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

by

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FOREWORD

The production of this users' manual was undertaken as part of the continuing effort to strengthen predictive capabilities used in support of blast studies. Work was performed during Fiscal Year 1981 and was funded by Director of Naval Laboratories Programs Task Assignment ZR000-01-01.

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

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

<div align="right">
JOHN PEARSON
Head, Detonation Physics Division
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26 September 1981
</div>

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None.

CONTENTS

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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.

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[1] M. Cowperthwaite and W. H. Zwisler. *The TIGER Computer Program.* Menlo Park, Calif., Stanford Research Institute, January 1973, 4 volumes. Republished by permission as NWC IDP 3518. China Lake, Calif., NWC, January 1978. Publication UNCLASSIFIED.

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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 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,O,6
        FORM,PETN,-121030,178.53,68.8,C,5,H,8,N,4,O,12

DESCRIPTION

        Usually the first or one of the first cards in the runstream
which gives the pertinent information needed to make various calcu-
lations. 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 BKW equation of state. The BKW 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 also 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 calculations 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.

---

[2] M. Cowperthwaite and W. H. Zwisler. *Improvement and Modification to TIGER Code.* Menlo Park, Calif., Stanford Research Institute, January 1973. Defense Technical Information Center AD B007911L, publication UNCLASSIFIED.

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

```
3835978*EX(1).C-J
        1       FORMULA,TNT,-17820,137.58,72.6,C,7,H,5,N,3,O,6
        2       TITLE, EXAMPLE OF C-J CONDITION                    .
        3       GEOS,BKW
        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.

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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

    3F35978*EX(1).HUG
        1   FORMULA,TNT,-17820,137.58,72.6,C,7,H,5,N,3,O,6
        2   TITLE, EXAMPLE OF HUGONIOT
        3   GEOS,BKW
        4   COMPOSITION,TNT,1,MOLE
        5   HUGONIOT,P,175000.25000,2500J,P,1,V,,6061,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
ISO,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

```
3F359780EX(1).ISO
       1      FORMULA,TNT,-17820,137.50,72.6,C.7,H,5,N,3,0,6
       2      TITLE, EXAMPLE OF ISOLINE
       3      GEOS,BKW
       4      COMPOSITION,TNT,1,MOLE
       5      ISOLINE,S,1.4,P,250000,10,25000,
       6      STOP
```

POINT

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

```
3835978*LX(1).POINT
    1       FORMULA,TNT,-17820,137.58,72.6,C,7,H,5,N,3,O,6
    2       TITLE, EXAMPLE OF POINT
    3       GEOS,GRW
    4       COMPOSITION,TNT,1,MOLE
    5       POINT,P,1,T,248.15
    6       STOP
```

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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
GRI,CORNER,V,.8,.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).

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EXAMPLE RUNSTREAM

```
3835978*EX(1).GRID
    1        FORMULA,TNT,-17820,137.58,72.6,C,7,H,5,N,3,O,6
    2        TITLE, EXAMPLE OF GRID
    3        GEOS,BKW
    4        COMPOSITION,TNT,1,MOLE
    5        GRID,CENTER,P,150000,10000,2,T,2700,100,2
    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,.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

```
3835978*EX(1).EXP
    1        FORMULA,TNT,-17820,137.58,72.6,C,7,H,5,N,3,O,6
    2        TITLE, EXAMPLE OF EXPLOSION
    3        GEOS,BKW
    4        COMPOSITION,TNT,1,MOLE
    5        EXPLOSION,RHO,1.65
    6        STOP
```

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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
    SAV,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*Ex(1).SAVE
     1      FORMULA,PETN,-121030,178,53,68.80,,,5,H,8,N,4,0,12
     2      FORMULA,TNT,-17820,137.56,72.6,C,7,H,5,N,3,0,6
     3      TITLE, EXAMPLE OF SAVE POINT - RECALL POINT
     4      GEOS,BKW
     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,,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

```
3835978*Ex(1).PRINT
     1    .  FORMULA,TNT,-17820,137.56,72.6,C,7,H,5,N,3,0,6
     2      TITLE, EXAMPLE OF PRINT SELECTION
     3      GEOS,BKW
     4      COMPOSITION,TNT,1,MOLE
     5      PRINT SELECTION,0
     6      POINT,P,1,T,298.15
     7      STOP
```

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CHECK

CHECK

EXAMPLES

CHECK
CHE

DESCRIPTION

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

```
3835978*EX(1).CHECK
      1       FORMULA,TNT,-17620,137.58,72.6,C,7,H,5,N,3,O,6
      2       TITLE, EXAMPLE OF CHECK
      3       GEOS,BKW
      4       COMPOSITION,TNT,1,MOLE
      5       POINT,P,1,T,300
      6       CHECK
      7       STOP
```

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 I.

