HOW TO MAKE TIGER PERFORM:
A SUPPLEMENTARY OPERATOR'S MANUAL
FOR THE TIGER CODE.

by

Edward P. Petkus
and
Kenneth J. Graham
Research Department

September 1981

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This is an informal report of the Naval Weapons Center
and is not part of the permanent records of the Depart-
ment of Defense.

NAVAL WEAPONS CENTER
China Lake, California 93555
FOREWORD

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The material in this report has been reviewed by M. Cowperthwaite, Stanford Research Institute, one of the authors of the original TIGER program.

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JOHN PEARSON
Head, Detonation Physics Division
Research Department
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INTRODUCTION

TIGER is a digital computer code written in FORTRAN IV for calculating the thermodynamic state of a nonideal heterogeneous system of known composition. It was developed at Stanford Research Institute specifically for detonation calculations after experience with the RUBY code at Lawrence Livermore Laboratory and the BKW code at Los Alamos Scientific Laboratory had led to the conclusion that a more versatile code was required to perform routine and research calculations on condensed explosives. While RUBY is limited by its inability to treat certain explosive compositions, both RUBY and BKW are restricted by the inflexibility of their interlocking subroutines which, for example, prevent use of a new equation of state in a calculation without complete reprogramming.

The TIGER code was constructed to avoid the problems associated with interdependent subroutines. The program was written in modular form so that the thermodynamics used to calculate the state, the hydrodynamics used to calculate detonation parameters, and the equations of state used to describe the properties of the system are treated separately in different parts of the code. Because of this separation, TIGER can be best described as a general code for calculating the thermodynamic properties of a nonideal heterogeneous mixture (described by an arbitrary equation of state), with the capability of calculating detonation parameters provided by the hydrodynamic option.¹

This manual was not written to replace the TIGER users' manual but to supplement it. The purpose of this manual is to create one that requires little programming experience to run the code. Numerous runstream examples are given for virtually every TIGER command so that better insight into their use in a typical run can be given. In Appendix A there are directions to run TIGER in demand mode from a Naval Weapons Center (NWC) remote terminal. Appendix B gives directions for running TIGER in batch mode from a demand terminal. Running in batch mode can save enormous amounts of money, so its use is advised when immediate output is not required.

A few notes on the format used in TIGER commands follow:

(a) The first three columns of each command will be read as the instruction. Therefore, only the first three characters of TIGER commands are necessary for execution; the rest of the characters are ignored.

(b) A comma is used to separate data entries.

(c) Two successive commas will be interpreted as if those data are missing, and the last computed or recalled value will be used for it.

(d) A comma at the end of a command will be ignored.

(e) Blanks are ignored in all instructions unless they occur in a numeric argument, in which case they will result in an error.

(f) Watch units on inputs and outputs as they are often different.

If the code has a problem calculating the C-J point, it probably is having difficulty with the initial value. The solution is to first guess an approximated C-J point, say at 2000 K and half the expected pressure. Use these values for a point calculation followed by a constant volume explosion calculation. Then try a C-J calculation and the system should function properly.

Please place this manual with TIGER, Volume IV.
A. INPUT CONTROL STATEMENTS

FORMULA

FORMULA, NAME, HfO, V, SO, A, #, B, #, C, #, .......

NAME- Unique name of substance with six or less characters.

HfO- Enthalpy change of reaction producing the given compound from its elements, with each substance in its standard state (298.15K, 1 atmosphere). The units are calories/mole.

V- Standard molar volume of substance (cubic centimeters/mole). This is simply the formula mass (grams/mole) divided by the density (gram/cubic centimeter).

SO- Standard molar entropy (calories/mole-K). (This value is not used in any calculation unless the REACTANTS REACTION option is used.)

A,B,C- Chemical symbol of element (must match library symbol).

#- Number of atoms of preceding element.

EXAMPLES

FORMULA, TNT, -17820, 137.58, 72.6, C, 7, H, 5, N, 3, 0, 6
FORM, PETN, -121030, 178.53, 68.8, C, 5, H, 8, N, 4, 0, 12

DESCRIPTION

Usually the first or one of the first cards in the runstream which gives the pertinent information needed to make various calculations. The maximum number of these cards is nine. Don't let the value of standard molar entropy scare you as it is only used when REACTANTS REACTION option has been chosen (explained later on). A FORMULA card must be given for every substance used in the COMPOSITION card (below).
COMPOSITION

COMPOSITION, NAME1, M1, NAME2, M2, ..., MOLE

NAME- Unique name from FORMULA card.

