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
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Dr. Robert C. Costen, Technical Monitor
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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-C₃F₇I iodine laser. The geometry of the amplifier is illustrated in Figure 1. In this figure

- $P_{in}$ - power density into the amplifier (watts/cm²),
- $W$ - transmission coefficient,
- $\epsilon$ - 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 $Z$

$$\rho^+(Z) \rho^-(Z) = K_0$$

(1)

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Figure 1. Geometry for Two Pass Amplifier.
where $K_0$ is a constant. At $Z = 0$ we have

$$\rho^+(0) \rho^-(0) = K_0$$

(2)

and at $Z = L$ we have

$$\rho^+(L) \rho^-(L) = K_0.$$ 

(3)

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

$$\rho^+(0) = \frac{P_{in} W}{\epsilon C}$$ 

(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
\[ \rho^-(L) = R_2 \rho^+(L). \]  \hspace{1cm} (5)

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

\[ R_2 \rho^+ \rho^+(L) = K_0 \quad \text{or} \quad \rho^+(L) = \sqrt{\frac{K_0}{R_2}} - \sqrt{\frac{\rho+(0) \rho^-(0)}{R_2}} \]  \hspace{1cm} (6)

Using the value (6) as the theoretical value for \( \rho^+(L) \) at \( Z = L \) we can compare this value with the calculated 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

\[ |\rho^+(L)_{\text{theoretical}} - \rho^+(L)_{\text{calculated}}| < E \]  \hspace{1cm} (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

\[ P_{\text{out}} = \rho^-(0) W \rho C \]  \hspace{1cm} (8)

and the gain is calculated from the relation

\[ \text{gain} = 10 \log_{10} \left( \frac{P_{\text{out}}}{P_{\text{in}}} \right) \text{ (decibels)}. \]  \hspace{1cm} (9)
The chemical reactions occurring in the laser tube are listed along with the values used for the rate constant. The assumed reactions are:

\[ RI + \hbar \nu \xrightarrow{\xi_1} R + I^* \]
\[ I_2 + \hbar \nu \xrightarrow{\xi_2} I+I^* \quad (51\% \text{ of the time}) \]
\[ I_2 + \hbar \nu \xrightarrow{\xi_2} I+I \quad (49\% \text{ of the time}) \]

Two Body Reactions

\[ I^* + R \xrightarrow{K_1} RI \quad , \quad K_1 = 1.0 \times 10^{-14} \]
\[ I + R \xrightarrow{K_2} RI \quad , \quad K_2 = 0.8 \times 10^{-11} \]
\[ R + R \xrightarrow{K_3} R_2 \quad , \quad K_3 = 2.0 \times 10^{-12} \]
\[ R + RI \xrightarrow{K_4} R_2 + I \quad , \quad K_4 = 3.0 \times 10^{-16} \]
\[ R + I_2 \xrightarrow{K_5} RI + I \quad , \quad K_5 = 1.0 \times 10^{-11} \]
\[ R + RI \xrightarrow{K_6} R_2 + I^* \quad , \quad K_6 = 0.0 \]
\[ I^* + RI \xrightarrow{K_7} R + I_2 \quad , \quad K_7 = 3.0 \times 10^{-9} \]
\[ I + RI \xrightarrow{K_8} I_2 + R \quad , \quad K_8 = 1.6 \times 10^{-23} \]
\[ I^* + RI \xrightarrow{Q_1} I + RI \quad , \quad Q_1 = 1.7 \times 10^{-17} \]
\[ I^* + I_2 \xrightarrow{Q_2} I + I_2 \quad , \quad Q_2 = 3.8 \times 10^{-11} e^{-4.4 \times 10^{-3} (T-300)} \]
\[ I^* + R \xrightarrow{Q_3} I + R \quad , \quad Q_3 = 3.7 \times 10^{-18} \]
\[ I^* + R_2 \xrightarrow{Q_4} I + R_2 \quad , \quad Q_4 = 4.7 \times 10^{-16} \]
\[ I^* + I \xrightarrow{Q_5} I + I \quad , \quad Q_5 = 1.6 \times 10^{-14} \]

Three Body Reactions

\[ I^* + I + RI \xrightarrow{C_1} I_2 + RI \quad , \quad C_1 = 1.6 \times 10^{-33} \]
\[ I + I + RI \xrightarrow{C_2} I_2 + RI \quad , \quad C_2 = 5.7 \times 10^{-33} e^{1310/T} \]
\[
\begin{align*}
I^* + I + I_2 & \rightarrow I_2 + I_2 , \quad C_3 = 0.0 \\
I + I + I_2 & \rightarrow I_2 + I_2 , \quad C_4 = 10^x \\
I + I + R_2 & \rightarrow I_2 + R_2 , \quad C_5 = 8.0(10^{-33})e^{1310/T} \\
I + I^* + R_2 & \rightarrow I_2 + R_2 , \quad C_6 = 0.0 \\
\end{align*}
\]

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 \( y_1, i=1,7 \) denote the normalized values of concentration. Define the quantities:

\[
\begin{align*}
X_1 &= B y_1 = [RI] \\
X_2 &= B y_2 = [R] \\
X_3 &= B y_3 = [R_2] \\
X_4 &= B y_4 = [I_2] \\
X_5 &= B y_5 = [I^*] \\
X_6 &= B y_6 = [I] \\
X_7 &= B y_7 = \rho^+(Z) \\
X_8 &= \rho^-(Z) = K_0/X_7 \\
\rho &= \rho(Z) = X_7 + X_8
\end{align*}
\]

