

MIE-GRUNEISEN EQUATION OF STATE
FOR LIQUID, UNREACTED CS_2

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Internal Report

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Calculation of $k_h \equiv -v \frac{dP_h}{dV}$ for the perturbation form of the Hugoniot for the universal liquid Hugoniot $U_S - U_p$ relation.*

Universal liquid Hugoniot

$$\frac{U_S}{c_0} = a_1 + \frac{bu_p}{c_0} - (a_1 - 1) e^{-2u_p/c_0}$$

where c_0 = sound speed at atmospheric pressure and ambient temperature
 $a_1 = 1.37$
 $b = 1.67$ (This is Sheffield's value. Woolfolk, et al., used $b = 1.62$. See Sheffield's thesis, p. 159).

This gives

$$\begin{aligned} U_S &= a + bu_p - c_0(a_1 - 1) e^{-2u_p/c_0} \\ &= a + bu - (a - c_0) \exp(-2u/c_0) \end{aligned} \quad (1)$$

where the subscript p has been dropped and the product $a_1 c_0$ has been replaced by

$$a \equiv a_1 c_0$$

Comparison of Eq. (1) with Eq. (15) of Internal Report Number 82-06 shows that

$$U_S = a + bu + \psi(u)$$

where

$$\psi(u) = - (a - c_0) e^{-2u/c_0} \quad (2)$$

* Internal Report 82-05 provides the framework for developing the Mie-Gruneison equation of state.

with

$$u_0 = \frac{a\eta}{1 - b\eta}, \quad \eta = 1 - V/V_0, \quad (3)$$

the perturbation form of the P-V Hugoniot is given by Eq. (22) of Internal Report No. 82-06:

$$P_h = P_h^0 (1 + \delta(u_0)) \quad (4)$$

$$\text{where } \delta(u_0) = \frac{2\psi(u_0)}{a - u_0(d\psi/du)_{u_0}} \quad (5)$$

$$P_h^0 = \frac{\rho_0 a^2 \eta}{(1 - b\eta)^2} \quad (6)$$

With ψ given by Eq. (2)

$$\frac{d\psi}{du} = -2\psi/c_0 \quad (7)$$

and Eq. (5) becomes

$$\delta(u_0) = \frac{2\psi(u_0)}{a + 2u_0\psi/c_0} \quad (8)$$

The Mie-Gruneisen equation of state described in Internal Report 82-05 requires the "Hugoniot modulus",

$$k_h = -V \frac{dP_h}{dV} = (1+\eta) \frac{dP_h}{d\eta} \quad (9)$$

with η defined in Eq. (3).

With P_h given by Eq. (4),

$$\frac{dP_h}{d\eta} = \frac{dP_h^0}{d\eta} (1 + \delta(u_0)) + P_h^0 \frac{d\delta}{du_0} \frac{du_0}{d\eta}. \quad (10)$$

Differentiation of Eq. (6) yields two terms:

$$\frac{dP_h^0}{d\eta} = \frac{\rho_0 a^2}{(1 - b\eta)^2} + \frac{2bP_h^0}{1 - b\eta} \quad (11)$$

From Eq. (5) the logarithmic derivative of $\delta(u_0)$ is readily calculated and the result is

$$\frac{1}{\delta} \frac{d\delta}{du_0} = -\frac{2}{c_0} \left(1 - \frac{u_0}{c_0} \delta(u_0)\right) \quad (12)$$

or

$$\frac{d\delta}{du_0} = -\frac{2\delta(u_0)}{c_0} \left(1 - \frac{u}{c_0} \delta(u_0)\right)$$

Differentiation of Eq. (3) yields

$$\frac{du_0}{d\eta} = \frac{a + bu_0}{1 - b\eta} \quad (13)$$

Combining Eqs. (10) - (13) gives

$$\frac{dP_h}{d\eta} = \frac{\rho_o a^2}{(1 - b\eta)^2} (1 + \delta) + \frac{2b}{1 - b\eta} P_h - \frac{2}{c_o} P_h^o \delta \left(1 - \frac{u}{c_o} \delta\right) \left(\frac{a + bu_o}{1 - b\eta}\right) \quad (14)$$

Computation in a subroutine will proceed as follows:

η is given

Define $d = 1 - b\eta$

$u_o = na/d$

$P_h^o = \rho_o a u_o / d$

$\psi = (c_o - a) e^{-2u_o/c_o}$

$\delta = 2\psi / (a + 2u_o\psi/c_o)$

$t_1 = \rho_o a^2 (1 + \delta) / (1 - b\eta)^2 = \rho_o a^2 (1 + \delta) / d^2$

$t_2 = 2bP_h / (1 - b\eta) = 2bP_h / d$

$t_3 = -2P_h^o \delta (1 - u\delta/c_o) (a + bu_o) / (c_o d)$

$\frac{dP_h}{d\eta} = t_1 + t_2 + t_3$

$k_h = (1 + \eta) dP_h / d\eta$

The complete Mie-Grüneisen subroutine is shown on pages 5 to 8, together with calling routine and output for an isentrope.

