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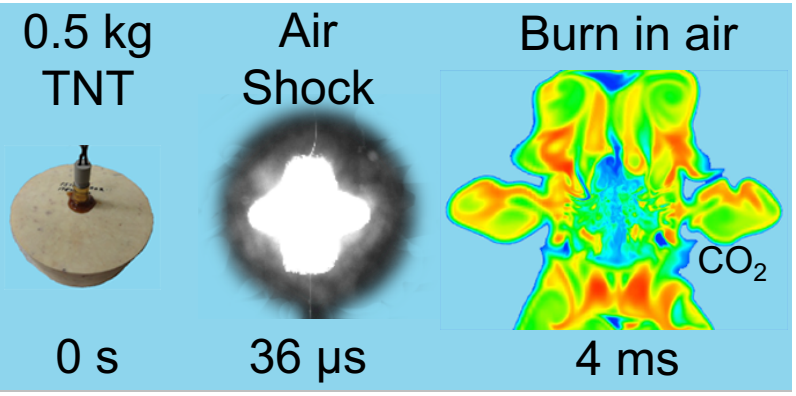

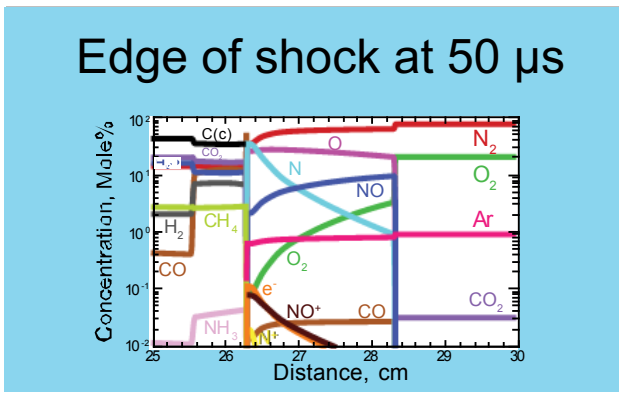

CTH-TIGER tutorial

(thermochemical equilibrium code distributed with CTH)

Michael L. Hobbs

Sandia National Laboratory, USA

U.S. DEPARTMENT OF ENERGY

National Nuclear Security Administration

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History of Equation of State at Sandia

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

[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)

Tanaka, K., 'Detonation Properties of High Explosives Calculated by Revised Kihara-Hikita Equation of State," *8th Detonation Symposium*, 548-557 (1985).

Hobbs, M. L. Tanaka, K., Iida, M. and Matsunaga, T., "Equilibrium Calculations of Firework Mixtures," *3rd (Beijing) International Symposium on Pyrotechnics and Explosives*, Beijing, China (1995).

High pressure, temperature EOS basics

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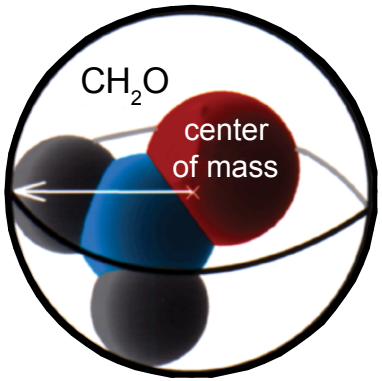
BKW, covolume based

