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Mid-Project Progress Report, NASA NAG-1-823

"Design of Catalytic Monoliths for Closed-Cycle Carbon Dioxide Lasers"

submitted by

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Summary

A computer program has been written that allows the design of catalytic monoliths for closed-cycle carbon dioxide lasers. Using design parameters obtained from workers at NASA Langley Research Center and from the literature, several specific monoliths have been designed and the results have been communicated to the research group working on this project at Langley. Two oral presentations have been made at NASA-sponsored workshops - at Langley in January, 1988 and in Gainesville, Florida in May, 1988.

Progress Report

A fully functional monolith design program has been written that inputs operating parameters and computes CO and O_2 conversions for specified a monolith length or, optionally, computes monolith length for specified reactant conversions. Currently, the program has more than 1,000 lines of standard FORTRAN code and has been run on both a Macintosh personal computer and a VAX/VMS minicomputer. A program listing is given in the appendix of this report.

Currently, a monolith geometry of parallel square channels is specified by the program. Variable thicknesses of active catalyst layers on the walls of the channels, as well as fully active walls, can be specified by the user. The program accounts for the following physical and chemical processes:

- laminar flow of gas in the channels
- mass transfer of reactants from the gas to the channel walls
- diffusion of reactants in the porous catalyst layer
- first-order-overall reaction kinetics in the porous catalyst layer
- option for adiabatic or isothermal modes of operation of the monolith
- heat release by the exothermic reaction in adiabatic operation mode
- effect of temperature on the reaction rate
- change in gas properties (viscosity, diffusivity, thermal conductivity) with temperature, pressure, and reactant conversion
- calculation of gas pressure drop

As an example of the use of the design program, a design study will be presented here in which a specific monolith was designed. For a given set of conditions including monolith face dimensions, the optimal channel wall thickness and channel opening size were determined that minimize the monolith length and, thus, overall volume.

Table 1 summarizes the parameters that were fixed and those that were varied in the design study. The face dimension of the monolith was fixed at 100 mm by 100 mm. For each design case, a wall thickness and a channel opening were chosen and the length of the monolith required to achieve 25% conversion of CO and O_2 at a pressure drop of 0.125 kPa (0.5 in. H_2O) was computed. Figure 1 shows how the total number of channels and the channel opening changed as the wall thickness was varied. Each of the points in Figure 1 represent a specific monolith design that achieves the requirements of 25% conversion at a pressure drop of 0.125 kPa. As the wall thickness is increased and the number of channels in the monolith decrease, the size of the channel openings must increase in order to stay within the pressure drop constraint.

Here, we use the term "% void" or void fraction to represent the volume of the total monolith that is taken up by the open channel passages. As shown in Figure 2, the void fraction of the monolith decreases as the wall thickness is increased. This decrease in void fraction means that the monolith tends to become more compact, that is, that the overall volume of the monolith decreases. The overall volume of the monolith, of course, is an important design criteria for aeronautical and space applications of closed-cycle carbon dioxide lasers.

However, there is a factor that tends to offset this decrease in void fraction. As the wall thickness and the channel opening increase, resistances to mass transfer of reactants also increase: reactant molecules have greater distances to travel from the center of a monolith channel to the channel wall and from the channel wall into the porous catalyst layer. This effect increases the amount of active catalyst required to do the required conversion and is shown in Figure 3.

Figure 4 shows how the two offsetting factors of decrease in void fraction and increase in mass transfer resistance couple to produce an optimal combination of wall thickness and channel opening that minimize the length and overall volume of the monolith. Figure 5 shows schematic representations of the relative dimensions of three of the design cases plotted in Figure 4: the left-most case (smallest wall thickness considered), the optimal case, and the right-most case in Figure 4 (largest wall thickness considered). The optimal case monolith is only two-thirds of the length of the case considered with the thinnest walls, and is only slightly more heavy, as Figure 6 shows.

Figure 7 compares the optimal design case considered here to a monolith with standard Corning Glass wall and channel dimensions. The optimal design is only about two-fifths the overall size of the monolith with off-the-self dimensions.

Future Work

The capabilities of the monolith design program will be expanded and the user interface will be enhanced. During the remainder of the project, the option to consider other channel geometries as well as parallel plate geometry will be added. In addition, the integration algorithm will be made more robust and efficient. Further designs will be performed using NASA catalyst kinetics.

Table 1

Design Study:
Minimize Monolith Length,
Keeping Pressure Drop Constant

Fix:

Square channels in square array

Face dimension = 100 mm x 100 mm (4 in x 4 in)

Gas flow rate = 1 liter/s (at inlet temperature of 300K)

Porous wall material is uniformly active, with kinetics from

Stark and Harris, J. Phys. E.: Sci. Instrum. 16, 492 (1983)

Adiabatic operation

CO and O_2 conversion = 25% (50 μmol O_2/s for 0.5% O_2 in)

Pressure drop across monolith = 0.125 kPa (0.5 in. H_2O)

Vary:

Wall thickness

Channel opening

Minimize:

Length of monolith

Figure 1

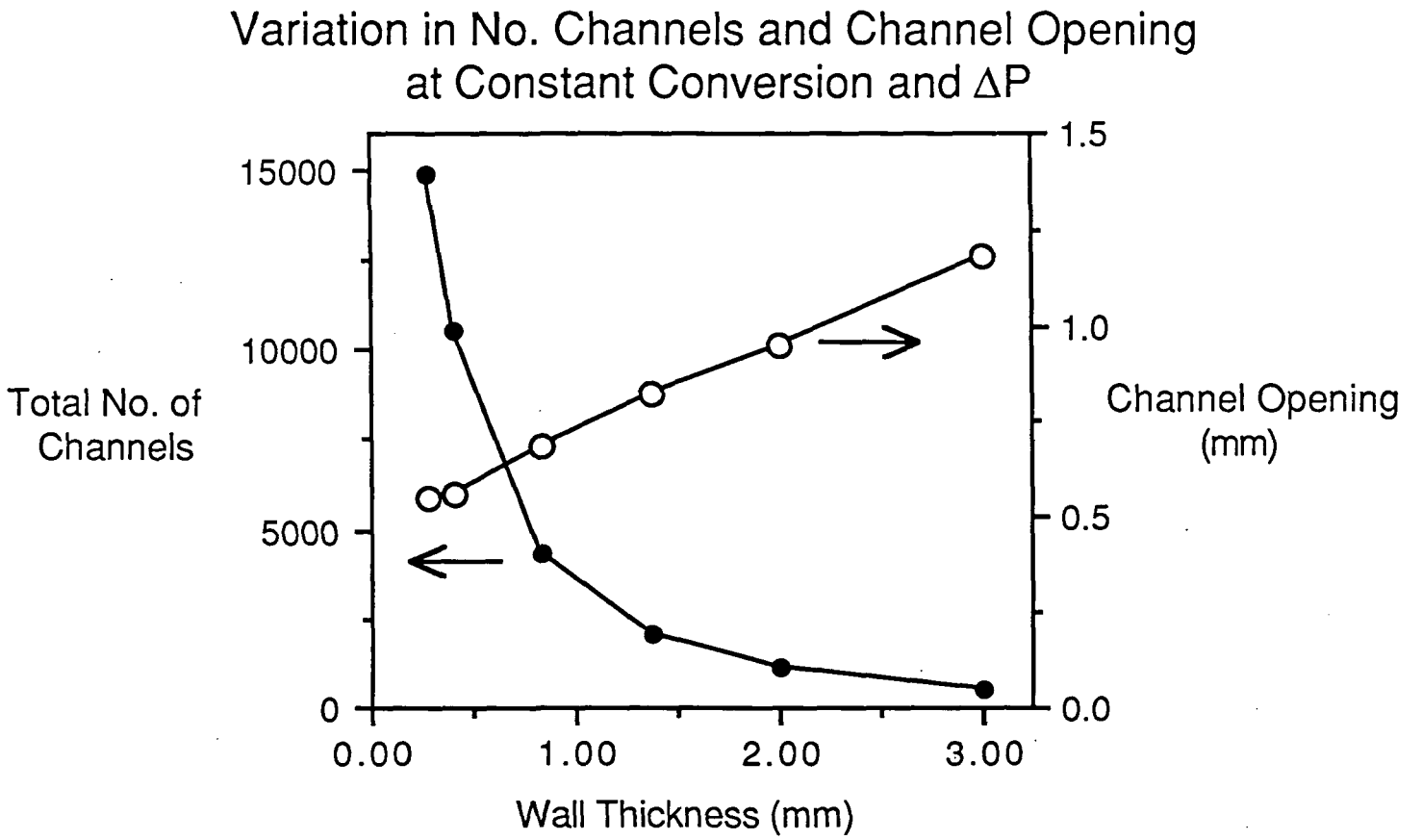

Variation in No. Channels and Channel Opening
at Constant Conversion and ΔP
Total No. of Channels
15000
10000
5000
0
1.5
1.0
0.5
0.0
Channel Opening (mm)
0.00
1.00
2.00
3.00
Wall Thickness (mm)