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```
c test of mie-gruneisen eosfor cs2---see internal report 82-05
)c and 82-06. Subroutine miecs2 is filed as /user/ged/POTD4/eosmiecs2.f
  px=0.
  vx=.7918
  vo=vx
  qx=0.
  ex=0.
  tx=293.
  m5=1
  cx=0.11530
  pf=.1200
  dv=-.01000
  write (6,100)
100 format(4x,'vx',8x,'px',8x,'ex',8x,'tx',6x,'cx',6x,'qx')
101 format(2x,2(f7.5,2x),e10.4,2x,f6.1,2x,f6.4,2x,f7.5)
  1 pt=px
  vn=vx+dv
  dq = 0.0
  qn=qx+dq
  call miecs2(vn,vx,px,qn,qx,ex,tx,m5,cx)
  write(6,101) vx, px, ex, tx, cx, qx
  if(px.lt.pf)go to 1
  stop
end
```

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```

subroutine miecs2(vn, vx, px, qn, qx, ex, tx, m5, cx)
real mu, kh, ks
if (m5.eq.2) go to 1
vo=.7918
co=.1153
a1=1.37
a=a1*co
b = 1.67
c eo=0, po=0, to=293.
gv = 2.108
cvo= .9845e-5
ro=1./vo
ac=31438.5
betta=2./co
alpha=co-a
m5 = 2
c
1 dv = vn - vx
eta=1.-vn/vo
vb=(vn+vx)/2.
ad=ac*exp(-2.*gv*(vb-vo))
c calculate Hugoniot pressure for eta
d=1.-b*eta
uo=a*eta/d
pho=ro*a*uo/d
psi=(co-a)*exp(-2.*uo/co)
delp=2.*psi/(a+2.*uo*psi/co)
ph=pho*(1.+delp)
c
eh = 0.5*ph * (vo - vn)
et = ex - 0.5*(px + qx + qn)*dv
pn = (ph + gv*(et - eh))/(1. + gv*dv/2.)
en = et - pn*dv/2.
de = en - ex
p = (pn + px)/2.
tn = tx
do 2 j = 1,4
t = (tn + tx)/2.
cv=cvo*(1.-ad/(t*t))
2 tn = tx + (de + (p - t*cv*gv)*dv)/cv
tx = tn
c calculate "Hugoniot modulus", -vdp/dv on hugoniot =kh
t1=ro*a*a*(1.+delp)/(d*d)
t2=2.*b*ph/d
t3=-2.*delp*(pho/co)*(1.-uo*delp/co)*(a+b*uo)/d
dpdeta=t1+t2+t3
kh=(1.-eta)*dpdeta
at = 0.5*vn*gv*(2.0*pn - ph - px)
ks = at + kh*(1.0 - gv*(vo - vn)/2.0)
cx2 = vn*ks
vx = vn
qx = qn
ex = en
px = pn
cx=sqrt(cx2)
c

```

return
end

ISENTROPE FOR CS₂ FROM MIE-GRUNEISEN EQUATION OF STATE

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v _x	p _x	e _x	t _x	c _x	q _x
0.78180	0.00020	0.9838e-06	299.2	0.1141	0.00000
0.77180	0.00042	0.4084e-05	305.6	0.1207	0.00000
0.76180	0.00068	0.9617e-05	312.1	0.1275	0.00000
0.75180	0.00098	0.1794e-04	318.8	0.1345	0.00000
0.74180	0.00132	0.2946e-04	325.6	0.1416	0.00000
0.73180	0.00171	0.4462e-04	332.5	0.1490	0.00000
0.72180	0.00215	0.6395e-04	339.6	0.1565	0.00000
0.71180	0.00266	0.8801e-04	346.8	0.1643	0.00000
0.70180	0.00323	0.1175e-03	354.2	0.1724	0.00000
0.69180	0.00388	0.1530e-03	361.8	0.1807	0.00000
0.68180	0.00462	0.1956e-03	369.5	0.1893	0.00000
0.67180	0.00546	0.2460e-03	377.3	0.1981	0.00000
0.66180	0.00641	0.3054e-03	385.4	0.2073	0.00000
0.65180	0.00749	0.3749e-03	393.6	0.2169	0.00000
0.64180	0.00871	0.4559e-03	402.0	0.2268	0.00000
0.63180	0.01009	0.5498e-03	410.5	0.2371	0.00000
0.62180	0.01165	0.6585e-03	419.3	0.2478	0.00000
0.61180	0.01342	0.7839e-03	428.2	0.2590	0.00000
0.60180	0.01543	0.9281e-03	437.3	0.2707	0.00000
0.59180	0.01770	0.1094e-02	446.7	0.2830	0.00000
0.58180	0.02028	0.1284e-02	456.2	0.2960	0.00000
0.57180	0.02321	0.1501e-02	465.9	0.3098	0.00000
0.56180	0.02654	0.1750e-02	475.8	0.3245	0.00000
0.55180	0.03034	0.2034e-02	486.0	0.3402	0.00000
0.54180	0.03468	0.2359e-02	496.3	0.3571	0.00000
0.53180	0.03966	0.2731e-02	506.9	0.3755	0.00000
0.52180	0.04539	0.3156e-02	517.7	0.3955	0.00000
0.51180	0.05201	0.3643e-02	528.7	0.4177	0.00000
0.50180	0.05971	0.4202e-02	540.0	0.4423	0.00000
0.49180	0.06871	0.4844e-02	551.5	0.4700	0.00000
0.48180	0.07933	0.5584e-02	563.2	0.5014	0.00000
0.47180	0.09197	0.6441e-02	575.2	0.5374	0.00000
0.46180	0.10717	0.7436e-02	587.5	0.5793	0.00000
0.45180	0.12568	0.8600e-02	600.0	0.6287	0.00000