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THEORETICAL STUDIES OF SOLAR LASERS AND CONVERTERS

By

John H. Heinbockel, Principal Investigator

Progress Report
For the period May 15, 1989 to December 31, 1989

Prepared for
National Aeronautics and Space Administration
Langley Research Center
Hampton, Virginia 23665

Under
Research Contract NAG-1-757
Dr. Robert C. Costen, Technical Monitor
SSD-High Energy Science Branch

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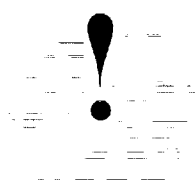
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Research for the period consisted of developing and refining the continuous flow laser model program. In addition, a working model for a two pass continuous wave amplifier was developed. The following is a summary of the mathematical development of a two pass amplifier for the $n\text{-C}_3\text{F}_7\text{I}$ iodine laser. The geometry of the amplifier is illustrated in Figure 1. In this figure

- P_{in} - power density into the amplifier (watts/cm^2),
- W - transmission coefficient,
- ϵ - radiation energy from I^* (watt-sec),
- C - speed of light,
- P_{out} - output power density,
- R_L - reflection coefficient for mirror,
- $\rho_+(Z)$ - photon density for wave motion in positive direction (cm^{-3}),
- $\rho_-(Z)$ - photon density for wave motion in negative direction (cm^{-3}).

The input power density P_{in} is assumed to be known. The photon density satisfies for all values Z

$$\rho_+(Z) \rho_-(Z) = K_0 \tag{1}$$

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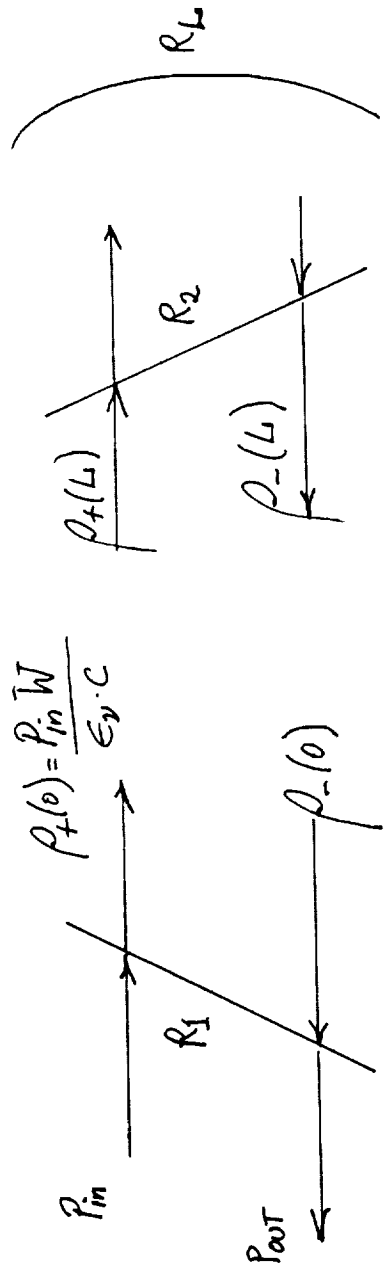


Figure 1. Geometry for Two Pass Amplifier.

where K_0 is a constant. At $Z = 0$ we have

$$\rho_+(0)\rho_-(0) = K_0 \quad (2)$$

and at $Z = L$ we have

$$\rho_+(L)\rho_-(L) = K_0. \quad (3)$$

The value of $\rho_+(0)$ is determined from the assumed value for the input power density P_{in} and from this we calculate

$$\rho_+(0) = \frac{P_{in} W}{\epsilon C} \quad (4)$$

and consequently from the relation (2) we have

$$\rho_-(0) = \frac{K_0}{\rho_+(0)} .$$

In the above relations W is the transmission coefficient of the Brewster windows and K_0 is an assumed initial value. At $Z = L$ we have $R_2 = W^2 R_L$ as the reflection coefficient from the Brewster window. We then are able to calculate the return photon density from the Brewster window at $Z = L$. We find that this density should have the value

$$\rho_-(L) = R_2 \rho_+(L). \quad (5)$$

Combining the equations (2) (3) and (5) we determine that

$$R_2 \rho_+^2(L) = K_0 \quad \text{or} \quad \rho_+(L) = \sqrt{\frac{K_0}{R_2}} = \sqrt{\frac{\rho_+(0)\rho_-(0)}{R_2}} \quad (6)$$

Using the value (6) as the theoretical value for $\rho_+(L)$ at $Z = L$ we can compare this value with the calculate value for $\rho_+(L)$ obtained from an integration of the differential equations defining the chemical reactions occurring in the amplifier. We adjust the value for $\rho_-(0)$ until

$$\left| \rho_+(L)_{\text{theoretical}} - \rho_+(L)_{\text{calculated}} \right| < E \quad (7)$$

where E is an error criteria.

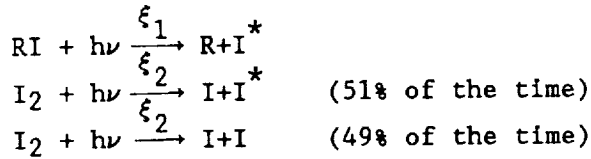
The above procedure is a shooting method for the determination of $\rho_-(0)$. When the error criteria is satisfied, the output power is obtainable from the relation

$$P_{\text{out}} = \rho_-(0) W \epsilon C \quad (8)$$

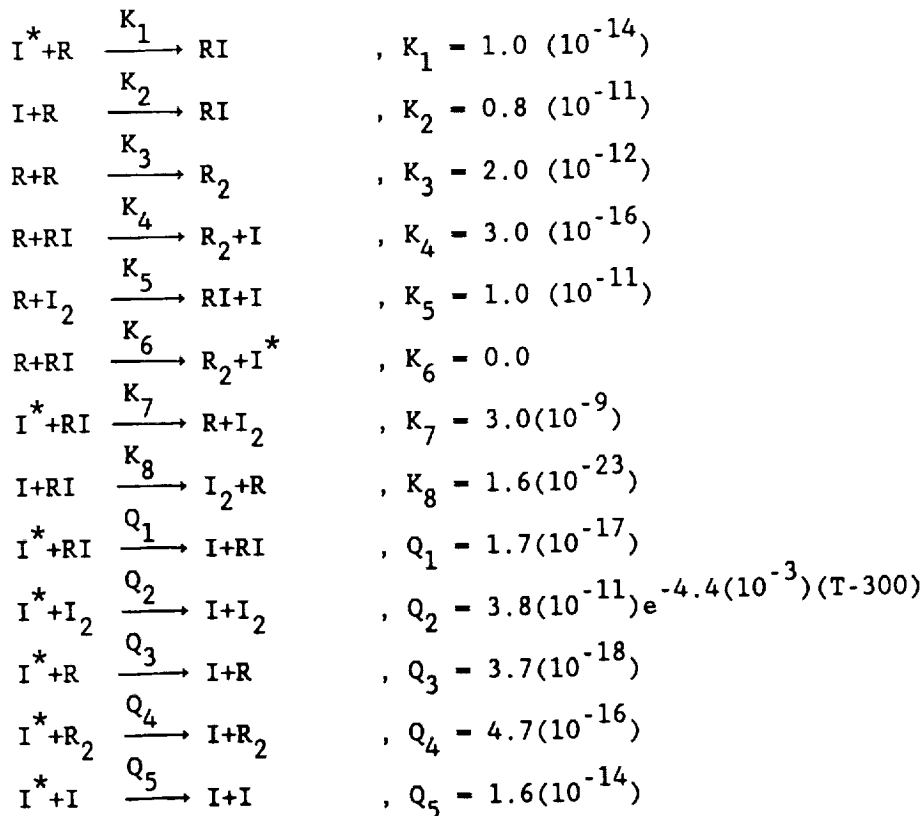
and the gain is calculated from the relation

$$\text{gain} = 10 \log_{10} \left(\frac{P_{\text{out}}}{P_{\text{in}}} \right) \text{ (decibels)}. \quad (9)$$

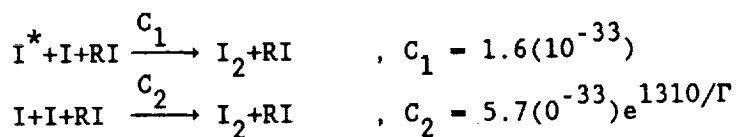
The chemical reactions occurring in the laser tube are listed along with the values used for the rate constant. The assumed reactions are:

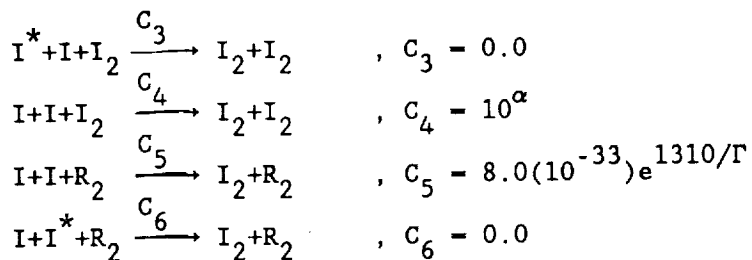


Two Body Reactions



Three Body Reactions





where

$$\alpha = -29.439 - 5.844 \log_{10} \left(\frac{T}{300} \right) - 2.163 \left[\log_{10} \frac{T}{300} \right]^2$$

Let B denote a scale factor and let y_i , $i=1,7$ denote the normalized values of concentration. Define the quantities:

$$\begin{aligned}
X_1 &= By_1 = [RI] \\
X_2 &= By_2 = [R] \\
X_3 &= By_3 = [R_2] \\
X_4 &= By_4 = [I_2] \\
X_5 &= By_5 = [I^*] \\
X_6 &= By_6 = [I] \\
X_7 &= By_7 = \rho + (Z) \\
X_8 &= \rho - (Z) = K_0/X_7 \\
\rho &= \rho(Z) = X_7 + X_8
\end{aligned}$$

where [] denotes concentration of substance, R is the iodide perfluoride radical $n-C_3F_7$, I is iodine and I^* denotes the excited state of iodine. For w the flow rate of $n-C_3F_7I$ in the Z direction (cm/sec) and ρ the total photon density, the differential equations defining the chemical kinetics of the amplifier are given by:

$$w \frac{dy_1}{dz} = K_1 B y_2 y_5 + K_2 B y_2 y_6 - \xi_1 y_1 - K_4 B y_1 y_2 + K_5 B y_2 y_4 - K_7 B y_5 y_1 - K_6 B y_2 y_1 - K_8 B y_1 y_6 - y_1 \frac{dw}{dz}$$

$$w \frac{dy_2}{dz} = \xi_1 y_1 - K_1 B y_2 y_5 - K_2 B y_2 y_6 - 2K_3 B y_2^2 - K_4 B y_1 y_2 - K_6 B y_1 y_2 - K_5 B y_2 y_4 \\ + K_7 B y_1 y_5 + K_8 B y_1 y_6 - y_2 \frac{dw}{dz} - y_2 / r_2$$

$$w \frac{dy_3}{dz} = K_3 B y_2^2 + K_6 B y_1 y_2 + K_4 B y_1 y_2 - y_3 \frac{dw}{dz} - y_3 / r_3$$

$$w \frac{dy_4}{dz} = C_1 B^2 y_1 y_5 y_6 + C_2 B^2 y_1 y_6^2 + C_3 B^2 y_4 y_5 y_6 + C_4 B^2 y_4 y_6^2 - \xi_2 y_4 + K_7 B y_1 y_5 \\ - K_5 B y_2 y_4 + C_5 B^2 y_6^2 y_3 + K_8 B y_6 y_1 + C_6 B^2 y_6 y_5 y_3 - y_4 \frac{dw}{dz} - y_4 / r_4$$

$$w \frac{dy_5}{dz} = \xi_1 y_1 + 0.51 \xi_2 y_4 - K_1 B y_2 y_5 - C_1 B^2 y_1 y_5 y_6 - C_3 B^2 y_4 y_5 y_6 - Q_1 B y_1 y_5 - Q_2 B y_4 y_5 \\ - C \sigma \cdot \rho \cdot (y_5 - \frac{1}{2} y_6) + K_6 B y_2 y_1 - Q_3 B y_5 y_2 - Q_4 B y_5 y_3 - Q_5 B y_5 y_6 \\ - K_7 B y_5 y_1 - C_6 B^2 y_6 y_5 y_3 - y_5 \frac{dw}{dz} - y_5 / r_5$$

$$w \frac{dy_6}{dz} = 1.49 \xi_2 y_4 + Q_1 y_1 y_5 + Q_2 B y_4 y_5 - 2C_5 B^2 y_6^2 y_3 - K_8 B y_6 y_1 + C \sigma \rho (y_5 - \frac{1}{2} y_6) \\ - C_1 B^2 y_1 y_5 y_6 - 2C_2 B^2 y_1 y_6^2 - C_3 B^2 y_4 y_5 y_6 - 2C_4 B^2 y_4 y_6^2 - K_2 B y_2 y_6 + K_4 B y_1 y_2 \\ + Q_3 B y_5 y_2 + Q_4 B y_5 y_3 + Q_5 B y_5 y_6 + K_5 B y_2 y_4 - C_6 B^2 y_6 y_5 y_3 - y_6 \frac{dw}{dz} - y_6 / r_6$$

$$\frac{dy_7}{dz} = L_c y_7 \left(y_5 - \frac{1}{2} y_6 \right) B \sigma$$

Normalizing the length of the amplifier by using the substitution $Z = SL$, $0 < S < 1$ the differential equations are solved numerically using a Runge-Kutta integration scheme. Appendix A contains the computer code for the simulation of a two pass continuous wave amplifier. Appendix B contains a representation of the output from the code. This Appendix contains figures illustrating how concentrations change with distance. Current research is directed toward the refining of this program and performing a systems study with the parameters involved in the code construction.