Figure 2

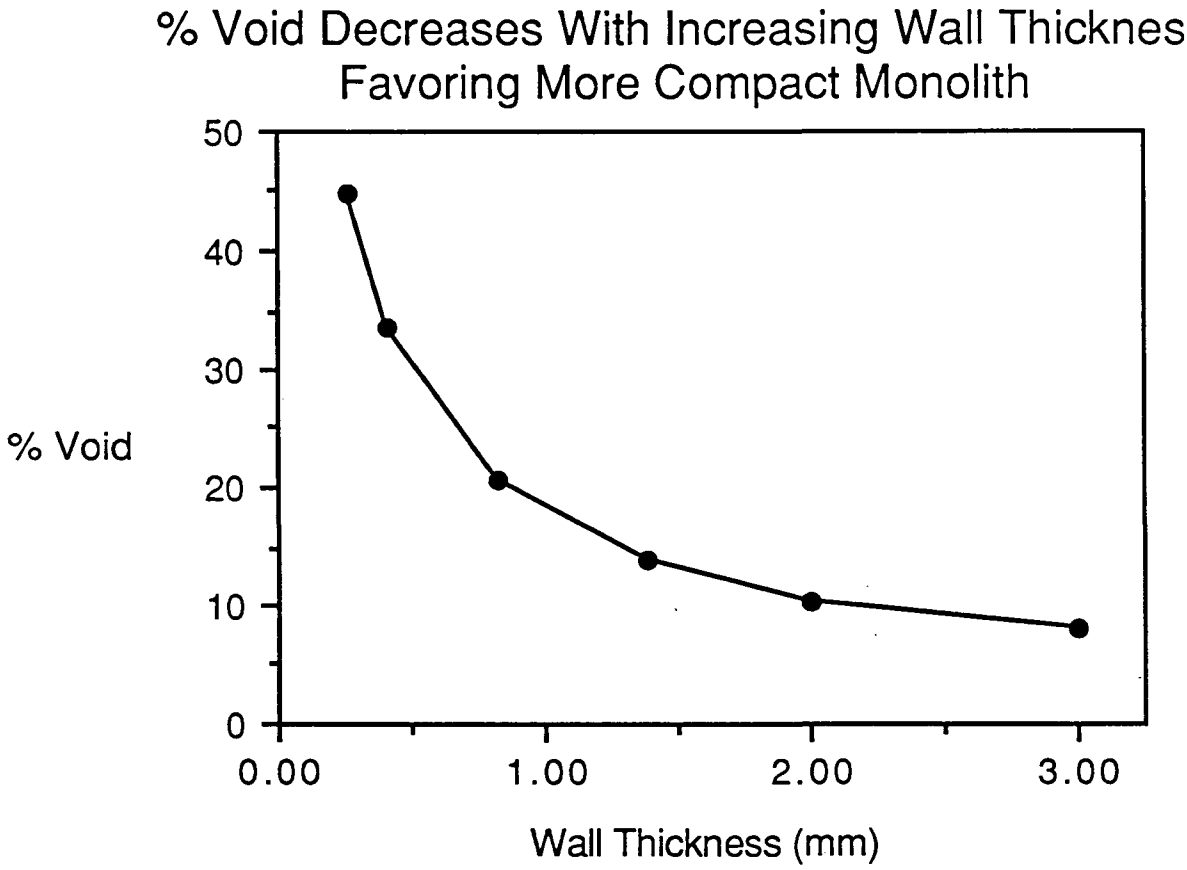

% Void Decreases With Increasing Wall Thickness -
Favoring More Compact Monolith
% Void
50
40
30
20
10
0
0.00
1.00
2.00
3.00
Wall Thickness (mm)

Figure 3

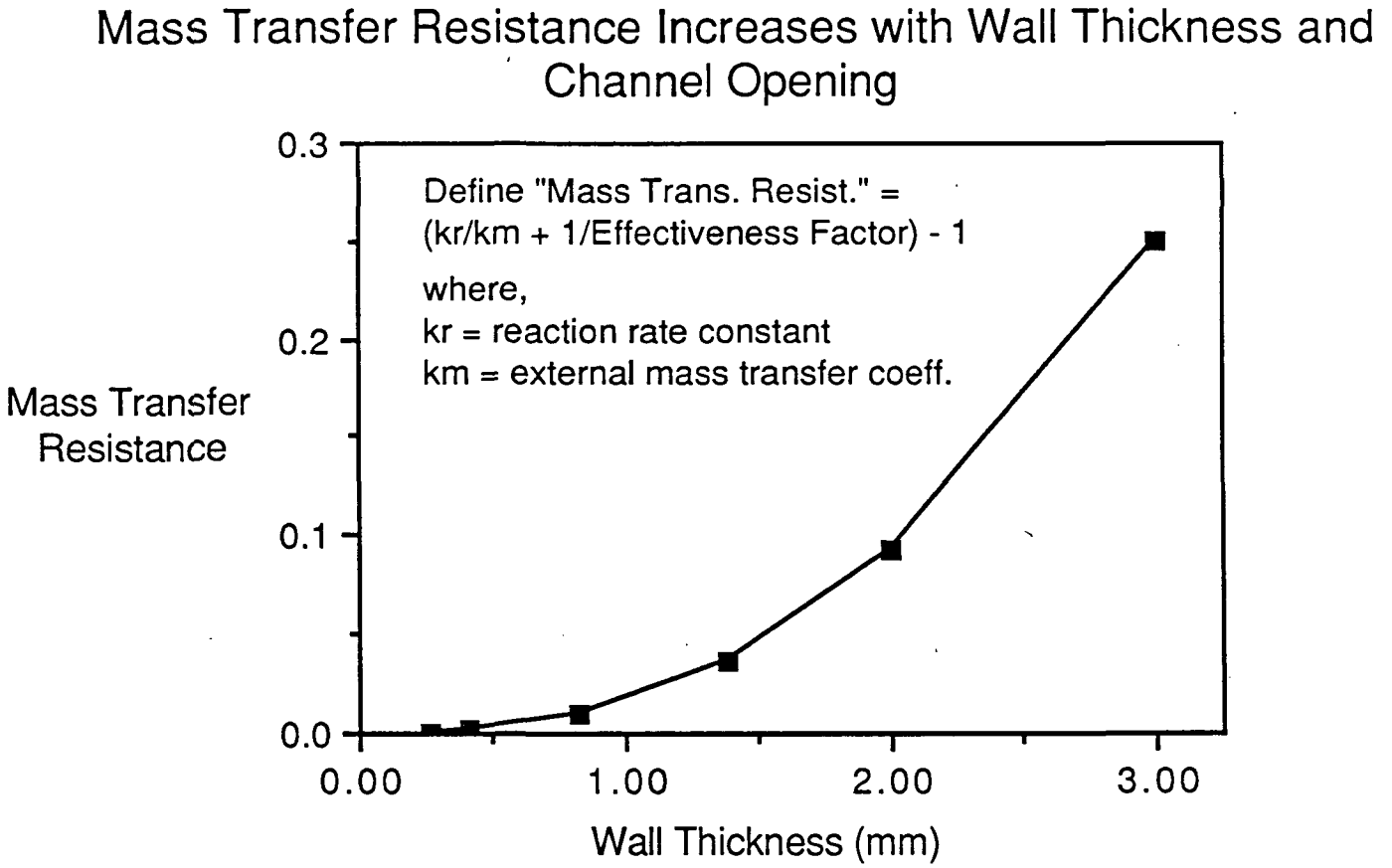

Mass Transfer Resistance Increases with Wall Thickness and Channel Opening
Define "Mass Trans. Resist." =
(kr/km + 1/Effectiveness Factor) - 1
where,
kr = reaction rate constant
km = external mass transfer coeff.
Mass Transfer Resistance
0.3
0.2
0.1
0.0
0.00
1.00
2.00
3.00
Wall Thickness (mm)

Figure 4

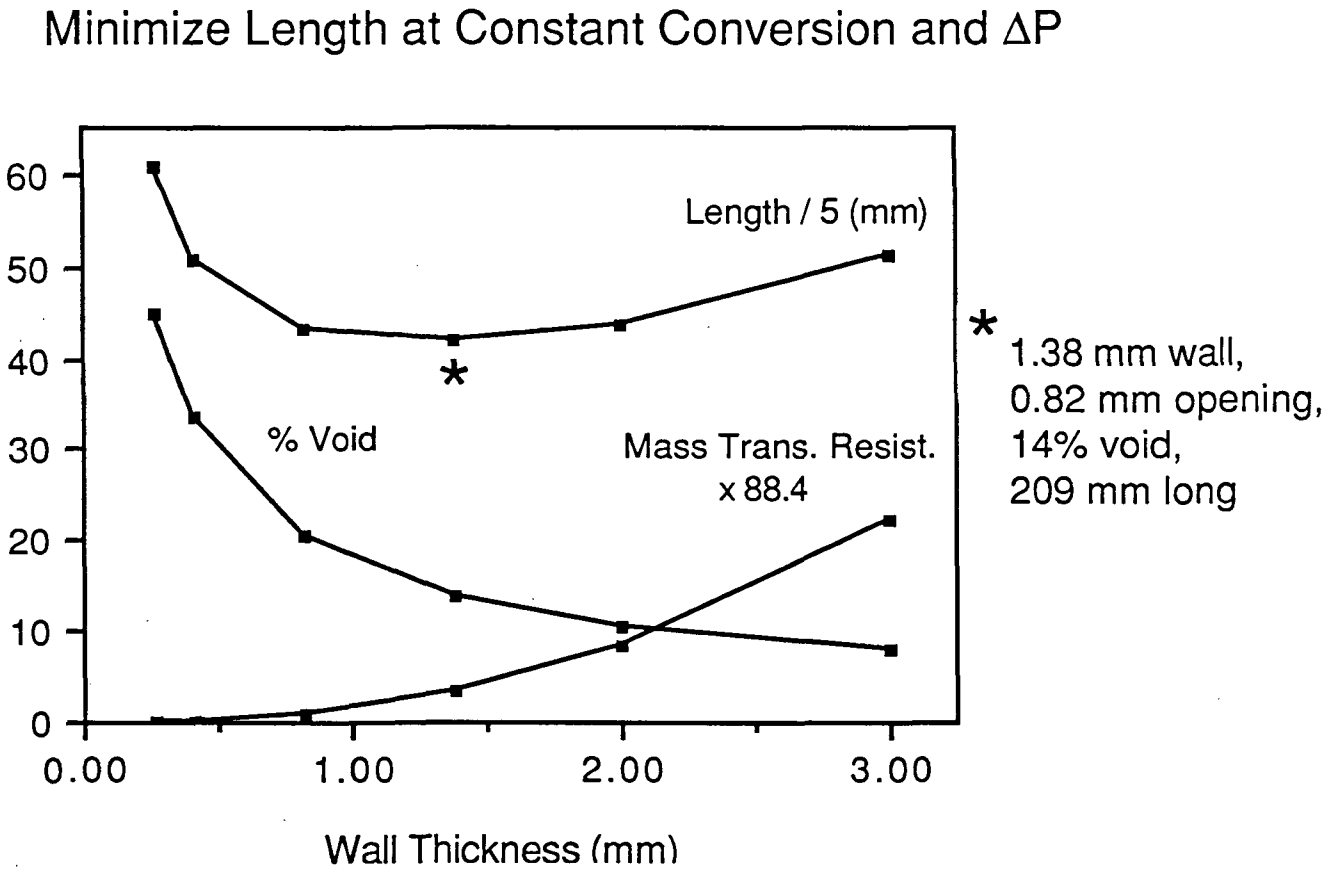

Minimize Length at Constant Conversion and ΔP
60
50
40
30
20
10
0
0.00
1.00
2.00
3.00
Length / 5 (mm)
% Void
Mass Trans. Resist.
x 88.4
*
Wall Thickness (mm)
* 1.38 mm wall,
0.82 mm opening,
14% void,
209 mm long