M- Amount of substance NAME to be used in mixture. Either in mass or moles. Amounts are relative only.

MOLE- Used if units of M are molar. Otherwise if by mass leave blank.

EXAMPLES

COMPOSITION, TNT, 1
COM, PETN, 1, TNT, 1, RDX, .5, MOLE

DESCRIPTION

This describes the initial composition of substances to be used for calculations. A FORMULA card must be previously defined before it can be used in the composition. This allows one to make many variations of mixtures with known substances.

GEOS

GEOS, EQNM

EQNM- Name of gaseous equation of state to be used. There are four choices: IDEAL, BKW, JCZ2, JCZ3.

EXAMPLES

GEOS, IDEAL
GEOS, JCZ3
DESCRIPTION

This command tells the code which equation of state to select. If this command is not used, the system will default and use the BW equation of state. The BW equation is the Becker-Kistiakowsky-Wilson equation of state. The IDEAL equation is simply the perfect gas law. The JCZ2,JCZ3 are equations of state developed by Jacobs-Cowperthwaite-Zwisler. The latter equations are an update to the code.2

STOP

STOP

EXAMPLE

STOP

DESCRIPTION

Used to end TIGER runstream and cease execution of program. Always the last card in runstream.

NOTE:

These first four commands are the basic commands needed on every run. They tell the system what type of mixture is being used and its needed parameters. The cards will normally be used with FORMULA card(s) first, followed by GEOS and COMPOSITION (order unimportant), then always ending with STOP. The following list of commands will usually be inserted before STOP in various order depending on type of calculation and options to be used. Some commands must precede the COMPOSITION card. The following command descriptions will also include example runstreams of each of the commands in use. Most of these runstreams are simple examples, but they should give insight as to order and command importance in various uses. The following TITLE command could be included in this group, but it is not a mandatory command. It is just an available option for keeping track of the output.

TITLE

TITLE, HEADING

HEADING- Title you wish to appear at top of every page of output following this command.

EXAMPLE

TITLE, C-J RUN WITH TNT, FEB. 13, 1981
TITLE, TRIAL RUN OF HUGONIOT (RDX)

DESCRIPTION

This command allows one to label centrally at top of every page of output. It provides a simple way to keep track of what is going on when referencing outputs. The command will continue until another TITLE command is encountered in the runstream.

B. CALCULATIONAL OPTIONS

C-J CONDITION

C-J CONDITION, P, A, V, B, E, C

P- "P" meaning pressure value follows.
A- Value of the initial pressure in atmospheres.
V- "V" or "RHO" depending on whether specifying initial specific volume or density of the explosive.
B- Value of initial specific volume or density. V (cubic centimeters/gram) or RHO (grams/cubic centimeter)
E- Optional for specifying specific energy of explosive. If explosive is in its standard state, a value need not be specified.
C- Value of specific energy of explosive if "E" has been chosen (calories/gram).
EXAMPLES

C-J CONDITION,P,1,V,.5
C-J,P,2,RHO,1.5,E,-750.

DESCRIPTION

This instructs the system to calculate the Chapman-Jouget point for the conditions prescribed. The output will include shock velocity, particle velocity, speed of sound, C-J pressure, volume, temperature, enthalpy, energy, and entropy. It will give constants used in equations. Also, it will list species of product gases and their concentrations, unless instructed not to (see PRINT SELECTION).

EXAMPLE RUNSTREAM

3835976*EX(1),C-J
1 FORMULA,TNT,17820,137.58,72.6,C,7,H,5-N,3,0,6
2 TITLE, EXAMPLE OF C-J CONDITION
3 GEOS,8K
4 COMPOSITION,TNT,1,MOLE
5 C-J CONDITION,P,1,V,6061
6 STOP

HUGONIOT

HUGONIOT,P,I,INC,F,P,A,V,B,E,C

P- "P" or "V" to either input pressure or specific volume to be used in step increments. Care should be exercised if specifying specific volume because iterations in small increments can cause system to fail.

I- First value of pressure (atmospheres) or specific volume (cubic centimeters/gram) on curve. If this is left blank, the last computed or recalled value will be used by default.

INC- Increment of pressure or specific volume to be used.

F- Final value of pressure or specific volume to be on curve.

P- "P" to specify pressure.
A- Value of pressure for unshocked material at center of Hugoniot curve that must be entered for a detonation Hugoniot. If left blank, the last computed or recalled value will be used, which could give a shock Hugoniot. (See TIGER Manual.)

V- "V" or "RHO" to specify specific volume or density.