APPENDIX A

COMPUTER PROGRAM FOR SIMULATION OF TWO PASS CONTINUOUS WAVE AMPLIFIER

PROGRAM TFAMP2(INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT,TAPE8)

MAIN PROGRAM
TWO PASS CONTINUOUS WAVE AMPLIFIER

AMPFAR IS THE DATA FILE WITH NAMELIST VARIABLES DEFINED

COMPRESSIBLE FLOW LASER MODEL WHICH INCLUDES
EQUATION OF STATE
CONTINUITY EQUATION
MOMENTUM EQUATION
ENERGY EQUATION

TAPE8 IS FOR DUPUT DATA---RENAME AND SAVE TAPE8 IF YOU WANT
TO SAVE THE OUTPUT DATA

PROBLEM IS SCALED IN THE AXIAL DIRECTION---LENGTH IS LC
SCALED LENGTH IS ZERO TO ONE

SPECIFIC HEAT AT CONSTANT VOLUME IS FUNCTION OF TEMPERATURE
OBTAINED FROM LEAST SQUARES FIT OF EMPIRICAL DATA
FOR N-C3F7I IODINE LASER

USED IN PREDICTION MODE---GIVEN CONDITIONS AT Z=0.

THIS VERSION CONTAINS AN AUTOMATICALLY CHOSEN VARIABLE STEP
SIZE. IT ALSO CONTAINS WALL EFFECT REACTIONS.(NOT USED THOUGH)

EFFECTS OF TEMPERATURE, FLOWRATE,DENSITY AND PRESSURE VARIATIONS
ARE CONSIDERED IN SUBROUTINES ARREN, PFLOW AND FLOW

COMMON/BLK2/K1,K2,K3,K4,K5,K6,K7,K8,C1,C2,C3,C4,C5
COMMON/BLK27/Q1,Q2,Q3,Q4,Q5
COMMON/BLK3/B,B2,B3,C,A00,B00,EPSNU,OMEGA,C6
COMMON/BLK4/CHSI10,CHSI20,ABARO,Z1BAR,LC,XK0
COMMON/BLK7/ABC,C00,C0,OMEG1,P,R1,R2,TM,XNRHO
COMMON/BLK8/ZOL,ZE,NG,TO,RAD,A,PIN,W
COMMON/BLK10/CF1,CF2,CF4,QFO,RSTAR,ZL,L,SF1,SF2,AR,AA0,BB0
COMMON/BLK22/AD,V1,V2,GG
COMMON/BLK23/W0,ETA0,PT0,FRAC
COMMON/BLK28/TAU2,TAU4,TAU5,TAU6,TAU3,SIG
COMMON/BLK299/TTT2,TTT3,TTT4,TTT5,TTT6
REAL K1,K2,K3,K4,K5,K6,K7,K8
REAL LC,L

WRITE(6,123)
123 FORMAT(1X,20H START OF PROGRAM)

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```
C   DEFAULT VALUES
IEND=0
ICOUNT=0
NG=0
FRAC=0.0
  AR=2.
  TLE=39.0
  PTO=20.0
  W0=15.8
  ETA0=.38
ZOL=7.50
  TO=300.
  AAO=147.23
C   AAO IN J/K MOL
C   BBO IN 1/K
  BBO=.0012
C   AAO,BBO USED IN LEAST SQ FIT OF SP.HEAT CONSTANT VOLUME
LC=15.0
C   LC IN CM
  XNRHO=1.0
RAD=0.0
V1=0.0
V2=0.0
  TTT2=1.0E18
  TTT3=1.0E18
  TTT4=1.0E18
  TTT5=1.0E18
  TTT6=1.0E18
C00=.5E12
  R1=0.0
  R2=.975
  TO=300.
  PIN=1.0
  W=0.98
  ZE=5.0
A=2.0
  TM= 1-R2
  OMEG1=5000.
C   OMEG1 IN CM/S
  CON=2.0E4
C
C
C   NAMELIST/PARAM/PTO, OMEG1, CON, C00, R1, R2, TM, XNRHO, LC, ZOL, A, ZE,
1  AR, IEND, FRAC, TO, RAD, V1, V2, TTT2, TTT4, TTT5, TTT6, TTT3, W, PIN
C
C
C   ASSUME PRESSURE PTO (TORR) AND TEMPERATURE TO( DEG K)
C   ARE GIVEN FOR LEFT END.  CALCULATE ETA0 TO SATISFY GAS LAW
55  CONTINUE
  IF(IEND.EQ. 1) GO TO 600
  IF(NG.EQ.8) GO TO 600
```

```
ICOUNT=ICOUNT+1
READ(5,PARAM)
IF(EOF(5))600,601
600 WRITE(6,603)
603 FORMAT(1X,28HEND OF FILE ENCOUNTERED-STOP)
CALL PSEUDO
DO 10 JJJ=1,9
CALL GRAPHS(JJJ)
10 CONTINUE
STOP 1313

C
C W=TRANSMISSION COEFFICIENT
C PIN=INPUT POWER DENSITY (WATTS/CM**2)
C
C P=PRESSURE, TORR
C AP=LASER BEAM DIAMETER CM
C A=RADIUS OF TUBE (CM)
C RAD=RADIUS OF TUBE WHERE CALCULATIONS ARE DONE.
C T=TEMPERATURE DEG K
C T0=TEMPERATURE LEFT END DEG K
C PTO= PRESSURE TORR LEFT END
C W0=FLOW RATE LEFT END M/SEC
C ETA0=DENSITY OF GAS KG/M**3
C OMEG1=FLOW RATE, CM/SEC , MAXIMUM FLOW RATE AT RAD=0
C TAU2,TAU4,TAU5,TAU6 ARE LIFETIMES FOR RADIAL DIFFUSION OF
C TTT2,TTT3,TTT4,TTT5,TTT6 ARE LIFETIME VALUES FOR TAU
C THE QUANTITIES [R],[I2],[I*] AND [I].
C TAU3 IS DIFFUSION COEFFICIENT FOR [R2]
C CON=PEAK CONCENTRATION , SOLAR CONSTANTS
C COO=INITIAL GUESS AT RHO-PLUS AT ZERO
C WHICH IS SQUARE OF (COO*R1)
C R1= REFLECTIVITY AT LEFT END
C R2= REFLECTIVITY AT RIGHT END
C ZE=DISTANCE FOR LIGHT INTENSITY TO DIMINISH BY FACTOR 1/E
C TM= TRANSMISSION COEFFICIENT (OUTPUT MIRROR)
C ZOL=POINT ALONG AXIS WHERE MAXIMUM ILLUMINATION OCCURS
C IN THE CASE ILLUMINATION IS A BELL SHAPED CURVE
C IN THE CASE OF A SQUARE WAVE, 2*ZOL IS CUT OFF POINT
C THE POINT 2*ZOL IS WHERE ILLUMINATION BEGINS TO DIMINISH
C LC=LENGTH OF LASER CAVITY IN CM
C S= SCALED LENGTH WHICH GOES FROM ZERO TO ONE
C LENGTH IS SCALED FROM ZERO TO ONE
C ZL=2*ZOL LENGTH WHICH IS ILLUMINATED
C FRAC=FRACTION OF PEAK CONCENTRATION WHICH GOES
C INTO HEAT
C DEFAULT VALUE IS FRAC=0.024 I.E. 2.40 PERCENT
C H IS STEP SIZE FOR NUMERICAL INTEGRATION OVER SCALED LENGTH
C
C
601 CONTINUE
F=PTO
T=T0
ETA0=P*(1.01325E5)*296./(8314.3*760.*T)
C PTO IS PRESSURE IN TORR
C ETA0 IS DENSITY IN KG/M**3
C ETA0 IN KG/M**3
```

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```
C      F IN TORR
C      T IN DEG K
      CMIN=1.0E4
      CMAX=1.0E20
ZL=2*ZOL
L=LC
C)=CON
C:1=CON
CALL COEFFS
C      W0 IN M/SEC
      W0=OMEGA/100.
C      OMEGA AND OMEGA ARE IN CM/SEC
      WRITE(6,198)
198     FORMAT(///)
      WRITE(6,199) ZE,ZOL,CON,OMEGA,FRAC,COO,R1,R2,F,T
199     FORMAT(1X, T5,5HZE = ,F10.3,T30,6HZOL = ,E15.7,T55,6HCON = ,
1 E15.7,T80,9HOMEGA = ,E15.7,T104,7HFRAC = ,F9.4,/,
2 1:,T5,6HCOO = ,E15.7, T30,6H R1 = ,F10.7, T55,6H R2 = ,F10.7,
3 T81,4H P = ,E15.7 ,T105,7HTEMP = ,F10.3)
C      SET UP COEFFICIENTS IN DIFFERENTIAL EQUATIONS
C      SET PRINTER OFF
C      IPRINT=0          PRINTER OFF
C      IPRINT=1          PRINTER ON
C      IPRINT=0
C      SET STEP SIZE H=.025 UNITS
      H=.025
C      INTEGRATE DIFFERENTIAL EQUATIONS FROM S=0 TO S=1.0
      X1=COO
      CALL INTEG(IPRINT,H)
C
C      INTERVAL HALVING SCHEME
C
      Y1=ABC
      IF(Y1.LT.0) PER=5.0
CC      IF(Y1.LT.0) PER=1.1
      IF(Y1.GT.0) PER=.1
CC      IF(Y1.GT.0) PER=.9
702     CONTINUE
C      IN THIS VERSION COO IS ASSUMED VALUE FOR RHO-(0)
      COO=(PER)*COO
      IF(COO .LT. CMIN) STOP 5432
      IF(COO .GT. CMAX) STOP 2345
      X2=COO
      CALL INTEG(IPRINT,H)
      Y2=ABC
C      ABC IS XKO INITIAL MINUS XKO CALCULATED (PERCENT ERROR)
      IF((Y1*Y2).LT. 0)GO TO 701
      X1=COO
      Y1=Y2
      GO TO 702
701     CONTINUE
      W1=.6
      W2=.4
      COO=W2*X1+W1*X2
708     CONTINUE
      CALL INTEG(IPRINT,H)
```



```

C      IC IS CODE TO DETERMINE NUMBER OF GRAPHS TO PLOT
C      IC=0 FOR MORE THAN ONE GRAPH
C      IC=1 FOR LAST GRAPH (USED FOR ONLY ONE GRAPH)
C
C      IC=0
C      NLAST=NG-1
C      SXC=5.0
C      SYC=5.0
C      SYCI=7.0
C      SXC=LENGTH OF XSCALE
C      SYC=LENGTH OF YSCALE
C      SYCI=LENGTH OF YSCALE FOR INVERSION
C      IF(NLAST .EQ. 0) IC=1
C      PLOT JJJ VS Z
C      IF(JJJ .GE. 6) GO TO 700
C      DO 10 I=1,NDMAX
C      X(I)=DATA(I,1)
C      DO 20 J=1,NG
C      NN=(J-1)*6
C      NCOL=NN+1+JJJ
C      YY(I,J)=DATA(I,NCOL)
20    CONTINUE
60    CONTINUE
C
C      FIND YMAX,YMIN
C
C      DMAX=0.0
C      YMAX=0.0
C      YMIN=0.0
C      ZMIN=0.0
C
C      FIND YMAX AND YMIN
C
C      DO 70 I=1,NDMAX
C      DO 71 J=1,NG
C      IF( YY(I,J) .GT. YMAX) YMAX=YY(I,J)
C      IF( YY(I,J) .LT. YMIN) YMIN=YY(I,J)
71    CONTINUE
70    CONTINUE
C
C      PLOT FIRST DATA CURVE
C
C      JJJ=1
C      ZMAX=1.00
C      DO 40 I=1,NDMAX
C      Y(I)=YY(I,1)
40    CONTINUE
C      LOGMAX=1+ALOG10(ABS(YMAX))
C      POWER1=10.**LOGMAX
C      TEST=YMAX/POWER1
C      YMAXX=0.025
C      IF(TEST .GT. 0.025) YMAXX=.05
C      IF(TEST .GT. 0.05) YMAXX=0.10
C      IF(TEST .GT. 0.10) YMAXX=0.25