    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

        3835978-LX(1).SET
            1   FORMULA,TNT,-17820,137.58,72.6,C.7,H,5,N,3,0,6
            2   TITLE, EXAMPLE OF SET
            3   GEOS,BKW
            4   COMPOSITION,TNT,1,MOLE
            5   SET,BKW,ALPHA,.50
            6   POINT,P,1,T,298.15
            7   STOP

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

```
3P3S978*LX(1).FIX
    1       FORMULA,TNT,-17820,137.58,72.6,C,7,H,5,N,3,O,6
    2       TITLE, EXAMPLE OF FIX CONCENTRATION
    3       GEOS,BKW
    4       COMPOSITION,TNT,1,MOLE
    5       FIX CONCENTRATION,H2O,10.0,
    6       POINT,P,1,1,298.15
    7       STOP
```

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,AL203,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=EX(1).MIX
      1      FOMM,ALUM,0.9.985R,6.769,AL,1
      2      TITLE, EXAMPLE OF MIXED PHASE
      3      COMP,ALUM,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)
CHO,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 for-
mats are identical, as is their order. Therefore, the REJECT com-
mand 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 bal-
ance cannot be obtained or where only one possible set of concen-
trations 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

    RETAIN

  EXAMPLES

    RETAIN
    RET

  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

    DESTROY

  EXAMPLES

    DESTROY
    DES

  DESCRIPTION

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

EXAMPLE RUNSTREAM

```
3835978*EX(1).CHO
        1       FORMULA,TNT,-17820,137.58,72.6,C,7,H,5,N,3,0,6
        2       TITLE, EXAMPLE OF CHOOSE-REJECT-ORDER-RETAIN-DESTROY
        3       GEOS,BKW
        4       COMPOSITION,TNT,1,MOLE
        5       POINT,P,10,T,820
        6       POI,P,20,T,820
        7       ORDER,H2O,N2,CO2,
        8       RETAIN
        9       COMPOSITION,TNT,1,MOLE
       10       POINT,P,10,T,820
       11       POI,P,20,T,820
       12       DESTROY
       13       REJECT,CO,OH,
       14       RETAIN
       15       COMPOSITION,TNT,1,MOLE
       16       POINT,P,10,T,820
       17       POI,P,20,T,820
       18       DESTROY
       19       CHOOSE,H2O,N2,CO2,C(S)
       20       RETAIN
       21       COMPOSITION,TNT,1,MOLE
       22       POI,P,10,T,820
       23       POI,P,20,T,820
       24       STOP
```

REACTANTS REACTION

REACTANTS REACTION

EXAMPLES

REACTANTS REACTION
REA

DESCRIPTION

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.)

PRODUCTS IN COMPUTED STATE

(R) ── REACTANTS IN STANDARD STATE

(E) ── ELEMENTS IN STANDARD STATE

(0) ── ZERO
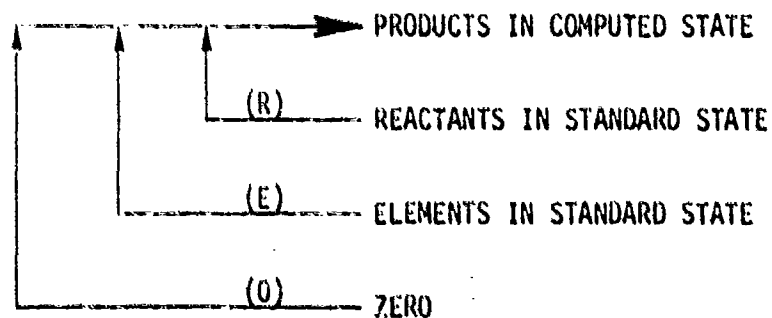
FIGURE 1. Relationships Between Thermodynamic States.

ELEMENTS REACTION

ELEMENTS REACTION

EXAMPLES

ELEMENTS REACTION
ELE

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 par-
ticular computation. It is shown on the output by "H(E), S(E), and
E(E)." (See Figure 1.)

ORIGINAL OUTPUT

ORIGINAL OUTPUT

EXAMPLES

ORIGINAL OUTPUT
ORI

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@35976*EX(1).REAC
      1       FORMULA,TNT,-17820.,137.5b,72.6,C,7,H,5,N,3,O,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,T,298.15
      7       REACTANTS REACTION
      F       POINT,P,1,T,298.15
      9       ORIGINAL OUTPUT
     10       POINT,P,1,T,298.15
     11       STOP
```

HISTORY

HISTORY

EXAMPLES

HISTORY
HIS

DESCRIPTION

This command allows one to process thermodynamic data calcu-
lated 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 manipu-
lations of TIGER variables already computed by the code. (See page
III-C-175 in the TIGER manual for listing of HISTRY.)

NOHISTORY

NOHISTORY

EXAMPLES

NOHISTORY
NOH

DESCRIPTION

This simply cancels any previous HISTORY command. Therefore,
the subroutine HISTRY is no longer called upon by the code.

DEBUG

>   DEBUG

>   EXAMPLES

>   DEBUG
>   DEB

>   DESCRIPTION

>   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.

>   EXAMPLES

>   FREEZE,H2O,CO,OH,
>   FRE

>   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 concen-
trations 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