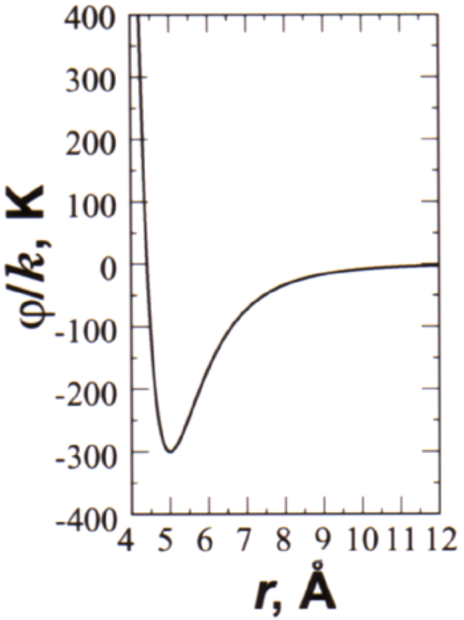
$$\frac{PV}{RT} = 1 + X\exp(\beta X)$$

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



JCZ, intermolecular potential based

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

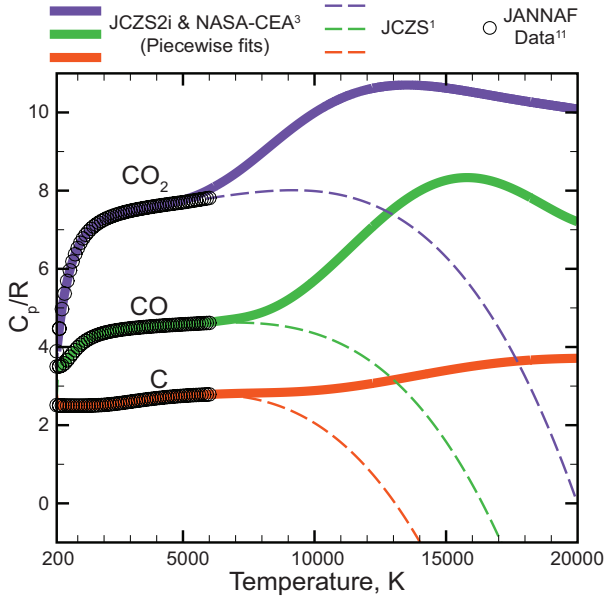


Thermodynamics

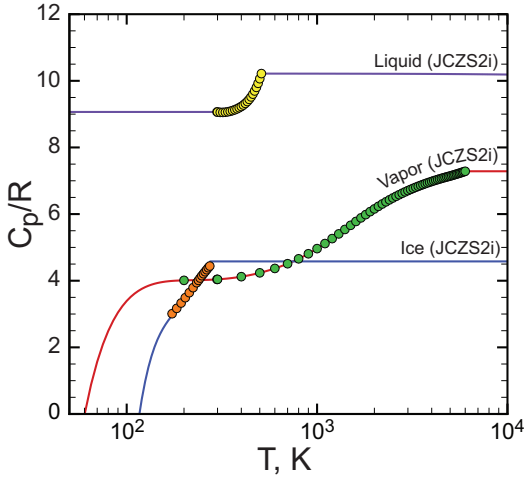
$$C_p/R = \sum_{i=1}^{7} a_i T^{i-3} \qquad \left(\partial S/\partial T\right) = C_p/T$$

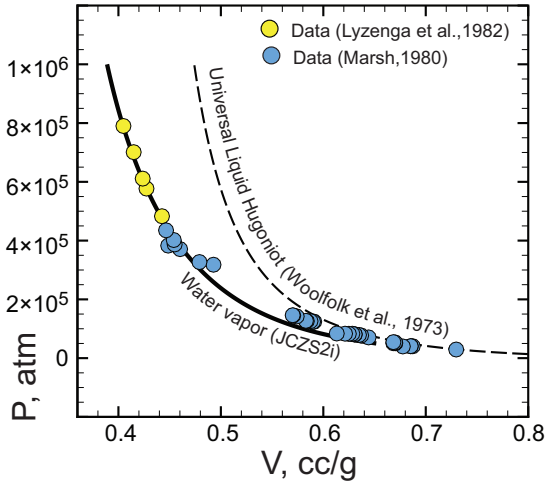
$$C_p = \left(\partial H/\partial T\right)_p \qquad S = \int \frac{C_p}{T} dT$$

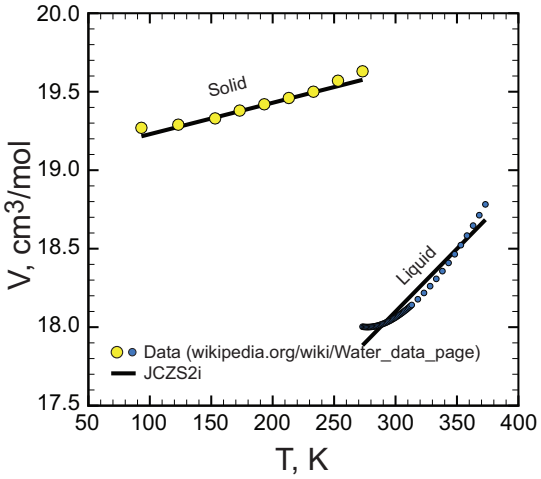
$$h = \int C_p dT \qquad \mu/RT = H/RT - S/R$$

