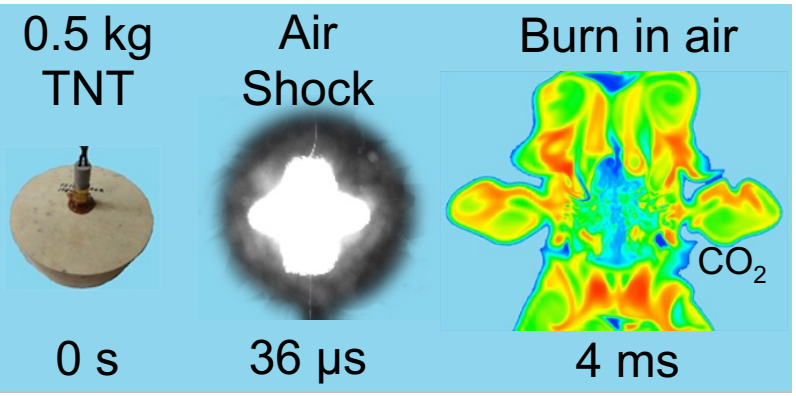
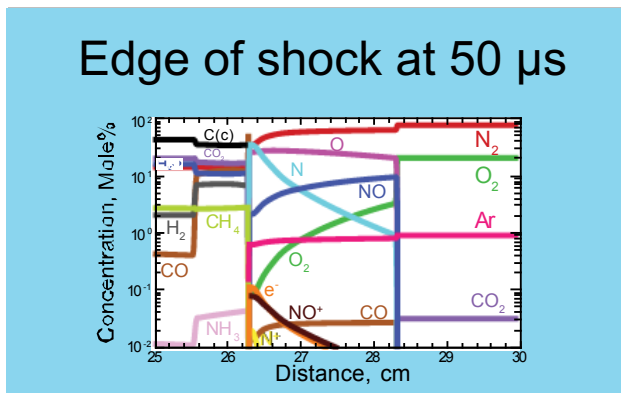
SAND2022-7946C

Exceptional service in the national interest

Sandia National Laboratories





TIGER Tutorial 2022

Michael L. Hobbs

Sandia National Laboratory, USA

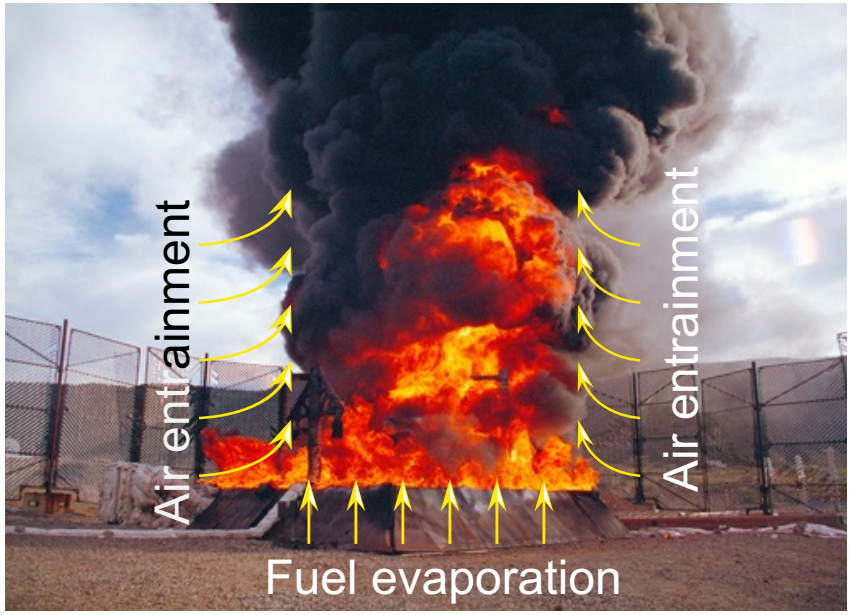
U.S. DEPARTMENT OF ENERGY

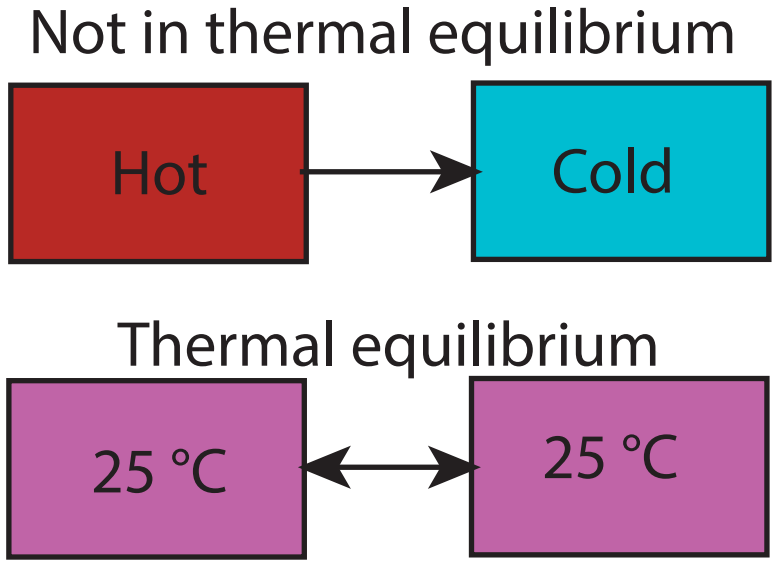
NNSA National Nuclear Security Administration

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000. SAND NO. 2014-19288 PER

Simple solutions to complex problems

- Complex problem is 3D fuel fire radiating to an object
- Simple solution is adiabatic flame assuming equilibrium and air entrainment.





Entrainment velocity is about 8% of vertical velocity

Equilibrium assumes well-mixed and no time dependence

Chemical equilibrium attained when the chemical potential is minimized

Sandia National Laboratories

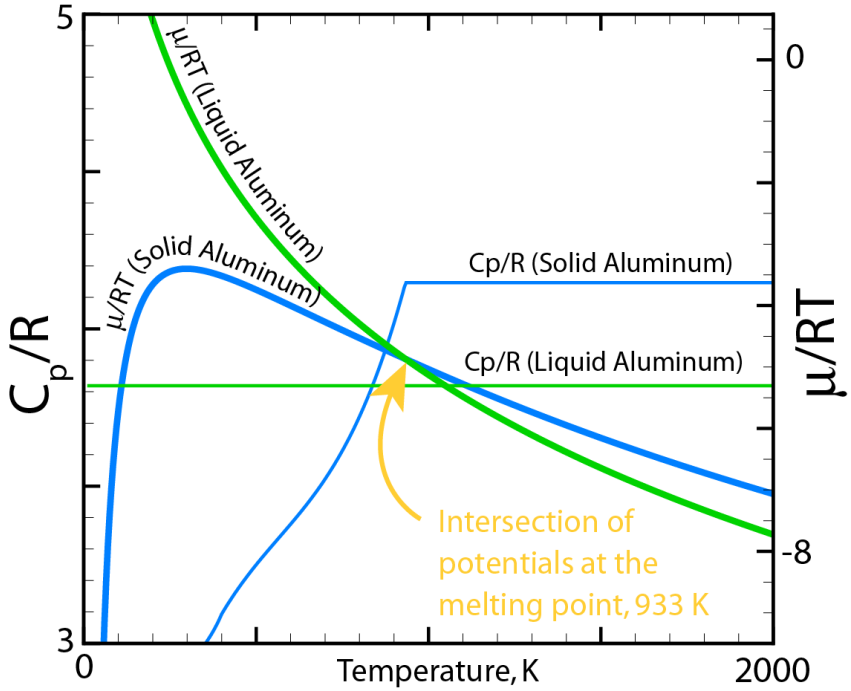
$$C_p = a_1 T^{-2} + a_2 T^{-1} + a_3 + a_4 T + a_5 T^2 + a_6 T^3 + a_7 T^4$$

$$H = \int C_p \, dT$$

$$S = \int \frac{C_p}{T} dT$$

Chemical Potential at 1 bar

$$\frac{\mu_o}{RT} = \frac{H_o}{RT} - \frac{S_o}{RT}$$



Chemical Potential:

$$\frac{\mu_i}{RT} = \frac{\mu_i^o}{RT} + \text{ imperfection terms which are functions of the EOS}$$

All we need is specific heat and an equation of state.

Melting point at elevated pressure is one way to test EOS!

