See pocket 2 for encl.

PDR-1 WM-10 (2)
PDR- WM-11 (2)
WM-16 (2)

ITASCA
Consulting Group, Inc.

20 July 1987

David Tiktinsky - SS623
U.S. Nuclear Regulatory Commission
Division of Waste Management
Washington, D.C. 20555

"NRC Technical Assistance
for Design Reviews"
Contract No. NRC-02-85-002
FIN D1016

Dear David,

Please find enclosed the following documents:

1. STRES3D Command List
2. FLAC Thermal-Mechanical Option documentation
3. MUDEC Thermal-Mechanical Option documentation
4. FLAC Creep Material Models documentation

This was accomplished under NRC Contract No. 02-85-002. The first document is supplied as requested under Task Order No. 001 (Task 2). The second and third are supplied as per Task Order No. 002 (Task 2). The fourth document is supplied as per Task Order No. 004 (Task 1).

Sincerely,

Roger D. Hart
Program Manager

WM-RES
WM Record File D1016
Itasca

WM Project 10, 11, 16
Docket No.
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LPDR ✓B, N, S

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Suite 210 • 1313 Fifth Street SE • Minneapolis, Minnesota 55414
Telephone: (612) 623-9599 • Telex: 201682

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F L A C

Fast Lagrangian Analysis of Continua

Supplement No. 1

THERMAL-MECHANICAL OPTION

F L A C
Fast Lagrangian Analysis of Continua

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THERMAL-MECHANICAL OPTION

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F L A C

Supplement No. 1

THERMAL-MECHANICAL OPTION

1.0 INTRODUCTION

This option of FLAC simulates the transient flow of heat in materials and the subsequent development of thermally-induced stresses.

This option has the following specific features.

1. There are two material models for the thermal behavior of the material —isotropic and anisotropic conduction.

2. As in the standard version of FLAC, different zones may have different models and properties.

3. Any of the mechanical models may be used with either thermal model.

4. Several different thermal boundary conditions may be prescribed.

5. Heat sources may be inserted into the material either as line sources or as volume sources. These sources may be made to decay exponentially with time.

2.0 THEORETICAL BACKGROUND

2.1 Basic Equation

The basic equation of conductive heat transfer is Fourier's law, which can be written in one dimension as

$$Q_x = - k_x \frac{\partial T}{\partial x} \qquad (1)$$

where Q_x = flux in the x-direction (W/m^2), and

k_x = thermal conductivity in the x-direction ($W/m°C$).

A similar equation can be written for Q_y. Also, for any mass, the change in temperature can be written as

$$\frac{\partial T}{\partial t} = \frac{Q_{net}}{C_p M} \qquad (2)$$

where Q_{net} = net heat flow into mass (W),

C_p = specific heat ($J/kg°C$), and

M = mass (kg).

These two equations are the basis of the thermal version of FLAC.

Equation (2) can be written as

$$\frac{\partial T}{\partial t} = \frac{1}{C_p \rho} \left[\frac{\partial Q_x}{\partial x} + \frac{\partial Q_y}{\partial y} \right]$$

Combining this with Eq. (1),

$$\frac{\partial T}{\partial t} = \frac{1}{C_p \rho} \frac{\partial}{\partial x} \left[k_x \frac{\partial T}{\partial x} \right] + \frac{\partial}{\partial y} \left[k_y \frac{\partial T}{\partial y} \right]$$

$$= \frac{1}{\rho C_p} \left[k_x \frac{\partial^2 T}{\partial x^2} + k_y \frac{\partial^2 T}{\partial y^2} \right]$$

if k_x and k_y are constant. This is called the Diffusion Equation.

Temperature changes cause stress changes according to the equation

$$\Delta \sigma_{ij} = - \delta_{ij} K \beta \Delta T \qquad (3)$$

where $\Delta \sigma_{ij}$ = change in stress ij,

δ_{ij} = Dirac delta function,

K = bulk modulus,

β = volumetric thermal expansion coefficient, and

ΔT = temperature change.

The mechanical changes can also cause temperature changes as energy is dissipated in the system. This effect is neglected because it is usually negligible.

2.2 Implementation in FLAC

Each zone is divided into four triangular subzones using the centroid as an extra gridpoint. In each triangle, one-third of the mass is assigned to each of the three gridpoints.

At each timestep, Eqs. (1) and (2) are solved numerically, using the following scheme.

(1) In each triangle, $(\partial T/\partial x)$ and $(\partial T/\partial y)$ are approximated using the equation

$$\frac{\partial T}{\partial x_i} = \frac{1}{A} \oint T \hat{n}_i \, ds$$

$$= \frac{1}{A} \sum_{n=1}^{3} \bar{T}^n \, \epsilon_{ij} \, \Delta x_j^n$$

where A = area of the triangle,

$\bar{T}^n$ = average temperature on side n,

Δx_j^n = difference in x_j between ends of side n, and

ϵ_{ij} = two-dimensional permutation tensor,

$$\epsilon_{ij} = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}$$

The heat flow into each gridpoint of the triangle is calculated from

$$F_i = A_j Q_i$$

where A_j is the width of the line perpendicular to the component Q_i, as shown in Fig. 1.

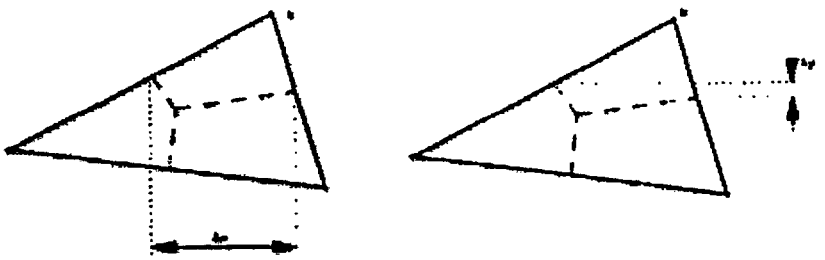

Fig. 1 Heat Flow Into Gridpoint k

$$F_{total} = F_x + F_y$$

$$= A_y Q_x + A_x Q_y$$

(2) For each gridpoint,

$$\Delta T = \frac{Q_{net}}{C_p M} \Delta t$$

where Q_{net} is the sum of F_{totals} from all zones affecting gridpoint i.

Steps (1) and (2) are repeated as necessary.

As thermal steps are taken, a cumulative temperature change ΔT_{tot} is maintained. When mechanical steps are taken, this temperature change is used to calculate stress increments using Eq. (3). These stresses are then used in the mechanical cycling.

3.0 THERMAL-MECHANICAL INSTRUCTIONS

The format of the thermal input commands is identical to that of the other commands in FLAC. This section is divided into two parts, the first describing commands available only with the thermal option and the second describing additions to commands already in the standard version of FLAC.

3.1 List of Thermal Input Commands

TFix <value> <range>

The temperature is fixed at all points in <range>. If a <value> is given, the temperature is fixed at that value.

TFREe <range>

The temperature at points in <range> is allowed to change.

THApp keyword value1 value2 <range>

This command is used to apply thermal boundary conditions and sources in the material. The keywords which can be used and the properties associated with value1 and value2 are listed below.

Keyword	Value1	Value2
Convection	convective heat transfer coefficient ($W/m^2°C$)	temperature of medium to which convection occurs
Flux	initial strength ($watts/m^2$)	decay constant (s^{-1})
Radiation	radiative heat transfer coefficient (for black bodies, this is the Stefan-Boltzmann constant, 5.668×10^{-8} $W/m^2 K^4$)	temperature of medium to which radiation occurs
Source	initial strength (watts)	decay constant (s^{-1})

Convection, radiation and flux conditions can be applied only over one row or column of gridpoints, either along a boundary or within the body. This feature enables the simulation of an internal line source, as a flux along an internal row or column of gridpoints. The **SOURCE** command results in a volume

THApp (continued)

source of the specified strength in the specified range of zones.

The decay constant in the SOURCE and FLUX options is defined by the equation

$$S_{curr} = S_{ini} * \exp[c_d(t_{curr} - t_{ini})]$$

where S_{curr} = current strength

S_{ini} = initial strength

c_d = decay constant

t_{curr} = current time

t_{ini} = initial time (when source was added)

To remove a CONVECTION or RADIATION boundary condition, the same condition should be applied, with the heat transfer coefficient of opposite sign.

CAUTION: It is not physically realistic to use negative heat transfer coefficients in any other circumstances.

THApp (continued)

To remove a FLUX or SOURCE condition, the condition should be applied with the strength replaced by s_{rep}, where

$$S_{rep} = -S_{ini} * \exp[c_d(t_{curr}-t_{ini})]$$

THis <Nstep=n> <keyword . . . I=il J=jl>

The history of the temperature is stored every NSTEP thermal timesteps for gridpoint il,jl. Up to 1,000 points per history may be kept for up to 25 histories at any time. Each history is numbered sequentially from 1. The user should keep track of the order of the histories, since a specific history number must be requested when plotting or printing. NSTEP must be the same for all thermal histories and need only be given once prior to timestepping; it defaults to 10 if not given.

The history values are stored on a direct access file on the hard disk. This file is erased when stopping FLAC; therefore, if the user wishes to save the history, a save file must be created or the history must be written to a formatted disk file (see **THIS WRITE N** command).

THis keyword

The following forms of the **THISTORY** command allow the user to plot, write or reset histories. History number nhis (nhis=1 to total number of histories) is written to the screen or to a disk file on the hard disk. The following choices of the keyword are possible.

Dump	nhis	The history (timestep number, history value) of history number nhis is written to the screen. If the history is greater than the page length, it will scroll past the screen. Use the cntrl-numlock keys to stop scrolling.
Write	nhis	The history (timestep number, history value) of history number nhis is written to a file FLACT.HIS on the hard disk. This file may be printed or manipulated after stopping FLAC. Successive **THIS WRITE** commands will sequentially add to the FLACT.HIS file. However, the first file written will overwrite any existing FLACT.HIS file.
Reset		All thermal histories are cleared.

THmod keyword <range>

This command associates a thermal model with an area of the grid. The models available are as follows.

Anisotropic	conduction and thermal expansion are anisotropic
Isotropic	conduction and thermal expansion are isotropic
Null	zone is null (Null zones model excavated material and can also model insulators)

THSolve <keyword <= value>...>

This command executes thermal timesteps. Calculation is performed until some limiting condition is reached. The limiting conditions may be the temperature increase at a point, the number of steps, the run time, or the simulated age. The limits are changed by the optional keywords listed below.

THSolve (continued)

Age = A	problem time (in days)
Noage	turns off the previously requested test for exceeding age A
Clock = t	run time (in minutes)
Temp = T	total temperature increase since the previous mechanical cycles
Step = s	timesteps

Defaults for these keywords are

T = 20 degrees
s = 500 timesteps
t = 5 minutes

The default for the age parameter is that the age is not tested until an age has been explicitly requested via an 'age = value' following a THSOLVE command.

