WASHINGTON STATE UNIVERSITY
Pullman, Washington

SHOCK DYNAMICS LABORATORY
Dept. of Physics

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A Program for Fitting Hugoniot Data to a Polynomial in (Vo/V-1)

George E. Duvall

I. Program Name: LIQUID COEFF. III

II. Program Description:

This program reads N data points (PH(I), BETA(I)), determines coefficients in the equation

$$PH = Ax + Bx^2 + Cx^3 , \qquad (1)$$

where x = (Vo/V)-1, and calculates sets of values PH from the coefficients A,B,C.

In order to use the program, punch the following data in the prescribed format:

N = number of data points

CØ2 = square of sound velocity, $K_o/\ _o$, at atmospheric pressure; $c_o = K_o/\ _o$ in cm/ sec. K_o in megabars

VØ = $1./\ _o$

SB = o/Vo . = Gruneisen coefficient

CV = specific heat at constant volume, Mbar cc/g^{o}K

NAME(I), I=1,3 = name of substance

FØRMAT (I2,8X,4F10.5,3A6)

PH(I) = pressure in megabars

BETA(I) = $\dot{V}/V_o$

FØRMAT (2F10.5)

The output of the computation consists of a listing of the material name and constants, the data pairs (PH, BETA), two sets of constants: B1, C1 and B2, 0.0, and two parameters of good fit: SUM1 and SUM2. V is incremented successively and PH = Y1 or Y2 is calculated from Eq. (1) for each set of constants and printed in tabular form.

SUM1 and SUM2 represent the total square deviations of calculated values of PH from the input values for (B1, C1) and (B2, 0.0), respectively. If SUM1 < SUM2, (B1, C1) represent the best fit.

III. Program Listing

The program consists of MAIN and 3 subroutines listed below. Binary and Source Decks are located in File G1, Room 102A, Dana.

```
$IBFTC MAIN
    1 CALL INPUT
      CALL SCHM1(B1,C1)
      CALL OUTPUT(B1,C1)
      CALL SCHM2(B2)
      CALL OUTPUT(B2,0.0)
      CALL PLOT(B1,C1,B2,0.0)
      GO TO 1
      END
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```
$IBFTC INOUT   DECK
      SUBROUTINE INPUT
C       INPUT SECTION BEGINS HERE
      DIMENSION NAME(3),BETA(100)
      COMMON PH(100), ETA(100), N, PO, CO2, VO, SB, CV
      COMMON /SUMS/ SUM1,SUM2
      DATA ISTOP/6HQUIT  /
      PO=0.
      READ(5,100) N,CO2,VO,SB,CV,(NAME(I),I=1,3)
      CV=CV*1.0E-3
      IF(NAME(1).EQ.ISTOP) CALL EXIT
      DO 1 I=1,N
      READ(5,101) PH(I),BETA(I)
    1 ETA(I)=1.0/BETA(I)
      INDEX=1
  100 FORMAT(I2,8X,4F10.5,3A6)
  101 FORMAT(2F10.5)
      RETURN
C       OUTPUT SECTION BEGINS HERE
      ENTRY OUTPUT(B,C)
      IF(INDEX.EQ.2) GO TO 2
      WRITE(6,103)(NAME(I),I=1,3),PO,CO2,VO,SB,CV,(PH(I),ETA(I),I=1,N)
    2 WRITE(6,104) INDEX,B,INDEX,C
      IF (INDEX.EQ.2) WRITE(6,105) SUM1,SUM2
      INDEX=2
      RETURN
  103 FORMAT(1H1,5X,3A6,3HPO=,E11.4,3X,7HCO**2 =,E11.4,3X,3HVO=,E11.4,3X
     1,4HSB =,E11.4,3X,4HCV =,E11.4//10X,2HPH10X,4HBETA//(7X,F8.5,4X,F8.
     25/))
  104 FORMAT(1H0,5X,1HB,I1,3H = ,E15.8,5X,1HC,I1,3H = ,E15.8)
  105 FORMAT(8HOSUM1 = ,E11.4,3X,7HSUM2 = ,E11.4)
      END
```

```
      SUBROUTINE PLOT(B1,C1,B2,C2)
      DIMENSION Y1(100), Y2(100)
      COMMON PH(100), ETA(100), N, PO, CO2, VO, SB, CV, A
      DELTAV=-VO/50.
      V=VO
      I=0
    1 V=V+DELTAV
      I=I+1
      X=VO/V-1.
      Y1(I)=PO+CO2/VO*X+B1*X**2+C1*X**3
      Y2(I)=PO+CO2/VO*X+B2*X**2
      IF(V-VO/2.) 5,5,1
    5 WRITE(6,100)
      V=VO
      DO 6 M=1,I
      V=V+DELTAV
      X=VO/V-1.
    6 WRITE(6,102) X, V, Y1(M), Y2(M)
      RETURN
  100 FORMAT(1H1,15X,1HX,15X,1HV,14X,2HY1,14X,2HY2/)
  102 FORMAT(1H0,6X,4(2X,E15.8))
      END
```

```
$IBFTC CALCS   DECK
      SUBROUTINE SCHM1(B,C)
      COMMON PH(100), ETA(100), N, PO, CO2, VO, SB, CV
      COMMON /SUMS/ SUM1,SUM2
      IF(N.LE.2) GO TO 20
C     SCHEME 1-A STARTS HERE
      A=CO2/VO
      SY2=0
      SYX=0
      SYX2=0.
      SX2=0.
      SYX3=0.
      SX3=0.
      SX4=0.
      SX5=0.
      SX6=0.
      DO 10 I=1,N
      X=ETA(I)-1.
      Y=PH(I)
      SYX2=SYX2+Y*X**2
      SY2=SY2+Y**2
      SYX=SYX+Y*X
      SX2=SX2+X**2
      SYX3=SYX3+Y*X**3
      SX3=SX3+X**3
      SX4=SX4+X**4
      SX5=SX5+X**5
   10 SX6=SX6+X**6
      S1=SYX2-PO*SX2-CO2/VO*SX3
      S2=SYX3-PO*SX3-CO2/VO*SX4
      C=(S1*SX5-S2*SX4)/(SX5**2-SX4*SX6)
      B=(S1-C*SX5)/SX4
      SUM1=SY2+SX2*A**2+2.0*A*B*SX3+(2.0*A*C+B**2)*SX4-2.0*A*SYX-2.0*B*
     -   SYX2-2.0*C*SYX3+2.0*B*C*SX5+SX6*C**2
      RETURN
C     SCHEME 1-B STARTS HERE
   20 X1=ETA(1)-1.
      X2=ETA(2)-1.
      S1=PH(1)-PO-CO2/VO*X1
      S2=PH(2)-PO-CO2/VO*X2
      C=(S1*X2**2-S2*X1**2)/((X2**2)*(X1**2)*(X1-X2))
      B=(S1-C*X1**3)/X1**2
      RETURN
C     SCHEME 2 STARTS HERE
      ENTRY SCHM2(B)
      A=CO2/VO
      SY2=0
      SYX=0
      SYX2=0.
      SX2=0.
      SX3=0.
      SX4=0.
      DO 100 I=1,N
      X=ETA(I)-1.
      Y=PH(I)
      SYX2=SYX2+Y*X**2
      SY2=SY2+Y**2
```

```
      SYX=SYX+Y*X
      SX2=SX2+X**2
      SX3=SX3+X**3
  100 SX4=SX4+X**4
      S1=SYX2-P0*SX2-C02/V0*SX3
      B=S1/SX4
      SUM2=SY2+SX2*A**2+2.0*A*B*SX3+(2.0*A*C+B**2)*SX4-2.0*A*SYX-2.0*B*
     -    SYX2-2.0*C*SYX3+2.0*B*C*SX5+SX6*C**2
      RETURN
      END
```