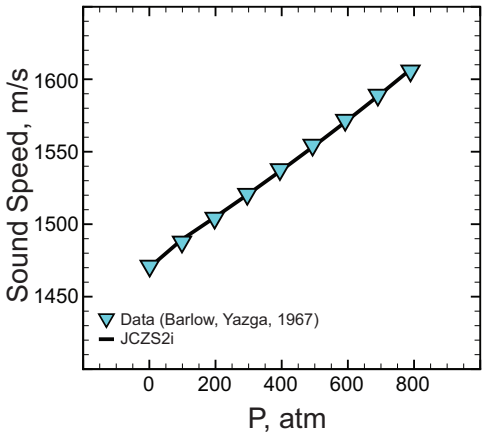


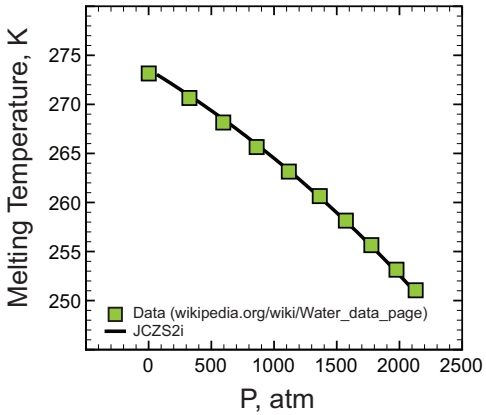
Water EOS

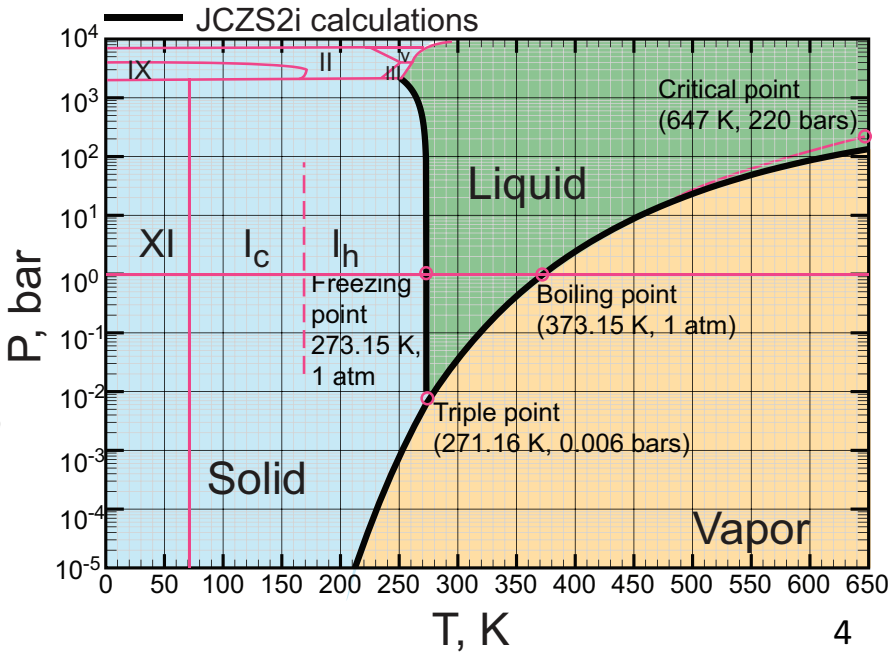






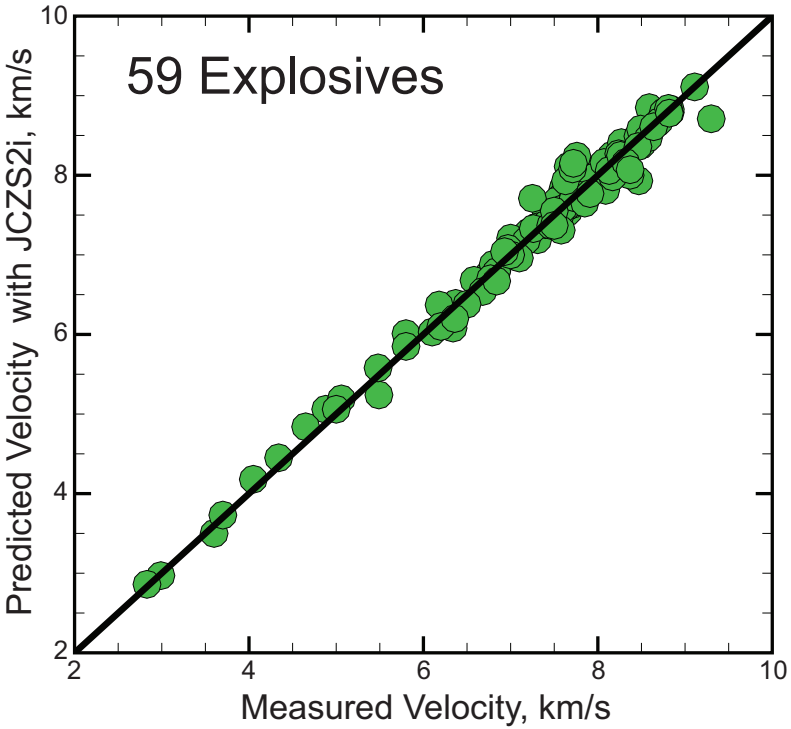






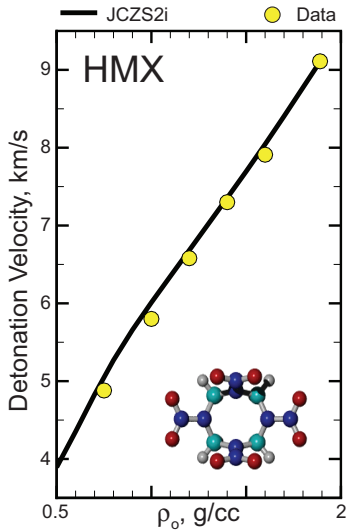
$$V = A + BT + CP\exp\left(1 - P/D\right)$$

