks of 50 (an arbitrarily selected but convenient number) until the entire temperature field is specified. This input option was included primarily to minimize the data preparation when temperature fields are computed using an in-house heat transfer code. The finite element mesh prepared in the SANDIA-BMINES code is transferred to the heat transfer code via permanent file and, following these computations, time-varying element centroidal temperatures are returned to the SANDIA-BMINES code for use in the stress analysis. This manner of "coupling" the heat transfer and stress computations is much more efficient for large scale computations.

Now with the temperatures appropriately specified, the thermal strains can be calculated. This is accomplished in subroutine TSTRAIN where the normal strain increments, $\Delta\epsilon_i$, due to a temperature change, T_1 to T_2 , are computed as

$$\Delta\epsilon_i = \int_{T_1}^{T_2} \alpha(T) dT . \quad (15)$$

The temperature dependent coefficient of thermal expansion is denoted as $\alpha(T)$. A substantial volume of experimental data on thermal expansion properties of rocks is contained in Ref. 4. Representative data from Ref. 4 which shows thermal expansion variation with temperature is reproduced in Fig. 3. Rather than allowing a completely general thermal expansion variation (i.e., table lookup) in the program, a specific form was selected for representing the data. The available data for a wide range of rock types can be well represented by a region of constant thermal expansion (low temperatures) followed by a region of higher temperature in which the coefficient varies linearly with temperature. This behavior is symbolically represented in Fig. 4 where it is noted that the linearly varying region begins at a reference temperature T_{ref} . The initial thermal expansion coefficients, α_0 , the gradient of the coefficients with temperature, $\frac{d\alpha}{dT}$, and the reference temperature, T_{ref} , are the material properties currently required to model the material behavior resulting from temperature effects. It is assumed in this formulation that only normal strains are generated as a result of thermal activity.

After computing the thermal strain increments, subroutine TSTRES is called. This routine has a threefold purpose. The first purpose is to modify the definition of the thermal strain increments for the plane strain case, i.e., the existing normal strain increments in the x- and y-directions

FIG. 3. COEFFICIENT OF THERMAL EXPANSION VARIATION WITH TEMPERATURE

Coeff. of
Thermal
Expansion

FIG. 4. ALLOWABLE THERMAL EXPANSION VARIATION
WITH TEMPERATURE

are multiplied by $(1 + \nu)$ where ν symbolically represents Poisson's ratio. The main purpose of this routine is to calculate the increment of "thermal stress" resulting from the previously calculated thermal strain increments. Equation 7, when written in incremental form, is used for this computation. The total thermal stress is updated to reflect the contribution of this new temperature increment. Finally, this subroutine determines the z-direction increments of stress and strain for the plane stress and strain options.

Equation 14 serves as the basis for the computations performed in subroutine TLOAD. For each element which has a nonzero temperature increment, an increment in the nodal loads vector is computed. This incremental load due to the temperature increment, ΔT , is then added to the other mechanical loads. Equation 14 is integrated over the volume of the element by assuming that the temperature increment, ΔT , is constant over the element hence the thermal stress will likewise be constant over the element. In addition, the B matrix evaluated at the element centroid is assumed constant in this integration except in the axisymmetric case. For axisymmetric problems, the integration is performed using B matrices evaluated at the four corners of the elements.

The final routine called in this major loop of the thermal computations is subroutine THTAPE. This routine stores the thermal information for each element (temperature, strain, stress, etc.) required in future computations or in the output section of the program (see the appendices for this format).

The only subroutine required for thermal calculations that is not called from TDRIVR is subroutine THSTRY. This routine is called from subroutine COMPUT to perform two jobs. The first task is to read the thermal information for the previous time step that was written by

subroutine THTAPE. The second task performed by this routine is to correct, in the manner described in Eq. 10, the stress and stress increment vectors that have been computed (for the previous time step) using the total strains as elastic strains. When the computations of this routine are completed, the correct values of the stress and stress increment vectors are returned to subroutine COMPUT.

Postprocessor Modifications

Minimal changes were required in the output section of the code as a result of adding thermoelastic capabilities. An optional output table is now available for thermoelastic problems. This table printed at each appropriate time step contains the element number, element temperature, thermal strain components, and thermal stress components. The information printed in this section is obtained by interrogating the files prepared during execution by subroutine THTAPE.

VERIFICATION STUDIES

The test problems used to validate changes in the program which were made to represent the thermoelastic behavior of the rocks are described in the following section. Results of the numerical analyses are in many cases compared with the response predicted by closed form solutions. Additional results for problems of interest in radioactive waste disposal are also described.

Whenever modifications are made to a computer program, verification or validation of the accuracy of these changes is mandatory. The matrix of test cases selected and run to validate the thermoelastic modifications is large enough to test virtually all regions of the code in which modifications were made. The element type, the temperature fields, initial geometry, the input options, and the boundary conditions were varied in the course of the checkout work.

Simple Test Problems

The first test problems which were run are depicted in Fig. 5.* These simple test cases required minimal amounts of computer time and yet allowed us to assess many facets of the modifications. Indeed because of the ease with which the results could be compared with the exact solutions obtained from continuum theory [5], these test problems served as an effective tool for debugging the modifications. In addition to the multi-element problems

* As explained in the footnote in Table I, any consistent set of units can be used in the SANDIA-BMINES program. For that reason, no indication of units is included in the dimensions of Fig. 5 or in the results of Table I. For example, if the dimensions in Fig. 5 are input as inches, the elastic modulus is specified in psi, and the thermal information is specified in terms of °F, the output stress and displacement quantities will be in psi and inches, respectively.

