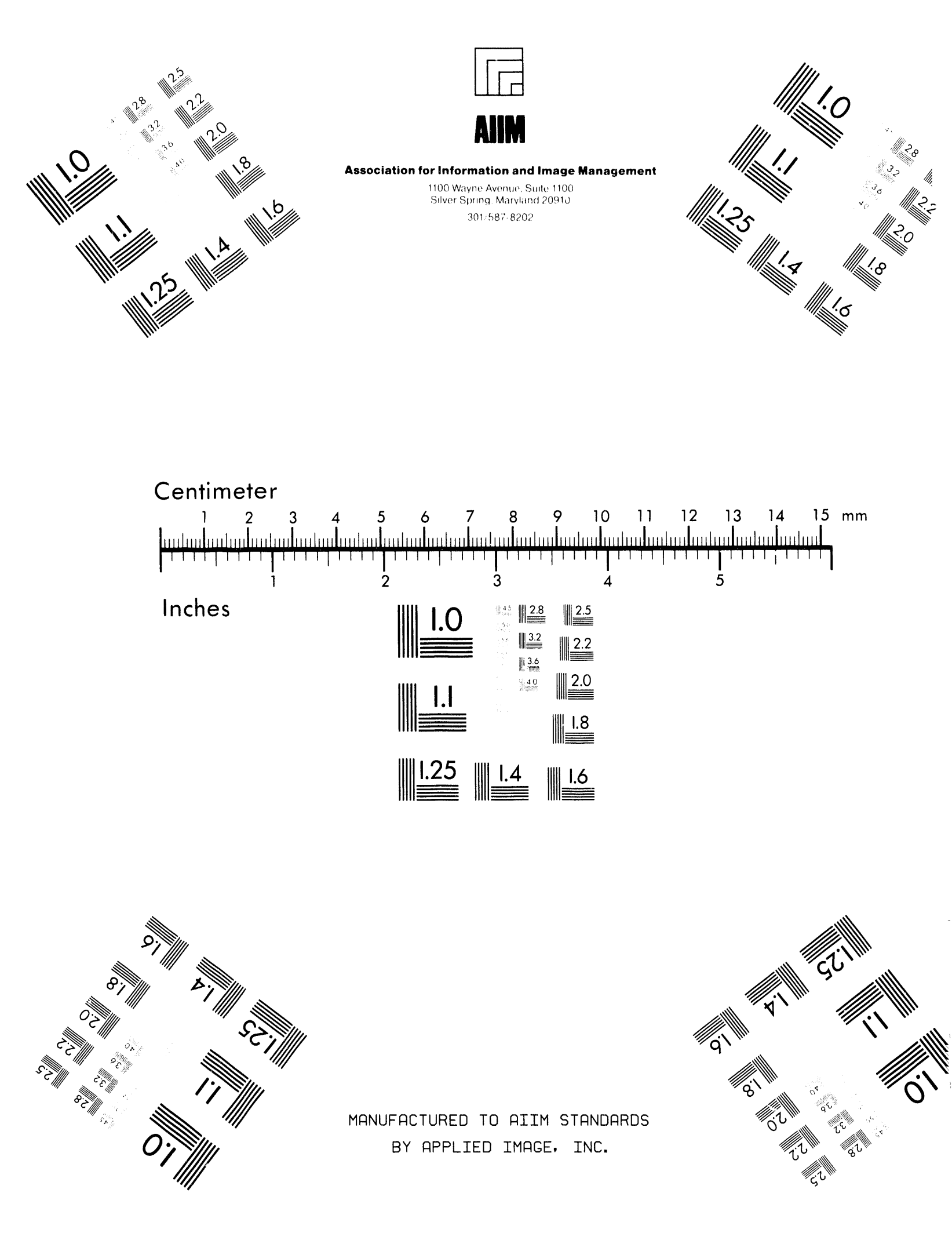
AIIM
Association for Information and Image Management
1100 Wayne Avenue, Suite 1100
Silver Spring, Maryland 20910
301/587-8202
Centimeter
Inches
MANUFACTURED TO AIIM STANDARDS
BY APPLIED IMAGE, INC.

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CHEETAH 1.0
User's Manual

Laurence E. Fried
Energetic Materials Center
Lawrence Livermore National Laboratory

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Contents

Section 1
Overview

CHEETAH is an effort to bring the TIGER thermochemical code[1] into the 1990s. A wide variety of improvements have been made in Version 1.0, and a host of others will be implemented in the future. In CHEETAH 1.0 I have improved the robustness and ease of use of TIGER. All of TIGER's solvers have been replaced by new algorithms. I find that CHEETAH solves a wider variety of problems with no user intervention (e.g. no guesses for the C-J state) than TIGER did. CHEETAH has been made simpler to use than TIGER; typical use of the code occurs with the new `standard run` command. I hope that CHEETAH makes the use of thermochemical codes more attractive to practical explosive formulators.

In the future I plan to improve the underlying science in CHEETAH. More accurate equations of state will be used in the gas and the condensed phase. A kinetics capability will be added to the code that will predict reaction zone thickness. CHEETAH is currently a numerical implementation of C-J theory. It will become an implementation of ZND theory. Further ease of use features will eventually be added; an automatic formulator that adjusts concentrations to match desired properties is planned.

1.1 What CHEETAH does

Below we give a non-technical explanation of what CHEETAH does. For a more technical discussion, see Section 8. CHEETAH is a thermochemical code. It solves thermodynamic equations between product species to find chemical equilibrium. For instance, in a system comprised solely of condensed carbon, gaseous CO, and gaseous CO_2, CHEETAH can find the equilibrium of the reaction

$$C + CO_2 \leftrightarrow 2CO$$

at a specified pressure and temperature. C-J theory says that the detonation point is a state in thermodynamic and chemical equilibrium, so CHEETAH can predict the properties of this state. From these properties and elementary detonation theory come the detonation velocity and other performance indicators. CHEETAH can calculate thermodynamic states where the pressure and temperature are not explicitly indicated. For instance, we can specify the volume and the entropy instead of the pressure and temperature. These types of calculations implicitly define pressure and temperature, i.e.

$$\begin{aligned} V(P,T) &= V_0 \\ S(P,T) &= S_0 \end{aligned}$$

(V,S) points play an important role when undertaking an adiabatic expansion from the C-J state.

Thermodynamic equilibrium can be found by balancing chemical potentials. The above carbon example leads to the equation

$$\mu_C + \mu_{CO_2} = 2\mu_{CO}$$

The chemical potentials of condensed species are just functions of pressure and temperature, while the potentials of gaseous species depend on concentrations:

$$\begin{aligned} \mu_C &= \mu_C(P,T) \\ \mu_{CO_2} &= \mu_{CO_2}(P,T,N_{CO_2},N_{CO}) \\ \mu_{CO} &= \mu_{CO}(P,T,N_{CO_2},N_{CO}) \end{aligned}$$

Here, N_{CO_2} is the number of molecules of CO_2. Just as a reminder, the chemical potential is the Gibbs free energy difference obtained from adding one more molecule into the system:

$$\mu_C = G(P,T,N_{CO_2},N_C+1,N_{CO}) - G(P,T,N_{CO_2},N_C,N_{CO})$$

Balancing the chemical potentials is the same as minimizing G. In fact many thermochemical codes (notably CHEQ[2]) numerically minimize G instead of bothering with chemical potentials.

When you start to use CHEETAH, you'll notice that there are no chemical reactions specified. How then, you might ask, does CHEETAH get the chemical reactions for balancing chemical potentials ? The answer is that the reactions used don't matter, as long as there are enough of them to change concentrations arbitrarily; the answer will come out the same no matter what reactions are used. CHEETAH manufactures a decomposition reaction for each product molecule. This reaction is an internal construct of the code and does not have to occur physically. The product molecule (called a "constituent" in the language of TIGER) decomposes into a small number of "component" molecules. The number of components is equal to the number of elements in the problem. For example CHEETAH might choose C and CO as components. The decomposition reactions would then be:

$$\begin{aligned} C &\leftrightarrow C \\ CO &\leftrightarrow CO \\ CO_2 &\leftrightarrow 2CO - C \end{aligned}$$

Since decomposition reactions in CHEETAH aren't real, they can have negative stoichiometric coefficients. The first two reactions are trivial and therefore have no effect on the chemical equilibrium.

The equations solved by CHEETAH are

$$\begin{aligned} \mu_{CO_2}(P,T,x_{CO},x_{CO_2}) &= 2\mu_{CO}(P,T,x_{rmCO},x_{CO_2}) - \mu_C(P,T) \\ x_{CO} + x_{CO_2} + x_C &= W_C \\ x_{CO} + 2x_{CO_2} &= W_O \end{aligned}$$

Here x_{CO_2} is the concentration of CO_2. W_C is the concentration of the element C in the system. In words the equations say: balance the chemical potentials while keeping the total moles of each element fixed. CHEETAH is nothing but a complicated chemical potential balancer.

1.2 The CHEETAH hotline

If you have any questions regarding CHEETAH, please send electronic mail to `cheetah@llnl.gov`. I am gently discouraging users from calling me on the

phone, unless you have an urgent problem or no other way to contact me. A CHEETAH electronic mailing list will be set up; you may subscribe by sending a request to `cheetah@llnl.gov`. Discussions on CHEETAH's features and documentation will occur through the mailing list. User's problems, and their resolution, will be posted in the hopes of alerting users to commonly encountered problems.

1.3 Bug reports

Users are strongly encouraged to report bugs. It is only through extensive user testing that CHEETAH will become a fully mature, error-free code. A bug ranges from behavior that you are sure is wrong, to behavior that you do not fully understand. Bug reports should be sent to the CHEETAH e-mail hotline. Please enclose a full input file, the output file, and any libraries or configuration files necessary to reproduce the bug. Also include a description of what you believe to be wrong.

1.4 New features

A list of changes made to CHEETAH is given below. A more detailed description of these changes is given in Chapter 5. Work on CHEETAH has fallen into one of three categories: enhanced user convenience, new algorithms, and new capabilities.

1.4.1 User convenience

- CHEETAH has a single command standard run. It is now possible to run CHEETAH by giving only the composition and density.
- The input routines of TIGER have been re-written. Longer, more logical, names can be used. Input files now accept comments.
- CHEETAH has a simple macro facility for frequently used commands.

- CHEETAH supports a startup file that loads initialization commands automatically.
- The output of CHEETAH can be exported to a spreadsheet file. This file is readable by Excel, Quattro, etc.
- CHEETAH supports user-defined and relative units for input.
- CHEETAH produces a single sheet summary of a run. The summary sheet has all the information that most users require.
- CHEETAH has a reactant database containing most frequently used explosives and binders. This saves the user the inconvenience of looking up thermodynamic constants.
- Product libraries now have titles. This allows the library used to be clearly identified in the output files.
- CHEETAH supports multiple product libraries.

1.4.2 Algorithmic improvements

- CHEETAH has a new solver for chemical equilibrium that is more reliable than TIGER's.
- Difficulties with freezing concentrations in TIGER have been fixed.
- CHEETAH has a new Hugoniot solver that is faster and more robust than TIGER's.
- CHEETAH has a new C-J solver that is more reliable than TIGER's.
- CHEETAH has a new solver for solid-liquid phase coexistence.
- CHEETAH can be dynamically resized to run large problems or accomodate small computers.

- A version of CHEETAH for MS-Windows was developed. The program is not limited to 640K of memory and can be resized to take advantage of available memory.

1.4.3 New capabilities

- CHEETAH has wide variety of thermodynamic point types. Most notably, T-S points are available for freezing along an adiabat.
- CHEETAH has a JWL fitting program built in. There is also a stand-alone program for fitting experimental cylinder test data to a JWL.
- CHEETAH estimates the portion of the detonation energy that is available for doing mechanical work.
- CHEETAH estimates cylinder test wall velocities for comparison with experiment.

1.5 Licensing and distribution

TIGER was a publicly available code, with modifications by users allowed. This arrangement has caused problems with the TIGER code; everyone has their own slightly modified version of TIGER. There is no way of verifying that the modifications made were correct, and it is difficult to know whether TIGER results quoted in the literature came from a modified version or not. CHEETAH will be more tightly controlled than TIGER to improve the code authentication and distribution process.

CHEETAH is distributed on an execute-only basis. Even if you have a copy of the source code, you may not modify it without permission. Redistribution of CHEETAH to others, even at your own institution, is prohibited. If someone you know wants CHEETAH, have them contact me (preferably by e-mail), and a separate copy of the code will be sent.

If you wish to modify CHEETAH, please send me an e-mail describing the project. I will then send you an agreement allowing you to become a CHEETAH developer. The purpose of development is to make changes to CHEETAH that can be

incorporated into future versions of the code. The developers will be recognized in future versions of the manual, and their contributions will be fully documented. Modified versions of CHEETAH must be renamed, with their relationship to CHEETAH acknowledged. The word CHEETAH should appear somewhere in the program's name. For instance, a typical journal article might read "In Table I we show results from CHEETAH-SNL, a modified version of the CHEETAH thermochemical code used at Sandia National Laboratory [reference to this manual]." Modified versions of CHEETAH are for your own personal use, and may not be distributed to others. Instead, the modified code should be sent to LLNL where it most probably will be incorporated into the latest version of CHEETAH.

In order to make code merging possible, please adhere to the following practices:

- Modifications should be implemented as new subroutines (functions) in CHEETAH. Avoid changing existing subroutines. If you really need to change something, copy and rename the subroutine, then modify the renamed version.
- Your modifications should be turned on and off with new commands. Do not change the behavior of existing commands. Make sure that the behavior of the original CHEETAH is preserved.
- Document what you do ! If I can't understand the code I won't use it.
- Never change the common blocks (external data structures). Create new common blocks specific to your modifications.
- It's preferable to explicitly pass all needed arguments to your subroutines rather than use common block variables. This ensures that your code will survive future changes in the common block structure.
- Write a mini-manual describing your changes at the same level of detail as the original CHEETAH manual.

1.6 Acknowledgements

CHEETAH owes an obvious debt to M. Cowperwaithe and W. H. Zwisler, the developers of TIGER[1]. Many of the capabilities that will be put into CHEETAH are inspired by the thermochemical code CHEQ, written by A. Nichols III and F. Ree. P. Clark Souers first advanced the idea of improving TIGER, and has been instrumental in testing the program. Clark has also assembled the reactant library described in Section 4. Randall Simpson has been a relentless proponent of the project. Milt Finger provided initial funding. Ed James and Mark Hoffman were the first brave users of the PC version. Mike Murphy loaned me computer hardware necessary to develop CHEETAH for the PC and helped with numerous file transfers. Craig Tarver has made several insightful suggestions. Finally, I have had many useful conversations with Albert Nichols III; his help has been invaluable. CHEETAH is supported under a Memorandum of Understanding between the Departments of Defense and Energy and is administered through the Office of the Secretary of Defense (Office of Munitions).

Section 2
Tutorial

CHEETAH was designed to be easy to use while retaining the flexibility of TIGER. In this section we will go through a number of example runs of increasing complexity. The first few example runs will serve the needs of most users. The user is encouraged to try the examples out while reading this section of the manual.

2.1 Standard Run

CHEETAH has a standard run that should meet the needs of most users in modeling detonation. The standard run calculates the C-J state, then models an adiabatic expansion. Finally, the end point of the detonation is calculated and the results are fit to a JWL equation of state. In this example we will do a calculation for PETN. We will name the input file `petn.in`. The input file is:

```
title, PETN example run 1
composition, petn, 100
standard run, rho, 1.763
```

Let us now say a few words about input in CHEETAH. Like TIGER, a CHEETAH input file is a series of commands, one on each line. Arguments to the commands are separated by commas. Unlike TIGER, all the characters of a CHEETAH command are significant. Commands can be abbreviated by truncation to the smallest string size that uniquely identifies the command. Usually this is three characters. Thus we could just as well have entered `com, petn, 100`.

The first line in the input file gives a title for the run. This title will be copied to the output. The second line in the input file says that the explosive is composed of 100 % PETN by weight. The third command makes CHEETAH execute the standard run, given that the initial density of the explosive is 1.763 g/cc.

CHEETAH is invoked by typing:

`cheetah petn.in petn.out`

at the command line. In the MS-Windows version of CHEETAH, double click on the file `petn.in`.

CHEETAH produces two output files. The main output file records detailed information about thermodynamic states calculated, including concentrations and values of many thermodynamic functions. The second output file is a single sheet summary of the run. We have found that the summary sheet meets the needs of many users in analyzing the results of the run. By default, the summary file is called `summary.out`.

The `summary.out` file is:

```
################################################################################
#                                                                              #
#                                                                              #
#                                                                              #
#                        CHEETAH SUMMARY SHEET          BKWR, LLNL Library     #
#                                                                              #
#                                                                              #
#                                                                              #
################################################################################

BKW eos used: alpha=  0.500, beta=  0.100 kappa= 11.850 theta=  400.0


The composition:
Name       % wt.    % mol  Heat of      Standard      Mol.    TMD
                           formation     volume        wt.     (g/cc)
                           (cal/mol)     (cc/mol)
petn       100.00 100.00  -128700      177.61      316.15    1.78

Density  =   1.763 g/cc   Mixture TMD =   1.780 g/cc   % TMD =  99.045


The C-J condition:
The pressure          =          31.00 GPa
The volume            =          0.423 cc/g
The density           =          2.361 g/cc
The energy            =           3.93 kJ/cc explosive
The temperature       =           3338 K
The shock velocity    =          8.330 mm/us
The particle velocity =          2.111 mm/us
The speed of sound    =          6.219 mm/us


Cylinder runs:                  % of standards
  V/V0      V        Energy     TATB      PETN      HMX    TRITON   half-wall  Full-wall
 (rel.)   (cc/g)    (kJ/cc)   1.83g/cc  1.76      1.89     1.70    v (mm/us)   v (mm/us)
   2.20     1.25      -7.30      143       100       86       154      2.09        1.58
   4.10     2.33      -8.81      148       100       87       148      2.28        1.72
   6.50     3.69      -9.38      150       100       89       143      2.38        1.78
  10.00     5.67      -9.73      151       100       89       139
```

```
  20.00    11.34    -10.10

Freezing occurred at T =      1800.0 K and relative V =    1.865
The mechanical energy of detonation =     -10.682 kJ/cc
The thermal energy of detonation    =       0.000 kJ/cc
The total energy of detonation      =     -10.682 kJ/cc

JWL Fit results:
A     =       1599.68 GPa, B     =         41.95 GPa , C      =          4.37 GPa
R[1] =           6.41,      R[2] =          1.88,       omega =          0.78
Gamma =     2.946
RMS fitting error =    0.00 %
```

Most of the summary sheet is self-explanatory. The energy listed under the C-J condition is *not* the energy of detonation. Instead, the energy listed there is the energy *absorbed* by the system in passing from the reactant state to the C-J state. CHEETAH lists all energies in reference to the reactants. Absorbed energy is positive, and released energy is negative.

In the `Cylinder runs` section of the summary sheet, we give information on the adiabat. The term `Cylinder run` is used, because the cylinder test is the best experimental measurement of the adiabat. Relative `V/V0` volumes are shown along with the calculated energy. The energies are then compared to TATB at 1.83 g/cc, PETN at 1.76 g/cc, HMX at 1.89 g/cc, and Tritonal at 1.70 g/cc. The comparison is given in terms of percentages, 100 percent indicating no difference. The last column of the cylinder run gives estimated half-wall and full-wall velocities for the cylinder test. These velocities are derived through the approximate relationship

$$V^2(PETN)/E(PETN) \approx V^2(X)/E(X), \tag{2.1}$$

where X is the new explosive under consideration. The wall velocities and energies of PETN are a standard determined by a combination of experiment and hydrodynamic modeling.

It has been found in the past that better results are obtained for the adiabat if reactions are frozen at 1800K. The summary sheet reports the volume along the adiabat where 1800K is obtained. Finally, the energy of detonation is given. The mechanical energy of detonation is the energy at the endpoint of the adiabat. We call it the "mechanical energy of detonation" because it represents the amount of energy available to do mechanical work (e.g. push metal). We define the adiabat endpoint to be the volume at which $P = 1$ atm. It sometimes happens, however, that adiabatic expansion out to 1 atm will produce gases that are colder than room

temperature. CHEETAH (and TIGER) do not produce reliable results for such conditions, so we cut the adiabat off at 298K if this temperature is reached before $P = 1$ atm. The "thermal energy of detonation" is the energy difference between $P = 1$ atm, $T = 298$ K, and the adiabat endpoint. It represents the amount of energy locked up as heat in the detonation products. Finally, the total energy of detonation is the sum of the mechanical and the thermal energy of detonation; i.e. it is the energy at $P = 1$ atm and $T = 298$K. This is the energy that a calorimeter experiment would measure.

The results of the standard run are fit to a JWL equation of state. The JWL equation of state is defined as:

$$P = A\exp[-R_1 v/v_0] + B\exp[-R_2 v/v_0] + C(\frac{v}{v_0})^{-(1+\omega)} \qquad (2.2)$$

Here v_0 is the specific volume of the explosive in its standard state (i.e. the inverse of the density).

Next we'll examine the long output file produced by CHEETAH for the same run. The long output file in this case is called `petn.out`:

```
Input from config/startup.in> ## These are startup commands, which are
Input from config/startup.in> ## run before every cheetah job.
Input from config/startup.in> gas eos, bkw
Input from config/startup.in> set, bkw, alpha, 0.5
Input from config/startup.in> set, bkw, beta, 0.176
Input from config/startup.in> set, bkw, kappa, 11.80
Input from config/startup.in> set, bkw, theta, 1850
Input from config/startup.in>
Input from config/startup.in>
Input from config/startup.in>
Input>
Input> # Specify the composition -- formulas are read from config/formula.in
Input> comp, petn, 100
                                The Composition

Name       % wt.    % mol  Heat of    Standard      Standard      Mol.    Formula
                           formation   volume        entropy       wt.
                           (cal/mol)   (cc/mol)     (cal/K/mol)
petn       100.00 100.00  -128700     177.61        0.000       316.15  c5h8n4o12

Heat of formation =    -407.090 cal/gm
Standard volume   =       0.562 cc/gm
Standard entropy  =       0.000 cal/k/gm
Standard energy   =    -407.104 cal/gm

The elements and percent by mole
     c              17.241
     h              27.586
```

```
     n              13.793
     o              41.379
The average mol. wt. = 316.146 g/mol


Input> standard run, rho, 1.763
                                The C-J condition

The shock velocity      =     8.32981e+03 m/s
The particle velocity =     2.11071e+03 m/s
The speed of sound      =     6.21910e+03 m/s

P0 = 1.000000 atm, V0 =  0.567215 cc/gm, E0 = -407.104001 cal/gm
                              Reference state = reactants
              H(R) = H--407.09, E(R) = E--407.10, S(R) = S- 0.00

          P            V          T        H(R)       E(R)       S(R)      VGS
       (ATM)       (CC/GM)      (K)     (CAL/GM)   (CAL/GM) (CAL/K/GM) (CC/GM)
 1.)  305915.3        .4235   3337.6    3669.88     532.42     1.557      .4235
Product concentrations
         Name     (mol/kg)     (mol gas/mol explosive)
      CO2 GAS     .9994E+01       .3160E+01
      H2O GAS     .6683E+01       .2113E+01
       N2 GAS     .6171E+01       .1951E+01
    HCOOH GAS     .5465E+01       .1728E+01
      NH3 GAS     .3073E+00       .9716E-01
       CO GAS     .3510E+00       .1110E+00
       NO GAS     .2472E-02       .7815E-03
       H2 GAS     .3281E-01       .1037E-01
       O2 GAS     .1186E-03       .3749E-04
    CH3OH GAS     .2108E-02       .6664E-03
      CH4 GAS     .3245E-02       .1026E-02
      HCN GAS     .9695E-08       .3065E-08
       *C SOLID   .0000E+00       .0000E+00
  Total Gas          29.0125


                              Reference state = reactants
              H(R) = H--407.09, E(R) = E--407.10, S(R) = S- 0.00

          P            V          T        H(R)       E(R)       S(R)      VGS
       (ATM)       (CC/GM)      (K)     (CAL/GM)   (CAL/GM) (CAL/K/GM) (CC/GM)
 1.)   25117.8        1.0577  1800.0    -252.51    -895.88     1.557     1.0577
Product concentrations
         Name     (mol/kg)     (mol gas/mol explosive)
      CO2 GAS     .1182E+02       .3736E+01
      H2O GAS     .1066E+02       .3369E+01
       N2 GAS     .6232E+01       .1970E+01
       CO GAS     .3560E+01       .1126E+01
       H2 GAS     .8882E+00       .2808E+00
      CH4 GAS     .3844E+00       .1215E+00
      NH3 GAS     .1885E+00       .5961E-01
    HCOOH GAS     .5320E-01       .1682E-01
    CH3OH GAS     .1263E-02       .3992E-03
      HCN GAS     .4857E-04       .1536E-04
       NO GAS     .2409E-06       .7617E-07
       O2 GAS     .1205E-09       .3810E-10
       *C SOLID   .0000E+00       .0000E+00
```

```
  Total Gas          33.7809
Freezing at v = 1.057673, t = 1800.000000

Constituent     *C has been indirectly frozen to zero

                              Reference state = reactants
                H(R) = H--407.09, E(R) = E--407.10, S(R) = S- 0.00

          P            V          T        H(R)        E(R)        S(R)       VGS
       (ATM)        (CC/GM)      (K)     (CAL/GM)    (CAL/GM)  (CAL/K/GM)  (CC/GM)
 1.)   16402.9       1.2479    1631.9    -493.71     -989.41     1.557      1.2479
Product concentrations
          Name      (mol/kg)      (mol gas/mol explosive)
 *    CO2 GAS      .1182E+02       .3736E+01
 *    H2O GAS      .1066E+02       .3369E+01
 *     N2 GAS      .6232E+01       .1970E+01
 *     CO GAS      .3560E+01       .1126E+01
 *     H2 GAS      .8882E+00       .2808E+00
 *    CH4 GAS      .3844E+00       .1215E+00
 *    NH3 GAS      .1885E+00       .5961E-01
 *  HCOOH GAS      .5320E-01       .1682E-01
 *  CH3OH GAS      .1263E-02       .3992E-03
 *    HCN GAS      .4857E-04       .1536E-04
 *     NO GAS      .2409E-06       .7617E-07
 *     O2 GAS      .1205E-09       .3810E-10
 *     *C SOLID    .0000E+00       .0000E+00
  Total Gas          33.7809

                              Reference state = reactants
                H(R) = H--407.09, E(R) = E--407.10, S(R) = S- 0.00

          P            V          T        H(R)        E(R)        S(R)       VGS
       (ATM)        (CC/GM)      (K)     (CAL/GM)    (CAL/GM)  (CAL/K/GM)  (CC/GM)
 1.)    3808.4       2.3256    1182.7    -980.14    -1194.62     1.557      2.3256
Product concentrations
          Name      (mol/kg)      (mol gas/mol explosive)
 *    CO2 GAS      .1182E+02       .3736E+01
 *    H2O GAS      .1066E+02       .3369E+01
 *     N2 GAS      .6232E+01       .1970E+01
 *     CO GAS      .3560E+01       .1126E+01
 *     H2 GAS      .8882E+00       .2808E+00
 *    CH4 GAS      .3844E+00       .1215E+00
 *    NH3 GAS      .1885E+00       .5961E-01
 *  HCOOH GAS      .5320E-01       .1682E-01
 *  CH3OH GAS      .1263E-02       .3992E-03
 *    HCN GAS      .4857E-04       .1536E-04
 *     NO GAS      .2409E-06       .7617E-07
 *     O2 GAS      .1205E-09       .3810E-10
 *     *C SOLID    .0000E+00       .0000E+00
  Total Gas          33.7809

                              Reference state = reactants
                H(R) = H--407.09, E(R) = E--407.10, S(R) = S- 0.00
```