B- Value of specific volume (cubic centimeter/gram) or density (grams/cubic centimeter) of unshocked material at center of Hugoniot curve, which must be entered for a detonation calculation. If left blank, last computed or recalled value will be used.

EOF- "EOF" to specify explosive is in its standard state. The option is to use E,C, the explanation of which follows below.

E- "E" to specify the specific energy of the material.

C- Value of specific energy (calories/gram).

EXAMPLES

HUGONIOT,P,250000,25000,25000,P,1,V,.8,EOF
HUG,P,,20000,200000,P,1.5,RHO,1.2,E,-66.

DESCRIPTION

This command instructs program to calculate points along a Hugoniot curve. This will be done for either increments of pressure or specific volume. Care should be exercised when incrementing in specific volume because it is easy to go out of the bounds of the program's capabilities. It should be noted that at the end of the command you can either specify "EOF" or you can put in the specific energy by "E,value of E".

EXAMPLE RUNSTREAM

3835976.4241.HUG
1 FORMULA,HIT,-17620,157,50,72,6,.7,.6,.5,.4,.3,.2,.1
2 TITLE,EXAMPLE OF HUGONIOT
3 GEOD,BKM
4 COMPOSITION,T47.1,MOLE
5 HUGONIOT,P,175060,25000,25000,P,1,V,.6001,E,-54.39
6 STOP
ISOLINE

ISOLINE,P,A,V,I,INC,F,LOG

P- "P", "V", "T", "H", "E", or "S" specifying which thermodynamic variable to be held constant.

A- Value of the constant variable. Units: P- atmospheres; V- cubic centimeters/gram; T- Kelvins; H- calories/gram; E- calories/gram; and S- calories/gram-Kelvin. If left blank, the last computed or recalled variable will be used.

V- Variable to be incremented. The constant variable and the incremented variable must come from one of the following pairs: (P,T), (P,H), (P,S), (P,V), (V,T), (V,E), or (V,S).

I- Initial value of incremented variable. If left blank, the last computed or recalled value will be used. Same units as "A".

INC- Number of increments to be calculated.

F- Final value of incremented variable.

LOG- "LOG" if increments to be logarithmic steps; otherwise, leave blank.

EXAMPLE

ISOLINE,T,900,P,100,9,1500
ISOL,H,75,P,100,5,1000,LOG

DESCRIPTION

This command allows calculation of different thermodynamic points along a specified constant variable. Thus isobars, isotherms, isentropes, etc., can be calculated quite easily with this command.

EXAMPLE RUNSTREAM

```
3435978e-12,1.50
1 FORKUPA,INT,-17620,137.50,72.62,7,10,5,4,3,0,6
2 TITLE, EXAMPLE OF ISOLINE
3 EOS,UKW
4 COMPOSITION,TNT,1,ROLE
5 ISOLINE,5,14,P,250000,10,25000,
6 STOP
```
POINT, P, A, T, B

P- "P" or "V" whether specifying pressure or specific volume.

A- Value of specific volume (cubic centimeters/gram) or pressure (atmospheres) of point to be calculated. If left blank, the last computed or recalled value will be used.

T- "T", "H", "S", "V", or "E", depending on whether the second variable is temperature (Kelvins), specific enthalpy (calories/gram), specific entropy (calories/gram-Kelvin), specific volume (cubic centimeters/gram), or specific energy (calories/gram).

B- The value of the previous variable in appropriate units. If left blank, the last computed or recalled value will be used. These variables must be chosen from the below set of variables and in the same order:

(P, T) (P, H) (P, S) (P, V) (V, T) (V, E) (V, S)

EXAMPLES

POINT, P, 3, T, 900
POI, V, 4, E, 125

DESCRIPTION

This command requests the system to calculate the thermodynamic properties given a pair of thermodynamic values. The output will include other thermodynamic properties at that point. Gaseous and condensed constituents of the products at that point from chemical equilibrium and concentrations will also be printed unless otherwise specified. (See PRINT SELECTION command.)

EXAMPLE RUNSTREAM

36359784*0A(1). POINT

1 FORMULA, INT. = 17820, 137.56, 72.6, 72.6, 2.5, 2.5, 2.5, 2.5, 2.5, 2.5, 2.5
2 TITLE, EXAMPLE OF POINT
3 GEOS, BAY
4 COMPOSITION, INT. 1, MOLE
5 POINT, P, 1, 1, 248, 15
6 STOP
GRID

GRID, CENTER, P, I, INC, NINC, V, I, INC, NINC

CENTER - "CENTER" or "CORNER", depending on whether specifying the initial point at the center or the corner of grid.