FIG. 5 SIMPLE THERMOELASTIC TEST PROBLEMS

TABLE I. COMPARISON OF NUMERICAL AND EXACT SOLUTIONS FOR SIMPLE THERMOELASTIC TEST PROBLEMS

QUANTITY	PLANE STRESS				PLANE STRAIN				AXISYMMETRIC				THREE DIMENSIONS			
	Free Expansion		Fixed Boundaries		Free Expansion		Fixed Boundaries		Free Expansion		Axial Restraint		Free Expansion		Fixed Boundaries	
	EXACT	COMPUTED	EXACT	COMPUTED	EXACT	COMPUTED	EXACT	COMPUTED	EXACT	COMPUTED	EXACT	COMPUTED	EXACT	COMPUTED	EXACT	COMPUTED
STRAINS																
ϵ_x^T	.002	.002	.002	.002	.0026	.0026	.0026	.0026	.002	.002	.002	.002	.002	.002	.002	.002
ϵ_y^T	.002	.002	.002	.002	.0026	.0026	.0026	.0026	.002	.002	.002	.002	.002	.002	.002	.002
ϵ_z^T	.002	.002	.002	.002	0.0	0.0	0.0	0.0	.002	.002	.002	.002	.002	.002	.002	.002
ϵ_x	.002	.002	0.0	0.0	.0026	.0026	0.0	0.0	.002	.002	.0026	.0026	.002	.002	0.0	0.0
ϵ_y	.002	.002	0.0	0.0	.0026	.0026	0.0	0.0	.002	.002	0.0	0.0	.002	.002	0.0	0.0
ϵ_z	.002	.002	.0037	.0037	0.0	0.0	0.0	0.0	.002	.002	.0026	.0026	.002	.002	0.0	0.0
STRESSES σ_f/t^2																
σ_x	0.0	0.0	-2857.	-2857.	0.0	0.0	-5000.	-5000.	0.0	0.0	0.0	0.0	0.0	0.0	-5000.	-5000.
σ_y	0.0	0.0	-2857.	-2857.	0.0	0.0	-5000.	-5000.	0.0	0.0	0.0	0.0	0.0	0.0	-5000.	-5000.
σ_z	0.0	0.0	0.0	0.0	-2000.	-2000.	-5000.	-5000.	0.0	0.0	-2000.	-2000.	0.0	0.0	-5000.	-5000.
DISPLACEMENTS u/t																
u	.002	.002	0.0	0.0	.0026	.0026	0.0	0.0	.004	.004	.0052	.0052	.002	.002	0.0	0.0
v	.001	.001	0.0	0.0	.0013	.0013	0.0	0.0	.001	.001	0.0	0.0	.001	.001	0.0	0.0

* The SANDIA-BMINES code will accept any consistent set of units such as SI units or inch-pound-second units. This table, therefore, indicates the values predicted (numerically and analytically) for stresses, strains, and displacements without regard to a particular system of units. The numerical values of the properties employed in these analyses were $E = 10^6$ (f/t²), $\nu = 0.3$, $\alpha = 2 \times 10^{-5}$ (deg⁻¹), and $\Delta T = 100$ (deg).

depicted in Fig. 5, the same geometries were employed in single element studies with each of these element types.

In Fig. 5a the geometry and finite element idealization for plane stress and plane strain problems are shown. Two sets of boundary conditions were applied in this problem. In the first case, free expansion of the outer boundaries was allowed for a temperature rise of 100° in each of the elements; the only nodal conditions specified were for the symmetry plane (no x-direction displacement) along the y-axis and no vertical deformation at node 2 so that rigid body motion in the y-direction is eliminated. Table I may be used to compare the numerical and exact results for this problem. The second case simulates complete confinement of the plane stress and plane strain bodies so that no displacement of any of the exterior nodes is allowed. This condition results in stresses imparted to the body as a result of the temperature rise. The agreement between the exact and numerical solutions (see Table I) is excellent for all of the previously described cases.

The axisymmetric element (Fig. 5b) was tested using 2 sets of boundary conditions. The first case was once again free expansion of the ring; this corresponds to a plane stress solution for a thin heated cylindrical disc with a hole in the center. In the second case no vertical (axial) deflection of the upper and lower boundaries is allowed. This condition simulates the response of a long heated cylinder which is axially constrained, i.e., a condition of plane strain exists in the y-direction. The results of both of these cases show that the axisymmetric option of the modifications is working correctly for these problems.

Similar boundary conditions were run for the three-dimensional body depicted in Fig. 5c. Simulation of the displacement, strain, and stress

response of the body was accurately accomplished (see Table I) for the free and constrained cases. In addition to the results depicted in Table I, this problem was used for successfully testing many of the ways in which temperature fields may be input to the program.

These simple test problems have provided a means of evaluating the accuracy of the thermoelastic modifications. While conducting these analyses the single and multi-element capabilities were tested, the input and output options were scrutinized for time varying temperature fields, and various element types were utilized. After obtaining the results of these simple problems more complex checkout problems were analyzed.

Cantilever Beam Studies

The cantilever beams depicted in Fig. 6 were analyzed for a variety of loading conditions. Two-dimensional, elastic, plane stress studies were run using a value of zero for Poisson's ratio in order to compare directly with beam theory results [5]. A vertical pressure loading was simulated along the top of the model to see how well the original program can simulate beam theory results. The displacements were computed to within 0.5% of the exact results at all points along the beam for both geometries using 5 elements through the thickness and 50 elements along the length of the model. The stresses were likewise in agreement with beam theory except near the cantilever points where the differences in the boundary conditions between this elasticity analysis and that of beam theory are greatest. As in the simple test problems, the input quantities may be interpreted in any consistent set of units so no units of displacement and stress are provided. This analysis firmly established that the finite element idealization is adequate to achieve excellent correlation

MATERIAL PROPERTIES:

$$E = 30 \times 10^6 \text{ (f/l}^2\text{)}$$

$$\alpha = 6 \times 10^{-6} \text{ (deg}^{-1}\text{)}$$

LOADING CONDITIONS

1. Vertical Pressure
2. Constant Temperature Rise ($\Delta T = 100^\circ$)
3. Linear Temperature Variation Through Thickness ($\Delta T = 150^\circ - 250^\circ$)

FIG. 6 CANTILEVERED BEAMS USED IN THERMOELASTIC TEST

with beam theory predictions in regions away from the cantilevered ends of the beams. The second loading condition was that of a temperature rise of 100° in each of the elements. For the simple cantilever, the predicted expansion of 0.06 units of length was accurate for at least four significant digits; the stresses predicted in the analysis were essentially zero (10^{-7} or 10^{-8}) which correctly indicates that free expansion has taken place. The axial deflections predicted for the doubly cantilevered problem were approximately 10^{-13} (effectively zero) while an axial stress of 18,000 was correctly computed in the central region of the model. When a linear temperature variation through the thickness of the model was simulated, the vertical displacement predicted by the computer program was within 0.1% of the beam solution at both the midpoint and the end of the beam. Since the temperature distribution within an element is assumed constant, the beam theory solution was obtained using a step function approximation of the linear distribution with the temperatures selected at the element centroids. The moment predicted from the axial stress distribution in the double cantilevered beam analysis was likewise in agreement with beam theory for this final loading case. The results of these analyses of stress and deformation fields in cantilevered beams indicate that the numerical results obtained using the tested options in the thermoelastic modifications are working correctly and can match theoretical results with good accuracy.

