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A Program for Calculating Zero Degree Isotherms
from Hugoniot Data

I. Program Name: COLD ISOTHERM

II. Program Description:

Material data and constants for calculating Hugoniot pressures are given as program statements in SUBROUTINE DECIM (See Listing, Paragraph IV). The necessary data are:

E_{K0} = specific internal energy at 0°K and at pressure P_{K0} . This may be taken to be zero

E_{KH} = specific internal energy at the foot of the Hugoniot, Mbcc/g

P_{K0} = ambient pressure, normally taken to be zero or 10^{-6} megabars

P_{H0} = P_{K0}

V_0 = specific volume at (0°K , P_{K0}), cc/g

GAMMA_0 = Γ_0 = Grüneisen parameter at (0°K , P_{K0})

V_{KH} = specific volume at the foot of the Hugoniot

A, B, C = constants of Eq. (9) below, megabars. If a different representation is used for Hugoniot pressure, the appropriate constants

will replace A,B,C and subroutine PH(V)
will be changed

VSTOP = specific volume at which the integration
is halted, cc/g.

Isothermal pressure, P_k , is calculated here by a
numerical process in which V is incremented by ΔV at succes-
sive steps, and at each step P_k is determined by an iteration.
This requires that two numbers be specified more or less
arbitrarily:

DELTA V = ΔV is $-V_0/100$ in the present listing. If
more than 100 steps are used in the integrat-
tion, DIMENSION must be changed

ACCUR = precision required for P_k in the iteration;
it is 10^{-4} in this listing.

Output consists of a table of values of P_k , E_k , Γ , and
V. The sample shown in the Listing (Paragraph IV), is for
lead.

III. Calculation of V_0 , E_0 , Γ

V_0 is obtained from handbook data in some instances,
or it may be calculated from thermal expansion coefficients:

$$\begin{aligned} V_0 - V_0 &= \int_0^{T_0} (\partial V / \partial T)_p dT \\ &= \int_0^{T_0} V \alpha dT \end{aligned} \quad (1)$$

where T_0 is temperature at the foot of the Hugoniot and $\alpha(T)$
is thermal expansion coefficient at one atmosphere.

The Dugdale-McDonald relation gives the Grincisen coefficient as: (1)

$$\Gamma = - \frac{V}{2} \frac{(PV^{2/3})''}{(PV^{2/3})'} - 1/3 \quad (2)$$

where ' denotes differentiation with respect to V and $P = P_k(V)$, the $0^\circ K$ isotherm. For

$$P = \bar{A}x + \bar{B}x^2 + \bar{C}x^3, \quad (3)$$

where

$$x = (V\phi/V) - 1, \quad \text{Eq. (2) becomes}$$

$$\Gamma = (F_1(x)/F_2(x)) - 1/3 \quad (4)$$

where

$$\begin{aligned} F_1(x) = & 3\bar{A} + 9\bar{B} + (5\bar{A} + 33\bar{B} + 27\bar{C})x \\ & + (2\bar{A} + 38\bar{B} + 90\bar{C})x^2 + (14\bar{B} + 98\bar{C})x^3 \\ & + 35\bar{C}x^4 \end{aligned} \quad (5)$$

$$\begin{aligned} F_2(x) = & 9\bar{A} + (12\bar{A} + 18\bar{B})x + (3\bar{A} + 30\bar{B} + 27\bar{C})x^2 \\ & + (12\bar{B} + 42\bar{C})x^3 + 21\bar{C}x^4. \end{aligned} \quad (6)$$

At $x = 0$, Eq. (4) becomes

$$\Gamma = \frac{3\bar{A} + 9\bar{B}}{9\bar{A}} = \bar{B}/\bar{A} \quad (7)$$

$$\frac{d\Gamma}{dx} = - \frac{11}{9} + \frac{23\bar{B}}{9\bar{A}} + \frac{\bar{C}}{\bar{A}} - \frac{2\bar{B}^2}{\bar{A}^2} \quad (8)$$

We are now faced with an awkward situation. If the cold isotherm were known, Γ could be calculated. In order to

determine the cold isotherm both r and dr/dV should be known at $V = V_0$.

