Final Project Report

Design of Catalytic Monoliths for Closed-Cycle Carbon Dioxide Lasers

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Submitted by

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*Each section pages individually numbered.
Abstract

Pulsed carbon dioxide (CO₂) lasers have many applications in aeronautics, space research, weather monitoring and other areas. Full exploitation of the potential of these lasers is hampered by the dissociation of CO₂ that occurs during laser operation. The development of closed-cycle CO₂ lasers require active CO-O₂ recombination (CO oxidation) catalyst and design methods for implementation of catalysts in CO₂ laser systems.

A monolith catalyst section model and associated design computer program, LASCAT, are presented to assist in the design of a monolith catalyst section of a closed cycle CO₂ laser system. Using LASCAT, the designer is able to specify a number of system parameters and determine the monolith section performance. Trade-offs between the catalyst activity, catalyst dimensions, monolith dimensions, pressure drop, O₂ conversion, and other variables can be explored and adjusted to meet system design specifications.

An introduction describes a typical closed-cycle CO₂ system, and indicates some advantages of a closed-cycle laser system over an open cycle system and some advantages of a monolith support over other types of supports. The development and use of a monolith catalyst model is presented. The results of a design study and a discussion of general design rules are given. Detailed instructions for the use of LASCAT is given in Appendices 1-4.
Monolith Catalyst Model Development and Implementation

1. INTRODUCTION

The design of a CO₂ laser system is made under constraints of energy consumption, operating cost, size, weight, pressure drop, loop O₂ conversion, catalyst activity, flow channel dimensions, particulate production, reliability, ease of operation, safety, and numerous others. Design decisions, made to satisfy one constraint, often push the limits imposed on other constraints. A means to design the monolith catalyst section of a closed-cycle CO₂ laser system under selected restraint conditions is presented.

A pulsed CO₂ laser produces useful laser light output when the laser gas volume is exposed to a high electrical potential for a period on the order of milliseconds. Low lying vibrational-rotational energy level CO₂ molecules are excited to higher energy levels. The relaxation of the excited molecules to low lying energy levels produces infrared radiation. The energy deposited by the electrical discharge alters the composition of the gas mixture by dissociation of CO₂ into stoichiometric ratios of CO and O₂.

In a high pulse repetition rate (PRR) CO₂ laser system, without a method of recombining the CO and O₂, the laser gas O₂ concentration would continue to increase with time. Depending on the particular system used, O₂ concentrations above a threshold level, on the order of 1%, severely degrades the laser output quality. The lasing process also raises the temperature of the laser gas volume. The output of the laser is sensitive to the temperature of the operating gas due to the effect of temperature on the distribution of CO₂ molecules among the rotational-vibrational energy levels.

An open-cycle laser system requires a continuous supply of fresh gas to maintain O₂ concentration below threshold levels. The higher the PRR, the higher the fresh gas flow rate required to maintain acceptable O₂ concentrations. If rare isotope CO₂ gases, such as ¹²C¹⁸O₂, were to be used in an open-cycle laser system, the cost of supplying large quantities of CO₂ gases would be prohibitive. The safety requirements for handling and for the disposal of CO, O₂, and CO₂ gases is another concern for open-cycle systems. Clearly, for portable uses, such as in satellites or in the field, open-cycle system operation is not feasible.

Closed-cycle systems can be envisioned to require an one time charge of the operating gas and to operate for a given number of pulses (>10⁷) at a specified PRR and power output. Portable closed-cycle systems would necessarily have power consumption constraints and, therefore, be limited in the output power and PRR. In a typical closed-cycle CO₂ laser system (Fig. 1), a gas mixture, comprised of CO₂ and other "inert" gases, is continuously recirculated through the system by a blower. The recombination of CO and O₂ is accomplished by the monolith catalyst section of the system (Fig. 2) and provides the laser section with a fresh supply of operating gas. The heat exchangers allow for the operation of the monolith catalyst section at elevated temperatures while maintaining moderate laser section temperatures. The monolith catalyst material is very porous (high surface area) and has catalytic material dispersed throughout. The performance of the monolith catalyst is measured by the section's ability to recombine CO and O₂, the size and weight of the monolith, and the pressure drop produced as a result of gas flow through the monolith. Monolith catalyst performance is dependent on a number of interrelated factors, such as, the catalyst's geometry, convective heat and mass transport rates from the bulk gas to the catalyst, inlet gas properties, inlet molar gas flow rate, and catalytic activity. A monolith support is chosen over other supports, e.g. powders, beads, etc., because of the reduced level of particulate production, and the sturdiness of the monolith under high volumetric gas flow conditions.
2. MONOLITH CATALYST SECTION MODEL

A flexible model of the monolith catalyst may be developed to determine the bulk-average gas temperature, composition, and pressure along the length of the monolith. The adjustable parameters required to specify the operating condition of the monolith are listed in Table 1. The model assumptions, balance equations, and model results follow.

2.1 Model Assumptions
- Steady state conditions.
- Identical conditions exist in each channel of the monolith.
• Channel gas flow is laminar and fully developed. The neglect of entrance effects for heat and mass transfer calculations provide for a conservative estimate of the amount of catalyst required. Pressure drop due to entrance and exit effects is neglected, therefore the actual pressure drops will be somewhat greater than calculated.

• The kinetics of the reaction, \( \frac{1}{2}O_2 + CO \rightarrow CO_2 \), is first order overall, reaction rate \( \propto [O_2]^a [CO]^b \) where sum of a and b equals one. \( O_2 \) and \( CO_2 \) appear in stoichiometric ratios, \( 2:1 \equiv CO:O_2 \). The concentration of \( O_2 \) is followed and the remaining species concentrations are calculated. The effect of temperature on the reaction rate is through an Arrhenius dependence of a reaction rate constant.

• Inlet gas composition, temperature and flow rate are known. Gas properties, viscosity, diffusivity, and thermal conductivity, are updated with changes in temperature, pressure, and reactant concentrations.

• Diffusivity in the porous catalytic layer is calculated using size and void fraction of micropores and macropores. Equimolar counterdiffusion in porous catalytic layer is assumed.

• Either adiabatic or isothermal monolith operating conditions can be selected by the operator. These two operating conditions provide the upper and lower bounds for oxygen conversion for a given inlet gas condition.

• Axial heat conduction in the porous catalytic layer and support is assumed to be negligible. For adiabatic monolith operation, transverse heat conduction the porous catalytic layer and support is assumed to be such that the porous catalytic layer and support temperature is uniform transversely.

• Slab geometry is used for calculation of the species concentration in the porous catalytic layer. A characteristic porous catalytic layer thickness is calculated to account for porous catalytic material in the channel corners.

• Heat and mass transport between the flowing gas and the channel walls are described using the limiting Sherwood (Sh) and Nusselt (Nu) numbers for constant wall concentration and temperature boundary conditions in square channels.

2.2 Model balance equations

The steady state conservation equations for \( O_2 \) in the flowing gas and \( O_2 \) in the porous catalytic layer are

\[
\frac{d\Phi_G}{d\zeta} = - \frac{\gamma}{\Gamma} \left[ \Phi_G - \Phi_W \right], \quad \text{and} \quad \frac{d^2\Psi}{d\lambda^2} = \phi \frac{d^2\Psi}{d\lambda^2},
\]

with initial and boundary conditions,

\[
\Phi_G = 1 \quad \text{at} \quad \zeta = 0 \quad , \quad \Psi = 1 \quad \text{at} \quad \lambda = 0 \quad \text{for all} \quad \zeta \quad , \quad \text{and} \quad \frac{d\Psi}{d\lambda} = 0 \quad \text{at} \quad \lambda = 1.
\]

\( \Phi_G \) is the dimensionless bulk-average \( O_2 \) molar flow rate in the flowing gas. Variables and parameters are defined in detail in the notation list. \( \Phi_W \) is the \( O_2 \) concentration at the channel wall times bulk-average volumetric flow rate divided by the inlet bulk-average \( O_2 \) molar flow rate. \( [\Phi_G - \Phi_W] \) is proportional to the concentration driving force for transport of \( O_2 \) from the flowing gas to the channel wall. \( \zeta \) is the dimensionless distance down the length of the monolith. \( \Psi \) is the dimensionless \( O_2 \) concentration inside the porous catalytic layer at a dimensionless depth \( \lambda \) into the layer. The solution to equation (2) yields an overall \( O_2 \) reaction rate in the porous catalytic layer as a function of \( \Phi_W \). At steady state, this reaction rate is equal to the rate of transport of \( O_2 \) from the flowing gas to the channel wall, and leads to

\[
\Phi_W = \Phi_G \left[ \frac{1}{\alpha + 1} \right].
\]

The steady state energy balance on the flowing gas relates the rise in the dimensionless bulk-average temperature of the flowing gas, \( \theta_G \), to the heat transferred to the gas from the channel wall and yields
where $\theta_G$ is the dimensionless bulk-average temperature of the flowing gas, and $\theta_w$ is the dimensionless temperature at the channel wall. An energy balance on the porous catalytic layer equates the heat generation from the oxygen consumption reaction to the heat transferred from the porous catalytic layer and yields

$$- \left[ \frac{\omega \alpha}{\Gamma} \right] \Phi_w = \left[ \theta_G - \theta_w \right].$$

Combining the two energy balance equations, (7) and (9), and substituting for $\Phi_w$ using equation (6) results in two final differential equations, to be integrated,

$$\frac{d\Phi_G}{d\zeta} = - \left[ \Gamma + \frac{\Gamma}{\alpha \gamma} \right]^{-1} \Phi_G,$$

and

$$\frac{d\theta_G}{d\zeta} = \frac{[d_h S \alpha \omega St]}{[1 + \alpha] \Gamma^2} \Phi_G,$$

with the same initial conditions for $\Phi_G$ and $\theta_G$ as above. Pressure drop for the laminar flow is calculated using the Hagen-Poiseuille equation,

$$\frac{d\phi}{d\zeta} = - \frac{32}{\text{Eu} \text{Re}},$$

with an initial condition of $\phi = 1$ at $\zeta = 0$.

2.3 Model results

The adjustable parameters required to specify the monolith catalyst section operating conditions are listed below in Table 1. They are used to compute the dimensionless parameters $\alpha$, $\omega$, $\Gamma$, $\gamma$, $\text{St}$, $\text{Eu}$, and $\text{Re}$, and to integrate the dimensionless variables in equations (10), (11), and (12). A computer program (see section 5) was written to perform integration using fourth order Runge-Kutta method. The program outputs $\theta_G$, $\theta_w$, $\Phi_G$, $\Phi_w$ and $\phi$ as $\zeta$ varies from zero to the desired dimensionless monolith catalyst section length. The computer program requires readily available parameters to calculate parameters such as mass and heat transfer coefficients, bulk-gas and effective diffusion coefficients, and thermal conductivity. Results for a monolith catalyst section operating under conditions specified in Table 1 are shown in Figs. 3, 4 and 5.