	P (ATM)	V (CC/GM)	T (K)	H(R) (CAL/GM)	E(R) (CAL/GM)	S(R) (CAL/K/GM)	VGS (CC/GM)
1.)	1475.5	3.6869	968.7	-1140.46	-1272.19	1.557	3.6869

Product concentrations

	Name	(mol/kg)	(mol gas/mol explosive)
*	CO2 GAS	.1182E+02	.3736E+01
*	H2O GAS	.1066E+02	.3369E+01
*	N2 GAS	.6232E+01	.1970E+01
*	CO GAS	.3560E+01	.1126E+01
*	H2 GAS	.8882E+00	.2808E+00
*	CH4 GAS	.3844E+00	.1215E+00
*	NH3 GAS	.1885E+00	.5961E-01
*	HCOOH GAS	.5320E-01	.1682E-01
*	CH3OH GAS	.1263E-02	.3992E-03
*	HCN GAS	.4857E-04	.1536E-04
*	NO GAS	.2409E-06	.7617E-07
*	O2 GAS	.1205E-09	.3810E-10
*	*C SOLID	.0000E+00	.0000E+00
Total Gas		33.7809	

Reference state = reactants
H(R) = H--407.09, E(R) = E--407.10, S(R) = S- 0.00

	P (ATM)	V (CC/GM)	T (K)	H(R) (CAL/GM)	E(R) (CAL/GM)	S(R) (CAL/K/GM)	VGS (CC/GM)
1.)	661.6	5.6721	820.1	-1228.44	-1319.31	1.557	5.6721

Product concentrations

	Name	(mol/kg)	(mol gas/mol explosive)
*	CO2 GAS	.1182E+02	.3736E+01
*	H2O GAS	.1066E+02	.3369E+01
*	N2 GAS	.6232E+01	.1970E+01
*	CO GAS	.3560E+01	.1126E+01
*	H2 GAS	.8882E+00	.2808E+00
*	CH4 GAS	.3844E+00	.1215E+00
*	NH3 GAS	.1885E+00	.5961E-01
*	HCOOH GAS	.5320E-01	.1682E-01
*	CH3OH GAS	.1263E-02	.3992E-03
*	HCN GAS	.4857E-04	.1536E-04
*	NO GAS	.2409E-06	.7617E-07
*	O2 GAS	.1205E-09	.3810E-10
*	*C SOLID	.0000E+00	.0000E+00
Total Gas		33.7809	

Reference state = reactants
H(R) = H--407.09, E(R) = E--407.10, S(R) = S- 0.00

	P (ATM)	V (CC/GM)	T (K)	H(R) (CAL/GM)	E(R) (CAL/GM)	S(R) (CAL/K/GM)	VGS (CC/GM)
1.)	207.3	11.3443	642.4	-1312.14	-1369.07	1.557	11.3443

Product concentrations

	Name	(mol/kg)	(mol gas/mol explosive)
*	CO2 GAS	.1182E+02	.3736E+01
*	H2O GAS	.1066E+02	.3369E+01
*	N2 GAS	.6232E+01	.1970E+01
*	CO GAS	.3560E+01	.1126E+01
*	H2 GAS	.8882E+00	.2808E+00

```
 *    CH4 GAS     .3844E+00      .1215E+00
 *    NH3 GAS     .1885E+00      .5961E-01
 *  HCOOH GAS     .5320E-01      .1682E-01
 *  CH3OH GAS     .1263E-02      .3992E-03
 *    HCN GAS     .4857E-04      .1536E-04
 *     NO GAS     .2409E-06      .7617E-07
 *     O2 GAS     .1205E-09      .3810E-10
 *     *C SOLID   .0000E+00      .0000E+00
  Total Gas          33.7809

                          Reference state = reactants
               H(R) = H--407.09, E(R) = E--407.10, S(R) = S- 0.00

         P           V          T        H(R)       E(R)       S(R)      VGS
       (ATM)       (CC/GM)     (K)     (CAL/GM)   (CAL/GM) (CAL/K/GM) (CC/GM)
 1.)     7.6     112.6217     298.0   -1427.42   -1448.08     1.557   112.6217
Product concentrations
         Name      (mol/kg)     (mol gas/mol explosive)
 *    CO2 GAS     .1182E+02      .3736E+01
 *    H2O GAS     .1066E+02      .3369E+01
 *     N2 GAS     .6232E+01      .1970E+01
 *     CO GAS     .3560E+01      .1126E+01
 *     H2 GAS     .8882E+00      .2808E+00
 *    CH4 GAS     .3844E+00      .1215E+00
 *    NH3 GAS     .1885E+00      .5961E-01
 *  HCOOH GAS     .5320E-01      .1682E-01
 *  CH3OH GAS     .1263E-02      .3992E-03
 *    HCN GAS     .4857E-04      .1536E-04
 *     NO GAS     .2409E-06      .7617E-07
 *     O2 GAS     .1205E-09      .3810E-10
 *     *C SOLID   .0000E+00      .0000E+00
  Total Gas          33.7809

                          Reference state = reactants
               H(R) = H--407.09, E(R) = E--407.10, S(R) = S- 0.00

         P           V          T        H(R)       E(R)       S(R)      VGS
       (ATM)       (CC/GM)     (K)     (CAL/GM)   (CAL/GM) (CAL/K/GM) (CC/GM)
 1.)     1.0     829.7420     298.0   -1428.04   -1448.12     1.693   829.7420
Product concentrations
         Name      (mol/kg)     (mol gas/mol explosive)
 *    CO2 GAS     .1182E+02      .3736E+01
 *    H2O GAS     .1066E+02      .3369E+01
 *     N2 GAS     .6232E+01      .1970E+01
 *     CO GAS     .3560E+01      .1126E+01
 *     H2 GAS     .8882E+00      .2808E+00
 *    CH4 GAS     .3844E+00      .1215E+00
 *    NH3 GAS     .1885E+00      .5961E-01
 *  HCOOH GAS     .5320E-01      .1682E-01
 *  CH3OH GAS     .1263E-02      .3992E-03
 *    HCN GAS     .4857E-04      .1536E-04
 *     NO GAS     .2409E-06      .7617E-07
 *     O2 GAS     .1205E-09      .3810E-10
 *     *C SOLID   .0000E+00      .0000E+00
  Total Gas          33.7809
The mechanical energy of detonation =    -10.682 kJ/cc
```

```
The thermal energy of detonation     =      0.000 kJ/cc
The total energy of detonation       =    -10.682 kJ/cc

JWL Fit results:
R[1] =      6.414, R[2] =      1.878, omega =      0.781
A    =   1599.676, B    =     41.953, C     =      4.374
Final fitting error = 0.000000

     V/V0      Actual E      Fit E     Actual P      Fit P
               (kJ/cc)      (kJ/cc)     (GPa)       (GPa)

     0.747       3.927       3.927      30.997     30.997
     2.200      -7.298      -7.298       1.662      1.749
     4.100      -8.812      -8.812       0.386      0.373
     6.500      -9.384      -9.384       0.150      0.156


Input> stop
```

The first lines of input begin with the prefix

```
Input from config/startup.in>
```

`config` is a directory where CHEETAH stores configuration files that are only infrequently (if at all) changed. The file `config/startup.in` is executed at the start of every job. The `startup.in` supplied with CHEETAH sets the equation of state parameters. These parameters may be changed by editing `startup.in`.

The first two lines of input from startup.in begin with a `#`. CHEETAH treats any line of input beginning with # as a comment, and simply passes it to the output file. Comments are useful in documenting your CHEETAH runs.

Each line of input in `petn.in` is repeated in `petn.out` with the prefix `Input>`. This helps you keep track of the relationship between the input entered into CHEETAH and the output. The `comp` command tells CHEETAH the explosive composition. Once the composition is known, CHEETAH reports the heat of formation, standard volume, and other properties of the unreacted explosive.

The second command entered is `standard run, rho, 1.763`. This produces a large quantity of output. First, the C-J point is found. The output line giving `P0, V0, and E0` describe the initial state of the explosive before detonation. These initial parameters enter into the shock Hugoniot formula of the explosive. The line `Reference state = reactants` indicates that thermodynamic potentials (H,E, and S) are given as changes from the reactant state.

CHEETAH evaluates states on the shock Hugoniot until the C-J point is found. The C-J properties listed from left to right, are the pressure, the specific volume, the

temperature, the enthalpy of reaction, the energy of reaction, the entropy of reaction, and the specific volume of the gas (VGS). VGS = V in this case, because there are no condensed species present at C-J. Below the thermodynamic functions, the concentrations of the product species are shown. Product concentrations are given both in mol / kg and mol gas / mol explosive.

The same description is repeated for a number of thermodynamic states along the adiabat. After the first adiabat point, CHEETAH freezes at 1800K. The volume at which the freeze occurred is reported. The following adiabat points occur with all concentrations frozen. The name of a frozen species is prefixed with a star. Sometimes a star is used as the first character of a product species' name. For instance, carbon in the example has been given the name *C. Care must be taken not to confuse this sort of star with the star indicating frozen concentration.

After the adiabat points have been calculated, a calculation at 298K, 1 atm is done to determine the total energy of detonation. As described above, the mechanical energy of detonation is defined as the energy at the endpoint of the adiabat.

Finally, the adiabat is fit to a JWL. The results of the fit are displayed, as well as a comparison of actual energy and pressures to the JWL energy and pressure. The fit minimizes the RMS difference of the energies, so calculated and fit energies usually match quite well. The fit is constrained to reproduce the exact C-J pressure, but there may be relatively large differences between the actual and the fit pressures at other points.

2.2 Adding a reactant

In the previous example CHEETAH "knew" what PETN was. CHEETAH knows about all the chemical compounds (explosives, binders, etc.) listed in `config/formula.in`. These compounds are given in Section 4 of this manual. It's likely that you will eventually require a compound that is not listed in `formula.in`. Let's try an example of an unknown explosive; we'll enter:

```
comp, wierdo, 100
```

This is what CHEETAH says:

```
Error in autoform: formula wierdo not found
```

There are two ways to fix this problem. If you don't expect to run compound "wierdo" again, you can enter the formula directly in the input file.

```
formula, wierdo, 5700., 68.92, 0., h, 4, n, 4, o, 4
comp, wierdo, 100
standard run, rho, 1.43
```

The `formula` command here acts just like the `formula` command in TIGER. The first argument is the name of the substance. The second is the heat of formation in calories/mole, the third is the standard molar volume in cc/mole. The fourth is the standard molar entropy in calories/mole/degree. Finally, the chemical formula of the substance is given in subsequent arguments. Use of the `formula` command in the input file disables the looking up of formulas in `config/formula.in`. Therefore, in a wierdo/tnt composite, you would give separate formula commands for wierdo and tnt, even though tnt is in the `formula.in` file.

If you intend to use "wierdo" again, it can be added as a line in your `formula.in` file. The syntax of the `formula` command is exactly the same in this case. Once a compound has been added to `formula.in`, CHEETAH will look up the name automatically.

2.3 Loading a new library

The library is handled similary in CHEETAH and TIGER; a library input file is run, and in subsequent runs that library is used. (If you want to get fancy, however, the `library file` command can be used to switch between pre-compiled libraries.) For instance, one could type

```
cheetah sandia.lib sandia.out
```

to load the Sandia BKW library. Be sure to check the `sandia.out` file for any errors in entering the library. Subsequent jobs will use the Sandia library, until another library is loaded.

CHEETAH can use the same library files as TIGER with minor modifications. For instance, the `CARDLIST` command in TIGER is called `card list` in CHEETAH. One important addition is that CHEETAH expects to have a title in the library file. The command `title, llnl bkwr` for instance, should appear right after the `start of library` command.

2.4 Shock Hugoniot calculation

In this example we will calculate the shock Hugoniot of reacted PETN. The input file is:

```
# You can use comments to document your input
# Any line that begins with a # is a comment.
#
comp, petn, 100
hug0, p, 1, rho, 1.763
spreadsheet, hugoniot.dat, v, p, space
point, p, 10000, t, 1000
isoline, hugoniot, , p, 1000, 20, 100000
stop
```

The `hug0` command is used to set the Hugoniot reference state to be $p = 1$ atm, $\rho = 1.763$ g/cc. This specifies the state of the unshocked material. The `spreadsheet` command is then used to save the pressure and the volume into the file `hugoniot.dat`. The `space` argument indicates that the data should be separated by spaces. Other possibilities are `tab` or the default `comma`. The `point` command calculates a thermodynamic state. In this case we calculate a state with $p = 10000$ atm and $t = 1000$K. It's a good idea to initialize CHEETAH witn a (P,T) point calculation before moving to more exotic point types.

Finally, we use the isoline command to specify a sequence of states along the shock Hugoniot, from 1000 atm to 100000 atm in 20 steps. The `hugoniot` point type always takes a blank argument. Instead, CHEETAH uses the `hug0` command to specify how the Hugoniot is to be calculated.

The spreadsheet file is:

```
     P          V
1.000000e+04 1.284903e+00
1.000000e+03 1.320219e+01
5.950000e+03 3.277776e+00
1.090000e+04 2.194625e+00
1.585000e+04 1.742692e+00
2.080000e+04 1.486159e+00
2.575000e+04 1.317648e+00
3.070000e+04 1.196997e+00
3.565000e+04 1.105542e+00
4.060000e+04 1.033344e+00
4.555000e+04 9.745841e-01
5.050000e+04 9.256133e-01
5.545000e+04 8.840159e-01
6.040000e+04 8.481244e-01
6.535000e+04 8.167477e-01
7.030000e+04 7.890106e-01
7.525000e+04 7.642549e-01
8.020000e+04 7.419759e-01
8.515000e+04 7.217799e-01
9.010000e+04 7.033552e-01
9.505000e+04 6.864521e-01
1.000000e+05 6.708679e-01
```

The first line indicates the quantities stored in the columns underneath.

The output file for an isoline calculation has each point along the hugoniot numbered; other than that the output is very similar to the C-J point described in previous sections.

```
Library Title: llnl bkwr
Input from startup.in> ## These are startup commands, which are
Input from startup.in> ## run before every cheetah job.
Input from startup.in> gas eos, bkw
Input from startup.in> set, bkw, alpha, 0.5
Input from startup.in> set, bkw, beta, 0.176
Input from startup.in> set, bkw, kappa, 11.80
Input from startup.in> set, bkw, theta, 1850
Input from startup.in>
Input from startup.in>
Input from startup.in>
Input>
Input> comp, petn, 100
Reactant library title:LLNL CHEETAH Reactant Library V1.01

                                The Composition

Name       % wt.    % mol  Heat of    Standard     Standard     Mol.    Formula
                           formation   volume       entropy      wt.
                           (cal/mol)   (cc/mol)     (cal/K/mol)
petn       100.00 100.00  -128700     177.61         0.000      316.15  c5h8n4o12

Heat of formation =    -407.090 cal/gm
Standard volume   =       0.562 cc/gm
Standard entropy  =       0.000 cal/k/gm
Standard energy   =    -407.104 cal/gm
```

```
The elements and percent by mole
     c              17.241
     h              27.586
     n              13.793
     o              41.379
The average mol. wt. = 316.146 g/mol


Input> hug0, p, 1, rho, 1.763
Input> spreadsheet, hugoniot.dat, v, p, space
Input> point, p, 10000, t, 1000

                          Reference state = reactants
               H(R) = H--407.09, E(R) = E--407.10, S(R) = S- 0.00

         P           V          T        H(R)       E(R)       S(R)      VGS
      (ATM)       (CC/GM)      (K)     (CAL/GM)   (CAL/GM)  (CAL/K/GM) (CC/GM)
 1.)  10000.0      1.2849    1000.0    -993.18    -1304.35     1.326     1.2849

Product concentrations
          Name      (mol/kg)     (mol gas/mol explosive)
    co2   Gas    1.420e+01   4.488e+00
    h2o   Gas    9.428e+00   2.981e+00
     n2   Gas    6.286e+00   1.987e+00
    ch4   Gas    1.483e+00   4.690e-01
     co   Gas    1.346e-01   4.257e-02
     h2   Gas    1.345e-01   4.251e-02
    nh3   Gas    8.076e-02   2.553e-02
  hcooh   Gas    1.934e-03   6.115e-04
  ch3oh   Gas    4.445e-05   1.405e-05
    hcn   Gas    1.012e-07   3.199e-08
     no   Gas    3.123e-14   9.874e-15
     o2   Gas    2.990e-20   9.454e-21
     *c Solid    0.000e+00   0.000e+00
  Total   Gas    3.174e+01


Input> isoline, hugoniot,, p, 1000, 20, 100000

0                                                          ISOLINE
                          Reference state = reactants
               H(R) = H--407.09, E(R) = E--407.10, S(R) = S- 0.00

         P           V          T        H(R)       E(R)       S(R)      VGS
      (ATM)       (CC/GM)      (K)     (CAL/GM)   (CAL/GM)  (CAL/K/GM) (CC/GM)
 1.)   1000.0     13.2022    3826.1     166.57    -153.15     2.199    13.2022
 2.)   5950.0      3.2778    3793.1     276.98    -195.33     2.050     3.2778
 3.)  10900.0      2.1946    3690.9     354.50    -214.82     1.989     2.1946
 4.)  15850.0      1.7427    3596.6     443.31    -225.62     1.947     1.7427
 5.)  20800.0      1.4862    3515.0     517.15    -231.46     1.913     1.4862
 6.)  25750.0      1.3176    3445.2     587.69    -234.00     1.885     1.3176

Product concentrations (mol/kg)
    Name            1.)         2.)         3.)         4.)         5.)         6.)
```

h2o	Gas	1.152e+01	1.177e+01	1.180e+01	1.181e+01	1.179e+01	1.178e+01
co2	Gas	8.797e+00	9.854e+00	1.011e+01	1.021e+01	1.027e+01	1.030e+01
co	Gas	7.017e+00	5.957e+00	5.694e+00	5.586e+00	5.526e+00	5.485e+00
n2	Gas	6.066e+00	6.209e+00	6.263e+00	6.288e+00	6.300e+00	6.305e+00
o2	Gas	6.495e-01	1.418e-01	4.723e-02	1.842e-02	8.091e-03	3.909e-03
h2	Gas	1.127e+00	8.779e-01	8.327e-01	8.206e-01	8.187e-01	8.194e-01
no	Gas	5.205e-01	2.327e-01	1.218e-01	6.908e-02	4.191e-02	2.687e-02
hcooh	Gas	7.804e-04	4.653e-03	9.517e-03	1.585e-02	2.401e-02	3.435e-02
nh3	Gas	3.790e-04	1.785e-03	3.644e-03	6.258e-03	9.823e-03	1.453e-02
hcn	Gas	7.400e-05	1.518e-04	1.724e-04	1.793e-04	1.783e-04	1.722e-04
ch4	Gas	5.494e-08	9.988e-07	4.274e-06	1.339e-05	3.517e-05	8.169e-05
ch3oh	Gas	3.522e-08	7.203e-07	2.637e-06	6.871e-06	1.508e-05	2.961e-05
*c	Solid	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00
Total	Gas	3.570e+01	3.505e+01	3.489e+01	3.482e+01	3.479e+01	3.476e+01

	P (ATM)	V (CC/GM)	T (K)	H(R) (CAL/GM)	E(R) (CAL/GM)	S(R) (CAL/K/GM)	VGS (CC/GM)
7.)	30700.0	1.1970	3385.2	655.82	-234.13	1.861	1.1970
8.)	35650.0	1.1055	3333.4	722.09	-232.40	1.840	1.1055
9.)	40600.0	1.0333	3288.3	786.86	-229.17	1.821	1.0333
10.)	45550.0	0.9746	3249.1	850.39	-224.70	1.804	0.9746
11.)	50500.0	0.9256	3214.8	912.85	-219.17	1.788	0.9256
12.)	55450.0	0.8840	3184.8	974.40	-212.72	1.773	0.8840

Product concentrations (mol/kg)

Name		7.)	8.)	9.)	10.)	11.)	12.)
h2o	Gas	1.175e+01	1.173e+01	1.169e+01	1.165e+01	1.161e+01	1.156e+01
co2	Gas	1.032e+01	1.034e+01	1.036e+01	1.038e+01	1.039e+01	1.042e+01
co	Gas	5.449e+00	5.413e+00	5.375e+00	5.333e+00	5.285e+00	5.229e+00
n2	Gas	6.307e+00	6.306e+00	6.303e+00	6.298e+00	6.292e+00	6.285e+00
o2	Gas	2.040e-03	1.136e-03	6.680e-04	4.121e-04	2.653e-04	1.776e-04
h2	Gas	8.204e-01	8.205e-01	8.193e-01	8.163e-01	8.112e-01	8.038e-01
no	Gas	1.804e-02	1.259e-02	9.080e-03	6.741e-03	5.136e-03	4.007e-03
hcooh	Gas	4.728e-02	6.322e-02	8.265e-02	1.060e-01	1.339e-01	1.668e-01
nh3	Gas	2.058e-02	2.818e-02	3.753e-02	4.883e-02	6.224e-02	7.788e-02
hcn	Gas	1.629e-04	1.517e-04	1.396e-04	1.271e-04	1.147e-04	1.027e-04
ch4	Gas	1.729e-04	3.400e-04	6.287e-04	1.103e-03	1.846e-03	2.963e-03
ch3oh	Gas	5.368e-05	9.152e-05	1.485e-04	2.311e-04	3.468e-04	5.038e-04
*c	Solid	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00
Total	Gas	3.474e+01	3.471e+01	3.468e+01	3.464e+01	3.460e+01	3.454e+01

	P (ATM)	V (CC/GM)	T (K)	H(R) (CAL/GM)	E(R) (CAL/GM)	S(R) (CAL/K/GM)	VGS (CC/GM)
13.)	60400.0	0.8481	3158.6	1035.14	-205.46	1.760	0.8481
14.)	65350.0	0.8167	3135.9	1095.15	-197.46	1.747	0.8167
15.)	70300.0	0.7890	3116.2	1154.49	-188.81	1.735	0.7890
16.)	75250.0	0.7643	3099.3	1213.22	-179.55	1.724	0.7643
17.)	80200.0	0.7420	3084.9	1271.40	-169.72	1.714	0.7420
18.)	85150.0	0.7218	3072.9	1329.05	-159.37	1.704	0.7218

Product concentrations (mol/kg)

Name		13.)	14.)	15.)	16.)	17.)	18.)
h2o	Gas	1.150e+01	1.143e+01	1.136e+01	1.127e+01	1.118e+01	1.108e+01
co2	Gas	1.044e+01	1.046e+01	1.049e+01	1.052e+01	1.056e+01	1.059e+01
co	Gas	5.166e+00	5.094e+00	5.011e+00	4.919e+00	4.816e+00	4.702e+00
n2	Gas	6.277e+00	6.267e+00	6.256e+00	6.244e+00	6.231e+00	6.217e+00
o2	Gas	1.231e-04	8.825e-05	6.526e-05	4.971e-05	3.894e-05	3.131e-05
h2	Gas	7.939e-01	7.814e-01	7.660e-01	7.480e-01	7.273e-01	7.041e-01

```
     no  Gas   3.194e-03  2.597e-03  2.153e-03  1.817e-03  1.560e-03  1.360e-03
  hcooh  Gas   2.051e-01  2.495e-01  3.002e-01  3.577e-01  4.222e-01  4.939e-01
    nh3  Gas   9.581e-02  1.160e-01  1.384e-01  1.627e-01  1.887e-01  2.160e-01
    hcn  Gas   9.137e-05  8.071e-05  7.086e-05  6.183e-05  5.365e-05  4.629e-05
    ch4  Gas   4.574e-03  6.805e-03  9.777e-03  1.359e-02  1.828e-02  2.385e-02
  ch3oh  Gas   7.109e-04  9.759e-04  1.306e-03  1.705e-03  2.176e-03  2.715e-03
     *c Solid  0.000e+00  0.000e+00  0.000e+00  0.000e+00  0.000e+00  0.000e+00
   Total Gas   3.448e+01  3.441e+01  3.433e+01  3.424e+01  3.414e+01  3.403e+01

          P          V          T        H(R)       E(R)       S(R)      VGS
       (ATM)    (CC/GM)        (K)   (CAL/GM)   (CAL/GM)  (CAL/K/GM) (CC/GM)
19.)    90100.0     0.7034   3062.9    1386.21    -148.53      1.695     0.7034
20.)    95050.0     0.6865   3054.9    1442.91    -137.24      1.686     0.6865
21.)   100000.0     0.6709   3048.7    1499.18    -125.51      1.678     0.6709

Product concentrations (mol/kg)
    Name            19.)       20.)       21.)
    h2o  Gas   1.097e+01  1.085e+01  1.072e+01
    co2  Gas   1.063e+01  1.067e+01  1.071e+01
     co  Gas   4.578e+00  4.446e+00  4.305e+00
     n2  Gas   6.203e+00  6.189e+00  6.175e+00
     o2  Gas   2.582e-05  2.179e-05  1.879e-05
     h2  Gas   6.789e-01  6.518e-01  6.233e-01
     no  Gas   1.205e-03  1.082e-03  9.849e-04
  hcooh  Gas   5.730e-01  6.593e-01  7.530e-01
    nh3  Gas   2.442e-01  2.730e-01  3.018e-01
    hcn  Gas   3.975e-05  3.397e-05  2.890e-05
    ch4  Gas   3.023e-02  3.726e-02  4.474e-02
  ch3oh  Gas   3.319e-03  3.977e-03  4.678e-03
     *c Solid  0.000e+00  0.000e+00  0.000e+00
   Total Gas   3.391e+01  3.378e+01  3.364e+01


Input> stop
```

2.5 C-J calculation

In this section we will execute a custom version of the standard run. Let's say that tritonal has been confined in a casing at a pressure of 1000 atm prior to detonation. Let's also assume that the tritonal volume is equal to 1 / TMD (theoretical maximum density) at this point. This means that the pressure and volume of the shock Hugoniot reference state is 1000 atm and 1 / TMD. Finally, since tritonal is an aluminized explosive we expect a slower release of energy than in non-aluminized explosives. This means that the JWL should be fit to larger volumes than in the standard run.