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 \( \omega \) the flow rate of \( n-C_3F_7I \) in the \( Z \) direction (cm/sec) and \( \rho \) the total photon density, the differential equations defining the chemical kinetics of the amplifier are given by:
\[
\begin{align*}
\omega \frac{\text{d}y_1}{\text{d}z} &= K_1 y_2 y_5 + K_2 y_2 y_6 - \xi_1 y_1 - K_4 y_1 y_2 + K_5 y_2 y_4 - K_7 y_5 y_1 - K_8 y_6 y_1 \frac{\text{d}w}{\text{d}z} \\
\omega \frac{\text{d}y_2}{\text{d}z} &= \xi_1 y_1 - K_1 y_2 y_5 - K_2 y_2 y_6 - 2K_3 y_2 y_4 - K_4 y_1 y_2 - K_6 y_1 y_2 - K_5 y_2 y_4 + K_7 y_5 y_1 - \frac{\text{d}w}{\text{d}z} - y_2/r_2 \\
\omega \frac{\text{d}y_3}{\text{d}z} &= K_3 y_2^2 + K_6 y_1 y_2 - K_4 y_1 y_2 - y_3/r_3 \\
\omega \frac{\text{d}y_4}{\text{d}z} &= C_1 B^2 y_1 y_5 y_6 + C_2 B^2 y_1 y_5 y_6 + C_3 B^2 y_4 y_5 y_6 + C_4 B^2 y_4 y_5 y_6 - \xi_2 y_4 + K_7 y_1 y_5 - K_5 y_2 y_4 + C_5 B y_3 y_5 y_6 + C_6 B y_3 y_5 y_6 - y_3/r_3 \\
\omega \frac{\text{d}y_5}{\text{d}z} &= \xi_1 y_1 + 0.5 \xi_2 y_4 - K_1 y_2 y_5 - C_1 B^2 y_1 y_5 y_6 - C_3 B^2 y_4 y_5 y_6 + Q_1 y_1 y_5 - Q_2 y_4 y_5 \\
&\quad - C_5 B y_3 y_5 y_6 + Q_3 y_2 y_5 - Q_4 y_5 y_3 - Q_5 y_5 y_6 \\
&\quad - K_7 y_5 y_1 - C_6 B^2 y_5 y_3 y_5 - y_5/r_5 \\
\omega \frac{\text{d}y_6}{\text{d}z} &= 1.49 \xi_2 y_4 + Q_1 y_1 y_5 + Q_2 y_4 y_5 - 2C_5 B^2 y_4 y_5 y_6 + K_8 y_6 y_1 + C_6 B y_3 y_5 y_6 + Q_3 y_2 y_5 y_3 + Q_4 y_5 y_3 y_6 + Q_5 y_2 y_6 + K_4 y_1 y_2 \\
&\quad - C_1 B^2 y_1 y_5 y_6 - 2C_2 B^2 y_1 y_6 - C_3 B^2 y_4 y_5 y_6 - 2C_4 B^2 y_4 y_5 y_6 - K_2 y_2 y_6 + K_4 y_1 y_2 + K_2 y_2 y_6 + K_4 y_1 y_2 \\
&\quad + Q_3 y_5 y_2 + Q_4 y_5 y_3 + Q_5 y_5 y_6 + K_5 y_2 y_4 - C_6 B^2 y_5 y_3 y_6 - y_6/r_6
\end{align*}
\]
\[
\frac{dy_7}{dz} = -L_c y_7 (y_5 - \frac{1}{2} y_6) B_0
\]

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 TPAMP2(INPUT, OUTPUT, TAPE5=INPUT, TAPE6=OUTPUT, TAPE8)

MAIN PROGRAM
TWO PASS CONTINUOUS WAVE AMPLIFIER

AMPFAA 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 OUTPUT 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 AREN, 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, ABAR0, ZBAR, LC, X0
COMMON/BLK7/ABC, CO0, CO, OMEGI, P, R1, R2, TM, XNRHO
COMMON/BLK8/ZDL, ZE, NG, TO, RAD, A, PIN, W
COMMON/BLK10/CFI, CF2, CF4, OF0, RSTAR, ZL, L, SF1, SF2, AR, AA0, BB0
COMMON/BLK22/AD, V1, V2, GG
COMMON/BLK23/W0, ETA0, PT0, FRAC
COMMON/BLK28/TAU2, TAU4, 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 )
C DEFAULT VALUES
IEND=0
ICOUNT=0
NG=0
FRAC=0.0
AR=2.
TLE=59.0
PTO=20.0
W0=15.8
ETA0=.58
ZDL=7.50
TO=300.
AAO=147.23
C AAQ IN J/K MOL
C BBO IN 1/K
BBO=.0012
C AAQ, 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=5.000.
C
OMEG1 IN CM/S
CON=2.0E4
C
C NAMELIST/FARAM/PTO, OMEG1, CON, C00, R1, R2, TM, XNRHO, LC, ZDL, A, ZE,
1 AR, IEND, FRAC, TO, RAD, V1, V2, TTT2, TTT4, TTT5, TTT6, W, PIN
C
C ASSUME PRESSURE PTO (Torr) AND TEMPERATURE TO (Deg K)
ARE GIVEN FOR LEFT END. CALCULATE ETAO TO SATISFY GAS LAW
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
WRITE(6,603)
600 FORMAT(1X,28HEND OF FILE ENCOUNTERED-STOP)
CALL PSEUDO
DO 10 JJJ=1,9
CALL GRAPHS(JJJ)
10 CONTINUE
STOP 1313

W=TRANSMISSION COEFFICIENT
FIN=INPUT POWER DENSITY (WATTS/CM**2)

F=PRESSURE, TORR
AF=LASER BEAM DIAMETER CM
A=RADIUS OF TUBE (CM)
RAD=RADIUS OF TUBE WHERE CALCULATIONS ARE DONE.
T=TEMPERATURE DEG K
TO=TEMPERATURE LEFT END DEG K
P0=PRESSURE TORR LEFT END
W0=FLOW RATE LEFT END M/SEC
ETA0=DENSITY OF GAS KG/M**3
OMEGA1=FLOW RATE CM/SEC , MAXIMUM FLOW RATE AT RAD=0
TAU2,TAU4,TAU5,TAU6 ARE LIFETIMES FOR RADIAL DIFFUSION OF
T,T,T,T,T,T,T ARE LIFETIME VALUES FOR TAU
THE QUANTITIES [R],[I2],[I*] AND [I].
TAU3 IS DIFFUSION COEFFICIENT FOR [R2]
CON=PEAK CONCENTRATION , SOLAR CONSTANTS
CO0=INITIAL GUESS AT RHO-PLUS AT ZERO
WHICH IS SQUARE OF (CO0*R1)
R1= REFLECTIVITY AT LEFT END
R2= REFLECTIVITY AT RIGHT END
ZE=DISTANCE FOR LIGHT INTENSITY TO DIMINISH BY FACTOR 1/E
TM=TRANSMISSION COEFFICIENT (OUTPUT MIRROR)
ZOL=POINT ALONG AXIS WHERE MAXIMUM ILLUMINATION OCCURS
IN THE CASE ILLUMINATION IS A BELL SHAPED CURVE
IN THE CASE OF A SQUARE WAVE, 2*ZOL IS CUT OFF POINT
THE POINT 2*ZOL IS WHERE ILLUMINATION BEGINS TO DIMINISH
L=LENGTH OF LASER CAVITY IN CM
S=SCALED LENGTH WHICH GOES FROM ZERO TO ONE
LENGTH IS SCALED FROM ZERO TO ONE
ZL=2*ZOL LENGTH WHICH IS ILLUMINATED
FRAC=FRACTION OF PEAK CONCENTRATION WHICH GOES
INTO HEAT
DEFAULT VALUE IS FRAC=0.024 I.E. 2.40 PERCENT
H IS STEP SIZE FOR NUMERICAL INTEGRATION OVER SCALED LENGTH