Internally Heated Cylinder

The cylinder depicted in Fig. 7 has been used as a test problem for the thermoelastic modifications to ensure that the capability exists for transferring geometry data from the SANDIA-BMINES to existing in-house

heat transfer computer programs and for transferring the temperature fields predicted by the heat transfer programs to the SANDIA-BMINES program for use in the thermal stress analysis. The geometry and material properties for this body are presented in Fig. 5 along with the finite element idealization used in the analysis. Axisymmetric ring elements were used. The restraint of axial movement of the elements corresponds to a condition of plane strain in the cylinder. After the finite element mesh was generated, the nodal coordinates and the element connectivity array were transferred to the MARC-HEAT program [6]. The temperature profiles determined by this program are presented for three selected points in time in Fig. 8. These temperatures were then used in the stress analysis. The results of this stress analysis are also presented in Fig. 8. These results were compared (see Tables II and III) with an exact solution presented in Ref. [5].* The agreement noted in Tables II and III is excellent for both the displacement and stress components. This provides further evidence that the axisymmetric option of the code is working correctly and that data transfer between the heat transfer program and the SANDIA-BMINES program has been successfully obtained.

A test of the plane strain capability of the program was then made using the same problem. A 90° segment of the cylinder as viewed in the $r-\theta$ plane was idealized using 16 elements through the thickness of the cylinder and 50 elements along the 90° segment. The axisymmetric temperature field predicted by the MARC-HEAT code [6] at $t = 60$ was used in the

* As in the beam problem the exact results were obtained by integrating the step function temperature used in the program rather than the smoother distribution seen in Fig. 8.

Material Properties:

$$E = 16.95 \times 10^6 \text{ (t/l}^2\text{)}$$

$$\nu = 0.345$$

$$\alpha = 9 \times 10^{-6} \text{ (1/deg)}$$

Ambient Temperature:

$$T = 70^{\circ}$$

Finite Element Idealization:

16 Square Ring Elements

Boundary Conditions:

Top and Bottom Surfaces are on
Rollers to Simulate Plane Strain
Condition

FIG. 7 INTERNALLY HEATED CYLINDER MODEL

FIG. 8 THERMOELASTIC RESPONSE OF AN INTERNALLY HEATED CYLINDER

TABLE II. DISPLACEMENT COMPARISONS FOR INTERNALLY HEATED CYLINDER

NODE NO.	RADIAL DISPLACEMENT $\times 10^4$	
	EXACT	COMPUTED
1	1.42	1.43
3	2.09	2.11
5	2.58	2.58
7	2.89	2.89
9	3.09	3.09
11	3.20	3.21
13	3.25	3.26
15	3.26	3.27
17	3.25	3.25
19	3.21	3.22
21	3.16	3.17
23	3.11	3.11
25	3.05	3.06
27	3.00	3.01
29	2.95	2.96
31	2.90	2.90
33	2.85	2.86

TABLE III. STRESS COMPARISONS FOR INTERNALLY HEATED CYLINDER

ELEM. NO.	TEMP.	σ_{rr}		σ_{zz}		$\sigma_{\theta\theta}$	
		EXACT	COMPUTED	EXACT	COMPUTED	EXACT	COMPUTED
1	134.6	-374	-364	-14095	-14094	-11920	-11931
2	118.7	-909	-903	-10396	-10397	-7686	-7693
3	106.3	-1187	-1185	-7509	-7507	-4522	-4522
4	96.7	-1297	-1296	-5276	-5274	-2181	-2179
5	89.4	-1297	-1297	-3572	-3570	-477	-473
6	83.9	-1230	-1231	-2288	-2288	739	743
7	79.8	-1124	-1124	-1336	-1336	1584	1588
8	76.8	-996	-997	-640	-640	2153	2156
9	74.7	-860	-861	-139	-140	2518	2521
10	73.1	-724	-724	215	215	2736	2738
11	72.1	-591	-591	464	461	2852	2852
12	71.3	-465	-465	634	631	2895	2896
13	70.9	-347	-347	748	746	2892	2893
14	70.5	-239	-238	829	843	2864	2863
15	70.3	-136	-137	886	880	2820	2816
16	70.1	-44	-43	928	920	2769	2764

analysis. The results were in complete agreement with the axisymmetric predictions shown in Tables II and III.

Analysis of Heated Shale Experiment

In recent months, the design of a shale formation heater experiment has been conducted. In support of this design, a preliminary analysis has been made to predict the stress field which surrounds the heater and to assess the potential for the occurrence of brittle fracturing near the heater. Several different models were used in this study with a variety of boundary conditions; the results obtained using one of these models are described in this section.

The model chosen to demonstrate the applicability of the code is depicted in Fig. 9. This one-dimensional, axisymmetric grid was used in some of the early analysis work. At the outer boundary of the model (4 meters from the cannister centerline), it is assumed that no radial deformation will occur while no vertical deformation is allowed along the top and bottom boundaries. The first two elements are used to simulate the heater; steel properties are used for these elements. The elastic material properties selected for the shale were a modulus of 13.8 GPa and a Poisson's ratio of 0.3. The coefficient of thermal expansion was used as $10 \times 10^{-6}/^{\circ}\text{C}$.

The radial distribution of the temperature field is shown at selected points in time in Fig. 10. These temperature profiles were used as input to the stress analysis. The thermoelastic stress field in the shale was computed for each of the temperature profiles shown in Fig. 10. A representative set of curves detailing this field is presented in Fig. 11 for a time equal to one year after the emplacement of the heater. These

FIG. 9 SIMULATION OF HEATED SHALE EXPERIMENT

FIG. 10 TEMPERATURE PROFILES FOR SHALE FORMATION SURROUNDING HEATER

stress components were used to assess the fracture potential of the shale formation according to a brittle fracture criteria employed previously by Ratigan [7]. This criteria is depicted in Fig. 12. A value of 69 MPa (10,000 psi) was selected as the uniaxial compressive strength of the shale while one-fifteenth ($1/15$) of that value was used for the tensile strength. Figure 12 presents the factors of safety (F.S.) for three different points in the mesh (time = 1 year). As anticipated, the lowest safety factor exists in the shale element closest to the steel while the element farthest from the heater is less likely to fail under the actions of this set of boundary conditions and this temperature field.

Heat Generating Radioactive Waste Storage Example

The SANDIA-BMINES program has recently been applied to a problem of interest in radioactive waste disposal. As will be reported in Ref. 8, several different models were used in this tradeoff study in which various ways of emplacing the heat generating waste in bedded salt formations were compared from a temperature field and room closure point of view. A variation of one of these models will be described in this section to demonstrate the use of the thermoelastic portion of this finite element code and to provide another "benchmark" problem which can be used for checkout or verification of thermoelastic modifications made to other programs. Only the loads due to the temperature field generated by the emplacement of the waste canister are considered in this example; this simplification of the loading conditions (i.e., neglecting extraction effects and overburden pressures) was made to keep from obscuring the thermal effects. In this configuration the waste cannisters are placed horizontally into the pillars at the pillar midheight. The details of the finite element simulation are provided in succeeding paragraphs.