P - "P" or "V" specifying either pressure (atmospheres) or specific volume (cubic centimeters/gram).

I - Initial value of previous specified variable. If left blank, the last computed or recalled value will be used.

INC - Value of the size of increment to be taken.

NINC - The number of increments to be taken in each direction if "CENTER" has been chosen. The value of the variable at the extremity of the grid if "CORNER" has been chosen.

V - "T", "H", "S", "V", or "E", depending on whether the second variable is temperature (Kelvins), specific enthalpy (calories/gram), specific entropy (calories/gram-Kelvin), specific volume (cubic centimeters/gram), or specific energy (calories/gram).

These variables must be chosen from the below set of variables and in the same order:

(P, T), (P, H) (P, S) (P, V) (V, T) (V, E) (V, S)

EXAMPLE

GRID, CENTER, P, 10000, 4, T, 20, 2
GRID, CORNER, V, 0.8, 0.05, 1.0, T, 3000, 100, 2500

DESCRIPTION

This requests that a grid of thermodynamic points be calculated. It is just a series of POINT calculations made in a specified grid setup. The output is similar to the point output except a series of points are listed instead of just one point. Care should be taken to make sure the calculations stay within allowable range of the code's capabilities (i.e., temperature range between 250K and 6500K).
EXAMPLE RUNSTREAM

3835978+EX(1), GRID
1 FORMULA, TNT, -17820, 137.58, 72.6, C, 2, H, 5, N, 3, O, 6
2 TITLE, EXAMPLE OF GRID
3 GEUS, BKW
4 COMPOSITION, TNT, 1, MOLE
5 GRID, CENTER, P, 150000, 100000, Z, 1703, 100, 2
6 STOP

EXPLOSION

EXPLOSION, V, A, E, B

V- "V" or "RHO", depending on whether specific volume or density is used.

A- Value of the specific volume (cubic centimeters/gram) or density (grams/cubic centimeter) of the intact explosive.

E- "E" to specify the specific energy. If left blank, it will be calculated from its standard state (E = H - PV).

B- Value of specific energy (calories/gram).

EXAMPLE

EXPLOSION, V, 0.8
EXP, RHO, 1.6, E, -77

DESCRIPTION

Requests the constant volume explosion point be calculated. Outputs thermodynamic variables and concentrations of products.

EXAMPLE RUNSTREAM

3835976+EX(1), EXP
1 FORMULA, TNT, -17820, 137.58, 72.6, C, 2, H, 5, N, 3, O, 6
2 TITLE, EXAMPLE OF EXPLOSION
3 GEUS, BKW
4 COMPOSITION, TNT, 1, MOLE
5 EXPLOSION, RHO, 1.65
6 STOP
C. UTILITY ROUTINES

SAVE POINT

SAVE POINT, NAME

NAME- Name you wish to assign to the computed point. It should have no more than six characters.

EXAMPLES

SAVE POINT, TNTCJ
SAVE, P1

DESCRIPTION

This command allows storing information about a computed point so that it may be used later on in other calculations. Only two points may be saved at any time. A third one may replace one of the two if the same name is used as one of the initial two saved points. This command can be useful when different isolines are to be plotted through a previously calculated point.

RECALL POINT

RECALL POINT, NAME

NAME- Name used in SAVE POINT command to initially store the point.

EXAMPLES

RECALL POINT, TNTCJ
REC, P1

DESCRIPTION

This recalls the point that was saved by the SAVE POINT command and treats it as if it were the last computed point by
the system. All commands following will treat it as the last computed point until another point is computed by the system.

EXAMPLE RUNSTREAM

```
3835978=E(j,jj),SAVE
1 FORMULA,PETN,-121030,178,53,88,80,5,9,8,4,0,12
2 FORMULA,TNT,-17820,137,50,72,6,7,3,7,5,3,0,6
3 TITLE, EXAMPLE OF SAVE POINT - RECALL POINT
4 EOS,UKY
5 COMPOSITION,TNT,5,PETN,5,MOLE
6 C,J,P,1,V,**,65
7 SAVE POINT,CJ
8 POINT,P,250000,V,**
9 RECALL POINT,CJ
10 ISOLINE,S,J,P,10,25000
11 STOP
```

PRINT SELECTION

```
PRINT SELECTION,OPT

OPT- "0" or "1", depending on the option to be selected. "0" means do not print the concentrations, and "1" means print the concentrations.

EXAMPLES

PRINT SELECTION,1
PRI,0

DESCRIPTION

This command tells the system to print or to stop printing constituent concentrations in succeeding operations where concentrations are calculated. The last PRINT SELECTION command will be read. If no PRINT SELECTION command is used, the system will default the "1" option.

EXAMPLE RUNSTREAM