601 CONTINUE
P=PT0
T=TO
ETA0=P*(1.01325E5)*296./(8314.3*760.*T)
PT0 IS PRESSURE IN TORR
ETA0 IS DENSITY IN KG/M**3
ETA0 IN KG/M**3
C F IN TORR
C \text{- IN DEG K}
C CMIN=1.0E4
C CMAX=1.0E20
C ZL=2*ZOL
C L=LC
C C=CON
C C=1=CON
C CALL COEFS
C \text{ IN M/SEC}
C \omega=\text{OMEGA/100.}
C \text{E=EG1 AND OMEGA ARE IN CM/SEC}
C \text{WRITE(6,199)}
C \text{FORMAT(//1)}
C \text{WRITE(6,199) ZE,ZOL,CJN,OMEGA,Frac,COO,R1,R2,F,T}
C \text{FORMAT(IX, TS,SHZE = ,F10.3,TSO,6HZDL = ,E15.7,TS5,6HCON = ,}
C \text{E15.7,T50,9HOMEGA = ,E15.7,T104,7HFRAC = ,F9.4,/,}
C \text{2 :TS,5HCOO = ,E15.7, T50,6H R1 = ,F10.7, T55,6H R2 = ,F10.7,}
C \text{3 T51,4H F = ,E15.7 ,T105,7HTEMP = ,F10.3;}
C \text{SET UP COEFFICIENTS IN DIFFERENTIAL EQUATIONS}
C \text{SET PRINTER OFF}
C \text{IPRINT=0 PRINTER OFF}
C \text{IPRINT=1 PRINTER ON}
C IPRINT=0
C \text{SET STEP SIZE H=.025 UNITS}
C \text{H=.025}
C \text{INTEGRATE DIFFERENTIAL EQUATIONS FROM S=0 TO S=1.0}
C X1=COO
C CALL INTEG(IPRINT,H)
C \text{INTERVAL HALVING SCHEME}
C \text{Y1=ABC}
C \text{IF(Y1.LT.0) PER=5.0}
C \text{IF(Y1.LT.0) PER=1.1}
C \text{IF(Y1.GT.0) PER=1.1}
C \text{IF(Y1.GT.0) PER=.9}
C 702 \text{CONTINUE}
C \text{IN THIS VERSION COO IS ASSUMED VALUE FOR RH0=(0)}
C \text{COO=(PER)*COO}
C \text{IF(COO.LT. CMIN) STOP 5432}
C \text{IF(COO.GT. CONAX) STOP 2345}
C X2=COO
C CALL INTEG(IPRINT,H)
C \text{Y2=ABC}
C \text{ABC IS XKO INITIAL MINUS XKO CALCULATED (PERCENT ERROR)}
C \text{IF((Y1*Y2).LT.0) GO TO 701}
C \text{X1=COO}
C \text{Y1=Y2}
C \text{GO TO 702}
C 701 \text{CONTINUE}
C \text{W1=.6}
C \text{W2=.4}
C \text{COO=W2*X1+W1*X2}
C 708 \text{CONTINUE}
C \text{CALL INTEG(IPRINT,H)
SUBROUTINE GRAPHS(JJJ)

AS THE NAME SUGGESTS THIS SUBROUTINE PLOTS GRAPHS OF THE NUMERICAL OUTPUT.

MULTIPLE PLOTS ON EACH GRAPH --- UP TO MAXIMUM OF EIGHT

COMMON/BLK4/CHS10,CHS120,ABARO,Z:BAR,LC,XKO
COMMON/BLK8/ZOL,ZE,N0,RAD,A,PIN,W
COMMON/BLK30/DATA(50,50),NDMAX,FLRATE(8),FDPTDAT(50,40)
DIMENSION X(50),Y(50),YY(50,8)
REAL LC

JJJ=1,9
JJJ=1 PLOT R VS Z
JJJ=2 PLOT I2 VS Z
JJJ=3 PLOT I* VS Z
JJJ=4 PLOT I VS Z
JJJ=5 PLOT INV VS Z
JJJ=6 PLOT FLOWRATE VS Z
JJJ=7 PLOT DENSITY VS Z
JJJ=8 PLOT PRESSURE VS Z
JJJ=9 PLOT TEMPERATURE VS Z

DATA ARRAY IS BY COLUMNS
ND=NUMBER OF DATA POINTS,=NUMBER OF ROWS IN DATA ARRAY
NG=NUMBER OF CURVES PER GRAPH
IC IS CODE TO DETERMINE NUMBER OF GRAPHS TO PLOT
IC=0 FOR MORE THAN ONE GRAPH
IC=1 FOR LAST GRAPH (USED FOR ONLY ONE GRAPH)

IC=0
NLAST=NG-1
SXC=5.0
SYC=5.0
SYCI=7.0

SXC=LENGTH OF XSCALE
SYC=LENGTH OF YSCALE
SYCI=LENGTH OF YSCALE FOR INVERSION

IF(NLAST .EQ. 0) IC=1
PLOT JJJ VS Z
IF(JJJ .GE. 6) GO TO 700
DO 10 I=1,NDMAX
X(I)=DATA(I,1)
DO 20 J=1,NG
NN=(J-1)*6
NCOL=NN+1+JJJ
YY(I,J)=DATA(I,NCOL)
20 CONTINUE
CONTINUE