FIG. 11 STRESS DISTRIBUTION IN SHALE AFTER ONE YEAR OF HEATING

**FACTORS OF SAFETY SHOWN APPLY AFTER
1 YEAR OF HEATING**

**FIG. 12 FAILURE CRITERIA AND FACTORS OF SAFETY
IN SHALE FORMATION**

The finite element mesh used in this analysis contained 336 plane strain quadrilateral elements with a total of 393 nodal points. This idealization provides a total of 688 degrees of freedom for this system after the application of the boundary conditions. The model extended 91.4 meters (300') above and below the opening. A portion of the mesh is shown in Fig. 13 to demonstrate the concentration of the elements in the vicinity of the room. Note that in this drawing only the 15.4 meters (50') above and below the opening is shown. Beyond this area the aspect ratios of the elements are gradually increased (over the next 30 meters) to 3:1; this ratio then remains constant over the final 45.7 meters (150') in the mesh. The rooms are roughly 9 meters (30') wide and 3 meters (10') high. As shown in Fig. 13, a cross section of the room indicates that the sides of the rooms have been assumed to be circular in shape with a 1.5 meter (5') radius. The distance from the center of one room to the center of the next one is 33.5 meters (110'). This combination of room and pillar sizes corresponds to an extraction ratio of 27%.

The nodes on the right and left (vertical) boundaries of the mesh are constrained to allow only vertical motion of these nodes in order to simulate the symmetry planes existing along the room and pillar centerlines. The top and bottom boundaries are not allowed to move vertically. The symmetry planes which are simulated on the sides of the model imply that there are several rooms of identical size and spacing in the repository. This explains the need for modeling only half of a room and a pillar. The plane strain assumption implies that the rooms or lanes are long in comparison with the cross section dimensions. These assumptions are reasonable for simulating current design configurations being considered for heat generating waste storage.

FIG.13 HORIZONTAL EMPLACEMENT MODEL - Mesh Near Room Opening

The conduction heat transfer subroutines in the COUPLEFLO finite element program [9] were used to compute the temperature histories at various points throughout the salt. These temperature fields serve as input to the thermoelastic stress analysis; since the COUPLEFLO program uses triangular elements and calculates nodal point values of the temperatures, a utility program was written to prepare the data for use in the SANDIA-BMINES program which requires temperatures at the center of the elements. The thermal conductivity was allowed to vary linearly with temperature in these calculations. The heat generation resulting from the horizontal emplacement of the waste canisters into the pillars was simulated by a series of point sources with a thirty year half life. The location of the canister is depicted in Fig. 13 by the heavy line in the pillar at the pillar midheight. The room was considered, for the heat transfer analysis, to be filled with air in which there was conduction heat transfer. The properties of the air and the properties of the salt that were used in this simulation are shown in Table IV. The temperature fields throughout the model are shown at selected points in time in Fig. 14.

The vertical, horizontal and shear stress fields generated near the opening by the temperature field are shown in Figs. 15-17, respectively, at 5, 11, and 21 years after emplacement of the waste. The growth of each stress component with time is immediately evident. The restrictive nature of the boundary conditions selected for this analysis is evident in the large magnitude of the stresses; the stresses in the column would be much lower if the top of the model were free to expand vertically. The restrictive boundary conditions also lead to a prediction of more closure

TABLE IV. MATERIAL PROPERTIES

SALT

Bulk Modulus	$K = 13.1 \text{ GPa}$	$(1.9 \times 10^6 \text{ psi})$
Shear Modulus	$G = 5.0 \text{ GPa}$	$(.73 \times 10^6 \text{ psi})$
Coefficient of Thermal Expansion	$\alpha = 1.2 \times 10^{-5} / ^\circ\text{C}$	$(2.2 \times 10^{-5} / ^\circ\text{F})$
Ambient Temperature	$T_0 = 32^\circ\text{C}$	(90°F)
Conductivity	$k = 5 \text{ W/m}\cdot^\circ\text{K @ } 300^\circ\text{K}$ $= 3 \text{ W/m}\cdot^\circ\text{K @ } 500^\circ\text{K}$	$(2.5 \times 10^4 \text{ Btu/yr}\cdot\text{ft}\cdot^\circ\text{F @ } 80.6^\circ\text{F})$ $(1.5 \times 10^4 \text{ Btu/yr}\cdot\text{ft}\cdot^\circ\text{F @ } 441^\circ\text{F})$
Density	$\rho = 2164 \text{ kg/m}^3$	$(135 \text{ lb}_m/\text{ft}^3)$
Heat Capacity	$c_p = 921 \text{ J/kg}\cdot^\circ\text{K}$	$(0.22 \text{ Btu/lb}_m\cdot^\circ\text{F})$

AIR

Conductivity	$k = 3.13 \times 10^{-2} \text{ W/m}\cdot^\circ\text{K}$	$(1.6 \text{ Btu/yr}\cdot\text{ft}\cdot^\circ\text{F})$
Density	$\rho = .962 \text{ kg/m}^3$	$(.06 \text{ lb}_m/\text{ft}^3)$
Heat Capacity	$c_p = 1010 \text{ J/kg}\cdot^\circ\text{K}$	$(.241 \text{ Btu/lb}_m\cdot^\circ\text{F})$

Temperatures are in $^{\circ}\text{C}$

Isotherms are spaced 25°C apart

FIG. 14 HORIZONTAL EMPLACEMENT MODEL - Temperature Fields

FIG. 15 HORIZONTAL EMPLACEMENT MODEL - Vertical Stress Contours

TIME = 5 YEARS

TIME = 11 YEARS

TIME = 21 YEARS

FIG. 16 HORIZONTAL EMPLACEMENT MODEL - Horizontal Stress Contours

TIME = 5 YEARS

TIME = 11 YEARS

TIME = 21 YEARS

FIG. 17 HORIZONTAL EMPLACEMENT MODEL - Shear Stress Contours

of the room than is expected if the top boundary were free to move. The vertical closure at the center of the room is 6.35 cm (2.5") at the end of 21 years in this confined configuration.

CONCLUSIONS AND RECOMMENDATIONS

The major conclusion that may be drawn from the document is that the necessary modifications have been successfully made to the SANDIA-BMINES finite element code which allow the prediction of the thermoelastic response of two- and three-dimensional structures. The credibility of this new capability has been established by demonstrating that correct solutions were obtained using the code in a variety of test problems. The application of the code in problems of current interest was demonstrated using two examples of radioactive waste disposal.

Recommendations for future development of this computer program include the addition of temperature dependent elastic and inelastic material properties. Additionally, for applications in which the long term response of waste repositories will be monitored, the effects of geometric nonlinearities should be added to the SANDIA-BMINES computer program.