The input file that does this is:

```
comp, tnt, 80, al, 20
```

```
point, p, 2000, t, 2000
hug0, p, 1000, sv,
c-j
units, sv
point, v, 2.2, s,
point, v, 4.1, s,
point, v, 6.5, s,
point, v, 10.0, s,
point, v, 20.0, s,
point, v, 50.0, s,
point, v, 100.0, s,
point, v, 200.0, s,
det energy, p, 1, t, 298
jwlfit, 7
stop
```

The `sv` argument in the `hug0` command is short for standard volume. This will set the density of the initial shock state to the TMD. Once the shock Hugoniot has been defined, the `c-j` command finds the C-J point on the Hugoniot.

We next do an adiabatic expansion from the C-J point. The adiabatic condition $dQ = 0$ implies that $dS = 0$, since $dQ = T\,dS$. Therefore each point on the adiabat has the same entropy as the C-J state.

The `units` command is used to set the input unit of volume. As in the `hug0` command, `sv` is short for standard volume. All the points that follow are relative to the standard volume (the reactant library is usually set so this is the inverse of the theoretical maximum density). Finally we find the detonation energy, with the final calorimetric state being $p = 1$ and $T = 298K$. We are now ready to fit the adiabat to a JWL equation of state with the `jwlfit` command. The argument of 7 indicates that the first 7 points previously calculated on the adiabat should be used in doing the fit.

The output file follows:

```
Library Title: llnl bkwr
Input from startup.in> ## These are startup commands, which are
Input from startup.in> ## run before every cheetah job.
Input from startup.in> gas eos, bkw
Input from startup.in> set, bkw, alpha, 0.5
Input from startup.in> set, bkw, beta, 0.176
Input from startup.in> set, bkw, kappa, 11.80
Input from startup.in> set, bkw, theta, 1850
Input from startup.in>
Input from startup.in>
Input from startup.in>
Input>
Input> comp, tnt, 80, al, 20
Reactant library title:LLNL CHEETAH Reactant Library V1.01
```

The Composition

Name	% wt.	% mol	Heat of formation (cal/mol)	Standard volume (cc/mol)	Standard entropy (cal/K/mol)	Mol. wt.	Formula
tnt	80.00	32.21	-17810	137.30	0.000	227.13	c7h5n3o6
al	20.00	67.79	0	9.98	0.000	26.98	al1

```
Heat of formation =    -62.729 cal/gm
Standard volume   =      0.558 cc/gm
Standard entropy  =      0.000 cal/k/gm
Standard energy   =    -62.743 cal/gm

The elements and percent by mole
     c             30.297
     h             21.641
     n             12.984
     o             25.969
     al             9.109
The average mol. wt. =  91.449 g/mol


Input> point, p, 2000, t, 2000
```

Reference state = reactants
H(R) = H--62.73, E(R) = E--62.74, S(R) = S- 0.00

	P (ATM)	V (CC/GM)	T (K)	H(R) (CAL/GM)	E(R) (CAL/GM)	S(R) (CAL/K/GM)	VGS (CC/GM)
1.)	2000.0	2.9897	2000.0	-907.68	-1052.48	1.369	2.8383

Product concentrations

Name		(mol/kg)	(mol gas/mol explosive)
co	Gas	9.966e+00	9.113e-01
n2	Gas	5.067e+00	4.634e-01
ch4	Gas	3.166e+00	2.896e-01
h2	Gas	2.225e+00	2.035e-01
hcn	Gas	4.164e-01	3.808e-02
co2	Gas	1.608e-02	1.470e-03
h2o	Gas	1.582e-02	1.447e-03
nh3	Gas	1.548e-02	1.416e-03
ch3oh	Gas	2.795e-05	2.556e-06
hcooh	Gas	5.557e-06	5.082e-07
no	Gas	8.909e-09	8.147e-10
alo	Gas	3.122e-12	2.855e-13
o2	Gas	4.201e-14	3.842e-15
*c	Solid	1.109e+01	1.014e+00
*o3al2	Solid	3.706e+00	3.390e-01
*al	Liquid	0.000e+00	0.000e+00
Total	Gas	2.089e+01	

```
Input> hug0, p, 1000, sv,
Input> c-j
```

The C-J condition

```
The shock velocity    =    6.61735e+03 m/s
The particle velocity =    1.61646e+03 m/s
The speed of sound    =    5.00089e+03 m/s

P0 = 1000.000000 atm, V0 =  0.557609 cc/gm, E0 = -62.742994 cal/gm
                        Reference state = reactants
               H(R) = H--62.73, E(R) = E--62.74, S(R) = S- 0.00


         P           V         T       H(R)       E(R)       S(R)      VGS
      (ATM)       (CC/GM)     (K)    (CAL/GM)   (CAL/GM) (CAL/K/GM) (CC/GM)
 1.)  190322.9      0.4214   4279.1   2257.88    315.56     1.465    0.2424

Product concentrations
         Name      (mol/kg)    (mol gas/mol explosive)
     n2  Gas    4.581e+00  4.189e-01
    h2o  Gas    3.746e+00  3.426e-01
     co  Gas    2.343e+00  2.143e-01
    nh3  Gas    1.401e+00  1.281e-01
  hcooh  Gas    8.478e-01  7.753e-02
    co2  Gas    1.089e+00  9.958e-02
     h2  Gas    9.842e-01  9.001e-02
    ch4  Gas    5.160e-01  4.719e-02
  ch3oh  Gas    4.692e-02  4.291e-03
     no  Gas    3.927e-03  3.591e-04
     o2  Gas    6.011e-05  5.497e-06
    hcn  Gas    1.150e-04  1.052e-05
    alo  Gas    5.073e-07  4.640e-08
     *c Solid   1.981e+01  1.812e+00
 *o3al2 Liquid  3.706e+00  3.390e-01
    *al Solid   0.000e+00  0.000e+00
   Total Gas    1.556e+01


Input> units, sv
Input> point, v, 2.2, s,

                        Reference state = reactants
               H(R) = H--62.73, E(R) = E--62.74, S(R) = S- 0.00


         P           V         T       H(R)       E(R)       S(R)      VGS
      (ATM)       (CC/GM)     (K)    (CAL/GM)   (CAL/GM) (CAL/K/GM) (CC/GM)
 1.)  12152.0       1.2267   2698.3   -266.95    -627.96     1.465    1.0708

Product concentrations
         Name      (mol/kg)    (mol gas/mol explosive)
     co  Gas    9.817e+00  8.977e-01
     n2  Gas    5.108e+00  4.671e-01
     h2  Gas    3.040e+00  2.780e-01
    ch4  Gas    2.700e+00  2.469e-01
    h2o  Gas    9.725e-02  8.894e-03
    nh3  Gas    9.081e-02  8.305e-03
    co2  Gas    4.922e-02  4.501e-03
  hcooh  Gas    2.767e-04  2.530e-05
  ch3oh  Gas    6.547e-04  5.987e-05
    hcn  Gas    2.596e-01  2.374e-02
```

```
     no  Gas    2.636e-06  2.410e-07
     o2  Gas    2.477e-10  2.265e-11
    alo  Gas    9.002e-09  8.232e-10
     *c Solid   1.183e+01  1.082e+00
 *o3al2 Liquid  3.706e+00  3.390e-01
    *al Solid   0.000e+00  0.000e+00
   Total Gas    2.116e+01
```

```
Input> point, v, 4.1, s,
```

```
                        Reference state = reactants
               H(R) = H--62.73, E(R) = E--62.74, S(R) = S- 0.00
```

	P (ATM)	V (CC/GM)	T (K)	H(R) (CAL/GM)	E(R) (CAL/GM)	S(R) (CAL/K/GM)	VGS (CC/GM)
1.)	3574.7	2.2862	2335.4	-595.47	-793.37	1.465	2.1325

```
Product concentrations
         Name      (mol/kg)    (mol gas/mol explosive)
     co  Gas    9.965e+00  9.113e-01
     n2  Gas    4.934e+00  4.512e-01
     h2  Gas    3.004e+00  2.747e-01
    ch4  Gas    2.701e+00  2.470e-01
    h2o  Gas    2.201e-02  2.013e-03
    nh3  Gas    2.763e-02  2.526e-03
    co2  Gas    1.333e-02  1.219e-03
  hcooh  Gas    1.341e-05  1.227e-06
  ch3oh  Gas    7.207e-05  6.590e-06
    hcn  Gas    6.715e-01  6.141e-02
     no  Gas    1.265e-07  1.157e-08
     o2  Gas    1.865e-12  1.705e-13
    alo  Gas    1.062e-09  9.709e-11
     *c Solid   1.130e+01  1.034e+00
 *o3al2 Liquid  3.706e+00  3.390e-01
    *al Liquid  0.000e+00  0.000e+00
   Total Gas    2.134e+01
```

```
Input> point, v, 6.5, s,
```

```
                        Reference state = reactants
               H(R) = H--62.73, E(R) = E--62.74, S(R) = S- 0.00
```

	P (ATM)	V (CC/GM)	T (K)	H(R) (CAL/GM)	E(R) (CAL/GM)	S(R) (CAL/K/GM)	VGS (CC/GM)
1.)	1654.8	3.6245	2149.8	-726.03	-871.27	1.465	3.4726

```
Product concentrations
         Name      (mol/kg)    (mol gas/mol explosive)
     co  Gas    9.988e+00  9.134e-01
     n2  Gas    4.867e+00  4.450e-01
     h2  Gas    2.990e+00  2.734e-01
    ch4  Gas    2.686e+00  2.457e-01
```

```
    h2o  Gas    1.099e-02  1.005e-03
    nh3  Gas    1.481e-02  1.354e-03
    co2  Gas    7.468e-03  6.829e-04
  hcooh  Gas    2.904e-06  2.656e-07
  ch3oh  Gas    2.152e-05  1.968e-06
    hcn  Gas    8.184e-01  7.484e-02
     no  Gas    2.153e-08  1.969e-09
     o2  Gas    1.181e-13  1.080e-14
    alo  Gas    1.857e-10  1.698e-11
     *c Solid   1.116e+01  1.020e+00
  Total Gas     2.138e+01

Input> point, v, 10.0, s,

                        Reference state = reactants
                H(R) = H--62.73, E(R) = E--62.74, S(R) = S- 0.00

          P           V          T        H(R)       E(R)       S(R)      VGS
       (ATM)       (CC/GM)      (K)     (CAL/GM)   (CAL/GM) (CAL/K/GM) (CC/GM)
 1.)     970.0       5.5761   2200.2    -804.63    -935.60     1.465     5.4244

Product concentrations
         Name      (mol/kg)     (mol gas/mol explosive)
     co  Gas    1.000e+01  9.146e-01
     n2  Gas    4.601e+00  4.208e-01
     h2  Gas    3.724e+00  3.406e-01
    ch4  Gas    2.191e+00  2.004e-01
    h2o  Gas    6.096e-03  5.575e-04
    nh3  Gas    1.039e-02  9.502e-04
    co2  Gas    3.223e-03  2.947e-04
  hcooh  Gas    8.794e-07  8.042e-08
  ch3oh  Gas    9.569e-06  8.750e-07
    hcn  Gas    1.353e+00  1.238e-01
     no  Gas    1.965e-08  1.797e-09
     o2  Gas    8.090e-14  7.398e-15
    alo  Gas    1.253e-09  1.146e-10
     *c Solid   1.111e+01  1.016e+00
 *o3al2 Solid   3.706e+00  3.390e-01
    *al Liquid  0.000e+00  0.000e+00
  Total Gas     2.189e+01

Input> point, v, 20.0, s,

                        Reference state = reactants
                H(R) = H--62.73, E(R) = E--62.74, S(R) = S- 0.00

          P           V          T        H(R)       E(R)       S(R)      VGS
       (ATM)       (CC/GM)      (K)     (CAL/GM)   (CAL/GM) (CAL/K/GM) (CC/GM)
 1.)     380.5      11.1522   2004.8    -912.76   -1015.52     1.465    10.9997

Product concentrations
         Name      (mol/kg)     (mol gas/mol explosive)
```

```
     co  Gas    1.001e+01  9.151e-01
     n2  Gas    4.684e+00  4.283e-01
     h2  Gas    3.853e+00  3.524e-01
    ch4  Gas    2.172e+00  1.986e-01
    h2o  Gas    3.401e-03  3.110e-04
    nh3  Gas    5.699e-03  5.211e-04
    co2  Gas    1.992e-03  1.821e-04
  hcooh  Gas    1.974e-07  1.805e-08
  ch3oh  Gas    2.654e-06  2.427e-07
    hcn  Gas    1.193e+00  1.091e-01
     no  Gas    2.809e-09  2.569e-10
     o2  Gas    4.187e-15  3.829e-16
    alo  Gas    8.214e-11  7.511e-12
     *c Solid   1.128e+01  1.032e+00
 *o3al2 Solid   3.706e+00  3.390e-01
    *al Liquid  0.000e+00  0.000e+00
   Total Gas    2.192e+01

Input> point, v, 50.0, s,

                        Reference state = reactants
              H(R) = H--62.73, E(R) = E--62.74, S(R) = S- 0.00

         P           V          T        H(R)       E(R)       S(R)      VGS
      (ATM)       (CC/GM)      (K)     (CAL/GM)   (CAL/GM) (CAL/K/GM) (CC/GM)
1.)    124.0      27.8[illegible]4   1800.0  -1016.28   -1100.02     1.465   27.7263

Product concentrations
         Name      (mol/kg)     (mol gas/mol explosive)
     co  Gas    1.001e+01  9.153e-01
     n2  Gas    4.862e+00  4.446e-01
     h2  Gas    4.016e+00  3.672e-01
    ch4  Gas    2.182e+00  1.995e-01
    hcn  Gas    8.391e-01  7.674e-02
    nh3  Gas    2.932e-03  2.681e-04
    h2o  Gas    1.915e-03  1.752e-04
    co2  Gas    1.295e-03  1.184e-04
  ch3oh  Gas    6.149e-07  5.623e-08
  hcooh  Gas    3.922e-08  3.587e-09
     no  Gas    2.644e-10  2.418e-11
    alo  Gas    1.858e-12  1.699e-13
     o2  Gas    1.217e-16  1.113e-17
     *c Solid   1.162e+01  1.063e+00
 *o3al2 Solid   3.706e+00  3.390e-01
    *al Liquid  0.000e+00  0.000e+00
   Total Gas    2.191e+01

Input> point, v, 100.0, s,

                        Reference state = reactants
              H(R) = H--62.73, E(R) = E--62.74, S(R) = S- 0.00
```

```
          P           V           T        H(R)       E(R)       S(R)      VGS
       (ATM)       (CC/GM)       (K)     (CAL/GM)   (CAL/GM) (CAL/K/GM) (CC/GM)
 1.)    55.5       55.7609    1666.5   -1079.95   -1154.86     1.465    55.6057

Product concentrations
         Name      (mol/kg)     (mol gas/mol explosive)
     co  Gas    1.001e+01   9.154e-01
     n2  Gas    4.990e+00   4.563e-01
     h2  Gas    4.076e+00   3.728e-01
    ch4  Gas    2.216e+00   2.027e-01
    hcn  Gas    5.846e-01   5.346e-02
    nh3  Gas    1.833e-03   1.676e-04
    h2o  Gas    1.338e-03   1.224e-04
    co2  Gas    1.037e-03   9.484e-05
  ch3oh  Gas    2.202e-07   2.014e-08
  hcooh  Gas    1.329e-08   1.215e-09
     no  Gas    4.439e-11   4.059e-12
    alo  Gas    7.930e-14   7.252e-15
     o2  Gas    8.779e-18   8.029e-19
     *c Solid   1.184e+01   1.083e+00
 *o3al2 Solid   3.706e+00   3.390e-01
    *al Liquid  0.000e+00   0.000e+00
  Total Gas     2.188e+01

Input> point, v, 200.0, s,

                        Reference state = reactants
              H(R) = H--62.73, E(R) = E--62.74, S(R) = S- 0.00

          P           V           T        H(R)       E(R)       S(R)      VGS
       (ATM)       (CC/GM)       (K)     (CAL/GM)   (CAL/GM) (CAL/K/GM) (CC/GM)
 1.)    25.2       111.5218   1545.0   -1136.24   -1204.35     1.465   111.3659

Product concentrations
         Name      (mol/kg)     (mol gas/mol explosive)
     co  Gas    1.001e+01   9.155e-01
     n2  Gas    5.092e+00   4.657e-01
     h2  Gas    4.055e+00   3.708e-01
    ch4  Gas    2.279e+00   2.084e-01
    hcn  Gas    3.807e-01   3.481e-02
    nh3  Gas    1.150e-03   1.052e-04
    h2o  Gas    9.708e-04   8.878e-05
    co2  Gas    8.935e-04   8.171e-05
  ch3oh  Gas    8.139e-08   7.443e-09
  hcooh  Gas    4.838e-09   4.424e-10
     no  Gas    6.993e-12   6.395e-13
    alo  Gas    2.440e-15   2.231e-16
     o2  Gas    5.957e-19   5.447e-20
     *c Solid   1.198e+01   1.096e+00
 *o3al2 Solid   3.706e+00   3.390e-01
    *al Liquid  0.000e+00   0.000e+00
  Total Gas     2.182e+01

Input> det energy, n, 1, t, 298
```

Reference state = reactants
H(R) = H--62.73, E(R) = E--62.74, S(R) = S- 0.00

	P (ATM)	V (CC/GM)	T (K)	H(R) (CAL/GM)	E(R) (CAL/GM)	S(R) (CAL/K/GM)	VGS (CC/GM)
1.)	1.0	1986.0038	1137.8	-1321.46	-1369.55	1.465	1985.8492

Product concentrations

Name		(mol/kg)	(mol gas/mol explosive)
co	Gas	1.001e+01	9.155e-01
n2	Gas	5.266e+00	4.815e-01
h2	Gas	3.086e+00	2.822e-01
ch4	Gas	2.851e+00	2.607e-01
hcn	Gas	3.502e-02	3.202e-03
co2	Gas	9.383e-04	8.581e-05
h2o	Gas	3.209e-04	2.934e-05
nh3	Gas	1.501e-04	1.373e-05
ch3oh	Gas	1.439e-09	1.316e-10
hcooh	Gas	1.169e-10	1.069e-11
no	Gas	1.178e-15	1.078e-16
alo	Gas	2.718e-23	2.485e-24
o2	Gas	2.527e-24	2.311e-25
*c	Solid	1.176e+01	1.075e+00
*o3al2	Solid	3.706e+00	3.390e-01
*al	Liquid	0.000e+00	0.000e+00
Total	Gas	2.125e+01	

Reference state = reactants
H(R) = H--62.73, E(R) = E--62.74, S(R) = S- 0.00

	P (ATM)	V (CC/GM)	T (K)	H(R) (CAL/GM)	E(R) (CAL/GM)	S(R) (CAL/K/GM)	VGS (CC/GM)
1.)	1.0	361.3808	298.0	-1788.04	-1796.78	0.785	361.2092

Product concentrations

Name		(mol/kg)	(mol gas/mol explosive)
n2	Gas	5.283e+00	4.831e-01
co2	Gas	5.007e+00	4.579e-01
ch4	Gas	4.403e+00	4.026e-01
co	Gas	7.135e-06	6.525e-07
h2o	Gas	6.837e-08	6.253e-09
h2	Gas	1.019e-08	9.318e-10
nh3	Gas	1.212e-10	1.108e-11
ch3oh	Gas	9.278e-20	8.485e-21
hcooh	Gas	8.658e-17	7.917e-18
hcn	Gas	2.463e-17	2.252e-18
no	Gas	0.000e+00	0.000e+00
o2	Gas	0.000e+00	0.000e+00
alo	Gas	0.000e+00	0.000e+00
*c	Solid	1.525e+01	1.394e+00
*o3al2	Solid	3.706e+00	3.390e-01
*al	Solid	0.000e+00	0.000e+00
Total	Gas	1.469e+01	

```
The mechanical energy of detonation =     -10.276 kJ/cc
The thermal energy of detonation    =      -3.206 kJ/cc
The total energy of detonation      =     -13.482 kJ/cc


Input> jwlfit, 7

JWL Fit results:
R[1] =       1.391, R[2] =       1.389, omega =       0.237
A    =   10000.000, B    =   -9964.565, C     =       1.396
Final fitting error = 0.095524

     V/V0      Actual E      Fit E     Actual P      Fit P
               (kJ/cc)      (kJ/cc)     (GPa)       (GPa)

     0.421       2.368       2.368      19.284      19.284
     2.200      -4.712      -6.087       1.231       0.206
     4.100      -5.953      -6.197       0.362       0.099
     6.500      -6.538      -6.505       0.168       0.127
    10.000      -7.020      -6.863       0.098       0.081
    20.000      -7.620      -7.380       0.039       0.034
    50.000      -8.254      -7.946       0.013       0.011
   100.000      -8.665      -8.299       0.006       0.005
Input> stop
```

The JWL fitting routine does poorly for Tritonal; giving a 9% error in the fit. This is because an aluminized explosive like tritonal has a slowly decreasing adiabat that is poorly fit by the JWL form. In this case the fitting routine has chosen the R_1 and R_2 terms so that they nearly cancel. More control over the fitting process can be obtained by using the stand-alone JWL fitter described in Section 7.1.

2.6 Constant volume explosion

The constant volume explosion command is used to describe a situation where an explosive sample is confined by a casing. The command gives the pressure and temperature obtained by the explosive, assuming that the casing holds for the timescale of chemical equilibration (usually for a microsecond or less). The constant volume explosion command can be used for a detonating or non-detonating material. The essential requirement for its use is the presence of an intact casing. There is sometimes confusion between the constant volume explosion state and the C-J state of a high explosive. The C-J state is a moving pressure pulse. Its energy is *higher* than that of the reactants. In other words shock energy is *absorbed* by the reactants at the C-J state. The constant volume explosion state is

stationary (non-propagating). It is at the same energy as the reactants. This is a thermodynamic consequence of containment by rigid insulating walls.

The `explosion` command is used to model constant volume explosion:

```
comp, petn, 100
explosion, rho, 1.60
units, v0
point, s, , v, 2.2
point, s, , v, 4.1
point, s, , v, 6.5
point, s, , v, 10.0
point, s, , v, 20.0
stop
```

The density `rho` given to the explosion command should be the weight of the explosive divided by the volume of the casing. The specific volume `v` can be given instead of density: `explosion, v, 0.80`. We do an adiabatic expansion of the constant volume explosion state to model what happens when the casing fails. The constant volume adiabat is different from the C-J adiabat, however, so the results should not be used in hydrodynamic modeling of detonation.