```

```

IF (TEST .GT. 0.25) YMAXX=0.50
IF (TEST .GT. 0.5) YMAXX=1.00
YMAX=YMAXX*POWER1
IF (JJJ.NE. 5) GO TO 507
506 CONTINUE
IF (YMIN .GE. 0) GO TO 507
IF (YMIN .LT. 0.0) LOGMAX2=1+ALOG10 (ABS (YMIN))
POWER=10.**LOGMAX2
TEST=ABS (YMIN)/POWER
YMINN=0.001
IF (TEST .GT. 0.001) YMINN=0.005
IF (TEST .GT. 0.005) YMINN=0.01
IF (TEST .GT. 0.01) YMINN=0.05
IF (TEST .GT. 0.05) YMINN=0.1
IF (TEST .GT. 0.10) YMINN=0.5
IF (TEST .GT. 0.5) YMINN=1.0
YMIN=-YMINN*POWER
SYC=SYCI
507 CONTINUE
ZMIN=0.0
IF (JJJ.GT.1) GO TO 50
C
C
CALL INFOPLT (IC,NDMAX,X,1,Y,1,ZMIN,ZMAX,YMIN,YMAX,1.0,
1 22,22HZ, SCALE DISTANCE,
2 11,11H [C3F7] ,0,
3 SXC,SYC,0.75,0.75)
GO TO 600
50 CONTINUE
IF (JJJ.GT.2) GO TO 100
C
C
C
JJJ=2 PLOT I2 VS Z

CALL INFOPLT (IC,NDMAX,X,1,Y,1,ZMIN,ZMAX,YMIN,YMAX,1.0,
1 23,23HZ, SCALE DISTANCE,
2 9,9H [I2] ,0,
3 SXC,SYC,0.75,0.75)
GO TO 600
100 CONTINUE
IF (JJJ.GT.3) GO TO 200
C
C
C
JJJ=3 PLOT I* VS Z

CALL INFOPLT (IC,NDMAX,X,1,Y,1,ZMIN,ZMAX,YMIN,YMAX,1.0,
1 23,23HZ, SCALE DISTANCE,
2 9,9H [I*] ,0,
3 SXC,SYC,0.75,0.75)
GO TO 600
200 CONTINUE
IF (JJJ.GT.4) GO TO 300
C
C
C
JJJ=4 PLOT I VS Z

CALL INFOPLT (IC,NDMAX,X,1,Y,1,ZMIN,ZMAX,YMIN,YMAX,1.0,
1 23,23HZ, SCALE DISTANCE,
2 8,8H [I] ,0,

```

```

3   SXC,SYC,0.75,0.75)
    GO TO 600
300  CONTINUE
C
C   JJJ=5   PLOT INV VS Z
C
    CALL INFOFLT(IC,NDMAX,X,1,Y,1,ZMIN,ZMAX,YMIN,YMAX,1.0,
1   23,23HZ, SCALE DISTANCE,
2   24,24H           [I*]-.5*[I] ,0,
3   SXC,SYC,0.75,0.75)
600  CONTINUE
C   PLOT REST OF CURVES OR EXIT IF ONLY ONE CURVE
C
    NLAST=NG-1
    IF(NG .EQ. 2) GO TO 5001
    IF(NLAST .EQ. 0) GO TO 601
    DO 500 J=2,NLAST
    DO 501 I=1,NDMAX
    Y(I)=YY(I,J)
501  CONTINUE
    CALL INFOFLT(IC,NDMAX,X,1,Y,1,ZMIN,ZMAX,YMIN,YMAX,1.0,
1   1,1H ,1,1H ,0,SXC,SYC,0.75,0.75)
500  CONTINUE
5001  CONTINUE
C
C   PLOT LAST CURVE
C
    DO 60 I=1,NDMAX
    Y(I)=YY(I,NG)
60   CONTINUE
    CALL INFOFLT(1,NDMAX,X,1,Y,1,ZMIN,ZMAX,YMIN,YMAX,1.0,
1   1,1H ,1,1H ,0,SXC,SYC,0.75,0.75)
601  CONTINUE
    CALL NFRAME
    RETURN
700  CONTINUE
C   GET DATA TO PLOT
    DO 701 I=1,NDMAX
    X(I)=FDPTDAT(I,1)
    DO 702 J=1,NG
    NN=JJJ-4+(J-1)*5
    YY(I,J)=FDPTDAT(I,NN)
702  CONTINUE
C   FDPTDAT IS STORED IN THE FORM:
C   Z, FLOWRATE, DENSITY, PRESSURE, TEMPERATURE, Z, FLOWRATE, ...
701  CONTINUE
C   FIND MAX AND MIN FOR Y VALUES
    YMIN=100.
    YMAX=0.0
    DO 703 I=1,NDMAX
    DO 704 J=1,NG
    IF(YY(I,J) .LT. YMIN) YMIN=YY(I,J)
    IF(YY(I,J) .GT. YMAX) YMAX=YY(I,J)
704  CONTINUE
703  CONTINUE
    MAX=10.*YMAX+1.0

```

```

      YMAX=FLOAT(MAX)/10.
      MIN=10.*YMIN-1.0
      YMIN=FLOAT(MIN)/10.
      ZMIN=0.0
      ZMAX=1.0
C     PLOT FIRST CURVEC
      DO 705 I=1,NDMAX
      NN=1
705   Y(I)=YY(I,NN)
C     PLOT JJJ VS Z
      IF(JJJ .GT. 6) GO TO 800
C     JJJ=6, PLOT FLOWRATE VS Z
      CALL INFOPLT(IC,NDMAX,X,1,Y,1,ZMIN,ZMAX,YMIN,YMAX,1.0,
1 25,25HZ, AXIAL DISTANCE, SCALED ,
2 15,15HFLOWRATE CM/SEC      , 0 ,
3 10.,5.,0.75,0.75)
      GO TO 820
800   CONTINUE
      IF(JJJ .GT. 7) GO TO 801
C     JJJ=7, PLOT DENSITY VS Z
      CALL INFOPLT(IC,NDMAX,X,1,Y,1,ZMIN,ZMAX,YMIN,YMAX,1.0,
1 25,25HZ, AXIAL DISTANCE, SCALED ,
2 16,16HDENSITY, KG/M**3      , 0 ,
3 10.,5.,0.75,0.75)
      GO TO 820
801   CONTINUE
      IF(JJJ .GT. 8) GO TO 802
C     JJJ=8, PLOT PRESSURE VS Z
      CALL INFOPLT(IC,NDMAX,X,1,Y,1,ZMIN,ZMAX,YMIN,YMAX,1.0,
1 25,25HZ, AXIAL DISTANCE, SCALED ,
2 14,14HPRESSURE, TORR        , 0 ,
3 10.,5.,0.75,0.75 )
      GO TO 820
802   CONTINUE
C     JJJ=9, PLOT TEMPERATURE VS Z
      CALL INFOPLT(IC,NDMAX,X,1,Y,1,ZMIN,ZMAX,YMIN,YMAX,1.0,
1 25,25HZ, AXIAL DISTANCE, SCALED ,
2 18,18HTEMPERATURE, DEG C    , 0 ,
3 10.,5.,0.75,0.75 )
820   CONTINUE
      IF(NLAST .EQ. 0) GO TO 901
C     PLOT REST OF THE CURVES
      IF(NG .EQ. 2) GO TO 5031
      DO 503 J=2,NLAST
      DO 504 I=1,NDMAX
      NN=J
      Y(I)=YY(I,NN)
504   CONTINUE
      CALL INFOPLT(IC,NDMAX,X,1,Y,1,ZMIN,ZMAX,YMIN,YMAX,1.0,
1 1,1H ,1,1H ,0,10.,5.,0.75,0.75 )
503   CONTINUE
5031  CONTINUE
C     PLOT LAST CURVE
      DO 505 I=1,NDMAX
      Y(I)=YY(I,NG)
505   CONTINUE

```

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OF POOR QUALITY

```

CALL INFOPLT(1,NDMAX,X,1,Y,1,ZMIN,ZMAX,YMIN,YMAX,1.0,
1 1,1H ,1,1H ,0,10.,5.,0.75,0.75 )
901 CONTINUE
CALL NFRAME
RETURN
END

SUBROUTINE PFLOW
C SUBROUTINE TO CALCULATE THE PARAMETERS FOR SUBROUTINE FLOW
C PARAMETERS STORE IN COMMON BLK10
COMMON/BLK7/ABC,C00,C0,OMEG1,P,R1,R2,TM,XNRHO
COMMON/BLK8/ZOL,ZE,NG,TO,RAD,A,PIN,W
COMMON/BLK10/CF1,CF2,CF4,QFO,RSTAR,ZL,L,SF1,SF2,AR,AAO,BBO
COMMON/BLK23/WO,ETA0,PTO,FRAC
COMMON/BLK29/ ZZZ,TZZ,PZZ,ETAZZ,WZZ
REAL L
C
C AR IS BEAM DIAMETER RADIUS IN CM
SF1=1000./296.
C SF1 =1/(M*1.E-03), WHERE M IS THE MOLECULAR WEIGHT
C CVS (J/K KG) =SF1*CV (J/K MOL)
SF2=(1.01325E5)/760.
C SF2 EQUALS 133.3 PA/TORR
C SF1,SF2 ARE SCALE FACTORS FOR THE CORRECT UNITS OF
C P=PRESSURE (N/M**2) , SF1 (MOLE/KG)
C PT=PRESSURE (TORR), SF2 (N/M**2)/TORR
C TEST TO SEE IF WO (M/SEC) IS NEAR MAX VALUE OF 5.30*SQRT(TO)
TEST=5.3*SQRT(TO)
TEST1=ABS(100.*(WO-TEST)/TEST)
IF(TEST1 .LT. 10.0) WRITE(6,778)
778 FORMAT(1X,52HWARNING WO VALUE IS WITHIN 10 PERCENT OF ITS MAXIMUM
1 ,/,1X,35ALLOWABLE VALUE OF 5.3*SQRT(TO) )
C ZL=LIGHT SOURCE LENGTH IN CM
C ETA=DENSITY (KG/M**3)
C L=TUBE LENGTH IN CM
C RSTAR=GAS CONSTANT (JOULE/KG DEG K)
C T=TEMPERATURE (DEG K)
C CV=SPECIFIC HEAT AT CONSTANT VOLUME
C RSTAR (J/K KG) = SF1*R(J/K MOL)
C WO,WL=FLOW VELOCITY (M/SEC) (SUBSCRIPTS O,L FOR START,END)
PO=SF2*PTO
RSTAR=8314.3/296.0
CF1=ETA0*WO
CF2=CF1*WO+PO
QFO=FRAC*(1.40E3)*C0 *2./(A*1.E-2)
C QFO IN W/M**3
C INPUT (W/M**2) DISTRIBUTED OVER VOLUME (2(PI)A)/PI(A**2) IN M2/M3
WZZ=WO
RETURN
END

SUBROUTINE FLOW(Z,T,PTORR,WSS,ETA,DWDZ)

```

```

COMMON/BLK8/ZOL, ZE, NG, TO, RAD, A, PIN, W
C SUBROUTINE TO CALCULATE T, P, WSS, ETA AS FUNCTION OF Z
COMMON/BLK10/CF1, CF2, CF4, QFO, RSTAR, ZL, L, SF1, SF2, AR, AAO, BBO
COMMON/BLK23/WO, ETAO, PTO, FRAC
C
COMMON/BLK29/ ZZZ, TZZ, PZZ, ETAZZ, WZZ
REAL L
ICOUNT=0
Q=QFO*Z/100.
C ENERGY INPUT TERM DETERMINED BY QFO
C Z IS IN CM AND QFO IS IN W/M**3
IF (Z.GT.ZL) Q=QFO*ZL/100.
XXX=BBO*(TO-300.)
CALL ETO (XXX, EEO)
WSS=WZZ
50 CONTINUE
T=((CF2/CF1)*WSS-WSS*WSS)/RSTAR
DTDW=((CF2/CF1)-2.*WSS)/RSTAR
XXX=BBO*(T-300.)
CALL ETO (XXX, EE1)
F=RSTAR*(T-TO)+(AAO/BBO)*SF1*(EE1-EEO)+
1 .5*(WSS*WSS-WO*WO)-Q/CF1
FP=(RSTAR+SF1*AAO*EE1)*DTDW+WSS
W1=WSS-F/FP
ERR=ABS(100.*(W1-WSS)/WSS)
IF (ERR .LT. .25) GO TO 100
IF (ICOUNT .GT. 95) WRITE (6, 357) ICOUNT, Z, WZZ, WSS, CF1, CF2, TO, Q, FM
357 FORMAT (1X, I5, 1X, (3E16.7, /))
WSS=W1
ICOUNT=ICOUNT+1
IF (ICOUNT .GT. 100) STOP 4444
GO TO 50
100 CONTINUE
WSS=W1
T=((CF2/CF1)*WSS-WSS*WSS)/RSTAR
TC=T-273
ETA=CF1/WSS
PNM2=ETA*RSTAR*T
PTORR=PNM2/SF2
ZZZ=Z
TZZ=TC
FZZ=PTORR
ETAZZ=ETA
WZZ=WSS
XXX=BBO*(T-300.)
CALL ETO (XXX, CV0)
CV=CV0*AAO
CVS=SF1*CV
XNUM=RSTAR*QFO
XDEN=(CF2-2.*CF1*WSS)*(CVS+RSTAR)+RSTAR*CF1*WSS
DWDZ=XNUM/XDEN
RETURN
END