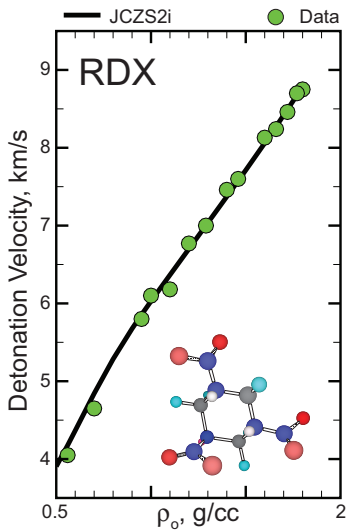
Detonation predictions

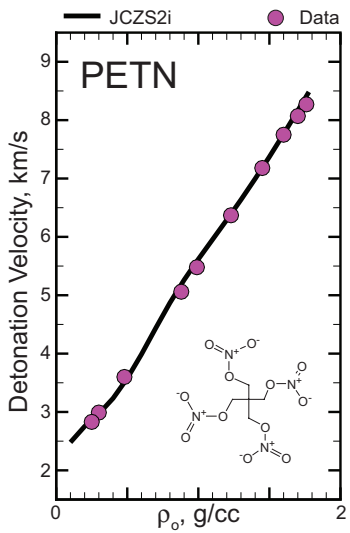


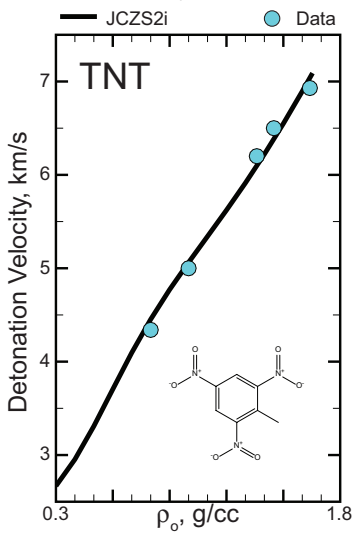
	Mean Absolute Error	RMS Error
JCZS[a]	1.76%	2.37%
Exp-6[b]	1.90%	2.51%
JCZS2i	1.73% Awesome!	2.34%

[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)