Fig. 3 shows the behavior of $\theta$, $\Phi$, and $\phi$ as $\zeta$ varies from 0 to 100. $\theta_G=\theta_w$ and $\Phi_G=\Phi_w$, therefore $\theta_G$, $\theta_w$, $\Phi_G$, and $\Phi_w$ are not shown individually on this small scale plot. The behavior of $\theta$, $\Phi$, and $\phi$ can be explained using equations (1)-(12), in which all parameters and variables are positive valued. The right side of equation (11) is positive, therefore, $d\theta_G/d\zeta > 0$. The left hand side of equation (9) is negative, therefore, $\theta_w > \theta_G$. Similar examination of equations (10) and (6) results in $d\Phi_G/d\zeta < 0$ and $\Phi_w > \Phi_G$. Equation (12) indicates that $d\phi/d\zeta < 0$. The drop in $\phi$ is negligible for the gas flow rate specified in Table 1. Pressure drop can be significant for higher gas flow rates.

Fig. 4 is an expansion of Fig. 3 in the $\zeta = 45$ to 50 region. The separation between $\theta_G$ and $\theta_w$ is now visible and provides an indication of the thermal driving force between the channel wall and the bulk-gas. Heat produced from the oxidation of CO in the active catalyst layer of the channel wall is transferred from the channel wall to the bulk-gas.

Fig. 5 is also an expansion of Fig. 3 in the $\zeta = 45$ to 50 region. An additional curve, $\Psi(\lambda=1)*\Phi_w$, is the scaled O$_2$ concentration at the centerline of the monolith channel support wall. O$_2$ is consumed in the porous catalytic layer as mass transport to the center of the monolith channel support wall occurs,
Figure 3. Results for Table 1 case. Dimensionless bulk-gas temp ($\theta$), pressure ($\varphi$), and O$_2$ concentration ($\Phi$) vs distance from monoinlet ($\zeta$).

Figure 4. Dimensionless temperatures for Table 1 case.

Figure 5. Dimensionless O$_2$ concentrations for Table 1 case.

Figure 6. Optimum design vs. standard commercial size.
therefore $\Psi(\lambda=1)\Phi_W$ is less than $\Phi_W$ or $\Phi_G$. The separation between the curves indicates the $O_2$ mass transport driving force. The difference between $\Phi_G$ and $\Phi_W$ is an indication of the driving force between the bulk gas and the channel wall. The difference between $\Phi_W$ and $\Psi(\lambda=1)\Phi_W$ is an indication of the driving force between the channel wall and the centerline of the monolith channel support wall.

Table 1: Monolith catalyst section operating parameters

<table>
<thead>
<tr>
<th>Monolith dimension</th>
<th>Catalyst properties</th>
</tr>
</thead>
<tbody>
<tr>
<td>Facial cross sectional area = 1.0e+4 mm$^2$</td>
<td>Void fraction as macropores = 0.25</td>
</tr>
<tr>
<td>Support wall thickness(including active layer) = 1mm</td>
<td>Void fraction as micropores = 0.48</td>
</tr>
<tr>
<td>Active layer thickness = 0.25mm</td>
<td>Macropore radius = 500nm</td>
</tr>
<tr>
<td>Gas inlet properties</td>
<td>Micropore radius = 12nm</td>
</tr>
<tr>
<td>Flowrate = 0.25 liters/sec</td>
<td>Active layer density = 0.5e-3 g/mm$^3$</td>
</tr>
<tr>
<td>Temperature = 300 K</td>
<td>Reaction rate constant = 123.4 mm$^3$/gcat sec</td>
</tr>
<tr>
<td>Pressure = 101.325 kPa</td>
<td>(at 298K)</td>
</tr>
<tr>
<td>Composition 37% CO$_2$, 2% CO, 1% O$_2$, 40% N$_2$, 20% He</td>
<td>Activation energy constant = 39700 J/mol</td>
</tr>
<tr>
<td>Thermal operation is adiabatic.</td>
<td></td>
</tr>
</tbody>
</table>

3. DESIGN STUDY

3.1 Design constraints

A design study for a monolith catalyst section, operating under parameters similar to those listed in Table 1, was performed. For the study, the support wall was assumed to be composed entirely of active catalytic material. Additional constraints, 25% $O_2$ conversion ($\Phi_G[\text{exit}]=0.75$) and a 0.125kPa (=0.5 in H$_2$O) pressure drop across the monolith section, were imposed. The monolith facial cross sectional area and inlet gas conditions (composition, temperature, flow, and pressure) were held constant. Active support wall thickness and channel opening dimensions were varied and the minimum monolith length determined under the imposed constraint conditions.

The rationale for minimizing the monolith length follows from the assertion that the smallest monolith leads to the smallest, lightest and least expensive laser system. In portable laser systems size, weight, and cost considerations are critical. The choice of the shortest monolith section reduces the system weight by reducing the required monolith section housing length. The housing material weight per unit length is typically an order of magnitude more than that of the monolith material. The monolith material can be quite expensive; a smaller system requires less materials and is less costly. The 25% conversion requirement ensures a constant gas temperature rise. A constant pressure drop across the monolith section ensures that an identical amount of energy is expended to circulate the gas through the system. Excluding laser pulse energy, system energy requirements (blower energy and heating and cooling loads) are fixed by the pressure drop and conversion requirements. Constant gas inlet conditions and 25% conversion ensure that a chosen laser PRR can be maintained without exceeding a the maximum allowable laser section inlet $O_2$ concentration.

3.2 Design results

Fig. 6 shows the optimum monolith section design geometry in comparison with a standard monolith design. The optimum monolith length is substantially less than the standard monolith length, whereas the optimum support wall thickness is substantially greater than standard thickness. As the monolith support wall thickness is increased, more catalytic material can be packed into a shorter monolith while conversion and pressure drop constraints are still satisfied. However, a thicker support wall has a larger $O_2$ mass transport resistance. A point is reached where the benefit of having thicker walls is negated by the large $O_2$ mass transport resistance and an optimum monolith length is determined.
4. DISCUSSION

The design study presented above shows that the use of off-the-shelf commercial monolith designs for CO₂ laser applications dramatically increases the overall monolith size required relative to the optimum design presented here. Off-the-shelf monoliths are designed for pollutant emission control and have been optimized for large gas flows and fast reactions at high temperatures. They have relatively thin monolith catalyst section dimensions and high % void volume. The slow reaction rates obtained over laser catalysts allow use of relatively thick monolith wall dimensions. With lower gas flow rates, low % void volume can be used to obtain compact monoliths, thereby reducing the size, weight, and cost of the laser system.

Using a computer program to generate variable and parameter values along the length of the monolith allows for rapid optimization of monolith section under a set of constraints. Use of a computer program also allows for complex channel geometries, such as cylindrical, hexagonal, triangular, etc., to be incorporated into the monolith design.

5. MODEL IMPLEMENTATION USING LASCAT

LASCAT, a computer program based on the monolith catalyst section model presented above, provides a means to design a monolith catalyst section that will satisfy a user specified set of design requirements. LASCAT requires the specification of the parameters listed in Table 1 and a few others. Values of key parameters (Re, CpG, ρₔ, DaB, DaBeff, and mole fractions) are provided at the inlet and exit of the monolith section. FG, T and P are integrated instead of the corresponding nondimensional parameters, ΦG, θG and ϕ. C, T and P values are provided along the length monolith. See Appendix 2, a step by step tutorial, for an example of the LASCAT output.

Appendix 1 gives detailed information on the implementation and compatibility of LASCAT. Appendix 3 details each menu operation of LASCAT. Appendix 4 is a program listing of LASCAT and provides a wealth of information on program structure, variable definitions and units, and physical properties computational methods and references.

6. NOTATION LIST

6.1 Variables and parameters

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>CO oxidation reaction rate constant (mm³ / g-cat s)</td>
</tr>
<tr>
<td>C</td>
<td>concentration of oxygen (mol / mm³)</td>
</tr>
<tr>
<td>CpG</td>
<td>bulk-average gas heat capacity (J / g K)</td>
</tr>
<tr>
<td>DaB</td>
<td>diffusion constant for O₂ in bulk gas mixture (mm² / s)</td>
</tr>
<tr>
<td>DaBeff</td>
<td>effective diffusion constant for oxygen in porous catalytic layer (mm²/s)</td>
</tr>
<tr>
<td>dh</td>
<td>hydraulic diameter of monolith channel, 4(cross sectional area)/(wetted perimeter) (mm)</td>
</tr>
<tr>
<td>Eu</td>
<td>Euler number, Eu = P₀ dh⁴ / ν² ρg</td>
</tr>
<tr>
<td>FG</td>
<td>bulk-average gas molar flow rate of oxygen, FG = CₚG ν (mol / s)</td>
</tr>
<tr>
<td>h</td>
<td>average heat transfer coefficient (W / mm² K)</td>
</tr>
<tr>
<td>ΔHₘ</td>
<td>heat of CO oxidation reaction (J / mol O₂ converted)</td>
</tr>
<tr>
<td>k</td>
<td>bulk-average gas thermal conductivity (J / m K)</td>
</tr>
<tr>
<td>kₘ</td>
<td>average mass transfer coefficient (mm / s)</td>
</tr>
<tr>
<td>Nu₀ ≡</td>
<td>limiting Nusselt number, Nu₀ = h dh / k</td>
</tr>
<tr>
<td>P</td>
<td>pressure in the channel at a position ζ (kPa)</td>
</tr>
<tr>
<td>ϕ</td>
<td>dimensionless pressure at position ζ, ϕ = P / P₀</td>
</tr>
<tr>
<td>Re</td>
<td>Reynolds number, Re = dh ν / ρg / μg dh²</td>
</tr>
<tr>
<td>S</td>
<td>Surface area of the channel wall per unit open volume of monolith channel (mm² / mm³)</td>
</tr>
<tr>
<td>Sh₀ =</td>
<td>limiting Sherwood number, Sh₀ = kₘ dh / DₐB</td>
</tr>
<tr>
<td>St =</td>
<td>Stanton number, St = h dh² / ν₀ ρg CₚG</td>
</tr>
<tr>
<td>tₙ</td>
<td>characteristic thickness of porous catalytic layer (mm)</td>
</tr>
</tbody>
</table>

6.2 Subscripts

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>C,c</td>
<td>in porous catalytic layer</td>
</tr>
<tr>
<td>G,g</td>
<td>in flowing gas</td>
</tr>
<tr>
<td>O,o</td>
<td>at inlet conditions</td>
</tr>
<tr>
<td>W,w</td>
<td>in gas at channel wall</td>
</tr>
</tbody>
</table>
T = temperature (K)
x = distance along the length of the monolith channel (mm)
z = depth into the porous catalytic layer (mm)