The output file is:

```
Library Title: llnl bkwr
Input from startup.in> ## These are startup commands, which are
Input from startup.in> ## run before every cheetah job.
Input from startup.in> gas eos, bkw
Input from startup.in> set, bkw, alpha, 0.5
Input from startup.in> set, bkw, beta, 0.176
Input from startup.in> set, bkw, kappa, 11.80
Input from startup.in> set, bkw, theta, 1850
Input from startup.in>
Input from startup.in>
Input from startup.in>
Input>
Input> comp, petn, 100
Reactant library title:LLNL CHEETAH Reactant Library V1.01

                                The Composition

Name       % wt.    % mol  Heat of    Standard      Standard      Mol.    Formula
                           formation   volume        entropy       wt.
                           (cal/mol)   (cc/mol)      (cal/K/mol)
petn       100.00 100.00  -128700     177.61        0.000       316.15  c5h8n4o12

Heat of formation =    -407.090 cal/gm
Standard volume   =       0.562 cc/gm
Standard entropy  =       0.000 cal/k/gm
Standard energy   =    -407.104 cal/gm

The elements and percent by mole
     c              17.241
     h              27.586
```

```
     n              13.793
     o              41.379
The average mol. wt. = 316.146 g/mol


Input> explosion, rho, 1.60


The Constant Volume Explosion State:

                          Reference state = reactants
               H(R) = H--407.09, E(R) = E--407.10, S(R) = S- 0.00


         P           V          T       H(R)       E(R)       S(R)      VGS
      (ATM)       (CC/GM)      (K)    (CAL/GM)   (CAL/GM) (CAL/K/GM) (CC/GM)
 1.)  120651.8      0.6250   3196.2    1826.21       0.00     1.679    0.6250

Product concentrations
         Name      (mol/kg)     (mol gas/mol explosive)
    co2  Gas    1.070e+01   3.383e+00
    h2o  Gas    1.036e+01   3.274e+00
     n2  Gas    6.149e+00   1.944e+00
     co  Gas    3.935e+00   1.244e+00
  hcooh  Gas    1.127e+00   3.563e-01
     h2  Gas    5.336e-01   1.687e-01
    nh3  Gas    3.531e-01   1.116e-01
    ch4  Gas    4.607e-02   1.456e-02
  ch3oh  Gas    6.273e-03   1.983e-03
     no  Gas    1.563e-03   4.942e-04
     o2  Gas    3.634e-05   1.149e-05
    hcn  Gas    1.969e-05   6.225e-06
     *c Solid   0.000e+00   0.000e+00
  Total Gas     3.321e+01


Input> units, v0
Input> point, s,, v, 2.2


                          Reference state = reactants
               H(R) = H--407.09, E(R) = E--407.10, S(R) = S- 0.00


         P           V          T       H(R)       E(R)       S(R)      VGS
      (ATM)       (CC/GM)      (K)    (CAL/GM)   (CAL/GM) (CAL/K/GM) (CC/GM)
 1.)     10.3     171.6000    660.5   -1397.61   -1440.26     1.679  171.6000

Product concentrations
         Name      (mol/kg)     (mol gas/mol explosive)
    co2  Gas    1.431e+01   4.523e+00
    h2o  Gas    9.296e+00   2.939e+00
     n2  Gas    6.324e+00   1.999e+00
    ch4  Gas    1.462e+00   4.622e-01
     h2  Gas    4.266e-01   1.349e-01
     co  Gas    4.641e-02   1.467e-02
    nh3  Gas    3.614e-03   1.142e-03
  hcooh  Gas    8.130e-07   2.570e-07
```

```
  ch3oh  Gas    1.639e-08  5.180e-09
    hcn  Gas    2.469e-09  7.804e-10
     no  Gas    6.625e-22  2.094e-22
     o2  Gas    6.632e-31  2.097e-31
     *c Solid   0.000e+00  0.000e+00
  Total Gas     3.187e+01

Input> point, s,, v, 4.1

                        Reference state = reactants
              H(R) = H--407.09, E(R) = E--407.10, S(R) = S- 0.00

         P          V          T       H(R)       E(R)       S(R)      VGS
      (ATM)      (CC/GM)      (K)    (CAL/GM)   (CAL/GM) (CAL/K/GM) (CC/GM)
1.)     4.7     319.8000    574.1   -1428.33   -1464.91     1.679  319.8000

Product concentrations
        Name      (mol/kg)    (mol gas/mol explosive)
    co2  Gas    1.428e+01  4.513e+00
    h2o  Gas    9.398e+00  2.971e+00
     n2  Gas    6.325e+00  2.000e+00
    ch4  Gas    1.533e+00  4.845e-01
     h2  Gas    1.861e-01  5.883e-02
     co  Gas    6.955e-03  2.199e-03
    nh3  Gas    1.989e-03  6.288e-04
  hcooh  Gas    1.231e-07  3.892e-08
  ch3oh  Gas    1.570e-09  4.962e-10
    hcn  Gas    4.973e-11  1.572e-11
     no  Gas    2.303e-25  7.282e-2[illegible]
     o2  Gas    1.132e-35  3.580e-36
     *c Solid   0.000e+00  0.000e+00
  Total Gas     3.173e+01

Input> point, s,, v, 6.5

                        Reference state = reactants
              H(R) = H--407.09, E(R) = E--407.10, S(R) = S- 0.00

         P          V          T       H(R)       E(R)       S(R)      VGS
      (ATM)      (CC/GM)      (K)    (CAL/GM)   (CAL/GM) (CAL/K/GM) (CC/GM)
1.)     2.6     507.0000    511.6   -1448.39   -1480.80     1.679  507.0000

Product concentrations
        Name      (mol/kg)    (mol gas/mol explosive)
    co2  Gas    1.425e+01  4.506e+00
    h2o  Gas    9.449e+00  2.987e+00
     n2  Gas    6.326e+00  2.000e+00
    ch4  Gas    1.561e+00  4.934e-01
     h2  Gas    8.084e-02  2.556e-02
     co  Gas    1.099e-03  3.473e-04
    nh3  Gas    1.166e-03  3.685e-04
  hcooh  Gas    2.254e-08  7.126e-09
```

```
  ch3oh  Gas    1.834e-10  5.799e-11
    hcn  Gas    1.246e-12  3.941e-13
     no  Gas    1.365e-28  4.317e-29
     o2  Gas    4.041e-40  1.278e-40
     *c Solid   0.000e+00  0.000e+00
  Total Gas     3.167e+01

Input> point, s,, v, 10.0

                        Reference state = reactants
              H(R) = H--407.09, E(R) = E--407.10, S(R) = S- 0.00

         P           V          T       H(R)       E(R)       S(R)      VGS
       (ATM)       (CC/GM)      (K)    (CAL/GM)   (CAL/GM) (CAL/K/GM) (CC/GM)
1.)      1.5     780.0000     455.6   -1465.21   -1493.98     1.679  780.0000

Product concentrations
         Name      (mol/kg)     (mol gas/mol explosive)
    co2  Gas    1.424e+01  4.502e+00
    h2o  Gas    9.474e+00  2.995e+00
     n2  Gas    6.326e+00  2.000e+00
    ch4  Gas    1.574e+00  4.975e-01
     h2  Gas    3.027e-02  9.568e-03
     co  Gas    1.293e-04  4.086e-05
    nh3  Gas    6.490e-04  2.052e-04
  hcooh  Gas    3.465e-09  1.095e-09
  ch3oh  Gas    1.676e-11  5.297e-12
    hcn  Gas    1.880e-14  5.942e-15
     no  Gas    3.038e-32  9.604e-33
     o2  Gas    0.000e+00  0.000e+00
     *c Solid   0.000e+00  0.000e+00
  Total Gas     3.165e+01

Input> point, s,, v, 20.0

                        Reference state = reactants
              H(R) = H--407.09, E(R) = E--407.10, S(R) = S- 0.00

         P           V          T       H(R)       E(R)       S(R)      VGS
       (ATM)       (CC/GM)      (K)    (CAL/GM)   (CAL/GM) (CAL/K/GM) (CC/GM)
1.)      0.6    1560.0000     372.4   -1488.59   -1512.04     1.679 1560.0000

Product concentrations
         Name      (mol/kg)     (mol gas/mol explosive)
    co2  Gas    1.423e+01  4.500e+00
    h2o  Gas    9.487e+00  2.999e+00
     n2  Gas    6.326e+00  2.000e+00
    ch4  Gas    1.581e+00  4.997e-01
     h2  Gas    3.835e-03  1.212e-03
    nh3  Gas    2.057e-04  6.503e-05
     co  Gas    1.501e-06  4.746e-07
  hcooh  Gas    8.411e-11  2.659e-11
```

```
  ch3oh  Gas    1.391e-13  4.399e-14
    hcn  Gas    3.558e-18  1.125e-18
     no  Gas    1.097e-39  3.467e-40
     o2  Gas    0.000e+00  0.000e+00
     *c Solid   0.000e+00  0.000e+00
  Total Gas     3.163e+01

Input> stop
```

2.7 Customizing the standard run

Clark Souers has standardized LLNL operating procedures for running thermochemical codes. The `standard run` is a distillation of this procedure. The C-J point is calculated, then adiabat points are found at relative volumes of 2.2, 4.1, 6.5, 10, and 20. The concentrations are frozen along the adiabat at a prescribed temperature (1800K is used for the BKWR[5] equation of state). Finally the energy of detonation is found. In this section we will look at how to customize the standard run to match operating procedures at your site.

The standard run is controlled by the file `config/standard.in`. Here is the default LLNL `standard.in`

```
5
2.2
4.1
6.5
10.0
20.0
1800.0
1
```

The first line is the number of points to calculate along the adiabat. In this case 5 adiabat points are specified. The next 5 numbers are the relative volumes. Following this is the freezing temperature. The last 1 indicates that a JWL equation of state should be produced from this set of points along the adiabat.

As an example, suppose that we have interest in the shape of the adiabat at very large volumes. Aluminized explosives, for example, have adiabats with long "tails". An appropriate set of points might be relative volumes of 2.2, 4.1, 6.5, 10, 20, 50, 100, 200. Freezing can be turned off by setting the freeze temperature to 0K. Finally, let's forego the JWL fitting step. The `standard.in` file that implements this is:

```
8
2.2
4.1
6.5
10.0
20.0
50.0
100.0
200.0
0.0
0
```

Here is the summary sheet for a calculation on PETN with the new `standard.in`:

```
################################################################################
#                                                                              #
#                          CHEETAH 1.0 SUMMARY SHEET                           #
#                          Energetic Materials Center                          #
#                     Lawrence Livermore National Laboratory                   #
#                     Technical Contact: Dr. Laurence E. Fried                 #
#                   Copyright 1994, Regents University of California           #
#                                All Rights Reserved                           #
#                                                                              #
################################################################################

Product library title: llnl bkwr
BKW eos used: alpha=  0.500, beta=  0.100 kappa= 11.850 theta=  400.0

Reactant library title: LLNL CHEETAH Reactant Library V1.01


The composition:
Name       % wt.    % mol  Heat of      Standard      Mol.    TMD
                           formation     volume        wt.     (g/cc)
                           (cal/mol)     (cc/mol)
petn       100.00 100.00  -128700      177.61      316.15    1.78

Density  =   1.763 g/cc   Mixture TMD =   1.780 g/cc   % TMD =  99.045


The C-J condition:
The pressure          =          31.00 GPa
The volume            =          0.423 cc/g
The density           =          2.361 g/cc
The energy            =           3.93 kJ/cc explosive
The temperature       =           3338 K
The shock velocity    =          8.330 mm/us
The particle velocity =          2.111 mm/us
The speed of sound    =          6.219 mm/us
Gamma                 =          2.946


Cylinder runs:                  % of standards
  V/V0      V        Energy    TATB     PETN      HMX   TRITON  half-wall Full-wall
 (rel.)   (cc/g)    (kJ/cc)  1.83g/cc  1.76      1.89    1.70   v (mm/us)  v (mm/us)
   2.20    1.25     -7.30      143      100       86      154     2.09       1.58
   4.10    2.33     -8.83      148      100       88      148     2.28       1.72
   6.50    3.69     -9.44      151      101       89      144     2.39       1.78
```

```
  10.00    5.67    -9.82    153     101      90     140
  20.00   11.34   -10.25
  50.00   28.36   -10.63
 100.00   56.72   -10.85
 200.00  113.44   -11.02

The mechanical energy of detonation =    -11.265 kJ/cc
The thermal energy of detonation    =      0.000 kJ/cc
The total energy of detonation      =    -11.265 kJ/cc
```

2.8 Customizing the summary sheet

The summary sheet is customizable. In particular, the number of points along the adiabat and the explosives which are used as standards can be modified. In the previous section we modified the standard run to calculate points at large expansion volumes. It is also convenient to compare the adiabat at large volumes to our standard explosives.

The form of the summary file is controlled by `config/summary.in`. The default `summary.in` is:

```
4
5
2.2
4.1
6.5
10.0
20.0
TATB
1.83
 -5.66
 -6.71
 -7.08
 -7.29
 -7.51
PETN
1.76
 -7.28
 -8.81
 -9.41
 -9.80
-10.23
HMX
1.89
  -8.51
 -10.12
 -10.69
 -11.02
 -11.36
TRITON
```

```
1.70
 -4.27
 -5.43
 -5.98
 -6.44
 -7.02
3
2.09 1.58 -7.30
2.28 1.72 -8.81
2.38 1.78 -9.39
```

The first line contains the number of standards to compare to, and the number of adiabat volumes to calculate. The relative value of the volume for each adiabat point is given next. For each standard a name line is given, followed by a standard value for the adiabat energy in kJ/cc. Finally we give the number of reference half and full wall velocities, and the square of the standard wall velocity in mm/μs divided by the adiabat energy in kJ/cc .

As an example, we will set up CHEETAH so that comparisons to the standards are made at relative volumes of 50, 100, and 200 in addition to the volumes in the default setup. The first question is: where do we get the adiabat energies for the standards ? There are two possible answers to the question. The results of cylinder tests can be used to obtain experimental adiabat energies. The problem here, however, is that calculated adiabat energies do not exactly match the experimental energies. This can lead to an apparent self-consistency problem: a calculation of HMX is not reported to have 100% the performance of HMX because the calculated adiabat energy is not equal to the experimental adiabat energy. This can be quite confusing to the novice.

Therefore, we use theoretical adiabat energies obtained from CHEETAH. One must be careful, however, when switching between various equations of state or parametrizations. Strictly speaking, you should change the `summary.in` file to match the equation of state and parameter values that you use. Then comparisons reported by CHEETAH will be self-consistent.

The new `summary.in` file is as follows, with results derived from the BKWR[5] equation of state:

```
4
8
2.2
4.1
6.5
10.0
20.0
```

```
50.0
100.0
200.0
TATB
1.83
 -5.66
 -6.71
 -7.08
 -7.29
 -7.51
 -7.68
 -7.77
 -7.83
PETN
1.76
 -7.28
 -8.81
 -9.41
 -9.80
-10.23
-10.61
-10.82
-11.00
HMX
1.89
  -8.51
 -10.12
 -10.69
 -11.02
 -11.36
 -11.62
 -11.76
 -11.85
TRITON
1.70
 -4.27
 -5.43
 -5.98
 -6.44
 -7.02
 -7.64
 -8.04
 -8.40
3
2.09 1.58 -7.30
2.28 1.72 -8.81
2.38 1.78 -9.39
```

The new summary sheet for a run of 80% HMX and 20% Al at TMD is as follows:

```
################################################################################
#                                                                              #
#                        CHEETAH 1.0 SUMMARY SHEET                             #
#                        Energetic Materials Center                            #
#                  Lawrence Livermore National Laboratory                      #
#                  Technical Contact: Dr. Laurence E. Fried                    #
#               Copyright 1994, Regents University of California               #
#                           All Rights Reserved                                #
```

```
#                                                                              #
################################################################################

Product library title: llnl bkwr
BKW eos used: alpha=  0.500, beta=  0.100 kappa= 11.850 theta=  400.0

Reactant library title: LLNL CHEETAH Reactant Library V1.01


The composition:
Name      % wt.   % mol  Heat of      Standard      Mol.    TMD
                         formation     volume        wt.     (g/cc)
                         (cal/mol)     (cc/mol)
hmx        80.00  26.71    17930      155.46      296.17   1.91
al         20.00  73.29        0        9.98       26.98   2.70

Density  =   2.025 g/cc   Mixture TMD =   2.025 g/cc   % TMD = 100.000


The C-J condition:
The pressure          =          35.79 GPa
The volume            =          0.381 cc/g
The density           =          2.622 g/cc
The energy            =           4.08 kJ/cc explosive
The temperature       =           4716 K
The shock velocity    =          8.809 mm/us
The particle velocity =          2.007 mm/us
The speed of sound    =          6.802 mm/us
Gamma                 =          3.389


Cylinder runs:              % of standards
  V/V0      Energy     TATB      PETN       HMX    TRITON  Half-wall Full-wall
 (rel.)    (kJ/cc)  1.83g/cc  1.76g/cc  1.89g/cc  1.70g/cc  v (mm/us)  v (mm/us)
   2.20     -8.57      151       118       101       201     2.26       1.71
   4.10    -10.65      159       121       105       196     2.51       1.89
   6.50    -11.61      164       123       109       194     2.65       1.98
  10.00    -12.25      168       125       111       190
  20.00    -13.01      173       127       115       185
  50.00    -13.75      179       130       118       180
 100.00    -14.21      183       131       121       177
 200.00    -14.60      186       133       123       174

The mechanical energy of detonation =    -15.855 kJ/cc
The thermal energy of detonation    =     -2.216 kJ/cc
The total energy of detonation      =    -18.071 kJ/cc
```

Note that the use of very large adiabat volumes is important in evaluating the change brought about by incorporating Al into HMX.

2.9 Customizing the startup file

The commands in `config/startup.in` are executed at the beginning of every CHEETAH run. Most commonly, equation of state parameters are set in the startup file. This ensures that all subsequent runs use the same equation of state parameters. The following `startup.in` file sets parameters for the BKWR[5] equation of state:

```
gas eos, bkw
set, bkw, alpha, 0.5
set, bkw, beta, 0.176
set, bkw, kappa, 11.80
set, bkw, theta, 1850
```

If the Sandia library[?] is used, however, the appropriate parameters in `startup.in` would have to be changed. Alternatively, the BKWR[5] startup file could be used and the Sandia parameters could be set in every input file. The startup file also sets the default gaseous equation of state. If we were performing a series of ideal gas calculations, the line `gas eos, ideal` could be the entire `startup.in`.

Other defaults can be set in the `startup.in`. Here's a fancier version:

```
gas eos, bkw
set, bkw, alpha, 0.5
set, bkw, beta, 0.176
set, bkw, kappa, 11.80
set, bkw, theta, 1850
summary, myfile.sum
spreadsheet, myfile.spr, p, v, t, co2
library file, bkwr.chl
units, v, v0
```

This file sets parameters appropriate for the BKWR[5] equation of state; sets the summary sheet to be `myfile.sum` instead of the default `summary.out`; outputs the pressure, volume, temperature, and co2 concentration of every thermodynamic point into a spreadsheet file; sets the default library file to be BKWR; and specifies that all volumes will be input relative to the initial explosive volume.

Section 3
Reference

CHEETAH accepts a large number of commands. The syntax of a CHEETAH command is:
command, *arg1*, *arg2*, *arg3*, . . .
Here *command* is the command name. Command names may be abbreviated to the smallest number of significant characters sufficient to resolve the command. In most cases a three character abbreviation will suffice. In some cases, however, more characters will be required. A command and its arguments are separated by commas. Arguments may be character strings or numerical values. Numerical values may be entered in either integer (e.g. 6) or floating point (6.0) format. Many CHEETAH commands interpret a blank argument to mean the current value of a variable. For instance,

```
units, v, 10.0
```

instructs CHEETAH to set the input unit of volume to 5 cc/gm. The command

```
units, v,
```

instructs CHEETAH to set the input unit of volume to be the current value of the volume. Subsequent volumes will then be relative to the current volume. Care should be taken in using blank arguments. For instance, the command

```
units, v
```

will produce an error message because the missing comma means that no second argument was given to the `units` command.

An & functions as a continuation character:

```
units, v, &
10
```

is valid input. This is helpful when entering long input lines. The # is a comment character. Any line beginning with # is treated as a comment by CHEETAH.

In Table 3.1 we have grouped CHEETAH's commands according to function. Next we give a list of all commands accepted by CHEETAH.

Run type selection	
c-j point	calculates the C-J point
det energy	Finds the energy of detonation.
explosion	Does a constant volume explosion calculation.
hug0	Defines the reference state of the shock Hugoniot.
grid	Calculates a grid of states.
isoline	Calculates a series of thermodynamic states.
mixed phase	Determines the mixed phase line for a condensed product.
point	Calculates a single thermodynamic state.
standard run	Calculates the C-J state and adiabat.
stop	Stops CHEETAH execution.
Product library	
card list	Turns on listing of library input.
constituent	Enters a new product species into the library.
element	Enters into the product library an element.
end of library	Denotes the end of the product library.
library file	Specify a compiled library file to use.
start of library	Denotes the beginning of the library commands.
stc	Enters the condensed equation of state name and constants.
stg	Enters constants necessary for the gaseous equation of state.
str	Enters the reference state constants.
Input/output	
details	Produces more detailed thermodynamic output.
load file	Executes the commands in the given file.
original output	Thermodynamic potentials are output as "raw" values.
print selection	To suppress or turn on printing of product concentrations.
reactants reaction	Makes CHEETAH report thermodynamic energies relative to the reactants.
spreadsheet	Saves variables into a file that is readable by a spreadsheet program.
summary	Sets the name of the summary file.
title	Gives a title to the current job.
units	Sets the input units of a specified quantity.
Product species	
choose	Selects which product species to use.
destroy	Overrides the retain command.
fix concentration	Fixes the concentration of specified products.
freeze	Freezes the concentrations of specified products to their current values.
melt	Undoes a freeze command.
order	Rearranges the ordering of gaseous products that have not been rejected.
reject	Prevents the specified products from being used in the calculation.
retain	Maintains the effects of the product selection commands.
Reactant species	
composition	Specifies the chemical composition of the reactants.
formula	Specifies the thermodynamic properties of a reactant.
Gaseous equation of state	
gas eos	Determines the gaseous equation of state.
set	Fixes equation of state parameters to specified values.
Miscellaneous	
jwlfit	Fits an adiabat calculated with CHEETAH to a JWL equation of state.
recall point	Recalls a point that has been saved.
save point	The current thermodynamic state is saved for later use.

Table 3.1: CHEETAH commands grouped by subject

3.1 c-j point

Purpose: Calculates the C-J point after the shock Hugoniot has been specified.

Syntax: c-j point
c-j point, *pmax*
c-j point, *pmax*, *pmin*
The C-J point is found by solving for the intersection of the Rayleigh line and the shock Hugoniot. If desired, an upper bound for the C-J pressure may be supplied by entering *pmax*. By default, the lower bound for the C-J pressure is the pressure at the constant volume explosion point. This can be changed by entering both *pmax* and *pmin*.

Example: The C-J point of PETN at 1 atm and a density of 1.763 g/cc is calculated.

```
comp, petn, 100
hug0, p, 1, rho, 1.763
c-j point
```

3.2 card list

Purpose: Turns on listing of library input. This does not occur by default.

Syntax: card list

3.3 choose

Purpose: The `choose` command allows the user to select which product species (call constituents in CHEETAH) will be used in the calculation. The product species can be either condensed or gaseous. Without the `choose` command, all possible products in the current library are used. The effect of the `choose` command is undone at the next `composition` command unless the `retain` command is used

Syntax: choose, *c1*, *c2*, ...
c1, *c2* are the names of product species.

Example: The standard state of reacted PETN with only H2, C02, N2, and O2 as products is calculated.

```
comp, petn, 100
choose, h2, co2, n2, o2
point, p, 1, t, 298
```

3.4 composition

Purpose: Specifies the chemical composition of the reactants.

Syntax: composition, *name1*, *f1*, *name2*, *f2*, mol
Names and fractions are given. The fractions are by weight, except if `mol` is given as the last argument, in which case mol fractions are given. The fractions do not have to add to 100 %.

Example: A mixture of 80 % TNT and 20 % Al is specified:

```
composition, tnt, 8, al, 2
```

3.5 constituent

Purpose: Enters a new product species into the library.

Syntax: constituent, *name*, *type*, *el*, *nl*, . . .
name is the name of the product (called a constituent in TIGER's language). *type* is either `gas` or `condensed`. *el* is an element name. *nl* is the number of atoms of element *el* in the chemical formula. The constituent command must be followed by the `str` and `stc` commands to make a complete definition.

Example: H2O is defined in the product library.

```
constituent, h2o, gas, h, 2, o, 1
```

3.6 destroy

Purpose: The `destroy` command overrides the `retain` command. After the `destroy` command the effects of `reject`, `order`, and `choose` are lost at the next specification of `composition`

Syntax: destroy

Example: A calculation of HMX and TATB is done first with a few selected products, then with all product species in the library

```
choose, co2, h2, h2o, n2, nh3
retain
# The chosen products are retained for subsequent runs.
comp, hmx, 100
point, p, 100000, t, 1000
comp, tatb, 100
point, p, 100000, t, 1000
# Retain is turned off.  All possible products will be selected.
destroy
```

```
comp, hmx, 100
point, p, 100000, t, 1000
comp, tatb, 100
point, p, 100000, t, 1000
```

3.7 det energy

Purpose: Finds the energy of detonation

Syntax: det energy, p, *x1*, t, *x2*
x1 is the value of the pressure at standard state (usually 1 atm), and *x2* is the value of the temperature at standard state (usually 298K).

This command evaluates the total amount of energy available in the detonation process. The `det energy` command must be used while on the C-J adiabat. It reports two energies of detonation; a mechanical energy of detonation given by the endpoint of and adiabat, and a thermal energy of detonation – which is the amount of energy tied up in heat at the endpoint of the adiabat. The mechanical energy of detonation is the amount of energy available to do pV work. The total energy of detonation is the sum of the mechanical and the thermal energy of detonation; it is equal to the energy at 298 K and 1 atm. The decomposition of the adiabat energy into thermal and mechanical parts can be important. Highly aluminized explosives (30 % Al) typically have a mechanical energy of detonation that is only one half the total energy of detonation. This means that 1/2 of the energy of such formulations is wasted (unless reactions with the environment are possible).

Example: The energy of detonation of TATB is calculated.

```
comp, tatb, 100
hug0, p, 1, sv
c-j point
isoline, s, , v, , 10, 10.0
det energy, p, 1, t, 298
```

3.8 details

Purpose: The `details` command produces more detailed thermodynamic output.

Syntax: details

After the `details` command, the following information is shown: the constant volume heat capacity, the hydrodynamic constants $\alpha, \beta, and \kappa$. κ was called ADEXP in TIGER.