```
3635978=E(j,jj),PRINT
1 FORMULA,TNT,-17820,137,50,72,6,7,3,7,5,3,0,6
2 TITLE, EXAMPLE OF PRINT SELECTION
3 EOS,UKY
4 COMPOSITION,TNT,1,MOLE
5 PRINT SELECTION,0
6 POINT,P,1,T,248,15
7 STOP
```
This command is used after a calculation to insure that the partial derivatives and imperfection integrals used to describe the gaseous phase and to do thermodynamic calculations are correct. It outputs all the variable values used and checks for equality of variables. OK is printed after the values if they equate. The output is quite lengthy.

**EXAMPLE RUNSTREAM**

```plaintext
3033978-2>1 CHECK
1 FORMULA T1=17620,137,5d72,6,c,7,n,5,h,3,0,6
2 TITLE EXAMPLE OF CHECK
3 GEOS,nkw
4 COMPOSITION,TNT,1,MUSE
5 POINT,P,1,1,360
6 CHECK
7 STOP
```
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SET

SET,EQN,NAME,VAL

EQN- Name of equation of state with constant(s) to be set. The three equations to choose from are: BKW, JCZ2, and JCZ3.

NAME- Name of the constant to be set for equation name above. The equations and their constant names are listed below:

- **BKW** - ALPHA, BETA, THETA, and KAPPA
- **JCZ2** - M, L, BL, BM, SR, Q, and A(I)
- **JCZ3** - M, L, BL, BM, SR, Q, A(I), and C

On the A(I) you use (A,Ivalue) where Ivalue is the integer number 1.

VAL- Value of the constant to be set.

EXAMPLES

- SET, BKW, KAPPA, 12.3
- SET, JCZ2, A, 3, 65.1
- SET, JCZ3, SR, .87

DESCRIPTION

This command allows setting certain constants used in the various equations of state in the code. This gives a way of overriding the code's calculation of these constants. (See Volume II in the TIGER Manual.)

EXAMPLE RUNSTREAM

```
3635978*Z=2(I).SET
  1  FORMULA,TIT,=17620,137.58,72.6,6.7,5.5,4.5,0.6
  2  TITLE, EXAMPLE OF SET
  3  EXP, BKW
  4  COMPOSITION,TIT,1,MOLE
  5  SET,UP+ALPHA,.50
  6  PINT,P1,17,248.15
  7  STOP
```

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FIX CONCENTRATION

FIX CONCENTRATION,NAME1,VAL1,NAME2,VAL2,...

NAME- Name of the constituent to have its concentration set.

VAL- Value of the concentration (grams of constituent per kilogram of explosive) of previous constituent name.

EXAMPLES

FIX CONCENTRATION,H2O,87,
FIX,CO2,98,H2O,105,N2,50

DESCRIPTION

This command precedes a calculation when a fixed concentration is desired for a certain constituent or certain number of constituents. It should be noted that input for this command is grams constituent/kilograms explosive, but on the output the concentrations are listed in moles constituent/kilograms explosive.

EXAMPLE RUNSTREAM

3P35976*EX(1).FIX
1 FORMULA,TNT,-17820,137.50,72.6,C7,H5,N3,O6
2 TITLE, EXAMPLE OF FIX CONCENTRATION
3 GEOS,TRAN
4 COMPOSITION,TNT,1,MOLE
5 FIX CONCENTRATION,H2O,10.0,
6 POINT,P1,1,246.15
7 STOP

19
MIXED PHASE

MIXED PHASE, NAME, P, I, INC, F, POINTS

NAME- Name of the condensed constituent for which calculation of mixed phase line is to be calculated. This constituent must have both solid and liquid data in the TIGER library.

P- "P" or "T", depending on whether pressure (atmospheres) or temperature (Kelvin) values and increments are to be chosen.

I- Initial value of pressure or temperature to be used.

INC- Increment of pressure or temperature to be used.

F- Final value of pressure or temperature to be used.

POINTS- "POINTS" if points option is selected; otherwise, leave blank. Points option will calculate phase boundaries in the pressure-volume plane instead of the pressure-temperature plane.

EXAMPLES

MIXED PHASE, AL(C), T, 300, 100, 2000
MIX, AL2O3, P, 30, 20, 200, POINTS

DESCRIPTION

This command will calculate mixed phase line in pressure-temperature plane or in a pressure-volume plane. This command can only be used with condensed constituents that have both liquid and solid data in the library that the code is using.

EXAMPLE RUNSTREAM