FIND YMAX,YMIN

DMAX=0.0
YMAX=0.0
YMIN=0.0
ZMIN=0.0

FIND YMAX AND YMIN

DO 70 I=1,NDMAX
DO 71 J=1,NG
IF(YY(I,J) .GT. YMAX) YMAX=YY(I,J)
IF(YY(I,J) .LT. YMIN) YMIN=YY(I,J)
71 CONTINUE
CONTINUE

PLOT FIRST DATA CURVE

JJJ=1
ZMAX=1.00
DO 40 I=1,NDMAX
Y(I)=YY(I,1)
40 CONTINUE
LOGMAX=1+ALOG10(ABS(YMAX))
POWER1=10.**LOGMAX
TEST=YMAX/POWER1
YMAXX=0.025
IF(TEST .GT. 0.025) YMAXX=.05
IF(TEST .GT. 0.05) YMAXX=0.10
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 * POWER
IF (JJJ .NE. 5) GO TO 507
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
JJJ = 1 PLOT R VS Z
CALL INFOPLT(IC, NDMAX, X, 1, Y, 1, ZMIN, ZMAX, YMIN, YMAX, 1.0, 1 22.22, SCALE DISTANCE, , 2 11.11, 'C3F7', 0, 3 SXC, SYC, 0.75, 0.75)
GO TO 600
50 CONTINUE
IF (JJJ .GT. 2) GO TO 100
JJJ = 2 PLOT I2 VS Z
CALL INFOPLT(IC, NDMAX, X, 1, Y, 1, ZMIN, ZMAX, YMIN, YMAX, 1.0, 1 23.23, SCALE DISTANCE, , 2 9.99, '12', 0, 3 SXC, SYC, 0.75, 0.75)
GO TO 600
100 CONTINUE
IF (JJJ .GT. 3) GO TO 200
JJJ = 3 PLOT I* VS Z
CALL INFOPLT(IC, NDMAX, X, 1, Y, 1, ZMIN, ZMAX, YMIN, YMAX, 1.0, 1 23.23, SCALE DISTANCE, , 2 9.99, 'I*', 0, 3 SXC, SYC, 0.75, 0.75)
GO TO 600
200 CONTINUE
IF (JJJ .GT. 4) GO TO 300
JJJ = 4 PLOT I VS Z
CALL INFOPLT(IC, NDMAX, X, 1, Y, 1, ZMIN, ZMAX, YMIN, YMAX, 1.0, 1 23.23, SCALE DISTANCE, , 2 8.88, 'I', 0, 3 SXC, SYC, 0.75, 0.75)
3   SX, SY, 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  23,24HZ, SCALE DISTANCE, ,
2  24,24H   [I*]-.5*[I] ,0,
3  SX, SY, 0.75, 0.75)
600  CONTINUE
C
C  PLOT REST OF CURVES OR EXIT IF ONLY ONE CURVE
C
LAST=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,SX, SY, 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,SX, SY, 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 CURVE
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
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 10,15FLOWRATE CM/SEC , 0,
3 10.,5.,0.75,0.75)
GO TO 820
800 CONTINUE
IF(JJJ.GT.7) GO TO 801
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
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
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(NL<LAST .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

A-10
SUBROUTINE PFLOW
SUBROUTINE TO CALCULATE THE PARAMETERS FOR SUBROUTINE FLOW
PARAMETERS STORE IN COMMON BLK10
COMMON/BLK7/ABC., C00, C0, OMEGI, P, R1, R2, TM, XNRHO
COMMON/BLK8/ZOL, ZE, NG, TO, RAD, A, PIN, W
COMMON/BLK10/CFL, CF2, CF4, OF0, RSTAR, ZL, SF1, SF2, AR, AA0, BB0
COMMON/BLK23/W0, ETA0, PT0, FRAC
COMMON/BLK29/ZZZ, TZZ, PZZ, ETAZZ, WZZ
REAL L

AR IS BEAM DIAMETER RADIUS IN CM
SF1 = 1/(M*1.E-03), WHERE M IS THE MOLECULAR WEIGHT
SJF (J/K KG) = SF1*CV (J/K MOL)
SF2 = (1.01325E5)/760,
SF2 EQUALS 133.3 PA/TORR
SF1, SF2 ARE SCALE FACTORS FOR THE CORRECT UNITS OF
P=PRESSURE (N/M**2), SF1 (MOLE/KG)
PT=PRESSURE (TORR), SF2 (N/M**2)/TORR
TEST TO SEE IF W0 (M/SEC) IS NEAR MAX VALUE OF 5.3*SQRT(T0)
TEST=5.3*SQRT(T0)
TEST1=ABS(100.*(W0-TEST)/TEST)
IF (TEST1 .LT. 10.0) WRITE (6,778)

778 FORMAT (1X,52H WARNING W0 VALUE IS WITHIN 10 PERCENT OF ITS MAXIMUM
1, /, 1X, 35HALLOWABLE VALUE OF 5.3*SQRT(T0)
C
ZL=LIGHT SOURCE LENGTH IN CM
ETA=DENSITY (KG/M**3)
L=TUBE LENGTH IN CM
RSTAR=GAS CONSTANT (JOULE/KG DEG K)
T=TEMPERATURE (DEG K)
CV=SPECIFIC HEAT AT CONSTANT VOLUME
RSTAR (J/K KG) = SF1*R(J/K MOL)
W0, WL=FLOW VELOCITY (M/SEC) (SUBSCRIPTS O,L FOR START,END)
PO=SF2*PT0
RSTAR=8314.3/296.0
CF1=ETA0*W0
CF2=CF1*W0+PO
QF0=FRAC*(1.40E3)*C0/(A*1.E-2)
QF0 IN W/M**3
INPUT (W/M**2) DISTRIBUTED OVER VOLUME (2(PI)A)/PI<A**2) IN M2/M3
WZZ=W0
RETURN
END

SUBROUTINE FLOW(Z,T,PTORR,WSS,ETA,DWDZ)
SUBROUTINE TO CALCULATE T, P, WSS, ETA AS FUNCTION OF Z

COMMON/BLK10/CF1, CF2, CF4, OF0, RSTAR, ZL, L, SF1, SF2, AR, AAO, BB0
COMMON/BLK23/W0, ETAO, PT0, FRAC

COMMON/BLK29/ ZZZ, TZZ, PZZ, ETAZZ, WZZ

REAL L
ICOUNT = 0
Q = OF0 * Z / 100.