Figure 5

Minimize Length at Constant Conversion and ΔP

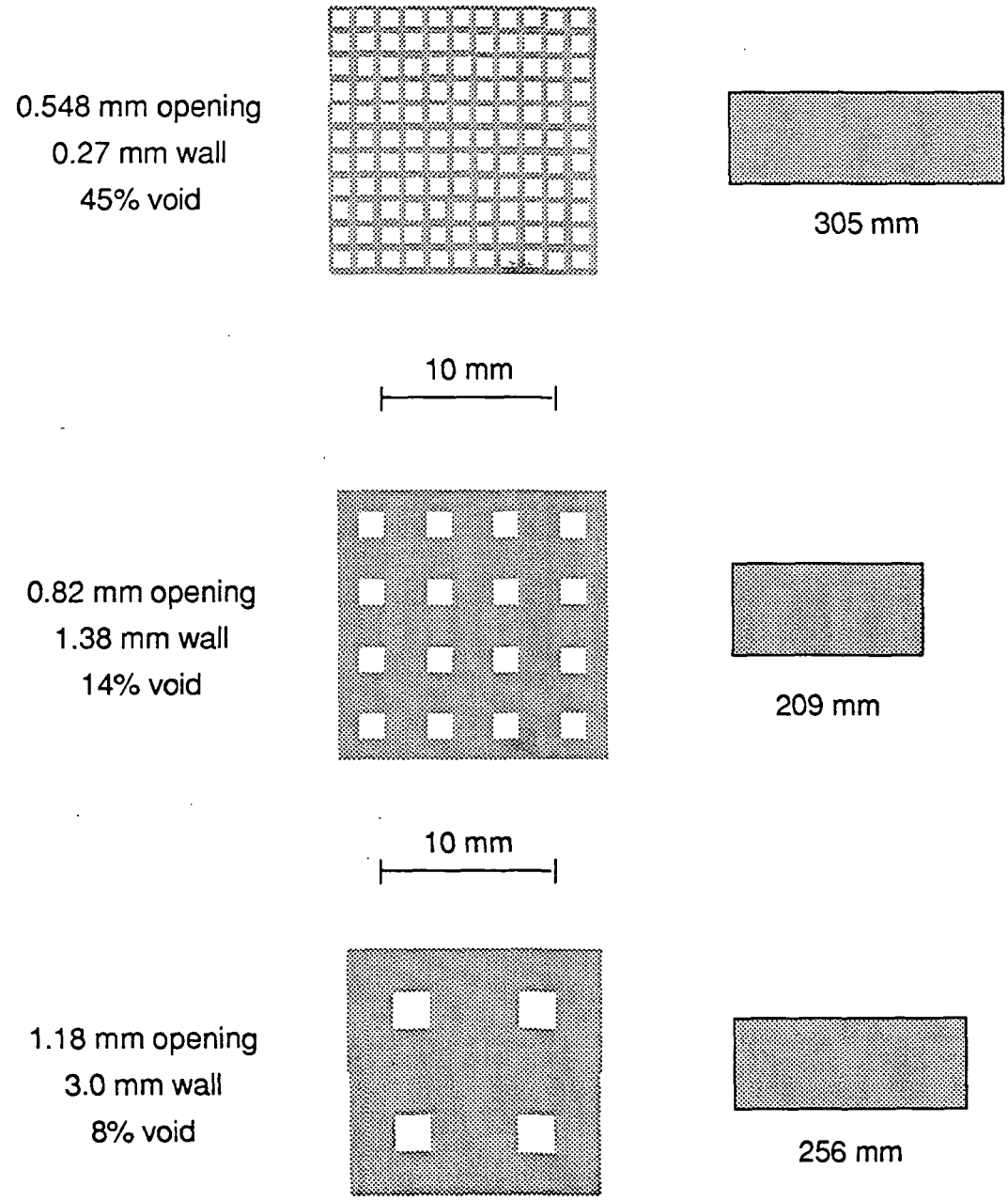


Figure 6

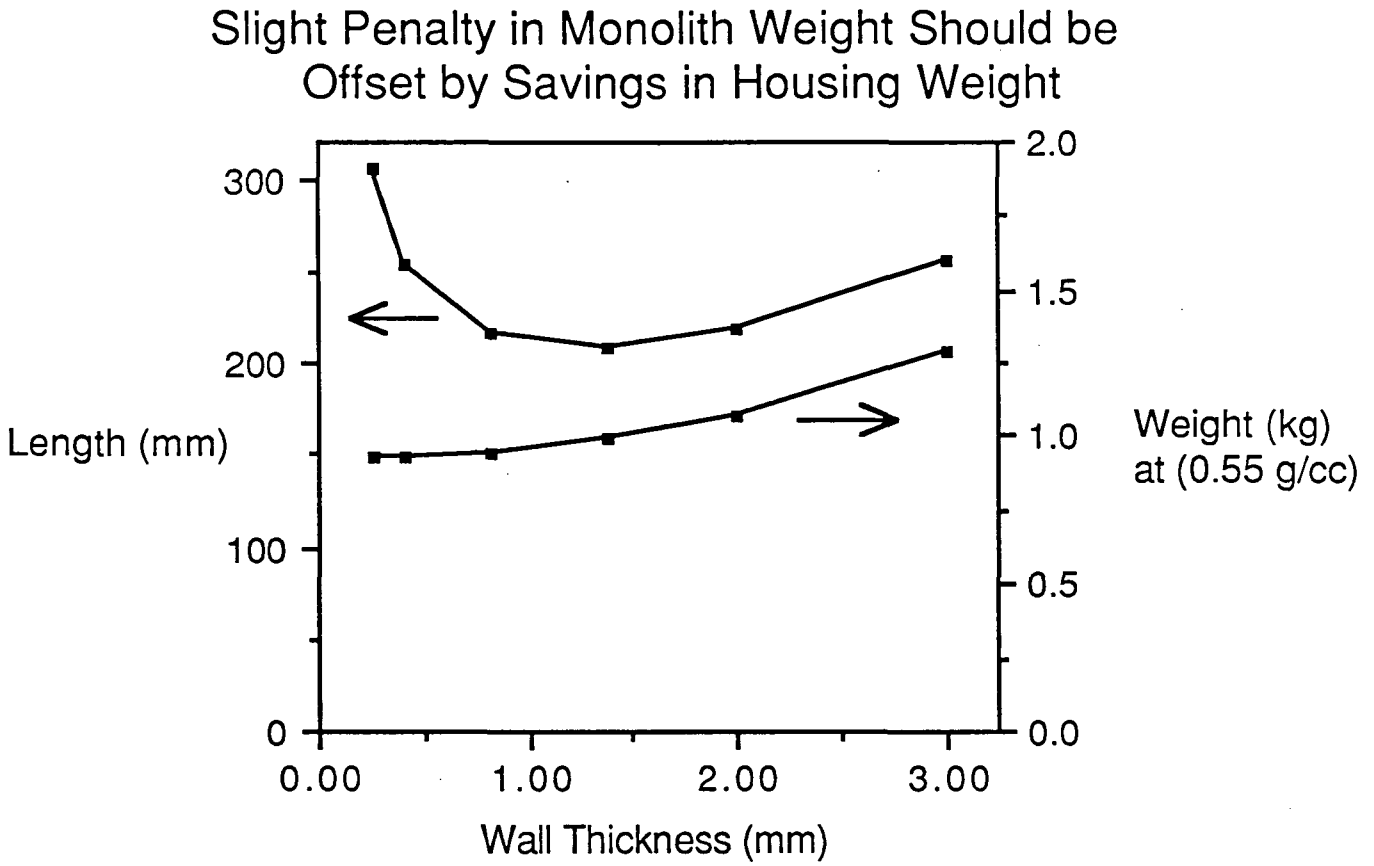
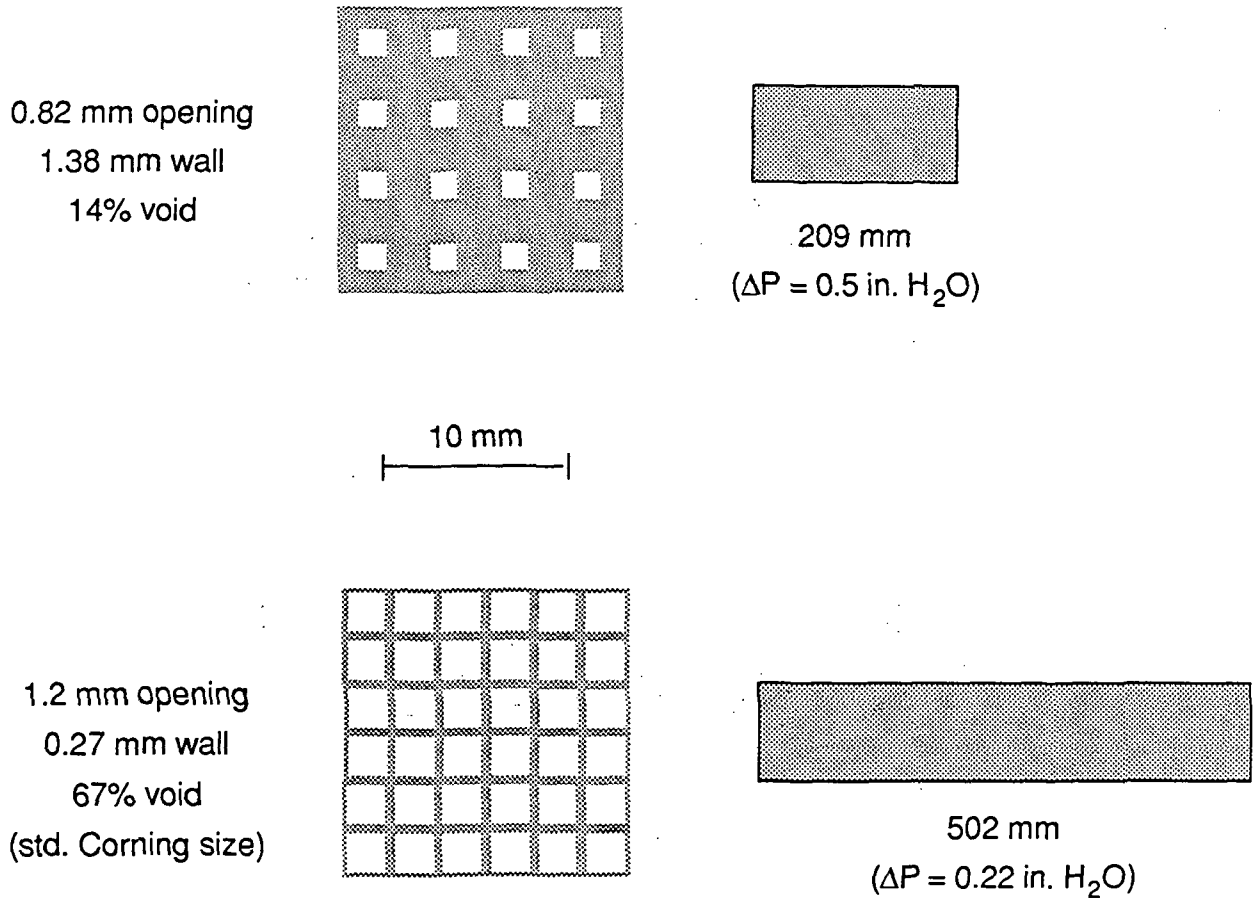