```
3635975=6*(1).MIX
  1 FORM, ALUN, 0.9, 0.9858, 0.769, AL, 1
  2 TITLE, EXAMPLE OF MIXED PHASE
  3 COMP, ALUN, 1, MOLE
  4 MIXED PHASE, AL(C), T, 300, 100, 1000
  5 STOP
```
NOTE:

The following five commands are used to put restrictions or directions on the selection process of the constituent products. Exercise care when using them as it is easy to "over" restrict the products so as mass balance cannot be satisfied or that only one mass balance is available. An example runstream is presented at the end of the five commands that incorporates them all. Order is extremely important. The "initial library" is set up by the first COMPOSITION command. Later commands must select from this initial library. Also, the selection/restriction commands must precede a COMPOSITION command, thus creating a "new library." The commands to utilize this library will follow the initial COMPOSITION card.

CHOOSE

CHOOSE,NAME1,NAME2,...

NAME- Names of constituents chosen from the library. If a constituent is a solid, include (S) after the name.

EXAMPLES

CHOOSE,CO2,H2O,N2,CO,OH,C(S)
CH0,H2O,CO2,N2,C(S)

DESCRIPTION

The use of this command allows preselecting the system of species to be considered in the products. Thus, a simplified or reduced set of constituents can be chosen that can be useful when trying to compare output with theories. Care should be used so as to choose enough constituents to allow for mass balance and also to allow for equilibrium to take place. If only one mass balance is available, all calculations will produce identical concentrations. This command must also precede a COMPOSITION command.
REJECT

REJECT, NAME1, NAME2, ...

NAME- Name(s) of constituent(s) from the library to be rejected. If a condensed constituent is rejected, all phases will be rejected.

EXAMPLES
REJECT, NH3
REJ, CO, OH, NO, H2

DESCRIPTION
This command is the opposite of the CHOOSE command because it rejects certain constituents instead of choosing them. Their formats are identical, as is their order. Therefore, the REJECT command must also precede a COMPOSITION card. The subsequent library will not include the species rejected. Again, care should be taken so as to not restrict the constituents to the point where mass balance cannot be obtained or where only one possible set of concentrations exists.

ORDER

ORDER, NAME1, NAME2, ...

NAME- Name(s) of constituent(s) from the library in the order in which they are to be considered.

EXAMPLES
ORDER, H2O, CO2, OH,
ORD, N2, H2O, CO, CO2

DESCRIPTION
There is usually no need for the use of this command because the program usually does a good job of ordering the species to begin with. This command need only be used when the system fails to provide an acceptable set of components. The command tells the system what order to consider the set of species. One may order any or all of the species. If you select a certain order for some of the constituents, the program will select the order for the rest of the constituents in the library. This command must also precede a COMPOSITION command.
RETAIN

DESCRIPTION

This command tells the system to keep in effect the CHOOSE, REJECT, or ORDER commands for the balance of the run. Otherwise, the next COMPOSITION card will destroy their effect. It can be cancelled by the DESTROY command.

DESTROY

DESCRIPTION

To override the effect of any previous RETAIN command when the next COMPOSITION card is encountered.
EXAMPLE RUNSTREAM

383597b*ex(1)*.cho
1 FORMULA,TNT,-17820,137.58,72.6,6,7,1,H,5,N,3,0,6
2 TITLE, EXAMPLE OF CHOOSE-REJECT-ORDER-RETAIN-DESTROY
3 GEOS,BK
4 COMPOSITION,TNT,1,MOLE
5 POINT,P,10,T,200
6 PO1,P,20,T,820
7 ORDER,H2O,N2,CO2
8 RETAIN
9 COMPOSITION,TNT,1,MOLE
10 POINT,P,10,T,200
11 PO1,P,20,T,820
12 DESTROY
13 REJECT,CO,OH
14 RETAIN