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APPENDICES

Appendix A. Input Data and User's Modifications

- A.1 "START" option--Automesh input data (Manual page 10, 13 Replacements)
- A.2 "EXECUTE" option--Calculation input data (Manual Insertion)
- A.3 "OUTPUT" option--Output tables input data (Manual Insertion)
- A.4 IWD Common Block Additions (Manual Replacements)

Appendix B. File Usage and Formats

- B.1 Heat transfer program input and SC-4020 plot input on unit 21
- B.2 Heat transfer program output on unit 23
- B.3 SC-4020 plot input on unit 20

Appendix C. Deck Setup Examples (SANDIA-BMINES)

- C.1 Temperature specified for each element (Card input)
- C.2 Temperature specified for element ranges (Card input)
- C.3 Temperature specified for each element (Tape input)
- C.4 SC-4020 plots

Appendix D. Updates to Modify SANDIA-BMINES Core Requirements

APPENDIX A

Input Data Modifications

The following pages are insertions and replacements for the original
BMINES user's manual [1].*

* See reference list at the end of the Appendices.

Replacement for Page 10
BUREAU OF MINES CODE MANUAL

Card Group	No. of Cards	Data and Definitions	Fortran Format
3.0		AUTOMESH INPUT DATA--OPTION "START"	
3.1	1	(HED(1), 1 = 1, 20) HED = An 80-column label of alphanumeric characters used to identify the problem. This label will appear at the top of each printed output page	(20A4)
3.2	1	NSPANY, NSPANX, NSPANZ, NMIDPT, NCOMFS, NCOMNP, ICOOR, NUMMAT, IPLOT, NSLIP, NPELAD, ITSHEL, IRENUM, JPLOT, IQUAD, ITHPLT NSPANY, NSPANX, NSPANZ = Number of "spans" or "blocks" in the y, x, and z directions, respectively, in the "key diagram." <u>NSPANZ is not meaningful in a two-dimensional problem, and the corresponding field must be left blank.</u> NMIDPT = Number of MIDPT's in key diagram. NCOMFS = Number of faces (3-D case) or sides (2-D case) to be formed by the face- or side-joining process described in card group 3.11 (page 16). NCOMNP ≥ Number of pairs of nodal points which will be joined by the face- or side-joining process in card group 3.11 (page 16). ICOOR = A numeric flag specifying the units of length in which the input data is given. = 0 if the units are in feet = 1 if the units are in inches	(16I5)

BUREAU OF MINES CODE MANUAL

Card Group	No. of Cards	Data and Definitions	Fortran Format
3.2 (cont)		<p>IQUAD = This variable is significant only in a two-dimensional run in which the mesh is automatically generated. It specifies if the quadrilaterals generated are plane strain, plane stress, or axisymmetric.</p> <p>= -3 or left blank. Quadrilaterals are plane strain.</p> <p>= 3 if the quadrilaterals are plane stress.</p> <p>= 4 if the quadrilaterals are axisymmetric.</p> <p>ITHPLT = Thermal tape creation flag</p> <p>= 0 if heat transfer program input tape <u>not</u> written</p> <p>= 1 if heat transfer program input tape written (unit 21)</p> <p>= 2 if heat transfer input tape written and input tape written for SC-4020 plots [1]. (units 20 and 21)</p>	
3.2.1	1	<p>ITHERM</p> <p>ITHERM = Thermal effects flag</p> <p>= 0 if thermal effects are <u>not</u> included</p> <p>= 1 if thermal effects are included</p>	(I5)
3.3	As req'd	<p>X (I, J) (or R(I, J) if axisymmetric mesh) in a 2-D case and</p> <p>X (I, J, K) in a 3-D case</p>	(8F10.0)

Replacement for Page 13 (Cont'd)

BUREAU OF MINES CODE MANUAL

Card Group	No. of Cards	Data and Definitions	Fortran Format
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X = X coordinates of the key diagram. Eight coordinates are given on a card, for as many cards as are necessary to define all the nodal points in the key diagram. They are given in the order: from the top to the bottom, from the left to the right, and in the 3-D case, from the front to the rear of the key diagram.

3.4 As req'd Y (I, J) (or Z(I, J) if axisymmetric mesh) in (8F10.0)
a 2-D case and

Y (I, J, K) in a 3-D case

Y = Y coordinates of the key diagram. Given in the order as stated in X.

BUREAU OF MINES CODE MANUAL

Card Group	No. of Cards	Data and Definitions	Fortran Format
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These modifications are applicable for thermoelastic analyses only.

4.9.5 9 (BCOEF(I),I=1,40),(YCOEF(I),I=1,25)

Cards 1-4 of this group are blank

Card 5 has the following information in the first
3 fields

3F10.0

α_o - coefficient of linear thermal expansion
applicable up to the reference temperature

$\frac{d\alpha}{dT}$ - slope of the α -T curve for temperatures
greater than the reference temperature

T_{ref} - reference temperature used in defining
these expansion properties

These material properties are graphically displayed
in Fig. 4 of the thermoelastic report.

Cards 6-9 of this group are blank

A.2 "EXECUTE" option---Input data for calculation phase when thermal effects are included (ITHERM = 1)

Card Group	No. of Cards	Data and Definitions	Fortran Format
5.1	1	<p>ITHRD, TAMBNT, TIMEMP, TCON</p> <p>ITHRD = Type of element temperature input</p> <p>= 0 if heat transfer program output file 23 supplies temperatures</p> <p>= +N if card reader contains temperature for element ranges (see card group 5.2)</p> <p>= -N if input cards contain temperatures for each element (see card group 5.2)</p> <p>Note N is a nonzero integer</p> <p>TAMBNT = Ambient temperature in the structure</p> <p>TIMEMP = The first time at which thermal stresses occur</p> <p>TCON = Time beyond which the temperatures of all elements become constant</p>	(I5, 3F10.0)

Card Group	No. of Cards	Data and Definitions	Fortran Format
5.2	As req'd	<p>OPTION ITHRD = -N</p> <p>(Temperatures specified for each element)</p> <p>Each time at which temperatures are specified requires the following data set:</p> <p>Card 1: TIMRD, NUMEL, NCARD</p> <p style="padding-left: 100px;">TIMRD = Time at which temperatures are provided</p> <p style="padding-left: 100px;">NUMEL = Number of elements in mesh</p> <p style="padding-left: 100px;">NCARD = Number of temperature cards</p> <p>Card 2 thru N card + 1: 8 temperatures/card in ascending element number ordering</p> <p>Card N card + 2: ⁷8₉ card to separate times.</p> <p style="padding-left: 100px;">Note the final time is <u>not</u> followed by a ⁷8₉ card</p>	<p>(F5.2, 2I5)</p> <p>(8E10.1)</p> <p>Column 1</p>

Card Group	No. of Cards	Data and Definitions	Fortran Format
5.2	As req'd	OPTION ITHRD = +N (Temperatures specified for element ranges) Each time at which temperatures are specified requires the following data set:	
	Card 1:	TIMRD, NUMEL, NCARD TIMRD = Time at which temperatures are provided NUMEL = Number of elements in mesh NCARD = Number of temperature cards	(F5.2, 2I5)
	Card 2 thru NCARD + 1:	NEL1, NEL2, TEMP NEL1 = First element of range for which temp. is given NEL2 = Final element of range for which temp. is given TEMP = Temperature for elements NEL1 to NEL2	(2I5, E10.1)
	Card NCARD + 2:	⁷ 8 ₉ card to separate times. Note the final time is <u>not</u> followed by a ⁷ 8 ₉ card	Column 1

A.3 "Output Option"--Allows selective printing of BMINES tables.