ENERGY INPUT TERM DETERMINED BY QFO
Z IS IN CM AND QFO IS IN W/M**3
IF (Z.GT.ZL) Q = QFO * ZL / 100.
XXX = BB0 * (TO - 300.)
CALL ETO(XXX, EE1)

WSS = WZZ

CONTINUE
T = (CF2 / CF1) * WSS - WSS * WSS) / RSTAR
DTDW = ((CF2 / CF1) - 2. * WSS) / RSTAR
XXX = BB0 * (T - 300.)
CALL ETO(XXX, EE1)
F = RSTAR * (T - TO) + (AAO / BB0) * SFI * (EE1 - EE0) +
1.5 * (WSS * WSS - W0 * W0) - O / CF1
FP = (RSTAR + SFI * 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, O, FM
357 FORMAT (IX, I5, IX, (3E16.7, /))

WSS = W1
ICOUNT = ICOUNT + 1
IF (ICOUNT .LT. 100) STOP 4444
GO TO 50

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
PZZ = PTO RR
ETA ZZ = ETA
WZZ = WSS
XXX = BB0 * (T - 300.)
CALL ETO(XXX, CV0)
CV = CV0 * AAO
CVS = SF1 * CV
XNUM = RSTAR * OF0
XDEN = (CF2 - 2. * CF1 * WSS) * (CVS + RSTAR) + RSTAR * CF1 * WSS
DWDZ = XNUM / XDEN
RETURN

END
SUBROUTINE ARREN(TEMP)
SUBROUTINE FOR ARRENHIUS EXPRESSION OF RATE COEFFICIENTS

BASIC ASSUMPTIONS
FOR QI TERMS QI=QIO*EXP(-BETA*(TEMP-TO))
TREAT KI TERMS LIKE CI TERMS

COMMON/BLK2/K1,K2,K3,K4,K5,K6,K7,K8,C1,C2,C3,C4,C5
COMMON/BLK27/01,02,03,04,05
COMMON/BLK27/B,B2,B3,C,A00,B00,EPNSU,OMEGA,C6
COMMON/BLK11/KK1,KK2,KK3,KK4,KK5,KK6,KK7,KK8
COMMON/BLK12/001,002,003,004,005
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
CALL ETO(XXX,YYY)
CALL ETO(XXX,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=001*SF1
Q2=002*EXP((-4.4E-3)*(TEMP-300.))
Q3=003*SF1
Q4=004*SF1
Q5=005*SF1
RETURN
END

SUBROUTINE ETO(X,Y)
NEGATIVE EXPONENTIAL FUNCTION
IF(X .LT. -470.) GO TO 100
FUNCTION CHSI1(Z)
C
ZIBAR 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,ZIBAR,LC,XK0
COMMON/BLK8/ZOL,ZE,NG,T0,RAD,A,PIN,W
REAL LC
IF(Z.LT.ABARO) GO TO 100
IF(Z.LT.ZIBAR) GO TO 200
C
Z GREATER THAN ZIBAR
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
ZIBAR 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,ZIBAR,LC,XK0
COMMON/BLK8/ZOL,ZE,NG,T0,RAD,A,PIN,W
REAL LC
IF(Z.LT.ABARO) GO TO 100
IF(Z.LT.ZIBAR) GO TO 200
C
Z GREATER THAN ZIBAR
C
XXX=-(Z-ZIBAR)/ZE
C
CALL ET0(XXX,YYY)
C
CHSI2=CHSI20*YYY
C
CHSI2 HAS UNITS OF SEC^-1
RETURN
100 CHSI2=0.0
RETURN
200 CONTINUE
CHSI2=CHSI20
RETURN
END

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

THIS SUBROUTINE DEFINES THE COEFFICIENTS IN THE DIFFERENTIAL EQUATIONS TO BE SOLVED.

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

COMMON/BLK22/AD,V1,V2,GG
COMMON/BLK3/BB,B2,B3,C,A00,B00,EPSNU,OMEGA,C6
COMMON/BLK4/CHSI10,CHSI20,ABAR0,ZIBAR,LC,XK0
COMMON/BLK7/ABC,C00,C0,OMEG1,F,R1,R2,TM,XNRH0
COMMON/BLK11/BB1,BB2,CC1,CC2,CC3,CC4,CC5,CC6
COMMON/BLK28/TAU2,TAU4,TAU5,TAU6,TAU3,SI
COMMON/BLK299/TTT2,TTT3,TTT4,TTT5,TTT6
REAL KK1,KK2,KK3,KK4,KK5,KK6,KK7,KK8
COMMON/BLK12/DO1,DO2,DO3,DO4,DO5
COMMON/BLK13/CC1,CC2,CC3,CC4,CC5,CC6
COMMON/BLK27/CHS10,CHS120,ABAR0,ZOL,LC,TIME
COMMON/BLK28/CHS10,CHS120,ABAR0,ZOL,LC,TIME
COMMON/BLK11/BB1,BB2,CC1,CC2,CC3,CC4,CC5,CC6
COMMON/BLK28/TAU2,TAU4,TAU5,TAU6,TAU3,SI
COMMON/BLK299/TTT2,TTT3,TTT4,TTT5,TTT6
REAL KK1,KK2,KK3,KK4,KK5,KK6,KK7,KK8,LC

COEFFICIENTS IN THE DIFFERENTIAL EQUATIONS

OMEGA=OMEG1

OMEGA=OMEG1 IS FLOW RATE IN CM/SEC
OMEGA IS FLOW RATE AT RADIUS R=RAD
SEE SUBROUTINE VELOC

CALL VELOC(OMEG1,RAD,OMEGA,A)

ABAR0=0.0
ABAR0 IS START OF ILLUMINATION
ZIBAR=2*ZOL IS THE POINT ON AXIS WHERE ILLUMINATION BEGINS TO DIMINISH
CHSI10=(3.04E-3)*C0*XNRH0
CHSI120=(3.38E-2)*C0/2.5
ZIBAR=2*ZOL
EPSNU=1.5E-19
WATTS*SEC
A00=2.0E17
B00=0.443
TAU2=TTT2
TAU3=TTT3
TAU4=TTT4
TAU5=TTT5
TAU6=TTT6

CHSI10+RI --> R + I
CHSI12 + I --> I* + I (51% OF THE TIME)
CHSI12 + I --> I + I (49% OF THE TIME)

(KK1) I* + R --> RI
(KK2) I + R --> RI
(KK3) R + R --> R2
(KK4) R + RI --> R2 + I
(KK5) R + I2 --> RI + I
(KK6) R + RI --> R2 + I*
(KK8) I**+R&I--->122+RR
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 (CC1)  I* + I + RI --> I2 + R1
C (CC2)  I + I + RI --> I2 + RI
C (CC3)  I* + I + I2 --> I2 + I2
C (CC4)  I + I + I2 --> I2 + I2
C (CC5)  I + I + I2 --> I2 + I2
C (CC6)  I + I* + R2 --> I2 + R2