Note that T depends on the units adopted for temperature. Old limits apply when set or on restart, but they are reset to defaults when a NEW command is given. A time limit of greater than 24 hours (1440 minutes) will not be accepted. When a

THSolve (continued)

THSOLVE command has been completed, the program will indicate which parameter has caused it to terminate. To ensure that it stops for the correct one, the values of the others should be set very high.

3.2 List of Changes to FLAC Input Commands

Initial keyword = value <range>

TEMPERATURE has been added to the list of keywords. The temperature is initialized to the given value at all gridpoints and zones in the range specified. The temperature at the center of the surrounding zones is set to the average of the four gridpoint temperatures for that zone.

Plot keyword <switch<=v>...>
<keyword <switch...>...>

TEMPERATURE has been added to the list of keywords.

THistory nhis plots thermal history nhis

Print keyword <keyword>

The keyword LIMITS, which is available in FLAC, prints out the limits on the THSOLVE command in addition to those printed in FLAC.

THerbou	thermal boundary conditions and sources

The following main grid keywords have also been added.

CONductivity	thermal conductivity
SPec_heat	specific heat
Temperature	
THEXp	volumetric thermal expansion coefficient
XConduct	thermal conductivity in x-direction
YConduct	thermal conductivity in y-direction

PROp keyword=value <keyword=value...> <range>

Properties can be assigned for models identified by the THMOD command. The property keywords and their meanings are given below.

Keyword	Description
SPec_heat	specific heat
Thexp	coefficient of volumetric thermal expansion

For the isotropic model:

CONductivity	thermal conductivity

For the anisotropic model:

XConductivity	thermal conductivity in x-direction
YConductivity	thermal conductivity in y-direction

SET keyword=value

Several new keywords have been added.

NMECH maximum number of mechanical steps executed between thermal steps when NTHER is non-zero (see below)

NOTE: The number of steps executed may be less than NMECH if the out-of-balance force gets low enough or the clock-time is exceeded. For the creep models (see FLAC Supplement No. 2), however, the number of mechanical steps is controlled by only two parameters—the clock-time and the problem time. The program will not stop after NMECH steps but will only stop when the CREEP problem time reaches the THERMAL problem time, unless the clock-time is exceeded. This is done so that the mechanical and thermal problems are always "in step" with each other. (default value = 500)

SET (continued)

NTHER — number of thermal steps to do before switching to mechanical steps

NOTE: The default value of NTHER is zero—in which case no interlinking occurs. If NTHER is not zero, the program will switch to mechanical steps every NTHER steps, or when the temperature change parameter (THSOLVE TEM=value) is exceeded. If the temperature change parameter is exceeded when NTHER=0, thermal cycling stops, and other thermal or mechanical cycling is user-controlled. To run a problem in which both thermal effects and creep occur, it is recommended that NTHER be set to one, so the the creep model is automatically accessed from the thermal model every thermal timestep. This allows the creep model to have access to the most accurate temperature history.

Caution: Geometry changes (in large-strain mode) are ignored by the thermal model until a THSOLVE command is given. This

SET (continued)

means that when the mechanical models are accessed automatically, the geometry changes are ignored on return to thermal steps. If large geometry changes occur, it is better to divide the run into several **THSOLVE** commands rather than having only one.

THDT = value

The thermal timestep is set to value.

NOTE: The program calculates the thermal timestep automatically. This keyword allows the user to choose a different timestep. If the program determines that the chosen step is too large, it will automatically reduce it to a suitable value when thermal steps are taken. It will not revert to a user-selected value until another **SET THDT** command is issued. The program selects a value which is usually one half the critical value for numerical stability.

SET (continued)

TOL = value

A thermal tolerance is set. This keyword is needed only for problems involving a slideline. If two points on opposite sides of the line are extremely close, the maximum thermal timestep for numerical stability will be controlled by these two points. To avoid this, interactions between points on opposite sides of the line are not calculated if they are within the tolerance. Instead, they are treated as one point for the thermal analysis.

The default for TOL is 0.5

4.0 SOLVING THERMAL-MECHANICAL PROBLEMS

The thermal option of FLAC has all the commands that FLAC has, as well as others, giving it the capability to solve transient thermal problems, and thermo-mechanical problems.

FLAC can be used in the usual way to model the excavation of material, change material properties, and change boundary conditions. The mechanical logic (the standard FLAC program) is also used in the thermomechanical program to take 'snapshots' of the mechanical state at appropriate intervals in the development of the transient thermal stresses. This logic is best explained by Fig. 2.

If creep models are being used, time is introduced into the mechanical model. There are then two different problem times, both of which have meaning. One is the THERMAL time; the other is called the CREEP time. (The second is only meaningful in mechanical analyses where time has meaning—not for equilibrium analyses.) The thermal and creep timesteps are normally very different, with the thermal one being greater. In this case, the mechanical logic is used not to take a snapshot at a fixed time but to let the stress state evolve with time. For the stress state to be calculated, as time proceeds, the temperature history is needed. This can be obtained by replacing steps 5 and 6 in Fig. 2 with the following steps.

1. SETUP . define grid,deform to desired shape . define material models and properties . define thermal models and properties . set boundary conditions (thermal and mechanical) . set initial conditions (thermal and mechanical) . set any internal conditions, such as heat sources
2. STEP TO EQUILIBRATE MECHANICALLY
3. PERFORM ANY DESIRED ALTERATIONS such as excavations
4. STEP TO EQUILIBRATE MECHANICALLY
REPEAT steps 3 and 4 until "initial" mechanical state is reached for thermal analysis.
5. TAKE THERMAL TIMESTEPS until (a) desired time is reached; or (b) temperature increases in grid cause "large" out-of-balance forces at gridpoints.
6. STEP TO EQUILIBRATE MECHANICALLY
REPEAT steps 5 and 6 until sufficient time has been simulated.
REPEAT steps 3 to 6 as necessary.

Fig. 2 General Solution Procedure for Thermal-Mechanical Analysis

1. Take one or more thermal steps, beginning at a time t_{ini}, and obtaining the temperatures at a time t_{later}.

2. Begin creep calculations from time t_{ini}, and take timesteps (usually much smaller than the thermal ones) until t_{later} is reached. At each timestep, obtain the temperature by linearly interpolating the temperature between the values at t_{ini} and t_{later}. The linear interpolation is done automatically by the program.

3. Repeat steps 1 and 2 until the desired time is reached.

4.1 Testing for Allowable Temperature Change

A difficulty associated with implementing this scheme lies in determining the meaning of "large" in Step 5(b). As described in the FLAC manual (Section 4.1), an advantage of explicit schemes is that the solution is reached in a physically meaningful manner, which is important for non-linear constitutive laws. In order to accomplish this in thermal analyses, the out-of-balance force caused by the temperature changes should not be allowed to adversely affect the accuracy of the solution. If the analysis being performed is linear, any temperature increase will be small enough, and FLAC need only equilibrate when the requested simulation time is reached. For non-linear problems, experimentation is necessary to obtain a feel for

what "large" means in a particular problem. Different allowable temperature increases must be tried with the **THSOLVE** command in the following manner.

1. Save the mechanical equilibrium state reached by FLAC (so that you can come back and try again).

2. Examine the plastic state of the grid using a **PRINT STATE** command.

3. Run thermal steps until a particular temperature increase is reported by the program (using a **THSOLVE TEM**=value command).

4. Use a **SOLVE** command to attain equilibrium.

   Again examine the state of the grid, using a **PRINT STATE** command.

   (a) If the plastic state has changed dramatically from that observed in Step 2, the temperature increase allowed was probably too great—in which case, restore the saved state and repeat from Step 3 using a smaller value of the temperature increase.

(b) If the plastic state has not changed much (say, in just a few zones), the allowed temperature increase was acceptable.

An important point to note is that the same temperature increase is not necessarily acceptable for all times in a problem. While the system is far from yield, large temperature increases will be acceptable, but near yield only relatively small increases can be tolerated.

4.2 Interlinking of Thermal and Mechanical Steps

For a problem in which many thermal steps can be taken before mechanical cycling is needed, thermal-mechanical analyses can be accomplished by executing a series of **THSOLVE** and **SOLVE** commands. If mechanical steps are required as often as thermal steps (e.g., for creep analysis), this procedure is impractical. Therefore, it has been made possible to switch to mechanical steps automatically during a series of thermal steps, using the **SET NTHER** and **SET NMECH** commands. If NTHER is set to a non-zero value, mechanical steps will be taken every NTHER steps, or whenever the temperature-change parameter (THSOLVE TEM=value) is exceeded.

An example of automatic linking of thermal and mechanical steps is given by the following commands.

```
set thdt = 1e5
set nmech = 100
set nther = 2
thsolve ste = 10
```

In this example, two thermal steps are taken to reach a thermal time of 2e5 secs. Then, 100 mechanical steps are taken, followed by two more thermal steps. This sequence is repeated until ten thermal steps have been taken.

5.0 EXAMPLE PROBLEM—A SIMPLIFIED MODEL OF A NUCLEAR WASTE REPOSITORY

We wish to determine the state of stress around a room excavation in a nuclear waste repository. The object of this example is to consider only the thermal effects—so gravity is ignored, as are in-situ stresses.

The material in which the excavation is made is assumed to be isotropic and linearly elastic. The thermal conductivity is assumed constant in all directions.

The heat source strength is approximated by the following equation (Hart et al, 1981):

$$Q(t) = 12.4 \exp(-3.5\times10^{-9}t) + 288.0 \exp(-7.1\times10^{-10}t) + 10.1 \exp(-9.6\times10^{-11}t)$$

where Q is the thermal output in watts, and t is the time in seconds after emplacement.

The heat transfer at the tunnel wall is assumed to be by convection to air at a temperature of 27°C. The initial rock temperature is also 27°C.

For the FLAC simulation, a simple 10x20 square-zone grid was used. Symmetry conditions were imposed on the left- and right-hand sides as well as the top and bottom. This corresponds to the situation in Fig. 3.