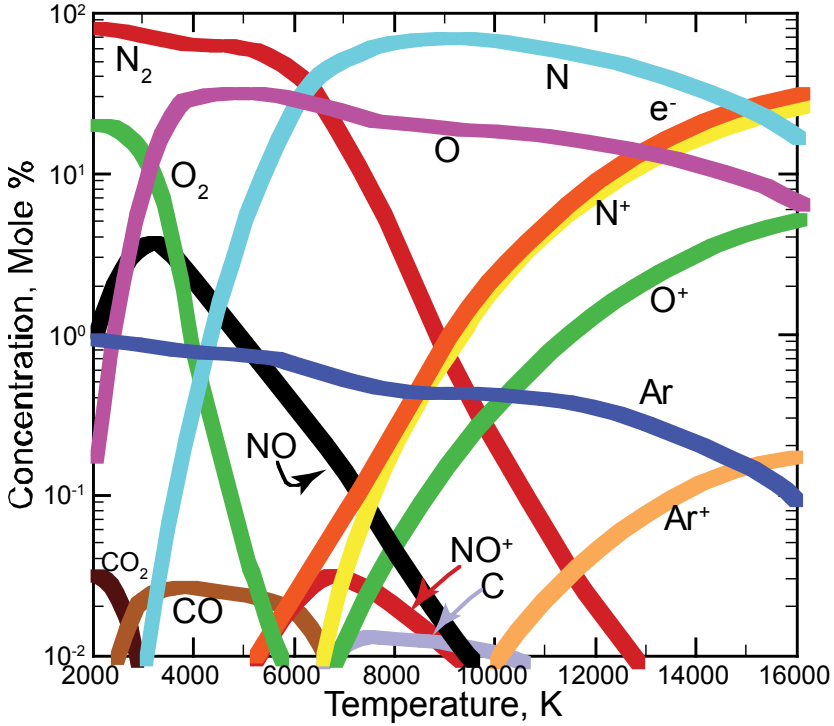




Air at low pressure, high temperature

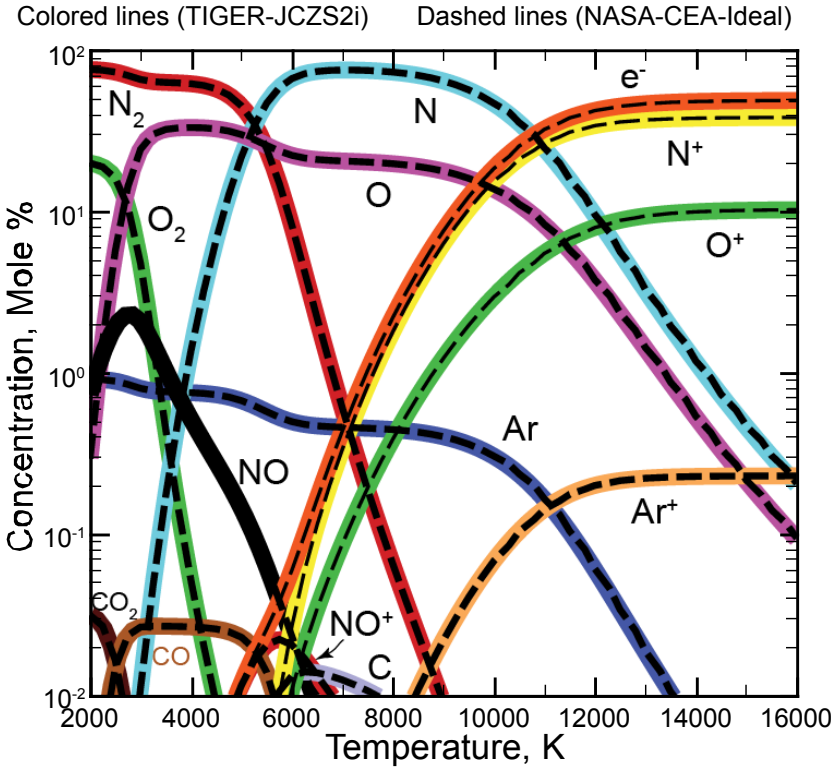
1950's

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