WALL REACTIONS

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

KK1 = 5.6E-13
COHEN AND JUDD (1984)
KK1 = .9E-13
VINOKUKROV AND ZALESSKII (1979)
KK1 = 1.0E-14

KK2 = 2.0E-11
BREDERLOW ET AL. (1983)
KK2 = .7E-11
COHEN AND JUDD (1984)
KK2 = .7E-11

KK3 = 2.6E-12
KK3 = 2.0E-12

KK4 = 3.0E-16

COHEN AND JUDD (1984)
KK5 = 1.0E-11

KK6 = 3.2E-17

A-16

\[ KK6 = 0. \]

COHEN AND JUDD (1984)

\[ KK7 = 3.0E-19 \]

COHEN AND JUDD (1984)

\[ KK8 = 1.6E-23 \]


\[ QQ1 = 2.0E-16 \]

COHEN AND JUDD (1984)

\[ QQ1 = 1.7E-16 \]

BREDERLOW ET AL. (1983)

\[ QQ1 = 1.7E-17 \]

COHEN AND JUDD (1984)

\[ QQ2 = 3.80E-11 * \exp(-4.4E-3 * (T-300.)) \]

SUBROUTINE ARREN ADDS TEMPERATURE EFFECT

BREDERLOW ET AL. (1983)

\[ QQ2 = 3.0E-11 \]


\[ QQ2 = 1.9E-11 \]

COHEN AND JUDD (1984)

\[ QQ3 = 3.7E-18 \]

COHEN AND JUDD (1984)

\[ QQ4 = 4.7E-16 \]

COHEN AND JUDD (1984)

\[ QQ5 = 1.6E-14 \]


\[ CC1 = 1.6E-32 \]


\[ CC1 = 3.2E-33 \]

HOHLA AND KOMPA (1976)

\[ CC1 = 1.6E-33 \]

COHEN AND JUDD (1984)

\[ CC2 = 5.7E-33 * \exp(1369./T) \]
$CC2 = 5.7E^{-33}$

SUBROUTINE ARREN ADDS TEMPERATURE EFFECT

HOHLA AND KOMPA (1976)

$CC2 = 2.1E^{-33}\times\exp(1600./T)$

BREDERLOW ET AL. (1983)

$CC2 = 3.8E^{-31}$


$CC2 = 8.5E^{-32}$


$CC3 = 8.0E^{-32}$


$CC3 = 0.0$


$CC4 = 3.8E^{-30}$

COHEN AND JUDD (1984)

$CC4 = 10.0\times(-29.437-5.844\times\log_{10}(T/300.))$

$CC4 = 10.0$

SUBROUTINE ARREN ADDS TEMPERATURE EFFECT

BREDERLOW ET AL. (1983)

$CC4 = 2.9E^{-30}$

COHEN AND JUDD (1984)

$CC5 = 8.0E^{-33}\times\exp(1310./T)$

$CC5 = 8.0E^{-33}$

SUBROUTINE ARREN ADDS TEMPERATURE EFFECT


$CC6 = 0.0$

$V1 = 0.0$

$V2 = 0.0$

KK1=.903E-13

KK2=80.E-12

KK3=.65E-12

KK4=1.000E-16

KK5=3.089E711

KK7=.1517E-18

KKB=1.6E-23

QQ1=.476E-16

QQ2=1.9E-11

QQ3=.1235E-17

QQ4=1.57E-16

A-18
Q5 = .53E-14

CC1 = 1.053E-33
CC2 = 45.0E-32
CC3 = .4447E-31
CC4 = 4.94E-30
CC5 = 3.6E-31
CC6 = 1.8E-32

V1 = 1.0E-12
V2 = 1.0E-11

GG = 2*(.18/LC)**2
C = 3.0E10

B = P*(3.5E16)
B = (9.66E18)*P/T0
B2 = B*B
B3 = B2*B
RETURN
END

SUBROUTINE VELOC(OMEG1,RAD,OMEGA,A)
VELOCITY PROFILE IS ASSUMED TO BE PARABOLIC
MAX VELOCITY AT RAD = 0.0
ZERO VELOCITY AT RAD = A
A IS RADIUS OF TUBE
OMEG1 IS MAXIMUM VELOCITY ALONG CENTERLINE

CALCULATE VELOCITY OMEGA AT R = RAD
0.0 .LE. RAD .LE. A

TYPE OF FLOW
OMEGA = (OMEG1/(A*A))*(RAD-A)**2
RETURN
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/B2,B3,C,A00,B00,EPSNU,OMEGA,C6
COMMON/BLK4/CHSI10,CHSI20,ABAR0,ZIBAR,LC,XKO
COMMON/BLK7/ABC,C00,C0,OMEG1,P,R1,R2,TM,XNRHO
COMMON/BLK22/AD/V1,V2,GG

A-19
COMMON/BK28/TAU2,TAU4,TAU5,TAU6,TAU3,SIG
COMMON/BK299/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,K2,K3,K4,K5,K6,K7,K8,
100 FORMAT(T5,5HKK1 = ,E15.7,T30,5HKK7 = ,E15.7,T60,5H001 = ,E15.7,
1 T85,5HCCS = ,E15.7,T103,7HTTT2 = ,E15.7 )
101 FORMAT(T5,5HKK2 = ,E15.7,T30,5HKK8 = ,E15.7,T60,5H002 = ,E15.7,
1 T85,5HV1 = ,E15.7, T103,7HTTT3 = ,E15.7 )
102 FORMAT(T5,5HKK3 = ,E15.7,T30,5HCC1 = ,E15.7,T60,5H003 = ,E15.7,
1 T85,5HV2 = ,E15.7, T103,7HTTT4 = ,E15.7 )
103 FORMAT(T5,5HKK4 = ,E15.7,T30,5HCC2 = ,E15.7,T60,5H004 = ,E15.7,
1 T85,8HSIGMA = ,E15.7 , T103,7HTTT5 = ,E15.7 )
104 FORMAT(T5,5HKK5 = ,E15.7,T30,5HCC3 = ,E15.7,T60,5H005 = ,E15.7,
1 T85,7TEMP = ,F9.2 , T103,7HTTT6 = ,E15.7 )
105 FORMAT(T5,5HKK6 = ,E15.7,T30,5HCC4 = ,E15.7,T60,5H006 = ,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 CHSII,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/B2,B3,C,A00,B00,EPSNU,OMEGA,C6
COMMON/BLK4/CHS110,CHS120,ABAR0,ZIBAR,LC,XK0
COMMON/BLK7/ABC,C00,C0,OMEG1,P,R1,R2,TM,XNRO0
COMMON/BLK22/AD,V1,V2,G6
COMMON/BLK28/TAU2,TAU4,TAU5,TAU6,TAU3,SIG
COMMON/BK299/TTT2,TTT3,TTT4,TTT5,TTT6
REAL K1,K2,K3,K4,K5,K6,K7,K8,LC
C
C
YQ=QUANTUM YIELD
YQ=1.0
C
C F(I),I=1,6 ARE RATES OF CHANGES FOR THE CONCENTRATIONS
F(1)=D[R1]/DZ         F(2)=D[R2]/DZ
F(3)=D[R3]/DZ         F(4)=D[R4]/DZ