Greek

\( \alpha \) = dimensionless rate constant, \( \alpha = \tau_c \rho_c \eta A / k_m \)
\( \gamma \) = dimensionless mass transfer coefficient, \( \gamma = d_h S k_m d_h^2 / \nu_0 \)
\( \Gamma \) = dimensionless volumetric flow rate, \( \Gamma = \nu / \nu_0 \)
\( \omega \) = dimensionless heat of reaction, \( \omega = -\Delta H_{\text{m}} k_m F_G / h T_{G_0} \nu_0 \)
\( \zeta \) = dimensionless distance along the length of the monolith channel, \( \zeta = x / d_h \)
\( \eta \) = effectiveness factor of the reaction in the monolith porous catalytic layer, \( \eta = \tanh (\varphi) / \varphi \)
\( \theta \) = dimensionless bulk gas temperature, \( \theta_G = T_G / T_{G_0}, \theta_W = T_W / T_{G_0} \)
\( \lambda \) = dimensionless depth into the porous catalytic layer, \( \lambda = z / t_c \)
\( \mu_g \) = viscosity of gas in channel (Pa·s)
\( \rho_c \) = density of porous catalytic layer material (g-cat / mm³)
\( \rho_g \) = density of flowing gas (g / mm³)
\( \nu \) = volumetric flow rate of flowing gas (mm³ / s)
\( \Phi_G \) = dimensionless bulk-average oxygen concentration in flowing gas, \( \Phi_G = F_G / F_{G_0} \)
\( \Phi_W \) = dimensionless channel wall surface oxygen concentration, \( \Phi_W = [C_w(\zeta) \nu(\zeta)] / F_{G_0} \)
\( \varphi \) = Thiele modulus, \( \varphi^2 = [\tau_c^2 \rho_c \eta A] / D_{\text{Aeff}} \)
\( \Psi \) = dimensionless O₂ concentration in the porous catalytic layer. \( \Psi(\lambda) = [C_G(\lambda) / C_w(\zeta)] \)

7. REFERENCES

Appendix 1: Program Implementation and Compatibility

The LASCAT program is written in the FORTRAN programming language and is compatible with FORTRAN 77 standards. Detailed implementation instructions are provided below for Apple Macintosh and Digital Equipment Corporation VAX computers. Familiarity with the particular operating system is assumed.

**Computer: Apple Macintosh SE or II**
Operating System: Apple System Version 6.0
Application Program: Absoft's MacFortran/020 Version 2.3
Compilation Options (Macintosh SE):
- Use compilation options B (Compile Using Long Addresses), E (Generate Errors List), and U (* = Unit 9).

Compilation Options (Macintosh II):
- Use compilation options B (Compile Using Long Addresses), E (Generate Errors List), M (68020/68030 instructions), P (68881/68882 instructions), and U (* = Unit 9).

Compilation and Execution:
- Place the LASCAT program in the **same folder** as the MacFortran/020 application and supporting files.
- Double click on MacFortran/020 application to launch the MacFortran/020 application.
- From the File Menu choose the "Select File" option. Select File LASCAT.
- From the Compile Menu choose the "Options" option and verify the compilation options selected are identical to the compilation options described above. If the options selected need to be changed, remember to save the new set of compilation options by clicking on the "Save" box. Exit the compilation options section by clicking on the "OK" box.
- From the Compile Menu choose the " Compile and Execute" option. The program will be compiled and executed. The output file, LDATA, and any selectable parameter files will be placed in the same folder as the LASCAT and MacFortran/020 files.

**Computer: Digital Equipment Corporation VAX 11/780**
Operating System: VAX/VMS Version 4.6
Application Program: VAX FORTRAN V4.8-276
Compilation and Execution:
- Rename the LASCAT program LASCAT.for
- To compile LASCAT.for, type for LASCAT.for
- To link LASCAT.for type link LASCAT
- To execute LASCAT.for type run LASCAT
- The output file, LDATA.DAT, and any selectable parameter files will be placed in the your directory. Use an editing program to examine files.
Appendix 2: LASCAT Tutorial

The LASCAT Tutorial provides a step by step example of the use of the program LASCAT. Required user input and comments are detailed on the left margin and the corresponding screen outputs are indented. Input(s) required by the operator are boldfaced. The example shown below was run on a Macintosh II using Absoft's MacFortran/020 Version 2.3 (Review the Program Implementation and Compatibility section for program compilation and execution details.). This tutorial will be of the greatest benefit if used while actually executing the program.

Compile and execute LASCAT application program.

"""
PROGRAM LASCAT ******
***
*****
The purpose of this program is to calculate the gas concentration and temperature profiles of a monolith catalyst section of a CO2 laser. The CO2 decomposes when the laser is pulsed. The CO and O2 produced as a result of pulsing are detrimental to the efficient operation of the laser. The recombination reaction is CO + 1/2 O2 -> CO. This program provides the means to model the performance of a monolith catalyst section under various gas compositions, temperatures, catalyst activities, gas flowrates, oxygen conversion, monolith face and length dimensions. Results can indicate if constraints such as conversion, maximum gas temperature, monolith weight are satisfied and how the system parameters may be altered to meet these constraints. Parameters and options may be altered to taylor the monolith design. Default values can also be used as a starting point for the design process. A review of the parameters and options chosen may be made prior to execution of the computational portion of the program.

(HIT RETURN TO CONTINUE)
""

A program introductory statement is presented. Type RETURN (key) after reading.

LASCAT Main Menu

1) Read in new operating parameters
2) Show current operating parameters
3) Change operating parameters
4) Run program
5) Exit program

Type in number corresponding to choice above.

The LASCAT Main Menu is presented. The main menu provides different options (1-5). Specific details for each option are provided in the Menu Description section. To choose one of these options, simply type in the desired number, then RETURN. For this example, type 2 and RETURN.

SELECTABLE PARAMETER SUMMARY
Monolith Dimensions(mm):
Support wall thickness: 1.00 Face dimension: 100.00 x 100.00
Channel inner dimension: 4.00  No. Face channels: 20.00 x 20.00  
Active layer thickness: .25  % monol. volume open: 64.0

Monolith inlet parameters:  
Gas Composition (mole fraction):  
CO2: .3700  CO: .0200  O2: .0100  
N2: .4000  He: .2000  Ar: 0.0000  
Gas Flow rate (liters/s): .250  Gas Temperature (K): 300.00  
Inlet Gas Pressure (kPa): 101.325

Catalyst Properties:  
Catalyst Density (g/mm^3): 0.500E-03  
Reaction rate constant at 298K (mm^3/gcat-s): 123.40  
Activation energy (J/mol): 39700.00  
Void-fraction as micropores: .24  Void-fraction as macropores: .48  
Average micropore radius (nm): .12E+02  Average macropore radius (nm): .50E+03  
Thermal Operation (adiabatic/isothermal): Adiabatic

Computational loop parameters:  
Output file (Full Profile/Summary): Full Profile  
Termination on (O2 conversion/Length): O2 conversion, %: 2.500  
Computation loop step size (mm): .5556  Display every 5.00 mm

==> Hit Return when finished viewing <==

The selectable parameter summary lists the parameter values that will be used in the computational portion of the program. When the program is initially run, default parameter values are assigned. As we'll see later, the values of the parameters can be changed. Hopefully, a review of the parameter summary above will hint to the meaning of each parameter. The use of each parameter is detailed in the Menu Description section. Let's assume the present values are satisfactory and proceed. Type RETURN.

LASCAT Main Menu

1) Read in new operating parameters  
2) Show current operating parameters  
3) Change operating parameters  
4) Run program  
5) Exit program

Type in number corresponding to choice above.

We have returned to the main menu. To save space, the main menu will listing will be abbreviated as "LASCAT Main Menu....". To run the computational portion of the program using the current parameter set listed in the selectable parameter summary type 4 and RETURN. Note: the program will alert you that it has completed computations by beeping three times.

*****SEE FILE LDATA FOR RESULTS*****

Initial values
Reynolds number = 9.880  
Gas Heat Capacity (J/K-g) = 1.797  
Gas Density (g/cm^3) = .0011817  
Gas Velocity (mm/s) = 39.063  
Effectiveness factor = .99969  
Bulk Gas Diffusivity (cm^2/s) = .22540
The information above provides initial and final values of important parameters along with values of key parameters along the length of the monolith. The units for each parameter are specified. A few minutes spent in reviewing the trend of each parameter, either initial vs. final or along the length of the monolith, is well worth the time. For example, the gas heat capacity increases from 1.797 to 1.799 due to the change in gas composition and the change in gas temperature. The gas temperature rises from 300.000 to 302.605 due to the exothermic nature of the reaction CO + 1/2O₂ -> CO₂. Type RETURN.

LASCAT Main Menu....

To change the value of a parameter or parameters, type 3 and RETURN.

Parameter Modification Menu

1) Change monolith physical dimensions
2) Change inlet gas composition
3) Change inlet gas volumetric flow rate
4) Change inlet gas temperature
5) Change inlet gas pressure
6) Change catalyst activation energy
You have entered the Parameter Modification Menu. The Parameter Modification Menu gives a number of options (1-18). The parameters are detailed in the Program Operations section. The Parameter Modification Menu will be abbreviated "Parameter Modification Menu....". Let's change the termination variable (option 12). Type 12 and RETURN.

Integration can be stopped by either specifying an amount of O2 conversion (O), or by specifying a monolith length (L).

Currently, integration will be stopped by specifying an amount of O2 conversion (O).

Type the letter O or the letter L. Hit return.

The letter L is for program computation section termination on monolith length. The letter O is for termination on O2 conversion and requires a conversion length specification. Type L and RETURN.

Current desired monolith length = 5.000 (mm)

Input desired monolith length (5 - 4000mm)

The current restriction on the desired monolith termination length is given. The restrictions presented must be followed. Attempts have been made to prevent out of bounds values from being input, however "nothing is perfect". Try entering 2 (this shorter than the minimum 5mm). The program will force a proper input. Type 100 and RETURN.

Parameter Modification Menu....

Let's see what has been changed. Type 14 and RETURN.

SELECTABLE PARAMETER SUMMARY
Monolith Dimensions (mm):
  Support wall thickness: 1.00  Face dimension: 100.00 x 100.00
  Channel inner dimension: 4.00  No. Face channels: 20.00 x 20.00
  Active layer thickness: .25  % monol. volume open: 64.0

Monolith inlet parameters:
Gas Composition (mole fraction): 
- CO₂: 0.3700 
- CO: 0.0200 
- O₂: 0.0100 
- N₂: 0.4000 
- He: 0.2000 
- Ar: 0.0000

Gas Flow rate (liters/s): 0.250 
Gas Temperature (K): 300.00 
Inlet Gas Pressure (kPa): 101.325

Catalyst Properties: 
- Catalyst Density (g/mm³): 0.500E-03 
- Reaction rate constant at 298K (mm³/g·cat·s): 123.40 
- Activation energy (J/mol): 39700.00 
- Void-fraction as micropores: 0.24 
- Void-fraction as macropores: 0.48 
- Avg. micropore radius (nm): 1.2E+02 
- Avg. macropore radius (nm): 5.0E+03 
- Thermal Operation (adiabatic/isothermal): Adiabatic

Computational loop parameters: 
- Change ==> Termination on (O₂ conversion/Length): Length. Length (mm): 100.000 
- Computation loop step size (mm): 0.5556 Display every 5.00 mm

===> Hit Return when finished viewing <==

Type RETURN. To avoid changing from the default parameter values to frequently used values, a parameter set can be saved to a file. These files can be read from at a later time. Type 15 and RETURN.

Would you like to save the current operating parameters to a New(N) or Existing(E) file?