Slight Penalty in Monolith Weight Should be Offset by Savings in Housing Weight
Length (mm)
300
200
100
0
2.0
1.5
1.0
0.5
0.0
Weight (kg) at (0.55 g/cc)
0.00
1.00
2.00
3.00
Wall Thickness (mm)

Figure 7

Optimum Design vs. Standard Corning Size

(25 % Conversion)



APPENDIX:

DRAFT OF COMPUTER PROGRAM LISTING, 6/30/88

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C PROGRAM LASER17 WRITTEN BY KEITH GUINN AND SETH GOLDBLUM UNDER
C THE DIRECTION OF PROF. RICHARD HERZ, CHEMICAL ENGINEERING, B-010
C AT THE UNIVERSITY OF CALIFORNIA AT SAN DIEGO, LA JOLLA, CA 92093
C    FUNDED BY NASA LANGLEY RESEARCH CENTER, TECHNOLOGY
C    UTILIZATION AND APPLICATIONS OFFICE
C    MICROSOFT FORTRAN V2.2   MACINTOSH PLUS
C    JUNE 30, 1988
C
C PURPOSE: See introduction below
C IDENTIFIERS:
C    A-REACTION RATE CONSTANT OF CATALYST(mm^3/g-cat s)
C    AMW-AVERAGE MOLECULAR WEIGHT OF GAS MIXTURE(g/mole)
C    AREF-VOL. PUMPING RATE OF CATALYST AT 298K(mm^3/g-cat s)
C    ASK-QUERY DIRECTION NUMBER
C    AX(i,j)-i,j=1->6** CROSS TERM MATRIX FOR THERMAL CONDUCTIVITY
C    BEEP-BEEP CHARACTER
C    CGX-MONOLITH CHAN. O2 GAS CONC. AT POSITION X (mol/mm^3)
C    CH - CHARACTER*1 Dummy Variable
C    CH1- CHARACTER*1 Dummy Variable
C    CHFLO-MONOLITH CHANNEL VOLUMETRIC FLOWRATE (mm^3/S)
C    CHGVEL-MONOLITH CHANNEL GAS VELOCITY (mm/s)
C    CHHD-MONOLITH CHANNEL HYDRAULIC DIAMETER (mm)
C    CHSTV-MONOLITH CHANNEL SURFACE AREA TO VOLUME (1/mm)
C    CHWP-MONOLITH CHANNEL WETTED PERIMETER (mm,R)
C    CMCWT-CHARACTERISTIC MCWT(mm)
C    CONST1,CONST2,CONST3,CONST4,CONST5-RESULT HOLDING CONSTANTS
C    CONST5,CONST6,CONST7,CONST8,CONST9-RESULT HOLDING CONSTANTS
C    CONSTA,CONSTB,CONSTC-RESULT HOLDING CONSTANT
C    CONV-CONVERSION OF OXYGEN IN MONOLITH CHANNEL (%)
C    CONVX-CONVERSION OF OXYGEN AS FUNCTION OF X(%)
C    CP(i),i=1,6-HEAT CAPACITY OF SPECIES i AT TEMP. TGX (J/K-g)
C    CPGAS-HEAT CAPACITY OF BULK GAS MIXTURE (J/K-g)
C    CPCAT-HEAT CAPACITY OF CATALYST WASHCOAT (J/K-g)
C    CPSUP-HEAT CAPACITY OF MONOLITH SUPPORT (J/K-g)
C    CSubS-SUTHERLAND INTERACTION COEFFICIENT,1 FOR NON-VERY POLAR
C         GASES
C    CSX-MONOLITH CHAN. WALL O2 GAS CONC AT POSIT. X (mol/mm^3)
C    D(i),i=1-6-BINARY DIFF. COEFF FOR SPECIES O2 & i,298K,1 atm
C         (mm^2/s)
C    DAB-DIFFUSIVITY OF O2 IN BULK GAS (mm^2/S)
C    DABEFF-EFFECTIVE DIFFUSIVITY OF O2 IN WASHCOAT (mm^2/S)
C    DABEFR-REF.EFFECTIVE DIFFUSIVITY OF O2 IN WASHCOAT,298K
C         (mm^2/S)
C    DCGX-CHANGE IN CGX FOR A CHANGE DX(mol/mm^3)
C    DENGAS-DENSITY OF BULK GAS MIXTURE (g/mm^3)
C    DENGSR-REFERENCE DENSITY OF BULK GAS MIXTURE (g/mm^3)
C    DENCAT-DENSITY OF CATALYST WASHCOAT (g/mm^3)
C    DENSUP-DENSITY OF MONOLITH SUPPORT (g/mm^3)
C    DP-CHANGE IN PRESS ASSOC. WITH A CHANGE IN CHANNEL POSITION
C         DX(atm)
C    DTGX-CHANGE IN TGX FOR A CHANGE DX(mol/mm^3)
C    DX-INCREMENTAL CHANGE IN MONOLITH CHANNEL POSITION X (mm)
C    DY5-CHANGE IN MOLE FRACT. OF O2 ASSOC. WITH A CHANGE DCGX IN
C         O2 CONC.
```

```
C     ENGACT-CATALYST REACTION ACTIVATION ENERGY(J/mol)
C     FACTOR-PROFILE STEP SIZE FACTOR(integer)
C     FILNAM - NAME OF DATAFILE CONTAINING DEFAULT PARAMETERS
C     H-HEAT TRANSFER COEFFICIENT FROM GAS TO WALL (J/mm^2-S-K)
C     HEATRX- NEG. CHANGE IN ENTHALPY FOR 02+2CO->CO2 (J/mol)
C     I-INTEGER COUNTER
C     K-THERMAL GAS CONDUCTIVITY (J/mm-S-K)
C     J-INTEGER COUNTER
C     KC-MASS TRANSFER COEFFICIENT(mm/S)
C     KREF-REFERENCE THERMAL GAS CONDUCTIVITY (J/mm^2-S-K)
C     MCH-MONOLITH CHANNEL HEIGHT (mm)
C     MCST-MONOLITH CHANNEL SUPPORT WALL THICKNESS (mm)
C     MCW-MONOLITH CHANNEL WIDTH (mm)
C     MCWT-MONOLITH CHANNEL WASHCOAT THICKNESS (mm)
C     MFD-MONOLITH FACE DIMENSION(mm)
C     MONOL-COMPUTATION LOOP COMPLETION MONOLITH LENGTH(mm)
C     MVFLO-MONOLITH VOLUMETRIC GAS FLOWRATE(mm^3/S)
C     MW(i)-i->1,6** MOLECULAR WEIGHT OF COMPONENT GASES(gms/mole)
C     N-EFFECTIVESS FACTOR FOR CATALYST WASHCOAL (NONDIM)
C     NOCHM-NUMBER OF CHANNELS IN MONOLITH (I)
C     NOCHV-NUMBER OF CHANNELS VERTICALLY IN MONOLITH
C     NOCHH-NUMBER OF CHANNELS HORIZONTALLY IN MONOLITH
C     O2ZERO-MONOLITH INLET OXYGEN CONCENTRATION (%O2)
C     P-DO LOOP VARIABLE
C     PHI(i,j)-i,j=1->6** CROSS TERM MATRIX FOR VISCOSITY
C     PRESS-PRESSURE OF GAS MIXTURE IN THE CHANNEL(atm)
C     PRESS1-HOLDING CONSTANT FOR PRESSURE OF GAS MIXTURE
C     Q-HOLDING CONSTANT
C     R-GAS CONSTANT  (J/mol-K)
C     Re - Reynold's number (dimensionless)
C     S-TAB CHARACTER
C     SS-CARRIAGE RETURM CHARACTER
C     SSS-A OR I FOR ADIABATIC OR ISOTHERMAL-CHARACTER
C     SSS1-P OR S FOR PROFILE OR SUMMARY-CHARACTER
C     SSS2-O OR L FOR O2 CONVERSION OR MONOLITH LENGTH-CHARACTER
C     SU(i)-i->1,6** SUTHERLAND CONSTANT OF COMPONENT
C          GASES(gms/mole)
C     SUINTER(i,j)-i,j=1->6** SUTHERLAND INTERACTION MATRIX
C     T-GAS TEMPERATURE FOR VISCOSITY AND THERMAL CONDUCTIVITY
C     TB(i)-i->1,6** BOILING POINT OF COMPONENT GASES(K)
C     TCON(i,j)-i->1,6**,j->2,7***,THERMAL COND. OF COMPONENT GASES
C       AT VARIOUS TEMPERATURES(mW/cm-K)
C     TCONT(i)-i->1,6** THERMAL COND.OF COMPONENT GASES AT TEMP
C          T(mW/cm-K)
C     TCONDC-COMPOSITE GAS THERMAL CONDUCTIVITY(mW/cm-K)
C     TGX-MONOLITH CHANNEL BULK GAS TEMPERATURE AT POSIT. X (K)
C     THIELE-SLAB THIELE MODULUS FOR CATALYST WASHCOAT (NONDIM)
C     TREF-PHYSICAL PROPERTIES REF TEMP=298K (K)
C     TSX-MONOLITH CHANNEL WALL TEMPERATURE AT POSIT. X (K)
C     TZERO-MONOLITH INLET GAS TEMPERATURE (K)
C     VISC(i,j)-i->1,6**,j->2,7***,VISCOSITY OF COMPONENT GASES
C       AT VARIOUS TEMPERATURES(centipoises)
C     VISCT(i)-i->1,6** VISCOSITY OF COMPONENT GASES AT TEMP
C          T(centipoises)
```