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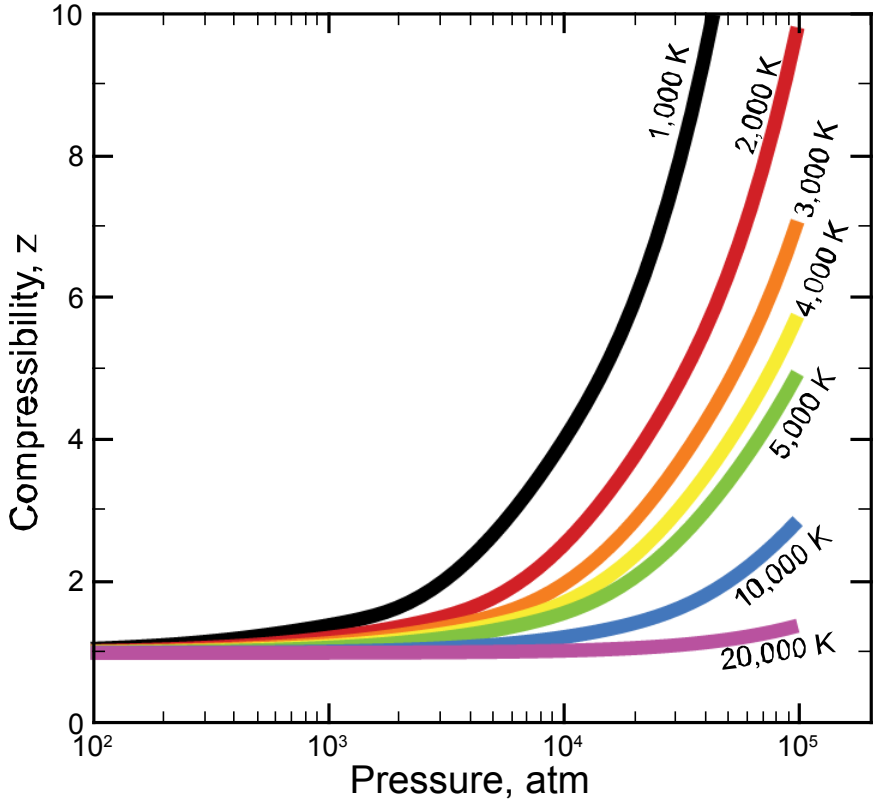
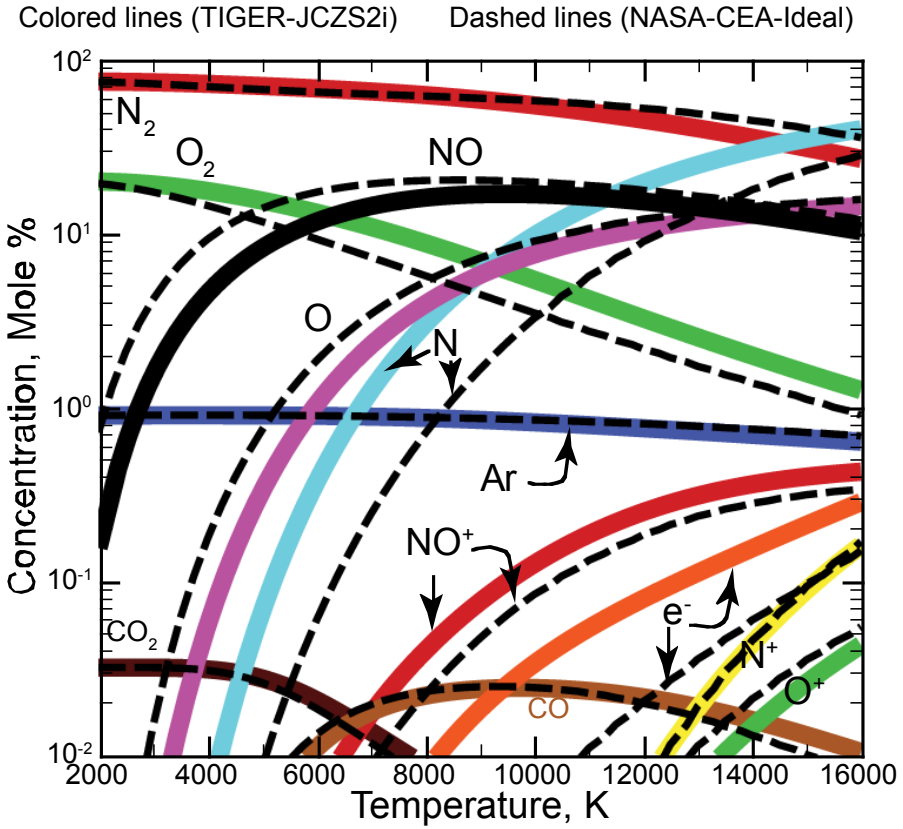
Air Compressibility