What is done in this program (Paragraph IV) is to assume

$$P_h(V) = Ax + Bx^2 + Cx^3, \quad (9)$$

and with these coefficients determine $GAMMA_0$ from Eq. (7).

It is also assumed that $dr/dV = 0$ at $V = V_0$.

E_{0H} can be determined from E_{KH} by integration of the First Law if specific heat at constant pressure, C_p , is known as a function of temperature:

$$E_{0H} = \int_0^{T_0} C_p dT - (P_0)(V_{0H} - V_0) \quad (10)$$

where $P_0 = P_{NH} = P_{KH}$. If $C_p(T)$ is not available, an alternative procedure is to integrate from (P_{KH}, V_0) to the Hugoniot at constant volume using Debye theory and correct the energy on the Hugoniot by means of the Rankine-Hugoniot equations:

$$E_H(V_0) = \left(\frac{U}{T}\right)T_h = E_{0H} + \frac{1}{2} \left[P_h(V_0) + P_{0H} \right] \cdot \left[V_{0H} - V_0 \right]$$

or

$$E_{0H} = \left(\frac{U}{T}\right)T_h - \frac{1}{2} \left[P_h(V_0) + P_{0H} \right] \cdot \left[V_{0H} - V_0 \right] \quad (11)$$

where $\frac{U}{T}$ is the Debye integral, tabulated in the AIP Handbook, and T_h is temperature on the Hugoniot at V_0 .

A third alternative is to calculate E_{0H} directly from

the Mie-Grüneisen equation of state. In general

$$P = P_h(V) + \frac{\Gamma}{V}(E - E_h(V)) \quad (12)$$

For the point on the Hugoniot at $V = V_0$ this becomes

$$P_h(V_0) = PK_0 + \frac{\Gamma_0}{V_0} [E_h(V_0) - EK_0].$$

Setting $PK_0 = EK_0 = 0$, this can be solved for E_{0H} :

$$E_{0H} = \frac{V_0}{\Gamma_0} P_h(V_0) - \frac{1}{2} P_h(V_0) (V_{0H} - V_0), \quad (13)$$

where the Rankine-Hugoniot equation has been used for $E_h(V_0)$.

Values of E_{0H} calculated from Eqs. (13) and (11) are compared in Table I. For the latter case, $T_h = 300^\circ\text{K}$ for all materials in the table. $E_h(V_0)$ is given

TABLE I
Comparison of E_{0H} from Eqs. (13) and (11)

Material	V_{0H} cc/g	V_0 cc/g	$P_h(V_0)$ Mbars	E_{0H}		$E_h(V_0)$ Mbcc/g
				Mbar cc/g Eq. (11)	Eq. (13)	
Cu	.1124	.1113	.0141	69×10^{-5}	75×10^{-5}	77×10^{-5}
Au	.05198	.05146	.0180	30 "	31 "	30 "
Pb	.08818	.08608	.0109	33 "	31 "	34 "
Mg	.5764	.5755	.0006	22 "	180 "	22 "
Ag	.09533	.09417	.0113	43 "	50 "	43 "
Ni	.1129	.1121	.0200	116 "	70 "	117 "
Al	.3591	.3545	.0079	130 "	160 "	132 "

for comparison. The second term on the right hand side of Eq. (13) contributes little to the total.