```
C     VISCTC-COMPOSITE GAS VISCOSITY(centipoises)
C     X-MONOLITH CHANNEL POSITION (mm)
C     Y(i)-i->1,6** MOLE FRACTION OF COMPONENT GASES(gms/mole)
C     Y10,Y20,Y30,Y40,Y50,Y60-HOLDING CONSTANTS FOR Y(i)'s
C     YT-SUM OF Y(i)-i->1,6
C     **1=He, 2=Ar, 3=CO2, 4=CO, 5=O2, 6=N2
C     ***2=200, 3=300, 4=400, 5=500, 6=600, 7=700K
C ALGORITHM:
C     -Declare variables, open data file
C     -Introduction
C     -Initialize physical and option parameters to default values
C     -Display Selectable Parameter Summary
C     -Input physical parameters (if required)
C       -Monolith face dimensions
C         -Perform monolith parameter calculations
C       -Gas composition
C       -Inlet gas temperature, inlet gas flowrate
C       -Catalyst volumetric pumping rate and activation energy
C     -Choose operation options(if required)
C       -Adiabatic or isothermal operation
C       -Complete conc. & temperature profile output or summary
C       -Loop completion criteria (conversion or monolith length)
C         -Input desired final conversion or monolith length
C       -Computation loop step size, profile output step size.
C     -Allow revision of parameters if desired
C     -Compute viscosity and thermal conductivity parameters
C     -Read in molecular weight,diffusion coeff, thermal
C               conductivity,
C        viscosity,boiling point data
C     -Prepare to compute thermal conductivity & viscosity
C     -Print to screen and file,inputted, computed, and option
C               parameters
C     -Computation loop
C       -Intialize computation loop parameters
C       -Print profile header
C       -Step through computation loop until loop conditions are
C          met
C         -Print to data file and screen profile results at this
C               step
C         -Update physical properties that may change
C     -Query for further runs using different parameters
C     -Exit program
C*************************************************************
C**********Declare variables**************************
C*************************************************************
      PROGRAM LASER17
      INTEGER  NOCHV,NOCHH,NOCHM,FACTOR
      REAL*8   MFD,MCW,MCH,MCWT,CMCWT,MCST,CHWP,CHSTV,CHHD
      REAL*8   TZERO,O2ZERO,MVFLO,CONV,CHFLO,CHGVEL,MONOL
      REAL*8   CGX,CSX,TGX,TSX,TREF,X,DX,DCGX,DTGX,AREF,A
      REAL*8   KC,DENGAS,DENGSR,DENCAT,DENSUP,CPGAS,CPCAT,CPSUP
      REAL*8   N,HEATRX,ENGACT,R,THIELE,DAB,DABR,DABEFF
      REAL*8   H,K,KREF,CONST1,CONST2,CONST3,P,Q,CONVX,ASK
      CHARACTER*1  S,SS,SSS,SSS1,SSS2,BEEP,CH,CH1
```

```
      CHARACTER*20 FILNAM
      REAL*8   T,Y(6),YT,TCONDC,VISCTC,Y10,Y20,Y30,Y40,Y50,Y60
      REAL*8   MW(6),TB(6),SU(6),CSub,DABEFR
      REAL*8   VISC(6,2:7),SUINTER(6,6),PHI(6,6)
      REAL*8   VISCT(6),TCONT(6),AX(6,6),AMW,PRESS,D(6),DY5,DP
      REAL*8   CONST5,CONST4,CONST6,CONST7,CONST8,CP(6)
      INTEGER I,J,CONSTA,CONSTB,CONSTC
C*************************************************************
C******Introduction*******************************************
C*************************************************************

C     Open Data file which will be used for output.

      OPEN( UNIT=25, FILE='LDATA', STATUS='NEW')
      WRITE(9,*)'                    ******PROGRAM LASER17*******'
      WRITE(9,*)
      WRITE(9,*)'  The purpose of Laser17 is to calulate the gas',
     2' concentration and temperature'
       WRITE(9,*)'profiles for a monolith catalyst section of a',
     2' CO2 laser.  The CO2 decomposes'
      WRITE(9,*)'when the laser is pulsed.  The  CO and O2',
     2' produced as a result of pulsing '
       WRITE(9,*)'are detrimental to the operation and efficiency',
     2' of the laser.  The '
       WRITE(9,*)'recovering rxn is CO+1/2 O2 -> CO2.  This program',
     2' provides the means to model '
       WRITE(9,*)'the performance of a monolith  catalyst section,',
     2' with various gas compositions,'
       WRITE(9,*)'temperatures, catalyst activities, gas flowrates',
     2', oxygen conversion, monolith'
       WRITE(9,*)'face and length dimensions.  Results can indicate',
     2' if constraints such as'
       WRITE(9,*)'conversion, max. gas temperature, monolith weight',
     2' are satisfied and how '
       WRITE(9,*)'the system parameters may be altered to meet
these',
     2' constraints. A number'
       WRITE(9,*)'of parameters may be altered to meet these',
     2' constraints.  A number'
      WRITE(9,*)'of parameters can be supplied and a number of',
     2' options chosen to'
       WRITE(9,*)'customize the monolith design process.  Default ',
     2'values can also be used.'
       WRITE(9,*)'A review of the parameters and options chosen may',
     2'be reviewed and altered'
       WRITE(9,*)'prior to execution of the computation portion of',
     2' the program'
      WRITE(9,*)
      WRITE(9,*)'                         (HIT RETURN TO CONTINUE)'
      PAUSE
      WRITE(9,*)
```

```
C*****************************************************************
C******Default values for parameters******************************
C*****************************************************************

C     First see if default parameters are already available in a data
C     file.

9000  WRITE(*,*)
      WRITE(*,*)'Read in Data from Existing Data File? (Y/N)'
      READ(*,*) CH
      IF ((CH.EQ.'Y').OR.(CH.EQ.'y')) THEN
           WRITE(*,*)'COOL... Thats Less Work for Both of Us.!!'
           WRITE(*,*)
           WRITE(*,*)'What`s the name of the Existing Data file'
           WRITE(*,*)'to be opened?'
           READ(*,*)FILNAM
           OPEN(UNIT=23, FILE=FILNAM, STATUS='OLD')

C     If existing data file exists, read in data.

           READ(23,*)MFD
           READ(23,*)MCST
           READ(23,*)MCW
           READ(23,*)MCH
           READ(23,*)MCWT
           READ(23,*)Y(1)
           READ(23,*)Y(2)
           READ(23,*)Y(3)
           READ(23,*)Y(4)
           READ(23,*)Y(5)
           READ(23,*)Y(6)
           READ(23,*)PRESS
           READ(23,*)SSS
           READ(23,*)SSS1
           READ(23,*)SSS2
           READ(23,*)CONV
           READ(23,*)ENGACT
           READ(23,*)AREF
           READ(23,*)TZERO
           READ(23,*)MVFLO
           READ(23,*)FACTOR
           READ(23,*)DX
           CLOSE (UNIT = 23)

C     If no external data file exists, then assign default values.

      ELSE
           WRITE(*,*)
           WRITE(*,*)' Default Values Being Assigned...'
11         MFD=100
           MCST=0.5
           MCW=4
           MCH=4
           MCWT=0.25
```

```
            Y(1)=0.2
            Y(2)=0.0
            Y(3)=0.37
            Y(4)=0.02
            Y(5)=0.01
            Y(6)=0.40
            PRESS=1.0
            SSS='A'
            SSS1='P'
            SSS2='O'
            CONV=5
            ENGACT=39700
            AREF=123.4
            TZERO=300
            MVFLO=0.25
            FACTOR=5
            DX=1.0
      ENDIF

C     Compute a few needed parameters:

      Y10=Y(1)
      Y20=Y(2)
      Y30=Y(3)
      Y40=Y(4)
      Y50=Y(5)
      Y60=Y(6)
      PRESS1=PRESS
      O2ZERO=100*Y(5)
      CHWP = 2 * ( MCW + MCH )
      CHSTV = CHWP / ( MCW * MCH )
      CHHD = 4 * ( MCW * MCH ) / CHWP
      NOCHV = INT(MFD / (MCW+2*MCST))
      NOCHH = NOCHV
      NOCHM = NOCHV * NOCHH

C*************************************************
C******** Print Out Main Menu ***************************
C*************************************************

9001  WRITE(*,*)
      WRITE(*,*)
      WRITE(*,*)
      WRITE(*,*)
      WRITE(*,*)
      WRITE(*,*)
      WRITE(*,*)
      WRITE(*,*)
      WRITE(*,*)
      WRITE(*,*)
      WRITE(*,*)
      WRITE(*,*)
      WRITE(*,*)
      WRITE(*,46)
```

```
46    FORMAT(1H ,T33,'Laser 17 Main Menu')
      WRITE(*,*)
      WRITE(*,*)
      WRITE(*,*) '  1) Read In New Operating Parameters'
      WRITE(*,*) '  2) Save Current Operating Parameters'
      WRITE(*,*) '  3) Show Current Operating Parameters'
      WRITE(*,*) '  4) Change Monolith Physical Dimensions'
      WRITE(*,*) '  5) Change Monolith Inlet Parameters'
      WRITE(*,*) '  6) Change Gas Flowrate and / or Temperature'
      WRITE(*,*) '  7) Change Catalyst Reaction Rate Constant'
      WRITE(*,*) '  8) Change Catalyst Activation Energy'
      WRITE(*,*) '  9) Change Thermal Operation (Adia./Isotherm)'
      WRITE(*,*) ' 10) Change Output Profile (Full / Summary)'
      WRITE(*,*) ' 11) Change Termination Parameter (Conv./Len.)'
      WRITE(*,*) ' 12) Change Computation Loop Step Size'
      WRITE(*,*)
      WRITE(*,*) ' 13) Compute Catalyst Profile'
      WRITE(*,*)' 14) Exit Program'
      WRITE(*,*)
      WRITE(*,*) 'Type in Number Corresponding to Choice Above.'
       Read(*,*) ASK

      If (ASK.EQ.1) GO TO 9000
      If (ASK.EQ.2) GO TO 11000
      If (ASK.EQ.3) GO TO 9002
      If (ASK.EQ.4) GO TO 101
      If (ASK.EQ.5) GO TO 110
      If (ASK.EQ.6) GO TO 114
      If (ASK.EQ.7) GO TO 118
      If (ASK.EQ.8) GO TO 119
      If (ASK.EQ.9) GO TO 235
      If (ASK.EQ.10) GO TO 236
      If (ASK.EQ.11) GO TO 237
      If (ASK.EQ.12) GO TO 309
      If (ASK.EQ.13) GO TO 348
      If (ASK.EQ.14) GO TO 99999
      WRITE(*,*) BEEP, BEEP, BEEP
      WRITE(*,*)
      WRITE(*,*) ' Invalid Choice, Ace.... '
      WRITE(*,*) ' Try Again & Follow Directions.'
      WRITE(*,*)
      WRITE(*,*) 'Hit Return for Another Chance! '
      PAUSE
      GOTO 9001
C*************************************************************
C******Output to screen for review*****************************
C*************************************************************
9002  Write(9,6000)
6000  FORMAT(20X,'SELECTABLE PARAMETER SUMMARY')
      WRITE(9,*)
      WRITE(9,*)' Monolith Dimensions(mm) :'
      WRITE(9,6001) MCST*2,MFD,MFD
6001  FORMAT('1. Support wall thickness :',F6.2,3X,'Face dimension
:',
```