```
3H35978*EX(1),MELT
    1      FORMULA,TNT,-17820,137.58,72.6,C,7,H,5,N,3,O,6
    2      TITLE, EXAMPLE OF FREEZE - MELT
    3      GEOS,BRW
    4      CHOOSE,H2O,CO2,N2,C(S),CO,N2,
    5      COMPOSITION,TNT,1,MOLE
    6      POINT,P,1,T,1298.15
    7      FREEZE,H2O,
    8      POINT,P,1,T,1000
    9      MELT,H2O
   10      POINT,P,1,T,1000
   11      STOP
```

Appendix A

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.)

```
                                        EXAMPLE
      @CAT,P runfilename.               @CAT,P RUNTIGER.
      @ED,C runfilename.elmname         @ED,C RUNTIGER.1
      1I:<RETURN>
      0:MSC .
      0:<RETURN>
      1I:.SUSPEND
      2I:.ASG,AX NWC*TIG.
      3I:.ASG,AX NWC*TIGER.
      4I:.ASG,AX datafilename.          .ASG,AX TIGERDATA.
      5I:.ASG,T 11,F2///999
      6I:.XQT NWC*TIGER.TIGER
      7I:.ADD,P NWC*TIG.LIBRARY
      8I:.ADD,P datafilename.dataname  .ADD,P TIGERDATA.TNT
      9I:.RESUME
      10I:<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.

EXAMPLE

```
@CAT,P datafilename.          @CAT,P TIGERDATA.
@ED,C datafilename.dataname   @ED,C TIGERDATA.TNT
1I:FORMULA,...
2I:TITLE,...
.
. (Balance of input statements)
.
?I:STOP
?I:<RETURN>
?:EXIT
```

The other file added in the first runstream is referenced as NWC*TIG.LIBRARY. This is the file that contains the library of thermo-dynamic 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 refer-ence 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.1
```

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 abe /e statement reappears. If you wish a printed output, you type PR; it w 11 reply with "WHERE?". For central site printing you type PR or you ma: 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:MSC .
0:<RETURN>
11:.RUN ID#,JO#5G,CODEID#...etc.
21:.ASG,AX NWC*TIG.
31:.ASG,T 11,F///999
51:.ASG,AX DATAFILE.
61:.ASG,AX NWC*TIGER.
71:.XQT NWC*TIGER.TIGER
81:.ADD,P NWC*TIG.LIBRARY
91:.ADD,P DATAFILE.NAME
10I:.FIN
11I:<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.

```
1:@RUN 978EXS,1380301KRS56,3635978
2:@ASG,AX NWC*TIGER.
3:@ASG,AX NWC*EX.
4:@ASG,T 11,F///999
5:@XQT NWC*TIGER.TIGER
6:@ADD 3246978*EPP.T-LIBR
7:@ADD,P NWC*EX.C-J
8:@XQT NWC*TIGER.TIGER
9:@ADD,P NWC*EX.HUG
10:@XQT NWC*TIGER.TIGER
11:@ADD,P NWC*EX.ISO
12:@XQT NWC*TIGER.TIGER
13:@ADD,P NWC*EX.POINT
14:@XQT NWC*TIGER.TIGER
15:@ADD,P NWC*EX.GRID
16:@XQT NWC*TIGER.TIGER
17:@ADD,P NWC*EX.EXP
18:@XQT NWC*TIGER.TIGER
19:@ADD,P NWC*EX.SAVE
20:@XQT NWC*TIGER.TIGER
21:@ADD,P NWC*EX.CHO
22:@XQT NWC*TIGER.TIGER
23:@ADD,P NWC*EX.PRINT
24:@XQT NWC*TIGER.TIGER
25:@ADD,P NWC*EX.MELT
26:@XQT NWC*TIGER.TIGER
27:@ADD,P NWC*EX.CHECK
28:@XQT NWC*TIGER.TIGER
29:@ADD,P NWC*EX.SET
30:@XQT NWC*TIGER.TIGER
31:@ADD,P NWC*EX.FIX
32:@XQT NWC*TIGER.TIGER
33:@ADD,P NWC*EX.MIX
34:@XQT NWC*TIGER.TIGER
35:@ADD,P NWC*EX.REAC
36:@FIN
```

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