```

```

SUBROUTINE ARREN(TEMP)
SUBROUTINE FOR ARRENIUS EXPRESSION OF RATE COEFFICIENTS
BASIC ASSUMPTIONS
FOR QI TERMS QI=QI0*EXP(-BETA*(TEMP-T0))
TREAT KI TERMS LIKE CI TERMS

COMMON/BLK2/K1,K2,K3,K4,K5,K6,K7,K8,C1,C2,C3,C4,C5
COMMON/BLK27/Q1,Q2,Q3,Q4,Q5
COMMON/BLK3/B,B2,B3,C,A00,B00,EPSNU,OMEGA,C6
COMMON/BLK11/KK1,KK2,KK3,KK4,KK5,KK6,KK7,KK8
COMMON/BLK12/Q01,Q02,Q03,Q04,Q05
COMMON/BLK13/CC1,CC2,CC3,CC4,CC5,CC6
REAL K1,K2,K3,K4,K5,K6,K7,K8,KK1,KK2,KK3,KK4,KK5,KK6,KK7,KK8

REFERENCE J.S. COHEN AND O.P. JUDD
J.APPL. PHYS., VOL 55, NO. 7, APRIL 1984
COEFFICIENTS MODIFIED TO ACHIEVE SPECIFIC VALUES AT TEMPERATURE
OF 276 DEGREES K.

BETA=4.4E-3
SF1=1.0
XXX=-BETA*(TEMP-300)
CALL ETO(XXX,YYY)
SF2=YYY
K1=KK1*SF1
K2=KK2*SF1
K3=KK3*SF1
K4=KK4*SF1
K5=KK5*SF1
K6=KK6*SF1
K7=KK7*SF1
K8=KK8*SF1
C1=CC1*SF1
C2=CC2*EXP(1360.00/TEMP)
C3=CC3*SF1
XYZ=-29.437-5.844*ALOG10(TEMP/300.)+2.163*(ALOG10(TEMP/300.))**2
C4=CC4**XYZ
C5=CC5*EXP(1310.000/TEMP)
C6=CC6*SF1
Q1=Q01*SF1
Q2=Q02*EXP((-4.4E-3)*(TEMP-300.))
Q3=Q03*SF1
Q4=Q04*SF1
Q5=Q05*SF1
RETURN
END

```

```

SUBROUTINE ETO(X,Y)
NEGATIVE EXPONENTIAL FUNCTION
IF(X.LT.-670.) GO TO 100

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OF POOR QUALITY

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        Y=EXP(X)
        RETURN
100    Y=0.
        RETURN
        END

```

```

FUNCTION CHSI1(Z)
C      Z1BAR IS CUTOFF POINT OF ILLUMINATION
C      ABARO IS FRONT CUTOFF POINT OF ILLUMINATION
C      CHSI1 IS A CONSTANT
C      IMPLICIT REAL*8(A-H,K,L,O-Z)
COMMON/BLK4/CHSI10,CHSI20,ABARO,Z1BAR,LC,XKO
COMMON/BLK8/ZOL,ZE,NG,TO,RAD,A,PIN,W
REAL LC
IF(Z.LT.ABARO) GO TO 100
IF(Z.LT.Z1BAR) GO TO 200
C      Z GREATER THAN Z1BAR
100    CHSI1=0.0
C      CHSI1 HAS UNITS OF SEC^-1
        RETURN
200    CONTINUE
        CHSI1=CHSI10
        RETURN
        END

```

```

FUNCTION CHSI2(Z)
C      ABARO IS FRONT CUTOFF POINT FOR ILLUMINATION
C      Z1BAR IS CUTOFF POINT FOR ILLUMINATION
C      CHSI2 IS A CONSTANT
C      IMPLICIT REAL*8(A-H,K,L,O-Z)
COMMON/BLK4/CHSI10,CHSI20,ABARO,Z1BAR,LC,XKO
COMMON/BLK8/ZOL,ZE,NG,TO,RAD,A,PIN,W
REAL LC
IF(Z.LT.ABARO) GO TO 100
IF(Z.LT.Z1BAR) GO TO 200
C      Z GREATER THAN Z1BAR
CC     XXX=-(Z-Z1BAR)/ZE
CC     CALL ETO(XXX,YYY)
CC     CHSI2=CHSI20*YYY
C      CHSI2 HAS UNITS OF SEC^-1
        RETURN
100    CHSI2=0.0
        RETURN
200    CONTINUE
        CHSI2=CHSI20
        RETURN
        END

```


C (001) I* + RI --> I + RI
 C (002) I* + I2 --> I + I2
 C (003) I* + R --> I + R
 C (004) I* + R2 --> I + R2
 C (005) I* + I --> I + I
 C
 CC (CC1) I* + I + RI --> I2 + R1
 CC (CC2) I + I + RI --> I2 + RI
 CC (CC3) I* + I + I2 --> I2 + I2
 CC (CC4) I + I + I2 --> I2 + I2
 CC (CC5) I + I + R2 --> I2 + R2
 CC (CC6) I + I* + R2 --> I2 + R2

WALL REACTIONS

C (V1) I + I + WALL --> I2 + WALL
 C (V2) R2 + I + WALL --> R + RI + WALL

CC

C
 C
 C WILSON ET AL. (1984) AND STOCK ET AL. (1986)
 C KK1 = 5.6E-13
 C COHEN AND JUDD (1984)
 C KK1 = .9E-13
 C VINOKKUROV AND ZALESSKKII (1979)
 C KK1 = 1.E-14

C
 C
 C WILSON ET AL. (1984) AND STOCK ET AL. (1986)
 C KK2 = 2.3E-11
 C BREDERLOW ET AL. (1983)
 C KK2 = .8E-11
 C COHEN AND JUDD (1984)
 C KK2 = .7E-11

C
 C
 C WILSON ET AL. (1984) AND STOCK ET AL. (1986)
 C KK3 = 2.6E-12
 C BREDERLOW ET AL. (1983) AND COHEN AND JUDD (1984)
 C KK3 = 2.0E-12

C
 C
 C WILSON ET AL. (1984), STOCK ET AL. (1986), AND COHEN AND JUDD (1984)
 C KK4 = 3.E-16
 C
 C
 C COHEN AND JUDD (1984)
 C KK5 = 1.0E-11

C
 C WILSON ET AL. (1984) AND STOCK ET AL. (1986)
 C KK6 = 3.2E-17

C BREDERLOW ET AL. (1983) AND COHEN AND JUDD (1984)
 KK6 = 0.
 C
 C
 C COHEN AND JUDD (1984)
 KK7 = 3.0E-19
 C
 C
 C
 C COHEN AND JUDD (1984)
 KK8 = 1.6E-23
 C
 C
 C WILSON ET AL. (1984) AND STOCK ET AL. (1986)
 QQ1 = 2.0E-16
 C COHEN AND JUDD (1984)
 QQ1 = 1.7E-16
 C BREDERLOW ET AL. (1983)
 QQ1 = 1.7E-17
 C
 C
 C
 C COHEN AND JUDD (1984)
 QQ2 = 3.80E-11*EXP(-4.4E-3*(T-300.))
 QQ2=3.8E-11
 C SUBROUTINE ARREN ADDS TEMPERATURE EFFECT
 C BREDERLOW ET AL. (1983)
 QQ2 = 3.0E-11
 C WILSON ET AL. (1984) AND STOCK ET AL. (1986)
 QQ2 = 1.9E-11
 C
 C
 C
 C COHEN AND JUDD (1984)
 QQ3 = 3.7E-18
 C
 C
 C COHEN AND JUDD (1984)
 QQ4 = 4.7E-16
 C
 C
 C COHEN AND JUDD (1984)
 QQ5 = 1.6E-14
 C
 C
 C
 C COHEN AND JUDD (1984) (A DIFFERENT REACTION, PERHAPS)
 CC CC1 = 1.E-32
 CC WILSON ET AL. (1984) AND STOCK ET AL. (1986)
 CC CC1 = 3.2E-33
 CC HOHLA AND KOMPA (1976)
 CC CC1 = 1.6E-33
 CC
 CC
 C COHEN AND JUDD (1984)
 C CC2 = 5.7E-33*EXP(1360./T)

```

      CC2 = 5.7E-33
C      SUBROUTINE ARREN ADDS TEMPERATURE EFFECT
CC      HOHLA AND KOMPA (1976)
CC      CC2 = 2.1E-33*EXP(1600./T)
C      BREDERLOW ET AL. (1983)
CC      CC2 = 3.8E-31
C      WILSON ET AL. (1984) AND STOCK ET AL. (1986)
CC      CC2 = 8.5E-32
C
C
C      WILSON ET AL. (1984) AND STOCK ET AL. (1986)
CC      CC3 = 8.E-32
C      BREDERLOW ET AL. (1983) AND COHEN AND JUDD (1984)
      CC3 = 0.
C
C
C      WILSON ET AL. (1984) AND STOCK ET AL. (1986)
CC      CC4 = 3.8E-30
C      COHEN AND JUDD (1984)
C      CC4 = 10.0**(-29.437-5.844*ALOG10(T/300.))
      CC4 = 10.0
C      SUBROUTINE ARREN ADDS TEMPERATURE EFFECT
C      BREDERLOW ET AL. (1983)
CC      CC4 = 2.9E-30
C
C
C      COHEN AND JUDD (1984)
C      CC5 = 8.E-33*EXP(1310./T)
      CC5 = 8.0E-33
C      SUBROUTINE ARREN ADDS TEMPERATURE EFFECT
C
C
C      BREDERLOW ET AL. (1983) AND COHEN AND JUDD (1984)
      CC6 = 0.0
C
C
C      V1 = 0.0
C
C
C      V2 = 0.0
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
C
C      KK1=.903E-13
C      KK2=80.E-12
C      KK3=.65E-12
C      KK4=1.000E-16
C      KK5=3.089E711
C      KK7=.1517E-18
C      KK8=1.6E-23
C
C      QQ1=.476E-16
C      QQ2=1.9E-11
C      QQ3=.1235E-17
C      QQ4=1.57E-16

```

```

C      Q05=.53E-14
C
CC     CC1=1.053E-33
CC     CC2=45.0E-32
CC     CC3=.4447E-31
CC     CC4=4.94E-30
CC     CC5=3.6E-31
CC     CC6=      1.8E-32
C
C      V1=      1.0E-12
C      V2=      1.0E-11
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC

```

```

C      GG=2*(.18/LC)**2
C      C=3.0E10
CC     B=P*(3.5E16)
C      B=(9.66E18)*P/T0
C      B2=B*B
C      B3=B2*B
C      RETURN
C      END

```

```

C      SUBROUTINE VELOC(OMEG1,RAD,OMEGA,A)
C      VELOCITY PROFILE IS ASSUMED TO BE PARABOLIC
C      MAX VELOCITY AT RAD=0.0
C      ZERO VELOCITY AT RAD=A
C      A IS RADIUS OF TUBE
C      OMEG1 IS MAXIMUM VELOCITY ALONG CENTERLINE
C
C      CALCULATE VELOCITY OMEGA AT R=RAD
C      0 .LE. RAD .LE. A
C
C      TYPE OF FLOW
C      OMEGA=(OMEG1/(A*A))*(RAD-A)**2
C      RETURN
C      END

```

```

SUBROUTINE PRINT(Z,TEMP)
COMMON/BLK2/K1,K2,K3,K4,K5,K6,K7,K8,C1,C2,C3,C4,C5
COMMON/BLK27/Q1,Q2,Q3,Q4,Q5
COMMON/BLK3/B,B2,B3,C,A00,B00,EPSNU,OMEGA,C6
COMMON/BLK4/CHSI10,CHSI20,ABARO,Z1BAR,LC,XK0
COMMON/BLK7/ABC,C00,C0,OMEG1,P,R1,R2,TM,XNRHO
COMMON/BLK22/AD,V1,V2,GG

```

```

COMMON/BLK28/TAU2,TAU4,TAU5,TAU6,TAU3,SIG
COMMON/BLK299/TTT2,TTT3,TTT4,TTT5,TTT6
REAL K1,K2,K3,K4,K5,K6,K7,K8,LC

```

```

C
IF(Z .EQ. 0.0) WRITE(6,10)
10  FORMAT(1X,20HCOEFFICIENTS AT Z=0      )
IF(Z .GE. 1.0) WRITE(6,11)
11  FORMAT(1X,20HCOEFFICIENTS AT Z=L     )
C
WRITE OUT COEFFICIENTS
WRITE(6,100) K1,K7,Q1,C5,TTT2
WRITE(6,101) K2,K8,Q2,V1,TTT3
WRITE(6,102) K3,C1,Q3,V2,TTT4
WRITE(6,103) K4,C2,Q4,SIG,TTT5
WRITE(6,104) K5,C3,Q5,TEMP,TTT6
WRITE(6,105) K6,C4,C6,LC
100  FORMAT(T5,5HKK1 = ,E15.7,T30,5HKK7 = ,E15.7,T60,5HQ01 = ,E15.7 ,
1 T85,5HCC5 = , E15.7 , T103,7HTTT2 = ,E15.7 )
101  FORMAT(T5,5HKK2 = ,E15.7,T30,5HKK8 = ,E15.7,T60,5HQ02 = ,E15.7 ,
1 T85,5HV1 = , E15.7 , T103,7HTTT3 = ,E15.7 )
102  FORMAT(T5,5HKK3 = ,E15.7,T30,5HCC1 = ,E15.7,T60,5HQ03 = ,E15.7 ,
1 T85, 5HV2 = , E15.7 , T103,7HTTT4 = ,E15.7 )
103  FORMAT(T5,5HKK4 = ,E15.7,T30,5HCC2 = ,E15.7,T60,5HQ04 = ,E15.7 ,
1 T85, 8HSIGMA = , E15.7 , T103,7HTTT5 = ,E15.7 )
104  FORMAT(T5,5HKK5 = ,E15.7,T30,5HCC3 = ,E15.7,T60,5HQ05 = ,E15.7 ,
1 T85,7HTEMP = ,F9.2 , T103,7HTTT6 = ,E15.7 )
105  FORMAT(T5,5HKK6 = ,E15.7,T30,5HCC4 = ,E15.7,T60,5HCC6 = ,E15.7 ,
1 T85, 4HL = ,F9.2 )
RETURN
END