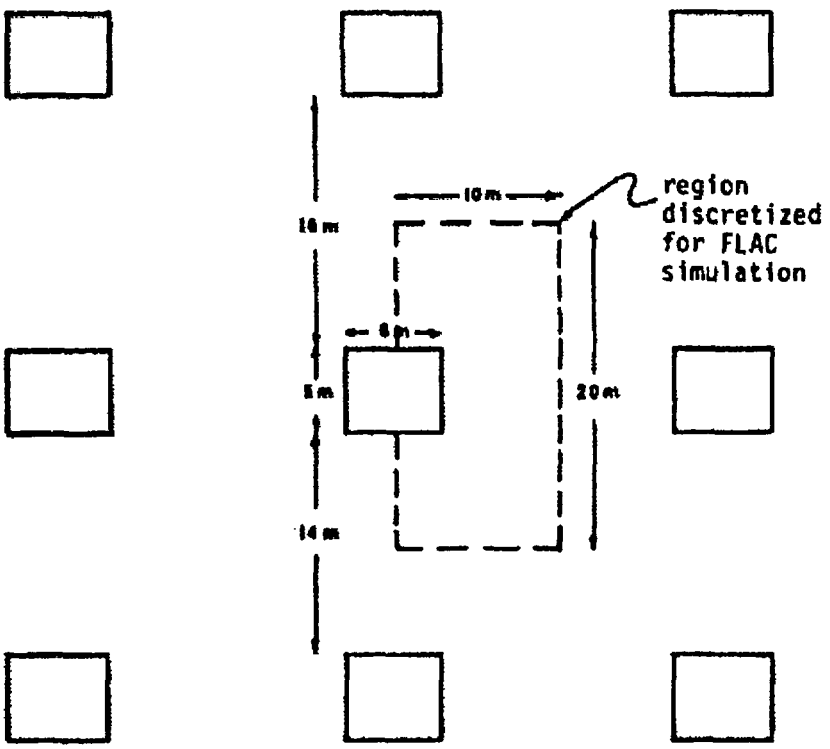

Fig. 3 Series of Excavations Modeled

The symmetry conditions are modeled by adiabatic boundaries (the default thermal boundary). If the problem really consisted of just one excavation, it would have been necessary to put the outer boundaries further away from the source and opening. In that case, it would have been desirable to run the simulation twice—first, with adiabatic outer boundaries and, then, with constant temperature outer boundaries. The correct result would be between these two; only if the two results were close would the boundaries be far enough away.

The mechanical boundary conditions for symmetry are that the top and bottom edges are prevented from moving in the y-direction, and the left and right edges cannot move in the x-direction.

The waste canister is represented by heat sources in two neighboring zones.

The rock mass material properties used for this simulation were

density	2200 kg/m^3
shear modulus	2.8×10^9 Pa
bulk modulus	4.7×10^9 Pa
specific heat	820 J/kg °C
thermal conductivity	2.1 W/m °C
coefficient of linear thermal expansion	1×10^{-5}/°C

The input is given in the following command sequence.

```
gr 10,20
mod elas
mod null i=1,3 j=8,12
thmod iso
thmod null i=1,3 j=8,12
prop bu=4.7e9 sh=2.8e9 dens=2200 cond=2.1 spec=820
     thexp=3e-5 * coeff. of volumetric expansion
fix y j=1
fix y j=21
fix x i=1
fix x i=11
* initialize rock temperature
ini te=27
* apply heat source in zones 5,10; 6,10
thapp source 6.2 -3.5e-9 i=5,6 j=10
thapp source 144.0 -7.1e-10 i=5,6 j=10
thapp source 5.05 -9.6e-11 i=5,6 j=10
* apply convective boundary conditions
thapp convec 1 27 i=4 j=8,13
thapp convec 1 27 i=1,4 j=8
thapp convec 1 27 i=1,4 j=13
set clo 180
set ste 1500
solve  * without gravity, so there should be no
     out-of balance forces
tit
     Heat Source in Tunnel Wall ( Initial State )
save year0.sav
set thdt=8.64e4 * thermal timestep of 24 hours
* solve thermal portion of problem
thsolve ste=365  tem=500 clo=180
* solve mechanical problem
solve
```

```
tit
     Heat Source in Tunnel Wall ( 1 Year )
save year1.sav
thsolve ste=365
solve
tit
     Heat Source in Tunnel Wall ( 2 Years )
save year2.sav
thsolve ste=1095
solve
tit
     Heat Source in Tunnel Wall ( 5 Years )
save Year5.sav
thsolve ste=1825
solve
tit
     Heat Source in Tunnel Wall ( 10 Years )
save Year10.sav
thsolve ste=3650
solve
tit
     Heat Source in Tunnel Wall ( 20 Years )
save Year20.sav
thsolve ste=10950
solve
tit
     Heat Source in Tunnel Wall ( 50 Years )
save Year50.sav
return
```

The saved states at times representing 1, 2, 5, 10 and 20 years can be restored to plot results such as those in Figs. 4 through 7.