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

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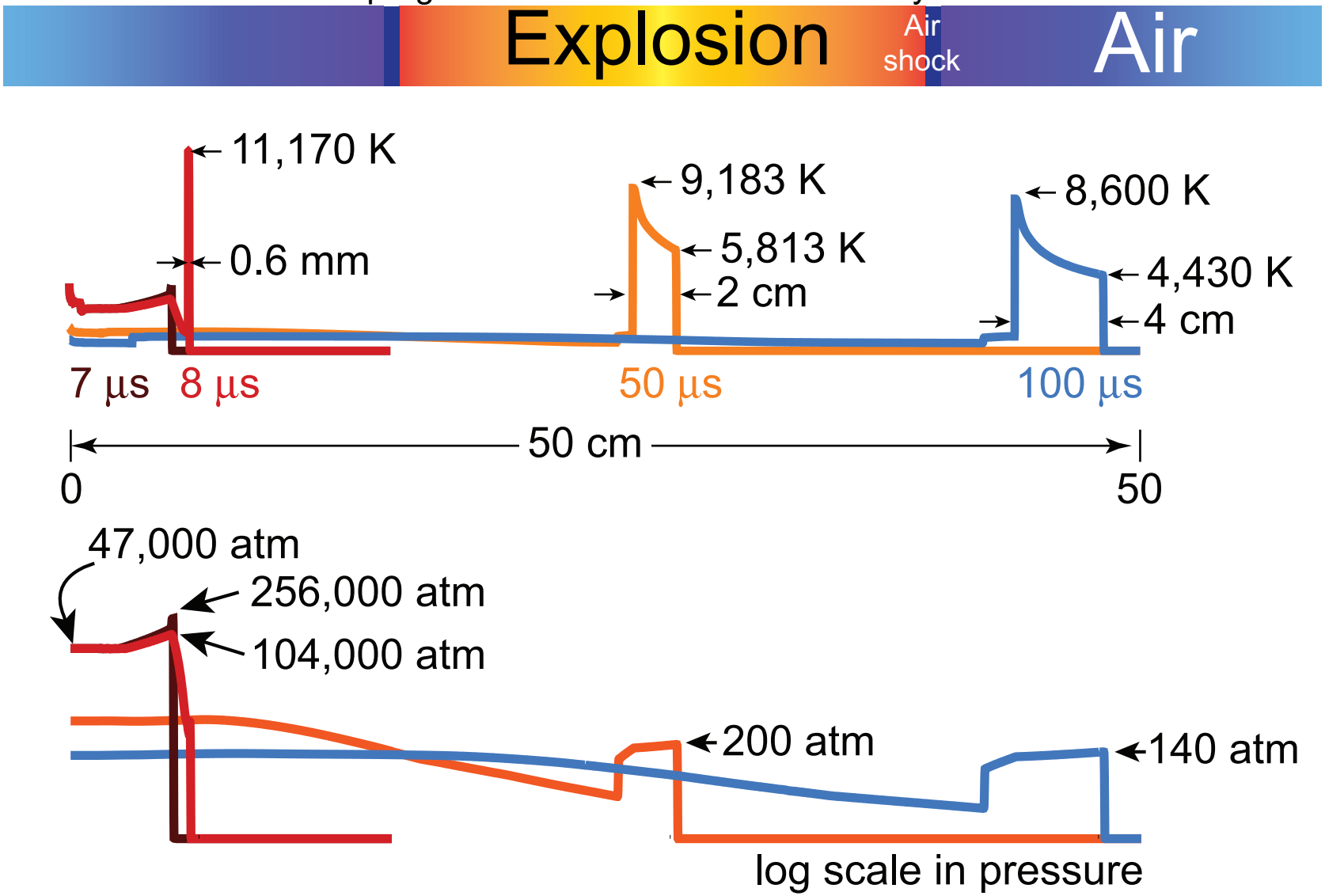
CTH programmed burn of a 5 cm radius cylinder.