History of Equation of State at Sandia

Sandia National Laboratories

1950's	1960's	1970's	1990's & 2000's		2010's
LRL[a]	SRI[c] Wiebenson et al.,[4] 1968	SRI[c] Cowperthwaite & Zwisler,[2,5] 1973	SNL[d] Hobbs & Baer,[7] 1992	LLNL[e] JCZS, Hobbs et al.,[1] 1999	SNL[d] JCZS2i
Ruby				BKWC, Fried et al.,[9] 1996	
LASL[b] BKW[6]	TIGER Modular (ideal,BKW)	TIGER Modular (ideal,BKW,JCZ)	TIGER BKWS[7] Large EOS database	Exp-6, Fried et al.,[10] 2002 CHEETAH Fried,[8] 1994 Graphical interface	CTH-TIGER Piecewise C_p fits Over 200 ions New water EOS Coupled shock code

[a]Lawrence Radiation Laboratory (LRL)
[b]Los Alamos Scientific Laboratory (LASL)
[c]Stanford Research Institute (SRI)
[d]Sandia National Laboratories (SNL)
[e]Lawrence Livermore National Laboratory (LLNL)

2020's JCZS4
Byers Brown EOS
Stand-alone code

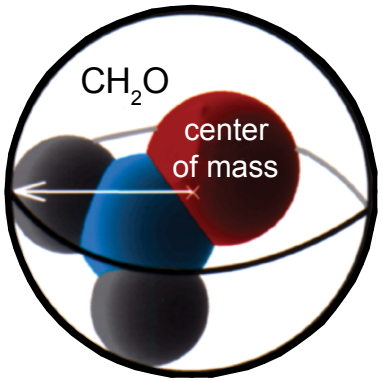
High pressure, temperature EOS basics

Sandia National Laboratories

BKW, covolume based

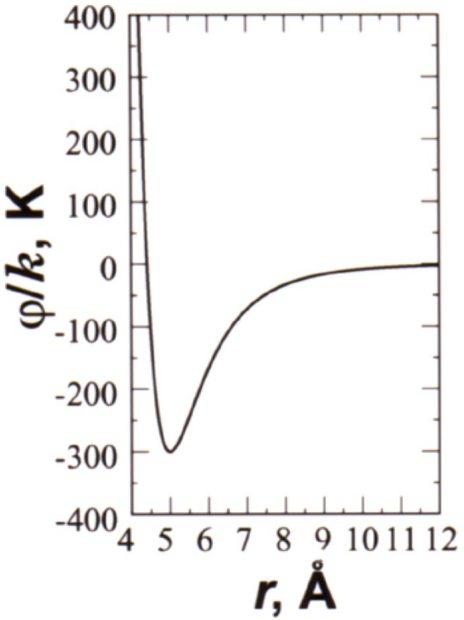
$$\frac{PV}{RT} = 1 + X\exp(\beta X)$$

$$X = \frac{\mathrm{K}\sum n_i k_i}{V\left(T+\theta\right)^{\alpha}}$$



JCZ, intermolecular potential based

$$P = \frac{G\left(V,T,\varphi\right)nRT}{V} + P_o\left(V,\varphi\right)$$

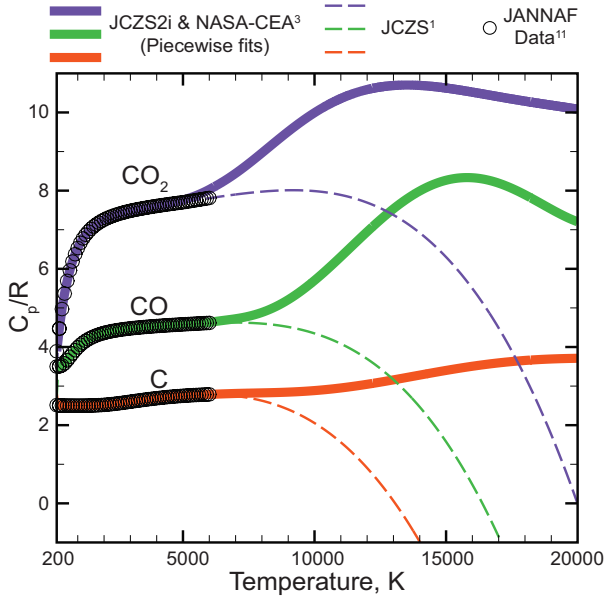


Thermodynamics

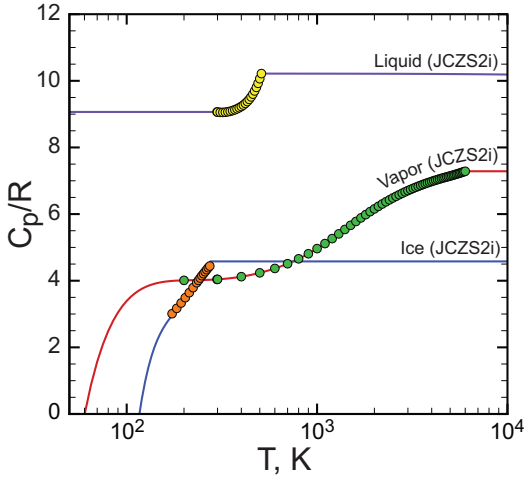
$$C_p/R = \sum_{i=1}^{7} a_i T^{i-3} \qquad \left(\partial S/\partial T\right) = C_p/T$$

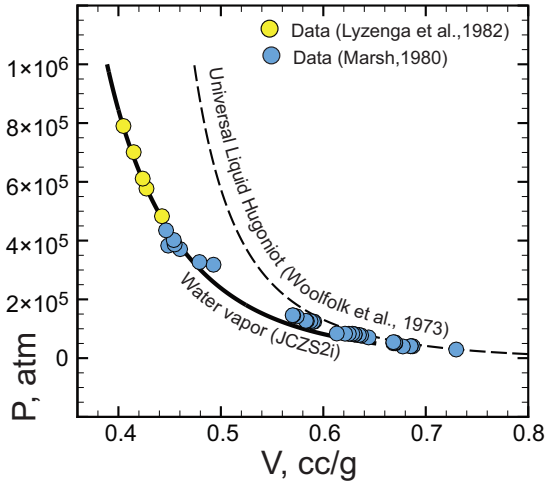
$$C_p = \left(\partial H/\partial T\right)_p \qquad S = \int \frac{C_p}{T} dT$$

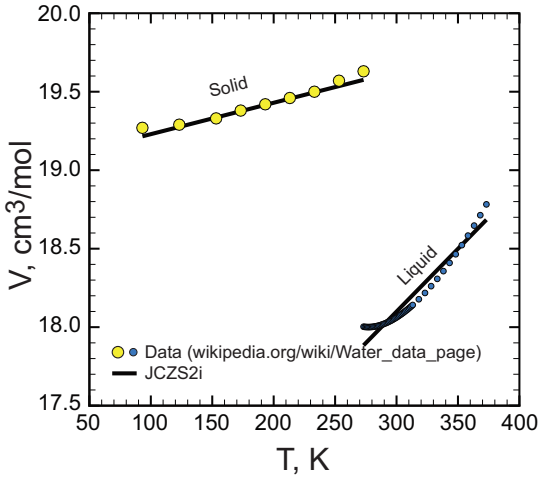
$$h = \int C_p dT \qquad \mu/RT = H/RT - S/R$$