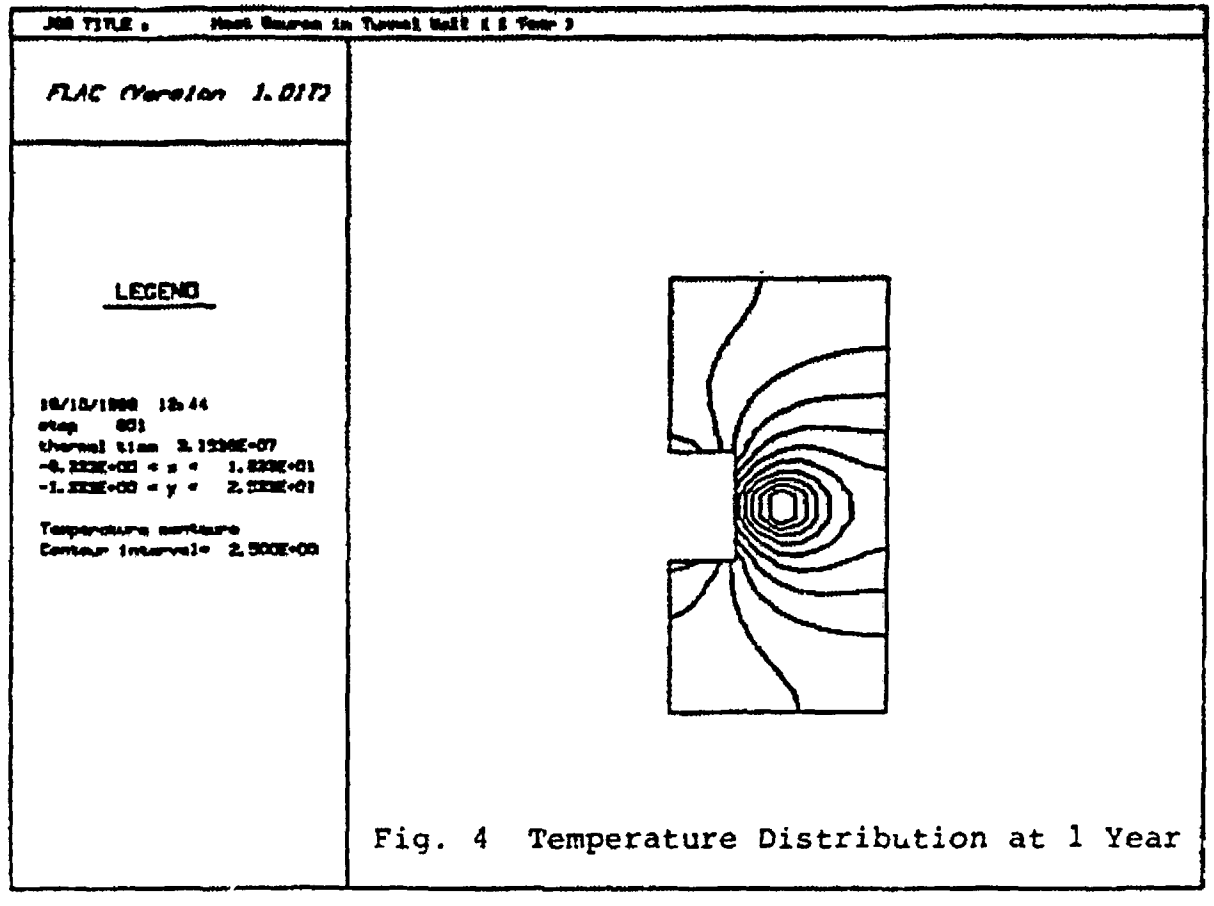

Fig. 4 Temperature Distribution at 1 Year

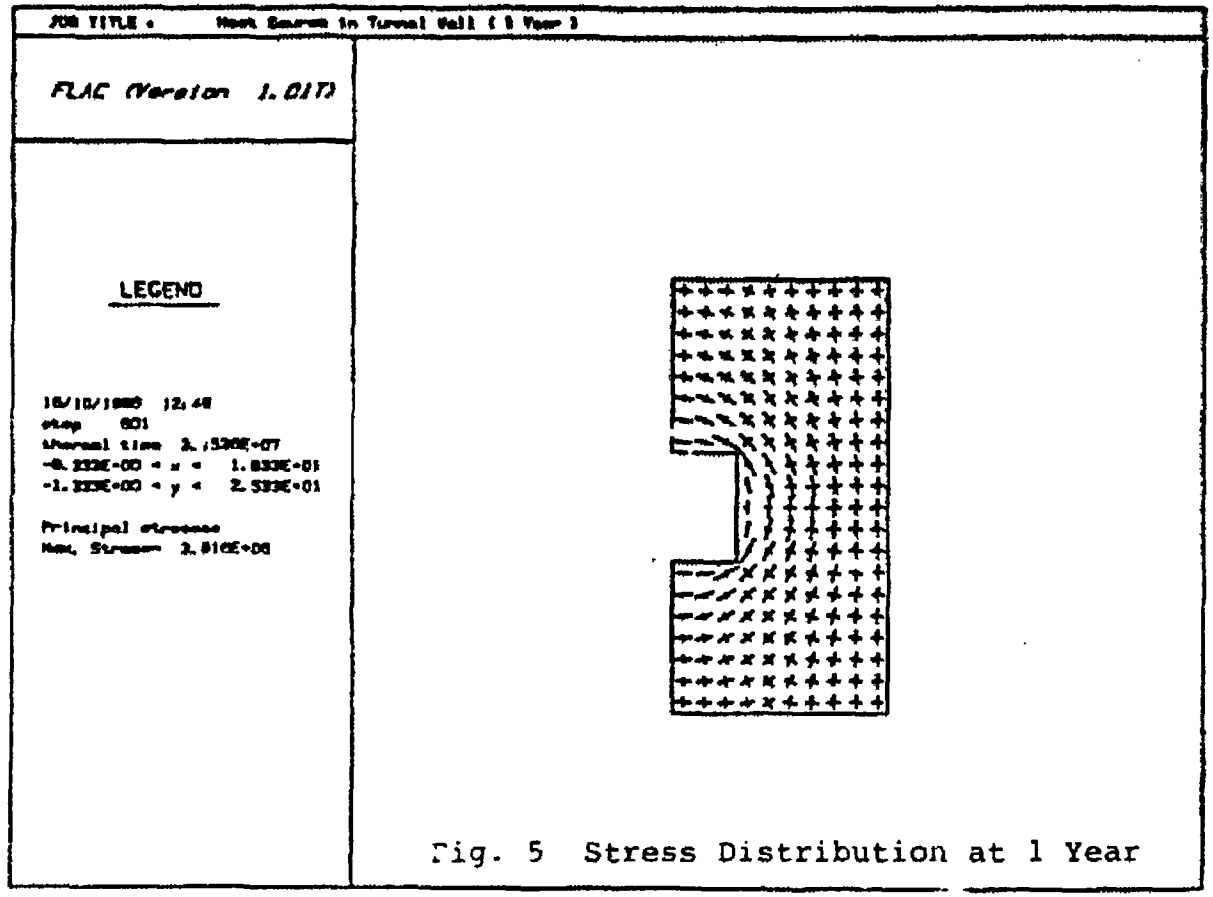

Fig. 5 Stress Distribution at 1 Year

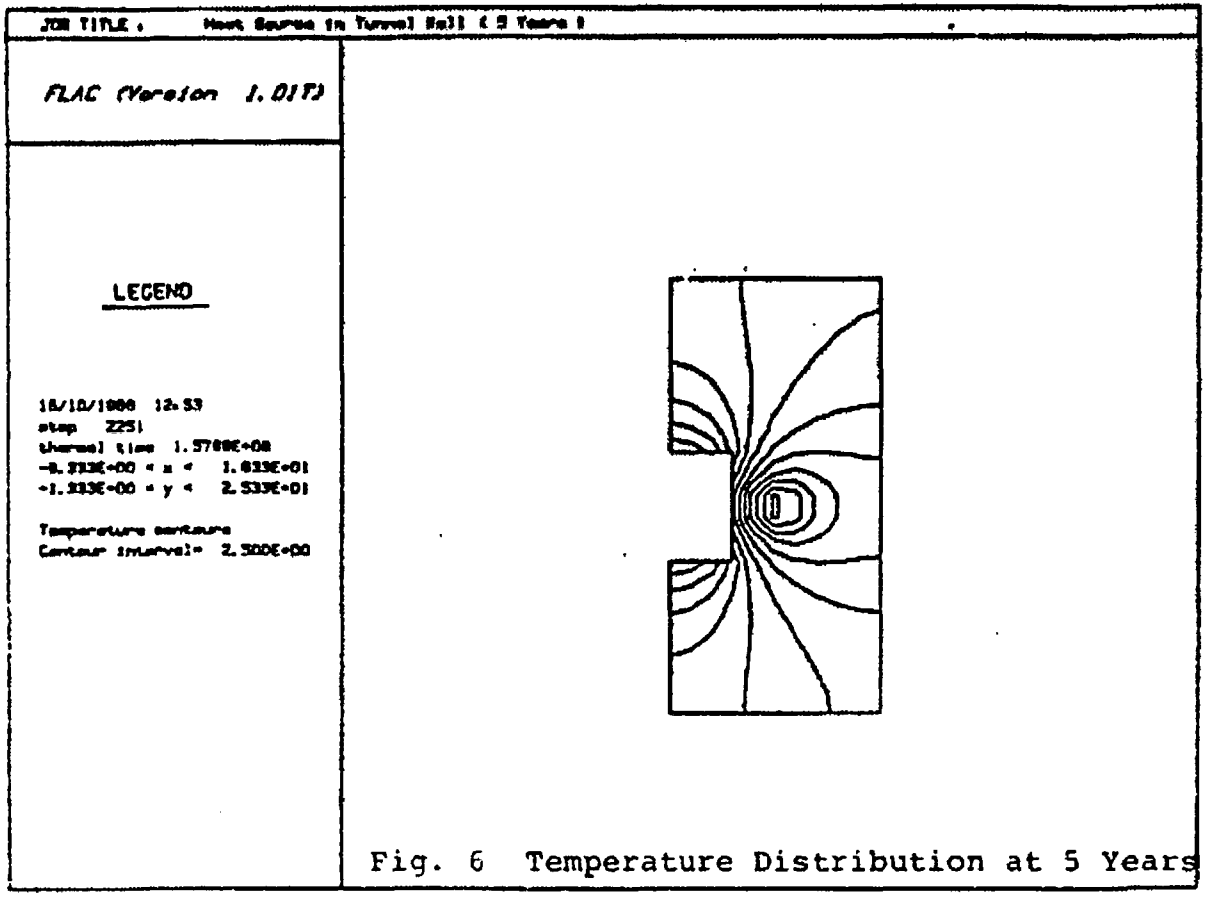

Fig. 6 Temperature Distribution at 5 Years

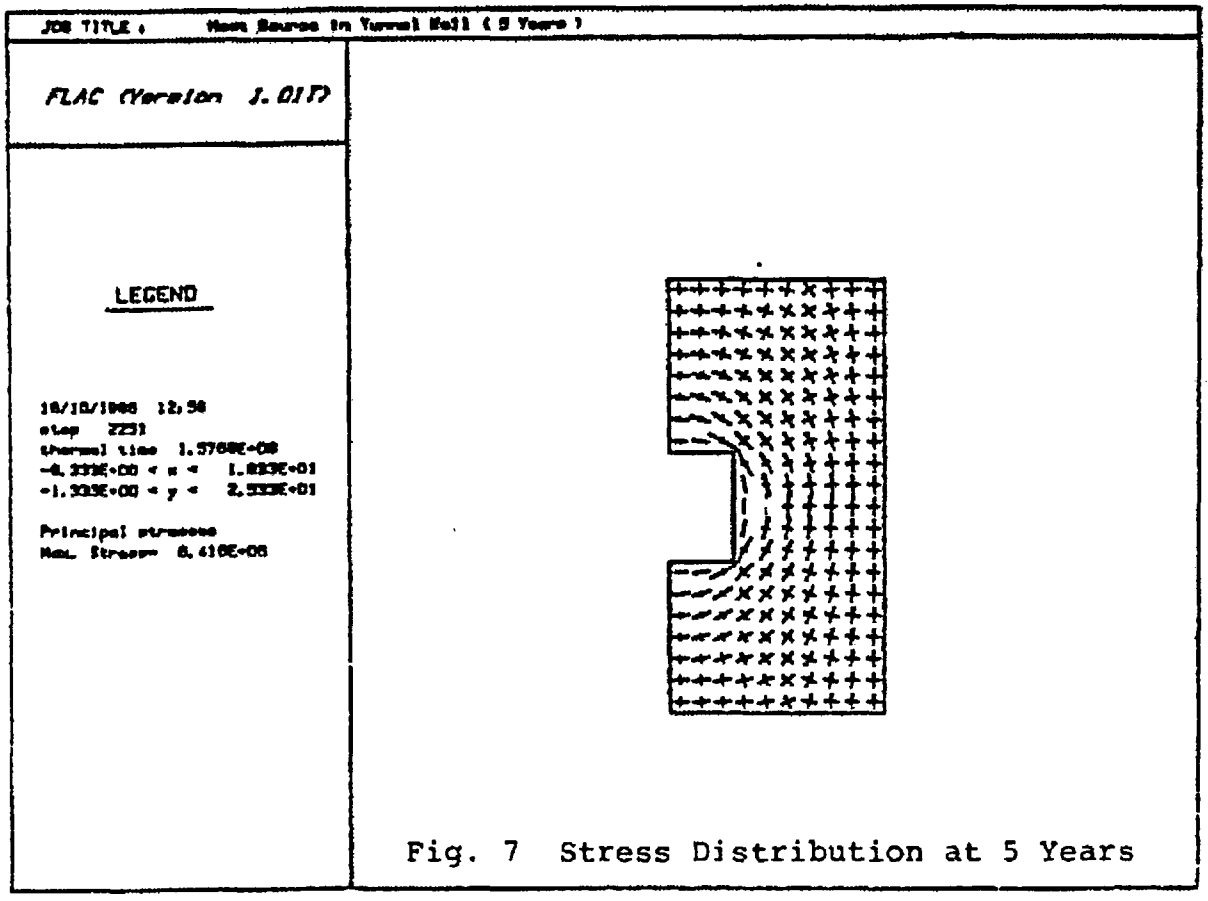

Fig. 7 Stress Distribution at 5 Years

As an example, type

```
flact> restore year1.sav
```

We now have the state after one year of simulation and can examine some of the conditions. Now, issue the command

```
flact> print temp
```

to see the temperatures in the grid. Follow this by

```
flact> plot temp  bound
```

or, for a hard copy, type

```
flact> plot pen  temp  red  bound
```

Also, issue the command

```
flact> plot stress  red  bound
```

to see the stresses developed around the opening. Recall that we had no initial stress or gravity so that the stresses shown are only those induced by the heat source.

We can restart from each of the saved states to see the changes as time progresses. Results at ages one and five years are shown in Figs. 4 through 7. The stress concentrations around the cavity are evident in Figs. 5 and 7.

REFERENCE

Hart, R. D., M. Christianson, W. Holman, and G. Hocking. "Numerical Modeling of Some Geotechnical Considerations Associated with Underground Isolation of Nuclear Wastes at the Savannah River Plant, South Carolina." Subcontract No. CNR3380 312, National Academy of Sciences, October 1981.

F L A C

Fast Lagrangian Analysis of Continua

Supplement No. 2

CREEP MATERIAL MODELS

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CREEP MATERIAL MODELS

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CREEP MATERIAL MODELS

1.0 INTRODUCTION

This option of FLAC can be used to simulate the behavior of materials which exhibit creep—i.e., time-dependent material behavior. Two creep models have been implemented in FLAC. These are:

(1) a classical visco-elastic model; and

(2) a reference creep formulation for nuclear waste isolation studies.

The second model is commonly used in thermomechanical analyses associated with studies for the underground isolation of nuclear waste in salt. A description of these models and their implementation is provided in this supplement.

2.0 DESCRIPTION OF CREEP CONSTITUTIVE MODELS

2.1 Classical Visco-Elasticity (Kelvin Substance)

The classical description of Newtonian viscosity is that the rate of strain is proportional to stress. Stress-strain relationships can be developed for viscous flow in exactly the same way as those developed for the theory of elasticity. The derivation of the equations in three dimensions can be found, for example, in Jaeger (1969).

Visco-elastic materials exhibit both viscous and elastic behavior. One such material is the Kelvin material, which can be represented in one dimension by a spring and dashpot in parallel, as shown in Fig. 1.