```

```

SUBROUTINE FUN(N,S,Y,F)

```

```

C THIS SUBROUTINE DEFINES THE RIGHT HAND SIDE
C OF THE DIFFERENTIAL EQUATIONS FOR THE CHEMICAL KINETICS
C IMPLICIT REAL*8(A-H,K,L,O-Z)
DIMENSION Y(7),F(7)
COMMON/BLK1/X7,POWER
EXTERNAL CHSI1,CHSI2
COMMON/BLK2/K1,K2,K3,K4,K5,K6,K7,K8,C1,C2,C3,C4,C5
COMMON/BLK27/Q1,Q2,Q3,Q4,Q5
COMMON/BLK3/B,B2,B3,C,A00,B00,EPSNU,OMEGA,C6
COMMON/BLK4/CHSI10,CHSI20,ABAR0,Z1BAR,LC,XK0
COMMON/BLK7/ABC,C00,C0,OMEG1,F,R1,R2,TM,XNRHO
COMMON/BLK22/AD,V1,V2,G6
COMMON/BLK28/TAU2,TAU4,TAU5,TAU6,TAU3,SIG
COMMON/BLK299/TTT2,TTT3,TTT4,TTT5,TTT6
REAL K1,K2,K3,K4,K5,K6,K7,K8,LC

```

```

C
C QY=QUANTUM YIELD
C QY=1.0

```

```

C
C F(I),I=1,6 ARE RATES OF CHANGES FOR THE CONCENTRATIONS
C F(1)=D[R1]/DZ F(2)=D[R1]/DZ
C F(3)=D[R2]/DZ F(4)=D[I2]/DZ
C

```

```

C          F(5)=D[I*]/DZ          F(6)=D[I]/DZ
C
C 20 CONTINUE
C     Z=LC*S
C     S IS SCALED LENGTH VARIABLE
C     O .LE. S .LE. 1
C     FLOW CALCULATES TEMPERATURE, PRESSURE, FLOWRATE
C     AND DENSITY RESPONSE AS FUNCTION OF Z
C
C     Z IS DISTANCE IN CM
C     CALCULATE GAS PARAMETERS AS FUNCTION OF Z
C     CALL FLOW(Z,TEMP,PRESS,FLOWR,DENSITY,DWDZ)
C     CALL FLOW(Z,TEMP,PRESS,FLOWR,DENSITY,DWDZ)
C     WRITE(6,357)Z,TEMP,PRESS,FLOWR,DENSITY,DWDZ
357  FORMAT(1X,3E16.7,/,3E16.7 )
C     TEMP IS TEMPERATURE DEG K
C     PRESS IS PRESSURE IN TORR
C     FLOWR IS FLOWRATE IN M/SEC
C     DENSITY IS GAS DENSITY IN KG/M**3
C     OMEGA=FLOWR*100.
C     OMEGA IS FLOW RATE IN CM/SEC
C     CALCULATE COEFFICIENTS AS FUNCTION OF TEMP AND Z
C     CALL ARREN(TEMP)
C     TAU5=(TTT5)*PRESS
C     TAU6=TAU5
C
C
C     CONSTANTS COME VIA COMMON BLKS 2 AND 3
C     K'S IN CM**3/SEC
C     C'S IN CM**6/SEC
C     Q'S IN CM**3/SEC
C     R0W0R0I5YI0W0C0M**2
C     X7STAR=Y(7)*B+X8
C     DIF=Y(5)-.5*Y(6)
C     CALL SIGMA(SIG2)
C     SIG=SIG2
C     F(1)=K1*B*Y(2)*Y(5)+K2*B*Y(2)*Y(6)-CHSI1(Z)*Y(1)-K4*B*Y(1)*Y(2)
1     +K5*B*Y(2)*Y(4) -K7*B*Y(5)*Y(1)-K6*B*Y(2)*Y(1) +V2*B*Y(3)*Y(6)
2     -K8*B*Y(6)*Y(1) -Y(1)*DWDZ
C     F(2)=CHSI1(Z)*Y(1)-K1*B*Y(2)*Y(5)-K2*B*Y(2)*Y(6)-2*K3*B*Y(2)*Y(2)
1     -K4*B*Y(1)*Y(2)-K6*B*Y(1)*Y(2)-K5*B*Y(2)*Y(4)+V2*B*Y(3)*Y(6)
2     +K7*B*Y(5)*Y(1) +K8*B*Y(6)*Y(1) -Y(2)*DWDZ-Y(2)/TAU2
C     F(3)=K3*B*Y(2)*Y(2)+K6*B*Y(1)*Y(2)+K4*B*Y(1)*Y(2)-V2*B*Y(3)*Y(6)-
1     Y(3)*DWDZ -Y(3)/TAU3
C     A1=C1*B2*Y(1)*Y(5)*Y(6)+C2*B2*Y(1)*Y(6)*Y(6)+C3*B2*Y(4)*Y(5)*Y(6)
C     A2=C4*B2*Y(4)*Y(6)*Y(6)-CHSI2(Z)*Y(4)+K7*B*Y(5)*Y(1)
1     -K5*B*Y(2)*Y(4) +V1*B*Y(6)*Y(6) +C5*B2*Y(6)*Y(6)*Y(3)
C     F(4)=A1+A2+K8*B*Y(6)*Y(1)+C6*B2*Y(6)*Y(5)*Y(3)-Y(4)*DWDZ-Y(4)/TAU4
C     A3=QY*CHSI1(Z)*Y(1)+0.51*CHSI2(Z)*Y(4)-K1*B*Y(2)*Y(5)
C     A4=-C1*B2*Y(1)*Y(5)*Y(6)-C3*B2*Y(4)*Y(5)*Y(6)-Q1*B*Y(1)*Y(5)
C     A5=-Q2*B*Y(4)*Y(5)-C*SIG*X7STAR*DIF +K6*B*Y(2)*Y(1)
C     F(5)=A3+A4+A5-Q3*B*Y(5)*Y(2)-Q4*B*Y(5)*Y(3)-Q5*B*Y(5)*Y(6)
1     -K7*B*Y(5)*Y(1)-C6*B2*Y(6)*Y(5)*Y(3)-Y(5)*DWDZ-Y(5)/TAU5
C     A6=1.49*CHSI2(Z)*Y(4)+Q1*B*Y(1)*Y(5)+Q2*B*Y(4)*Y(5)
1     -2*C5*B2*Y(6)*Y(6)*Y(3) -K8*B*Y(6)*Y(1)
C     A7=C*SIG*X7STAR*DIF -C1*B2*Y(1)*Y(5)*Y(6)

```

```

A8=-2*C2*B2*Y(1)*Y(6)*Y(6)-C3*B2*Y(4)*Y(5)*Y(6)
A9=-2*C4*B2*Y(4)*Y(6)*Y(6)-K2*B*Y(2)*Y(6)+K4*B*Y(1)*Y(2)
A10=Q3*B*Y(5)*Y(2)+Q4*B*Y(5)*Y(3)+Q5*B*Y(5)*Y(6)
1 +K5*B*Y(2)*Y(4) -V2*B*Y(3)*Y(6) -2*V1*B*Y(6)*Y(6)
F(6)=A6+A7+A8+A9+A10-C6*B2*Y(6)*Y(5)*Y(3) -Y(6)*DWDZ-Y(6)/TAU6
C   SCALED EQUATIONS IN THE Z-DIRECTION
DO 10 I=1,6
10  F(I)=LC*F(I)/OMEGA
    F(7)=LC*Y(7)*DIF*B*SIG
RETURN
END

```

```

C   SUBROUTINE SIGMA(SIG)
    THIS SUBROUTINE DEFINES THE CROSS SECTION SIGMA
COMMON/BLK3/B, B2, B3, C, A00, B00, EPSNU, OMEGA, C6
COMMON/BLK7/ABC, C00, C0, OMEG1, P, R1, R2, TM, XNRHO
REAL NU, NUS, NU0, NU1, NU2, NU3, NU4, NU5
PI=3.14159
FIS=PI*PI
NU=C/1.315246E-4
NUS=NU*NU
FISNUS=FIS*NUS*4.
G=0
CS=C*C
NU0=NU
NU1=NU0+.141*C
NU2=NU1+.068*C
NU3=NU0-.427*C
NU4=NU3-.026*C
NU5=NU4-.068*C
DELTA23=NU-NU5
DELTA22=NU-NU4
DELTA21=NU-NU3
DELTA34=NU-NU0
DELTA33=NU-NU1
DELTA32=NU-NU2
TEMPO=293
TWALL=TEMPO
T1=TWALL
A=5.434
A1=A*2.4/7.7*CS
A2=A*3.0/7.7*CS
A3=A*2.3/7.7*CS
A4=A*5.0/7.7*CS
A5=A*2.2/7.7*CS
A6=A*0.6/7.7*CS
FUGTEMP=SQRT(T1/300.)
ALPHAM=1.88E7*FUGTEMP
DELDOF=2.51E8*FUGTEMP
DELNU=DELDOF+ALPHAM*P
SIGMA23=A1/(FISNUS*DELNU)/(1+(2.*DELTA23/DELNU)**2)*5./12.
SIGMA22=A2/(FISNUS*DELNU)/(1+(2.*DELTA22/DELNU)**2)*5./12.
SIGMA21=A3/(FISNUS*DELNU)/(1+(2.*DELTA21/DELNU)**2)*5./12.

```



```

SIGMA34=A4/(FISNUS*DELNU)/(1+(2.*DELTA34/DELNU)**2)*7./12.
SIGMA33=A5/(FISNUS*DELNU)/(1+(2.*DELTA33/DELNU)**2)*7./12.
SIGMA32=A6/(FISNUS*DELNU)/(1+(2.*DELTA32/DELNU)**2)*7./12.
SIGMAT=SIGMA23+SIGMA22+SIGMA21+SIGMA34+SIGMA33+SIGMA32
SIG=SIGMAT
RETURN
END

```

```

SUBROUTINE INTEG(IPRINT,H)

```

```

C THIS SUBROUTINE INTEGRATES THE SYSTEM OF DIFFERENTIAL EQUATIONS
C DEFINING THE CHEMICAL KINETICS OF N-C3F7I IODINE LASER

```

```

C USING A VARIABLE STEP SIZE 7TH ORDER RUNGE KUTTA-FEHLBERG METHOD.

```

```

C IMPLICIT REAL*8(A-H,K,L,O-Z)

```

```

C DIMENSION YD(7),X(7),WK(84)

```

```

C COMMON/BLK1/X7,POWER

```

```

C COMMON/BLK3/B,B2,B3,C,A00,B00,EPSNU,OMEGA,C6

```

```

C COMMON/BLK4/CHSI10,CHSI20,ABARO,Z1BAR,LC,XK0

```

```

C COMMON/BLK7/ABC,C00,C0,OMEG1,P,R1,R2,TM,XNRHO

```

```

C COMMON/BLK8/ZOL,ZE,NG,TO,RAD,A,PIN,W

```

```

C COMMON/BLK22/AD,V1,V2,GG

```

```

C COMMON/BLK23/W0,ETA0,PT0,FRAC

```

```

C COMMON/BLK29/ZZZ,TZZ,FZZ,ETAZZ,WZZ

```

```

C COMMON/BLK30/DATA(50,50),NDMAX,FLRATE(8),FDPTDAT(50,40)