Card Group	No. of Cards	Data and Definitions	Fortran Format
6.1	1	IPHASB, IPHASC, IPHA ST IPHASB $\neq$ 0 or blank suppresses strain tables IPHASC $\neq$ 0 or blank suppresses displacement tables IPHA ST $\neq$ 0 or blank suppresses thermal stress tables IPHASB = 0 or blank prints strain tables IPHASC = 0 or blank prints displacement tables IPHA ST = 0 or blank prints thermal stress tables Note: Selective printing is not allowed when ITHPLT = 2 (SC-4020 plots are to be made). Thermal stress tables are not created when ITHERM = 0. Stress tables cannot be suppressed.	(3I5)

A.4 IWD Common Block Additions to BMINES Code

Replaces Page 39

Bureau of Mines Code Manual

<u>Location</u>	<u>Name</u>	<u>1108 Default Value</u>	<u>Meaning</u>
31	IWLUN(9)	11	(Tape or drum logical unit number)
32	IWLUN(10)	12	
33	IWLUN(11)	13	
34	IWLUN(12)	14	
35	IWLUN(13)	15	
36	IWLUN(14)	16	
37	IWLUN(15)	17	
38	IWLUN(16)	18	
39	IWLUN(17)	19	
40	IWLUN(18)	20	
41	IWLUN(19)	21	
42	IWLUN(20)	22	
43-62	IWHDR(1)- IWHDR(20)	Blanks	Contain run title
63	IWNNP	Not set	Number of node points
64	IWNEL	Not set	Number of elements
65	IWNMAT	Not set	Number of materials
66	IWBAND	Not set	Bandwidth
67	IWNEQ	Not set	Number of equations (DOF's)
68	IWNLDB	Not set	Number of entries/load coefficient block
69	IWNREC	Not set	Number of load coefficient blocks
70	IWNCF	3	Number of columns in load vector
71	IWNEQB	Not set	Number of equations/block
72	IWNEU	Not set	Size of element data block
73	IWERR	0	Error flag
74	IWLPPG	50	Maximum lines/page
75	IWKEN	27000	Length of ATOMSH common

Replaces Page 39 (Cont'd)

<u>Location</u>	<u>Name</u>	<u>1108 Default Value</u>	<u>Meaning</u>
76	ITHPLT	Not set	Thermal tape creation flag (Card group 3.2)
77	MAXDIF	Not set	Maximum node number difference for any element in renumbered mesh (written on logical unit 21)
78	ITHERM	Not set	Thermal effects flag (Card group 3.2.1)
79-100	IWDUM	Not used	
101	LMSTRT	21	Pointer to start of LM array
102	NRSTRT	Not set	Restart step number

APPENDIX B

File Usage Additions and Formats

The following files have been added to the BMINES program for use in the plotting options and in the thermoelastic calculations. The plot information is for two-dimensional cases only when written in these formats.

- Logical Unit 20-----1. Idealization scratch tape in subroutines PRINT and THMTAP
2. Thermal scratch tape (ITSCH) in subroutines THTAPE, TDRIVR, etc.
3. Output phase writes stresses, strains and displacements for SC-4020 plotting (see B.3 for format)
- Logical Unit 21----- Geometric idealization data written by subroutines PRINTE and THMTAP for input to both heat transfer code and SC-4020 plots. (see B.1 for format)
- Logical Unit 22----- Written by subroutine THTAPE for Output phase thermal stress tables (ITHOUT)
- Logical Unit 23----- Contains time-temperature histories written by heat transfer program. Read by subroutines TEMP and TINITL (see B.2 for format).

B.1 Heat Transfer Program Input and SC-4020 Plot Input Format on Unit 21

File 21 is written as an unblocked file.

Record 1. Write (21) (COMMENT(I), I = 1, 8)

COMMENT = A comment packed 10 characters per word.

Record 2. Write (21) IWNEL, IWNNP, NFF, MAXDIF

IWNEL = Number of elements in the mesh

IWNNP = Number of nodes in the mesh

NFF = Dummy parameter

MAXDIF = Maximum node number difference for any element pair in
the renumbered mesh

Record 3. Write (21) ((IX(I,J), I = 1, 4), MAT(J), J = 1, IWNEL)

IX = Node numbers for the Jth element in counter-clockwise order

MAT = Material number for Jth element

Record 4. Write (21) (X(K), Y(K), K = 1, IWNNP)

X = X coordinate of the Kth node (in renumbered order)

Y = Y coordinate of the Kth node (in renumbered order)

END FILE

B.2 Heat Transfer Program Output Format on Unit 23
(Time-Temperature Histories)

File 23 is written as an unblocked file.

For each time the following sequence is required:

Record 1. Read (23) TIME, NUMEL

TIME = Time at which temperatures exist

NUMEL = Number of elements for which temperatures are written

Record 2 thru NREC + 1

Read (23) (TEMP(I), I = 1, NBLK)

NREC = Number of records necessary to write all the element
temperature data for a given time

$(NREC = (NUMEL - 1)/50 + 1)$

NBLK = 50 for all records except the last

= NUMEL - (NREC - 1)*50 for the last record

END FILE

The temperatures for the final time are followed by an additional END FILE

B.3 SC-4020 Plot Input Format on Unit 20

File 20 is written as an unblocked file. For each time cycle the following sequence is repeated:

1. DO 1 J = 1, IWNEL

1 Write (20) (SIG(I, J), I = 1, 4), IACT(J)

SIG(1,J) = x component of stress for Jth element

SIG(2,J) = y component of stress for Jth element

SIG(3,J) = z component of stress for Jth element

SIG(4,J) = xy component of stress for Jth element

IACT(J) = Activity of Jth element

(0 = active and 1 = inactive)

2. Write (20) ITIME

ITIME = TIME

3. DO 2 J = 1, IWNEL

2 Write (20) (EPS(I,J), I = 1, 4)

EPS(1,J) = x component of strain for Jth element

EPS(2,J) = y component of strain for Jth element

EPS(3,J) = z component of strain for Jth element

EPS(4,J) = xy component of strain for Jth element

4. DO 3 K = 1, IWNNP

3 Write (20) (U(I,K), I = 1, 2)

U(1,K) = x displacement for Kth node

U(2,K) = y displacement for Kth node

The final time is followed by an END FILE.