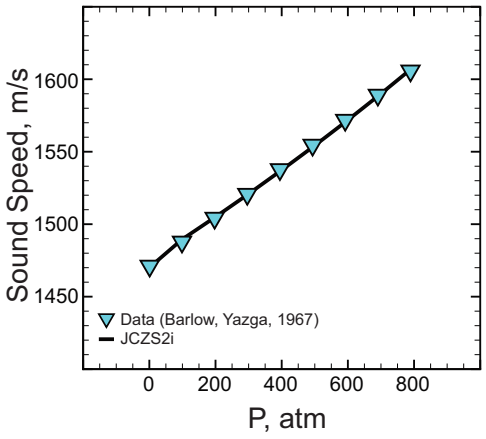


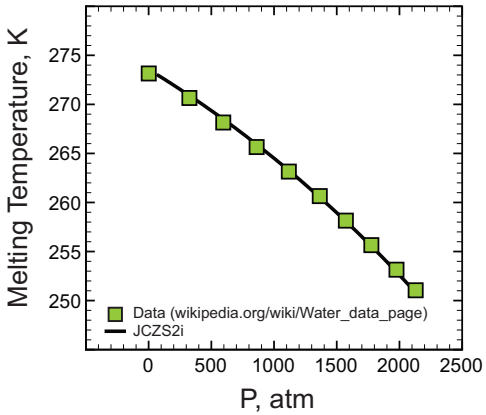
Water EOS

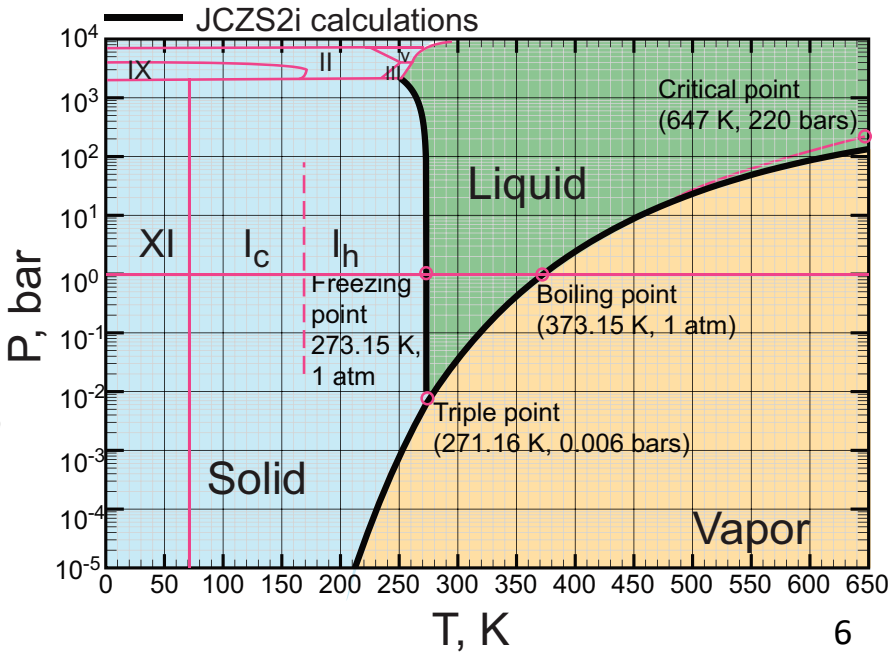






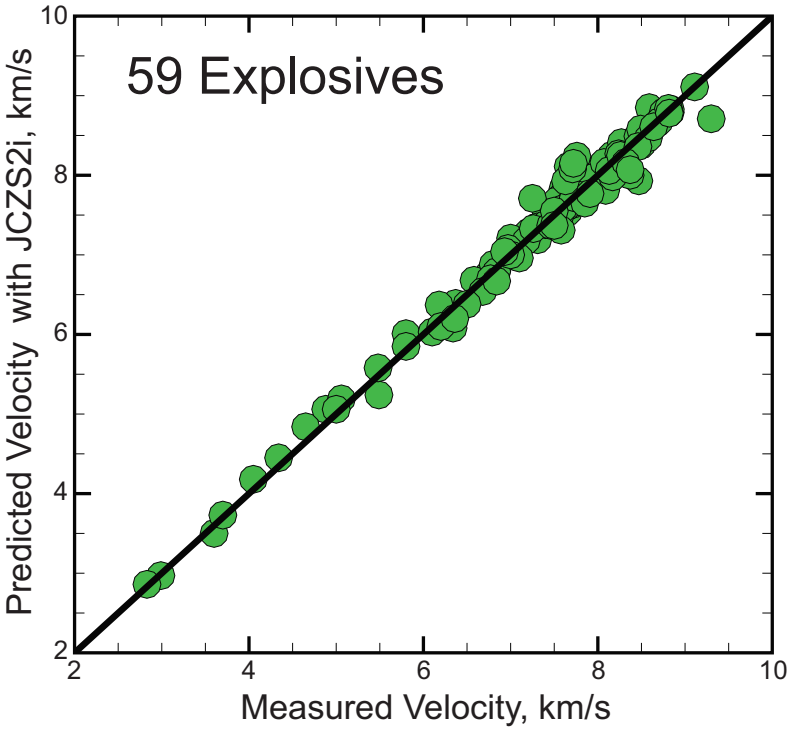






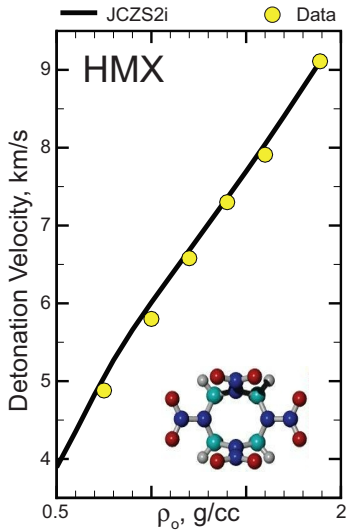
$$V = A + BT + CP\exp\left(1 - P/D\right)$$

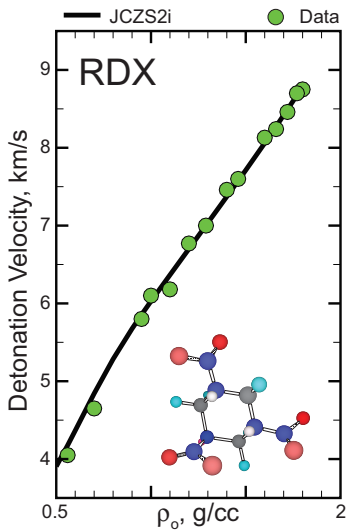
Detonation predictions

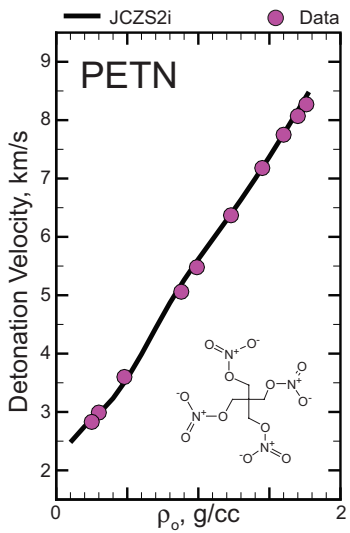


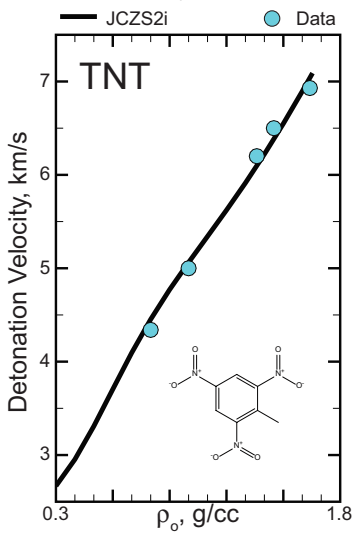
	Mean Absolute Error	RMS Error
JCZS[a]	1.76%	2.37%
Exp-6[b]	1.90%	2.51%
JCZS2i	1.73% Awesome!	2.34%

[a]Hobbs, M. L., Baer, M. R., McGee, B. C., Propellants, Explosives, Pyrotechnics, 24, 269-279 (1999).
[b]Fried, L. E., Howard, W. M., Souers, P. C. 12th International Detonation Symposium, San Diego, CA p. 567 (2002)







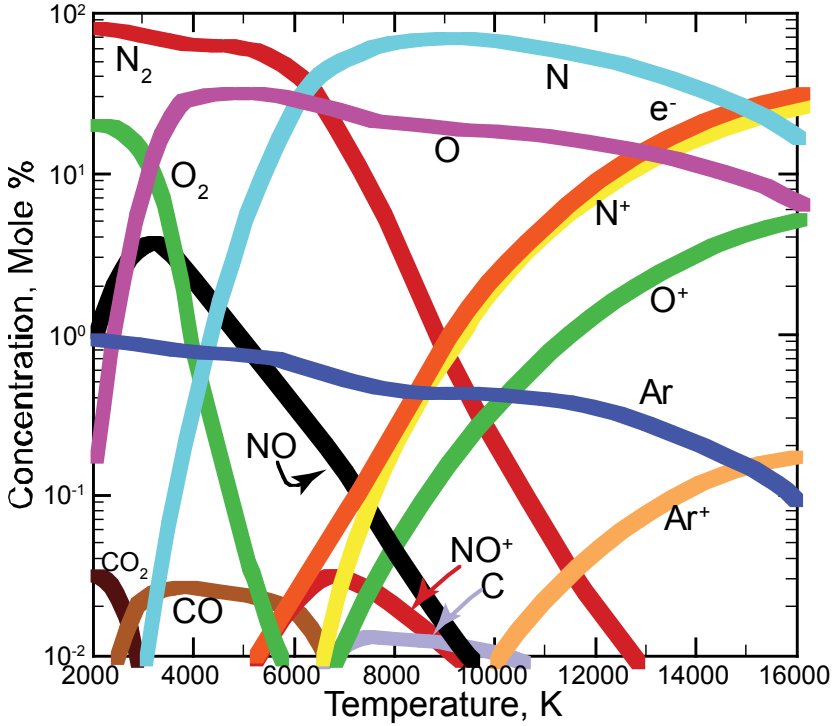


Air at low pressure, high temperature

Sandia National Laboratories

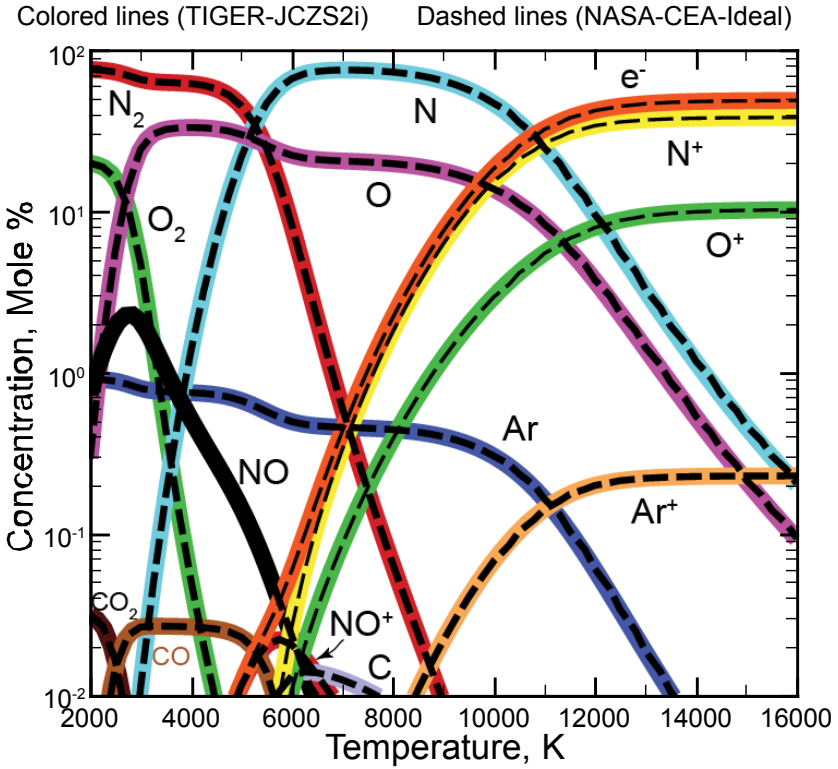
1950's

P = 0.01 atm, (Vincenti, Kruger, 1967)