A-20
CONTINUE

Z = LC*S
S IS SCALED LENGTH VARIABLE
0 .LE. S .LE. 1
FLOW CALCULATES TEMPERATURE, PRESSURE, FLOW RATE
AND DENSITY RESPONSE AS FUNCTION OF Z

Z IS DISTANCE IN CM
CALCULATE GAS PARAMETERS AS FUNCTION OF Z
CALL FLOW(Z, TEMP, PRESS, FLOWR, DENSITY, DWDZ)
CALL FLOW(Z, TEMP, PRESS, FLOWR, DENSITY, DWDZ)
WRITE(6, 357) Z, TEMP, PRESS, FLOWR, DENSITY, DWDZ
357 FORMAT(1X, 3E16.7, /, 3E16.7 )
TEMP IS TEMPERATURE DEG K
PRESS IS PRESSURE IN TORR
FLOWR IS FLOW RATE IN M/SEC
DENSITY IS GAS DENSITY IN KG/M**3
OMEGA = FLOWR * 100.
OMEGA IS FLOW RATE IN CM/SEC
CALCULATE COEFFICIENTS AS FUNCTION OF TEMP AND Z
CALL ARREN(TEMP)
TAU5 = (TTT5) * PRESS
TAU6 = TAU5

CONSTANTS COME VIA COMMON BLKS 2 AND 3
K'S IN CM**3/SEC
C'S IN CM**6/SEC
Q'S IN CM**3/SEC
Q'R'S IN CM**2/SEC
X7STAR = Y(7) * B + X8
DIF = Y(5) - .5 * Y(6)
CALL SIGMA(SIG2)
SIG = SIG2
F(1) = K1 * B * Y(2) * Y(5) + K2 * B * Y(2) * Y(6) - CHSII(Z) * Y(1) - K4 * B * Y(1) * Y(2)
1 + K5 * B * Y(1) * 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
F(2) = CHSII(Z) * Y(1) - K1 * B * Y(2) * Y(5) - K2 * B * Y(2) * Y(6) - 2 * K3 * B * Y(2) * Y(2)
- K3 * B * Y(1) * Y(2) - K5 * B * Y(2) * Y(3) * Y(4) + V2 * B * Y(3) * Y(6)
+ K7 * B * Y(5) * Y(1) - K8 * B * Y(6) * Y(1) - Y(2) * DWDZ - Y(2) / TAU2
F(3) = K3 * B * Y(2) * Y(2) + K6 * B * Y(1) * Y(2) + K4 * B * Y(1) * Y(2) - 2 * V2 * B * Y(3) * Y(6)
- 1 Y(3) * DWDZ - Y(3) / TAU3
A1 = C1 * B * Y(1) * Y(5) + C2 * B * Y(1) * Y(6) + C3 * B * Y(4) * Y(5) + Y(6)
A2 = C4 * B * Y(4) * Y(6) + C5 * B * Y(4) * Y(6) - CHSII(Z) * Y(4) + K7 * B * Y(5) * Y(1)
- K5 * B * Y(2) * Y(4) - V1 * B * Y(6) * Y(6) + C5 * B * Y(6) * Y(6)
F(4) = A1 + A2 + K8 * B * Y(6) * Y(1) + C6 * B * Y(6) * Y(5) * Y(3) - Y(4) * DWDZ - Y(4) / TAU4
A3 = QY * CHSII(Z) * Y(1) + 0.5 * CHSII(Z) * Y(4) - K1 * B * Y(2) * Y(5)
A4 = - C1 * B * Y(1) * Y(5) - C3 * B * Y(4) * Y(5) * Y(6) - Q1 * B * Y(1) * Y(5)
A5 = - Q2 * B * Y(4) * Y(5) + C6 * B * Y(6) * Y(5) * Y(3) - Y(5) * DWDZ - Y(5) / TAU5
A6 = 1.49 * CHSII(Z) * Y(4) + Q1 * B * Y(1) * Y(5) + Q2 * B * Y(4) * Y(5)
1 - 2 * C5 * B * Y(6) * Y(6) + Y(5) * Y(3) - K8 * B * Y(6) * Y(1)
A7 = C * SIG * X7STAR * DIF - C1 * B * Y(1) * Y(5) * Y(6)
A-21
**C** SCALED EQUATIONS IN THE Z-DIRECTION

```fortran
DO 10 I=1,6
  F(I)=LC*F(I)/OMEGA
  F(7)=LC*Y(7)*DIF*B*SIG
RETURN
END
```

**SUBROUTINE SIGMA(SIG)**

This subroutine defines the cross section SIGMA.

```fortran
COMMON/BLK3/B,B2,B3,C,A00,B00,EPSNU,OMEGA,C6
COMMON/BLK7/ABC,C00,C0,C01,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
FISNU=2*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
TI=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
DELDOP=2.51E8*FUGTEMP
DELNU=DELDOP+ALPHAM*P
SIGMA23=A1/(FISNU*DELNU)/(1+(2.*DELTA23/DELNU)**2)*5./12.
SIGMA22=A2/(FISNU*DELNU)/(1+(2.*DELTA22/DELNU)**2)*5./12.
SIGMA21=A3/(FISNU*DELNU)/(1+(2.*DELTA21/DELNU)**2)*5./12.
```