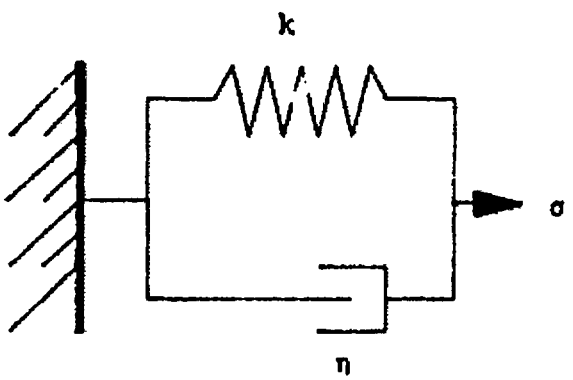

Fig. 1 One-Dimensional Kelvin Model

The stress-strain law for this material can be written as

$$\sigma_{ij} = \overset{(e)}{\sigma}_{ij} + \overset{(v)}{\sigma}_{ij} \qquad (1)$$

where $\overset{(e)}{\sigma}_{ij} = 2G\overset{(d)}{e}_{ij} + K\delta_{ij}\, e_{kk}$,

$\overset{(v)}{\sigma}_{ij} = 2n\, \dot{\overset{(d)}{e}}_{ij}\, \delta_{ij}$,

G = shear modulus,

K = bulk modulus,

n = dynamic viscosity,

$\overset{(d)}{e}_{ij}$ = deviatoric strain = $e_{ij} - \frac{1}{3} e_{kk}\, \delta_{ij}$,

$\dot{\overset{(d)}{e}}_{ij}$ = deviatoric rate = $\dot{e}_{ij} - \frac{1}{3} e_{kk}\, \delta_{ij}$,

e_{ij} = ij strain component,

$\overset{(e)}{\sigma}_{ij}$ = elastic part of stress, and

$\overset{(v)}{\sigma}_{ij}$ = viscous part of stress.

The material properties required for this model are the shear and bulk moduli (for the elastic behavior) and the viscosity.

2.2 A Reference Creep Law for Nuclear Waste Isolation Studies

An empirical law has been developed (Senseny, 1985) to describe the time- and temperature-dependent creep of natural rock salt. In addition to the elastic component, the material is assumed to undergo creep, based on the equation

$$\frac{d\dot{\epsilon}}{dt} = -\zeta\,(\dot{\epsilon} - \dot{\epsilon}_{ss})$$

—i.e.,

$$\dot{\epsilon} = \dot{\epsilon}_{ss} + e_a\,\zeta\,\exp(-\zeta t) \qquad (2)$$

where $\dot{\epsilon}$ = creep rate,

$\dot{\epsilon}_{ss}$ = steady-state creep rate,

ζ = a rate parameter,

e_a = an integration constant, and

t = time.

Based on experiments, Senseny observed two re-

gimes. For steady-state creep rates above a critical value $\dot{\epsilon}^{*}_{ss}$, e_a is a constant ϵ_a, and $\zeta = B\dot{\epsilon}_{ss}$, where B is a constant.

For steady-state creep rates below $\dot{\epsilon}^{*}_{ss}$,

$$e_a = \left[\frac{\dot{\epsilon}_{ss}}{\dot{\epsilon}^{*}_{ss}}\right]\epsilon_a \qquad \text{and} \qquad \zeta = B\,\dot{\epsilon}^{*}_{ss}$$

Thus, Eq. (2) can be written as

$$\dot{\epsilon} = \begin{cases} \dot{\epsilon}_{ss} + \epsilon_a B\dot{\epsilon}_{ss}\exp(-B\dot{\epsilon}_{ss}t) & \dot{\epsilon}_{ss} \geq \dot{\epsilon}^{*}_{ss} \\ \dot{\epsilon}_{ss} + \epsilon_a B\dot{\epsilon}_{ss}\exp(-B\dot{\epsilon}^{*}_{ss}t) & \dot{\epsilon}_{ss} \leq \dot{\epsilon}^{*}_{ss} \end{cases}$$

Also, the steady-state strain rate is assumed to be given by

$$\dot{\epsilon}_{ss} = A\sigma^{n}\exp(-Q/RT) \qquad (3)$$

where σ = applied stress,

A, n, Q = parameters of the model,

R = universal gas constant, and

T = temperature (in Kelvin).

This formulation of the creep law is known as the RE/SPEC baseline creep law.

Another formulation, known as the WIPP reference creep law, can be written as

$$\dot{\varepsilon} = \dot{\varepsilon}_s + \dot{\varepsilon}_p \qquad (4)$$

where

$$\dot{\varepsilon}_p = \begin{cases} (A - B\varepsilon_p)\,\dot{\varepsilon}_s & \dot{\varepsilon}_s \geq \dot{\varepsilon}^* \\ \left(A - B\dfrac{\dot{\varepsilon}_s^*}{\dot{\varepsilon}_s}\varepsilon_p\right)\dot{\varepsilon}_s & \dot{\varepsilon}_s < \dot{\varepsilon}^* \end{cases}$$

$$\dot{\varepsilon}_s = D(\bar{\sigma})^n \exp(-Q/RT)$$

where ϵ_p = primary creep strain,

ϵ_s = secondary creep strain,

n, A, B, D, Q = parameters of the model,

R = universal gas constant,

$\bar{\sigma}$ = deviatoric stress, and

T = temperature (in Kelvin).

The WIPP and RE/SPEC formulations are different expressions of the same law, using slightly different notations. The WIPP formulation is better-suited for implementation in explicit computer codes such as FLAC because the effect of temperature and stress histories is automatically built into the formulation. The RE/SPEC formulation is only valid for constant stresses and temperatures, although it can be modified to account for stress and temperature histories.

The relationship between the notations used in the two laws is given in Table 1.

Table 1

NOTATION FOR WIPP AND RE/SPEC FORMULATIONS

WIPP Notation	RE/SPEC Notation	Units	Typical Value
A	Bc_a	—	4.56
B	B	—	127
D	A	$Pa^{-n}\ s^{-1}$	5.79×10^{-36}
n	n	—	4.9
Q	Q	cal/mol	1200
R	R	cal/mol K	1.987
$\dot{\varepsilon}^{*}_{ss}$	$\dot{\varepsilon}^{*}_{ss}$	—	5.39×10^{-8}

3.0 INPUT INSTRUCTIONS

All commands have the same structure as those in the standard version of FLAC. No new commands have been added, but many keywords have been added to existing commands. The new keywords for each command are described below.

Model	keyword <range>	
	Viscous	classical viscosity
	Wipp	WIPP reference creep formulation

Print <keyword> <keyword>

The following keywords have been added:

Main Grid Keywords

ACt_energy	Q
A_wipp	A
B_wipp	B
D_wipp	D
E_dot_star	$\dot{\epsilon}^{*}_{ss}$
GAs_c	R
N_wipp	n
VIscosity	n

PROp keyword=value

In addition to the bulk and shear moduli, the creep models require the following properties:

Keyword	Description	Model
ACt_energy	activation energy (Q)	WIPP
A_wipp	A	WIPP
B_wipp	B	WIPP
D_wipp	D	WIPP
E_dot_star	$\dot{\epsilon}^{*}_{ss}$	WIPP
GAs_c	gas constant (R)	WIPP
N_wipp	n	WIPP
VIscosity	dynamic viscosity	classical

SET <keyword=value>

The timestep for the creep model is controlled using the following keywords. A description of the automatic timestep controller appears in Section 3.

DT = value

The timestep is set manually to value. Whenever the timestep changes, the velocities are changed, to accomadate the fact that the FLAC velocities represent distance per step. (default=0.0)

DT=AUTO The timestep will change automatically, according to the value of the maximum unbalanced force. In this case the following keywords can also be used.

MAXDT = value

The maximum timestep allowed is set to value. (default = 1e4)

MINDT = value

The minimum timestep allowed is set to value. (default = 1e2)

SET (continued)

FOBL = value

The timestep will be increased if the maximum unbalanced force falls below this value. (default = 1e4)

FOBU = value

The timestep will be decreased if the maximum unbalanced force goes above this value. (default = 1e5)

LMUL = value

The timestep will be multiplied by value if the unbalanced force falls below FOBL. (LMUL should be greater than 1, default = 2.0)

UMUL =value

The timestep will be multiplied by value if the unbalanced force exceeds FOBU. (UMUL should be less than 1, default = 0.5)

SET (continued)

LATENCY = value

the minimum number of timesteps which must elapse between timestep changes. (default = 100)

SOLVE <keyword = value>

Two keywords have been added to control when timestepping is stopped. These are:

Age = A problem time (in days)

Noage turns off the previously-requested test for exceeding age A.

The age parameter is not tested until an age has been explicitly requested via an "age=value" following a **SOLVE** command.

4.0 SOLVING CREEP PROBLEMS WITH FLAC

4.1 Introduction

The creep option of FLAC offers the same features as, and is run in the same manner as, the standard FLAC program. The major difference between creep and other constitutive models in FLAC is the concept of problem-time in the simulation. For creep runs, the problem-time and timestep represent real time, while in the other constitutive models the timestep is an artificial quantity, used only as a means of stepping to equilibrium. This also has an effect on the velocities—velocities in FLAC are actually measured in units of distance per step rather than distance per time. The timestep, and how to control it in FLAC, are described below.

4.2 Timesteps in FLAC

For time-dependent phenomena such as creep, FLAC allows the user to define a timestep. The default for this timestep is zero, in which case, the program treats the material as linearly elastic. This can be used to attain equilibrium before starting a creep simulation. Although velocities are still in units of distance per timestep, the constitutive laws for creep make use of the timestep in their equations, so timestep may affect the response.

Although the user may set the timestep, it is not arbitrary. If a system is desired to always be in mechanical equilibrium (as in a long-term creep

simulation), the time-dependent stress changes produced by the constitutive law must not be large compared to the strain-dependent stress changes, otherwise out-of-balance forces will be large. The timestep must therefore be chosen small enough that the maximum unbalanced force is smaller than some tolerance. FLAC allows the user to set the timestep manually, or allow the program to control it automatically. If the timestep is changed automatically, it can be decreased whenever the maximum unbalanced force exceeds some threshold, and increased whenever it goes below some other level. It has been found that continuous adjustment of the timestep creates mechanical "noise" in the system, so a different scheme has been introduced. After a timestep change has occured, there is a user-defined "latency period" (e.g., 100 steps) during which no further adjustments are made, allowing the system to settle. Normally, the timestep will start at a small value, to accommodate transients such as excavation, and then increase as the simulation proceeds. If a new transient is introduced, it may be desirable to reduce the timestep manually, and then let it increase again automatically.

The SET command is used to set the timestep, and the parameters required to allow it to change automatically. The new keywords are listed in Section 2.

NOTE: In order to accomodate the concept of problem time in FLAC runs, all previous TIME keywords (used to control the real time used by the computer) have been changed to CLOCK—i.e.,

```
SET CLOCK=value
SOLVE <CLOCK=value>
THSOLVE <CLOCK=value>
```

5.0 EXAMPLE PROBLEMS

5.1 Example 1: Parallel Plate Viscometer — Classical Model

Suppose that a material with viscosity η is steadily squeezed between two parallel plates which are moving at a constant velocity V_0. The two plates have length $2l$ and are a distance $2h$ apart. The material is prevented from slipping at the plates. The approximate analytical solution, given by Jaeger (1969), is

$$v_x = 3V_o x(h^2 - y^2)/2h^3$$

$$v_y = V_o y(y^2 - 3h^2)/2h^3$$

$$\sigma_{xx} = 3\eta V_o[3(h^2 - y^2) + (x^2 - l^2)]/2h^3$$

$$\sigma_{yy} = 3\eta V_o(y^2 - h^2 + x^2 - l^2)/2h^3$$

$$\sigma_{xy} = -3(V_o \eta x y)/h^3$$

The problem is illustrated in Fig. 2.