Air at 0.01 atm

P = 0.01 atm, improved C_p

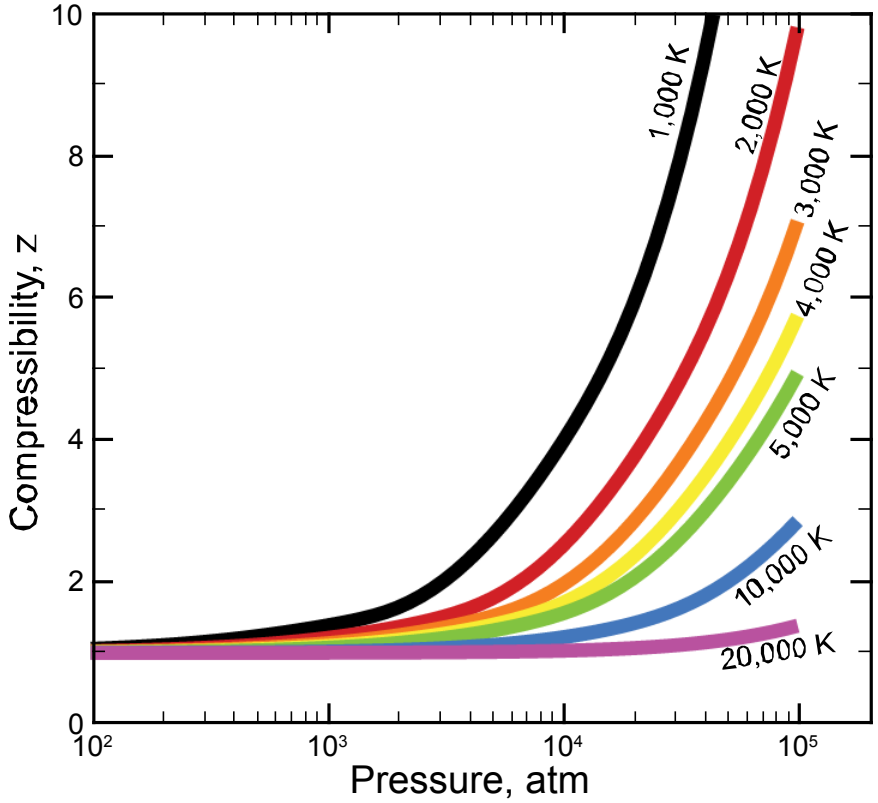


NASA-CEC and CTH-TIGER give same results at low pressure.

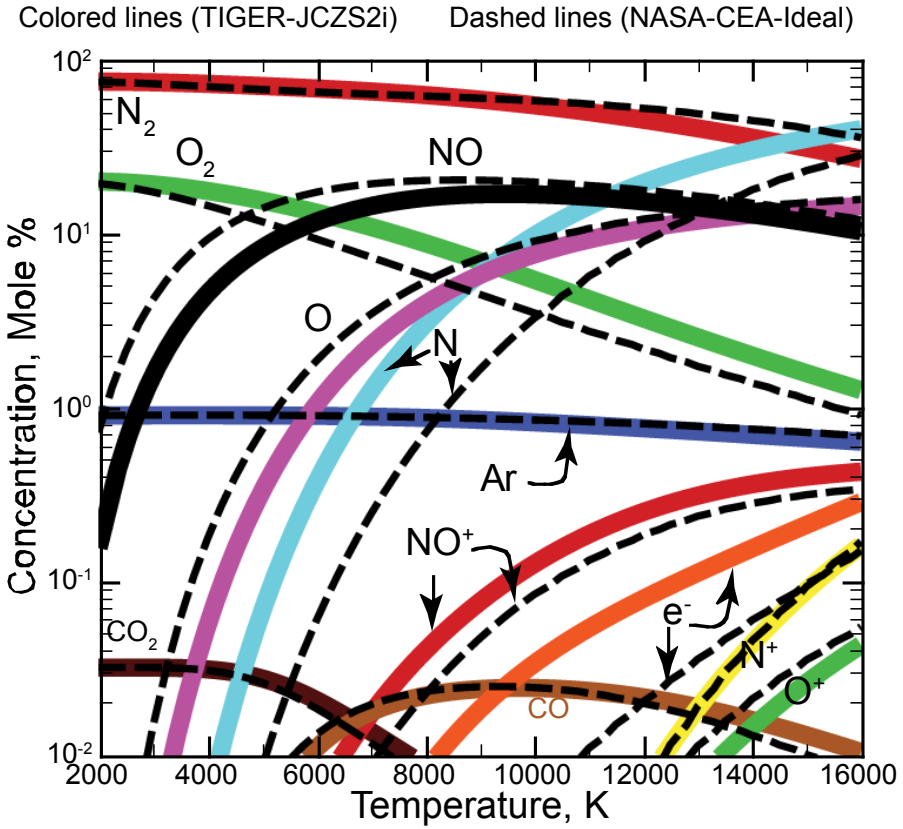
Air at high temperature and pressure

Sandia National Laboratories

Air Compressibility



Air at 100,000 atm

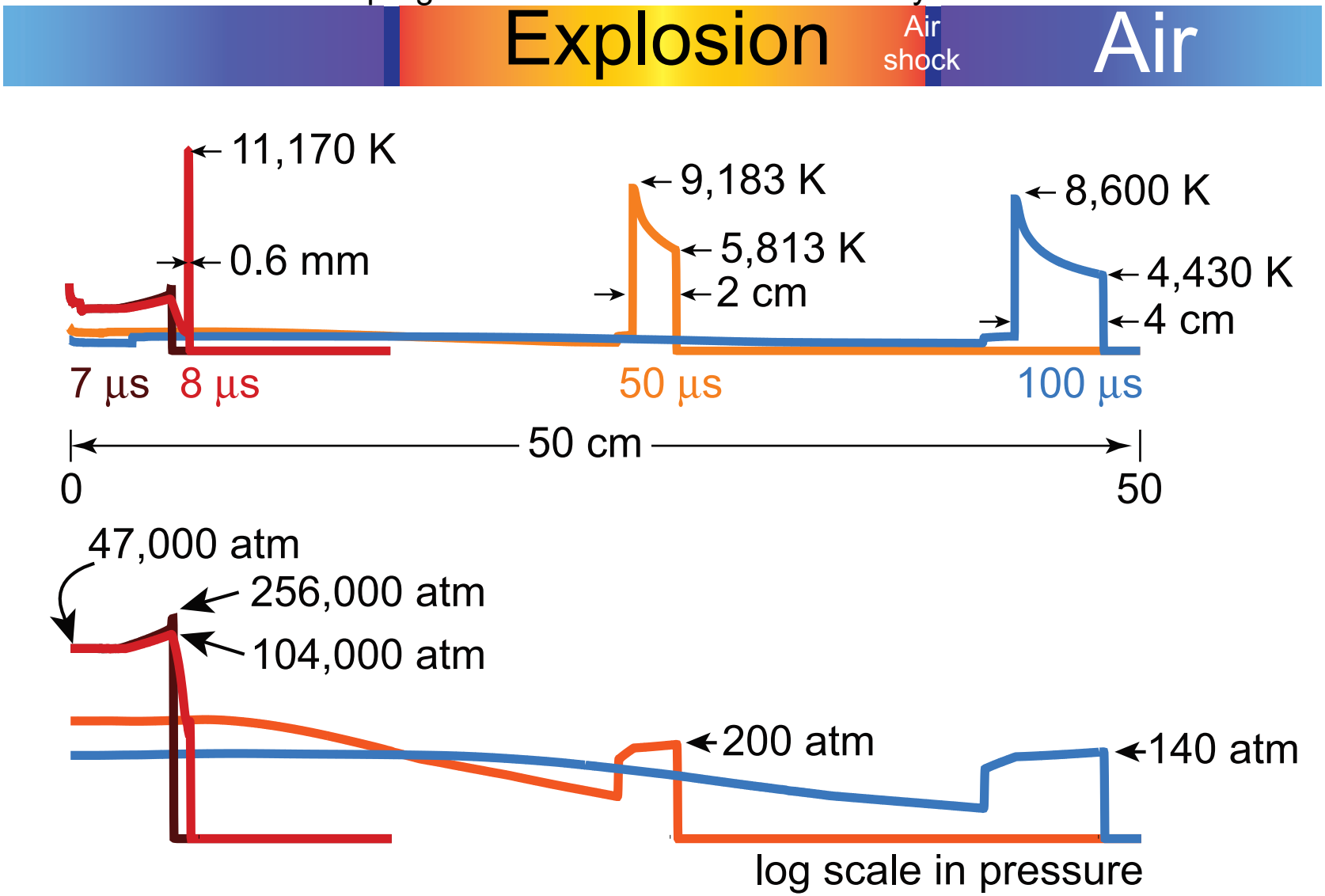


*Debye-Hückel effect is negligible on air compressibility. Calculation from Hilsenrath J. and Klein M., National Bureau of Standards, Washington, D.C. (1965).