```

```

C EXTERNAL FUN,CHSI1,CHSI2

```

```

C REAL LC

```

```

C INTEGRATE SYSTEM FROM S=0 TO S=1.0 USING RUNGE-KUTTA METHOD

```

```

C X(1)=RI

```

```

C X(2)=R

```

```

C X(3)=R2

```

```

C X(4)=I2

```

```

C X(5)=I*

```

```

C X(6)=I

```

```

C X(7)=RHO+

```

```

C X8=RHO-

```

```

C X9=I*-.5*I

```

```

C INITIALIZE CONSTANTS FOR FLOW EQUATIONS

```

```

C SEE COMMON BLK10 FOR THESE CONSTANTS--NEEDED FOR SUB FLOW

```

```

C CALL PFLOW

```

```

C ND=0

```

```

C TEST FOR PRINT CONDITIONS

```

```

C IF(IPRINT.EQ. 0) GO TO 229

```

```

C NG=NG+1

```

```

C NG IS THE NUMBER OF GRAPHS TO BE SAVED

```

```

C MAXIMUM NG=8

```

```

C FLOWRATE(NG) IS LABEL FOR DATA SAVED

```

```

C SEE ALSO PROGRAM PLOTD--WHICH CAN PLOT THE SAVED DATA

```

```

C FLRATE(NG)=OMEGA

```

```

C WRITE(8,331) LC

```

```

331     FORMAT(1X,11H   LC   =  ,F10.2)
229     CONTINUE
55      CONTINUE
      N=7
      TOL=1.0E-5
      PD=1.0
      MTH=1
      WZZ=W0
C      H IS STEP SIZE IN SCALED UNITS BETWEEN PRINT OUTS
C      IPRINT=0 OFF, IPRINT=1 ON
      HMIN=1.0E-9
      HMAX=H/100.
      HUSE=HMIN*1000.
      IERR=0
C      INITIAL CONDITIONS
      Z0=0.0
      Y0(1)=1.0
      Z1=0.0
      DO 9 I=2,6
9      Y0(I)=0.0
C      INITIALIZE FLOW,DENSITY,PRESSURE AND TEMPERATURE AT Z=0
      CALL FLOW(Z0,TEMP,PRESS,FLOWR,DENSITY,DWDZ)
C      GUESS AT INITIAL CONDITIONS FOR X(8)
      X70=PIN*W/(EPSNU*C)
C      X70 IS RHO+(0) WHICH IS GIVEN
C      INITIAL CONDITION FOR RHO-(0) IS UNKNOWN--ASSUME C00 VALUE
      XK0=X70*C00
      X8=XK0/X70
      Y0(7)=X70/B
      IF(IPRINT .EQ. 0) GO TO 300
      CALL FUN(N,Z0,Y0,F)
      TEMP=TZZ+273.
      IF(Z0.EQ.0.0)CALL PRINT(Z0,TEMP)
      WRITE(6,191)
191    FORMAT(///,T7,1HZ,T20,4H[R1],T32,4H[R1],T45,5H[R2],T57,4H[C1],
1     T69,4H[C1*],T80,4H[C1] ,T91,6H[RHO+],T103,6H[RHO-],T112,
2     9HINVERSION      )
300    CONTINUE
      DO 10 I=1,7
10     X(I)=B*Y0(I)
C
      X8=XK0/X(7)
      X9=X(5)-.5*X(6)
      X7STAR=X(7)+X8
C      USE SUBROUTINE SIGMA TO CALCULATE CROSS SECTION SIGMA
      CALL SIGMA(SIG2)
      IF(IPRINT .EQ. 0) GO TO 222
      WRITE(6,199)Z0,(X(I),I=1,7),X8,X9
      WRITE(6,303)ZZZ,TZZ,PZZ,ETAZZ,WZZ
      CALL FUN(N,Z0,Y0,F)
      TEMP=TZZ+273.
      IF(Z0.EQ.1.0)CALL PRINT(Z0,TEMP)
222    CONTINUE
C      SAVE THE DATA FOR FUTURE PLOT ROUTINES
C      DATA ARRAYS ARE DATA(50,50) AND FDPTDAT(50,40)
C

```

```

IF(IPRINT .EQ. 0) GO TO 227
ICOL=(NG-1)*6
ND=ND+1
DATA(ND,ICOL+2)=X(2)
DATA(ND,ICOL+1)=Z0
DATA(ND,ICOL+3)=X(4)
DATA(ND,ICOL+4)=X(5)
DATA(ND,ICOL+5)=X(6)
DATA(ND,ICOL+6)=X9
NNN=(NG-1)*5
FDPTDAT(ND,NNN+1)=Z0
FDPTDAT(ND,NNN+2)=WZZ
FDPTDAT(ND,NNN+3)=ETAZZ
FDPTDAT(ND,NNN+4)=PZZ
FDPTDAT(ND,NNN+5)=TZZ
C WRITE(Z,R,I2,I*,I,INV)
WRITE(8,6773) Z0,X(2),X(4),X(5),X(6),X9
WRITE(8,6773) Z0,WZZ,ETAZZ,PZZ,TZZ
6773 FORMAT(1X,F6.3,2X,5(2X,E15.6))
227 CONTINUE
IF(Z0.LE.0.0) GO TO 3567
IF(IPRINT .EQ. 0) GO TO 223
WRITE(6,303) ZZZ,TZZ,PZZ,ETAZZ,WZZ
223 CONTINUE
303 FORMAT(1X,T2,3HZ=,F10.3,2X,T15,3HT=,F7.3,2X,T30,
1 7HPTORR=,F9.4,2X,
2 T55,9HDENSITY =,F9.6,2X,T80,3HW=,E14.7 )
3567 CONTINUE
199 FORMAT(1X,E12.5,8E12.5,E12.5,E12.5 )
C
C
C USE 7TH ORDER RUNGE KUTTA INTEGRATION SCHEME WITH VARIABLE STEP
C STEP SIZE CAN VARY FROM HMIN TO HMAX
C Z0 IS STARTING VALUE FOR Z
C Z1 IS NEXT STOPPING POINT IN INTEGRATION SCHEME
C TOL IS TOLERANCE
C IERR IS ERROR CODE TO DETERMINE IF INTEGRATION WAS SUCCESSFUL
C
C
100 CONTINUE
Z1=Z1+H
IF(Z1 .GT. 1.00) GO TO 111
CALL RKF7(N,Z0,Z1,Y0,TOL,FUN,PD,MTH,HMIN,HMAX,HUSE,WK,IERR)
IF(IERR .NE. 0) WRITE(6,444) IERR,Z0,Z1,(Y0(I),I=1,7)
IF(IERR .NE. 0) STOP 1717
444 FORMAT(1X,18HIERR IS NOT ZERO ,I5,(4E16.7,/))
200 CONTINUE
X(7)=B*Y0(7)
XB=XK0/X(7)
60 FORMAT(1X,5(2X,E14.6))
GO TO 300
500 CONTINUE
DO 110 I=1,7
110 X(I)=B*Y0(I)
XB=XK0/X(7)
X9=X(5)-.5*X(6)

```

```

111     CONTINUE
        XX7L=X(7)
C      X(7) IS CALCULATED RHO+(L) VALUE
        XKCAL=R2*X(7)*X(7)
C      XKCAL IS CALCULATED VALUE FOR XK0
C      ABC IS DIFFERENCE BETWEEN CALCULATED AND INITIAL VALUE
        DIF=((XK0-XKCAL)/XKCAL)*100.
        ABC=DIF
        IF(IPRINT .EQ. 0) GO TO 224
        WRITE(6,202)DIF,XKCAL,XK0,C00
224     CONTINUE
202     FORMAT(1X,13HDIFFERENCE = ,E18.9,2X,12HXKCAL = ,E18.9,
1 2X,10HXK0 = ,E18.9,2X,6HC00 = ,E18.9 )
237     CONTINUE
C
C      RHOMIN=RHO-(0)=XK0/RHO+(0)=XK0/X70
        RHOMIN=XK0/X70
        FOUT=RHOMIN*W*EPSNU*C
        GAINDB=10.*ALOG10(FOUT/PIN)
        GAIN=FOUT/PIN
        IF(IPRINT .EQ. 0) GO TO 226
        WRITE(6,193)R1,R2,P,PIN,FOUT,GAINDB,GAIN
226     CONTINUE
193     FORMAT(1X,5HR1 = ,F10.7,2X,5HR2 = ,F10.7,1X,
1 6HPRESS = ,F10.7,2X,6HPIN = ,E14.7,3X,7HPOUT = ,E14.7,/,
2 1X,9HGAINDB = ,E14.7,3X,7HGAIN = ,E14.7 )
501     CONTINUE
        NDMAX=ND
C      NDMAX IS THE MAXIMUM NUMBER OF DATA POINTS
        RETURN
        END

```

APPENDIX B

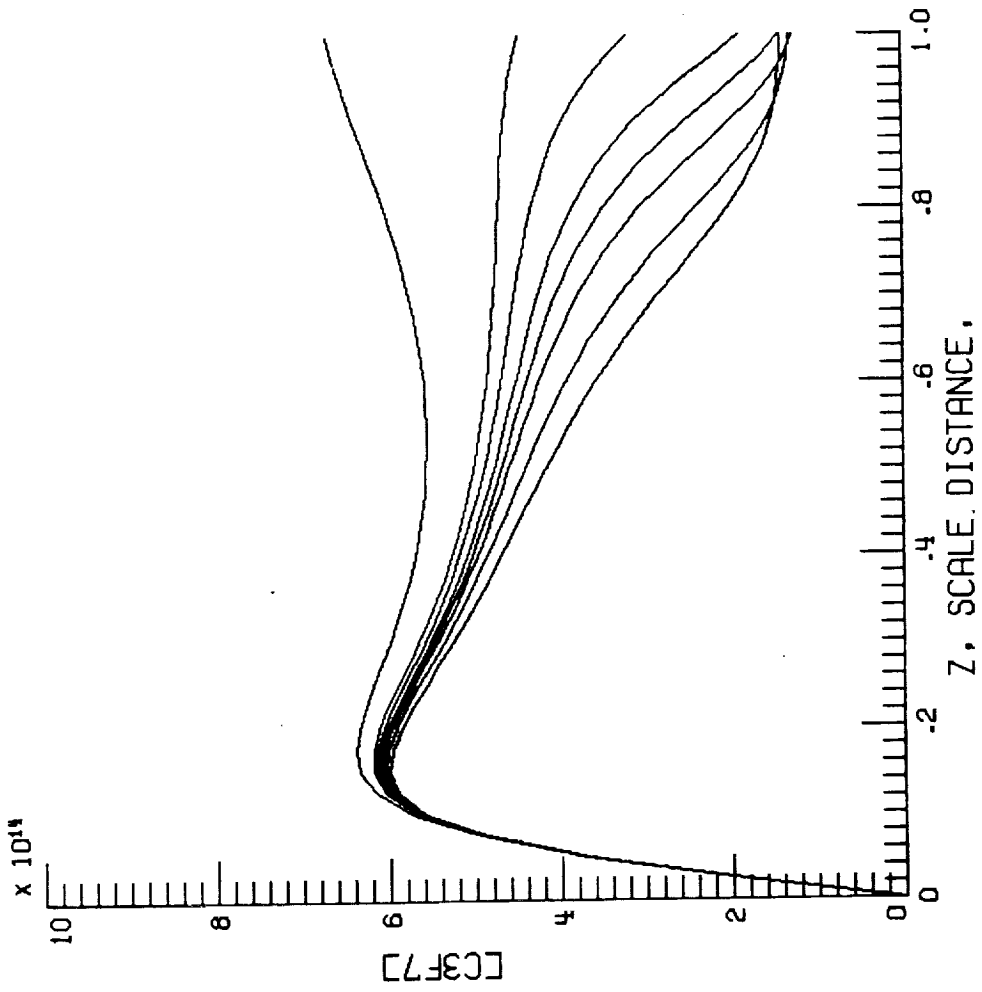
OUTPUT FROM SIMULATION MODEL

INPUT PARAMETERS

PTO - 15.0
 OMEG1 - 3000
 CON - 1689
 COO - 2,13398E8
 R1 - 0.00
 R2 - 0.9584792
 LC - 1000
 ZOL - 500
 XNRHO - 1.0
 TO - 300.0

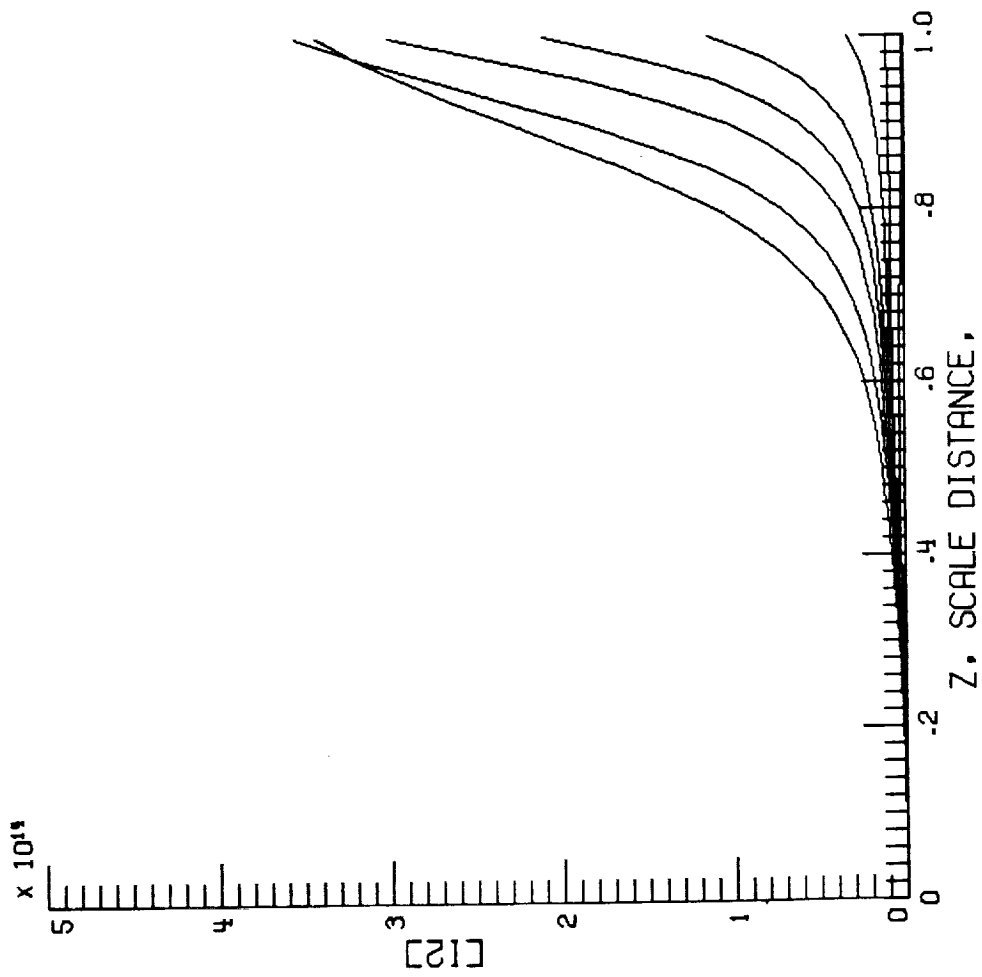
OUTPUT

<u>P_{in}</u>	<u>P_{out}</u>	<u>Gain</u>	<u>Gain db</u>
10.0	128.4570	12.8457	11.0875
5.0	124.9000	24.9801	13.97595
2.0	122.2330	61.1166	17.8616
1.0	119.9611	119.9611	20.7904
0.5	116.9325	233.8649	23.6895
0.2	111.3596	556.798	27.4570
0.1	105.7950	1057.954	30.2446
0.01	80.3968	8039.678	39.0524