We're creating a new file. Type N and RETURN.

What's the name of the NEW parameter file to be opened?

Name this file CATONE (abbreviation for CATALYST-ONE). Type CATONE and RETURN.

Parameter Modification Menu....

Using the revised parameter set, run the computational portion of the program by typing 16 and RETURN.

*****SEE FILE LDATA FOR RESULTS*****

Initial values
- Reynolds number = 9.880
- Gas Heat Capacity (J/K·g) = 1.797
- Gas Density (g/cm³) = 0.0011817
- Gas Velocity (mm/s) = 39.063
- Effectiveness factor = 0.99969
- Bulk Gas Diffusivity (cm²/s) = 0.22540
- Effective Diffusivity (cm²/s) = 0.053407
- Step size (mm) = 0.555556

Distance % Conversion O₂ Gas O₂ Wall O₂ Center Tgas Twall DPress (mm) <== (mMOL/L) ==> (Kelvin) (Kelvin) (kPa)
0.000 0.0000 0.4065 0.4060 0.4058 300.000 300.179 -0.000E+00
Final values
Mole fractions:
- \( \text{He} = 0.2001 \)
- \( \text{Ar} = 0.0000 \)
- \( \text{CO}_2 = 0.3712 \)
- \( \text{CO} = 0.0190 \)
- \( \text{O}_2 = 0.0095 \)
- \( \text{N}_2 = 0.4002 \)

Gas Pressure (kPa): 101.325
Reynolds number = 9.753
Gas Heat Capacity \((\text{J/K-g})\) = 1.800
Gas Density \((\text{g/cm}^3)\) = 0.0011624
Gas Velocity \((\text{mm/s})\) = 39.693
Effectiveness factor = 0.99961
Bulk Gas Diffusivity \((\text{cm}^2/\text{s})\) = 0.23125
Effective Diffusivity \((\text{cm}^2/\text{s})\) = 0.054566
Step size \((\text{mm})\) = 0.55556

--- Hit Return when finished viewing ---

In addition to the screen output the selectable parameter summary and the section above are written to file LDATA (Macintosh) or LDATA.DAT (VAX). (For Macintosh only: Any additional "runs" in this session will be tacked on to the end of LDATA. If the program is terminated and rerun the old LDATA file will be erased and a new LDATA file started. If you desire to keep the information in LDATA, rename LDATA prior to running LASCAT again.) Type RETURN.

LASCAT Main Menu....

After each computational run, you are returned to the main menu. Let's change another parameter. Type 3 and RETURN.

Parameter Modification Menu....

To change the inlet gas volumetric flow rate, type 3 and RETURN.

Current inlet volumetric flow rate = 0.250 \((\text{l/s})\)
Input monolith inlet volumetric flow rate

The desired flowrate is 2.5 liters/sec. Type 2.5 and RETURN.

Parameter Modification Menu....

Let's examine the change to the parameter set. Type 14 and RETURN.

SELECTABLE PARAMETER SUMMARY
Monolith Dimensions(mm):
Support wall thickness: 1.00  Face dimension: 100.00 x 100.00
Channel inner dimension: 4.00  No. Face channels: 20.00 x 20.00
Active layer thickness: .25  % monol.volume open : 64.0

Monolith inlet parameters:
Gas Composition (mole fraction): CO2: .3700  CO: .0200  O2: .0100
N2: .4000  He: .2000  Ar: 0.0000
Gas Flow rate(liters/s): 2.500  Gas Temperature(K): 300.00
Inlet Gas Pressure (kPa): 101.325

Catalyst Properties:
Catalyst Density (g/mm^3): 0.500E-03
Reaction rate constant at 298K(mm^3 /gcat-s): 123.40
Activation energy(J/mol): 39700.00
Void-fraction as micropores: .24  Void-fraction as macropores: .48
Avg. micropore radius (nm): .12E+02  Avg. macropore radius (nm): .50E+03
Thermal Operation (adiabatic/isothermal): Adiabatic

Computational loop parameters:
Output file (Full Profile/Summary): Full Profile
Termination on (O2 conversion/Length): Length.  Length(mm): 100.000
Computation loop step size(mm): 5.0000  Display every 5.00 mm

==> Hit Return when finished viewing <==

Type RETURN.

Parameter Modification Menu....

Run computational portion of the program by typing 16 and RETURN

*****SEE FILE LDATA FOR RESULTS*****
Initial values
Reynolds number = 98.802
Gas Heat Capacity (J/K-g) = 1.797
Gas Density (g/cm^3) = .0011817
Gas Velocity (mm/s) = 390.625
Effectiveness factor = .99969
Bulk Gas Diffusivity(cm^2/s)= .22540
Effective Diffusivity(cm^2/s)= .053407
Step size(mm) = 5.000000

Distance  %Conver  O2gas  O2wall  O2center  Tgas  Twall  DPress
(mm)  <=(mMOL/L)===>  (Kelvin)  (Kelvin)  (kPa)
.000  .0000  .4065  .4060  .4058  300.000  300.179  -0.000E+00
5.000  .0156  .4064  .4059  .4057  300.024  300.203  -0.730E-04
10.000  .0391  .4062  .4058  .4056  300.047  300.227  -0.146E-03
15.000  .0624  .4061  .4057  .4055  300.071  300.250  -0.219E-03
20.000  .0855  .4060  .4055  .4054  300.095  300.274  -0.292E-03
25.000  .1086  .4059  .4054  .4052  300.119  300.298  -0.365E-03
30.000  .1317  .4057  .4053  .4051  300.142  300.322  -0.438E-03
35.000  .1549  .4056  .4052  .4050  300.166  300.346  -0.511E-03
40.000  .1781  .4055  .4050  .4049  300.190  300.370  -0.584E-03
45.000  .2013  .4054  .4049  .4047  300.214  300.394  -0.657E-03
50.000  .2245  .4052  .4048  .4046  300.238  300.418  -0.730E-03
55.000  .2478  .4051  .4047  .4045  300.261  300.442  -0.803E-03
60.000  .2711  .4050  .4045  .4043  300.285  300.466  -0.877E-03
65.000  .2944  .4049  .4044  .4042  300.309  300.490  -0.950E-03
70.000  .3177  .4047  .4043  .4041  300.333  300.514  -0.102E-02
75.000  .3411  .4046  .4041  .4040  300.357  300.538  -0.110E-02
80.000  .3644  .4045  .4040  .4038  300.381  300.562  -0.117E-02
85.000  .3879  .4043  .4039  .4037  300.405  300.587  -0.124E-02
90.000  .4113  .4042  .4038  .4036  300.429  300.611  -0.132E-02
95.000  .4347  .4041  .4036  .4034  300.453  300.635  -0.139E-02
100.000  .4582  .4040  .4035  .4033  300.477  300.659  -0.146E-02

=> Hit Return to Return to Main Menu <=

Notice that the program computation terminated when the monolith length reached 100 mm,
whereas, previously, the termination condition was an oxygen conversion of 2.5 %. Type RETURN.

LASCAT Main Menu....

The parameter set has been changed from the CATONE set. Let's return to the CATONE parameter
set by reading in the CATONE set file. Type 1 and RETURN.

Read in data from existing parameter file?(Y/N)

Type Y and RETURN.

What is the name of the existing parameter file to be opened?

Type CATONE and RETURN (Note that the required file name to be inputted may be lower
/upper case sensitive).

LASCAT Main Menu....

Let's review the parameter set. Type 2 and RETURN.

SELECTABLE PARAMETER SUMMARY

Monolith Dimensions(mm):
Support wall thickness: 1.00  Face dimension: 100.00 x 100.00
Channel inner dimension: 4.00  No.Face channels: 20.00 x 20.00
Active layer thickness: .25  % monol.volume open : 64.0

Monolith inlet parameters:
Gas Composition (mole fraction): CO2: .3700 CO: .0200 O2: .0100
N2: .4000 He: .2000 Ar: 0.0000
Gas Flow rate(liters/s): .250 Gas Temperature(K): 300.00
Inlet Gas Pressure (kPa): 101.325

Catalyst Properties:
- Catalyst Density (g/mm^3): 0.500E-03
- Reaction rate constant at 298K(mm^3/gcat-s): 123.40
- Activation energy(J/mol): 39700.00
- Void-fraction as micropores: .24
- Void-fraction as macropores: .48
- Avg. micropore radius (nm): .12E+02
- Avg. macropore radius (nm): .50E+03
- Thermal Operation (adiabatic/isothermal): Adiabatic

Computational loop parameters:
- Output file (Full Profile/Summary): Full Profile
- Termination on (O2 conversion/Length): Length. Length(mm): 100.000
- Computation loop step size(mm): .5556 Display every 5.00 mm

Type RETURN.

LASCAT Main Menu....

Let’s explore the use of some other parameters. Type 3 and RETURN.

Parameter Modification Menu....

Type 11 and RETURN.

Full concentration and temperature profile (P) or summary (S)?
Type the letter P or the letter S. HIT RETURN.

Choose summary by typing S and RETURN.

Parameter Modification Menu....

Type 16 and RETURN.

*****SEE FILE LDATA FOR RESULTS*****

Initial values
- Reynolds number = 9.880
- Gas Heat Capacity (J/K-g) = 1.797
- Gas Density (g/cm^3) = 0.0011817
- Gas Velocity (mm/s) = 39.063
- Effectivness factor = .99969
- Bulk Gas Diffusivity(cm^2/s)=.22540
- Effective Diffusivity(cm^2/s)=.053407
- Step size(mm) = .555600

<table>
<thead>
<tr>
<th>Distance (mm)</th>
<th>%Conver</th>
<th>O2gas</th>
<th>O2wall</th>
<th>O2center</th>
<th>Tgas</th>
<th>Twall</th>
<th>DPress (kPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>.000</td>
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<td>.4065</td>
<td>.4060</td>
<td>.4058</td>
<td>300.00</td>
<td>300.179</td>
<td>-0.000E+00</td>
</tr>
<tr>
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<td>5.0878</td>
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<td>.3787</td>
<td>.3785</td>
<td>305.180</td>
<td>305.395</td>
<td>-0.148E-03</td>
</tr>
</tbody>
</table>
Final values
Mole fractions:
He = .2001 Ar = 0.0000 CO2 = .3712
CO = .0190 O2 = .0095 N2 = .4002
Gas Pressure (kPa): 101.325
Reynolds number = 9.753
Gas Heat Capacity (J/K-g) = 1.800
Gas Density (g/cm^3) = .0011624
Gas Velocity (mm/s) = 39.693
Effectivness factor = .99961
Bulk Gas Diffusivity(cm^2/s)= .23125
Effective Diffusivity(cm^2/s)= .054566
Step size(mm) = .555600

==> Hit Return to Return to Main Menu <==

The key parameters along the length of the monolith are presented for the initial and final (termination condition met) monolith distances. The file LDATA also has this summary form. Type RETURN.

LASCAT Main Menu....

Please feel free to play around with the program. To exit the program by type 5 and RETURN. Take a look at files, LDATA and CATONE. A listing of both files is given below. The table entries are separated by tab characters for further processing by programs such as Cricket Graph and Excel (these are both Macintosh programs). Adjusting the tabs to 1 space may help to align the table.