```
     2F7.2,' x ',F7.2)
     WRITE(9,6002) MCW,NOCHV,NOCHV
6002 FORMAT('2. Channel inner dimension:',F6.2,3X,'No.Face
channels',
     2':',I4,'   x  ',I4)
     WRITE(9,6003) MCWT,100*(MCW**2/(MCST*2+MCW)**2)
6003 FORMAT('3. Washcoat thickness     :',F6.2,'  % open face',F6.1)
     WRITE(9,*)
     WRITE(9,*)' Monolith inlet parameters:'
     WRITE(9,6004) Y(3),Y(4),Y(5),Y(6),Y(1),Y(2)
6004 FORMAT('4. Gas Composition(mole fraction): CO2-',F5.3,2X,
     2'CO -',F5.3,2X,'O2 -',F5.3,/,35X,'N2 -',F5.3,2X,'He -
',F5.3,2X,
     3'Ar -',F5.3)
      WRITE(9,6005) MVFLO,TZERO
6005 FORMAT('5. Gas Flowrate(l/s):',F7.3,9X,'Gas Temperature(K):',
     2F7.2)
     WRITE(9,*)
     WRITE(9,*)' Catalyst Properties:'
     WRITE(9,6006) AREF
6006 FORMAT('6. Reaction rate constant(mm^3 O2/gcat-s):',F8.2)
     WRITE(9,6007) ENGACT
6007 FORMAT('7. Activation energy(J/mol)              :',F10.2)
     IF (SSS.EQ.'A')      WRITE(9,6008)
6008 FORMAT('8. Thermal Operation (adiabatic/isothermal):Adiabatic')
     IF (SSS.EQ.'I')   WRITE(9,6009)
6009 FORMAT('8. Thermal Operation
(adiabatic/isothermal):Isothermal')
     WRITE(9,*)
     WRITE(9,*)' Computational loop parameters:'
     IF (SSS1.EQ.'S')     WRITE(9,6010)
6010 FORMAT('9. Output file (Full Profile/Summary): Summary')
     IF (SSS1.EQ.'P')     WRITE(9,6011)
6011 FORMAT('9. Output file (Full Profile/Summary): Full Profile')
     IF (SSS2.EQ.'O')     WRITE(9,6012) CONV
6012 FORMAT('10. Termination on (O2 conversion/Length):',
     2'O2 conversion.  %O2:', F7.3)
     IF (SSS2.EQ.'L')     WRITE(9,6013) MONOL
6013 FORMAT('10. Termination on (O2 conversion/Length):',
     2'Length.  Length(mm):', F7.3)
      IF (SSS1.EQ.'P') WRITE(9,6015) DX,FACTOR
6015 FORMAT('11. Computation loop step size(mm)= ',F6.3,
     2'    Step size factor= ',I4)
      IF (SSS1.EQ.'S') WRITE(9,60150) DX
60150     FORMAT('11. Computation loop step size(mm)= ',F6.3)
     WRITE(*,*)
     WRITE(*,*)     '==> Hit Return When Finished Viewing <=='
     PAUSE
     GOTO 9001

CC*************************************************************
C******Parameter input section*********************************
C*************************************************************
101  WRITE(9,*)
```

```
      WRITE(9,*)' For a square face, input monolith face ',
     2'dimension(mm)'
       READ(9,*) MFD
       IF (MFD.LE.0.0)    GO TO 101
102   WRITE(9,*)
      WRITE(9,*)' Input the monolith channel support wall'
       WRITE(9,*)' thickness(mm). This includes the washcoat.'
       READ(9,*)  MCST
       IF (MCST.LE.0.0)    GO TO 102
       MCST = MCST / 2.0
       IF (MCWT.GT.MCST)  GO TO  104
103   WRITE(9,*)
      WRITE(9,*)' For a square monolith channel, input monolith'
      WRITE(9,*)' inner channel dimension(mm).'
       READ(9,*)  MCW
       IF (MCW.LE.0.0)     GO TO 103
       MCH = MCW
104   WRITE(9,*)
      WRITE(9,*)' Input monolith channel washcoat thickness(mm).'
      WRITE(9,*)' Washcoat cannot be >1/2  support wall thickness.'
      WRITE(9,*)' Support wall thickness is', MCST*2,' (mm)'
       READ(9,*)  MCWT
       IF ((MCWT.EQ.0).OR.(MCWT.GT.MCST))    GO TO 104
C**********Perform monolith parameter calculations
8900  CHWP = 2 * ( MCW + MCH )
      CHSTV = CHWP / ( MCW * MCH )
      CHHD = 4 * ( MCW * MCH ) / CHWP
      NOCHV = INT(MFD / (MCW+2*MCST))
      NOCHH = NOCHV
      NOCHM = NOCHV * NOCHH
      GO TO 9001
C********Gas composition
C     Define Mole fractions of species Y(i)
C     The index of Y(i) correspond to the species.
C     Species: 1=He,2=Ar,3=CO2,4=CO,5=O2,6=N2.
110   Write(9,*) 'Input section for gas composition'
      Write(9,*) 'The mixture can consist of only the following'
      Write(9,*) 'species: He, Ar, CO2, CO, O2, N2. The mole '
      Write(9,*) 'fractions must add up to >=.99 to <=1.01.'
      Write(9,*) 'All mole fractions must be > or = zero.'
      WRITE(9,*)
      Write(9,*) 'Input gas mole fraction for He'
           Read(9,*) Y(1)
      Write(9,*) 'Input gas mole fraction for Ar'
           Read(9,*) Y(2)
      Write(9,*) 'Input gas mole fraction for CO2'
           Read(9,*) Y(3)
      Write(9,*) 'Input gas mole fraction for CO'
           Read(9,*) Y(4)
      Write(9,*) 'Input gas mole fraction for O2'
           Read(9,*) Y(5)
           O2ZERO=Y(5)*100
      Write(9,*) 'Input gas mole fraction for N2'
           Read(9,*) Y(6)
```

```
      YT=  Y(1) +Y(2) +Y(3) +Y(4) +Y(5) +Y(6)
           Y10=Y(1)
           Y20=Y(2)
           Y30=Y(3)
           Y40=Y(4)
           Y50=Y(5)
           Y60=Y(6)
C     Check if restrictions are met.If not, force user to reinput
C     values
      Do 112 I=1,6
        IF ((Y(I).LT.0).or.(Y(I).GT.1.0))  GOTO 110
112   Continue
      IF ((YT.GT.1.01) .or. (YT.LT.0.99 )) GOTO 110
      GO TO 9001
C********Inlet gas temperature
114   WRITE(9,*)
      WRITE(9,*)'Input monolith inlet gas temperature(K)'
      WRITE(9,*)'Temperature must be >200K and <700K.'
       READ(9,*)  TZERO
       IF ((TZERO.EQ.0).OR.(TZERO.LT.200)) GO TO 114
       IF (TZERO.GT.700)  GO TO 114
C********Inlet gas flowrate
116   WRITE(9,*)
      WRITE(9,*)' Input monolith inlet volumetric flowrate(l/S)'
       READ(9,*)  MVFLO
       IF (MVFLO.EQ.0)  GO TO 116
      GO TO 9001
C********Catalyst reaction rate constant and activation energy
118   WRITE(9,*)
      WRITE(9,*)'Catalyst reaction rate constant-298K(mm^3/gcat-s)'
       READ(9,*)  AREF
       IF (AREF.EQ.0)  GOTO 118
      GO TO 9001
119   WRITE(9,*)
      WRITE(9,*)'Catalyst activation energy(J/mol)'
       READ(9,*)  ENGACT
       IF (ENGACT.EQ.0)  GOTO 119
      GO TO 9001
C******Adiabatic or isothermal operation
235   WRITE(9,*)'Isothermal(I) or Adiabatic(A) operation?'
      WRITE(9,*)'Type the letter I or the letter A. HIT RETURN'
       READ(9,*)  SSS
       IF (SSS.EQ.'i') SSS = 'I'
       IF (SSS.EQ.'a') SSS = 'A'
      IF ((SSS.NE.'I').AND.( SSS.NE.'A')) GO TO 235
      GO TO 9001
C*******FULL CONCEN. AND TEMP. PROFILE(P) OR SUMMARY ONLY'
236   WRITE(9,*)
      WRITE(9,*)'Full concentration and temperature profile (P) OR'
      2'summary(S)?'
      WRITE(9,*)'Type the letter P or the letter S. HIT RETURN '
       READ(9,*)  SSS1
       IF (SSS1.EQ.'p') SSS1 = 'P'
       IF (SSS1.EQ.'s') SSS1 = 'S'
```

```
      IF ((SSS1.NE.'P').AND.( SSS1.NE.'S')) GO TO 236
      GO TO 9001
C********COMPUTATION LOOP COMPLETION CRITERIA
237   WRITE(9,*)
      WRITE(9,*)'Computation loop completion criteria can be '
      WRITE(9,*)'chosen to depend on oxygen conversion(O) or'
      WRITE(9,*)'monolith length(L).'
       WRITE(9,*)'Type the letter O or the letter L. HIT RETURN.'
       READ(9,*)  SSS2
       IF(SSS2.EQ.'o') SSS2 = 'O'
       IF(SSS2.EQ.'l') SSS2 = 'L'
      IF ((SSS2.NE.'O').AND.( SSS2.NE.'L')) GO TO 237
      IF (SSS2.EQ.'O') THEN
238     WRITE(9,*)'Input desired %oxygen conversion,0 TO 100%'
        READ(9,*) CONV
        IF ((CONV.GT.100.0).OR.(CONV.LT.0)) GOTO 238
      ENDIF
239   IF (SSS2.EQ.'L') THEN
        WRITE(9,*)'Input desired monolith length(10 TO 500mm)'
        READ(9,*) MONOL
        IF (MONOL.LT.0) GOTO 239
        IF (MONOL.GT.500) GOTO 239
      ENDIF
      GO TO 9001
C******COMPUTATION LOOP STEP SECTION
309   WRITE(9,*)
      WRITE(9,*)'Input computation loop step size(mm).'
      WRITE(9,*)'Maximum loop step size 1mm.'
       READ(9,*) DX
      IF (DX.GT.1.0) GO TO 309
      WRITE(9,*)
320   IF (SSS1.EQ.'P') THEN
323     WRITE(9,*)
      WRITE(9,*)'Input profile step size factor.'
      WRITE(9,*)'Profile step size factor must be >=1.'
            READ(9,*) CONST1
        IF (CONST1.LT.1.0) GOTO 323
        FACTOR=CONST1/1
       ENDIF
      WRITE(9,*)
      GO TO 9001

11000  WRITE(9,*)

C     Give user option to save present default parameters.


           WRITE(*,*)
           WRITE(*,*)' Would you like to save the data to a'
           WRITE(*,*)' NEW or EXISTING data file? (N/E)'
           WRITE(*,*)
           READ(*,*)CH1
           IF ((CH1.EQ.'E').OR.(CH1.EQ.'e')) THEN
                WRITE(*,*)
```

```
            WRITE(*,*)'What`s the name of the EXISTING'
            WRITE(*,*)'Data file to be opened?'
            READ(*,*) FILNAM
            OPEN( UNIT=24, FILE=FILNAM, STATUS='OLD')
      ELSE
            WRITE(*,*)
            WRITE(*,*)'What`s the name of the NEW'
            WRITE(*,*)'Data file to be opened?'
            READ(*,*) FILNAM
            OPEN( UNIT=24, FILE=FILNAM, STATUS='NEW')
      ENDIF

C     Write  default parameters to data file.