IV. Program Listing and Output for Lead

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SIRFTC C:D150
COMMON VOH, EOH, A, B, C
DIMENSION PK(100), EK(100), V(100), GAMMA(100)
C*****SET CONSTANTS AND WRITE OUT CONSTANTS*****
EKO=0.
PKO=0.
PHO=0.
ACCUR=.0001
VO=.08608
DELTAV=-VO/100.
VSTOP=VO/2.
GAMMAO=2.78
VOH=.08818
EOH=.000326
A=.417
B=1.159
C=1.01
WRITE(6,100)A,ACCUR,B,C,DELTAV,EKO,EOH,GAMMAO,PHO,PKO,VO,VOH,VSTOP
100 FORMAT(1H1,4X,2HA=,E15.8/5X,6HACCUR=,E15.8/5X,2HB=,E15.8/5X,2HC=,
-E15.8/5X,7HDELTAV=,E15.8/5X,4HEKO=,E15.8/5X,4HEOH=,E15.8/5X,4HVOH=,
-AO=,E15.8/5X,4HPHO=,E15.8/5X,4HPKO=,E15.8/5X,3HVO=,E15.8/5X,4HVOH=,
-,E15.8/5X,6HVSTOP=,E15.8//)
C
C*****INITIALIZING PROCEDURE FOLLOWS*****
V1=VO
PK1=PKO
EK1=EKO
GAMMA1=GAMMAO
PH1=PH(V1)
V2=V1+DELTAV
PH2=PH(V2)
EH2=EH(V2,PH2)
C
C*****SET STARTING VALUE FOR ITERATION TO DETERMINE PK(V2)*****
PKT=PH2-PH1
C
C*****STORE VALUES OF PK,EK,V, AND GAMMA*****
N=1
PK(N)=PK1
EK(N)=EK1
V(N)=V1
GAMMA(N)=GAMMA1
C
C*****ITERATION TO DETERMINE PK(V2)*****
1 EK2=EK1-(PKT+PK1)*DELTAV/2.
PK2=PH2-GAMMA1*(EH2-EK2)/V2
IF (ABS((PK2-PKT)/PKT).LE.ACCUR) GO TO 2
PKT=PK2
GO TO 1
2 EK2=EKO-(PK2+PK1)*DELTAV/2.

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C*****STORE VALUES OF PK, EK, V, AND GAMMA*****
      N=2
      PK(N)=PK2
      EK(N)=EK2
      V(N)=V2
      GAMMA(N)=GAMMA1

C*****INITIALIZE FOR ITERATION TO DETERMINE PK(V2)*****
      V3=V2
      3 N=N+1
      V3=V3+DELTAV
      PH3=PH(V3)
      EH3=EH(V3,PH3)
      PKT=PK2+(PK2-PK1+PH3-PH2)/2.

C
C*****ITERATION TO DETERMINE PK3=PK(V3)*****
      4 PK3=PKK(V3,V2,V1,PK2,PK1,DELTAV,GAMMA1)
      EK3=EK2-(PK3+PK2)*DELTAV/2.
      GAMMA1=V3*(PH3-PK3)/(EH3-EK3)
      IF (ABS((PK3-PKT)/PK3).LE.ACCUR) GO TO 5
      PKT=PK3
      GO TO 4

C
C*****STORE VALUES OF PK, EK, V, AND GAMMA*****
      5 PK(N)=PK3
      EK(N)=EK3
      V(N)=V3
      GAMMA(N)=GAMMA1

C
C*****DETERMINE IF ALL ITERATIONS COMPLETED*****
C*****IF NOT, GO BACK AND DO IT AGAIN*****
      IF (V3.LE.VSTOP) GO TO 6
      V1=V2
      V2=V3
      PK1=PK2
      PK2=PK3
      EK2=EK3
      GO TO 3

C
C*****AT THIS POINT THE CALCULATIONS ARE COMPLETE AND THE RESULTS MAY BE
C*****USED IN ANY DESIRED MANNER*****
      6 WRITE(6,101) (PK(I),EK(I),V(I),GAMMA(I),I=1,N)
      101 FORMAT(4(5X,E15.8))
      RETURN
      END

*IBFTE FUNCT1
      FUNCTION PH(V)
      COMMON VOH,EOH,A,B,C
      X=VOH/V-1.
      PH=A*X+B*X**2+C*X**3
      RETURN
      END

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)STATIC FUNCT2
  FUNCTION FHV(V,P)
  COMMON VDH,EDH,A,B,C
  FH=EDH+.5*P*(VDH-V)
  RETURN
  END