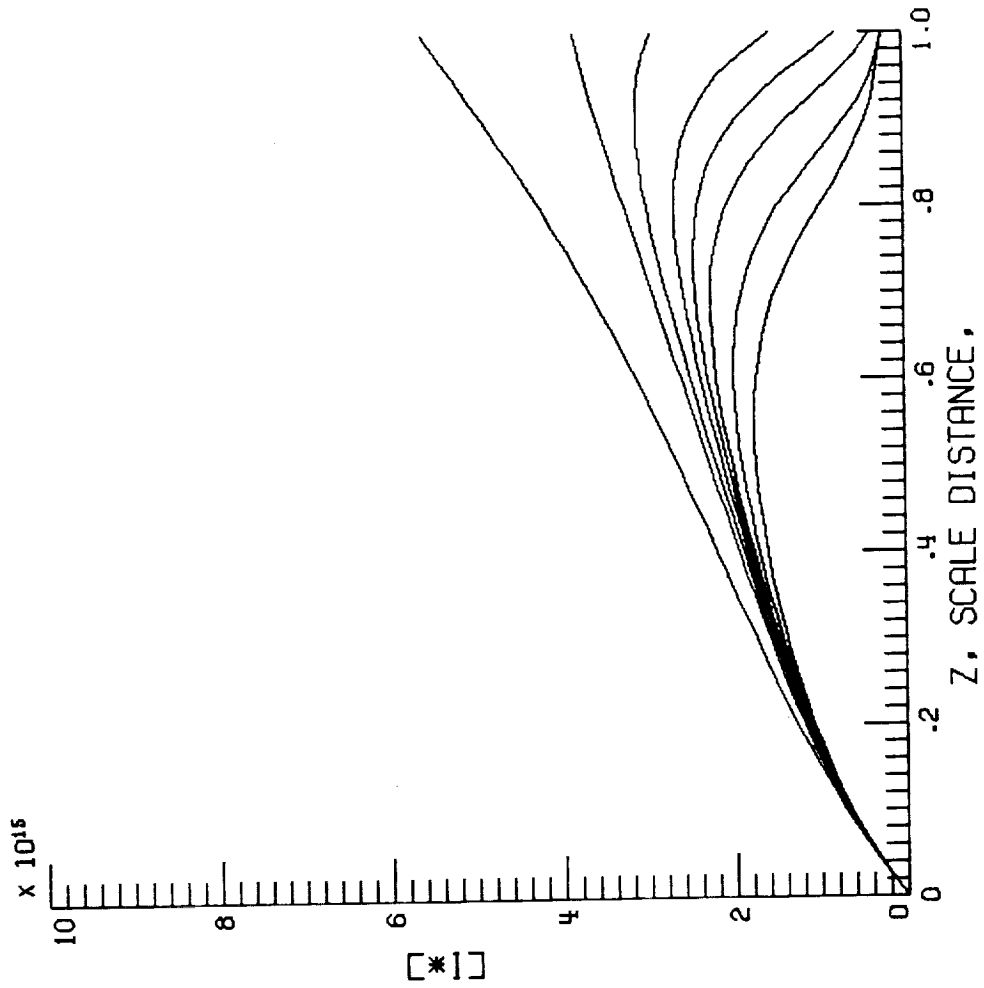
INFOPLT 1

Figure 1.



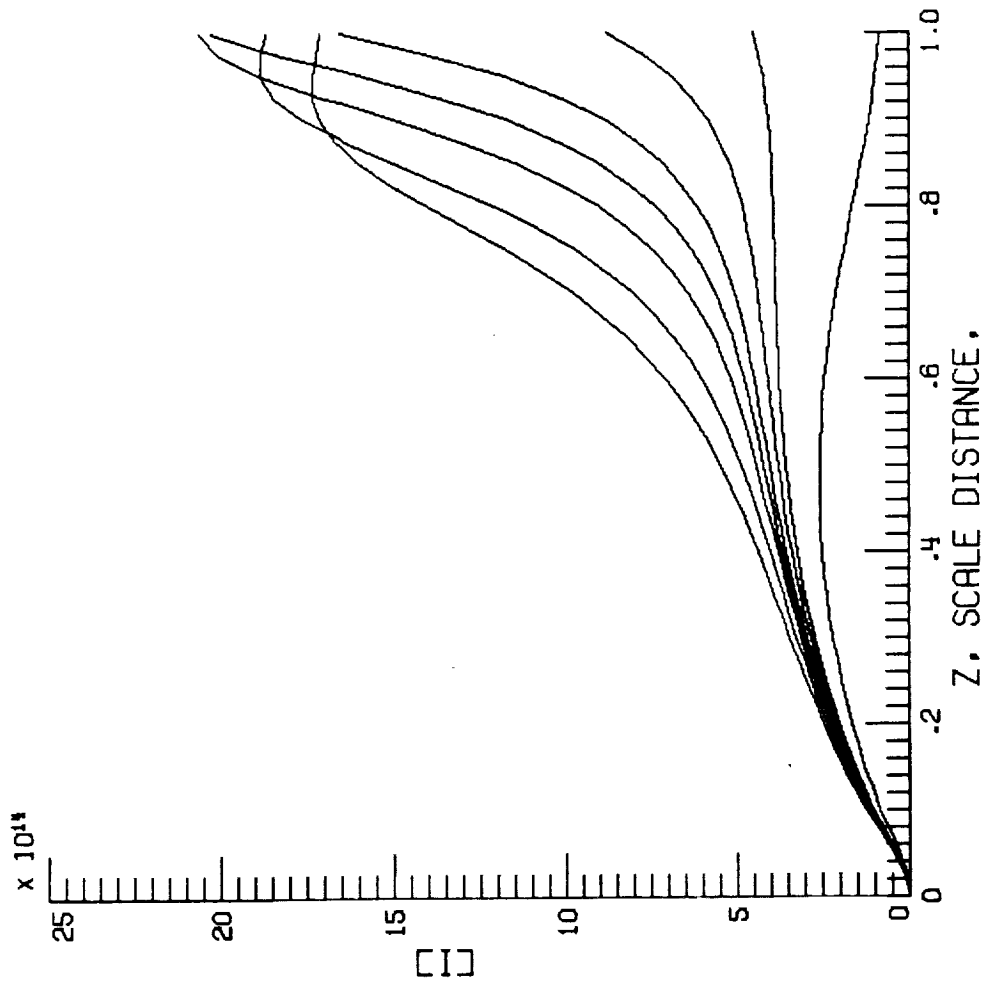
INFOPLT 2.

Figure 2.



INFOPLT 3.

Figure 3.



INFOPLT 4.

Figure 4.

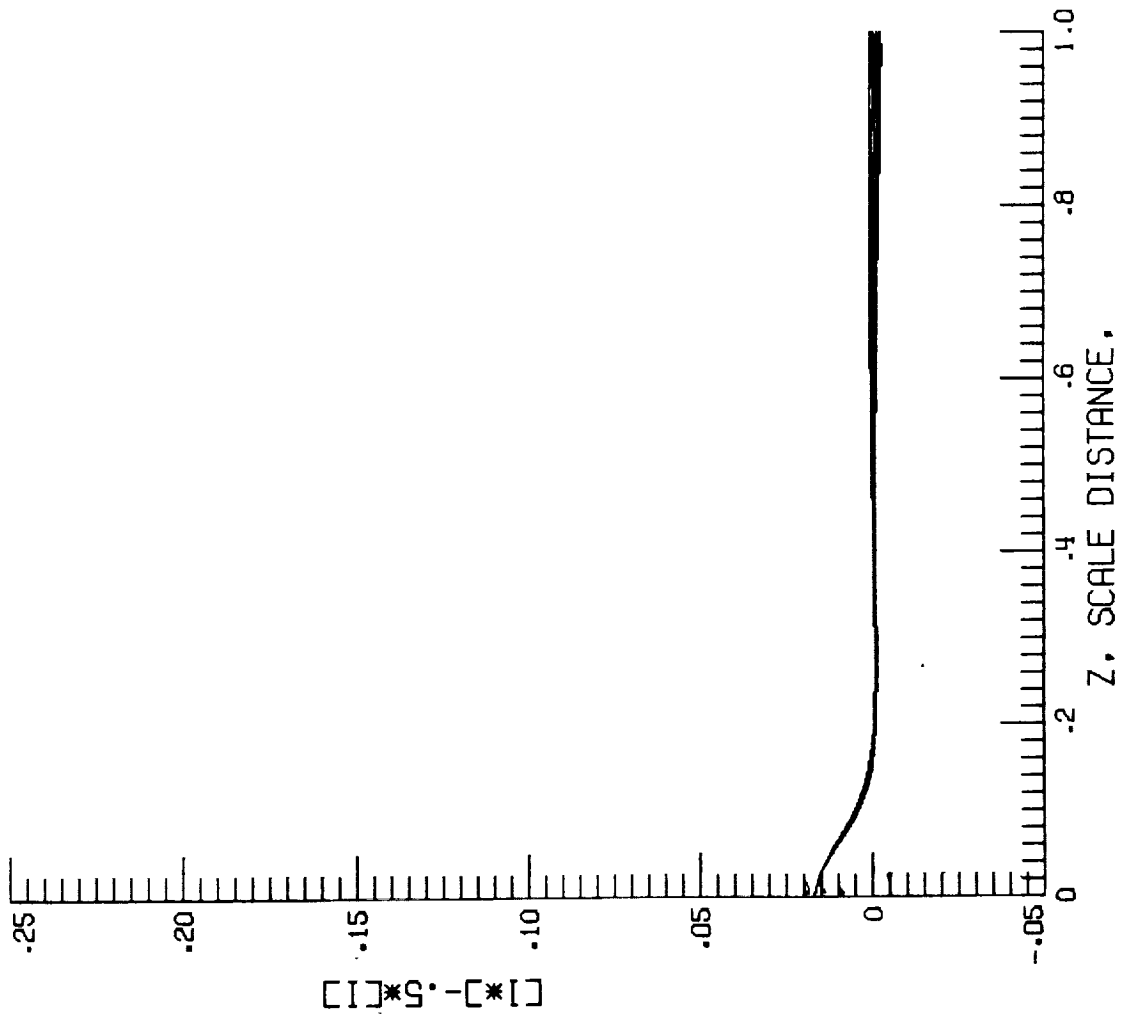


Figure 5.

INFOPLT 5.

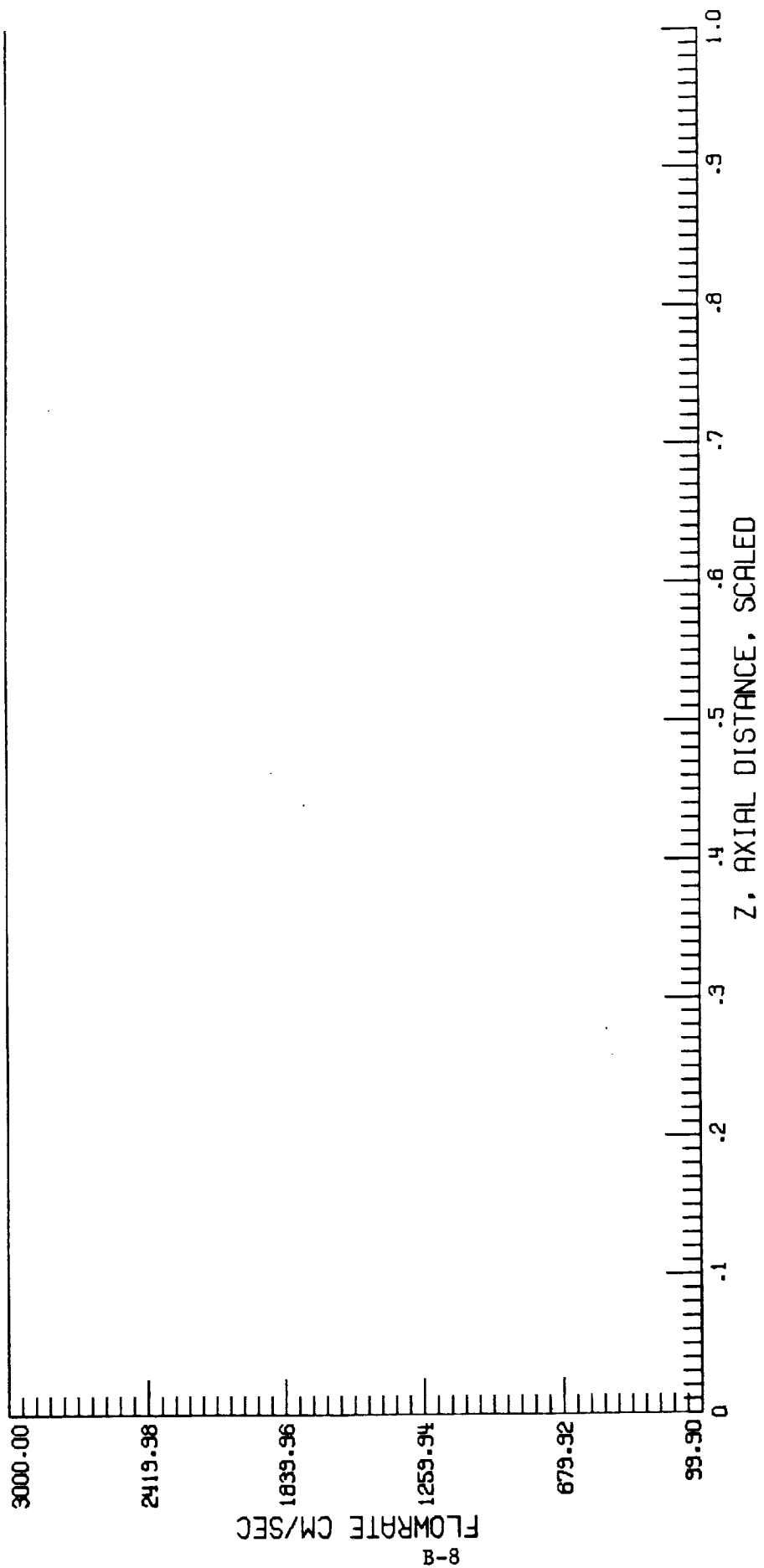


Figure 6.