_file LDATA

SELECTABLE PARAMETER SUMMARY
Monolith Dimensions(mm):
Support wall thickness: 1.00 Face dimension: 100.00 x 100.00
Channel inner dimension: 4.00 No.Face channels: 20.00 x 20.00
Active layer thickness: .25 % monol.volume open : 64.0
Monolith inlet parameters:
Gas Composition (mole fraction): CO2: .3700 CO: .0200 O2: .0100
N2: .4000 He: .2000 Ar: 0.0000
Gas Flowrate(liters/s): .250 Gas Temperature(K): 300.00
Inlet Gas Pressure (kPa): 101.325
Catalyst Properties:
Catalyst Density (g/mm^3): 0.500E-03
Reaction rate constant at 298K(mm^3 /gcat-s): 123.40
Activation energy(J/mol): 39700.00
Void-fraction as micropores: .24 Void-fraction as macropores: .48
Avg. micropore radius (nm): .12E+02 Avg. macropore radius (nm): .50E+03
Thermal Operation (adiabatic/isothermal): Adiabatic
Computational loop parameters:
Output file (Full Profile/Summary): Full Profile
Termination on (O2 conversion/length): O2 conversion. %: 2.500
Computation loop step size(mm): .5556 Display every 5.00 mm

Initial values
Reynolds number = 9.880
Gas Heat Capacity (J/K-g) = 1.797
Gas Density (g/cm^3) = .0011817
Gas Velocity (mm/s) = 39.063
Effectivness factor = .99969
Bulk Gas Diffusivity(cm^2/s)=.22540
Effective Diffusivity (cm^2/s) = 0.053407
Step size (mm) = 0.55556

<table>
<thead>
<tr>
<th>Distance (mm)</th>
<th>%Conv</th>
<th>O2gas</th>
<th>O2wall</th>
<th>O2center</th>
<th>Tgas (Kelvin)</th>
<th>Twall (Kelvin)</th>
<th>DPRESS (kPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.000</td>
<td>0.000</td>
<td>0.4065</td>
<td>0.4058</td>
<td></td>
<td>300.00</td>
<td>300.179</td>
<td>-0.000E+00</td>
</tr>
<tr>
<td>5.000</td>
<td>0.2239</td>
<td>0.4052</td>
<td>0.4046</td>
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<td>300.236</td>
<td>300.416</td>
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<td>0.4033</td>
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<tr>
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<td>0.3955</td>
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<td>0.3920</td>
<td></td>
<td>302.605</td>
<td>302.801</td>
<td>-0.776E-04</td>
</tr>
</tbody>
</table>

Final values

Mole fractions:
- He = 0.2000
- Ar = 0.0000
- CO = 0.3706
- CO2 = 0.0200
- O2 = 0.0100
- N2 = 0.4000
- He = 0.2000
- Ar = 0.0000

Gas Pressure (kPa): 101.325
Reynolds number = 9.817
Gas Heat Capacity (J/K-g) = 1.799
Gas Density (g/cm^3) = 0.0011720
Gas Velocity (mm/s) = 39.378
Effectiveness factor = 0.99965
Bulk Gas Diffusivity (cm^2/s) = 0.22832
Effective Diffusivity (cm^2/s) = 0.053988
Step size (mm) = 0.55556

SELECTABLE PARAMETER SUMMARY

Monolith Dimensions (mm):
- Support wall thickness: 1.00
- Face dimension: 100.00 x 100.00
- Channel inner dimension: 4.00
- No. Face channels: 20.00 x 20.00
- Active layer thickness: 0.25
- % monol. volume open: 64.0

Monolith inlet parameters:
- Gas Composition (mole fraction): CO2 = 0.3700, CO = 0.0200, O2 = 0.0100, N2 = 0.4000, He = 0.2000, Ar = 0.0000
- Gas Flowrate (liters/s): 0.250
- Gas Temperature (K): 300.00
- Inlet Gas Pressure (kPa): 101.325

Catalyst Properties:
- Catalyst Density (g/mm^3): 0.500E-03
- Reaction rate constant at 298K (mm^3/gcat-s): 123.40
- Activation energy (J/mol): 39700.00
- Void fraction as micropores: 0.24
- Void fraction as macropores: 0.48
- Avg. micropore radius (nm): 0.12E+02
- Avg. macropore radius (nm): 0.50E+03

Thermal Operation (adiabatic/isothermal): Adiabatic

Computational loop parameters:
- Output file (Full Profile/Summary): Full Profile
- Termination on (O2 conversion/Length): Length = 100.000
- Computation loop step size (mm): 0.5556
- Display every 5.00 mm

Initial values

- Reynolds number = 9.880
- Gas Heat Capacity (J/K-g) = 1.797
- Gas Density (g/cm^3) = 0.0011817
- Gas Velocity (mm/s) = 39.063
- Effectiveness factor = 0.99969
- Bulk Gas Diffusivity (cm^2/s) = 0.22540
- Effective Diffusivity (cm^2/s) = 0.053407
- Step size (mm) = 0.55556
<table>
<thead>
<tr>
<th>Distance (mm)</th>
<th>%Conv</th>
<th>O2gas</th>
<th>O2wall</th>
<th>O2center</th>
<th>Tgas (Kelvin)</th>
<th>Twall (Kelvin)</th>
<th>DPress (kPa)</th>
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<td>20.000</td>
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Final values
Mole fractions:
- He = 0.2001
- Ar = 0.0000
- CO2 = 0.3712
- CO = 0.0190
- O2 = 0.0095
- N2 = 0.4002

Gas Pressure (kPa): 101.325
Reynolds number = 9.753
Gas Heat Capacity (J/K-g) = 1.800
Gas Density (g/cm³) = 0.0011624
Gas Velocity (mm/s) = 39.693
Effectiveness factor = 0.99961
Bulk Gas Diffusivity (cm²/s) = 0.23125
Effective Diffusivity (cm²/s) = 0.054566
Step size (mm) = 0.55556

SELECTABLE PARAMETER SUMMARY
Monolith Dimensions (mm):
- Support wall thickness: 1.00
- Face dimension: 100.00 x 100.00
- Channel inner dimension: 4.00 x 200.00
- Active layer thickness: 0.25
- % monol. volume open: 64.0

Monolith inlet parameters:
- Gas Composition (mole fraction):
  - CO2: 0.3700
  - CO: 0.0200
  - O2: 0.0100
  - N2: 0.4000
  - He: 0.0000
- Gas Flowrate (liters/s): 2.500
- Gas Temperature (K): 300.00
- Inlet Gas Pressure (kPa): 101.325
- Catalyst Properties:
  - Catalyst Density (g/mm³): 0.500E-03
  - Reaction rate constant at 298K (mm³/g-cat-s): 123.40
  - Activation energy (J/mol): 39700.00
  - Void-fraction as micropores: 0.24
  - Void-fraction as macropores: 0.48
  - Avg. micropore radius (nm): 0.12E+02
  - Avg. macropore radius (nm): 0.50E+03
- Thermal Operation (adiabatic/isothermal): Adiabatic

Computational loop parameters:
- Output file (Full Profile/Summary): Full Profile
- Termination on (O2 conversion/Length): Length
- Length (mm): 100.000
- Computation loop step size (mm): 5.0000
- Display every 5.00 mm

Initial values
- Reynolds number = 98.802
- Gas Heat Capacity (J/K-g) = 1.797
- Gas Density (g/cm³) = 0.0011817
Gas Velocity (mm/s) = 390.625
Effectivness factor = .99969
Bulk Gas Diffusivity(cm²/s) = .22540
Effective Diffusivity(cm²/s) = .053407
Step size(mm) = 5.000000

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Final values
Mole fractions:
- He = .2000  Ar = 0.0000  CO2 = .3701  CO = .0199  O2 = .0100  N2 = .4000
Gas Pressure (kPa): 101.324
Reynolds number = 98.705
Gas Heat Capacity (J/K-g) = 1.798
Gas Density (g/cm³) = 1.011800
Gas Velocity (mm/s) = 391.188
Effectivness factor = .99969
Bulk Gas Diffusivity(cm²/s) = .22540
Effective Diffusivity(cm²/s) = .053407
Step size(mm) = 5.000000

SELECTABLE PARAMETER SUMMARY
Monolith Dimensions(mm):
- Support wall thickness: 1.00  Face dimension: 100.00 x 100.00
Channel inner dimension: 4.00  No. Face channels: 20.00 x 20.00
Active layer thickness: 0.25  % monol.volume open : 64.0
Monolith inlet parameters:
- Gas Composition (mole fraction): CO2: .3700  CO: .0200  O2: .0100  N2: .4000  He: .2000  Ar: 0.0000
Gas Flowrate(liers/s): .250  Gas Temperature(K): 300.00
Inlet Gas Pressure (kPa): 101.325
Catalyst Properties:
- Catalyst Density (g/mm³): 0.500E+03
- Reaction rate constant at 298K(mm³/gcat-s): 123.40
- Activation energy(J/mol): 39700.00
Void-fraction as micropores: .24  Void-fraction as macro pores: .48
Avg. micropore radius (nm): .12E+03  Avg. macropore radius (nm): .50E+03
Thermal Operation (adiabatic/isothermal): Adiabatic
Computational loop parameters:
- Output file (Full Profile/Summary): Summary
- Termination on (O2 conversion/Length): Length  Length(mm): 100.000
Computation loop step size (mm): .5556

Initial values
Reynolds number = 9.880
Gas Heat Capacity (J/K-g) = 1.797
Gas Density (g/cm³) = .0011817
Gas Velocity (mm/s) = 39.063
Effectiveness factor = .99969
Bulk Gas Diffusivity (cm²/s) = .22540
Effective Diffusivity (cm²/s) = .053407
Step size (mm) = .555600

Distance %Conv O₂gas O₂wall O₂center Tgas Twall DPress
(mm) <===(mMOL/L)===> (Kelvin) (Kelvin) (kPa)
0.000 0.000 .4065 .4060 .4058 300.000 300.179 -0.000E+00
100.008 5.0878 .3792 .3787 .3785 305.180 305.395 -0.148E-03

Final values
Mole fractions:
He = .201 Ar = 0.0000 CO₂ = .3712
CO = .0190 O₂ = .0095 N₂ = .4002
Gas Pressure (kPa): 101.325
Reynolds number = 9.753
Gas Heat Capacity (J/K-g) = 1.800
Gas Density (g/cm³) = .0011624
Gas Velocity (mm/s) = 39.693
Effectiveness factor = .99961
Bulk Gas Diffusivity (cm²/s) = .23125
Effective Diffusivity (cm²/s) = .054566
Step size (mm) = .555600

File CATONE. See if you can pick out some of the parameters listed below. The program listing will show the structure of the parameter file.
Appendix 3: Menu Description

LASCAT Main Menu

The LASCAT Main Menu section provides detailed instructions on the use of the main menu. It is assumed that the LASCAT Tutorial has been reviewed. The LASCAT Main Menu is first encountered upon program execution and has five options available. Each option is detailed below. To select an option type the desired choice (1-5) and then RETURN (key). A number other than 1-5 will cause an input requirement message to appear and another chance to enter 1-5 is made available.