The definitions are as follows:

$$C_V \equiv (\frac{\partial e}{\partial T})_V \tag{3.1}$$

$$\alpha \equiv \frac{1}{p}(\frac{\partial e}{\partial v})_p \tag{3.2}$$

$$\beta \equiv \frac{1}{v}(\frac{\partial e}{\partial p})_v \tag{3.3}$$

$$\kappa \equiv -(\frac{\partial \ln p}{\partial \ln v})_s = \frac{\alpha + 1}{\beta} \tag{3.4}$$

Example: The constant volume heat capacity is calculated along the C-J isentrope of HNB

```
comp, hnb, 1
details
hug0, p, 1, sv
c-j point
isoline, s, , v, , 10, 100
```

3.9 element

Purpose: Enters an element into the product library.

Syntax: element, *name*, *wt*, *name*, *nmol*, V, *vol*, S, *ent*
name is the name of the element. It is repeated twice for compatibility with TIGER. *wt* is the atomic weight of the element. *nmol* is the number of atoms per molecule of the element in its standard state. *vol* is the specific volume of the standard state in cc/mole. *ent* is the specific entropy of the standard state in calories/mole/degree.

Example: Carbon is defined in the library.

```
element, c, 12.01, c, 1, v, 27.02, s, 1.359
```

3.10 end of library

Purpose: Denotes the end of the product library.

Syntax: end of library

3.11 explosion

Purpose: Does a constant volume explosion calculation.
A constant volume explosion calculation describes a confined quantity of explosion that has undergone complete chemical reaction, whether through combustion or confined detonation.

Syntax: explosion, v, *x*

Syntax: explosion, rho, *x*

Example: 100 g of TNT is contained in a 200 cc vessel. The explosion command gives pressure and temperature of the vessel after the TNT is ignited.

```
comp, tnt, 100
explos, v, 2.0
```

3.12 fix concentration

Purpose: This command fixes the concentration of specified products

Syntax: fix concentration, *c1*, *x1*, *c2*, *x2*, . . .
c1, *c2*, etc. are the names of product species. *x1*, *x2*, etc. is the mass fraction of the product species expressed in grams/kg of the total mixture

Example: The C-J state of tritonal with unreacted aluminum is found.

```
comp, tnt, 80, al, 20
fixcon, al, 200
hug0, p, 1, sv
c-j
```

The `al` in the fixcon command is different from the `al` in the `comp` command. In the `comp` command we are referring to a reactant named `al`. In the `fixcon` command we are referring to a product named `al`. Of course, sane naming conventions require that both should be aluminum metal.

3.13 formula

Purpose: The chemical composition and thermodynamic properties of a reactant is specified
This command is usually found in the reactant library, although it can be entered directly in the input file. Use of the `formula` command in the input file disables use of the reactant library.

Syntax: formula, *name*, *hof*, *mvol*, *sof*, *el*, *nl*, ...
Here *name* is the name of the reactant. *hof* is the heat of formation in calories/mole, *mvol* is the standard molar volume in cc/mole, *sof* is the standard molar entropy in calories/mole/degree. Finally the chemical formula is given as a series of elements and stoichiometric coefficients.

Example: PETN is defined.

```
for, petn, -128700., 177.61, 0., c, 5, h, 8, n, 4, o, 12
```

3.14 freeze

Purpose: The concentrations of specified products are frozen to their current values. With no arguments all concentrations are frozen.

Syntax: freeze, *name1*, *name2*, ...

Example: Concentrations along the adiabat are frozen at the C-J point of TNT.

```
comp, tnt, 100
units, sv
hug0, p, 1, v, 1
c-j point
freeze
```

```
isoline, s, , v, 2, 10, 20
```

3.15 gas eos

Purpose: Determines the gaseous equation of state.

Syntax: gas eos, *eosname*
eosname is the name of the equation of state. Choices are `ideal`, `bkw`[4], or `jcz3`[6].

Example: The BKW[4] equation of state is specified.

```
gas eos, bkw
```

3.16 grid

Purpose: Calculates a grid of states centered about or cornered at a specific point

Syntax: grid, center, *q1*, *x1*, *d1*, *n1*, *q2*, *x2*, *d2*, *n2*
grid, corner, *q1*, *x1*, *d1*, *x2*, *q2*, *y1*, *d2*, *y2*
In the first form a grid of points formed of thermodynamic variables *q1*, *q2* is calculated. *q1* and *q2* may be any two variables chosen from the list (P,V,T,H,S,E,G,Hugoniot,A). The center of the grid is at values *x1*, *x2*. The grid step sizes are *d1* and *d2*, respectively. The number of steps to take in either direction are *n1* and *n2*.

In the second form a grid of points is calculated by specifying two corners. *x1* and *y1* define one corner, while *x2* and *y2* define the other. *d1* and *d2* are the step sizes to take in each direction.

Example: Generate a p-v grid for p ranging from 1600 to 2400 atm in steps of 50 and for v ranging from 0.8 to 1.2 cc/gm in steps of 0.05. This is done twice, once

with the `center` variant and once with the `corner` variant. The results are the same.

```
comp, petn, 100
grid, center, p, 2000, 50, 8, v, 1, 0.05, 4
grid, corner, p, 1600, 50, 2400, v, 0.8, 0.05, 1.2
```

3.17 hug0

Purpose: Defines the reference state of the shock Hugoniot.

Syntax:
hug0, p, *x1*, v, *x2*
hug0, p, *x1*, rho, *x2*
hug0, p, *x1*, sv,
hug0, p, *x1*, v, *x2*, eof
hug0, p, *x1*, v, *x2*, e, *x3*

If only p,v (or equivalently p, ρ) are specified, the energy E_0 in the Hugoniot is taken to be the energy of the explosive in its standard state. In the second example, the `sv` argument indicates that the explosive is initially at its standard volume. In the third example the energy of the reference state is set to be the energy of formation of the explosive. This is also done automatically if no energy arguments are given. In the fourth example, the E_0 value is directly specified.

Example: The shock Hugoniot of HNB is calculated.

```
comp, hnb, 100
hug0, p, 1, sv
isoline, p, 1000, 20, 100000
```

3.18 isoline

Purpose: Calculates a series of thermodynamic states.

Syntax: isoline, *Q1*, *x1*, *Q2*, *x2*, *nsteps*, *x3*
isoline, *Q1*, *x1*, *Q2*, *x2*, *nsteps*, *x3*, log
Here *Q1* is a thermodynamic variable chosen from the list (P,V,T,H,S,E,G,Hugoniot,A). States will be calculated with *Q1* = *x1*. The second thermodynamic variable *Q2*, again chosen from the above list, will be varied from *x2* to *x3* in *nsteps* steps. If log is specified, equal logarithmic steps are taken.

Example: The C-J isentrope of TATB is calculated

```
comp, tatb, 100
hug0, p, 1, v, sv
c-j point
isoline, s, , v, , 10, 100.0
```

3.19 jwlfit

Purpose: Fits an adiabat calculated with CHEETAH to a JWL equation of state.

Syntax: jwlfit, *npoints*
npoints is the number of points on the adiabat to use in the JWL fit. If this argument is omitted, all previous adiabat points are used in the fit. At least three points along the adiabat are required. The `jwlfit` command must be proceeded by the `det energy` command.

Example: The adiabat of HMX is fit to a JWL equation of state using 4 points

```
comp, hmx, 100
```

```
hug0, p, 1, sv
c-j
point, s, , v, 1.247
point, s, , t, 1800.0
freeze
point, s, , v, 2.325
point, s, , v, 3.687
point, s, , v, 5.672
point, s, , v, 11.344
det energy, p, 1.0, t, 298.0
jwlfit, 4
```

3.20 library file

Purpose: Specify a compiled library file to use

Syntax: library file, *filename*
CHEETAH can keep track of more than one pre-compiled library file at a time through the use of the `library file` command. This command needs to be used twice. First, it should be inserted into the top of the input file describing the library. This will save the library into the named file instead of the default `cheetah.chl` file. Secondly, the `library file` command is used to load the named library at the beginning of the normal input file. It is often convenient to put this command in the `startup.in` file, since it is likely to be used repeatedly. Library files are conventionally named with the `.chl` suffix.

Example: Two runs are performed, one with the BKWR[5] equation of state, the other with the BKWS[?] equation of state

```
libary file, bkwr.chl
comp, petn, 100
standard run, rho, 1.763
```

```
library file, bkws.chl
comp, petn, 100
standard run, rho, 1.763
```

3.21 load file

Purpose: The commands in the given file will be executed. This provides a simple macro facility.

Syntax: load file, *filename*
filename is the name of the file containing input commands.

3.22 melt

Purpose: Undoes a freeze command.

Syntax: melt, *c1*, *c2*, ...
c1, *c2* are the names of products. With no arguments `melt` unfreezes the concentrations of all products.

Example: A calculation of the C-J isentrope of PETN is done with and without freezing at 1800K

```
comp, petn, 100
hug0, p, 1, sv
c-j point
point, s, , t, 1800
freeze
isoline, s, , v, 5.0, 10, 20.0
melt
```

```
isoline, s, , v, 5.0, 10, 20.0
```

3.23 mixed phase

Purpose: To determine the mixed phase line for a particular condensed product in the pressure-temperature plane, or the corresponding mixed phase region in the pressure-volume plane

Syntax: mixed, *c1*, *q1*, *x1*, *d1*, *x2*
mixed, *c1*, *q1*, *x1*, *d1*, *x2*, points
c1 is the name of a condensed product. *q1* is either `P` or `T`. *x1* is the starting value of *q1*, *d1* is the increment, and *x2* is the final value. In the second form, the `points` argument specifies that phase boundaries in the pressure-volume plane are required.

Example: The solid-liquid phase boundary of Al2O3 is calculated from 10 to 100 atm in steps of 5 atm

```
mix, al2o3, p, 10, 5, 100
```

3.24 order

Purpose: To rearrange the ordering of gaseous products that have not been rejected so that those most likely to be accepted as components will be tried first. Components are products that serve to describe the stoichiometry in CHEETAH. This subroutine should only be used when the program has failed to find an acceptable set of components.

Syntax: order, *c1*, *c2*, *c3*
c1, *c2*, *c3* are the names of gaseous products.

Example: Try H20 as the first component, then CO2

```
order, h2o, co2, o2, n2
comp, petn, 100
point, p, 10000, t, 100
```

3.25 original output

Purpose: Thermodynamic potentials are printed as "raw" values, rather than as changes from the reactants or elements, as in the `reactants reaction` or `elements reaction` command.

Syntax: original output

Example: The enthalpy of PETN will be found as an absolute value, then as the change from the reactants in their standard state, and finally as a change from the elements in their standard state.

```
comp, petn, 100
original output
comp, petn, 100
point, p, 100, t, 100
reactants reaction
point, p, 100, t, 100
elements reaction
point, p, 100, t, 100
```

3.26 point

Purpose: Calculates a single thermodynamic state.

Syntax: point, *Q1*, *x1*, *Q2*, *x2*
Q1 and *Q2* are thermodynamic variables chosen from the list `(P,V,T,H,S,E,G,Hugoniot,A)`. If `Hugoniot` is selected, the shock Hugoniot reference state must have previously been specified with the `hug0` command. *x1* and *x2* are the desired values of *Q1* and *Q2*, respectively. If *x1* or *x2* are left blank, their current values are used instead.

Example: Calculate the products of HMX combustion after expansion and cooling.

```
comp, hmx, 100
point, p, 1, t, 298
```

3.27 print selection

Purpose: To suppress or turn on printing of product concentrations.

Syntax: print selection, *i1*
i1 is either 0 or 1. 0 turns on printing of product concentrations. 1 turns off printing of the concentrations.

Example: Product concentrations are found for a constant volume explosion of TATB, but not for the adiabat

```
comp, tatb, 1
explosion, rho, 2.50
print selection, 1
isoline, s, , v, , 20, 40.0
```

3.28 reactants reaction

Purpose: The specific enthalpy, energy, and entropy changes for the reaction converting the reactants in their standard states into the products is reported. This is the default in CHEETAH.

Syntax: reactants reaction

Example: The enthalpy of PETN will be found as an absolute value, then as the change from the reactants in their standard state, and finally as a change from the elements in their standard state.

```
comp, petn, 100
original output
comp, petn, 100
point, p, 100, t, 100
reactants reaction
point, p, 100, t, 100
elements reaction
point, p, 100, t, 100
```

3.29 recall point

Purpose: To recall a point that has been saved. This point will be treated as if it were the last point computed.

Syntax: recall, *n1*
n1 is the name of a saved point.

Example: Adiabatic expansion and constant volume cooling of a constant volume

explosion is performed. This examines situations where the confinement vessel did or did not fail.

```
comp, tnt, 100
explos, rho, 2.5
save, cvexplos
isoline, s, , v, , 10, 20.0
recall, cvexplos
isoline, v, , t, , 20, 298.0
```

3.30 reject

Purpose: The reject command prevents the specified condensed or gaseous products from being used in the calculation.

Syntax: reject, *n1*, *n2*, ...
n1, *n2* are the products to be rejected.

Example: Perform a standard run on TNT without carbon condensation

```
reject, *c
comp, tnt, 100
standard run, rho, 1.5
```

3.31 retain

Purpose: `retain` maintains the effects of the product selection commands `reject`, `order`, and `choose` command for subsequent compositions. Without `retain` the

effect of the product selection commands is lost with the next `composition` command.

Syntax: retain

Example: Point calculations are performed on TNT and HMX without carbon condensation.

```
reject, *c
retain
comp, tnt, 100
point, p, 10000, t, 1000
comp, hmx, 100
point, p, 10000, t, 1000
```

3.32 save point

Purpose: The current thermodynamic state is saved for later use with the `recall` command.

Syntax: save point, *name*

Example: See the example for `recall`.

3.33 set

Purpose: Fixes equation of state parameters to specified values.

Syntax: set, *eosname*, *value*

Example: Set the BKW parameters to the BKWR[5] values.

```
set, bkw, alpha, 0.5
set, bkw, beta, 0.176
set, bkw, kappa, 11.80
set, bkw, theta, 1850
```

Example: Set the JCZ3[6] parameters.

```
set, jcz3, m, 7
set, jcz3, l, 15
set, jcz3, bm, 13.8
set, jcz3, bl, 15.1
set, jcz3, sr, 0.95
set, jcz3, se, 1.03
set, jcz3, q, 4
set, jcz3, c, 0.573
set, jcz3, a, 4, 92.1
```

The last example changes the JCZ3 parameter a_4.

3.34 standard run

Purpose: Calculates the C-J state and adiabat; fits the results to a JWL equation of state

standard run, rho, *x1*
Syntax: standard run, v, *x1*
standard run

The standard run requires only that the composition and the density or specific volume by specified.

The purpose of the standard run is to automate the use of CHEETAH as much as possible. The calculations performed under the standard run should meet the needs of the majority of users. CHEETAH can be run with only two commands using the standard run. If no arguments are given, a calculation at TMD is performed. For a more thorough discussion of the standard run, see Section 2.1 and 2.7.

Example: Do a standard run for HNS

```
comp, hns, 100
standard run, rho, 1.8
```

3.35 start of library

Purpose: Denotes the beginning of the library commands.

Syntax: start of library

3.36 stop

Purpose: Stops CHEETAH execution. `Stop` should be given at the end of every CHEETAH input file.

Syntax: stop

3.37 stc

Purpose: Enters into the product library the condensed equation of state name and condensed equation of state constants.

Syntax: stc, *name*, *type*, *ncall*, *eosname*, *x1*, *x2*, *x3*
name is the name of the product species. *type* is either `solid` or `liquid`. *ncall* is the number of times that the `stc` command has been used; it is either 1, 2, 3, or 4. *eosname* is the name of the equation of state. Currently, only `old` is accepted. *x1*, *x2*, and *x3* are three equation of state constants.

The `old` equation of state has the form:

$$V = (A_{11} + A_{12}T + A_{13}T^2) + P(A_{21} + A_{22}T + A_{23}T^2) + P^2(A_{31} + A_{32}T + A_{33}T^2) \quad (3.5)$$

The first term in parenthesis are entered in the first call to STC, The linear term in P is entered in the second call to STC, and the quadratic term is entered in the third call. A fourth call to STC with all zeros is necessary.

Example: The condensed phase equation of state of carbon is set.

```
stc, *c ,solid,1,old,4.99259,3.9628e-5,1.191359e-9
stc, *c ,solid,2,old,-6.377527e-6,1.1924995e-10,-3.7557816e-15
stc, *c ,solid,3,old, 3.58287e-12,-1.00976e-16,0.0
stc, *c ,solid,4,old,0.0,0.0,0.0
```

3.38 stg

Purpose: Enters into the product library constants necessary for the evaluation of the gaseous equation of state.

Syntax: stg, *eosname*, *c1*, *x1*, *x2*, *x2*, ...
eosname is the name of the equation of state. Currently BKW[4] or JCZ3[6] are accepted. The ideal gas EOS does not require any parameters. *c1* is the name of the product species. *x1*, *x2* are the equation of state parameters.

Example: Set the BKW covolume for h2o.

```
stg, bkw, h2o, 360.0
```

Example: Set the JCZ3 constants for h2o.

```
stg, jcz3, h2o, 9.3, 260
```

3.39 str

Purpose: Enters into the product library the constants necessary to compute thermodynamic properties at the reference state (1 atm).

Syntax: str, *name*, *type*, *icall*, *c1*, *c2*, *c3*
name is the name of the product species. *type* is either `gas`, `liquid`, or `solid`. *icall* is the number of times that `str` has been called for this species. It is either 1, 2, or 3. `str` must be called three times to enter in the nine thermodynamic constants. *c1*, *c2*, and *c3* are the values of the thermodynamic constants, which are input three at a time. The `str` command must be preceded by the `constituent` command.

The constants C_i ($i = 1, \ldots 9$) are obtained from thermodynamic reference data, such as the JANAF tables. The first seven constants are obtained by fitting specific heat capacity data to the following equation:

$$C_p = R(C_1 + C_2\theta + C_3\theta^2 + C_4\theta^3 + C_5\theta^{-1} + C_6\theta^{-2} + C_7\theta^{-3}), \qquad (3.6)$$

where C_p is the specific heat capacity in calories/mole/degree, and $\theta = T/1000$, where T is in degrees Kelvin.

The last two constants may be computed from the first seven plus the heat of formation, $H^0_{f\,298}$ at 298.15 K, in calories/mole and the entropy S^0_{298} in calories/mole/degree:

$$C_8 = H^0_{f\,298} - 298.15R[C_1 + \frac{C_2 x}{2} + \frac{C_3 x^2}{3} + \frac{C_4 x^3}{4} + \frac{C_5 \log x}{x} - C_6 x^{-2} - \frac{C_7 x^{-3}}{2}] \quad (3.7)$$

$$C_9 = S^0_{298} - R[C_1 log x + C_2 x + \frac{C_3 x^2}{2} + \frac{C_4 x^3}{3} - C_5 x^{-1} - \frac{C_6 x^{-2}}{2} - \frac{C_7 x^{-3}}{3}] \quad (3.8)$$

where $x = 0.29815$.

Example: The reference data for CO2 is entered into the library.

```
str, co2, gas, 1,  8.8154827e+00, -2.9677816e-01, 4.1121392e-02
str, co2, gas, 2, -1.4369961e-03, -2.4642032e+00, 4.7372105e-01
str, co2, gas, 3, -3.5108985e-02, -1.0241280e+05, 6.0435569e+01
```

3.40 spreadsheet

Purpose: Saves variables into a file that is readable by a spreadsheet program.

Syntax: spreadsheet, *filename*, *Q1*, *Q2*, *N1*, ...
spreadsheet, *filename*, *Q1*, *Q2*, *N1*, ..., tab
Q1 and *Q2* are variables chosen from the list (p, v, t, h, s, e, v, vgs, alpha, beta, cv, and adexp.) Any number of variables can be saved. *N1* is the name of any product species. More than one product species can also be saved. In the second example, the last argument of `tab` indicates that columns are to be separated by tabs. Other possibilities are comma or space separated columns (the default).

Example: Save the concentration of CO2 for the C-J adiabat of TATB.

```
composition, tatb, 100
hug0, p, 1, sv
c-j
spreadsheet, plot.dat, v, co2
isoline, s, , v, , 20, 100
```

3.41 summary

Purpose: Sets the name of the summary file.

Syntax: summary, *filename*
filename is the name of the summary file. The summary file contains the initial composition, C-J parameters, and the volumes and energies of any subsequent S-V points. The S-V points correspond to cylinder test results. Subsequent `summary` commands close the previous summary file. The `summary` command with a blank argument closes the current summary file.

The form of the summary file is controlled by the file `summary.in`. This file should be set up before using the summary command for the first time. The first line contains the number of standards to compare to, and the number of adiabat volumes to calculate. The relative value of the volume for each adiabat point is given next. Then, for each standard a name line is given, followed by a standard value for the adiabat energy in kJ/cc. Finally we give the number of reference half and full wall velocities, and the square of the standard wall velocity in mm/μs divided by the adiabat energy in kJ/cc .

Example: A possible `summary.in` file is:

```
4
5
2.2
4.1
6.5
```

```
10.0
20.0
TATB
-5.11
-5.96
-6.26
-6.44
-6.64
PETN
-7.30
-8.81
-9.39
-9.74
-10.10
HMX
-8.52
-10.08
-10.60
-10.90
-11.18
TRITON
-4.73
-5.96
-6.56
-7.02
-7.62
3
-0.286 -0.216
-0.258 -0.195
-0.253 -0.190
```

3.42 title

Purpose: Gives a title to the current job. The title is echoed to the main output and summary files.

Syntax: title, *name*

Example: A Tritonal run is labeled.

```
title, An easy tritonal run.
comp, tnt, 80, al, 20
standard run, rho, 1.8
```

3.43 units

Purpose: Sets the input units of a specified quantity Units can be set for p, v, ρ, E and T. If E units are specified, all quantities with the dimensions of energy (E, H, G) are input with the new E units. The unit of S is the unit of E divided by the unit of T.

Syntax: units, *Q1*, *X1*
Q1 is one of the thermodynamic quantities p, v, ρ, E and T. The unit of ρ is the inverse of the unit of v. *X1* is the new unit of quantity *Q1*, in atm, cc/gm, gm/cc, cal/gm, or K (depending on whether p, v, ρ, E, or T is given, of course).

There are two special ways to set the unit of volume. The command `units, sv` indicates that the standard volume is the new input unit of volume. The standard volume is defined as:

$$V_s = \sum_i x_i V_i \tag{3.9}$$

where x_i is the mole fraction of reactant i and V_i is the molar volume of the reactant in its standard state. The molar volume in the standard state is usually the same as the inverse of the TMD divided by the molecular weight, so V_s can generally be regarded as the TMD of the reactant mixture.

The second way to define the unit of volume is through the command `units, v0`. In this case the unit of volume is set to be the shock Hugoniot reference volume v_0. This volume should have been previously set through the `hug0` command or the `standard run` command. The `v0` command gives volumes in reference to the initial explosive volume; therefore it is of particular use in specifying expansion volumes.

Section 4
Reactant library

CHEETAH comes bundled with a library of reactants in the file `config/formula.in`. The library is simply a long list of `formula` commands. When a reactant is specified in the `composition` command, CHEETAH searches the reactant library for a species of the same name. *All* of the characters of a reactant name are significant in CHEETAH. This allows the use of longer and less confusing names. The reactant library is not read with CHEETAH normal input routine; this allows for fast scanning of the library. This also means that more restrictive rules must be followed when writing entries in the `formula.in` file. This `formula` command must be abbreviated as `for`. The command must be followed by a comma, a single space, and the name of the compound, as in the following example:

```
for, adn,          -35700.,  68.92, 0., h, 4, n, 4, o, 4
```

Below is the current LLNL reactant database. We are attempting to verify all values here through an exhaustive literature search. For the time being, however, the reported values are "historical" ones used for the last several years at LLNL. If you have a serious disagreement with reported densities or heats of formation in this file, please inform Laurence Fried by sending e-mail to `cheetah@llnl.gov`. Please try to send a a literature citation for what you feel the correct value to be. This will be of great help in improving future CHEETAH releases.