Air shock from TNT detonation

Sandia National Laboratories

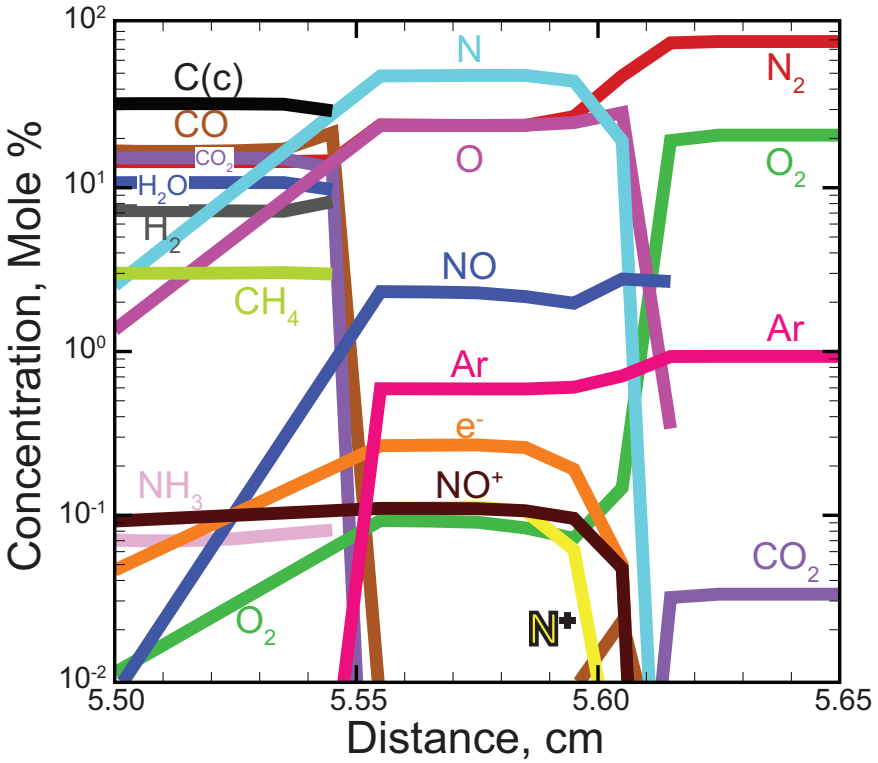
CTH programmed burn of a 5 cm radius cylinder.



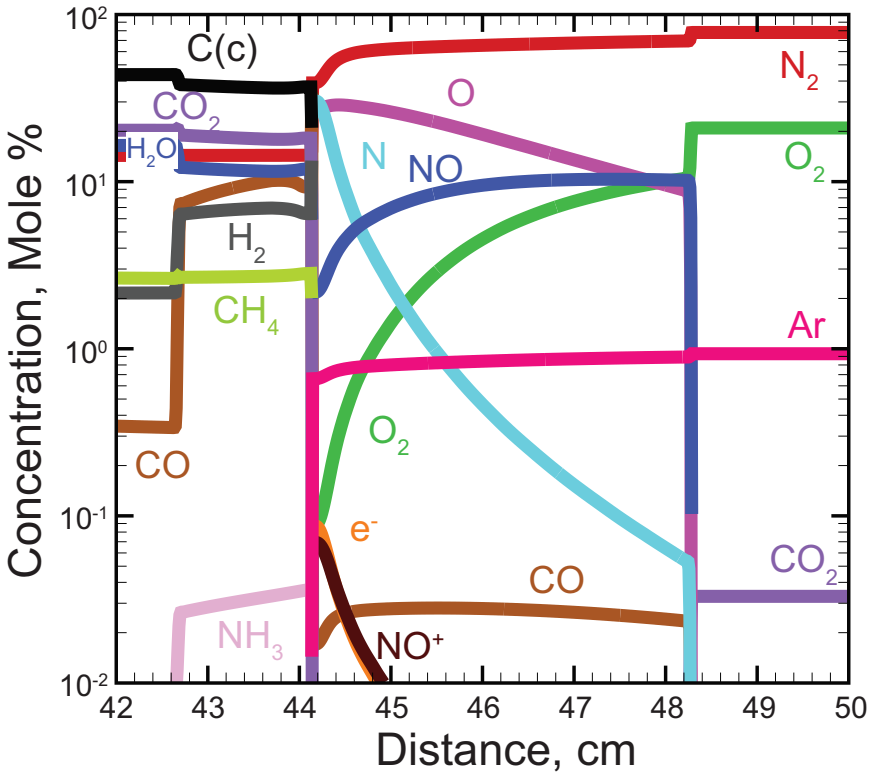
Edge of shock at 8 µs and 100 µs

Sandia National Laboratories

8 µs



100 µs



CTH programmed burn with JCZS-EOS fit with CTH TIGER JWL fitter. Initial geometry is a 5 cm radius cylinder. Profiles plotted at 8 and 100 µs.

reflected wave | air shock | quiescent air

Quick hands on tutorial
(best to do while running TIGER)

- CTH-TIGER is distributed with CTH
- CTH-TIGER can be coupled to CTH or run as a stand-alone-code.
- The users manual is built into the code.
- Philosophy for code is to provide a fast, robust, explosives calculator to answer many questions. We'll discuss a few.

```
INPUT > help
 help
 Type 'help, command' where command can be any of the following:*
    aft, p, 1             === Adiabatic flame temperature
    cardlist              === Library command to list library cards
    c-j, p, 1, rho, 1.9   === Chapman Jouget (CJ) point calculation
    check                 === EOS checking flag
    choose, n2, co2, h2o  === Choose constituents
    composition, hmx, 1   === Composition of mixture
    cve, rho, 1.9         === Constant volume explosion giving TNT equivalence
    debug                 === Turns on extra printing
    det, p, 1, rho, 1.9   === CJ point calculation giving TNT equivalence
    element,o,16,o,2,v,24464,s,49,0B,-1 === Element definition card
    end                   === End calculations
    exit                  === Exit calculations
    exp, rho, 1.9         === Constant volume explosion calculation
    fixcon, al, 5, mole   === fix concentration to given mol/kg-mix
    for,hmx,17925,155,0,n,8,p,8,c,4,h,8 === Formula definition card
    freeze, o2, co        === Freeze constituents
    geos, ideal           === Set the gaseous equation of state
    grid,corner,p,1,10,4e5,t,300,10,6e3 === Calculate a grid of points
    help, c-j             === print out help information (e.g. about c-j)
    hug,p,35000,5000,45000,p,,v,0.39,eof === points along a Hugoniot curve
    ion                   === include ions in jczs3 library
    iso,s,,p,,1000,1,log  === points along an isoline
    jou                   === toggle to save commands in tiger.jou
    jwl, p, 1, rho, 1.89  === Compute C-J pt, isentropic expansion, fit JWL
    lib, jczs3            === Change product library to jczs3
    lim, 50               === Limit products mw to be less than 50 g/mol
    melt, co2, co         === Melt overrides previous freeze commands
    mixed,al2o3,t,3000,100,6000 === Compute mixed phase line
    noi                   === do not include ions in jczs3
    nol                   === Do not limit product selection by molecular wt.
    order,co,h2,co2       === Order gases for better component guesses
    original output       === Print thermodynamic variables as absolute values
    plot, h2o(c)          === Print T_K Cp/R h/RT S/R u/RT for h2o(c)
    plt, p, t, h2o        === Print p, t, and h2o to tiger.plt file
    point, p, 1, t, 3000  === (p,t);(p,h);(p,s);(p,v);(v,t);(v,e);(v,s);(s,t)
    reactants output      === Print thermodynamic variables as differences
    recall, old           === Recall point named 'old' (see 'save' command)
    reject, al,al2o3      === Reject constituents from calculations
    reset                 === Resets with a p=3000,t=3000 point calculation
    rxn                   === Toggle to print reaction stoichiometry
    save, old             === Save point named 'old' (used with 'recall' command)
    set, jcz3,l,13        === Change gaseous EOS constants
    start of library      === Specifies beginning of library commands
    stop                  === Stop calculations

*Only the first 3 characters are significant and case does not matter.
```

Adiabatic flame calculation ($H_2 + 0.5O_2$)

```
INPUT > help, aft
 help, aft
 ********** Help with 'aft' help screen **********

 The 'aft' command is used to calculate the adiabatic flame
 temperature at a given pressure. If no argument is given
 the adiabatic flame temperature is calculated at 1 atm.
 Otherwise, the adibatic flame temperature is calculated
 at the given pressure.

 Some examples:
   1) Most common:     aft
   2) Same command:    aft,p,1
   3) Higher pressure: aft,p,20

 Here are results* from Glassmans 1987 Combustion Book, pg 25:
 Fuel              Pressure  T(K)  jcz jczs jczs2 jczs2i
 C2H2+2.5O2+9.4N2   1 atm   *2600 2548 2539  2538   2538
 C2H2+2.5O2         1 atm   *3410 3522 3342  3338   3338
 CO+0.5O2+1.88N2    1 atm   *2400 2388 2384  2383   2383
 CO+0.5O2           1 atm   *3220 3043 2977  2975   2975
 C7H16+11O2+41.38N2 1 atm   *2290 2276 2274  2273   2273
 C7H16+11O2         1 atm   *3100 3178 3107  3102   3102
 H2+0.5O2+1.88N2    1 atm   *2400 2385 2382  2380   2380
 H2+0.5O2           1 atm   *3080 3126 3079  3073   3073
 CH4+2O2+7.5238N2   1 atm   *2210 2226 2225  2224   2224
 CH4+2O2+7.5238N2  20 atm   *2270 2276 2275  2275   2275
 CH4+2O2            1 atm   *3030 3109 3054  3048   3048
 CH4+2O2           20 atm   *3460 3506 3455  3448   3448
 NOTE: I believe there is something wrong with Glassmans
       CO+0.5O2 calculation. Everything else is close.

 Here is how to do the last two calculations in this table:

     lib, jczs2i
     com, ch4,1,o2,2,mole
     aft
     aft,p,20
     stop
```

```
INPUT > help, com
 help, com
 ********** Help with composition **********

 Two examples:
   1) Mass basis: com, hmx, 1, rdx, 1, tnt, 1, petn, 1
   2) Mole basis: com, hmx, 1, rdx, 1, tnt, 1, petn, 1, mole

 NOTES:
 A) These examples assumed that the individual ingredients are defined
    in formula.lib. If they are not in formula.lib, they can be defined
    using the 'formula' command (type 'help, formula' for more info).
 B) The arguments are alternating alpha and numeric where the formula
    name is followed by the relative amount in the mixture.
 C) If the last argument is alpha, then the relative amounts are assumed
    to be based on moles, else they are assumed to be based on mass.
 D) The examples show 25% by mass (example 1) or 25% by mole (example 2).
```

```
INPUT > com, h2, 1, o2, 0.5, mole
 com, h2, 1, o2, 0.5, mole

 Reactants:

   Name  % weight   % mole   % volume   mol. wt.   Formulas
 h2       11.195    66.667    66.855     2.0169    h2e2
# h2,          hydrogen gas
 o2       88.805    33.333    33.145     32.000    o2e2
# o2,          oxygen gas

   Name  rho[g/cc]  hf[cal/mol]  V[cc/mol] S[cal/K mol]
 h2        0.000      0.000        0.2467E+05     0.000
 o2        0.001      0.000        0.2446E+05     0.000

 Initial mixture:
   Heat of formation =    0.000    cal/g
   Standard energy   =   -49.61    cal/g
   Standard volume   =    2048.    cc/g
   Standard entropy  =   0.000     cal/(g-K)
   Standard density  =   0.4882E-03g/cc

 Number of gaseous constituents   =  10
 Number of condensed constituents =   1
 Molecular formula of mixture (ave. mw =  12.0112    g/mol)
   Elements    moles        % moles      % mass
   h           1.3333       33.333       11.188
   e           2.0000       50.000      0.91345E-02
   o          0.66667       16.667       88.802
Oxygen balance:    0.00 %
```