)STATIC FUNCT3
  FUNCTION PKK(V3,V2,V1,P2,P1,DELTA,GAMMA)
  PKK=((GAMMA+1.0/3.0+V2/DELTA)*P1*V1**((2.0/3.0)+2.0*V2/P2*V2**((2.0/3.0)
  -DELTA)/((GAMMA+1.0/3.0+V2/DELTA)*V3**((2.0/3.0)))
  RETURN
  END

```

A= 0.41700000E 00
ACCUR= 0.10000000E-03
B= 0.11590000E 01
C= 0.10100000E 01
DELTA=-0.86079999E-03
EDH= 0.
EKO= 0.
GAMMA= 0.32600000E-03
)GMMO= 0.27800000E 01
PHO= 0.
PKO= 0.
V0= 0.86080000E-01
VDH= 0.88180000E-01
VSTOP= 0.43040000E-01

1st Col. is P_k , Mbar
2nd Col. is E_k , Mb cc/g
3rd Col. is V , cc/g
4th Col. is r

0.	0.	0.86080000E-01	0.27800000E 01
0.45898298E-02	0.19754627E-05	0.85219200E-01	0.27800000E 01
0.95420406E-02	0.80578196E-05	0.84358400E-01	0.27796317E 01
0.14886578E-01	0.18571897E-04	0.83497600E-01	0.27720222E 01
0.29555082E-01	0.33869027E-04	0.82636800E-01	0.27556061E 01
0.26880761E-01	0.54328453E-04	0.81776000E-01	0.27292103E 01
0.33598008E-01	0.80358514E-04	0.80915200E-01	0.26921719E 01
0.40842180E-01	0.11239757E-03	0.80054400E-01	0.26444088E 01
0.48549336E-01	0.15091472E-03	0.79193600E-01	0.25864383E 01
0.57056026E-01	0.19641030E-03	0.78332799E-01	0.25193544E 01
0.656997150E-01	0.24941629E-03	0.77471999E-01	0.24447573E 01
0.75815931E-01	0.31049654E-03	0.76611199E-01	0.23646222E 01
0.85244011E-01	0.38024714E-03	0.75750399E-01	0.22811426E 01
0.97421672E-01	0.45929684E-03	0.74889599E-01	0.21965556E 01
0.10938819E 00	0.54830781E-03	0.74028799E-01	0.21129763E 01
0.12218429E 00	0.64797660E-03	0.73167999E-01	0.20322565E 01
0.13585267E 00	0.75903571E-03	0.72307199E-01	0.19558833E 01
0.15043858E 00	0.88225546E-03	0.71446399E-01	0.18849244E 01

0.15599043E 00	0.10184465E-02	0.70885592E-01	0.13970722E-01
0.10295035E 00	0.11584628E-02	0.69724799E-01	0.13964000E-01
0.20020479E 00	0.13332049E-02	0.68863999E-01	0.17070272E-01
0.21398482E 00	0.15136239E-02	0.68003199E-01	0.16281000E-01
0.23696618E 00	0.17107259E-02	0.67142399E-01	0.15874000E-01
0.26022214E 00	0.19255755E-02	0.66281599E-01	0.15855000E-01
0.28289310E 00	0.21593066E-02	0.65420799E-01	0.15840000E-01
0.30587609E 00	0.24131174E-02	0.64559999E-01	0.15824000E-01
0.33245578E 00	0.26882867E-02	0.63699199E-01	0.14975000E-01
0.35968406E 00	0.29851750E-02	0.62838399E-01	0.14827600E-01
0.38861109E 00	0.33082326E-02	0.61977599E-01	0.14501400E-01
0.41941540E 00	0.36560063E-02	0.61116799E-01	0.14287000E-01
0.45219709E 00	0.40311474E-02	0.60255999E-01	0.14081000E-01
0.48709793E 00	0.44354199E-02	0.59395199E-01	0.13881000E-01
0.52426238E 00	0.48707094E-02	0.58534399E-01	0.13681000E-01
0.56384830E 00	0.53390322E-02	0.57673599E-01	0.13481000E-01
0.60602596E 00	0.58425460E-02	0.56812799E-01	0.13281000E-01
0.65097691E 00	0.63835608E-02	0.55951999E-01	0.13100000E-01
0.69890522E 00	0.69645509E-02	0.55091199E-01	0.12910000E-01