            WRITE(24,*)MFD
            WRITE(24,*)MCST
            WRITE(24,*)MCW
            WRITE(24,*)MCH
            WRITE(24,*)MCWT
            WRITE(24,*)Y(1)
            WRITE(24,*)Y(2)
            WRITE(24,*)Y(3)
            WRITE(24,*)Y(4)
            WRITE(24,*)Y(5)
            WRITE(24,*)Y(6)
            WRITE(24,*)PRESS
            WRITE(24,*)SSS
            WRITE(24,*)SSS1
            WRITE(24,*)SSS2
            WRITE(24,*)CONV
            WRITE(24,*)ENGACT
            WRITE(24,*)AREF
            WRITE(24,*)TZERO
            WRITE(24,*)MVFLO
            WRITE(24,*)FACTOR
            WRITE(24,*)DX
            CLOSE ( UNIT = 24)

      GOTO 9001
348   CONTINUE
C**Computation of parameters needed for thermal cond. calcuation
C     Read in molecular weights MW(I) into array.
C     The index of MW correspond to the species.
C     Species: 1=He,2=Ar,3=CO2,4=CO,5=O2,6=N2.
      DATA MW(1),MW(2),MW(3),MW(4),MW(5),MW(6)
     +     / 4.0026,39.948,44.01,28.0105,31.9988,28.0134/
C     Read in binary diffusion coefficients D(I) into array.
C     The index of D correspond to the species in which O2 is
C     diffusiving
C     Note: There is no D(5) defined. These are reference values at
C     298K,
C          1 atm,units(mm^2/s)
C     Species: 1=He,2=Ar,3=CO2,4=CO,6=N2.
      DATA D(1),D(2),D(3),D(4),D(6)
```

```
     +     /72.9,21.2,16.4,15.6,22.5/

C    Read in viscosity (VISC) values into matrix.
C    Units on VISC are centipoises. The values are read off a
C    nomagraph
C    in Perry's Chemical Engineering Handbook, 5th ed., p3-210.
C    The first index of VISC corresponds to the species.
C    Species: 1=He,2=Ar,3=CO2,4=CO,5=O2,6=N2.
C    The second index of VISC corresponds to the temperature.
C    Temperature:  2=200K,3=300K,4=400K,5=500K,6=600K,7=700K
     DATA
VISC(1,2),VISC(1,3),VISC(1,4),VISC(1,5),VISC(1,6),VISC(1,7)
     +/.014,.0188,.022,.027,.031,.034/
     DATA
VISC(2,2),VISC(2,3),VISC(2,4),VISC(2,5),VISC(2,6),VISC(2,7)
     +/.0164,.0223,.0278,.0327,.0376,.041/
     DATA
VISC(3,2),VISC(3,3),VISC(3,4),VISC(3,5),VISC(3,6),VISC(3,7)
     +/.0105,.0147,.019,.023,.027,.031/
     DATA
VISC(4,2),VISC(4,3),VISC(4,4),VISC(4,5),VISC(4,6),VISC(4,7)
     +/.0138,.018,.022,.0255,.029,.0325/
     DATA
VISC(5,2),VISC(5,3),VISC(5,4),VISC(5,5),VISC(5,6),VISC(5,7)
     +/.0155,.02,.0247,.0288,.0327,.0368/
     DATA
VISC(6,2),VISC(6,3),VISC(6,4),VISC(6,5),VISC(6,6),VISC(6,7)
     +/.013,.0175,.0218,.026,.029,.0332/

C    Read in boiling point (TB) data into array.
C    The index of TB corresponds to the species.
C    Species: 1=He,2=Ar,3=CO2,4=CO,5=O2,6=N2.
C    Units are K. The values are taken from "Properties of Gases
C    and Liquids", 3rd ed.,Reid, Prausnitz,& Sherwood, p629-633
C    and p509 (Note says to use 79K for He).
     DATA TB(1),TB(2),TB(3),TB(4),TB(5),TB(6)
     +/79,87.3,194.7,145.2,90.2,77.4/
C    Compute Sutherland  (SU) constant for each species
C    The index of SU corresponds to the species.
C    Species: 1=He,2=Ar,3=CO2,4=CO,5=O2,6=N2.
C    The Sutherland constant is defined on p509 of "Properties of
C    Gases
C    and Liquids", 3rd ed.,Reid, Prausnitz,& Sherwood.
SU(i)=1.5*TB(i).
     DO 150 I=1,6
          SU(I)=1.5*TB(I)
150  CONTINUE
C    Compute the Sutherland interaction constants,SUINTER
C    The indexes of SUINTER corresponds to the species.
C    Species: 1=He,2=Ar,3=CO2,4=CO,5=O2,6=N2.
C    The Sutherland interaction constant is defined on p509 of
C    "Properties of Gases and Liquids", 3rd ed.,Reid, Prausnitz,
C    & Sherwood. SU(i)=1.5TB(i). None of the species are "very
C    polar,
```

```
C     therefore, CSubS=1.0, see p509-510.
      CSubS=1.0
      DO 175 I=1,6
           DO 170 J=1,6
           SUINTER(I,J)=CSubS*(SU(I)*SU(J))**0.5
170        CONTINUE
175   CONTINUE
C        COMPUTE ADDITIONAL MONOLITH PARAMETERS
C        CONVERT MVFLO FROM l/S TO mm^3/S
      MVFLO = MVFLO *1.0E+06
      CHFLO = MVFLO / NOCHM
      CHGVEL = CHFLO / ( MCW * MCH)
C*****************************************************************
C**Output of selectable parameter to data file*********************
C*****************************************************************
      WRITE(9,*)'              *****SEE FILE LDATA FOR RESULTS*****'
      WRITE(25,6100)
6100  FORMAT(20X,'SELECTABLE PARAMETER SUMMARY')
      WRITE(25,*)' Monolith Dimensions(mm) :'
      WRITE(25,6101) MCST*2,MFD,MFD
6101  FORMAT('1. Support wall thickness :',F6.2,3X,'Face dimension
:',
      2F7.2,' x ',F7.2)
      WRITE(25,6102) MCW,NOCHV,NOCHV
6102  FORMAT('2. Channel inner dimension:',F6.2,3X,'No.Face
channels',
      2':',I4,'   x  ',I4)
      WRITE(25,6103) MCWT,100*(MCW**2/(MCST*2+MCW)**2)
6103  FORMAT('3. Washcoat thickness    :',F6.2,'  % open face',F6.1)
      WRITE(25,*)
      WRITE(25,*)' Monolith inlet parameters:'
      WRITE(25,6104) Y(3),Y(4),Y(5),Y(6),Y(1),Y(2)
6104  FORMAT('4. Gas Composition(mole fraction): CO2-',F5.3,2X,
      2'CO -',F5.3,2X,'O2 -',F5.3,/,35X,'N2 -',F5.3,2X,'He -
',F5.3,2X,
      3'Ar -',F5.3)
       WRITE(25,6105) MVFLO/1.0E+06,TZERO
6105  FORMAT('5. Gas Flowrate(l/s):',F5.3,9X,'Gas Temperature(K):',
      2F7.2)
      WRITE(25,*)
      WRITE(25,*)' Catalyst Properties:'
      WRITE(25,6106) AREF
6106  FORMAT('6. Reaction rate constant(mm^3 O2/gcat-s):',F8.2)
      WRITE(25,6107) ENGACT
6107  FORMAT('7. Activation energy(J/mol)              :',F10.2)
      IF (SSS.EQ.'A')      WRITE(25,6108)
6108  FORMAT('8. Thermal Operation (adiabatic/isothermal):Adiabatic')
      IF (SSS.EQ.'I')    WRITE(25,6109)
6109  FORMAT('8. Thermal Operation
(adiabatic/isothermal):Isothermal')
      WRITE(25,*)
      WRITE(25,*)' Computational loop parameters:'
      IF (SSS1.EQ.'S')     WRITE(25,6110)
6110  FORMAT('9. Output file (Full Profile/Summary): Summary')
```

```
      IF (SSS1.EQ.'P')     WRITE(25,6111)
 6111 FORMAT('9. Output file (Full Profile/Summary): Full Profile')
      IF (SSS2.EQ.'O')     WRITE(25,6112) CONV
 6112 FORMAT('10. Termination on (O2 conversion/Length):',
     2'O2 conversion.  %O2:', F7.3)
      IF (SSS2.EQ.'L')     WRITE(25,6113) MONOL
 6113 FORMAT('10. Termination on (O2 conversion/Length):',
     2'Length.  Length(mm):', F7.3)
       WRITE(25,6115) DX,FACTOR
 6115 FORMAT('11. Computation loop step size(mm)= ',F6.3,
     2'    Step size factor= ',I4)
 6114  WRITE(25,*)
C*****************************************************************
C******INTIALIZE PHYSICAL PROPERTIES PARAMETERS********************
C*****************************************************************
      HEATRX=5.64E+05
      TREF=298
      DENCAT=5.0E-04
      DABEFR=1.0
      R=8.3144
C*****************************************************************
C*******EULER'S METHOD COMPUTATION OF CG(X),TG(X),CS(X),&TS(X)*****
C*****************************************************************
      TGX= TZERO
      CGX= 4.092E-08 * O2ZERO /100.0 * (298/TGX)
      CONST3=CGX
      CGXEND =CGX * ( 1 - CONV/100)
      S = CHAR(9)
      SS = CHAR(13)
      BEEP= CHAR(7)
      X=0
      CMCWT= ((MCH+2*MCWT)*(MCW+2*MCWT)-(MCH*MCW))/2/(MCH+MCW)
         WRITE(9,9950)
        WRITE(25,9950)
 9950  FORMAT('  X-mm  ',2X,'%CONVER',2X,' O2gas<-mMOL/L->O2surf ',
     +'  Tgas<-K->Tsurf    ETA    DP(KPA) ')
C*************************************************************
C**********  LOOP UNTIL REQUIRED CONDITION IS MET************
C*************************************************************
      CONSTA=0
      DO 8000 P=0,1000,DX
        IF (SSS2.EQ.'O') THEN
          IF (CGX .LT. (CGXEND /(TZERO/TGX))) GO TO 9900
            GO TO 8250
          ENDIF
        IF (SSS2.GE.'L') THEN
          IF (P.GT. MONOL) GO TO 16900
          IF (CGX.LE.0.0)  GO TO 16900
        ENDIF
 8250 AMW=0
      DO 8350 I=1,6
           AMW=MW(I)*Y(I)+AMW
 8350 CONTINUE
      DENGAS=AMW*(PRESS/9896)/R/TGX
```