Adiabatic flame calculation ($H_2 + 0.5O_2$)

Sandia National Laboratories

1 atm: Glassman says 3080 K

3073 K

Cheetah V8 gives 2990 K

```
INPUT > aft
 aft

 ************************************
 **  adiabatic flame temperature   **
 **         3072.86 K              **
 **           1.0000     Atm       **
 ************************************
 Current library is jczs3
 Using JCZ3 EOS with reference state based on reactants (R):

   H(R) = H - (    0.000)    E(R) = E - (  -49.608)       S(R) = S - (    0.000)

   1.) Thermodynamic STATE of products:
       P [atm]:                    1.000000
       V [cc/g]:                   16997.93
       Rho [g/cc]:                0.5883069E-04
       T [K]:                      3072.859
       H(R) [cal/g]:              0.2702163E-04
       E(R) [cal/g]:              -362.0488
       S(R) [cal/(gK)]:            4.358922
       Vg [cc_gas/g_gas]:          16997.93
       Rho_g [g_gas/cc_gas]:      0.5883069E-04
       V_hat [cc_gas/g_mix]:       16997.93
       Rho_hat [g_mix/cc_gas]:    0.5883069E-04
       wgas [g_gas/g_mix]:         1.000000
       wcond [g_cond/g_mix]:     -0.6698359E-08
       phigas [v_gas/v_mix]:       1.000000
       phicond [v_cond/v_mix]:     0.000000
       rhoc [g_cond/cc_cond]:      0.000000
       Speed of sound [m/s]:       1383.616     = sqrt(dP/drho)_s = sqrt(adexp*P*V)
       Cv [cal/(gK)]:              3.993507     = (de/dT)_v
       Cp [cal/(gK)]:              4.777393     = cv+T(dV/dT)_p(dP/dT)_v
       Alpha [(1/P)*(dE/dV)_p]:    13.21073
       Beta [(1/V)*(dE/dP)_v]:     12.78491
       ADEXP [-(dlnP/dlnV)_s]:     1.111524     = -(V/P)*(dP/dV)_s = (Alpha+1)/Beta
       z (imperfection):           1.000080
       gas mol. wt. [g/mol]:       14.83532
       cond. mol. wt. [g/mol]:     0.000000
       mix mol. wt. [g/mol]:       14.83532

       Product YIELD (mol/kg_mix) and CONCENTRATION (gas mole %, mixture mole %)
       Name                 Phase   [mole/kg_mix]    [gas mole %]    [mix mole %]          mw
       h2o                  GAS      3.90011E+01      57.859          57.859          18.017
       h2                   GAS      1.01137E+01      15.004          15.004          2.0169
       oh                   GAS      7.63657E+00      11.329          11.329          17.008
       h                    GAS      5.13791E+00      7.6223          7.6223          1.0084
       o2                   GAS      3.34561E+00      4.9633          4.9633          32.000
       o                    GAS      2.16885E+00      3.2176          3.2176          16.000
       ho2                  GAS      2.73809E-03     0.40620E-02     0.40620E-02      33.008
       h2o2                 GAS      1.71646E-04     0.25464E-03     0.25464E-03      34.017
       o3                   GAS      1.17975E-06     0.17502E-05     0.17502E-05      48.000
       e-                   GAS      0.00000E+00      0.0000          0.0000         0.54858E-03
       h2o(c)               LIQUID   0.00000E+00   not applicable     0.0000          18.017
       TOTAL                GAS(g)   6.74067E+01
       TOTAL                COND(c)  0.00000E+00
       TOTAL                g+c      6.74067E+01
       h1.333e2o0.667 --> 0.80964     Gas +    0.0000      Cond
       Hrxn = -7.486E+06 J/kg exothermic at tref = 298.15
```

20 atm

Cheetah V8 gives 3427 K

```
INPUT > aft, p, 20
 aft, p, 20

 ************************************
 **  adiabatic flame temperature   **
 **         3490.74 K              **
 **           20.000     Atm       **
 ************************************
 Current library is jczs3
 Using JCZ3 EOS with reference state based on reactants (R):

   H(R) = H - (    0.000)    E(R) = E - (  -49.608)       S(R) = S - (    0.000)

   2.) Thermodynamic STATE of products:
       P [atm]:                    20.00006
       V [cc/g]:                   928.3045
       Rho [g/cc]:                0.1077233E-02
       T [K]:                      3490.739
       H(R) [cal/g]:              0.2128617E-01
       E(R) [cal/g]:              -400.0067
       S(R) [cal/(gK)]:            3.965276
       Vg [cc_gas/g_gas]:          928.2994
       Rho_g [g_gas/cc_gas]:      0.1077239E-02
       V_hat [cc_gas/g_mix]:       928.3045
       Rho_hat [g_mix/cc_gas]:    0.1077233E-02
       wgas [g_gas/g_mix]:         1.000006
       wcond [g_cond/g_mix]:     -0.5535194E-05
       phigas [v_gas/v_mix]:       1.000000
       phicond [v_cond/v_mix]:     0.000000
       rhoc [g_cond/cc_cond]:      0.000000
       Speed of sound [m/s]:       1456.031     = sqrt(dP/drho)_s = sqrt(adexp*P*V)
       Cv [cal/(gK)]:              2.615973     = (de/dT)_v
       Cp [cal/(gK)]:              3.114478     = cv+T(dV/dT)_p(dP/dT)_v
       Alpha [(1/P)*(dE/dV)_p]:    10.95807
       Beta [(1/V)*(dE/dP)_v]:     10.61105
       ADEXP [-(dlnP/dlnV)_s]:     1.126945     = -(V/P)*(dP/dV)_s = (Alpha+1)/Beta
       z (imperfection):           1.001412
       gas mol. wt. [g/mol]:       15.44993
       cond. mol. wt. [g/mol]:     0.000000
       mix mol. wt. [g/mol]:       15.44993

       Product YIELD (mol/kg_mix) and CONCENTRATION (gas mole %, mixture mole %)
       Name                 Phase   [mole/kg_mix]    [gas mole %]    [mix mole %]          mw
       h2o                  GAS      4.15301E+01      64.163          64.163          18.017
       h2                   GAS      8.75825E+00      13.531          13.531          2.0169
       oh                   GAS      7.33472E+00      11.332          11.332          17.008
       h                    GAS      3.08384E+00      4.7645          4.7645          1.0084
       o2                   GAS      2.60968E+00      4.0319          4.0319          32.000
       o                    GAS      1.39820E+00      2.1602          2.1602          16.000
       ho2                  GAS      9.49608E-03     0.14671E-01     0.14671E-01      33.008
       h2o2                 GAS      1.25994E-03     0.19466E-02     0.19466E-02      34.017
       o3                   GAS      8.58868E-06     0.13269E-04     0.13269E-04      48.000
       e-                   GAS      0.00000E+00      0.0000          0.0000         0.54858E-03
       h2o(c)               LIQUID   0.00000E+00   not applicable     0.0000          18.017
       TOTAL                GAS(g)   6.47256E+01
       TOTAL                COND(c)  0.00000E+00
       TOTAL                g+c      6.47256E+01
       h1.333e2o0.667 --> 0.77743     Gas +    0.0000      Cond
       Hrxn = -8.748E+06 J/kg exothermic at tref = 298.15
```

CJ Calculation (HMX at 1.89 g/cc)