Option 1 - Read in new operating parameters:
If you have a file containing a selectable parameter set that you want to use, choose this option. This file would have been previously generated by saving the parameter set using option 15 of the parameter modification menu. You will first be queried whether the file is New (N) or Existing (E). If you indicate that the file is existing, you will be queried for the file name. Some systems are sensitive to upper and lowercase differences in file names. After specifying the filename, you are returned to the main menu. If you indicate that the file is new, default file parameters are assigned.

Option 2 - Show current operating parameters:
This option lists the current selectable parameter set. Use this option to verify the proper selectable parameter set prior to execution of the program. After parameter set review, you are returned to the main menu.

Option 3 - Change operating parameters:
This option leads to the parameter modification menu described below. The options similar to main menu options 1-5 are available in the parameter modification menu. You can return to the main menu from the parameter modification menu.

Option 4 - Run program:
The Run program option executes the computational portion of the program, using the current selectable parameter set. Results obtained are output to the screen for review and to the file LDATA for further processing or review. Any additional "runs" in the session will be tacked onto the end of file LDATA. (Macintosh only: If the program is terminated and run the old LDATA file will be erased and a new LDATA file started. If you desire to keep the information in contained in LDATA, rename LDATA prior to running LASCAT again.) After computations are completed or a termination condition is met, the program returns to the main menu.

Option 5 - Exit program:
The program is exited. If using the Macintosh remember the caution concerning LDATA, as noted above in the Option 4 section.

LASCAT Parameter Modification Menu

The LASCAT parameter modification menu section provides detailed instructions on the use of the parameter modification menu. It is assumed that the LASCAT Tutorial has been reviewed. The LASCAT parameter modification menu is encountered when option 3 of the main menu is chosen and has eighteen options available. Each option is detailed below. To select an option type the desired choice (1-18) and then RETURN. A number other than 1-18 will cause an input requirement message to appear and another chance to enter 1-18 is made available. The default file parameter set is the parameter set is instituted at the start of the program.
Option 1 - Change monolith physical dimensions:
A number of physical dimensions (see diagram below) are queried for in this section. A description of each dimension and the associated restrictions are listed. Values that represent a valid physical situation and meet the listed restrictions should not cause any problems. A number of constraint for given below. The program assumes monolith channels are square. Remember that the system under study can be scaled up or down. For instance, a monolith with an inlet gas flow rate of 1 liters/sec and a face (H x V) of 100 x 100 mm can be scaled up to an inlet gas flow rate of 4 liters/sec and a face of 200 x 200 mm. The other dimensions (H, W, and A) are held the same.

- Monolith horizontal face dimension (mm), H, \( 10 \leq H \leq 1000 \)
- Monolith vertical face dimension (mm), V, \( 10 \leq V \leq 1000 \)
- Monolith channel wall thickness (mm), T, \( T \leq H, T \leq V \)
- Monolith channel opening dimension (mm), W, \( W \leq H, W \leq V \)
- Monolith active layer thickness (mm), A, \( A \leq W/2 \)

Default file dimension values (mm) are \( H=V=100.0, T=0.50, W=4.00, \) and \( A=0.25 \) mm. Monoliths with square channels but with circular, oval, etc., shaped faces can be modelled. For these nonstandard shapes, determine the dimensions (H x V) of a square faced monolith that has an equivalent facial area and use the calculated H and V in the program.

Option 2 - Change inlet gas composition:
The program allows for the laser operating gas to contain He, Ar, CO₂, O₂, CO, and N₂ gases. The species mole fraction is defined as the mole percent divided by 100. For example, 10 mole% N₂ corresponds to a mole fraction of 0.10. Each mole fraction must be between 0 and 1. Mole fractions for He, Ar, CO₂, O₂ are queried for when this option is chosen. Stoichiometric ratios of O₂:CO (1:2) are assumed; the input mole fraction of O₂ is used to calculate the CO mole fraction. The mole fraction of O₂ is limited to 0.03 (3%). The sum of the mole fractions must add up to 1; N₂ mole fraction is calculated using the mole fractions of the other species. The default file values for mole fractions are \( \text{He}=0.20, \text{Ar}=0.0, \text{CO}_2=0.37, \text{O}_2=0.01, \text{CO}=0.02, \) and \( \text{N}_2=0.40 \).

Option 3 - Change inlet gas volumetric flow rate:
Inlet gas volumetric flow rate (liters/sec) is queried for in this option. The inlet flow rate is assumed to be at the temperature specified in option 4. Although there is no upper limit on the inlet gas flow rate, if the flow rate results in a Reynolds (Re) number > 2300, the computational portion of the program will be terminated. The default file value is 0.25 liters/sec.

Option 4 - Change inlet gas temperature:
Inlet gas temperature (K) is queried for in this option. The acceptable range of temperature is 200 to 700 K. Gas temperature is updated along the length of the monolith. If the gas temperature reaches 700 K along the length of the monolith the computational portion of the program will be terminated. The default file inlet gas temperature is 300 K.

Option 5 - Change inlet gas pressure:
Inlet gas pressure (kPa) is queried for in this option. The acceptable range for inlet gas pressure is 0.1 to 350 kPa. The pressure is updated along the length of the monolith. If the gas pressure exceeds 350 kPa or drops below 0.1 kPa along the length of the monolith the computational portion of the program will be terminated. The default file value is 101.325 kPa (1 atm).

Option 6 - Change catalyst activation energy:
Catalyst activation energy (J/mol) is queried for in this option. The acceptable range for catalyst activation energy is between 0 and 300,000 J/mol. The default file value is 39700 J/mol.

Option 7 - Change catalyst reaction rate constant:
Catalyst reaction rate constant (mm\(^3\)/gcat-sec) [referenced to 298 K] is queried for. The catalyst activation energy must be greater than zero. The default file value is 123.4 mm\(^3\)/gcat-sec.

**Option 8 - Change catalyst active layer density:**
Catalyst active layer density (g/mm\(^3\)) is queried for in this option. The catalyst active layer density must be greater than zero. The default file value is 5e-04 g/mm\(^3\).

**Option 9 - Change macro/micro pore radius & void-fraction:**
Four quantities, macropore and micropore radius and macropore and micropore void-fractions, are queried for in this option.
- Define macropore radius (nm) = RMACRO Default value= 500 nm
- Define micropore radius (nm) = RMICRO Default value= 12 nm
- Define macropore void-fraction = EMACRO Default value= 0.48
- Define micropore void-fraction = EMICRO Default value= 0.24
Acceptable ranges: RMICRO < RMACRO, EMACRO + EMICRO ≤ 1.0

**Option 10 - Change thermal operation (Adiabatic/ Isothermal):**
The type of monolith thermal operation (adiabatic/isothermal) is queried for in this option. For isothermal operation the gas and the monolith section are maintained at (or very close to) the gas inlet temperature specified in option 4. Default file operation mode is adiabatic.

**Option 11 - Change output profile (Full/Summary):**
The type of output profile is queried for in this option. Only the initial and final values (temperature, pressure, and O\(_2\) concentration) are output in the summary option. In the full option, the values are specified for each display interval as specified in option 13. Default file value is Full. See LASCAT Tutorial for an example.

**Option 12 - Change termination variable (Conversion/Length):**
The termination condition (O\(_2\) conversion or monolith length) is queried for in this option. If O\(_2\) conversion is chosen, the termination percent conversion (0-100%) is required to be specified. The default O\(_2\) conversion is 2.5%. If the monolith length option is chosen, the monolith length (5-4000mm) is required to be specified. The default monolith length is 5mm. See LASCAT Tutorial for an example.

**Option 13 - Change computation display interval:**
Computation display interval (CDI) is queried for in this option. The display interval specifies the reporting interval for temperature, pressure, and O\(_2\) concentration. The specified display interval may be overrodden if too many computational loop iterations (>250) are required to meet the specified display interval. The default file value is 5mm.

**Option 14 - Show current operating parameters:**
This option lists the current selectable parameter set. Use this option to verify the proper selectable parameter set prior to execution of the program. After parameter set review, you are returned to the parameter modification menu. This option is similar to option 2 of the main menu.

**Option 15 - Save current operating parameters:**
This option allows the user to save the current operating parameter set to file. The file name and the file status (new or existing) are required to be specified. The main menu's option 1 allows parameter set files to be installed as the current selectable parameter set.

**Option 16 - Run program:**
The "Run program" option executes the computational portion of the program, using the current selectable parameter set. Results obtained are output to the screen for review and to the file LDATA for further processing or review. Any additional "runs" in this session will be tacked on to the end of file LDATA. (Macintosh only: If the program is terminated and rerun the old LDATA file will be erased and a new LDATA file started. If you desire to keep the information in contained in LDATA, rename LDATA prior to running LASCAT again.) After computations are completed or a termination condition is met, the program returns to the main menu. This option is identical to option 4 of the main menu.

**Option 17 - Return to main menu:**
Returns to the main menu. See main menu section above.

**Option 18 - Exit program:**
The program is exited. If using the Macintosh remember the caution concerning LDATA, as noted above.
C******************************PROGRAM LASCAT******************************
C Written by
C Keith Guinn, Seth Goldblum Dr. Richard Herz, and Ed Noskowski
C Department of AMES / Chemical Engineering B-010
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C
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C
C Fortran Software Compatibility
C MICROSOFT FORTRAN Version 2.2 (MACINTOSH PLUS, SE, & II)
C ABSOFT MacFORTRAN/020 Version 2.3 (MACINTOSH II)
C This program is FORTRAN 77 compatible.
C
C Editing program used: QUED Version 1.53 (MACINTOSH)
C
C Program listing outline
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C
C****************************** IDENTIFIERS ******************************
C
C A-REACTION RATE CONSTANT OF ACTIVE CATALYST MATERIAL (mm^3/g-cat s)
C AMW-AVERAGE MOLECULAR WEIGHT OF GAS MIXTURE (g/mole)
C AREF-VOLUMETRIC PUMPING RATE OF ACTIVE 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 CDI=COMPUTATION DISPLAY INTERVAL (mm)
C CGX-MONOLITH CHANNEL O2 GAS CONC. AT POSITION X (mol/mm^3)
C CGXTMP-MONOLITH CHANNEL O2 GAS CONC. AT POSITION X-DX (mol/mm^3)
C THIS IS A HOLDING CONSTANT TO DETERMINE DCGX
C CGXZ-MONOLITH CHANNEL O2 GAS CONC. AT POSITION X=0 (mol/mm^3)
C CH,CH1,CH2 - 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)
C CMCTW-CHARACTERISTIC MCWT (mm)
C CONST1,CONST2,CONST3,CONST4,CONST5-RESULT HOLDING CONSTANTS
C CONST5,CONST6,CONST7,CONST8,CONST9-RESULT HOLDING CONSTANTS
C CONSTA,CONSTB,CONSTD,CONSTE,CONSTF,CONSTC-RESULT HOLDING CONSTS
<table>
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<td>EMACRO</td>
<td>FRACTION OF TOTAL VOIDS IN PELLETS AS MACROPORES</td>
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<td>CATALYST REACTION ACTIVATION ENERGY (J/mol)</td>
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<td>NAME OF DATAFILE CONTAINING DEFAULT PARAMETERS</td>
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<td>FIXST</td>
<td>LOGICAL *1 IS TRUE IF FIRST TIME THROUGH LOOP, AND FALSE IF ANYTHING ELSE</td>
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<td>H-HEAT</td>
<td>TRANSFER COEFFICIENT FROM GAS TO WALL (J/mm^2-s-K)</td>
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<td>K</td>
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<td>MASS TRANSFER COEFFICIENT (mm/s)</td>
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<td>LAMMX</td>
<td>THERMAL CONDUCTIVITY OF THE BULK GAS MIXTURE (mW/cm K)</td>
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<td>MAIN</td>
<td>BOOLEAN EXPRESSION. TRUE WHEN USER IS IN MAIN MENU</td>
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<td>MONOLITH CHANNEL HEIGHT (mm)</td>
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<td>MONOLITH CHANNEL SUPPORT WALL THICKNESS (mm)</td>
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<td>MCW</td>
<td>MONOLITH CHANNEL WIDTH (mm)</td>
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<td>MVFL</td>
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<tr>
<td>100</td>
<td>MW(i)</td>
<td>MOLECULAR WEIGHT OF COMPONENT GASES (g/mol)</td>
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<tr>
<td>101</td>
<td>N</td>
<td>EFFECTIVNESS FACTOR FOR CATALYST WASHCOAL (NODIM)</td>
</tr>
</tbody>
</table>
Appendix 4 - program listing