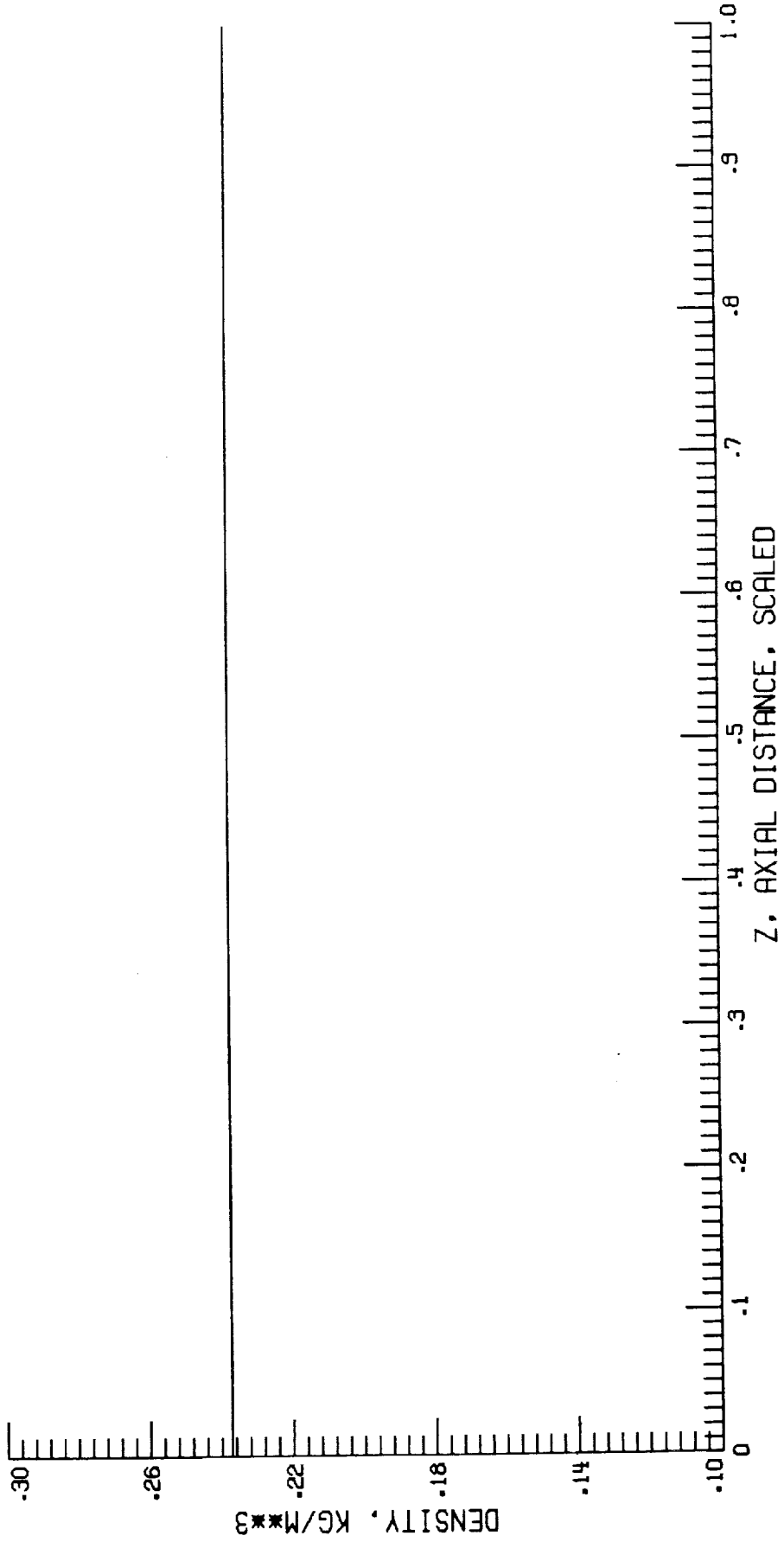


Figure 7.

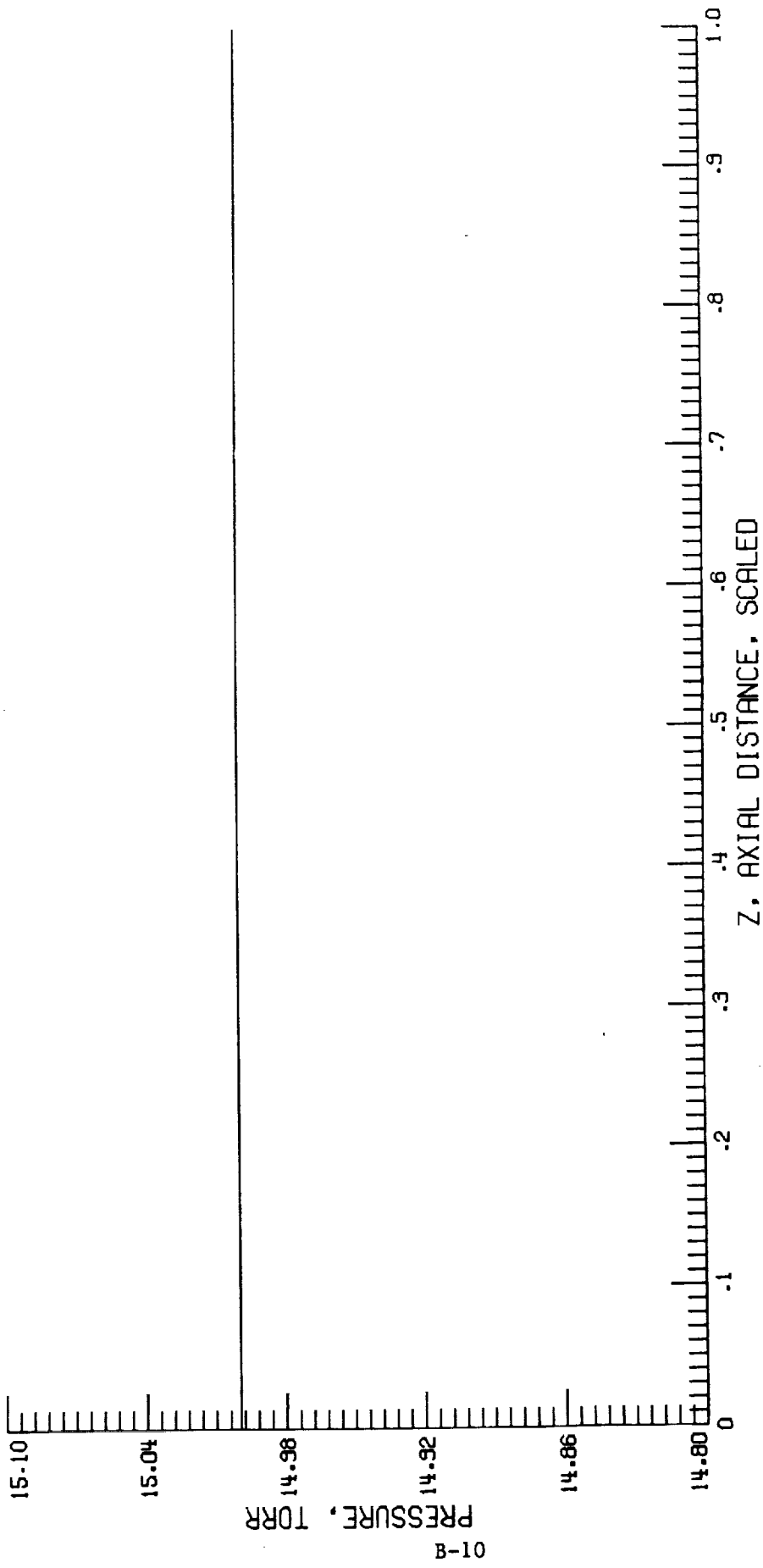


Figure 8.

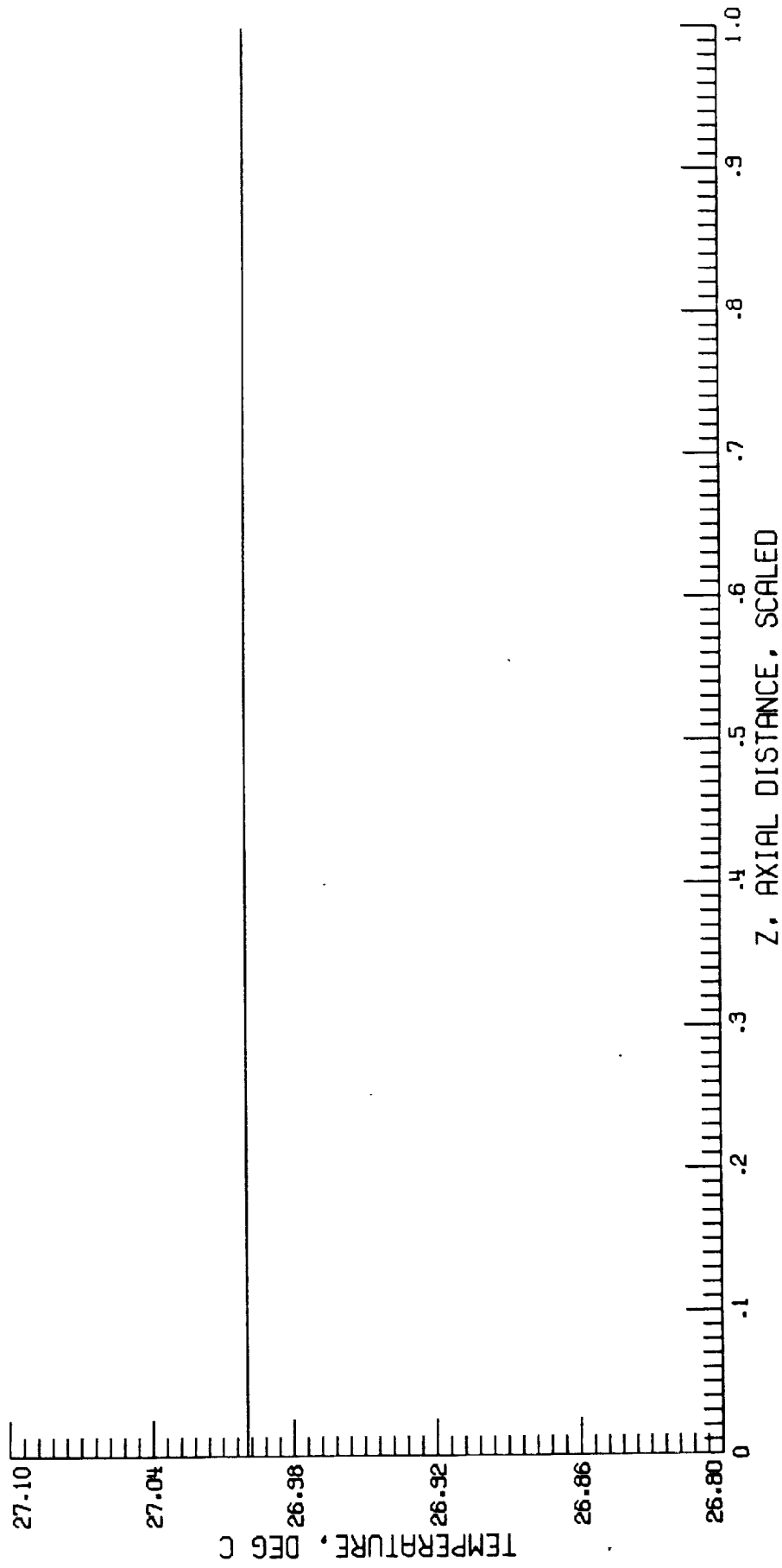


Figure 9.