15 COMPOSITION,TNT,1,MOLE
16 POINT,P,10,T,200
17 PO1,P,20,T,820
18 DESTROY
19 CHOOSE,H2O,N2,CO2,CC(S)
20 RETAIN
21 COMPOSITION,TNT,1,MOLE
22 PO1,P,10,T,820
23 PO1,P,20,T,820
24 STOP
This command only affects the output of a calculation. This is the only command where the standard molar entropy from the FORMULA card is used. It requests that the specific enthalpy change, specific energy change, and specific entropy change be computed for the reaction converting the reactants in their standard states into the products in the thermodynamic state computed by the particular calculation. Signified on the output by "E(R), H(R), or S(R)." (See Figure 1.)

FIGURE 1. Relationships Between Thermodynamic States.
ELEMENTS REACTION

EXAMPLES

DESCRIPTION

This command is quite similar to the REACTANTS REACTION except this command instructs the code to compute thermodynamic changes for the reaction converting the elements in their standard states into the products in the thermodynamic state computed by the particular computation. It is shown on the output by "H(E), S(E), and E(E)." (See Figure 1.)

ORIGINAL OUTPUT

EXAMPLES

DESCRIPTION

This command cancels any previous REACTANTS REACTION command or ELEMENTS REACTION command. The output then becomes the default output of the code. This output is the thermodynamic state of the products. It is not a change in thermodynamic properties as is the case in the REACTANTS REACTION option or the ELEMENTS REACTION option. It is simply the thermodynamic state of the products at the conditions specified referenced to zero. (See Figure 1.) The following runstream is an example of these three commands in use.
EXAMPLE RUNSTREAM

3*597b+2x(1), REAC
1 FORMULA,TNT,-17620,137.5b,72.6,C,7,H,5,N,3,0.6
2 TITLE, EXAMPLE OF REACTANTS REACTION-ELEMENTS REACTION-ORIGINAL OUTPUT
3 GEOS.IDEAL
4 COMPOSITION,TNT,1,MOLE
5 ELEMENTS REACTION
6 POINT,P,1,7,298.15
7 REACTANTS REACTION
8 POINT,P,1,7,298.15
9 ORIGINAL OUTPUT
10 POINT,P,1,7,298.15
11 STOP

HISTORY

HISTORY

EXAMPLES

HISTORY

DESCRIPTION

This command allows one to process thermodynamic data calculated by TIGER code to a further extent. When HISTORY is used, the data are sent to a subroutine. This subroutine only has comments on input variables that can be included in a common block. Then, these data can be processed by any program that you put in. It is simply an option that allows you to do calculation or manipulations of TIGER variables already computed by the code. (See page III-C-175 in the TIGER manual for listing of HISTORY.)

NOHISTORY

NOHISTORY

EXAMPLES

NOHISTORY

DESCRIPTION

This simply cancels any previous HISTORY command. Therefore, the subroutine HISTRY is no longer called upon by the code.
To use this command one must reference the TIGER volumes I-III. This command will allow the user to write intermediate results if trouble is encountered in receiving the final results.

**FREEZE**

FREEZE,NAME1,NAME2,...

NAME- Name(s) of constituent(s) whose concentration(s) are to be frozen. If left blank, all concentrations will be frozen.

**DESCRIPTION**

This command will hold all concentrations of listed species to their last computed values. The instruction will be in effect for all subsequent calculations or until a MELT command is encountered.

**NOTE:** At the time of this writing (March 1981) this command was not working properly so its use should be observed closely.
MELT

MELT, NAME1, NAME2, ...

NAME- Name(s) of constituent(s) whose concentration(s) are no longer to be frozen. If left blank, all frozen concentrations will be unfrozen.

EXAMPLES

MELT
MEL, H2O, OH,

DESCRIPTION

This command simply negates the FREEZE command. It will override the effect of any prior FREEZE command for the species listed.

EXAMPLE RUNSTREAM