APPENDIX C

Deck Setup Examples (SANDIA-BMINES Code)

Sample deck setups for runs with thermal effects (ITHERM = 1 in card group 3.2.1) are shown in this appendix. These cards must be preceded by an appropriate *START data card.

Example 1-----Temperatures specified for each element (card reader input).

The simple 3-D example problem shown in Fig. 5 has temperatures specified at times 0, 1, and 3. All output tables will be printed. The input data for this problem is shown on the following page.


```

*START
3-D TEST PROBLEM - THERMAL - 8 ELEMENT
1 1 1 0 0 0 1 1 0 0 0 0 0 0
1
0.0 0.0 1.0 1.0 0.0 0.0 1.0 1.0
1.0 0.0 1.0 0.0 1.0 0.0 1.0 0.0
1.0 1.0 1.0 1.0 0.0 0.0 0.0 0.0
1
2
2
2
000050 7
5 010111
11 111111
13 001111
14 011111
15 001111
17 011111
23 010111
000006
-1.0
0
1 0
5
0.0 1.0 0.0
1.0 1.0 0.0
2.0 1.0 0.0
3.0 1.0 0.0
4.0 1.0 0.0
.8333E+06 .3846E+06

```

} 9 Blank Cards

20.E-6

} 4 Blank Cards

```

*EXECUTE
-1 0. 1 1.0 10.
0. 8 1 100. 100. 100. 100. 100. 100.
7-8-9 1. 8 1 200. 200. 200. 200. 200. 200.
7-8-9 3.0 8 1 300. 300. 300. 300. 300. 300.
300. 300. 300. 300. 300. 300.
*OUTPUT
0 0 0
*EXIT

```

Example 2-----Temperatures specified for element ranges (card
input).

The input data for the cantilever beam example (see Fig. 6)
is shown below. All output tables will be printed.

```

*START
THERMAL PROBLEM 2 2-D ANALYSIS OF BEAM DEFLECTIONS AND STRESSES
1 1 0 0 0 0 1 1 0 0 0 0 0 0 -3 0
1
-2.5 -2.5 2.5 2.5
100.0 0.0 100.0 0.0
1
50
5
0200 6
1 111111
52 111111
103 111111
154 111111
205 111111
256 111111
0004
1.0 1.0
0
1 0
1
1.0 0. 0.0
10.E+6 15.00E+6
} 9 Blank Cards

6.E-6
} 4 Blank Cards

*EXECUTE
1 0. 1. 6.
0. 250 5
1 50 240.
51 100 220.
101 150 200.
151 200 180.
201 250 160.
*OUTPUT
0 0 0
*EXIT

```

Example 3-----Temperatures specified for each element (File 23 from
heat transfer program).

The input data for the axisymmetric hollow cylinder
example problem described in Fig. 7 is shown below.

All output tables will be printed.

```

*START
THERMAL TAPE CALC HOLLOW CYLINDER PROB 1 0 0 0 0 0 4 2
1 1 0 0 0 1 1 0 0 0 0 0 0 0 4 2
1 1.0 1.0 2.0 2.0
0.0625 0.0 0.0625 0.0
1 1
1 1
16
1200 0
2
1 0.5 0.0 0.0
2 0.5 0.0 0.0
1 0.125 0.0 0.0
2 0.125 0.0 0.0
0
2 0 0.0 0.0 0.0
3
20. 1.0 0.0
60. 1.0 0.0
180. 1.0 0.0
18.23E+6 6.30E+6 1.0

} 9 Blank Cards

9.0E-06
} 4 Blank Cards

*EXECUTE 1 70. 0. 60.
*OUTPUT 0 0 0
*EXIT

```

C.4 SC-4020 Plots

Contour, mesh, and time history plots are obtained by reformatting BMINES logical unit 20 and 21 output into the format for input to the Structural Mechanics Plots Package, [2, page 13].

A program such as the following (RANGE) can be used for reformatting. Note array dimensions will require enlargement for problems with more than 600 elements or 800 nodes.

MADSEN,T100,CM100000.

MARCELLA MADSEN OX 128 BLDG 806

ACCOUNT,5476464575,D5162,G2103,A0395320,RT,KUNC.

FTN.

COLLECT,LGO,FTNLIR.

ATTACH,TAPE21,JRT-KARL-PLOT2,CY=5.

ATTACH,TAPE20,JRT-KARL-PLOT1,CY=5.

PRESET,PIND.

REDUCE,OFF.

LGO.

ATTACH,DMESH,LGO1540-PLOTS,CY=40.

PRESET,PIND.

DMESH.