Edge of shock at 8 µs and 100 µs

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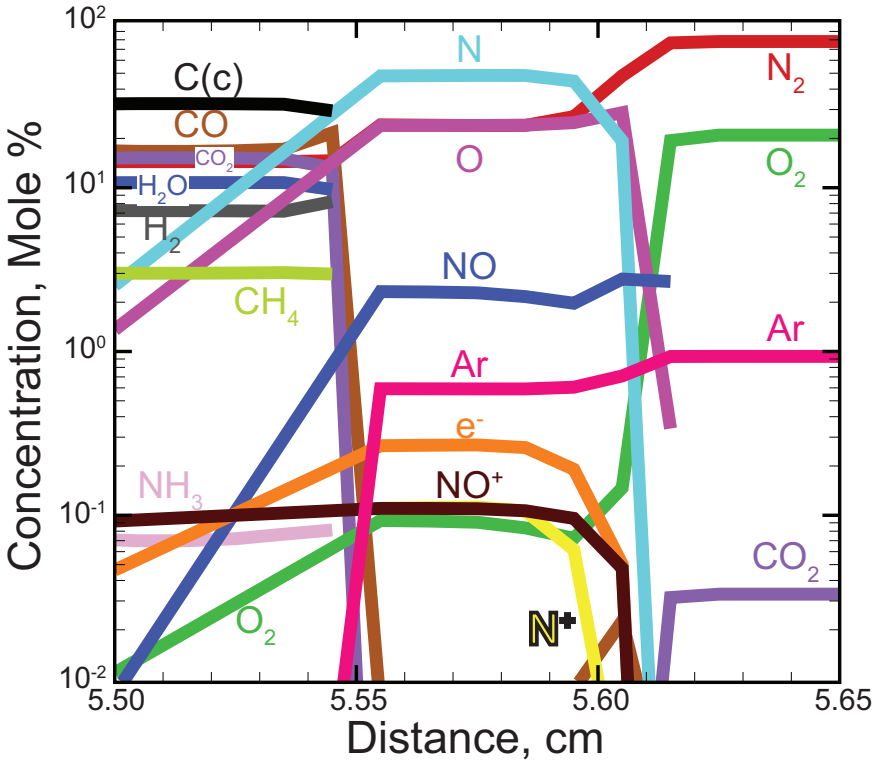
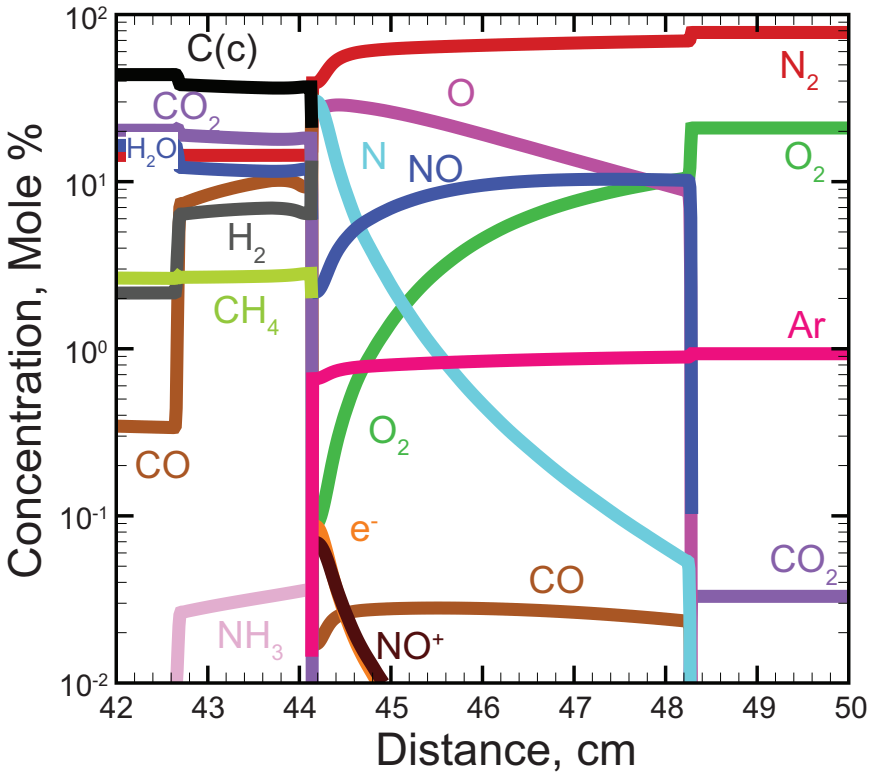
8 µs



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,OB,-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 ($H_2 + 0.5O_2$)

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```
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)

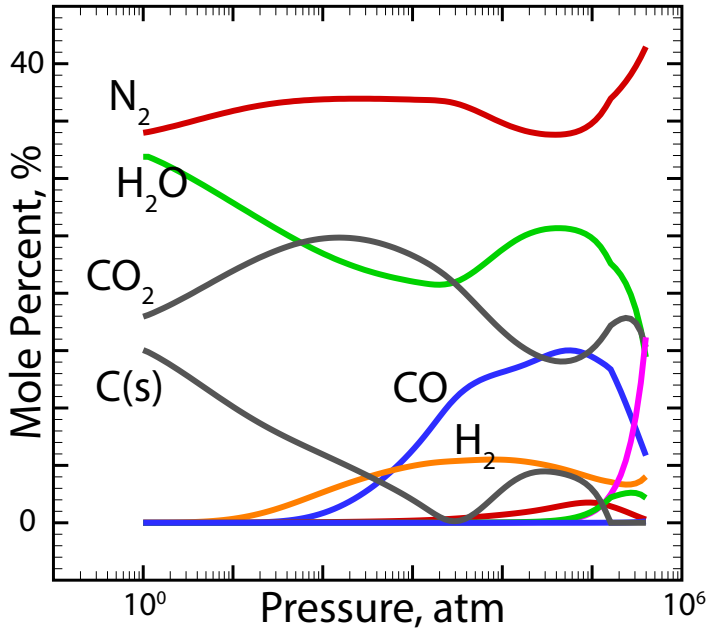
```
INPUT > c-j, p , 1, rho, 1.89
 c-j, p , 1, rho, 1.89
       ****** The Chapman-Jouguet condition ******
       The shock velocity     =   9.1058018E+03 m/s
       The particle velocity  =   2.3379814E+03 m/s
       The speed of sound     =   6.7678204E+03 m/s
       ****** The Hugoniot reference 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

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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

Summary and Conclusions

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- 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 currently collecting EOS data to fine tune the JCZS3 database. Got any data?