Sandia National Laboratories

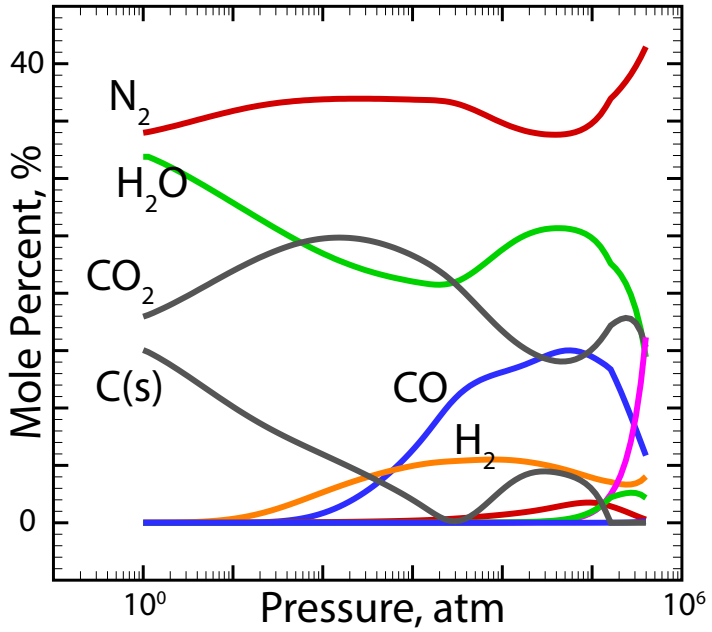
```
INPUT > c-j, p , 1, rho, 1.89
 c-j, p , 1, rho, 1.89
       ****** The Chapman-Jouguet condition ******
       The shock velocity    =   9.1058018E+03 m/s
       The particle velocity =   2.3379814E+03 m/s
       The speed of sound    =   6.7678204E+03 m/s
       ****** The Hugoniot reference state *******
       P0 =                      1.0000000E+00 atm
       V0 =                      5.2910053E-01 cc/g
       E0 =                      6.0511298E+01 cal/g
 Current library is jczs3
 Using JCZ3 EOS with reference state based on reactants (R):

   H(R) = H - (    60.524)    E(R) = E - (    60.511)        S(R) = S - (     0.000)

   2.) Thermodynamic STATE of products:
       P [atm]:                   397105.0
       V [cc/g]:                 0.3932501
       Rho [g/cc]:                2.542911
       T [K]:                     3653.203
       H(R) [cal/g]:              4435.161
       E(R) [cal/g]:              653.2454
       S(R) [cal/(gK)]:           1.699270
       Vg [cc_gas/g_gas]:        0.3932501
       Rho_g [g_gas/cc_gas]:      2.542911
       V_hat [cc_gas/g_mix]:     0.3932501
       Rho_hat [g_mix/cc_gas]:    2.542911
       wgas [g_gas/g_mix]:        1.000000
       wcond [g_cond/g_mix]:     0.2492935E-08
       phigas [v_gas/v_mix]:      1.000000
       phicond [v_cond/v_mix]:    0.000000
       rhoc [g_cond/cc_cond]:     0.000000
       Speed of sound [m/s]:      6767.819     = sqrt(dP/drho)_s = sqrt(adexp*P*V)
       Cv [cal/(gK)]:            0.5448616     = (de/dT)_v
       Cp [cal/(gK)]:            0.5730764     = cv+T(dV/dT)_p(dP/dT)_v
       Alpha [(1/P)*(dE/dV)_p]:   4.562902
       Beta [(1/V)*(dE/dP)_v]:    1.921741
       ADEXP [-(dlnP/dlnV)_s]:    2.894721     = -(V/P)*(dP/dV)_s = (Alpha+1)/Beta
       z (imperfection):          16.07668
       gas mol. wt. [g/mol]:      30.86111
       cond. mol. wt. [g/mol]:    0.000000
       mix mol. wt. [g/mol]:      30.86111

       Product YIELD (mol/kg_mix) and CONCENTRATION (gas mole %, mixture mole %)
       Name                Phase  [mole/kg_mix]   [gas mole %]   [mix mole %]          mw
       n2                  GAS     1.34362E+01      41.466         41.466          28.014
       h2o                 GAS     4.67967E+00      14.442         14.442          18.017
       co                  GAS     1.89751E+00      5.8559         5.8559          28.011
       co2                 GAS     4.95728E+00      15.299         15.299          44.011
       h2                  GAS     1.30393E+00      4.0241         4.0241          2.0169
       hcooh               GAS     5.23517E+00      16.156         16.156          46.028
       nh3                 GAS     9.19321E-02     0.28371        0.28371          17.033
```

9.1 km/s

Use plt to plot and isoline to expand

```
INPUT > plt, p,n2,h2o,co,co2,h2,hcooh,nh3,c2h6,oh,c(c),h2o(c)
 plt, p,n2,h2o,co,co2,h2,hcooh,nh3,c2h6,oh,c(c),h2o(c)
INPUT > iso,s,,p,,100,1,log
 iso,s,,p,,100,1,log
```

This creates a text file, tiger.plt, with columns that can be plotted with excel, tecplot, etc.)



Point calculations for quick cookoff mechanism

Sandia National Laboratories

Run with input file, in

```
s984441:tutorial mlhobbs$ cat in
com,hmx,1,rdx,1,tnt,1,wax,0.1
rxn
poi,p,1,t,400
s984441:tutorial mlhobbs$ tiger < in > out
```

```
INPUT >  com,hmx,1,rdx,1,tnt,1,wax,0.1

 Reactants:

   Name  % weight   % mole   % volume   mol. wt.   Formulas
 hmx      32.258    27.012    29.255     296.17    c4h8n8o8e28
# hmx,          octahydro--tetranitro-1,3,5,7-tetrazocine
 rdx      32.258    36.016    30.859     222.13    c3h6n6o6e21
# rdx,          hexahydro-1,3,5-trinitro-1,3,5-triazine
 tnt      32.258    35.220    33.694     227.14    c7h5n3o6e21
# tnt,          trinitrotoluene
 wax       3.226     1.752     6.192     456.61    c36h24e60
# wax,          wax

   Name  rho[g/cc]  hf[cal/mol]  V[cc/mol] S[cal/K mol]
 hmx       1.905    0.1793E+05     155.5         0.000
 rdx       1.806    0.1650E+05     123.0         0.000
 tnt       1.654   -0.1506E+05     137.3         0.000
 wax       0.900   -0.1781E+05     507.3         0.000

 Initial mixture:
   Heat of formation =    20.84    cal/g
   Standard energy   =    20.82    cal/g
   Standard volume   =   0.5788    cc/g
   Standard entropy  =   0.000     cal/(g-K)
   Standard density  =    1.728    g/cc

 Number of gaseous constituents   =  65
 Number of condensed constituents =   2
 Molecular formula of mixture (ave. mw =  248.003    g/mol)
   Elements     moles        % moles      % mass
   c           5.2571        11.150       25.460
   h           6.5034        13.794       2.6430
   n           5.3785        11.408       30.377
   o           6.4351        13.649       41.515
   e           23.574        50.000      0.52146E-02
Oxygen balance:  -47.30 %
```

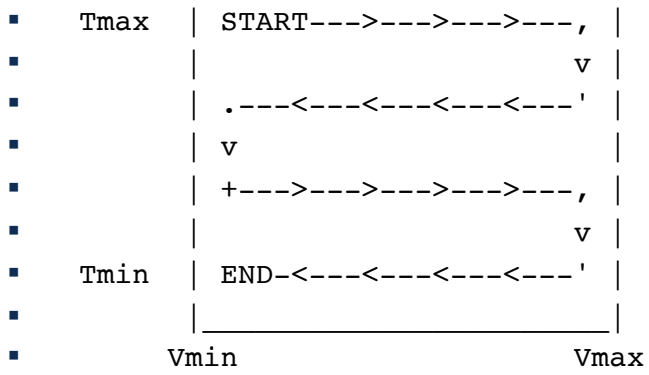
```
INPUT >  rxn
 Reaction stoichiometry will be printed.
INPUT >  poi,p,1,t,400
 Current library is jczs3
 Using JCZ3 EOS with reference state based on reactants (R):

   H(R) = H - (    20.838)    E(R) = E - (    20.824)        S(R) = S - (     0.000)

   1.) Thermodynamic STATE of products:
       P [atm]:                      1.000000
       V [cc/g]:                     999.0308
       Rho [g/cc]:                  0.1000970E-02
       T [K]:                        400.0000
       H(R) [cal/g]:                -1351.575
       E(R) [cal/g]:                -1375.756
       S(R) [cal/(gK)]:              1.589506
       Vg [cc_gas/g_gas]:            1191.713
       Rho_g [g_gas/cc_gas]:        0.8391282E-03
       V_hat [cc_gas/g_mix]:         998.9633
       Rho_hat [g_mix/cc_gas]:      0.1001038E-02
       wgas [g_gas/g_mix]:          0.8382583
       wcond [g_cond/g_mix]:        0.1617417
       phigas [v_gas/v_mix]:        0.9999325
       phicond [v_cond/v_mix]:      0.6751029E-04
       rhoc [g_cond/cc_cond]:        2.398133
       Speed of sound [m/s]:         355.2444     = sqrt(dP/drho)_s = sqrt(adexp*P*V)
       Cv [cal/(gK)]:               0.2478129     = (de/dT)_v
       Cp [cal/(gK)]:               0.3083655     = cv+T(dV/dT)_p(dP/dT)_v
       Alpha [(1/P)*(dE/dV)_p]:      4.100189
       Beta [(1/V)*(dE/dP)_v]:       4.090979
       ADEXP [-(dlnP/dlnV)_s]:       1.246692     = -(V/P)*(dP/dV)_s = (Alpha+1)/Beta
       z (imperfection):             1.001901
       gas mol. wt. [g/mol]:         27.59490
       cond. mol. wt. [g/mol]:       12.01135
       mix mol. wt. [g/mol]:         22.80864

       CONCENTRATION (mixture mole%), STOICHIOMETRY, hf at 298 K
       Name                Phase  [mix mole%]     [rxn. stoic]    [hfo, kJ/mol]         mw
       h2o                 GAS      11.793          2.9247          -241.81          18.017
       n2                  GAS      10.843          2.6892          0.61142E-08      28.014
       co2                 GAS       7.0773         1.7552          -393.49          44.011
       ch4                 GAS      0.65473         0.16237         -74.595          16.045

       c(c)                SOLID   1.34657E+01      3.3395         0.99805E-08      12.011
       h2o(c)              LIQUID  0.00000E+00      0.0000         -285.81          18.017
       TOTAL               GAS(g)                   7.5337
       TOTAL               COND(c)                  3.3395
       c5.257h6.503n5.378o6.435e23.574 -->  7.5337    Gas +    3.3395     Cond
       Hrxn = -5.773E+06 J/kg exothermic at tref = 298.15
```