IV. Program Notes

Subroutine INPUT
Statement 1: ETA (I) = 1.0/BETA (I)

It is assumed that the input data are punched as BETA (I) = V (I)/Vo. Since the fitting variable is (V∅/V) -1, ETA (I) defined in this statement. In the rest of the program

ETA (I) = V∅/V (I)
ETA∧I and
X = ETA (I) - 1.0

Subroutine SCHM1 (B, C)

Scheme 1A computes B and C by least squares. A is determined directly by the normal-density sound speed.

Scheme 1B assumes that there are only 2 data points and B and C are calculated exactly.

Scheme 2. C = 0 and B is obtained from least squares, even when there are only 2 data points.

SUM1 is the total square deviation of data points from calculated values of P, using B and C determined by 1A

$$SUMI = \sum_{L=1}^{N} \left[y_i - (AX_i + BX_i^2 + CX_i^3) \right]^2$$

SUM2 is total deviation for Scheme 2

$$SUM2 = \sum_{L=1}^{N} \left[y_i - (AX_i + BX_i^2) \right]^2$$

The cubic or quadratic coefficient should be used, depending on which set gives the smaller value of SUM.

V. Results for Several Liquids*

Liquid	N	C_0^2 $(Cm/\mu sec)^2$	Vo CC/g	o/Vo g/CC	Cv MbCC/g°	B_1 Mbarr	C_1 Mbar	B_2 Mbar	SUM1	SUM2
Acetone	2	.01447	1.266	.7717	$.2210 \times 10^{-4}$	.06664	.06529	.12057	*	
Ethyl Alcohol	2	.01350	1.266	.500	.2390 "	.01272	.18343	.15044		
Mercury	3	.02105	.07390	37.14	.0140 "	.33709	5.2384	2.1931		
Glycerine	2	.03625	.7950	.9770	.2360 "	.18572	.39734	.40461		
Benzene	2	.01726	1.139	1.105	.1700 "	.07614	.13401	.17368		
Ethyl Ether	2	.01012	1.405	.5270	.2260 "	.03693	.08276	.10653		
Methanol	2	.01257	1.264	.4750	.2510 "	.04493	.11398	.13558		
CC/44	2	.009025	.6260	2.114	.08400 "	.17873	.15974	.20732		
Water	16	.02199	1.002	.1070	.4180 "					

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P-V Data from J.M. Walsh and M.H. Rice, J. Chem. Phys, 26 (Apr 57) p 815