To solve the problem with FLAC, advantage can be taken of the symmetry about the x- and y- axes. The top right quadrant only need be modeled. For compatibility with the approximations of the analytical solution, artificial forces have to be applied at the "free" right-hand edge, and small strain logic is used.

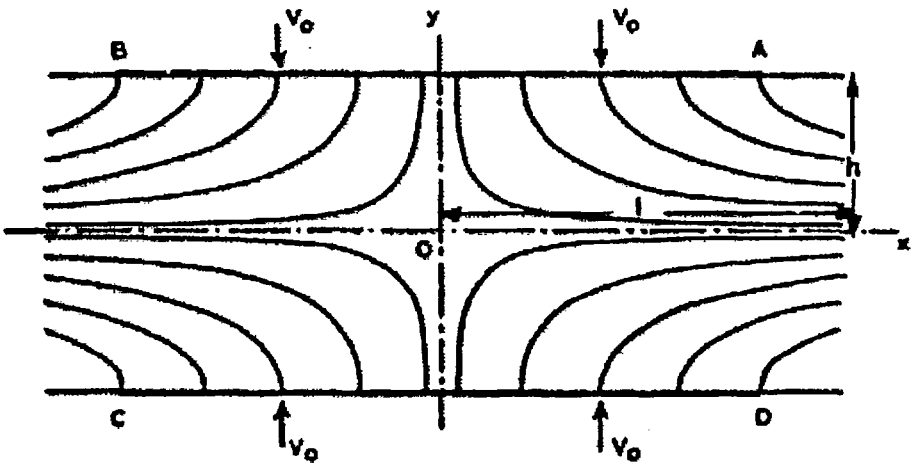

Fig. 2 Parallel Plate Viscometer [Jaeger, 1969]

The material properties are:

Density	1 kg/m^3
Shear modulus	$5x10^8$ Pa
Bulk modulus	$1.5x10^9$ Pa
Viscosity	$1x10^{10}$ kg/ms

The input is given in the following command sequence:

```
* parallel plate test viscous model
g 10 5
m vis
title
parallel-plate viscometer with viscous model
fix x i 1
fix y j 1
fix x y j 6
ini yv -1e-4 j 6
ini tem 300
appl xf 4.5e5 i 11 j 1
appl xf 8.64e5 yf -2.4e5 i 11 j 2
appl xf 7.56e5 yf -4.8e5 i 11 j 3
appl xf 5.76e5 yf -7.2e5 i 11 j 4
appl xf 3.24e5 yf -9.6e5 i 11 j 5
prop d 1 sh .5e9 bu 1.5e9 vis 1e10
set dt 1
wind -1 15 -4 8
c 900
return
```

Figure 3 is a plot of σ_{xx} contours. Other variables can be plotted and compared with the analytical solutions.

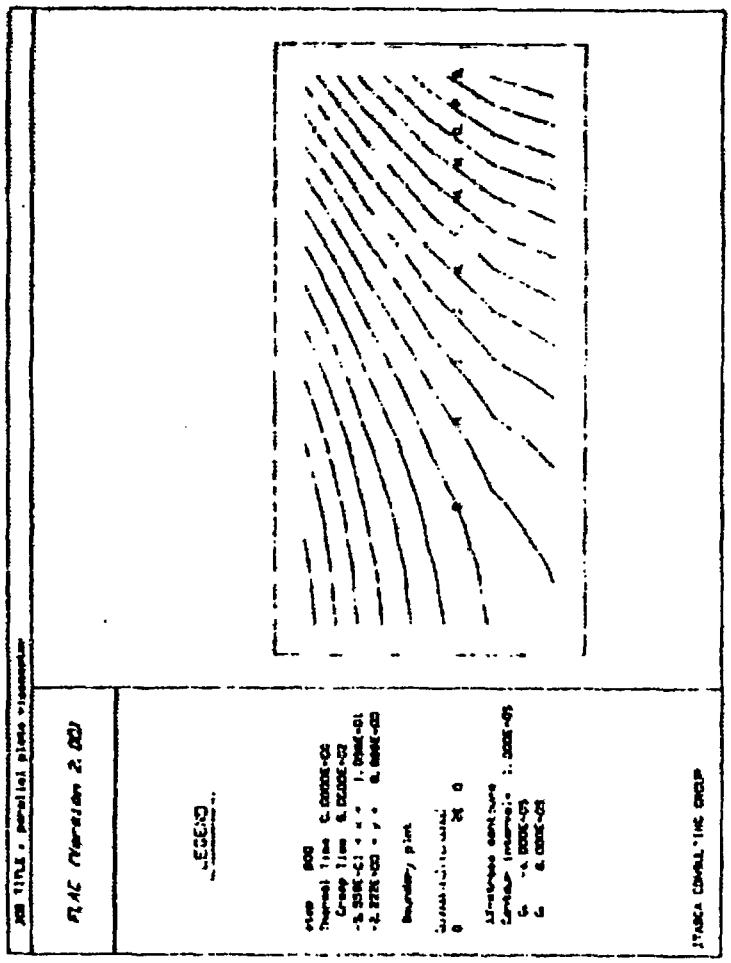

Fig. 3 σ_{xx} Contours for Example Problem 1

5.2 Example 2: Parallel Plate Viscometer—WIPP Model

The same problem can be modeled using the WIPP model. The following data file contains the commands necessary to run this problem. Note that, for this problem, it is essential to have the temperatures in the grid available, because they are used by the WIPP creep law. In this case, the **ini tem** command is used to input a uniform temperature of 300K.

```
* parallel plate test WIPP model
g 10 5
m wipp
title
parallel-plate viscometer with WIPP model
fix x i 1
fix y j 1
fix x y j 6
ini yv -1e-5 j 6
ini tem 300
appl xf 4.5e5 i 11 j 1
appl xf 8.64e5 yf -2.4e5 i 11 j 2
appl xf 7.56e5 yf -4.8e5 i 11 j 3
appl xf 5.76e5 yf -7.2e5 i 11 j 4
appl xf 3.24e5 yf -9.6e5 i 11 j 5
prop d 2600 sh 12.4e9 bu 20.7e9
prop gas 1.987 act 12e3 n_wipp 4.9 D_wipp 5.79e-36
prop a_wip 4.56 b_wip 127 e_dot 5.39e-8
set dt 1e4
wind -1 15 -4 8
c 900
ret
```

REFERENCES

Jaeger, J. C. Elasticity, Fracture and Flow (3rd Ed.). New York: John Wiley & Sons, Inc., 1969.

Senseny, Paul, E. "Determination of a Constitutive Law for Salt at Elevated Temperature and Pressure," American Society for Testing and Materials Reprint 869, 1985.

M U D E C
(Version 1.02)

A P P E N D I X T

THERMAL-MECHANICAL OPTION

T1. INTRODUCTION

This option of MUDEC simulates the transient flow of heat in materials and the subsequent development of thermally-induced stresses. This option has the following specific features.

1. Heat flow is modeled as conduction—either isotropic or anisotropic, depending on the user's choice of material properties.

2. Several difierent thermal boundary conditions may be imposed.

3. Heat sources may be inserted into the material either as line sources or as volume sources. The sources may be made to decay with time.

T2. THEORETICAL BACKGROUND

T2.1 Basic Equation

The basic equation of conductive heat transfer is Fourier's law, which can be written in one dimension as

$$Q_x = - k_x \frac{\partial T}{\partial x} \qquad (1)$$

where Q_x = flux in the x-direction (W/m^2), and

k_x = thermal conductivity in the x-direction ($W/m°C$).

A similar equation can be written for Q_y. Also, for any mass, the change in temperature can be written as

$$\frac{\partial T}{\partial t} = \frac{Q_{net}}{C_p M} \tag{2}$$

where Q_{net} = net heat flow into mass (W),

C_p = specific heat (J/kg°C), and

M = mass (kg).

These two equations are the basis of the thermal version of MUDEC.

Equation (2) can be written as

$$\frac{\partial T}{\partial t} = \frac{1}{C_p \rho} \left[\frac{\partial Q_x}{\partial x} + \frac{\partial Q_y}{\partial y} \right]$$

Combining this with Eq. (1),

$$\frac{\partial T}{\partial t} = \frac{1}{C_p \rho} \frac{\partial}{\partial x} \left[k_x \frac{\partial T}{\partial x} \right] + \frac{\partial}{\partial y} \left[k_y \frac{\partial T}{\partial y} \right]$$

$$= \frac{1}{\rho C_p} \left[k_x \frac{\partial^2 T}{\partial x^2} + k_y \frac{\partial^2 T}{\partial y^2} \right]$$

if k_x and k_y are constant. This is called the Diffusion Equation.

Temperature changes cause stress changes according to the equation

$$\sigma_{ij} = - \delta_{ij} K \beta \Delta T \tag{3}$$

where $\Delta\sigma_{ij}$ = change in stress ij,

δ_{ij} = Dirac delta function,

K = bulk modulus,

β = volumetric thermal expansion coefficient, and

ΔT = temperature change.

The mechanical changes can also cause temperature changes as energy is dissipated in the system. This effect is neglected because it is usually negligible.

T2.2 Implementation in MUDEC

MUDEC divides blocks into triangular zones which are also used for the thermal analysis.

At each timestep, Eqs. (1) and (2) are solved numerically, using the following scheme.

(1) In each triangle, $(\partial T/\partial x)$ and $(\partial T/\partial y)$ are approximated using the equation

$$\frac{\partial T}{\partial x_i} = \frac{1}{A} \oint T n_i \, ds$$

$$= \frac{1}{A} \sum_{n=1}^{3} \bar{T}^n \, \epsilon_{ij} \, \Delta x_j^n$$

where A = area of the triangle,

$\bar{T}^n$ = average temperature on side n,

Δx_j^n = difference in x_j between ends of side n, and

ϵ_{ij} = two-dimensional permutation tensor,

$$\epsilon_{ij} = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}$$

The heat flow into each gridpoint of the triangle is calculated from

$$F_i = A_j Q_i$$

where A_j is the width of the line perpendicular to the component Q_i, as shown in Fig. T1.