Here's the generic reaction and reaction enthalpy

Some TIGER updates since 2017

Sandia National Laboratories

- We have been improving TIGER's solvers. Our main code developer is the author of Cantera open source software.
- We have added native SESAME table generation (this will be the remainder of the discussion).
- Here is the old methodology:



Creating SESAME tables with TIGER

Sandia National Laboratories

- Old method of generating table (input deck):
  - composition, hmx, 1
  - geos, bkw
  - point, T, 1000, p, 1000
  - plt, T, V, P, E, S
  - isoline, T, 6000.0, V, 0.3, 177, 1000.0,log
  - isoline, T, 5937.5, V, 1000.0, 177, 0.3,log
  - isoline, T, 5875.0, V, 0.3, 177, 1000.0,log
  - …
  - isoline, T, 325.0, V, 1000.0, 177, 0.3,log
  - isoline, T, 300.0, V, 0.3, 177, 1000.0,log
  - isoline, T, 298.0, V, 1000.0, 177, 0.3,log
  - exit
- New method: create input deck using “mkin. The new calculation order is the same, but the input deck only considers point calculations. As such, failures can be easily restarted with new P,T guesses.

TIGER SESAME Help

mkin

```
INPUT > help, mki
 help, mki
 ***** Help for mki (makes in0 for generating SESAME data) *****

 mki produces an input deck (in0) for creating EOS data for SESAME
 tables. This can be done using a variety of isolines that take
      advantage of the previous TIGER solution in this fashion:

                 ._________________________.
           Tmax  | START--->--->--->---, | 1st isoline (Tmax isotherm)
                 |                     v |
                 | .---<---<---<---<---' | 2nd isoline
                 | v                     |
                 | +--->--->--->--->---, | ...
                 |                     v |
           Tmin  | END-<---<---<---<---' | last isoline (Tmin isotherm)
                 |_________________________|
                Vmin                    Vmax

      BCAT requires this format of output from TIGER. However,
      periodically the TIGER solver fails in the middle of the isoline.
      Starting up the calculation in the middle of the failed
      isotherm is difficult and a bookkeeping nightmare. One solution is
      to substitute point calculations for the isoline calculations.
      The new calculation order is the same, but the input deck only
      considers point calculations. As such, failures can be easily
      restarted with new P,T guesses.

      The volumes are incremented logarithmically and the temperatures
      are evenly spaced.

      INPUT PARAMETERS:
      t0 [=] initial temperature              (default is 298 K)
      tf [=] final temperature                (default is 6000 K)
      nt [=] number of temperature increments (default is 110)
      v0 [=] initial volume                   (default is 0.35 cc/g)
      vf [=] final volume                     (default is 1000 cc/g)
      nv [=] number of volume increments      (default is 177)

      EXAMPLE INPUT: mki, t, 298, 6000, 110, v, 0.35, 1000, 177
      1) mki, t, 298, 6000, 110, v, 0.35, 1000, 177
      2) mki

      NOTES: the t and v can be interchanged
      1) the t and v can be interchanged
      2) if just mki is input, then the default values above are used
      3) default composition is HMX. Change Composition in in0 as desired
```

Procedure

```
      help, ses
       ********************** Help with ses **********************


       Create both an ascii and binary (201, 301) SESAME file using
       data in all.plt located in the local directory. The (ses)
       command assumes the reference state is 1 atm and 298 K. The
       reference density is used to numerically calculate the
       isothermal bulk modulus (bref). The SESAME files are created
       without an energy shift (ESFT). If desired, the energy shift
       should be performed within either BCAT or CTH.


       An example using TIGER's ses command:
       ses,nv,178,nt,110,fz,152,mw,296.17,ro,0.5,id,1234,dt,111321
          nv is the number of volumes (178) in the all.plt file.
          nt is the number of temperatures (110) in the all.plt file.
          fz is the formula number giving the number of electrons
             in the reactant mixture. This is output after every
             composition command.
          mw is the molecular weight of the reactant mixture. Similar
             to fz, this is output after every composiiton command.
          ro is the ref. density from which the isothermal bulk
             modulus, 'kref' is calculated.
          id is the four digit matid for the SESAME table.
          dt is the six digit date.
```

TIGER SESAME Help (continued)

Sandia National Laboratories

```
Procedure for creating a SESAME table from scratch
   1) Create TIGER input deck using 'mkin' to generate EOS data.
   2) Create tiger.plt file: tiger < in0 > out0
   3) Rename tiger.plt all.plt, remove 2nd header, use 'sfix' command.
      if 'number of v changes' > 0, mv fixed.plt to all.plt.
   4) Run 'ses' command.
NOTE: step 2 may require some iteration if TIGER fails to converge.
Split in0 into small files and use better TP guesses for failed points.
Concatonate tiger.plt files into all.plt file with single header.


Procedure for checking a SESAME table: check TIGER cj with BCAT cj:
    1) Use 'eos' part of a CTH input deck as BCAT input deck, bcat.in:
        eos
          mat1 sesame user eos=1234 feos='./b1234' esft = 1
        endeos
    2) Run BCAT with these commands
       OPTION?
       set eos
       ENTER NAME OF CTH INPUT FILE.
       bcat.in
       OPTION?
       cj mat 1
       ENTER RZRO, PZRO, AND EZRO FOR UNBURNED EXPLOSIVE
       1,0,0
    3) BCAT returns the CJ state. Note that 'esft' in the bcat.in
       was set to 1. Do not set this to zero, since zero is a flag
       within BCAT to use a large energy shift. Energy units in BCAT
       are in ergs, so 1 is essentially zero. You could also use
       something like 1e-6 if you want, but don't use zero.
    4) Compare the BCAT cj velocity with the TIGER cj velocity.
```

Example of generating a SESAME Table

- Do a CJ calculation to see range for V

```
INPUT > com, hmx,91, etc.
 com, hmx,91,etc.


 Reactants:
```

```
 Initial mixture:
   Heat of formation =    42.16    cal/g
   Standard energy   =    42.15    cal/g
   Standard volume   =   0.5381    cc/g
   Standard entropy  =   0.000     cal/(g-K)
   Standard density  =    1.858    g/cc
 Number of gaseous constituents    =  66
 Number of condensed constituents =   1
 Molecular formula of mixture (ave. mw =  286.748    g/mol)
   Elements     moles        % moles      % mass
   c            4.4565       16.264       18.667
   h            7.9571       29.039       2.7969
   n            7.3292       26.748       35.801
   o            7.6583       27.949       42.730
   e            27.401       0.0000      0.52421E-02
Oxygen balance:  -29.20 %
Formula number (FZ):     147.27      number of electrons in mixture formula
```

```
INPUT > c-j, p, 1, rho, tmd
      ****** The Chapman-Jouguet condition ******
      The shock velocity    =   8.8173500E+03 m/s
      The particle velocity =   2.2206835E+03 m/s
      The speed of sound    =   6.5966665E+03 m/s
```

Make input deck (mkin):

- `mki, t,275,6000,230,v,0.35,1000,100`
- This creates in0 with 23000 point calculations. Make sure the composition is correct and then run this file with tiger.
- Run tiger until failure:
  - `Tiger < in0 > out0`
  - Out TP solvers are robust enough to easily restart this calculation.
  - cp in0 in1 and run again, repeat
- `cat tiger*.plt > all.plt`
- vi all.plt to remove all header files except on line 1.
- INPUT > `sfix`, nt,230,nv,100
- mv fixed.plt all.plt
- INPUT > `ses,nv,100,nt,230,fz, 147.27,mw,286.748,ro,1.8,id,3333,dt,060722`

- Took me about 30 minutes to make EDC SESAME table.

Summary and Conclusions

Sandia National Laboratories

- JCZS database was improved with piecewise specific heat fits of NASA's latest specific heat parameters (15th Det. Symp). Two new databases were created: JCZS2 (no ions) and JCZS2i (ions).
- We have combined these two databases into one: JCZS3. A key word is used to toggle ions on or off. We have also implemented a molecular weight limiter when selecting possible product species.
- We have refit all *condensed* specific heat fits to avoid spurious roots when calculating the chemical potential. All melting points have been checked with data.
- We are creating TIGER SESAME tables for a variety of materials
  - Make T,V grid more dense for better convergence in expanded states.