CHEETAH Reactant Library Version 1.0

Assembled by P. Clark Souers

E = explosive, B = binder, P = plasticizer, R = reducer

Name		Full Name	Mol. wt. g/mol	TMD g/cc	H_f cal/mol	V cc/mol	c	h	n	o	Other
adn	E	ammonium dinitramide	124.1	1.80	-35,700	68.92		4	4	4	
adnbf	E	4-amino-5,7-dinitrobenz[1,2-c][1,2,5]oxadiazole-3-oxide	241.1	1.90	36,790	126.80	6	3	5	6	
ammazide	E	ammonium azide	60.1	1.35	20,400	44.62		4	4		
ammpicrate	E	ammonium picrate	246.1	1.72	-94,000	143.27	6	6	4	7	
anpz	E	3,5-diamino-2,6-dinitropyrazine	200.1	1.80	-5,400	111.00	4	4	6	4	
anta	E	5-amino-3-nitro-1,2,4-triazole	129.1	1.82	14,400	70.96	2	3	5	2	
bicyclohmx	E	bicyclo-hmx	294.1	1.87	25,000	157.46	4	6	8	8	
btf	E	benzotrifuroxan	252.1	1.90	144,500	132.62	6		6	6	
cl-12	E	4,4'-diamino-2,2',3,3',5,5',6,6'-octanitrobiphenyl	438.2	2.04	81,000	214.80	6	6	12	12	
cl-14	E	5,7-diamino-4,6-dinitrobenzofuroxan	256.1	1.94	20,630	131.89	6	4	6	6	
cl-20	E	hexanitroazaisowurzitane (HNIW)	438.2	2.04	90,000	214.38	6	6	12	12	
datb	E	diaminotrinitrobenzene	243.1	1.84	-29,230	132.35	6	5	5	6	
dftnb	E	difluorotrinitrobenzene	249.1	1.87	-49,690	132.90	6	1	3	6	f, 2
dina	E	dioxyethylnitramine dinitrate	240.1	1.49	-75,400	161.36	4	8	4	8	
dipam	E	3,3'-diamino-2,2'-4,4'-6,6'-hexanitrobiphenyl	454.2	1.82	-20,100	249.03	12	6	8	12	
dipehn	E	hexanitrodiphenylerithytol	524.3	1.63	-233,790	321.64	10	16	6	19	
dnb	E	m-dinitrobenzene	168.1	1.58	-6,200	106.73	6	4	2	4	
dnbt	E	dinitrobistriazole	226.1	1.80	94,000	125.60	4	2	8	4	
dnbtzl	E	dinitrobenzotriazole	209.1	1.84	0	113.70	6	3	5	4	
dni24	E	2,4-dinitroimidizole	158.1	1.45	4,900	108.96	3	2	4	4	
dnpa	E	2,2'-dintropropylacrylate	204.1	1.47	-110,000	138.84	6	8	2	6	
dnt	E	2,4-dinitrotoluene	182.1	1.52	-16,300	119.75	7	6	2	4	
dp12	E	1,2-bis(difluoroamino)propane	146.1	1.26	-48,000	116.00	3	6	2		f, 4
edd	E	ethylenediamine dinitrate	186.1	1.58	-255,766	118.01	2	10	4	6	
edna	E	ethylene dinitramine	150.1	1.71	-24,706	87.78	2	6	4	4	
ednp	E	ethyl-4,4'-dinitropentanoate	220.2	1.28	-140,000	172.02	7	12	2	6	
ethcarb	E	ethylene carbonate	88.1	1.32	-138,900	66.66	3	4		3	
ethpicrate	E	ethyl picrate	257.2	1.55	-48,020	165.91	8	7	3	7	
fefo	E	bis(2-fluoro-2,2-dinitroethyl)formal	320.1	1.61	-177,530	199.20	5	6	4	10	f, 2
hk6	E	3,5-dinitro-2-oxo-1,3,5-hexahydrotriazine	191.1	1.66	25,000	115.10	3	5	5	5	
hmx	E	octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine	296.2	1.91	17,930	155.46	4	8	8	8	
hnab	E	bis(2,4,6-trinitrophenyl)diazene; phase I used	452.2	1.80	57,800	251.37	12	4	8	12	
hnb	E	hexanitrobenzene	348.1	2.02	15,700	172.33	6		6	12	
hndp	E	2,4,6,2',4',6'-hexanitrodiphenylamine	439.2	1.64	9,570	267.81	12	5	7	12	
hne	E	hexanitroethane	300.1	1.85	28,600	162.19	2		6	12	
hns	E	2,2'-4,4'-6,6'-hexanitrostilbene	450.2	1.74	18,700	258.80	14	6	6	12	
hnx	E	4,6-bis[1-(3-amino-5-nitro-1,2,4-triazoyl)]-5-nitropyrimidine	393.2	1.91	104,000	206.10	8	5	6	13	
hydrazine	E	hydrazine	32.0	1.68	12,050	19.02		4	2		
hyd nitrate	E	hydrazine mononitrate	95.1	1.69	-59,000	56.41		5	3	3	
k-6	E	2-oxo-1,3,5-trinitro-1,3,5-triazacyclohexane	236.1	1.93	-10,000	122.20	3	4	6	7	
medina	E	methylenedinitramine	136.1	1.74	-13,840	78.42	1	4	4	4	
mf-1	E	(2-fluoro-2,2-dinitroethyl-2,2-dinitropropyl)formal	316.2	1.53	-160,115	206.10	6	9	4	10	f, 1
ng	E	nitroglycerin(1,2,3-propanetriol trinitrate)	227.1	1.60	-88,600	142.29	3	5	3	9	
nglycol	E	nitrogylcol	152.1	1.48	-58,250	102.50	2	4	2	6	
nibtn	E	nitroisobutylglycerol trinitrate	286.1	1.68	-54,600	170.30	4	6	4	11	

Name		Full Name	Mol. wt. g/mol	TMD g/cc	H_f cal/mol	V cc/mol	c	h	n	o	Other
nm	E	nitromethane	61.0	1.13	-27,030	54.02	1	3	1	2	
nq	E	nitroguanidine	104.1	1.77	-22,100	58.63	1	4	4	2	
nto	E	5-nitro-1,2,4-triazol-2-one	130.1	1.93	-28,000	67.39	2	2	4	3	
petn	E	pentaerythritol tetranitrate	316.1	1.78	-128,700	177.61	5	8	4	12	
petrin	E	pentaerythritol trinitrate	271.1	1.54	-134,000	176.04	5	9	3	10	
picchloride	E	picryl chloride (2,4,6-trinitrochlorobenzene)	247.6	1.80	6,410	137.79	6	2	3	6	cl, 1
picfluoride	E	picryl fluoride (2,4,6-trinitrofluorobenzene)	231.1	1.83	-62,000	126.10	6	2	3	6	f, 1
picric acid	E	picric acid(2,4,6-trinitophenol)	229.1	1.77	-59,400	129.44	6	3	3	7	
pran	E	2-(5-amino-3-nitro-1,2,4-triazolyl)-3,5-dinitropyridine	296.2	1.87	50,000	158.40	7	4	8	6	
pzo	E	3,5-diamino-2,6-dinitropyrazine-1-oxide	216.1	1.91	-3,100	113.00	4	4	6	5	
rdx	E	hexahydro-1,3,5-trinitro-1,3,5-triazine	222.1	1.81	14,710	122.99	3	6	6	6	
styph acid	E	styphnic acid; 2,4,6-trinitro-1,3-dihydroxybenzene	245.1	1.83	-105,900	133.93	6	3	3	8	
tacot	E	tetranitro-benzotrizolo-benzotriazol-ium, hydroxide	388.2	1.85	110,500	209.85	12	4	8	8	
tatb	E	2,4,6-trinitro-1,3,5-triaminobenzene	258.2	1.94	-36,850	133.21	6	6	6	6	
tena	E	2,3,4,6-tetranitroaniline	273.1	1.87	-11,690	146.29	6	3	5	8	
tetrazene	E	tetrazene	188.2	1.70	45,200	110.68	2	8	10	1	
tetryl	E	N-methyl-N,2,4,6-tetranitroaniline	287.1	1.73	4,670	165.98	7	5	5	8	
tna	E	2,4,6-trinitroaniline	228.1	1.76	-17,790	129.47	6	4	4	6	
tnan	E	2,4,6-trinitroanisole	243.1	1.61	-36,610	151.01	7	5	3	7	
tnaz	E	1,33-trinitroazetidine	192.1	1.84	8,700	104.40	3	4	4	6	
tnb	E	trinitrobenzene	213.1	1.76	-8,480	121.08	6	3	3	6	
tnc	E	trinitrocresol	243.1	1.68	-60,290	144.72	7	5	3	7	
tneb	E	trinitroethylbenzene	241.2	1.62	-21,650	148.87	8	7	3	6	
tneoc	E	trinitroethylorthocarbonate	732.2	1.84	-282,130	397.90	9	8	12	28	
tngu	E	tetranitroglycoluril	322.1	2.04	12,000	157.90	4	2	8	10	
tnm	E	tetranitromethane	196.0	1.65	13,000	118.81	1		4	8	
tnp	E	2,4,6-trinitropyridine	214.1	1.77	79,000	120.96	5	2	4	6	
tnt	E	trinitrotoluene	227.1	1.65	-17,810	137.30	7	5	3	6	
urea	E	urea	60.1	1.32	-79,610	45.39	1	4	2	1	
ureanit	E	urea nitrate	123.1	1.68	-130,610	73.21	1	5	3	4	
cabosil	B	silica powder	60.1	2.20	-215,940	27.31				2	si, 1
cellulose	B		162.1	0.90	-230,800	179.96	6	10		5	
estane	B	polyurethane solution	194.7	1.18	-184,820	165.02	10	15	0.4	3.4	
ethglycol	B	ethylene glycol	58.1	1.04	-108,700	55.97	2	6	2		
eva	B	ethylene vinylacetate	3966.1	1.01	250,000	3942.40	240	440		40	
for	B	formadide	45.0	1.13	-60,700	39.72	1	3	1	1	
gap	B	glycidylazide polymer	100.0	1.32	28,200	75.79	3.1	5.3	2.9	1.1	
hdi	B	hexamethylene diisocyanate	164.2	1.24	9,400	132.82	8	8	2	2	
ipdi	B	isophorone diisocyanate	222.3	1.06	-58,000	210.11	12	18	2	2	
kel-f	B	chlorotrifluoroethylene/vinylidine fluoride copolymer	413.4	2.02	-578,000	204.68	8	2			f, 11, cl, 3
kraton	B	a rubber	700.2	0.91	-161,230	769.52	51	87			
lecithin	B	rdx sensitivity additive	677.0	0.94	-252,860	720.24	36	76	4	7	
melamine	B		126.1	1.57	-20,810	80.18	3	6	6		
n-100	B	commercial isoceprate	478.6	1.14	9,082	419.82	23	38	6	5	
ncellulose-11	B	nitrocellulose (11% nitrogen)	252.1	1.53	-180,000	164.80	6	8	2	9	
ncellulose-12	B	nitrocellulose (12% nitrogen)	263.8	1.65	-174,000	159.61	6	7.7	2.3	9.5	

Name		Full Name	Mol. wt. g/mol	TMD g/cc	H_f cal/mol	V cc/mol	c	h	n	o	Other
ncellulose-13	B	nitrocellulose (13.35% nitrogen)	283.9	1.66	-183,000	171.45	6	7.3	2.7	10	
ncellulose-14	B	nitrocellulose (14.14% nitrogen)	297.1	1.66	-156,000	179.10	6	7	3	11	
paraffin	B	wax	352.7	0.89	-183,000	396.28	25	52			
pcl	B	polycaprolactone	993.1	1.07	-371,008	928.11	46	72		23	
pe	B	polyethylene	28.1	0.93	-12,700	30.16	2	4			
pgn	B	polygylcidyl nitrate	119.1	1.45	68,000	82.12	3	5	1	4	
phenoxy	B	polymeric epoxy of bis phenol A	284.4	1.18	-110,000	240.98	18	20		3	
pnimmo	B	poly(-3-nitratomethyl-3-methyl oxetane)	147.1	1.28	73,900	114.94	5	9	1	4	
pvc	B	polyvinylchloride	62.5	1.40	-19,750	44.64	2	3			cl, 1
pvf	B	polyvinylformal	830.0	1.23	-479,740	676.42	38	69		19	
saran	B	polyvinylidene chloride	28.5	1.12	-1,200	25.50	1	1.3	0.2		cl, 0.4
sylgard	B	silicone resin	72.2	1.02	-24,900	70.62	2	6	1		si, 1
viton	B	vinylidine fluoride/hexafluoropropylene copolymer	187.1	1.83	-332,700	102.50	5	3.5			f, 6.5
water	B		18.0	1.00	-68,315	18.02		2		1	
an	O	ammonium nitrate	80.0	1.73	-87,280	46.40		4	2	3	
ap		ammonium perchlorate	117.5	1.95	-70,580	60.25		4	1	4	cl, 1
calcium nit	O	calcium nitrate	164.1	2.50	-224,200	65.53			2	6	ca, 1
lithium nit	O	lithium nitrate	68.9	2.38	-115,500	28.97			1	3	li, 1
lithium per	O	lithium perchlorate	106.4	2.43	-91,060	43.78				4	cl, 1, li, 1
magnesium per	O	magnesium perchlorate	223.2	2.21	-140,600	101.00				8	cl, 2, mg, 1
nitric acid	O	nitric acid	63.0	1.50	-41,610	41.92		1	1	3	
potassium nit	O	potassium nitrate	101.1	2.11	-118,200	47.94			1	3	k, 1
potassium per	O	potassium perchlorate	138.5	2.52	-103,400	55.00				4	cl, 1, k, 1
sodium nit	O	sodium nitrate	85.0	2.26	-111,800	37.59			1	3	na, 1
sodium per	O	sodium perchlorate	122.4	2.50	-91,610	48.98				4	cl, 1, na, 1
bdnpa	P	bis(2,2-dinitropropyl)acetal	326.2	1.39	-151,300	234.69	8	14	4	10	
bdnpf	P	bis(2,2-dinitropropyl)formal	312.2	1.39	-142,700	224.60	7	12	4	10	
cef	P	tris-b-chloroethylphosphate (Used in PBX-9404)	285.5	1.42	-300,000	200.35	6	12		4	cl, 3, p, 1
dop	P	di-2-ethylhexylphthalate	390.6	0.99	-268,200	396.15	24	38		4	
tegdn	P	tetraethyleneglycol dinitrate	240.2	1.33	-145,400	180.58	6	12	2	8	
tmetn	P	trimethylol ethane trinitrate	255.1	1.47	-105,800	173.56	5	9	3	9	
al	R	elemental aluminum	27.0	2.70	0	9.99					al, 1
b	R	elemental boron	10.8	2.34	0	4.62					b, 1
fuel oil	R	fuel oil used by Dyno Nobel in ANFO (1994)	96.2	0.83	70,000	115.90	7	12			
graphite	R	graphite	12.0	2.25	0	5.34	1				

Section 5
New features

The following sections describe changes to TIGER made in CHEETAH. The descriptions assume that you are familiar with the behavior of TIGER. If you are not a TIGER expert, the tutorial and reference sections will probably be more helpful.

5.1 New input routines

TIGER was written before FORTRAN had character string types. Because of this, the authors translated character strings into floating point numbers. This had nightmarish consequences for the readability of the code. For instance, the string 'ALPHA' appears as the number 1526302215.0 in TIGER. It also had subtle consequences for the user. Single-precision versions of TIGER, (like Dan Calef's PC version) were limited to recognizing only the first three characters of a string. This made the creation of constituent libraries very error-prone, since one had to be sure that no two constituents shared the same first three letters.

To solve this problem, a set of modifications were made to the entire code that replaced all the input with a modern token-based input system. While commands may be abbreviated to three letters, further letters are now significant. Spaces in words are now recognized. Thus,

```
set, bkw, alpha, 0.5
```

is valid input, as is

```
set, bkw, alp, 0.5.
```

But,

```
s e t, bkw, al p, 0.5
```

worked with the old program, but not with the new input. Similarly,

```
set, bkw, alphalfa, 0.7
```

worked with the old program, but not with the new one.

Although commands can be abbreviated, user-defined names cannot. This is to help reduce errors in library files. For instance, previously

```
for, petn,      -128700., ....
```

would conflict with

```
for, petroleum, -128700, .....
```

Now ALL the characters in a user-defined name are significant.

You can have spaces in user-defined names if you want.

```
for, alpha olefin, ....
```

is valid input.

CHEETAH keeps a "dictionary" of strings that it has learned in previous runs and while loading the library, in the file string.in. You should probably delete string.in before loading a new library to avoid overfilling the dictionary. The maximum dictionary length is currently 5000 words.

An '&' is a continuation character for long lines. The '&' must be the last character on the line. For example,

```
comp, petn, 100, ammazide, 10, bicyclohmx, 10, cl-20, 10, ethpicrate, 10, &
      hmx, 10, hnb, 10, hns, 10
```

5.2 Comments in input files

Any input line beginning with a "#" character is a comment. Comments are echoed into the output file but are otherwise ignored.

5.3 Load file command

The command

```
load file, myfile.in
```

instructs CHEETAH to execute the commands contained in `myfile.in`. After the commands are executed, it returns to running commands from the original input file. The `load file` command is particularly useful in conjunction with relative units (see below). For instance, the input file

```
c-j, p, 1.0, rho, 1.894
load, cylinder.in
```

with the file `cylinder.in` containing

```
units, v,
point, s, , v, 1.5
point, s, , v, 2.0
point, s, , v, 2.5
```

would run a standard set of points along the C-J adiabat at 1.5, 2.0, and 2.5 times the C-J volume.

5.4 Startup file

Any commands in the file `startup.in` will be executed before the regular input file. Favorite input units, equation of state `set` commands, or frequently used reactants are good candidates for inclusion into the startup file.

5.5 Spreadsheet output

CHEETAH can create an auxiliary output file consisting of specified thermodynamic variables, in a form readable by most spreadsheets and plotting packages. For example,

```
spreadsheet, myfile.dat, p, v, t, s, tab
isoline, s, v, , 10 0.5
spreadsheet, close
point, t, 3000, p, 20000
spreadsheet, myfile2.dat, h, e
point, t, 1200, p, 200000
stop
```

specifies that a spreadsheet file `myfile.dat` be created, containing values of p,v,t, and s. The columns in the file are to be separated by tabs. Other separator options are `comma` and `space`. By default, columns are separated by commas. The first argument to spreadsheet must be either a filename or `close`.

The `close` command is necessary to make sure that unwanted points do not end up in the spreadsheet file. In the above example, the point at 3000K and 20000 atm would be put in the spreadsheet file were it not for the `close` command. `Spreadsheet` commands can follow one another without an intervening `close`, in which case the set of variables used in the first `spreadsheet` command is inherited by the second. `Spreadsheet` can report the following variables: p, t, v, h, s, e, v_{gas}, α, *beta*, C_v, and κ.

In addition, CHEETAH can report the concentrations of selected constituents, by giving the constituent name. For example,

```
spreadsheet, myfile.dat, co2
```

will put the concentration of CO2 into myfile.dat. Up to 20 constituents (either gaseous or condensed) can be followed at one time.

5.6 Improvements to the freeze command

The freeze command in TIGER used an algorithm that was susceptible to roundoff errors. The consequence of this to the user was that TIGER would frequently refuse to freeze concentrations, so that freezing had to be done in multiple steps. The freezing algorithm was modified in CHEETAH to make it more reliable.

5.7 Reformulated concentration solver

For every calculation type (point, c-j, isoline), TIGER solves at least once for the concentrations of the non-frozen constituents at a specified thermodynamic state (e.g. P,T). The original solver would often fail to converge. This occurred for two reasons: the two-step solver used in TIGER could get trapped in local minima that a single-step solver would avoid. Secondly, the Newton solvers in TIGER used a poor backtracking mechanism that often led to poor convergence.

In the two-step solver the concentrations were adjusted at fixed η values (the η were related to chemical potentials), then the ηs were adjusted. The problem with the two-step scheme is that if a difficult or unphysical set of η's was chosen, the inner concentration solver would fail.

The ηs have now been eliminated as basic variables in CHEETAH. Instead, the log concentrations, temperature, and specific volume are adjusted simultaneously in a single solver. The new solver implements a different set of equations than TIGER. The new equations are given below. The new thermo solver also incorporates bounds so that no concentration can exceed the maximum allowed by stoichiometry. The new solver is more robust than the TIGER solver, and maintains the exceptional speed of the original TIGER solver.

5.8 New point types

CHEETAH allows the user to specify the thermodynamic state ("point") by giving any two functions from the list (p,v,t,e,h,s,a,Hugoniot). See section 5.10 for information on Hugoniot points. Most notably, T-S points can be given. This should be useful for freezing along an isentrope. Other exotica, such as H-S points, are possible. Currently, the new point types require that you first run an ordinary point, such as p-t, p-v, etc. Sometimes the state specified does not exist (e.g., not all p-v states are attainable), in which case CHEETAH will be unable to find a solution.

5.9 New isoline types

Corresponding to the new point types, isolin accepts new variables. Any thermodynamic variable from the list (p,v,t,e,h,s,Hugoniot) can be held constant, while any other variable from the list can be changed. Isentrope integrals are only calculated for p-s or v-s lines, as in TIGER.

5.10 New Hugoniot solver

TIGER used a simple iteration scheme to find a point on a shock Hugoniot. The same iteration was used within the C-J solver. Unfortunately, iterative methods don't always converge; the C-J and Hugoniot solvers in TIGER often ran into difficulties. CHEETAH implements a Hugoniot point in a different way than TIGER: rather than solving for a successive number of (p, v) points, it uses the equation

$$e_1 - e_0 = (p_1 + p_0)(v_0 - v_1)/2 \tag{5.1}$$

as an implicit definition of the thermodynamic state. Thus, saying that we are on the Hugoniot plays the same role in CHEETAH as saying that the pressure is 100kBar.

The reference state (p_0, v_0, e_0) is specified through the new `hug0` command. It behaves very similarly to the specification of the reference state in TIGER's `c-j` or `hugoniot` command. The syntax is

```
hug0, p, 1, v, 0.529
hug0, p, 1, rho, 1.890
hug0, p, 1, rho, 1.5, e, 66.0
hug0, p, , rho, , e,
hug0, p, 1, sv,
```

The first command sets the reference pressure and volume. The second command specifies the inverse reference volume `rho`. By default, the reference energy is calculated from the heats of formation given in the `formula` instruction. The third command overrides this default and sets the reference energy. The fourth command sets the reference state to be the current thermodynamic state. The fifth command sets the reference volume to be the standard volume of the explosive.

Once the reference state is set, the `hugoniot` keyword specifies that the given state is to be on the Hugoniot. The `hugoniot` point always takes an empty argument. For example,

```
## Don't forget to set the initial state !
hug0, p, 1, v, 0.529
## Point along the Hugoniot at 400kBar
point, p, 400000, hugoniot,
## Give me points along the Hugoniot up to 1800 K.
isolin, hugoniot, t, , 10, 1800
```

5.11 New C-J solver

CHEETAH has a new C-J solver that should be more robust than TIGER's solver. CHEETAH's solver takes advantage of the `hugoniot` point type. A series of `p, hugoniot` calculations are performed until a pressure is found that satisfies the equation

$$v = v_0[(1 - p_0/p)/\kappa + 1]^{-1} \tag{5.2}$$

is satisfied. Here, v is the volume at the specified pressure on the Hugoniot line, and κ is the adiabatic exponent. The detonation pressure is assumed to be between the constant volume explosion point and 500kBar. Using these points as brackets, it finds the root of Eq. (5.2) with Brent's method.

The `c-j` command also has a new syntax. The reference point on the Hugoniot is specified with the `hug0` command described in Sec. 5.10. The `c-j` command doesn't take any arguments. For example,

```
hug0, p, 1, rho, 1.890
c-j
```

5.12 User-defined units

Units to use when entering pressures or volumes can be specified with the commands

```
units, p, 100
units, v, 2
units, p,
```

The first command sets the input unit of pressure to be 100 Atm. The second command sets the input unit of relative volume to be 2 cc / gm. The third command sets the unit of pressure to be the current pressure. This is particularly useful when specifying pressures or volumes relative to the last thermodynamic state in the calculation. The units in the output file are unaffected by the `units` command.

Units can be set for p, v, ρ, E and T. If E units are specified, all quantities with the dimensions of energy (E, H, G) are input with the new E units. The unit of S is the unit of E divided by the unit of T.

There are two special ways to set the unit of volume. The command `units, sv` indicates that the standard volume is the new input unit of volume. The standard volume is defined as:

$$V_s = \sum_i x_i V_i \tag{5.3}$$

where x_i is the mole fraction of reactant i and V_i is the molar volume of the reactant in its standard state. The molar volume in the standard state is usually the same as the inverse of the TMD divided by the molecular weight, so V_s can generally be regarded as the TMD of the reactant mixture.

The second way to define the unit of volume is through the command `units, v0`. In this case the unit of volume is set to be the shock Hugoniot reference volume v_0. This volume should have been previously set through the `hug0` command or the `standard run` command. The `v0` command gives volumes in reference to the initial explosive volume; therefore it is of particular use in specifying expansion volumes.

5.13 New `gas eos` command

The old `geos` command has been given the less cryptic name `gas eos`.

5.14 Summary sheet output

A file summarizing the run can be generated by using the command:

```
summary, myfile.sum
```

where `myfile.sum` is the name of the summary file. The file `summary.out` is created as the default summary file if the summary command is not given. The summary file contains the initial composition, C-J parameters, and the volumes and energies of any subsequent S-V points. The S-V points correspond to cylinder test results. Subsequent `summary` commands close the previous summary file. The `summary` command with a blank argument closes the current summary file.

The form of the summary file is controlled by the file `summary.in`. This file should be set up before using the summary command for the first time. The first line contains the number of standards to compare to, and the number of cylinder runs to calculate. Then, for each standard a name line is given, followed by a standard value for the cylinder energy in kJ/cc. Finally we give the number of reference half and full wall velocities, and the standard wall velocity in $mm/\mu s$ squared divided by the cylinder energy in kJ/cc . An example `summary.in` file is

```
BKWR, LLNL Library
4
5
TATB
-5.11
-5.96
-6.26
-6.44
-6.64
PETN
-7.30
-8.81
-9.39
-9.74
-10.10
```

```
HMX
-8.52
-10.08
-10.60
-10.90
-11.18
TRITON
-4.73
-5.96
-6.56
-7.02
-7.62
3
-0.286 -0.216
-0.258 -0.195
-0.253 -0.190
```

5.15 JWL Fitting

CHEETAH will automatically determine a JWL fit to the C-J point and the adiabat. The appropriate command is `jwlfit`. This command should be given after finding the C-J point and at least 3 points along the adiabat. This should be followed by the `det energy` command, which finds the detonation energy. An example is:

```
c-j
point, s, , v, 1.247
point, s, , t, 1800.0
freeze
point, s, , v, 2.325
point, s, , v, 3.687
point, s, , v, 5.672
point, s, , v, 11.344
det energy, p, 1.0, t, 298.0
jwlfit, 4
```

More than 3 points along the adiabat can also be used, in which case the JWL fitter will find the best possible fit to the points. `jwlfit` takes a single argument, which is the number of cylinder runs to use in the fit. At least three runs must be used. By default, all the previous cylinder runs are used.