```
      DAB=0
      DO 8450 I=1,6
           IF (I.EQ.5) GO TO 8450
           DAB=Y(I)/(D(I)*(TGX/298)**1.5)+DAB
8450  CONTINUE
      DAB=(1-Y(5))/DAB/PRESS
      DABEFF=DABEFR*(TGX/298)**1.5
C*************************************************************
C********* COMPUTE THERMAL CONDUCTIVITY**********************
C*************************************************************
      IF (MOD( CONSTA,2) .GT. 0.0 ) GO TO 6666
        T=TGX
C     Compute viscosity (VISCT(i)) for a given species at temp. T
C     Units on VISCT are centipoises.
C     The index of VISC corresponds to the species.
C     Species: 1=He,2=Ar,3=CO2,4=CO,5=O2,6=N2.
C     CONST5 is a temporary value holding constant
      DO 200 I=1,6
           CONST5=VISC(I,INT(1+T/100.0))-VISC(I,INT(T/100.0))
           CONST5=CONST5*(T/100.0-INT(T/100))
           VISCT(I)=VISC(I,INT(T/100.0)) + CONST5
200   CONTINUE
C     Compute thermal cond.(TCONT(i)) for a given species at temp. T
C     Units on TCON are mW/cM-K.
C     The index of TCONT(i) corresponds to the species.
C     Species: 1=He,2=Ar,3=CO2,4=CO,5=O2,6=N2.
C     The following polynomial equations used to compute the
C     thermal conductivity of each species at temperature T
C     have been taken from page 515 of "Properties of Gases and
C     Liquids"
C     4th Ed. Reid, Prausnitz, & Sherwood

C     CONST5 is a temporary value holding constant

      TCONT(1) = (3.722E-2 + 3.896E-4*T - 7.450E-8*T**2 +
     1   1.290E-11*T**3)*10.0
      TCONT(2) = (2.714E-3 + 5.540E-5*T - 2.178E-8*T**2 +
     1   5.528E-12*T**3)*10.0
      TCONT(3) = (-7.215E-3 + 8.015E-5*T + 5.477E-9*T**2 -
     1   1.053E-11*T**3)*10.0
      TCONT(4) = (5.067E-4 + 9.125E-5*T - 3.524E-8*T**2 +
     1   8.199E-12*T**3)*10.0
      TCONT(5) = (-3.273E-4 + 9.966E-5*T - 3.743E-8*T**2 +
     1   9.732E-12*T**3)*10.0
      TCONT(6) = (3.919E-4 + 9.816E-5*T - 5.067E-8*T**2 +
     1   1.504E-11*T**3)*10.0



C     Compute parameter matrix AX(i,j)
C     The indexes of A(i,j) correspond to the species.
C     Species: 1=He,2=Ar,3=CO2,4=CO,5=O2,6=N2.
C     The A(i,j) matrix is defined on p509 of "Properties of Gases
C     and
```

```
C     Liquids", 3rd ed.,Reid, Prausnitz,& Sherwood.
C     CONST5 is a temporary value holding constant
      CONST5=0
      DO 260 I=1,6
           DO 270 J=1,6
                CONST5=(T+SU(I))/(T+SU(J))*(MW(J)/MW(I))**0.75
                CONST5=(1+(CONST5*VISCT(I)/VISCT(J))**0.5)**2.0
                AX(I,J)=CONST5/4.0*(T+SUINTER(I,J))/(T+SU(I))
270        CONTINUE
260   CONTINUE
C     Compute the thermal conductivity of the mixture at TGX
C     CONST4,CONST5 are holding constants
      CONST4=0
      DO 550 I=1,6
           CONST5=0
           DO 650 J=1,6
                CONST5=CONST5 + Y(J)*AX(I,J)
650        CONTINUE
           CONST4=CONST4 + Y(I)*TCONT(I)/CONST5
550   CONTINUE
         TCONDC=CONST4
        K=TCONDC/10000.0
C     Compute parameter matrix PHI(i,j)
C     The indexes of PHI(i,j) correspond to the species.
C     Species: 1=He,2=Ar,3=CO2,4=CO,5=O2,6=N2.
C     The PHI(i,j) matrix for WIlke's Approximation method
C     is defined on p411 of "Properties of Gases and
C     Liquids", 3rd ed.,Reid, Prausnitz,& Sherwood.
C     CONST5 is a temporary value holding constant
      DO 280 I=1,6
       DO 290 J=1,6
        CONST5=(VISCT(I)/VISCT(J))**0.5*(MW(J)/MW(I))**0.25
        PHI(I,J)=(1+CONST5)**2.0/(8*(1+MW(I)/MW(J)))**0.5
290    CONTINUE
280   CONTINUE
C     Compute the viscosity of the mixture at TGX
C     CONST4,CONST5 are holding constants
      CONST4=0
      DO 750 I=1,6
           CONST5=0
           DO 850 J=1,6
           CONST5=CONST5 + Y(J)*PHI(I,J)
850        CONTINUE
        CONST4=CONST4 + Y(I)*VISCT(I)/CONST5
750   CONTINUE
      VISCTC=CONST4
6666     KC = 3.66 * DAB / CHHD
         H = 3.66 * K / CHHD
C*************************************************************
C*********COMPUTE HEAT CAPACITY OF GAS MIXTURE AT TGX********
C*************************************************************
      CP(1)=20.786
      CP(2)=20.786
      CP(3)=20.712+6.2501E-02*TGX-1.188E-5*TGX*TGX
```

```
     +      -5.5773E-08*TGX*TGX*TGX + 4.1875E-11*TGX*TGX*TGX*TGX
     CP(4)=28.777  +  5.5297E-03*TGX  -3.1851E-5*TGX*TGX
     +     +7.0946E-08*TGX*TGX*TGX  -4.2501E-11*TGX*TGX*TGX*TGX
          CP(5)=31.033  -  2.0261E-02*TGX  +6.3410E-5*TGX*TGX
     +     -4.9951E-08*TGX*TGX*TGX +9.1266E-12*TGX*TGX*TGX*TGX
          CP(6)=28.567  +  7.3978E-03*TGX  -3.5831E-05*TGX*TGX
     +     +6.9415E-08*TGX*TGX*TGX -3.8499E-11*TGX*TGX*TGX*TGX
      CPGAS = Y(1)*CP(1)/MW(1) + Y(2)*CP(2)/MW(2) +
     +        Y(3)*CP(3)/MW(3) + Y(4)*CP(4)/MW(4) +
     +        Y(5)*CP(5)/MW(5) + Y(6)*CP(6)/MW(6)
        A = AREF * EXP ( -ENGACT / R * ( 1 / TGX -1 / TREF))
        THIELE = CMCWT * (  A  * DENCAT / DABEFF) ** 0.5
        N = TANH ( THIELE ) / THIELE
        CONST1= N*A*CMCWT*DENCAT
        CSX = CGX * ( KC) / (KC+CONST1)
        TSX =TGX + HEATRX*CSX*CONST1/H
        DCGX = DX*KC*CHSTV*MCH*MCW/CHFLO*(CSX-CGX)
        IF (SSS.EQ.'I')  DTGX=0
        IF (SSS.EQ.'A')   THEN
          DTGX = DX*H* CHSTV*MCH*MCW/CHFLO*(TSX-TGX)/DENGAS/CPGAS
        ENDIF
        CONVX = 100 * ( CONST3-CGX*(TZERO/TGX))/CONST3

C      WRITE RESULTS TO SCREEN
       IF (MOD( CONSTA,FACTOR) .GT. 0.0) GO TO 7777
       WRITE(25,10) X,S,CONVX,S,CGX*1E+09,S,CSX*1E+09,S,TGX,S,TSX,S,N
     +,S,(PRESS-PRESS1)*101.33
10     FORMAT(' ',F6.1,A1,1X,F5.2,A1,2(3X,F7.4,A1),2(3X,F8.3,A1),F6.4
     +,A1,F7.3)
       WRITE(9,10) X,S,CONVX,S,CGX*1E+09,S,CSX*1E+09,S,TGX,S,TSX,S,N
     +,S,(PRESS-PRESS1)*101.33
7777        CGX = (CGX +DCGX)*(TGX/(TGX+DTGX))
            TGX = TGX +DTGX
            X   = X +  DX
            DP  = 32*(VISCTC/1000)*CHGVEL*DX/CHHD/CHHD/101330.0
            PRESS   = PRESS - DP
            CONST7 = Y(1)+Y(2)+Y(3)+Y(4)+Y(5)+Y(6)
            DY5 = DCGX*R*TGX/(PRESS/9869)
            CONST8 = Y(1)+Y(2)+Y(3)+Y(4)+Y(5)+Y(6)-3*DY5
            Y(1) = Y(1)*CONST7/CONST8
            Y(2) = Y(2)*CONST7/CONST8
            Y(3) = Y(3)*CONST7/CONST8
            Y(4) = (Y(4)-2*DY5)*CONST7/CONST8
            Y(5) = (Y(5)-DY5)*CONST7/CONST8
            Y(6) = Y(6)*CONST7/CONST8
            CONSTA=CONSTA + 1
C     Check to make sure that Temperature, Pressure, and Reynold's
C     number are still in valid range.

C     Temperature must be between 200-700 K
C     Pressure must be between 10E-03 and 3.45 bar
C     Reynolds number must be in laminar region. < 2300

            RE=1000.0*CHHD*CHGVEL*DENGAS/VISCTC
```

```
            IF ((RE.GT.2300.0).OR.(TGX.GT.700.).OR.(TGX.LT.200.)
     1                .OR.(PRESS.LT.0.001).OR.(PRESS.GT.3.45)) THEN
                  WRITE(*,*)
                  WRITE(*,*)'Error: Parameters have exceeded'
                  WRITE(*,*)'allowable Range... '
                  WRITE(*,*)' Returning to Main Menu'
                  WRITE(*,*)
                  WRITE(*,*) 'Hit Return When Finished Viewing'
                  PAUSE
                  GOTO 9001
            ENDIF

8000        CONTINUE
9900   WRITE(25,10) X,S,CONVX,S,CGX*1E+09,S,CSX*1E+09,S,TGX,S,TSX,S,N
      +,S,(PRESS-PRESS1)*101.33
       WRITE(9,10) X,S,CONVX,S,CGX*1E+09,S,CSX*1E+09,S,TGX,S,TSX,S,N
      +,S,(PRESS-PRESS1)*101.33
16900  WRITE(25,*)
      WRITE(9,*) BEEP,BEEP,BEEP
17000       WRITE(*,*)
      WRITE(*,*) '  ==> Hit Return to Return to Main Menu <=='
      PAUSE
        MVFLO=MVFLO/1E+6
        Y(1)=Y10
        Y(2)=Y20
        Y(3)=Y30
        Y(4)=Y40
        Y(5)=Y50
        Y(6)=Y60
        PRESS=PRESS1
        GOTO 9001

99999 END
```