**A-22**
SUBROUTINE INTEG(IPRINT,H)
   THIS SUBROUTINE INTEGRATES THE SYSTEM OF DIFFERENTIAL EQUATIONS
   DEFINING THE CHEMICAL KINETICS OF N-C3F7I IODINE LASER
   USING A VARIABLE STEP SIZE 7TH ORDER RUNGE KUTTA-FEHLMAN METHOD.
   IMPLICIT REAL*8(A-H,K,L,O-Z)
   DIMENSION YO(7),X(7),WK(84)
   COMMON/BLK1/X7,POWER
   COMMON/BLK3/B2,B3,C,A00,B00,EFSNU,OMEGA,C6
   COMMON/BLK4/CHSI10,CHSI20,ABAR0,Z1BAR,LC,XK0
   COMMON/BLK7/ABC,C00,C0,OMEG1,P,R1,R2,TM,XNRHO
   COMMON/BLK8/ZOL,ZE,NG,T0,RAD,A,PIN,W
   COMMON/BLK22/AD,V1,V2,GG
   COMMON/BLK23/W0,ETA0,PTO,FRAC
   COMMON/BLK29/ZZZ,TZZ,PZZ,ETA2Z,WZZ
   COMMON/BLK30/DATA(50,50),NDMAX,FLRATE(8),FDFTDAT(50,40)
   EXTERNAL FUN,CHSI1,CHSI2
   REAL LC

   INTEGRATE SYSTEM FROM S=0 TO S=1.0 USING RUNGE-KUTTA METHOD
   X(1)=RI
   X(2)=R
   X(3)=R2
   X(4)=I2
   X(5)=I*
   X(6)=I
   X(7)=RHO+
   X8=RHO-
   X9=I*-.5*I

   INITIALIZE CONSTANTS FOR FLOW EQUATIONS
   SEE COMMON BLK10 FOR THESE CONSTANTS--NEEDED FOR SUB FLOW
   CALL PFLOW
   ND=0
   TEST FOR PRINT CONDITIONS
   IF(IPRINT.EQ.0) GO TO 229
   NG=NG+1
   NG IS THE NUMBER OF GRAPHS TO BE SAVED
   MAXIMUM NG=8
   FLOWRATE(NG) IS LABEL FOR DATA SAVED
   SEE ALSO PROGRAM PLOTD--WHICH CAN PLOT THE SAVED DATA
   FLOWRATE(NG)=OMEGA
   WRITE(8,331) LC
FORMAT(1X,11H LC = ,F10.2)
CONTINUE
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
YO(1)=1.0
Z1=0.0
DO 9 I=2,6
YO(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=FIN*W/(EPSNU*C)
C X70 IS RHO+(0) WHICH IS GIVEN
C INITIAL CONDITION FOR RHO-(0) IS UNKNOWN—ASSUME COO VALUE
X70=X70*C00
XB=XK0/X70
YO(7)=X70/B
IF(IPRINT .EQ. 0) GO TO 300
CALL FUN(N,Z0,Y0,F)
TEMP=TZZ+273.
IF(ZO.EQ.0.0) CALL PRINT(ZO,TEMP)
WRITE(6,191)
CONTINUE
DO 10 I=1,7
X(I)=B*YO(I)
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) TZZ,TZZ,ETAZZ,WZZ
CALL FUN(N,Z0,Y0,F)
TEMP=TZZ+273.
IF(ZO.EQ.1.0) CALL PRINT(ZO,TEMP)
CONTINUE
C SAVE THE DATA FOR FUTURE PLOT ROUTINES
C DATA ARRAYS ARE DATA(50,50) AND FDPTDAT(50,40)
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
WRITE(6,6773) Z0,X(2),X(4),X(5),X(6),X9
WRITE(6,6773) Z0,WZZ,ETAZZ,PZZ,TZZ
6773 FORMAT(1X,F6.3,2X,5(2X,15.6))
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 T7HPTORR=,F9.4,2X,
2 T55,9H DENSITY =,F9.6,2X,TB8,3HW=,E14.7 )
3567 CONTINUE
199 FORMAT(1X,E12.5,8E12.5,E12.5,E12.5)
USE 7TH ORDER RUNGE KUTTA INTEGRATION SCHEME WITH VARIABLE STEP
STEP SIZE CAN VARY FROM HMIN TO HMAX
Z0 IS STARTING VALUE FOR Z
Z1 IS NEXT STOPPING POINT IN INTEGRATION SCHEME
TOL IS TOLERANCE
IERR IS ERROR CODE TO DETERMINE IF INTEGRATION WAS SUCCESSFUL
CONTINUE
100 CONTINUE
ZI=ZI+H
IF(ZI .GT. 1.00) GO TO 111
CALL RKF7(N,ZO,Z1,YO,TOL,FUN,PD,MTH,HMIN,HMAX,HUSE,WK,IERR)
IF(IERR .NE. 0) WRITE(6,444) IERR,Z0,Z1,(YO(I),I=1,7)
444 FORMAT(1X,18HIERR IS NOT ZERO ,15,(4E16.7,/) )
200 CONTINUE
X(7)=B*YO(7)
X8=XK0/X(7)
60 FORMAT(1X,5(2X,E14.6))
GO TO 300
500 CONTINUE
DO 110 I=1,7
110 X(I)=B*YO(I)
X8=XK0/X(7)
X9=X(5)-.5*X(6)

A-25
CONTINUE
XX7L=X(7)
C X(7) IS CALCULATED RHO+(L) VALUE
XXCAL=R2*X(7)*X(7)
C XXCAL IS CALCULATED VALUE FOR XK0
C ABC IS DIFFERENCE BETWEEN CALCULATED AND INITIAL VALUE
DIF=((XK0-XXCAL)/XXCAL)*100.
C ABC=DIF
IF(IPRINT .EQ. 0) GO TO 224
WRITE(6,202)DIF,XXCAL,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(POUT/PIN)
GAIN=POUT/PIN
IF(IPRINT .EQ. 0) GO TO 226
WRITE(6,193)R1,R2,P,PIN,POUT,GAINDB,GAIN
226 CONTINUE
193 FORMAT(1X,5HR1 = ,F10.7,2X,5HR2 = ,F10.7,1X,
1 8HPRESS = ,F10.7,2X,6HPIN = ,E14.7,3X,7HPOUT = ,E14.7,/,
2 1X,9HGAINDB = ,E14.7,3X,7HGAIN = ,E14.7 )
501 CONTINUE
NDMAX=ND
C ND MAX IS THE MAXIMUM NUMBER OF DATA POINTS
RETURN
END
APPENDIX B

OUTPUT FROM SIMULATION MODEL
INPUT PARAMETERS

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<tr>
<td>LC</td>
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<td>ZOL</td>
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<td>TO</td>
<td>300.0</td>
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OUTPUT

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<th>Gain db</th>
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Figure 2.