5.16 `Det energy` command

This command is used to find the detonation energy. The energy of detonation is broken out into a mechanical and a thermal part. See Sections 3 and 2 for a more detailed explanation. An example is:

```
det energy, p, 1.0, t, 298.0
```

5.17 `Standard run` command

The standard CHEETAH run performed at LLNL can be executed with the `standard run` command. The syntax is:

```
standard run, rho, 1.82
```

where 1.82 is the density of the formulated explosive. Without the `rho` argument, `standard run` assumes that the density is equal to TMD. The command first finds the C-J point, assuming a reference pressure of 1 atm for the Hugoniot. It then proceeds along the adiabat, calculating points at relative volumes equal to 2.2, 4.1, 6.5, 10.0, and 20.0. The composition is frozen at 1800K along the adiabat. The energy of detonation is then found and finally, the adiabat points are fit to a JWL equation of state.

The `standard run` can be customized by modifying the file `config/standard.in`. The first line of the `standard.in` file is the number of points to calculate along the adiabat. Next follows the relative volumes at each of the points. Next the freezing temperature is given; enter 0.0 if freezing is not desired. The last line of the `standard.in` file controls whether JWL fitting is done or not. A 1 indicates that the adiabat is to be fit to a JWL equation of state, while a 0 indicates that fitting is not to be done. For an example of the `standard.in` file, see Section 2.7.

5.18 New default reference state

By default, CHEETAH reports thermodynamic quantities as differences between the products and the standard state of the reactants. This makes it unnecessary to use the `reactants` command.

5.19 Formula library

The old `for, ...` command to specify the reactant formulas is no longer necessary. Instead, these commands have been put into a database file `config/formula.in`. When the `components` command is given, the database is searched for the appropriate formula. The first line of the database gives a title that will be echoed to the main output and summary files. Formulas in the database must begin with the command `for,` starting with the first character in the line. Longer versions of the command (e.g. `formula, `) cannot be used in the database file. The `formula` command can be used in the input file to override database values. The use of a `formula` command in the input file discontinues searching of the database for all formulas.

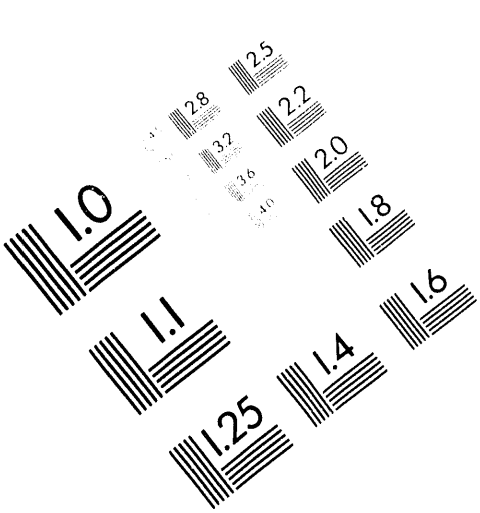
5.20 Configuration directory

All startup and configuration files are now put in a configuration directory. By default, the directory is `config`. You can change this default, however, by adding the following line to your `.cshrc` file on UNIX systems:

```
setenv CHCONFIG /usr/people/fried/myconfig
```

If you use the Bourne shell of Korn shell instead of csh (if you don't know what this means, it probably doesn't apply to you), then instead add to your `.profile` file the line

```
export CHCONFIG=/usr/people/fried/myconfig
```



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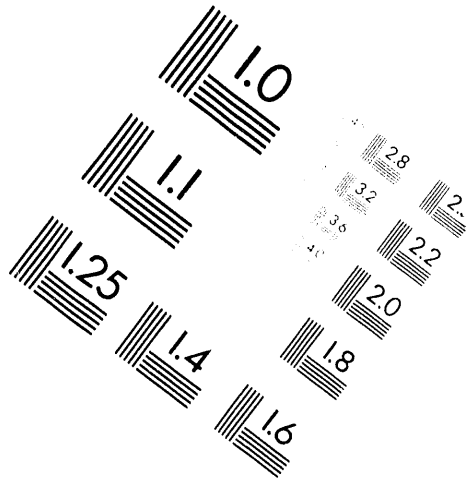

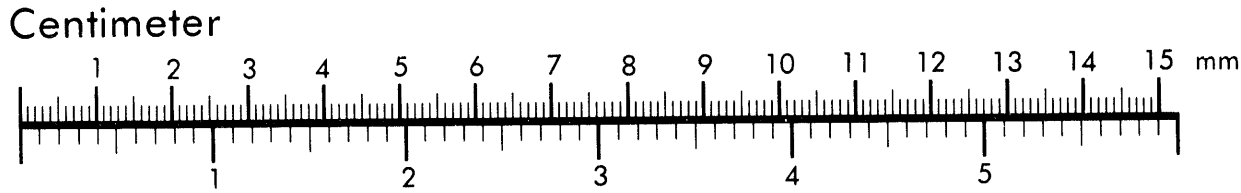

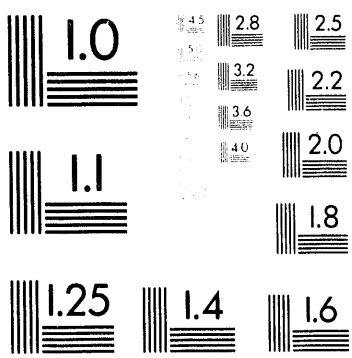

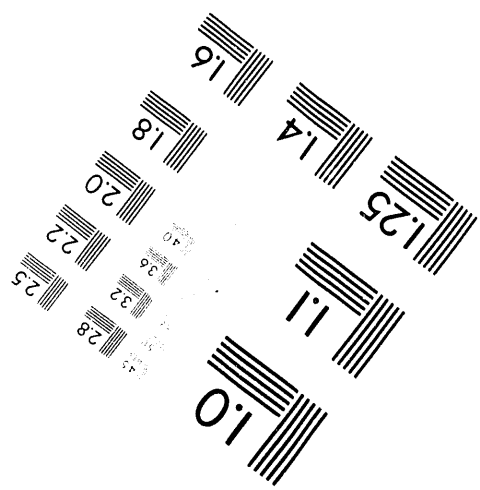

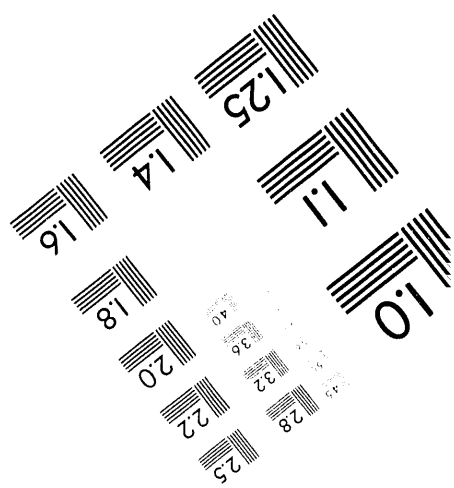

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2 of 2

On an IBM PC, add the following line to your `autoexec.bat`:

```
set CHCONFIG=c:\cheetah\myconfig
```

Then the directory `/usr/people/fried/myconfig` will be used as the CHEETAH configuration directory. It is best to give a full pathname The following files are now located there: `startup.in, formula.in, string.in, summary.in.`

5.21 New mixture solver

The mixture solving and detection routines from TIGER have been replaced with new routines in CHEETAH. The old subroutine CHKPHA has been replaced by the C subroutine checkphase. The following algorithm is used to check the condensed phase assumptions: if condensed phase assumptions are violated, new assumptions are generated which are correct for the current (T, P) values. The thermodynamic state (and hence (T, P)) are recalculated using these assumptions. If the assumptions are again incorrect, a unique set of new assumptions are generated, until all possible assumptions are exhausted. At this point, checkphase() concludes that the state of the system must be a solid-liquid mixture. checkphase() then looks through all previously tried guesses to find a candidate for the melting compound.

The melting compound is identified when the following conditions are met: there exists two guesses identical in all assumptions except the ith. For these two guesses the chemical potential conditions are satisfied for all but the ith condition, which is violated in both of the guesses. It is then concluded that the ith condensed constituent should be in a mixture state.

The liquid fraction f_l is then determined in a new subroutine, called mixmaster. This subroutine uses Brent's method to find the value of f_l such that the chemical potential of the solid is equal to that of the liquid for condensed constituent i. In general, the mixmaster() routine is somewhat slower than the iteration method used in TIGER, but it should be more reliable.

5.22 Dynamic memory allocation

The size of internal arrays in CHEETAH can be easily changed by the user. Large numbers of products or reactants can be run on computers with sufficient memory (RAM), while CHEETAH can be kept small for PC's or other systems with little memory. CHEETAH's array sizes are controlled by the file `config/alloc.in`. The first number is the maximum number of gaseous products (called constituents in the language of TIGER) The second is the maximum number of condensed products. The third number is the maximum number of elements (called components in TIGER). Finally the fourth number is the maximum number of reactants. The `alloc.in` file can be edited to change the default array sizes, and the changes then take effect upon running CHEETAH.

5.23 Obsolete TIGER commands

In the interest in keeping the code size of CHEETAH as small as possible (thus improving maintainability and performance on small systems like PC's), little used or obsolete commands were eliminated. The following commands that were present in TIGER have been dropped from CHEETAH:

- `HISTORY` This was supposed to record a history of all thermo points executed in TIGER. It was not functional in the version of TIGER that CHEETAH grew from.
- `HUGONT` This calculated points on a shock Hugoniot. It has been made obsolete by the new `hugoniot` point type.
- `JCZ2` EOS. The JCZ2[6] EOS was not widely used in TIGER, and has been eliminated.
- `GEOS` This specified the gaseous equation of state. It has been renamed `gas eos` in CHEETAH.
- `LEE` TIGER had the option of specifying a JWL for the condensed equation of state. This was eliminated from CHEETAH due to disuse.

- NOHISTORY This turned HISTORY off.
- TESTSG This command tested new gaseous equations of state.

5.24 Library file command

CHEETAH can keep track of more than one pre-compiled library file at a time through the use of the `library file` command. The command `library file, mylib.chl` should be placed in the library prior to running it with CHEETAH. You then run CHEETAH on a library file:

```
cheetah library.in library.out
```

The `library file` command specifies that the compiled library will be stored in `mylib.chl`, rather than the default `cheetah.chl`.

Then, library files may be selected with the command `library file, mylib.chl` in the input file or `config/startup.in`. If the `library file` command is not used, CHEETAH will store and read the library in the file `cheetah.chl`.

5.25 Library titles

Product libraries can now be titled. CHEETAH prints the title of the current library in the output and summary files. Naming libraries is highly recommended as a mechanism for documenting the library associated with a particular output file, especially when using the `library file` command above to switch between libraries.

To give a library a title, enter the command

```
title, an example library
```

immediately after the `start of library` command in the library input file. This title is recorded in the binary library file and is reported for each subsequent CHEETAH run using that library.

5.26 `Details` command

By default, CHEETAH shows fewer thermodynamic functions than TIGER did. By using the `details` command, the reporting of these functions is restored. After the `details` command, the following information is shown: the constant volume heat capacity, the hydrodynamic constants $\alpha, \beta, and \kappa$. κ was called `ADEXP` in TIGER.

The definitions are as follows:

$$C_V \equiv (\frac{\partial e}{\partial T})_V \tag{5.4}$$

$$\alpha \equiv \frac{1}{p}(\frac{\partial c}{\partial v})_p \tag{5.5}$$

$$\beta \equiv \frac{1}{v}(\frac{\partial e}{\partial p})_v \tag{5.6}$$

$$\kappa \equiv -(\frac{\partial \ln p}{\partial \ln v})_s = \frac{\alpha + 1}{\beta} \tag{5.7}$$

5.27 Configuration directory

CHEETAH reads "configuration" input files which are kept in a separate directory. By default, this directory is called `config`, and is a subdirectory of the same directory that CHEETAH is executed in. It is preferable, however, to use the `CHCONFIG` environment variable to set the configuration directory once and for all. The same configuration directory will then be used regardless of where CHEETAH is executed.

On UNIX systems, the following line should be put in your `.cshrc` file:

```
setenv CHCONFIG /usr/people/fried/cheetah/config
```

where `/usr/people/fried/cheetah/config` the full pathname of the config directory. The exact pathname will probably be different on your system.

For MS-DOS systems, the following line should be put in your `autoexec.bat` file:

```
set CHCONFIG=c:\cheetah\config
```

Section 6
CHEETAH for the IBM PC

A version of CHEETAH for the IBM PC has been prepared. CHEETAH-PC requires an Intel 386 or higher processor and a math coprocessor. The code runs under Microsoft Windows 3.1. CHEETAH-PC takes advantage of Windows memory management facilities, so that it is not limited to 640K of memory. Unlike TIGER-PC, CHEETAH-PC does full double precision calculations, so that the results of CHEETAH-PC are identical to those of the UNIX version of CHEETAH.

In order to run CHEETAH-PC, double click on the file `cheetah.exe`. A window will appear on this screen containing the CHEETAH output. Commands can be entered directly into this window by typing. A typical run would be as follows:

```
summary, sum.out
comp, petn, 100
standard run, rho, 1.763
stop
```

Alternatively, the commands can be put into a file with a text editor. Then type `load, file.in` into the CHEETAH window and the commands in `file.in` will be executed. Execution of CHEETAH can be stopped and started with commands in the menu bar. Cut and paste commands are useful in transferring CHEETAH's output to other applications.

Section 7
Utility program

In addition to the main CHEETAH program we have included a JWL fitting program, which is discussed here.

7.1 JWLFIT

The JWLFIT program fits experimental or theoretically derived cylinder data to the JWL adiabat equation of state:

$$P = A\exp(-R_1 v) + B\exp(-R_2 v) + Cv^{-(1+\omega)}. \tag{7.1}$$

The program is invoked with the command:

```
jwlfit > jwlfit.out
```

You will be prompted to enter the explosive name, the density of the explosive, the detonation velocity, the energy of detonation, the C-J pressure, and cylinder energies. If desired, you can prepare an input file with the answers, and then run JWLFIT with the command:

```
jwlfit < jwlfit.in > jwlfit.out
```

This is useful when running several jobs with similar parameters.

The program reports the set of JWL parameters that best matches the cylinder energies while exactly matching the CJ pressure, energy, and Grüneisen parameter. The C-J pressure and total energy of detonation can be measured by supracompression and bomb calorimetry, respectively. If measured values are not available for the explosive, it is best to treat P_{cj} and E_0 as adjustable fitting parameters. The user must enter a number of cylinder energies equal to or greater than the number of adjustable parameters. The number of independently adjustable parameters is 3 if P_{cj} and E_0 are fixed, 4 if one if adjustable and the other isn't, and 5 if both P_{cj} and E_0 are adjustable.

Section 8
The thermochemical equations

8.1 Overview

CHEETAH solves the same physical model as TIGER: there are t chemical species present, composed of c elements. A single gaseous phase composed of s species is in chemical equilibrium with $t - s$ condensed phases. Each condensed phase is comprised of a single chemical species. Condensed phases may undergo solid-liquid phase transitions. Of the t condensed species (referred to as "constituents" in the TIGER documentation, p are assumed to have nonzero concentrations at equilibrium, while the remaining $t - p$ condensed constituents are assumed absent.

CHEETAH solves for the concentrations in the gaseous phase given the guesses about the presence or absence of condensed constituents, then checks if these guesses are valid. Stoichiometry is then used to determine the mole numbers of the condensed constituents. CHEETAH uses the following variables to describe the gaseous phase: the mole numbers of each gaseous constituent n_i, the temperature T, and the inverse volume of gas per unit mass of mixture $\hat{\rho}$.

The Newton solver in CHEETAH operates with logarithmic variables, so the quantities $\xi_i \equiv \ln n_i$, $\ln T$, and $\ln \hat{\rho}$ are the independent variables in the solver. CHEETAH has the capability to freeze the mole numbers of given species, in which case the corresponding ξ_i are simply omitted from the solver. We will establish the notation that F_i is the ith equation in the Newton solver. The variables in CHEETAH must satisfy stoichiometric equations, balance of chemical potentials, and two thermodynamic conditions. These equations are discussed in more detail below.

8.2 Stoichiometry

There are c equations which express the conservation of the mole number of each element. Stoichiometry is usually expressed in terms of the total amount of each element:

$$\sum_{j=1}^{s} \alpha_{i,j} n_i + \sum_{j=1}^{t-s} \alpha_{i,j+s} N_j = Q_i, \tag{8.1}$$

where $\alpha_{i,j}$ is the formula matrix, N_j is the mole number of condensed constituent j, and Q_i is the number of moles of element i.

In CHEETAH, however, stoichiometry is handled through the selection of c reference species. This is the same scheme used in TIGER. These species are referred to as "components". The formulas of the component species serve as basis vectors for the description of the stoichiometry. Matters are further specialized by the convention that condensed constituents assumed to have nonzero concentrations are always chosen to be components. We have:

$$\sum_{m=p+1}^{p'} \beta_{i'(m),j} N_m + \sum_{i=1}^{s} \beta_{i,j} n_i + N_j = q_j \quad j = 1 \cdots p \tag{8.2}$$

$$\cdots = q_j \quad j = p+1 \cdots c. \tag{8.3}$$

Here, $p' - p$ is the number of frozen condensed constituents. CHEETAH solves for Eq. (8.3) as part of the Newton solver, while Eq. (8.2) is used to determine the N_j for each set of $\{n_j\}$. This gives us

$$F_j \equiv q_j - \sum_{m=p+1}^{p'} \beta_{i'(m),j} N_m - \sum_{i=1}^{s} \beta_{i,j} n_i = 0, \quad j = 1 \cdots c - p \tag{8.4}$$

In TIGER, Eq. (8.4) is substituted into the equations for the ηs.

8.3 Chemical potential balance

CHEETAH solves for chemical equilibrium between the constituents by balancing chemical potentials. The balance equations can be understood by constructing a

set of fictitious decomposition reactions:

$$Y_j \Leftrightarrow \sum_{i=1}^{c} \beta_{j,i} Y_i \quad j = 1 \cdots t. \tag{8.5}$$

The final chemical equilibrium obtained is unaffected by the use of fictitious reactions, as long as t linearly independent reactions are used. The decomposition reaction is trivial if constituent j is a component:

$$Y_j \Leftrightarrow Y_j \quad \text{if } j \text{ is a component} \tag{8.6}$$

Gibb's condition for chemical equilibrium of these reactions is

$$\mu_j = \sum_{i=1}^{c} \beta_{j,i} \mu_i \quad j = 1 \cdots t. \tag{8.7}$$

CHEETAH uses the non-trivial chemical potential balance equations in the Newton solver:

$$F_{j+c-p} = \mu_{j'} - \sum_{i=1}^{c} \beta_{j',i} \mu_i \quad \text{if } j' \text{ is not a component,} \tag{8.8}$$

where $j = 1 \cdots s - c + p$, and $j' = j + c - p$.

8.4 Thermodynamic state

The last two equations in CHEETAH defines the thermodynamic state. CHEETAH allows the user to specify any two variables from the list (p, v, T, E, H, S). Depending on what variables are specified, CHEETAH evaluates the apropriate thermodynamic function. The following equations are used:

8.4.1 p specified

The equation to be solved is

$$F_j = \ln(p/p_0), \tag{8.9}$$

where p_0 is the specified value of p. p is evaluated in subroutine STATEG through the equation of state relation:

$$p = \frac{nRT}{M_0}\hat{\rho}(\hat{\rho}, T, n_1, \ldots, n_s), \tag{8.10}$$

where n is the total mole number, M_0 is the total mass of the sample, and is the gas imperfection factor.

8.4.2 v specified

The equation to be solved is

$$F_j = \frac{pM_0}{RT}(v - v_0), \tag{8.11}$$

where the specific volume v is evaluated as:

$$\frac{pM_0 v}{RT} = \frac{pM_0}{\hat{\rho}RT} + \sum_{j=1}^{p'} N_j \phi_j^*, \tag{8.12}$$

where ϕ_j^* is the reduced molar volume of the jth condensed constituent, defined by

$$\phi^*{}_j = \frac{pV_j^*}{RT}, \tag{8.13}$$

where V_j^* is the molar volume of the jth condensed constituent.

8.4.3 T specified

In this case the equation is simply

$$F_j = \ln T - \ln T_0 \tag{8.14}$$

8.4.4 H specified

The equation is

$$F_j = \frac{M_0}{RT}(h - h_0), \tag{8.15}$$

where h_0 is the specified enthalpy and

$$\frac{M_0 h}{RT} = \sum_{j=1}^{p} N_j {\chi^*}_j + \sum_{i=1}^{s} n_i {\chi^0}_i + \frac{pM_0}{RT} + \epsilon - n. \tag{8.16}$$

${\chi^*}_j \equiv H_j^*/RT$ is the reduced molar enthalpy of condensed constituent j. ${\chi^0}_j$ is the reduced enthalpy of the jth gaseous constituent at the standard pressure of 1 Atm. ϵ is the nonideality correction factor for the enthalpy, defined as

$$\epsilon = \int_0^{\hat{\rho}} \frac{M_0}{RT\hat{\rho}^2}\left[p - \frac{\partial p}{\partial \ln T}\right] d\hat{\rho}, \tag{8.17}$$

where the integral is along an isotherm.

8.4.5 S specified

The equation used is

$$F_j = \frac{M_0}{RT}(TS_0 - H + G), \tag{8.18}$$

where the Gibbs free energy is evaluated with

$$M_0 G = \sum_{j=1}^{p'} N_j {\mu^*}_j + \sum_{i=1}^{s} n_i \mu_i. \tag{8.19}$$

8.4.6 E specified

The equation used is

$$F_j = \frac{M_0}{RT}(H - pv - E_0), \tag{8.20}$$

where E_0 is the specified energy.

8.5 The Jacobian matrix

The partial derivatives of the F_j with respect to system variables χ_i, $\ln T$, $\ln \hat{\rho}$ are called the Jacobian matrix. The Jacobian matrix, used in the Newton solver, is evaluated analytically in CHEETAH. This subsection gives the formulas used in evaluating the Jacobian matrix.

8.5.1 Stoichiometric equations

The derivatives are quite simple for these equations:

$$\frac{\partial F_j}{\partial \xi_k} = -\beta_{k,j} n_k \tag{8.21}$$

$$\frac{\partial F_j}{\partial \ln \hat{\rho}} = 0 \tag{8.22}$$

$$\frac{\partial F_j}{\partial \ln T} = 0 \tag{8.23}$$

8.5.2 Chemical potential balance

The relation

$$\mu_i/RT = \mu_i^0/RT + \xi_i + {}_i + \ln(RT\hat{\rho}/M_0), \tag{8.24}$$

is used to re-write the chemical potential balance equations. Here, ${}_i$ is a non-ideality term. This leads to the form:

$$\begin{aligned} F_j &= \xi_j - {}_j + \sum_{k=1}^{p} \beta_{jk} \frac{\mu_k^*}{RT} + \sum_{k=p+1}^{c} \beta_{jk}(\xi_{i*(k)} + {}_{i*(k)}) \\ &\quad + \beta_{j,c+1} \ln(RT\hat{\rho}/M_0) - \frac{\mu_j^0}{RT} + \sum_{k=p+1}^{c} \beta_{jk} \frac{\mu_k^0}{RT} \end{aligned} \tag{8.25}$$

Here $\beta_{i,c+1} \equiv \sum_{j=p+1}^{c} \beta_{ij}$. The resulting derivatives are

$$\frac{\partial F_j}{\partial \xi_k} = -\delta_{jk} - \frac{\partial {}_j}{\partial \xi_k} + \sum_{l=1}^{p} \beta_{jl} \phi_l^* \frac{\partial \ln p}{\partial \xi_k} + \sum_{l=p+1}^{c} \beta_{jl} (\delta_{i*(l),j} + \frac{\partial {}_{i*(l)}}{\partial \xi_l}) \tag{8.26}$$

$$\frac{\partial F_j}{\partial \ln \hat{\rho}} = -\frac{\partial_j}{\partial \ln \hat{\rho}} + \frac{\partial \ln p}{\partial \ln \hat{\rho}} \sum_{k=1}^{p} \beta_{jk}\phi^*_k + \sum_{k=p+1}^{c} \beta_{jk} \frac{\partial_{i*(k)}}{\partial \ln \hat{\rho}} + \beta_{i,c+1} \tag{8.27}$$

$$\frac{\partial F_j}{\partial \ln T} = \frac{\partial_j}{\partial \ln T} - \sum_{k=1}^{p} \beta_{jk}\chi^*_k + \sum_{k=p+1}^{c} \frac{\partial_{i*(k)}}{\partial \ln T}\beta_{jk} + \beta_{j,c+1} + \chi^0_j$$
$$- \sum_{k=p+1}^{c} \beta_{jk}\chi^0_k + \sum_{k=1}^{p} \beta_{jk}\phi^*{}_k \frac{\partial \ln p}{\partial \ln T} \tag{8.28}$$

8.5.3 Thermodynamic state equations

The thermodynamic functions in CHEETAH are linear combinations of the variables p, v, H, and G. These variables serve as a basis for the evaluation of derivatives of thermodynamic functions. We begin with the pressure derivatives:

$$\frac{\partial \ln p}{\partial \xi_k} = n_k \left[\frac{\partial}{\partial n_k} + 1/n\right] \tag{8.29}$$

$$\frac{\partial \ln p}{\partial \ln \hat{\rho}} = 1 + \frac{\partial}{\partial \ln \hat{\rho}} \tag{8.30}$$

$$\frac{\partial \ln p}{\partial \ln T} = 1 + \frac{\partial}{\partial \ln T} \tag{8.31}$$

where is the equation of state imperfection factor, and n is the total gaseous mole number.