```
1 FORMULA, TNT, -17820, 137.58, 2.72, 6.3, 7, N, 5, N, 3, 0.6
7 TITLE, EXAMPLE OF FREEZE - MELT
3 GEOS, bkW
4 CHOOSE, H2O, CO2, H2, C(S), CO, N2, H2
5 COMPOSITION, TNT, 1, Mole
6 POINT, P, 1, T, 1296.15
7 FREEZE, H2O
8 POINT, P, 1, T, 1000
9 MELT, H2O
10 POINT, P, 1, T, 1000
11 STOP
```
DEMAND TIGER RUN FROM NWC TERMINAL

1. Dial up computer (if required).
2. Enter site identifier.
3. Enter i.d./password.
4. Enter @RUN statement.

This puts you in demand access on the Central Computing Facility (CCF) system. For more in-depth information on the above statements reference "1110 EXEC CONTROL LANGUAGE AND DEMAND TERMINAL USE" available from the computing center library as CCF-36. Now we may create a run-file as follows: (Note: All spaces are significant.)

```
@CAT,P runfilename.
@ED,C runfilename.elmname
11:<RETURN>
0:<MSC>
0:<SUSPEND>
11:<ASG,A
21:<ASG,A NWC*TIG.
31:<ASG,A NWC*TIGER.
41:<ASG,A datafilename.
51:<ASG,T "F2//999
61:<KQT NWC*TIGER.TIGER
71:<ADD,P NWC*TIG.LIBRARY
81:<ADD,P datafilename.dataname .ADD,P TIGERDATA.TNT
91:<RESUME
101:<RETURN>
10:EXIT
```

This will now be your runfile and it need not be created again, but it may be necessary to edit, using @ED,C runfilename.elmname.

Another file must be created referenced above as datafilename.dataname. This element inputs the TIGER runstream. It is here where either the example runstreams or your actual runstream is included. The procedure is similar to above.
The other file added in the first runstream is referenced as NWC*TIG.LIBRARY. This is the file that contains the library of thermodynamic information for the species in TIGER. There is a file called NWC*TIG.LIBRARY that is available to you on the system. If you wish to create your own library or update the current library you should reference the Type III commands in the TIGER user manual section IV, and store your library under a different name.

Now once all this has been accomplished you have a simple way of receiving a printed output of a TIGER run from a demand terminal. You simply sign on, enter your @RUN statement followed by:

@ADD runfilename.elmname  ADD RUNTIGER

System replies with
SUSPENDED

After some time you will see on the screen:
EXAMINE, PRINT, or DROP?

If you wish to examine output, you type EX (SEND) to enter edit mode in the output file. When you are finished, you type EXIT and above statement reappears. If you wish a printed output, you type PR; it will reply with "WHERE?". For central site printing you type PR or you may use a remote printer by putting in its calling code. If you do not wish output, you simply type DR.

At the end of the run, type:
@FIN

The CCF charges will be printed on the screen. Then type
@TERM

and turn off the terminal.
Appendix B

BATCH RUN FROM A DEMAND TERMINAL

This appendix is similar to Appendix A except this one describes the use of a batch run from a demand terminal. There is no output on the terminal screen. Printed output at CCF or other batch printer is often delayed, but the costs are much lower for the run time used. It is as simple as the demand run once the runfile is created.

The runfile may be created as follows:

```
@CAT,P RUN-FILE.
@ED,C RUN-FILE.
11:<RETURN>
0:<RETURN>
11:RUN ID1,JO15G,CODEID1...etc.
21:ASG,AX NWC*TIG.
31:ASG,T 11,999
51:ASG,AX DATAFILE.
61:ASG,AX NWC*TIGER.
71:XTT NWC*TIGER,TIGER
81:ADD,P NWC*TIG.LIBRARY
91:ADD,P DATAFILE.NAME
101:<FIN
111:<RETURN>
10:EXIT
```

Use a DATAFILE.NAME identical to that created in Appendix A. To run this batch runstream you simply sign on, enter @RUN, then type

```
@START RUN-FILE.
```

It will output the number in line you are.

An example called EX-RUN. follows. This file can be run by you to receive the output for all the example runstreams in the text (the cost is approximately $24.00). To do so, simply create the file on the following page with your own run card statement.
NWC TM 4650

1: #RUN 97665S, 1387030KRSKS6, 3635978
2: #ASG, AX NWC*TIGER
3: #ASG, AX NWC*EX
4: #ASG, T 11, F//F999
5: #XGT NWC*TIGER
6: #ADD3 2649758=EPP,T-LIER
7: #ADD,P NWC*EX.C-J
8: #XGT NWC*TIGER
9: #ADD,P NWC*EX.HUG
10: #XGT NWC*TIGER
11: #ADD,P NWC*EX.IJS
12: #XGT NWC*TIGER
13: #ADD,P NWC*EX.POINT
14: #XGT NWC*TIGER
15: #ADD,P NWC*EX.GRID
16: #XGT NWC*TIGER
17: #ADD,P NWC*EX.EX
18: #XGT NWC*TIGER
19: #ADD,P NWC*EX.SAVE
20: #XGT NWC*TIGER
21: #ADD,P NWC*EX.CH0
22: #XGT NWC*TIGER
23: #ADD,P NWC*EX.PRINT
24: #XGT NWC*TIGER
25: #ADD,P NWC*EX.MELT
26: #XGT NWC*TIGER
27: #ADD,P NWC*EX.CHECK
28: #XGT NWC*TIGER
29: #ADD,P NWC*EX.SET
30: #XGT NWC*TIGER
31: #ADD,P NWC*EX.FIX
32: #XGT NWC*TIGER
33: #ADD,P NWC*EX.MIX
34: #XGT NWC*TIGER
35: #ADD,P NWC*EX.REAC
36: *FIN

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