0.75001867E 00	0.75881677E-02	0.54230399E-01	0.12715000E-01
0.80455013E 00	0.82572540E-02	0.53369599E-01	0.12520000E-01
0.86274909E 00	0.89748595E-02	0.52508799E-01	0.12324000E-01
0.92488538E 00	0.97442573E-02	0.51647999E-01	0.12127000E-01
0.99125107E 00	0.10568962E-01	0.50787199E-01	0.11928000E-01
0.10621625E 01	0.11452752E-01	0.49926399E-01	0.11729000E-01
0.11379626E 01	0.12399685E-01	0.49065599E-01	0.11529000E-01
0.12190237E 01	0.13414132E-01	0.48204799E-01	0.11329000E-01
0.13057503E 01	0.14500795E-01	0.47343999E-01	0.11128000E-01
0.13985820E 01	0.15664739E-01	0.46483199E-01	0.10927000E-01
0.14979975E 01	0.16911427E-01	0.45622399E-01	0.10725000E-01
0.16045189E 01	0.18246750E-01	0.44761599E-01	0.10524000E-01
0.17187150E 01	0.19677070E-01	0.43900799E-01	0.10323000E-01
0.18412082E 01	0.21209260E-01	0.43039999E-01	0.10122000E-01

V. Program Notes

The integration starts at $V = V_0$ and proceeds to smaller values of V . Since the equation is second order, three points are involved in the integration. These are labelled V_1, V_2, V_3 and they are all advanced by ΔV after each iteration. Also required are $P_h(V_1), P_h(V_2), P_h(V_3)$, given by Eq. (9).

E_{k1} = specific internal energy on the $0^\circ K$ isotherm at $V = V_1$, etc.

E_{h1} = specific internal energy on the Hugoniot at $V = V_1$, etc.

$GAMMA(N)$ = $\Gamma(V_n)$

The equations on which the integration is based are Eqs. (2), (9), (12) and the following:

$$E_h = E_{oh} + 1/2 P_h (V_{oh} - V) \quad (14)$$

$$E_k = - \int_{V_0}^V P_k dV \quad (15)$$

Define $P_3 > P_2 > P_1, V_3 < V_2 < V_1$; $(P_3, V_3), (P_2, V_2), (P_1, V_1)$ are pairs on $P_k(V)$. Then write Eq. (2) in difference form:

$$\Gamma = - \frac{V_2 P_3 V_3^{2/3} - 2P_2 V_2^{2/3} + P_1 V_1^{2/3}}{\Delta V^2 (P_3 V_3^{2/3} - P_1 V_1^{2/3})} - 1/3 \quad (16)$$

$2\Delta V$

Solve Eq. (16) for P_3 :

$$P_3 = \frac{\left(\Gamma + \frac{1}{3} - \frac{V_2}{\Delta V}\right) P_1 V_1^{2/3} + \frac{2V_2}{\Delta V} P_2 V_2^{2/3}}{\left(\Gamma + \frac{1}{3} + \frac{V_2}{\Delta V}\right) V_3^{2/3}} \quad (17)$$

The integration procedure is to calculate P_3 from Eq. (17), using an old Γ , then calculate a new Γ from Eq. (12), then a new P_3 from Eq. (17), etc. The obvious procedure, in which P is calculated from Eq. (12) and Γ from Eq. (16), is unstable.

References

1. Rice, McQueen and Walsh, Vol. VI, Solid State Physics, Seitz and Turnbull, Eds.

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1. J.N. Johnson, "Basic Theory of Irreversible Thermodynamics with Applications to the Anelastic Solid", Internal Report 01-67, October, 1967.
2. R. White, "Effect of Valve Opening Time on Gas Gun Performance", Internal Report 02-67, May, 1967.