It is most convenient to express the volume derivatives in terms of the reduced volume $v^* \equiv pM_0 v/RT$. The reduced volume is equal to

$$v^* = \frac{pM_0}{\rho RT} + \sum_{j=1}^{p'} N_j \phi^*{}_j. \tag{8.32}$$

The partial derivatives are given by

$$\frac{\partial v^*}{\partial \xi_k} = \frac{pM_0}{\rho RT}\frac{\partial \ln p}{\partial \xi_k} - \sum_{j=1}^{p} \beta_{kj} n_k \phi^*{}_j + \sum_{j=1}^{p'} N_j \phi^*{}_j (1 + \beta^*_j)\frac{\partial \ln p}{\partial \xi_i} \tag{8.33}$$

$$\frac{\partial v^*}{\partial \ln \hat{\rho}} = \frac{pM_0}{\rho RT}\left(\frac{\partial \ln p}{\partial \ln \hat{\rho}} - 1\right) + \sum_{j=1}^{p'} N_j \phi^*{}_j (1 + \beta_j) \tag{8.34}$$

$$\frac{\partial v^*}{\partial \ln T} = \frac{pM_0}{\rho RT}\left(\frac{\ln p}{\ln T} - 1\right) + \sum_{j=1}^{p'} N_j \phi^*{}_j \left[\alpha_j - 1 + \frac{\partial \ln p}{\partial \ln T}(\beta_j + 1)\right] \tag{8.35}$$

The enthalpy equations are expressed in terms of the reduced enthalpy $H^* \equiv M_0 H/RT$. We then have

$$H^* = \sum_{j=1}^{p} \chi^*{}_j \left(q_j - \sum_{i=1}^{s} \beta_{ij} n_i\right) + \sum_{i=1}^{s} n_i \chi_i^0 + \frac{pM_0}{\hat{\rho} RT} + \epsilon - n + \sum_{m=p+1}^{p'} N_m \chi^*{}_m \tag{8.36}$$

The resulting derivatives are

$$\frac{\partial H^*}{\partial \xi_k} = -\sum_{j=1}^{p} \beta_{kj} n_k \chi^*{}_j + \sum_{j=1}^{p'} N_j \phi^*{}_j (1 - \alpha_j) \frac{\partial \ln p}{\partial \xi_k} + \frac{pM_0}{\rho RT} \frac{\ln p}{\xi_k} - n_k \frac{\partial_k}{\partial \ln T} + n_k (\chi_i^0 - 1) \tag{8.37}$$

$$\frac{\partial H^*}{\partial \ln \hat{\rho}} = \sum_{j=1}^{p'} N_j \phi^*{}_j (1 - \alpha_j) \frac{\partial \ln p}{\partial \ln \hat{\rho}} + \frac{pM_0}{\rho RT}\left(\frac{\partial \ln p}{\partial \ln \hat{\rho}} - \frac{\partial \ln p}{\partial \ln T}\right) + \frac{\partial \epsilon}{\partial \ln \hat{\rho}} \tag{8.38}$$

$$\frac{\partial H^*}{\partial \ln T} = \sum_{j=1}^{p'} N_j \left(\frac{C_{pj}^*}{R} - \chi^*{}_j + \frac{\partial \ln p}{\partial \ln T}[\phi^*{}_j - phis_j \alpha_j]\right) \tag{8.39}$$

$$+ \sum_{i=1}^{s} n_i \left(\frac{C_{pi}}{R} - \chi_i^0\right) + \frac{pM_0}{\rho RT}\left(\frac{\partial \ln p}{\partial \ln T} - 1\right) + \frac{\partial \epsilon}{\partial \ln T} \tag{8.40}$$

We finally consider the reduced Gibbs free energy $G^* \equiv M_0 G/RT$. We have

$$G^* = \sum_{j=1}^{p'} N_j \mu_j^* + \sum_{i=1}^{s} n_i \mu_i, \tag{8.41}$$

and the following derivatives:

$$\frac{\partial G^*}{\partial \xi_k} = \sum_{j=1}^{p'} N_j \phi^*{}_j \frac{\partial \ln p}{\partial \xi_k} - \sum_{j=1}^{p} \beta_{kj} n_k \frac{\mu_j^*}{RT}$$
$$+ n_k \left(\frac{\mu_k^0}{RT} + \xi_k + {}_k + \ln(RT\hat{\rho}/M_0) + \sum_{i=1}^{s} n_i (\delta_{ki} + \frac{\partial_i}{\partial \xi_k}) \right) \quad (8.42)$$

$$\frac{\partial G^*}{\partial \ln \hat{\rho}} = \sum_{j=1}^{p'} N_j \phi^*{}_j \frac{\partial \ln p}{\partial \ln \hat{\rho}} + \sum_{i=1}^{s} n_i \left(\frac{\partial_i}{\partial \ln \hat{\rho}} + 1 \right) \quad (8.43)$$

$$\frac{\partial G^*}{\partial \ln T} = \sum_{j=1}^{p'} N_j \phi^*{}_j \frac{\partial \ln p}{\partial \ln T} + \sum_{i=1}^{s} n_i \left(\frac{\partial_i}{\partial \ln T} - \chi_i^0 + 1 \right) - \sum_{j=1}^{p'} N_j \chi^*{}_j \quad (8.44)$$

Section 9
Error messages

One common source of errors in entering CHEETAH commands is misplaced commas. For instance, the command `point, p, , t, 2000` specifies the calculation of a thermodynamic point at the current pressure and a temperature of 2000K. It is easy to forget the comma and enter `point, p, t, 2000` instead. It is also important to remember that CHEETAH recognizes all the characters of a command. This is different from TIGER, in which only the first few were significant. For instance, CHEETAH will report an error if the library command `constituent` is misspelled as `constitent`. A greater degree of consistency is required with the names of chemical compounds. In TIGER, `aloxide` and `aloxid` were the same material. CHEETAH, on the other hand, distinguishes between long names. The following is an alphabetical listing of the error messages produced by CHEETAH.

cheetah error - instruction is not acceptable
You have entered a command that CHEETAH does not understand. Check for typographical errors or mispelling.

cheetah error - too many constituents chosen, maximum is N
You have entered too many product molecules with the `choose` command. The maximum number of product molecules can be increased by changing `config/alloc.in`.

cheetah error - too many constituents ordered, maximum is N
You have entered too many product molecules with the `order` command. The `order` command should not be necessary in CHEETAH.

cheetah error - too many constituents rejected, maximum is N
You have rejected more product molecules than CHEETAH is capable of handling. Make a temporary version of the product library with the rejected molecules deleted instead.

compos error - composition card not acceptable

You have made a mistake in entering the `composition` command. Check to make sure that all the required arguments are given.

compos error - constituents selected can not satisfy mass balance equations
The reactant mixture has a mass ratio that cannot be obtained with the current set of products. For instance, if we have 10% oxygen by mole and 50% Fe by mole, the reactant mixture cannot be described with Fe2O3 alone. The usual solution to this error is adding more product species.

compos error - formula name has not been defined
A formula name was used as an argument to the `composition` command that has not been defined. Check carefully for misspellings. Also, remember that a `formula` command disables use of the reactant library, so all reactants must be entered explicitly once `formula` is used.

compos error - no gaseous constituents selected
CHEETAH requires that at least one gaseous species is present. Purely condensed problems cannot be treated. This limitation can be worked around by choosing a gaseous product that is will be present only in very small concentrations; e.g. gaseous C.

compos error - not all ordered constituents are in the library
A compound was used in the `order` command that is not present in the product library.

compos error - too many condensed constituents
The specified composition requires more condensed constituents than CHEETAH allows.

compos error - too many gaseous constituents
The specified composition requires more gaseous constituents than CHEETAH allows.

error in allocate: could not open alloc.in
The `alloc.in` file is required for CHEETAH to dimension its arrays on startup. If the `alloc.in` file is in your `config` directory, be sure that the CHCONFIG environment variable is set to the full pathname of the `config` directory.

error in autoform: the file formula.in does not exist
The file `config/ formula.in` is searched for data on reactants. `formula.in` either does not exist or could not be opened. If the `formula.in` file is in your `config` directory, be sure that the CHCONFIG environment variable is set to the full pathname of the `config` directory.

error in autoform: formula S not found
The autoform subroutine looks up a formula name in the reactant library `config/ formula.in`. If the formula name is not in the database, either add the corresponding `formula` command to `formula.in` or add explicit `formula` commands to the input file.

error in calculating a thermo point: the state equations must be different
The point command was given with two identical arguments (e.g. `point, t, 100, t, 200`).

error in checkphase: couldn't identify k3
This is an internal error. Please file a bug report if it occurs.

error in chemeqn: temperature got too low
The parametrization of the 1 atm heat capacity in CHEETAH is not accurate at temperatures substantially below room temperature. CHEETAH will not calculate points in the low temperature regime.

error in cjbrent: couldn't bracket root
The C-J point solver failed. This is an internal error; please file a bug report if it occurs.

error in cjfunc: n is not 1
This is an internal error. Please file a bug report if it occurs.

error in cjsolve: the reference state must be specified first
The `C-J` command was given without first specifying the shock Hugoniot reference state through the `hug0` command.

error in compos: the maximum number of reactants was exceeded
Too many reactants were specified in the `composition` command. The maximum number of reactants can be increased by editing `config/ alloc.in`.

error in convrt: argument out of range
This is an internal error. Please file a bug report if it occurs.

error in convrt: bad index
This is an internal error. Please file a bug report if it occurs.

error in dumpstrings: could not open string.in
The file `config/ string.in` contains all character strings known to CHEETAH. For some reason CHEETAH was unable to write to this file. Be sure that you have write permission to the `config` directory.

error in etanewt: ludcmp2 failed
The chemical equilibrium equations were singular.

error in etanewt: solution violated maximum bounds
The solution of the chemical equilibrium equations violated bounds based on stoichiometry. This is an internal error. Please file a bug report if it occurs.

error in findeta, continuing ...
Chemical equilibrium was not found. Another attempt will be made.

error in formla: the maximum number of reactants was exceeded
The maximum number of reactants can be increased by modifying `config/ alloc.in`.

error in freader: bad index
This is an internal error. Please file a bug report if it occurs.

error in hug0: first argument must be 'p'
The pressure must be the first argument to `hug0`.

error in hug0: not enough arguments
The initial pressure and specific volume must be specified in the hug0 command.

error in hug0: pressure must be positive

error in hug0: rho must be positive

error in hug0: specific volume must be positive

error in inputfile: the specified input file could not be opened
The `load file` command specified a file that did not exist or could not be opened.

error in inststr: bad index
This is an internal error. Please file a bug report if it occurs.

error in jwlerr: ludcmp failed
Linear equations solved in the JWL fitting process became singular.

error in jwlerr: solution check failed
This is an internal error. Please file a bug report if it occurs.

error in jwlfit: not enough cylinder runs performed
More points along the adiabat must be calculated to uniquely determine the JWL equation of state.

error in libfile: need an argument for the library file command

error in libray: too many condensed products defined
The maximum number of condensed products can be increased by changing the `config/ alloc.in` file.

error in libray: too many elements defined.
The maximum number of elements can be increased by changing the `config/ alloc.in` file.

error in libray: too many gaseous products defined.
The maximum number of condensed products can be increased by changing the `config/ alloc.in` file.

error in mixfunc: ecompo failed
Chemical equilibrium could not be found for a mixed phase calculation.

error in opensummary: couldn't open summary file
The specified summary file could not be opened. This typically occurs when a

non-writable file of the specified name already exists.

error in print_inst: bad index
This is an internal error. Please file a bug report if it occurs.

error in printout: bad mode
This is an internal error. Please file a bug report if it occurs.

error in reader: line begins with a number
An input line began with a digit. Since CHEETAH commands begin with alphabetic values, this is an error.

error in reader: unrecognized character
A character outside of CHEETAH's character set was used in the input file. For example, a % is not allowed in the input file.

error in reader: unrecognized command
An invalid command was encountered in the input file.

error in standardrun: couldn't open config/ standard.in
The file `config/ standard.in` controls the standard run. It could not be opened. If `standard.in` exists in your `config` directory, make sure that the CHCONFIG environment variable is set to the full pathname of the `config` directory.

error in standardrun: end of file reached in config/ standard.in
Lines were missing from the `config/ standard.in` file.

error in units: unrecognized command
A bad argument was given to the `units` command.

explos error - input not acceptable
A mistake was made in entering the explos command. Check for the right number of arguments.

findrh error - excessive iterations for rho
The iteration procedure to invert the gaseous equation of state to find the density failed to converge.

findtp error - excessive iterations for t

The iteration procedure to invert the gaseous equation of state to find the temperature failed to converge.

fixcon error - input card error
The input to the `fix concentration` command was incorrect.

fixcon error - no such constituent
An attempt was made to fix the concentration of a product molecule that was not defined.

formla error - formula card not acceptable
The `formula` command was not entered correctly.

freadj error - frozen constituents violate mass balance
Mass balance could not be achieved with the frozen set of constituents. Please report it if this error occurs.

freeze error - no such constituent
An undefined product molecule was used in the `freeze` command.

meltit error - no such constituent

mixxed error - error in field
A bad argument was given to mixed phase.

mixxed error - next point did not converge
CHEETAH was unable to calculate a thermodynamic point in a mixed phase calculation.

mixxed error - no such species
The requested species was misspelled or not defined.

mixxed error - wrong number of fields on card

poinnt error - input not acceptable
The `point` command was invoked with bad or missing arguments. Check for missing commas.

recall error - this point not saved

savept error - too many points saved

select error - no acceptable components
A linearly independent set of products could not be chosen as a basis to represent the stoichiometry. Try adding more species to the product library.

statec error - condensed equation of state did not converge

thermo error - iteration exceeded
A thermodynamic point could not be calculated within the maximum number of tries.

thermo error - mixed phase error
A thermodynamic point in the solid-liquid phase coexistence region could not be calculated.

a floating point error occurred in cheetah
Divide by zero or some other floating point problem occurred.

error: bad argument to hug0

error: bad argument to spreadsheet

error: c-j velocity went imaginary
This is an internal error. Please file a bug report if it occurs.

error: the hugoniot reference state was not initialized
The C-J command was called before the shock Hugoniot was defined with the `hug0` command.

error: unable to find good phase presence assumptions in chekpres
A set of phase presence equations satisfying thermodynamic stability with positive

concentrations could not be found. This is an internal error. Please file a bug report if it occurs.

internal error in checkpres: didn't set condensed assumptions correctly
This is an internal error. Please file a bug report if it occurs.

internal error in newguess
This is an internal error. Please file a bug report if it occurs.

Section 10
Source code

Extensive changes have been made to TIGER in the writing of CHEETAH. The most obvious of these is that CHEETAH is written entirely in the C programming language, whereas TIGER was written in FORTRAN. FORTRAN routines from TIGER were converted to C with the f2c FORTRAN to C converter. C was chosen partly due to the author's taste and partly due to the ready availability of dynamic memory allocation in C. New code being added to CHEETAH is written directly in C.

The converted FORTRAN code is still readable (or at least no more unreadable than TIGER was) if one keeps in mind the relationship between C and FORTRAN constructs. Common block FORTRAN variables have been placed into external C data structures. For instance, the FORTRAN code

```
common / junk / a, b, c

a = 10.0
```

is replaced by the C code

```
extern struct {
     Real a, b, c ;
} junk ;

junk.a = 10.0 ;
```

Variables in CHEETAH are declared as either Real or integer. Currently these are typedefs to double and long. A future single precision version of CHEETAH for PC's, however, would use alternative typedefs.

Arrays have been converted to pointers which are dynamically allocated. For instance, the FORTRAN code

```
common / junk / a(100), b(100,100)

a(i) = 2.0
b(j,k) = 4.0
```

is replaced by

```
struct {
     Real *a, *b ;
}

a[i-1] = 2.0 ;
b_ref(j,k) = 4.0 ;
```

Here, `b_ref` is a macro defined in `cheetah.h`. `a` and `b` are allocated in the function `allocate` when CHEETAH starts up.

Below we give a briefly annotated list of the C functions in CHEETAH.

allocate
This function allocates memory upon startup.

bkweqn
This function evaluates the BKW[4] equation of state.

brent2
This function is a modified version of the Numerical Recipes one dimensional minimizer.

calcgd
This function calculates the Gibbs free energy and its partial derivatives.

calcgd2
This function calculates the Gibbs free energy. It is a new version of calcgd.

calchd
This function calculates the enthalpy and its derivatives.

calchd2
This function calculates the enthalpy.

calcnd
This function calculates the concentrations.

calcnd2
This is a new version of calcnd.

calcvd
This function calculates the specific volume and its derivatives.

calcvd2
This function calculates the specific volume.

checktraces
This sets trace concentrations, and checks to see if constituents assumed to be present in trace quantities actually were.

cheetah_alloc
This allocates memory. It's an interface to malloc, etc.

cheetah_free
This frees memory. It's an interface to free.

chemeqn
This evaluates the chemical equilibrium equations.

cjbrent
This is a modified version of the Numerical Recipes[8] brent solver. It finds the C-J state.

cjsolve
This is a wrapper for cjbrent. It does preliminary work, calls cjbrent, and prints the output.

cjsummary
This outputs C-J state information to the summary state.

compos
This selects constituents for the system.

compsummary

This prints the composition to the summary file.

coneqn
This evaluates the condensed equation of state.

cosh_
The hyperbolic cosine.

cylsum
This writes a summary of adiabat ("cylinder") points.

dcjfunc
This evalutates the equation solved by cjbrent.

denthalpy
Derivatives of the enthalpy with respect to the concentrations, etc. are evaluated.

dgibbs
Derivatives of the Gibbs free energy with respect to the concentrations, etc. are evaluated.

dmatrix
This is a Numerical Recipes[8] routine to allocate a double precision matrix.

do_exit
Exits the program.

dpressure
Derivatives of the pressure with respect to the concentrations, etc. are evaluated.

dumpstrings
This function writes currently known character strings to `config/ string.in`.

dvector
This is a Numerical Recipes[8] routine to allocate a double precision matrix.

dvolume
Derivatives of the volume with respect to the concentrations, etc. are evaluated.

ecompo

This is a driver for solving the composition equations.

ecompout
This prints output after ecompo is finished.

edet
This calculates the energy of detonation.

etainit
This initializes the etas and thermodynamic variables before solving the equilibrium equations.

etaupdate
This updates derivatives with respect to the etas after findmol has been called.

explos
This calculates a constant volume explosion point.

explossum
This puts information about the constant volume explosion point in the summary file.

f1dim
This is a wrapper function used by linmin.

f1dim2
This is another linmin wrapper.

feasib
Determines whether a feasible solution exists to a linear programming problem. This is used to find whether a good set of constituents exits.

findeta
This solves the chemical equilibrium equations. It is called by ecompo.

findmax
This finds the maximum possible values of the gaseous mole numbers.

findrh
This inverts the gaseous equation of state to find the density

findtp
This inverts the gaseous equation of state to find the temperature.

fixcon
This sets flags and concentrations of the frozen constituents.

formla
This sets data regarding a reactant.

freadj
This readjusts concentrations if the frozen concentrations violate mass balance.

freeze
This freezes the concentration of a given constituent.

gridle
This runs a grid of thermodynamic points.

guessx
This guesses initial concentrations.

idealg
This evaluates the ideal gas equation of state.

imatrix
This allocates an integer matrix (Numerical Recipes[8] style).

indexx
This produces a set of sort keys for a given array.

inststring
This returns the string associated with a given token number.

invert
This inverts a matrix

isolin
This executes the isoline command.

ivector

This allocates an integer vector (Numerical Recipes[8] style).

jcz3eq
This evaluates the JCZ[6] equation of state.

libray
This reads and writes a library file.

linear
This determines whether the ith column of a matrix is linearly independent of those preceding it.

linmin
This minimizes a function of many variables along a line.

loadstrings
This reads in character strings from `config/ string.in`

lvector
This allocates a vector of long integers (Numerical Recipes style).

main
The main program.

mapvar
This establishes a mapping between active variables in the Newton solver and gaseous constituents.

matrix
This allocates an integer matrix (Numerical Recipes[8] style).

max
The maximum of two numbers.

meltit
This unfreezes a concentration.

min
The minimum of two numbers.

mixfunc
This evaluates the equation to be solved when in the mixed solid/liquid regime.

mixxed
This calculates the solid-liquid phase coexistence line for a particular materical.

mnbrak
This brackets a minimum.

mnbraks
This is a minimum bracketer used in linmin.

nint
This calculates the nearest integer to a floating point number.

oldcon
The evaluates the "old" (polynomial) equation of state.

pagecheck
This checks if a page header should be printed.

poinnt
This calculates a thermodynamic point.

prelement
This prints information regarding an element.

prinnt
This prints thermodynamic variables, etc. after a thermodynamic point has been calculated.

print_head
This prints the header for the thermodynamic variables.

print_inst
This prints a text string given a token number.

print_lhead
This prints the long header for the thermodynamic variables.

prtcon
This prints concentrations.

read_libtitle
This reads the title from the compiled library file.

recall
This executes the recall command.

rorder
This executes the rorder command.

savept
This executes the save command.

select
This selects a linearly independent set of constituents as a basis for representing the system.

set_state0
This sets the desired value of a thermodynamic variable.

setpha
This sets initial solid/liquid phase assumptions.

setunits
This sets up user-defined units.

sigfdie
This makes the program die upon floating point errors.

sigidie
This makes the program die upon integer errors.

solveq
This solves a set of simultaneous linear equations using the triangularized matrix produced by subroutine linear.

solvex
This solves N linear equations with N unknowns by Gaussian elimination with partial

pivoting.

spreadout
This writes data out to a spreadsheet file.

statec
This calculates condensed equation of state data.

stateg
This calculates gaseous equation of state data.

stater
This calculates reference (1 atm) equation of state data.

store_ccon
This stores condensed concentrations for later printing.

store_cj
This stores the C-J state for the JWL fitter.

store_con1
This stores the names and concentrations of the first equilibrium point in an isolin.

store_con2
This stores the names and concentrations of a subsequent equilibrium point in an isolin.

storefreeze
This stores the state variables that freezing occurred at.

storestate
This stores the current thermodynamic state.

thermo
This solves a thermodynamic point.

thermoeqn
This evaluates the

titlepage

This prints out the CHEETAH banner.

vector
This allocates a floating point vector (Numerical Recipes style).

work
Calculates the gas phase PV work.

zbrac
This brackets a root of a one dimensional equation.

zbrent
This solves a one dimensional equation.

Section 11
Caveats and limitations

CHEETAH is an ongoing project to produce the next generation of thermochemical code. There are many problems to address, and not enough time or manpower to fix all of them in a single year. In this section we will outline some issues which the careful user should be aware of.

The first is that CHEETAH is a pure thermochemical code. It gives answers based on the C-J theory of plane-wave detonation in an infinite system. Unfortunately, finite size effects are often important in an explosive. CHEETAH can give a good answer (i.e. an accurate prediction of detonation in the infinite size limit), but the answer doesn't always match up to the problem you are interested in. As a practical illustration, Clark Souers at LLNL[7] ran CHEETAH on a mixture of AN and fuel oil (ANFO), and predicted a detonation velocity of 7 mm / μs. This value was far higher than any previous measurements. A large-scale test was conducted with 2.8 million pounds of ANFO. A detonation velocity of 7 mm / μs was indeed observed, along with a distance to steady-state detonation of 4 meters. The lesson is that thermochemical codes can give accurate infinite-size predictions, but that real experimental situations are often far from the infinite size limit. We intend to extend CHEETAH to give finite size predictions the future. This is a complicated problem, however, since such predictions will require a combination of kinetic information and reactive flow hydrodynamic modeling. Until that time, however, caution should be used in applying predictions of CHEETAH to small scale tests of highly non-ideal explosives.

A second problem is that condensed species in CHEETAH's product libraries are poorly parametrized. As far as we know, this problem is shared by all current TIGER libraries. The condensed species in the large product library of Hobbs and Baer[3] are virtually the same (where overlap exists) as the much smaller BKWR[5] library used at LLNL. The problem is this: reference state information (e.g. thermodynamics at 1 ATM) has been entered for the condensed species from JANAF tables. This information is sound. The condensed phase equation of state comes

into play when predicting properties away from 1 ATM. Most condensed species have "minimalist" condensed equations of state: only a volume is entered, without compressibility or a coefficient of thermal expansion. This can have serious consequences when there is a substantial portion of condensed material at the C-J state. As an example, Al2O3 has been set with 0 compressibility in many TIGER libraries. As a consequence, it is treated as having an infinite sound speed. If the C-J point contains a substantial fraction of Al2O3, there will be a corresponding overestimate of the detonation velocity. Obviously, what is needed is a comprehensive condensed library that fits the latest shock Hugoniot data. We are working on such a library, but it will not be available in this version of CHEETAH.

In CHEETAH Version 1.0 we have replaced TIGER's solvers with an improved set of equation solvers. Our goal has been to maintain most of the speed of TIGER while enhancing the reliability and ease of use of the program. The treatment of condensed species in the underlying equations, however, is similar to that of TIGER. Assumptions are made about the presence or absence of condensed species. The gaseous concentrations first found given the assumptions; then the condensed concentrations are determined at the end. This methodology is very fast when there are only one or two condensed species. Unfortunately, there are some inherent limitations in the procedure. One is that only "linearly independent" condensed species can appear at once. For instance, it is impossible to have Fe2O3, Fe, Al2O3, and Al present at once in CHEETAH, because Al2O3 = Fe2O3 – Fe + Al. Another issue is the dramatic slowdown of the code as the number of condensed species increases. Future versions of CHEETAH will most likely have a more robust "slow solver" that works by minimizing free energy, in addition to the present "fast solver". The fast solver will be used by default, while the slow solver will be used for problems involving a large number of condensed species.

Index

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CHEETAH commands

Run type selection

c-j point
det energy
explosion
hug0
grid
isoline
mixed phase
point
standard run
stop

Product library

card list
constituent
element
end of library
library file
start of library
stc
stg
str

Input/output

details
load file
original output
print selection
reactants reaction
spreadsheet
summary
title
units

Product species

choose
destroy
fix concentration
freeze
melt
order
reject
retain

Reactant species

composition
formula

Gaseous equation of state

gas eos
set

Miscellaneous

jwlfit
recall point
save point

DATE

FILMED

8/9/94

END