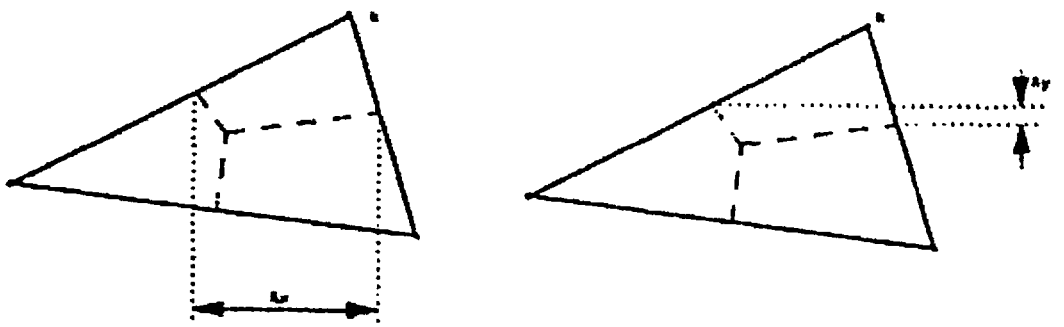

Fig. T1 Heat Flow Into Gridpoint k

$$F_{total} = F_x + F_y$$
$$= A_y Q_x + A_x Q_y$$

(2) For each gridpoint,

$$\Delta T = \frac{Q_{net}}{C_p M} \Delta t$$

where Q_{net} is the sum of F_{totals} from all zones affecting gridpoint i.

Steps (1) and (2) are repeated as necessary.

Joints are assumed to offer no resistance to heat flow and, for thermal calculations, gridpoints on opposite sides of the joints are used as if they were all part of one block.

As thermal steps are taken, a cumulative temperature change ΔT_{tot} is maintained. When mechanical steps are taken, this temperature change is used to calculate stress increments using Eq. (3). These stresses are then used in the mechanical cycling.

T3. THERMAL-MECHANICAL INPUT INSTRUCTIONS AND COMMAND DESCRIPTIONS

The format of the input commands is the same as that of other commands in MUDEC. Table T-1 illustrates examples of consistent sets of units. As in the standard version of MUDEC, no conversions are performed by the program.

The rest of this section is divided into two parts—the first describing commands available only with the thermal option and the second describing additions to commands already in the standard version of MUDEC.

Table T-1

SYSTEM OF UNITS FOR THERMAL PROBLEMS

	METRIC			BRITISH		
Length	m	m	m	cm	ft	in
Density	kg/m^3	$10^3 kg/m^3$	$10^6 kg/m^3$	$10^6 g/cm^3$	$slugs/ft^3$	$snails/in^3$
Stress	Pa	kPa	MPa	bar	lb_f/ft^2	psi
Temperature	K	K	K	K	R	R
Time	s	s	s	s	hr	hr
Specific Heat	J/(kgK)	10^{-3}J/(kgK)	10^{-6}J/(kgK)	10^{-6}cal/(gK)	$(32.17)^{-1}$Btu/(lbR)	$(32.17)^{-1}$Btu/(lbR)
Thermal Conductivity	W/(mK)	kW/(mK)	MW/(mK)	(cal/s)/(cmK)	(Btu/hr)/(ftR)	(Btu/hr)/(inR)
Thermal Modulus	Pa/K	KPa/K	MPa/K	bar/K	$(lb_f/ft^2)/R$	psi/R
Convective Heat Transfer Coefficient	$W/(m^2K)$	$W/(m^2K)$	$W/(m^2K)$	$(cal/s)/(cm^2K)$	$(Btu/hr)/(ft^2R)$	$(Btu/hr)/(in^2R)$
Radiative Heat Transfer Coefficient	$W/(m^2K^4)$	$W/(m^2K^4)$	$W/(m^2K^4)$	$(cal/s)/cm^2K^4$	$(Btu/hr)/(ft^2R^4)$	$(Btu/hr)/(in^2R^4)$
Flux Strength	W/m	W/m	W/m	(cal/s)/cm	(Btu/hr)/ft	(Btu/hr)/in
Source Strength	W/m^2	W/m^2	W/m^2	$(cal/s)/cm^2$	$(Btu/hr)/ft^2$	$(Btu/hr)/in^2$
Decay Constant	s^{-1}	s^{-1}	s^{-1}	s^{-1}	hr^{-1}	hr^{-1}
Stefan-Boltzmann Constant	$5.67 \times 10^{-8} W/m^2K^4$			1.356×10^{-12} $cal/(cm^2sK^4)$	1.713×10^{-9} $Btu/(ft^2hrR^4)$	1.19×10^{-11} $Btu/(in^2hrR^4)$

where 1K = 1.8R

1J = 0.239 cal = 9.48×10^{-4} Btu

1J/kgK = 2.39×10^{-4} Btu/lbR

1W = 1 J/s = 0.239 cal/s = 3.412 Btu/hr

1W/mK = 0.578 Btu/(ft/hrR)

$1W/m^2K$ = 0.176 Btu/ft^2hrR

Note that unless radiation is being used, temperatures may be quoted in the more common units of °C (instead of K) or °F (instead of R).

where Temp(°C) = $\frac{5}{9}$ * (Temp(°F) - 32)

Temp(°F) = (1.8 Temp(°C)) + 32

Temp(°C) = Temp(K) - 273

Temp(°F) = Temp(R) - 460

List of Thermal Input Commands

INITEM value xl xu yl yu

The temperature is set to value at all corners and gridpoints in the range xl<x<xu, yl<y<yu. Thermal stresses are not induced by this method of setting the temperature.

TFIX value xl x2 yl y2

The temperature at all corners and gridpoints in the range xl<x<xu,yl<y<yu is held fixed at value during the simulation. If value is not the current temperature, stresses are induced by the difference between value and the current temperature. (NOTE: by default, all temperatures are free to change initially.)

TFREE xl xu yl yu

The temperature at all corners and gridpoints in the range xl<x<xu,yl<y<yu is allowed to change during the simulation. Note: by default all temperatures are free to change initially.

THAPP <x1 xu y1 yu> keyword parameter1 parameter2 <region x1,y1 x2,y2 x3,y3 x4,y4>

This command is used to apply thermal boundary conditions and sources in the range x1<x<xu,y1<y<yu or in the region defined by (x1,y1), (x2,y2), (x3,y3), and (x4,y4). The keywords which can be used and the properties associated with parameters 1 and 2 are listed below.

Keyword	Parameter 1	Parameter 2
Convection	convective heat transfer coefficient	temperature of medium to which heat transfer occurs
Flux	initial strength	decay constant
Radiation	radiative heat transfer coefficient (For black bodies, this is the Stefan-Boltzmann constant)	temperature of medium to which occurs
Source	initial strength	decay constant

The convection, radiation, and flux commands are used to apply the stated boundary condition between corners in the range x1<x<xu,y1<y<yu. Convection, radiation and flux conditions are meaningful only along lines. The program ensures that this condition is achieved by only applying the boundary condition between two corners in the range (x1<x<xu,y1<y<yu) if they are consecutive corners on the block. This condition is only checked during cycling—so, some corners listed when the boundary conditions are printed out may not be subject to the boundary condition if the next corner either clockwise or anticlockwise on the block is not also listed.

The SOURCE keyword results in a volume source of the stated strength in all blocks with centroids in the range x1<x<xu,y1<y<yu.

Consistent units for the various quantities listed above are summarized in Table T-1.

The decay constant in the SOURCE and FLUX options is defined by the equation

$$S_{curr} = S_{ini} * \exp[c_d(t_{curr} - t_{ini})]$$

where S_{curr} = current strength

S_{ini} = initial strength

c_d = decay constant

t_{curr} = current time

t_{ini} = initial time (when source was added)

To remove a CONVECTION or RADIATION boundary condition, the same condition should be applied with the heat transfer coefficient of opposite sign.

CAUTION: It is not physically realistic to use negative heat transfer coefficients in any other circumstances.

To remove a FLUX or SOURCE condition, the condition should be applied with the strength replaced by S_{rep}, where

$$S_{rep} = -S_{ini} * \exp[c_d(t_{curr}-t_{ini})]$$

RUN <<keyword=value>...>

This command executes thermal timesteps. Calculation is performed until some limiting condition is reached. The limiting conditions may be the temperature increase at any point, the number of steps, the run time, or the simulated age. The limits are changed by the optional keywords listed below.

Age = A	problem time (in consistent units)
Noage	turns off the previously requested test for exceeding age A
Clock = t	run time (in minutes)
Temp = T	total temperature increase since the previous mechanical cycles
Step = s	timesteps
delt = Δt	thermal timestep

The thermal timestep is calculated automatically by the program. This parameter allows the user to change the timestep. If the program determines that this value is too large, it will automatically reduce the timestep to a suitable value when it begins the analysis. The value determined by the program is usually one half the critical value for numerical stability.

One other keyword is available i.e.,

TOL = tol	points in this tolerance merged for thermal calculations

Defaults for these keywords are:

T = 20 degrees
s = 500 timesteps
t = 5 minutes
tol = 0.1

The default for the age parameter is that the age is not tested until an age has been explicitly requested via an 'age = value' following a **RUN** command.

Old limits apply when set or on restart. A time limit of greater than 24 hours (1440 minutes) will not be accepted. When a **RUN** command has been completed, the program will indicate which parameter has caused it to terminate. To ensure that it stops for the correct one, the values of the others should be set very high.

THIST keyword <keyword> ...

This command is similar to the **HIST** command in the standard version of MUDEC. A history may be kept of the temperature at positions in the grid. Temperatures are accessed by their "thermal-history" number, which corresponds to the order in which the histories were requested by the user. The temperature is stored every Nlcyc thermal steps. A time history of of the temperature may be made at up to twenty points. A maximum of twenty **RUN** command may follow a **THIST** command. For more thermal steps, the history must be reset with the **RESET** command followed by new **THIST** commands. The keywords available are:

NTCYC n thermal histories are sampled every n steps. (default is n=10)

TYPE n displays the value of temperature history n on the screen during thermal stepping. Only one point can be selected with this command.

WRITE n fname

write temperature history number n to file fname

Temperature x y

temperature at location nearest to x,y

List of Changes to MUDEC Input Commands

PLOT keyword

Keywords which have been added are:

Temperature
temperature contours

THist n1 <n2...>

temperature histories n1,n2 ... assigned by THIST command.

PRINT keyword

The new properties relevant to the thermal model (and described under the PROP command below) are printed out in addition to the properties printed out by the standard version of MUDEC.

THERMAL Thermal boundary conditions and sources are printed.

THIST n1 <n2...>

Temperature histories n1, n2, . . . are printed.