**NOCHM**-NUMBER OF CHANNELS IN MONOLITH

**NOCHV**-NUMBER OF CHANNELS VERTICALLY IN MONOLITH

**O2ZERO**-MONOLITH INLET OXYGEN CONCENTRATION (%O2)

**ONCE**-INTEGER-DETERMINES IS THIELE STATEMENT HAS BEEN WRITTEN

**P**-DO LOOP VARIABLE

**PZERO**-INLET PRESSURE OF GAS MIXTURE (atm)

**PRESS**-PRESSURE OF GAS MIXTURE IN THE CHANNEL (atm)

**Q**-HOLDING CONSTANT

**R**-GAS CONSTANT (J/mol-K)

**RMICRO**-AVERAGE MICROPOROUS RADIUS (cm)

**RMACRO**-AVERAGE MACROPOROUS RADIUS (cm)

**S**-TAB CHARACTER

**SS**-CARRIAGE RETURN CHARACTER

**SSS**-A OR I FOR ADIABATIC OR ISOTHERMAL-CHARACTER

**SSS1**-P OR S FOR PROFILE OR SUMMARY-CHARACTER

**SSS2**-O OR L FOR O2 CONVERSION OR MONOLITH LENGTH-CHARACTER

**T**-GAS TEMPERATURE FOR VISCOSITY AND THERMAL CONDUCTIVITY

**TCON(i,j)**-i->1,6**, j->2,7***, THERMAL COND. OF COMPONENT GASES AT VARIOUS TEMPERATURES (mW/cm-K)

**TCONT(i)**-i->1,6** THERMAL COND. OF COMPONENT GASES, @ TEMP T (mW/cm*K)

**TGX**-MONOLITH CHANNEL BULK GAS TEMPERATURE AT POSIT. X (K)

**THIELE**-SLAB THIELE MODULUS FOR CATALYST WASHCOAT (NONDIM)

**TREF**-PHYSICAL PROPERTIES REF TEMP=298K (K)

**TSX**-MONOLITH CHANNEL WALL TEMPERATURE AT POSIT. X (K)

**TSXZ**-MONOLITH CHANNEL WALL TEMPERATURE AT POSIT. X=0 (K)

**TZERO**-MONOLITH INLET GAS TEMPERATURE (K)

**VISC(i,j)**-i->1,6**, j->2,7***, VISCOSITY OF COMPONENT GASES AT VARIOUS TEMPERATURES (centipoises)

**VISC(i)**-i->1,6** VISCOS OF COMP GASES @ TEMP T (centipoises)

**VISCTC**-COMPOSITE GAS VISCOSITY (centipoises)

**X**-MONOLITH CHANNEL POSITION (mm)

**XZ**-MONOLITH CHANNEL POSITION AT X=0 (mm)

**Y(i)**-i->1,6** MOLE FRACTION OF COMPONENT GASES (gms/mole)

**Y10**, **Y20**, **Y30**, **Y40**, **Y50**, **Y60**-HOLDING CONSTANTS FOR Y(i)'s

*****2**=200, 3=300, 4=400, 5=500, 6=600, 7=700K

**C**

************ PROGRAM ALGORITHM/RESTRICTIONS ************

**C**-Declare variables

**C**-Open output data file "LDATA" using unit 25

**C**-Display introduction on screen

**C**-Read in values of default operating parameters

**C**-Compute some geometric and record starting values using default parameters

**C**-Display main menu, query for desired option (1-5)

**C**-Read in new operating parameters

**C**-Query for file from which to read from

**C**-Read in values from file

**C**-Return to main menu

**C**-Show current operating parameters

**C**-Display operating parameter summary table, this includes some calculated values

**C**-Return to main menu

**C**-Change operating parameters

**C**-Drop to submenu, query for desired option (1-18), if not 1-18
query again. After each section is completed return to the submenu.

-1 Change monolith physical dimensions (mm)
  - Input monolith face dimensions (vertical & horizontal)
    range: >10mm, <=1000mm
  - Input monolith channel wall thickness, inner channel dimension, active layer thickness
    range: support wall thickness
    < either vert. or horiz face
    range: inner channel dimension
    < either vert or horiz face
    range: active layer thickness < 0.5 * (support wall)
  - Recompute some geometric parameters using new dimensions

-2 Change Inlet Gas Composition (mole fractions)
  - Input mole fractions of He, Ar, CO2, and O2
  - Mole fraction of CO is set to twice that of O2
  - Mole fraction of N2 is computed to make mole fraction sum equal to one
    range: each mole fraction >=0 and <=1, sum mole fractions = 1

-3 Change inlet gas volumetric flowrate (l/s)
  - Input inlet volumetric flowrate
    range: volumetric flowrate > 0

-4 Change inlet gas temperature (Kelvin)
  - Input inlet gas temperature
    range: temperature >=200K and <=700K

-5 Change inlet gas pressure (kPa)
  - Input inlet gas pressure (kPa)
    range: pressure 0.1-350 kPa

-6 Change catalyst activation energy (J/mol)
  - Input catalyst activation energy (J/mol)
    range: activation energy > 0 and < 300000

-7 Change catalyst reaction rate constant (mm^3/gcat-s)
  - Input reaction rate constant
    range: reaction rate > 0

-8 Change catalyst active layer density (g/mm^3)
  - Input density
    range: density > 0

-9 Change macro/micro pore radius & void-fraction
  - Input macro/micro pore radius
    range: radius > 0, micro<macro
  - Input macro/micro void-fractions
    range: sum <= 1, void-fractions >= 0

-10 Change thermal operation (Adiabatic/Isothermal)
  - Input option A/I or a/i

-11 Change output profile (Full/ Summary)
  - Input option P/S or p/s

-12 Change termination variable (Conversion/Length)
  - Input termination option O2 conversion (O) or monolith length (L). If (O) is chosen, specific termination conversion (%O2). If (L) is chosen specify monolith length (mm). O2% conversion range > 0, < 100%. Monolith length range > 5, < 4000 mm.

-13 Change computation display interval (mm)
  - Input computation display interval (mm)
    range: computation display interval <= 100 mm

-14 Show current operating parameters
Program listing

- Displays current operating parameters
- 15 Save current operating parameters
- Query for name of file which current operating parameters will be saved. Unit 24 is used.
- 16 Run program
- Executes computational loop until desired termination condition is reached. See below for details.
- 17 Return to main menu
- See above for options in main menu
- 18 Exit program
- Terminates program

4 - Run program
- Executes computational loop until desired termination condition is reached. See below for details.

5 - Exit program

Run program details:
- Computation of average molecular weight and gas density
- Computation of parameters needed for thermal conductivity and viscosity calculations
- Computation of channel volumetric flowrate and channel gas velocity
- Initialize some physical properties parameters
- Step size computational loop (2 loop passes)
- Compute gas density, channel flow and velocity
- Compute bulk diffusivity and thermal conductivity
- Compute viscosity of gas and heat capacity of gas
- Compute transport parameters and rxn rate
- Compute thiele modulus and effectiveness factor
- Compute Reynolds number and conversion
- Perform Runge-Kutta integration
- Update variables
- Return to beginning of step size computational loop
- Compute step size to produce approx. 0.04% change per loop iteration
- Initialize some physical properties parameters
- Main computational loop (continue until termination criteria met)
- Check if termination criteria are met, if so exit loop
- Compute gas density, channel flow and velocity
- Compute bulk diffusivity and thermal conductivity
- Compute viscosity of gas and heat capacity of gas
- Compute transport parameters and rxn rate
- Compute thiele modulus and effectiveness factor
- Compute Reynolds number and conversion
- Print (to screen and file) header if first time through
- Print (to screen and file) parameters at desired interval
- Perform Runge-Kutta integration
- Update variables
- Step size check section, if conversion per step is < 0.08%, then reduce step size (/5) and increase display factor (*5)
- Parameter value boundary check, if out of bounds, exit loop
- Return to beginning of main computational loop
- Final computed values output section
- Reset some important variable values
- End of program
- Subroutines
- RK4, fourth order Runge-Kutta
- FUNC, support for RK4
C -LINES, writes a specified no. of lines
C -HEADER, writes a portion of the header to screen and file
C -TCON, computes thermal cond. of each species and a specified temp
C -PROP, computed viscosity and thermal conductivity of gas
C -VIS, computes the viscosity of each species at a specified temp
C -OUTPUT, writes a portion of the header to screen and file
C -FXN1, computes effective diffusivity of gas mixture
C -FXN2, computes heat capacity of gas mixture
C -FXN3, computes diffusivity of O2 in mixture
C -FXN4, computes average molecular weight