7-8 0

```
PROGRAM RANGE (INPUT,OUTPUT,TAPE20,TAPE21,TAPE10)
DIMENSION HFD(8),P(800),Z(800),IX(6,600),U(1600)
1  .SIG(4,600),EPS(4,600)
CALL FTNRIN(1,1,10)
READ (21)HFD
PRINT 20,HFD
20  FORMAT(1X,8A10)
READ (21)NUMEL,NUMNP,NUL,NULL
PRINT 10,HFD,NUMNP,NUMEL
10  FORMAT(1X,8A10/* NUMNP,NUMEL*2I5)
WRITE(10)HFD,NUMEL,NUMNP
READ (21)((IX(I,J),I=1,5),J=1,NUMEL)
PRINT 11,IX(1,1),IX(1,NUMEL)
11  FORMAT(* IX*2I5)
READ (21)(R(I),Z(I),I=1,NUMNP)
PRINT 12,R(1),Z(1),R(NUMNP),Z(NUMNP)
12  FORMAT(* R,Z* 4E15.4)
WRITE(10)(R(I),I=1,NUMNP),(Z(I),I=1,NUMNP),((IX(I,J),J=1,NUMEL),
1  I=1,5)
5  DO 1 J=1,NUMEL
READ (20)(SIG(I,J),I=1,4),IX(6,J)
IF(FOUR(20))4.1
1  CONTINUE
PRINT 15,SIG(1,1),SIG(1,NUMEL)
15  FORMAT(* SIG*2E15.4)
READ (20)TIME
37  PRINT 13,TIME
DO 2 J=1,NUMEL
2  READ (20)(EPS(I,J),I=1,4)
PRINT 14,EPS(1,1),EPS(1,NUMEL)
14  FORMAT(* EPS* 2E15.4)
NEQ=2*NUMNP
DO 3 I=1,NEQ,2
3  READ (20)U(I),U(I+1)
PRINT 16,U(1),U(2)
16  FORMAT(* U* 2E13.4)
13  FORMAT(* TIME* F15.4)
WRITE(10)TIME
WRITE(10)(U(I),I=1,NEQ),(U(I),I=1,NEQ),(U(I),I=1,NEQ)
WRITE(10) (IX(6,J),J=1,NUMEL)
WRITE(10) ((SIG(I,J),J=1,NUMEL),I=1,4)
WRITE(10) ((EPS(I,J),J=1,NUMEL),I=1,4)
```

```

      GO TO 5
4     PRINT 6
6     FORMAT(* PLOT TAPE WRITTEN*)
      ENDFILE 10
      REWIND 10
      READ (10)HED,NUMEL,NUMNP
      PRINT 10,HED,NUMNP,NUMEL
      READ (10)((R(I),I=1,NUMNP),(Z(I),I=1,NUMNP),((IX(I,J),J=1,NUMEL),
1      I=1,5)
      PRINT 11,IX(1,1),IX(1,NUMEL)
32    READ (10)TIME
      IF (EOF(10)) 30,31
31    PRINT 13, TIME
      READ (10)((U(I),I=1,NEQ),(U(I),I=1,NEQ),(U(I),I=1,NEQ)
      PRINT 16,U(1),U(2)
      READ (10) (IX(6,J),J=1,NUMEL)
      PRINT 33,IX(6,1),IX(6,NUMEL)
33    FORMAT(1X*ACTIVITIES* 2E15.6)
      READ (10)((SIG(I,J),J=1,NUMEL),I=1,4)
      PRINT 15,SIG(1,1),SIG(1,NUMEL)
      READ (10)((EPS(I,J),J=1,NUMEL),I=1,4)
      PRINT 14,EPS(1,1),EPS(1,NUMEL)
      GO TO 32
30    CONTINUE
      REWIND 10
      END

```

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```

NTIMES      1
TMAX        0.
TMIN        0.
DYNAMIC
ENDDATA

```

The following set of updates should be applied to permanent file CNTR, cy = 6 to allow excavation sequencing. CNTR is the permanent file which contains the contour plot program in update format.

```

*IDENT,EXSEQ
*DELETE,CNTR.45
    N2 = NEXT+6*NUMEL
*DDELETE,CNTR.427
    DIMENSION      TX(1),SS(6,1),EE(6,1),DD(6,1),IX(6,1),R(1),Z(1),
*DELETE,CNTR.523
    2000 CONTINUE
    READ (KR) (IX(6,K),K=1,NUMEL)
    READ (KK) ((SIG(I,J),J=1,NUMEL),I=1,4)
*DELETE,CNTR.605
    DIMENSION      IX(6,1),SE(6,1),R(1),Z(1),V(1),IND(1),
*DELETE,CNTR.627
    DIMENSION      TX(1),SE(6,1),TX(6,1),R(1),Z(1),IND(1),V(1),
*INSERT,CNTR.688
    READ (KK) (IX(6,K),K=1,NUMEL)
*DELETE,CNTR.741
    DIMENSION      IX(6,1),R(1),Z(1)
*DELETE,CNTR.794
    DIMENSION      IZ(6,1),R(1),Z(1),IQ(1),IM(1)
*DELETE,CNTR.994
    DIMENSION IX(6,1),IQ(1),IM(1),IA(5)
*DDELETE,CNTR.1037
    DIMENSION      DD(6,1),IX(6,1),R(1),Z(1),V(1),SIG(4,1),CMX(2,1)
*DELETE,CNTR.1071
    DIMENSION      SE(6,1),LAB(1),IX(6,1),R(1),Z(1),V(1),IND(1),
*DELETE,CNTR.1130
    DIMENSION      IX(6,1),R(1),Z(1),V(1),IND(1),SIG(4,1)
*INSERT,CNTR.1145
    IF (IX(6,N).EQ.1) GO TO 90
*DDELETE,CNTR.1189
    DIMENSION      IX(6,1),R(1),Z(1),V(1),LAB(1)
*INSERT,CNTR.1211
    IF (IX(6,N).EQ.1) GO TO 70

```

The following CDC 6600 control cards will perform a SANDIA-BMINES calculation, reformat tapes 20 and 21, and produce deformed mesh plots.

JOBNAME,CM152000,T100.

(Name, Box Number)

ACCØUNT.....

ATTACH,BMINES.

MAP,ØFF.

BMINES.

ATTACH,RANGE.

MAP,ØFF.

RANGE.

RFL,100000.

ATTACH,DMESH.

MAP,ØFF.

DMESH.

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BMINES input data

7-8-9

DMESH input data

6-7-8-9

APPENDIX D

Updates to Modify SANDIA-BMINES Core Requirements

Larger problems can be run with the following updates. Note that the core memory (CM) increases to 230K.

BMINES,CM230000,T100. MARCELLA MADSEN BOX 128 BLDG 806
ACCOUNT,S476464575,D5162,G2103,A0395320,RT,KUNG.
ATTACH,OLDPL,MMM-BMINES-UPDATE-5-27-77.
REQUEST,NEWPL,*PF.
UPDATE,N,W.
FIN,S,I=COMPILE.
REWIND,LGO.
ATTACH,LGO1,MMM-BMINES-LGO-5-27-77.
REQUEST,NEWLGO,*PF.
COPYL,LGO1,LGO,NEWLGO.
CATALOG,NEWLGO,JRT-BMINES-LGO-COR40,CN=JRT,CY=1,RP=365.
NEWLGO.

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*IDENT COR40
*D CORMOD.4
COMMON/BMCMN/A(40000)
*D CORMOD.3
COMMON/EKCMN/E(40000)
*D CORMOD.5
DIMENSION IBUF(40000)
*D CORMOD.6
ICR=40000
*D CORMOD.1,CORMOD.2
IWCORE=40000
IWKEN=40000
*COMPILE BMCALC,ATOMSH,OUTPUT,SETIW,NB3

7-8-9

APPENDIX REFERENCES

1. Isenberg, Jeremy, "Users Guide for a Computer Program for Analytic Modeling of Rock Structure Interaction," Final Technical Report, Volume 2, Agbabian Associates, 250 N. Nash Street, El Segundo, CA, 90245, April 1973.
2. Beisinger, Zelma, and Benzley, Steven, "Structural Mechanics Computer Plotting Handbook," Sandia Laboratories, Albuquerque, SAND 75-0038, September 1975.

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