PROP material n keyword v <keyword v>

Keywords which have been added are:

CONd	thermal conductivity
SPecheat	specific heat
THMOD	thermal modulus (explained below)
XCOnd	thermal conductivity in x-direction
YCOnd	thermal conductivity in y-direction
XTHMod	thermal modulus in x-direction
YTHMod	thermal modulus in y-direction

The thermal modulus is a derived quantity relating induced stresses to temperature changes. It is related to the thermal expansion coefficient and moduli of elasticity of the intact material; for discontinuous materials, however, the thermally-induced stresses are affected by the presence of joints, so we define the thermal modulus in the i-direction (E_{Ti}) such that, for a temperature increase ΔT, the stress change $\Delta\sigma_{ii}$ is

$$\Delta\sigma_{ii} = -E_{Ti}\,\Delta T \qquad i=1,2$$

The actual properties used by the program are the thermal conductivities and moduli in the x- and y-directions. The COND keyword simply sets the conductivities in both directions equal to the set value. The THMOD keyword acts similarly on the thermal moduli in the x- and y-directions.

RESET keyword

The new keyword THIST has been added. The effect of this command is to set the current values of the thermal histories to zero. This command must be used if more than 20 **RUN** commands follow a **THISTORY** command.

SET keyword = value

Several new keywords have been added.

NMECH maximum number of mechanical steps executed between thermal steps, when NTHER is non-zero (see below). NOTE: The number of steps executed may be less than NMECH if the out-of-balance force gets low enough or the clock-time is exceeded (default value = 500).

NTHER number of thermal steps to do before switching to mechanical steps.

NOTE: The default value of NTHER is zero, in which case no interlinking occurs. If NTHER is not zero, the program will switch to mechanical steps every NTHER steps, or when the temperature change parameter (THSOLVE TEM = value) is violated. If the temperature change parameter is violated when NTHER=0, thermal cycling stops, and further thermal or mechanical cycling is user-controlled.

Caution: Geometry changes are ignored by the thermal model until a RUN command is given. This means that when the mechanical models are accessed automatically, the geometry changes are ignored on return to thermal steps. If large geometry changes occur, it is better to divide the run into several RUN commands rather than having only one.

THDT The thermal timestep is set to value.

NOTE: The program calculates the thermal timestep automatically. This keyword allows the user to choose a different timestep. If the program determines that the chosen step is too small, it will automatically reduce it to a suitable value when thermal steps are taken. It will not revert to a user-selected value until another SET THDT command is issued. The program selects a value which is usually one half the critical value for numerical stability.

T4. SOLVING THERMAL-MECHANICAL PROBLEMS

The thermal option of MUDEC has all the commands that MUDEC has, as well as others, giving it the capability to solve transient thermal problems, and thermo-mechanical problems.

MUDEC can be used in the usual way to model the excavation of material, change material properties, and change boundary conditions. The mechanical logic (the standard MUDEC program) is also used in the thermomechanical program to take 'snapshots' of the mechanical state at appropriate intervals in the development of the transient thermal stresses. This logic is best explained by Fig T-2.

1. SETUP

. define problem geometry
. define material properties
. define thermal properties
. set boundary conditions (thermal and mechanical)
. set initial conditions (thermal and mechanical)
. set any internal conditions, such as heat sources

2. STEP TO EQUILIBRATE MECHANICALLY

3. PERFORM ANY DESIRED ALTERATIONS such as excavations

4. STEP TO EQUILIBRATE MECHANICALLY

REPEAT steps 3 and 4 until "initial" mechanical state is reached for thermal analysis.

5. TAKE THERMAL TIMESTEPS until

(a) desired time is reached; or

(b) temperature increases cause "large" out-of-balance forces in blocks.

6. STEP TO EQUILIBRATE MECHANICALLY

REPEAT steps 5 and 6 until sufficient time has been simulated.

REPEAT steps 3 to 6 as necessary.

Fig. T-2 General Solution Procedure for Thermal-Mechanical Analysis

A difficulty associated with implementing this scheme lies in determining the meaning of "large" in Step 5(b). As described in the MUDEC manual (Section 2.1), an advantage of explicit schemes is that the solution is reached in a physically meaningful manner, which is important for non-linear constitutive laws. In order to accomplish this in thermal analyses, the out-of-balance force caused by the temperature changes should not be allowed to adversely affect the accuracy of the solution. If the analysis being performed is linear, no temperature increase will be too great, and MUDEC need only equilibrate when the simulation time is such that you want to know the stresses. For non-linear problems, experiment to obtain a feel for what "large" means in the particular problem you are trying to solve, by trying different allowable temperature increases on the **RUN** command as follows:

1. Save the mechanical equilibrium state reached by MUDEC (so that you can come back and try again).

2. Plot the stresses and shear displacements. If the tresses are near yield, the thermal stressses caused by the temperature changes should not be large. If the stresses are far from yield, larger stresses can be tolerated.

3. Run thermal steps until a particular temperature increase is reported by the program (using a **RUN TEM** =value command).

4. Cycle mechanically to attain equilibrium.

5. again, plot the stresses and shear displacements. If the area where the stresses are at or near yield is not much larger than at step 2 and the shear displacements are not very different, the temperature increase allowed was acceptable. If the changes are judged to be too great, the run must be repeated with a smaller allowed temperature change.

An important point to note is that the same temperature increase is not necessarily acceptable for all times in a problem. While the system is far from yield, large temperature increases will be acceptable, but near yield only relatively small increases can be tolerated.

Interlinking of Thermal and Mechanical Steps

For a problem in which the number of thermal steps before mechanical cycling is needed is large, analyses can be accomplished by executing a series of RUN and STEP commands. If the number of thermal steps is small, however, this is impractical. It has therefore been made possible to automatically switch to mechanical steps during a series of thermal steps using the SET NTHER and SET NMECH commands. If NTHER is set to a non-zero value, mechanical steps will be taken every NTHER steps, or whenever the temperature-change parameter (RUN TEM = value) is exceeded.

S T R E S 3 D

COMMANDS

CALL filename

loads command file from disk. **RET** must be last command.

CAN type, clen, nsorc, depth

canister definition:

type	number to be associated with canister type
clen	length of canister (m)
nsorc	number of pont sources to represent canister
depth	distance from z = 0 to canister center (m)

Note: **CAN** command must precede **DECAY** command for each canister type.

DECAY type, icomp, qta, qca, qexpa

defines decay parameters for canister:

type	canister type associated with the decay parameters
icomp	decay component number
qta	time at which this component starts (years)
qca	initial strength of this component ($C \cdot m^1$/year)
qexpa	decay const : (` 0) (1/year)

$$Q = QCAe^{-QExp \cdot t}$$

HEAd plot title input command.

INIT forces recalculation of stress, displacement, and temperature data.

MODEL <keyword>

specifies if there is to be a free surface

INF	no free surface
SEMI	z = 0 is a free surface

QGRID n, m, type, x1,y1, x2,y2, time

places regular grid of canisters

n	number of columns of canisters
m	number of rows of canisters
type	type of canisters
x1,y1	lower-left corner of grid
x2,y2	upper-right corner of grid
time	time of canister emplacement

QLINE n, type, x1,y1, x2,y2, time

n	number of canisters to place
type	type of canister
x1,y1	start of line
x2,y2	end of line
time	time of canister emplacement

QSINGLE type, x,y, time

Place single-TYPE canister at (x,y)

time time of canister emplacement

QUIT stops code execution (same as STOP).

RESTART filename

restarts saved data. Data must be saved with a SAVE filename command.

RETurn last command in the command file. It returns control to the keyboard.

RMP e, pr, den

rock mechanics properties

e Young's modulus (Pa)

pr Poisson's ratio

den rock density (N/m^3)*

*Due to an error in stress calculation, the user must multiply density by gravity to get a proper vertical stress gradient (den = density * 9.8).

RTP diff, tsurf, tgrad, alpha

rock thermal properties:

diff thermal diffusivity (m^2/year)

tsurf rock surface temperature (°C)

tgrad thermal rock gradient (C/m)

alpha coefficient of thermal expansion (1/K)

SAVE filename

saves data to disk file. Data may be reloaded with RESTART command.

START re-initializes all data.

SGRID xc,yc, nrow, ncol, sw

shear stress removal grid

xc	grid x-center
yc	grid y-center
nrow	number of rows of elements
ncol	number of columns of elements
sw	spacing length (m)

Note: nrow·ncol < 1600

STOP stops code execution (same as QUIT).

STRess ratio, sigo

stress ratio command:

ratio	ratio of horizontal to vertical stress gradient
sigo	horizontal stress at z = 0 (Pa)

S T R E S 3 D

COMMANDS TO CONTROL OUTPUT

GRID n, m, x1,y1,z1, x2,y2

sets output for horizontal grid

N*	number of rows of points
M*	number of rows of columns
x1,y1,z1	coordinates of lower-left corner of output grid
x2,y2,z2	coordinates of upper-right corner of output grid

*N·M < 1000

LINE n, x1,y1,z1, x2,y2,z2

sets line output mode

n*	number of calculation points along line
x1,y1,z1	coordinates of start of line
x2,y2,z2	coordinates of end of line

*N < 1000

POINT x1,y1,z1

sets point output mode

x1,y1,z1	coordinates of output point

TIME tim

sets time of calculation.

tim time for output (years)

PDEV name

assigns plot devices for plots.

Name com1 or com2 (Default is com1.)

Note: Baud rate is 9600 and must be set externally by

mode com1:9600,n,8,1,p

or

mode com2:9600,n,8,1,p.

Also, the plots may be sent to a text file (except for the contour plots and the T3D plots) by specifying PDEV filename.

PLOT <keyword> <s1> <s2>

Plots are controlled by **LINE** or **GRID** command. If **LINE** is selected, x-y plots will be produced. If **GRID** is selected, contour plots will be produced. s1 and s2 represent ranges in values for contour and x-y plots.

TEMp **SXX** **SYY** **SZZ** **SXY** **SXZ** **SYZ** **XDIsp** **YDIsp** **ZDIsp**	plots contour of value

CAN plots canister locations

?ECay <1Q>

generates plot of power output of canister type 1Q.

DISp displacement vector plot in horizontal plane

PEN causes plots to be sent to plotter. PEN must be first keyword.

STRess principal stress plot

T3D generates 3-D plot with temperature as z-axis data.

WINdow plot window on screen

PRINT <keyword>

prints data on screen.

TEMp SXX SYY SZZ SXY SXZ SYZ XDIsp YDIsp ZDIsp	prints table of values

CAN	canister parameters
LOC	canister locations
MAX	prints minimum or maximum values for all data
PROp	material properties
RES	prints calculated results as specified by **POINT**, **LINE**, or **GRID** commands.

Note: Output locations and form are controlled by **POINT**, **LINE**, or **GRID** commands.

ROT xrot, zrot

changes rotation angles for T3D plots.

xrot	angle of rotation about x-axis
zrot	angle of rotatin about z-axis

Note: The program will rotate around the z-axis (temperature axis) first and then rotate around the x-axis. (Default values are xrot = 80° and zrot = 45°.)

WINDOW <x1,x2 y1,y2>

overrides automatic plot window. **WINDOW** command with no parameters resets automatic windowing.