PROGRAM LASCAT

C******Declare variables***************************************************************************
COMMON /BLK1/ KC, CHSTV, MCH, MCW, CSX, CGX, CHFLO, CPAGS
COMMON /BLK2/ VISCTC, CHGVEL, CHHD, H, TSX, DENGAS
INTEGER FACTOR, ONCE
REAL*8 MFDH, MOW, MCH, MCWT, CMCT, CHWP, CHSTV, CHHD
REAL*8 TZERO, O2ZERO, MVFLO, CONV, CHFLO, CHGVEL, MONOL, SUM
REAL*8 CGX, CSX, TGX, TSX, TREF, X, DX, DCGX, DTGX, AREF, A, CDI
REAL*8 KC, DENGAS, DENGSR, DENCAT, DENSUP, CPAGS, CPACAT, CPSUP
REAL*8 N, HEATRX, ENGACT, R, THIELE, DAB, DABR, DABEFF, LAMBMX
REAL*8 H, K, KREF, CONST1, CONST2, CONST3, P, Q, CONVX, ASK
REAL*8 CONSTD, CONSTE, CONSTF, X0 (3), XNEW(3)
REAL*8 EMICRO, EMACRO, RMICRO, RMACRO, MFDV
REAL*8 DMICR, DRMACR, DMICRO, DMACRO
CHARACTER*1 SS, SSS, SSS1, SSS2, BEEP, CH1, CH2
CHARACTER*20 FILNAM,
REAL*8 T, Y (6), TCONDC, VISCTC, X10, Y20, Y30, Y40, Y50, Y60
REAL*8 MW (6), MOLFLO, MVFLZ, PZERO
REAL*8 VISC (6,2:7), AX (6,6)
REAL*8 VISCT (6), TCONT (6), AMW, PRESS, D (6), DP
REAL*8 CONST5, CONST4, CONST6, CONST7, CONST8, CP (6)
REAL*8 FGX, DFGX, PZERO, FGXEND, NOCHV, NOCHH, NOCHM
REAL*8 CONVXZ, X2, CGXZ, CSXZ, TSXZ, RE
INTEGER I, J, CONST, CONSB, CONSTC, DXCHK, JUMP
LOGICAL*, FIRST, MAIN

C******Introduction******************************************************************************

C Open Data file which will be used for output.
OPEN( UNIT=25, FILE='LDATA', STATUS='NEW')
WRITE(*,*), " ***** PROGRAM LASCAT *****
WRITE(*,*), " The purpose of this program is to calculate ',
2 'the gas concentration and'
WRITE(*,*), 'temperature profiles of a monolith catalyst section',
2 'of a CO2 laser. The'
WRITE(*,*), 'CO2 decomposes when the laser is pulsed. The CO ',
2 'and O2 produced as a result'
WRITE(*,*), 'of pulsing are detrimental to the efficient opera',
2'tion of the laser. The'
WRITE(*,*), 'recombination reaction is CO +1/2 O2 -> CO2. ','
2 'This program provides the'
WRITE(*,*), 'means to model the performance of a monolith ',
2'catalyst section under various'
WRITE(*,*), 'gas compositions, temperatures, catalyst ',
2'activities gas flowrates, oxygen '
WRITE(*,*), 'conversion, monolith face and length dimensions. ',
2'Results can indicate if constraints such as conversion, maximum gas temperature, 
are satisfied and how the system parameters may be altered to meet these constraints. Parameters and options may be altered to tailor the monolith design. Default values can also be used as a starting point for the design process. A review of the parameters and options may be chosen to meet these constraints. To execute the computational portion of the program,

CALL LINES(5) 
WRITE(*,*)' Programm' (HIT RETURN TO CONTINUE)' 

C First time through, skip over query for reading parameter file
GO TO 2119
C Default values for parameters
C First see if operating parameters are already available in a data file.
C
9000 WRITE(*,*)' Read in data from existing parameter file? (Y/N)'
READ(*,621) CH
IF ((CH.EQ.'Y').OR.(CH.EQ.'y')) THEN
WRITE(*,*) 
WRITE(*,*)' What is the name of the existing parameter file?'
WRITE(*,*)' To be opened?'
READ(*,621) FILNAM
OPEN(UNIT=23, FILE=FILNAM, STATUS='OLD')
C If existing data file exists, read in data.
READ(23,*), MFDH
READ(23,*), MFDV
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,*), PZERO
READ(23,622), SSS
READ(23,622), SSS1
READ(23,622), SSS2
READ(23,*), CONV
READ(23,*), MONOL
READ(23,*), ENGA4CT
READ(23,*), AREF
READ(23,*), TZERO
READ(23,*), MVFLZ
Appendix 4 - program listing

```
400   READ (23, *) FACTOR
401   READ (23, *) DX
402   READ (23, *) DENCAT
403   READ (23, *) EMICRO
404   READ (23, *) EMACRO
405   READ (23, *) RMICRO
406   READ (23, *) RMACRO
407   CLOSE (UNIT = 23)
408   C If no external data file exists, then assign default values.
409   ELSE
410   WRITE(*, *) ' Default values being assigned...
411   MFDH = 100.0
412   MF DV = 100.0
413   MCST = 0.5
414   MCW = 4.0
415   MCH = 4.0
416   MCWT = 0.25
417   Y (1) = 0.2
418   Y (2) = 0.0000001
419   Y (3) = 0.37
420   Y (4) = 0.02
421   Y (5) = 0.01
422   Y (6) = 0.40
423   PZERO = 1.0
424   SSS = 'A'
425   SSS1 = 'P'
426   SSS2 = 'O'
427   CONV = 2.5
428   MONO = 5.0
429   ENGACT = 39700.0
430   AREF = 123.4
431   TZZERO = 300.0
432   MF1Z = 0.25
433   FACTOR = 50
434   DX = 0.1
435   DENCAT = 5.0E-04
436   EMICRO = 0.24
437   EMACRO = 0.48
438   RMICRO = 1.2E+1
439   RMACRO = 5.0E+2
440   ENDIF
441   C Compute a few needed parameters:
442   Y10 = Y(1)
443   Y20 = Y(2)
444   Y30 = Y(3)
445   Y40 = Y(4)
446   Y50 = Y(5)
447   Y60 = Y(6)
448   O2ZERO = 100 * Y(5)
449   CHWP = 2 * (MCW + MCH)
450   CHSTV = CHWP / (MCW * MCH)
451   CHHD = 4 * (MCW * MCH) / CHWP
452   NOCHH = (MFDH / (MCH + 2*MCST))
453   NOCHV = (MF DV / (MCW + 2*MCST))
454   NOCHM = NOCHV * NOCHH
455   CDI = DX * FACTOR
```
457 9001 CONTINUE
458 C Set FIRST equal to true the first time through the loop
459 C so that initial parameters may be viewed.
460 FIRST = .TRUE.
461 C Print Out Main Menu
462 CALL LINES(17)
463 WRITE(*,46)
464 46 FORMAT(1H ,T20,'LASCAT Main Menu')
465 MAIN = .TRUE.
466 9011 WRITE(*,*)
467 WRITE(*,*) ' 1) Read in new operating parameters'
468 WRITE(*,*) ' 2) Show current operating parameters'
469 WRITE(*,*) ' 3) Change operating parameters'
470 WRITE(*,*) ' 4) Run program'
471 WRITE(*,*) ' 5) Exit program'
472 WRITE(*,*)
473 WRITE(*,*) ' Type in number corresponding to choice above.'
474 CALL LINES(12)
475 ASK=0
476 Read(*,*) ASK
477 IF (ASK.EQ.1) GO TO 9000
478 IF (ASK.EQ.2) GO TO 9002
479 IF (ASK.EQ.3) GO TO 100
480 IF (ASK.EQ.4) GO TO 348
481 IF (ASK.EQ.5) GO TO 99999
482 WRITE(*,*) BEEP, BEEP, BEEP
483 WRITE(*,*)
484 WRITE(*,**) ' A number, 1 to 5, is required.'
485 WRITE(*,*)
486 WRITE(*,*)
487 GOTO 9011
488 C Output parameters to screen for review
489 9002 CALL OUTPUT(0, MCST, MFH, MFV, MCW, NOCHV, NOCHH, MCWT, 
490 + Y, MFLZ, TZERO, PZERO, DENCAT, AREF, ENGACT, 
491 + EMICRO, EMACRO, RMICRO, RMACRO, SSS, SSS1, SSS2, 
492 + CONV, MONOL, DX, CDI)
493 IF (MAIN) THEN
494 GOTO 9001
495 ELSE
496 GOTO 100
497 ENDIF
498 C******Parameter Modification Section********_____________
499 100 MAIN = .FALSE.
500 CALL LINES(9)
501 WRITE(*,73)
502 73 FORMAT(1H ,T20,'Parameter Modification Menu')
503 WRITE(*,*)
504 334 WRITE(*,*)
505 WRITE(*,**) ' 1) Change monolith physical dimensions'
506 WRITE(*,**) ' 2) Change inlet gas composition'
507 WRITE(*,**) ' 3) Change inlet gas volumetric flowrate'
508 WRITE(*,**) ' 4) Change inlet gas temperature'
509 WRITE(*,**) ' 5) Change inlet gas pressure'
510 WRITE(*,**) ' 6) Change catalyst activation energy'
511 WRITE(*,**) ' 7) Change catalyst reaction rate constant'
512 WRITE(*,**) ' 8) Change catalyst active layer density'
513 WRITE(*,**) ' 9) Change macro/micro pore radius & void-fraction'
10 WRITE(*,*),'10) Change thermal operation (Adiabatic/Isothermal)'
11 WRITE(*,*),'11) Change output profile (Full/Summary)'
12 WRITE(*,*),'12) Change termination variable (Conversion/Length)'
13 WRITE(*,*),'13) Change computation display interval'
14 WRITE(*,*),'14) Show current operating parameters'
15 WRITE(*,*),'15) Save current operating parameters'
16 WRITE(*,*),'16) Run program'
17 WRITE(*,*),'17) Return to main menu'
18 WRITE(*,*),'18) Exit program'

Type in number corresponding to choice above

ASK=0
READ(*,*) ASK

IF (ASK.EQ.1) GOTO 101
IF (ASK.EQ.2) GOTO 110
IF (ASK.EQ.3) GOTO 120
IF (ASK.EQ.4) GOTO 130
IF (ASK.EQ.5) GOTO 140
IF (ASK.EQ.6) GOTO 150
IF (ASK.EQ.7) GOTO 160
IF (ASK.EQ.8) GOTO 170
IF (ASK.EQ.9) GOTO 180
IF (ASK.EQ.10) GOTO 200
IF (ASK.EQ.11) GOTO 210
IF (ASK.EQ.12) GOTO 220
IF (ASK.EQ.13) GOTO 230
IF (ASK.EQ.14) GOTO 9002
IF (ASK.EQ.15) GOTO 11000
IF (ASK.EQ.16) GOTO 348
IF (ASK.EQ.17) GOTO 9001
IF (ASK.EQ.18) GOTO 99999
WRITE(*,*)'A number, 1 to 18, is required.'
WRITE(*,*)
GOTO 334

C************** PARAMETER INPUT SECTION************************************
C INPUT MONOLITH PHYSICAL DIMENSIONS
101 WRITE(*,*)
102 MCST=MCST*2.0
103 WRITE(*,*)'Current monolith horizontal'
104 WRITE(*,1075) MFH
105 WRITE(*,*)
106 1075 FORMAT('face dimension (mm) = ',F8.3)
107 WRITE(*,*)'Input new monolith horizontal face dimension.'
108 WRITE(*,*)'Value must be >=10mm and <=1000mm.'
109 READ(*,*) MFH
110 IF ((MFH.LT.10.0).OR.(MFH.GT.1000.0)) GOTO 1136
111 WRITE(*,*)
112 WRITE(*,*)'Current monolith vertical'
113 WRITE(*,1076) MFV
114 WRITE(*,*)
115 1076 FORMAT('face dimension (mm) = ',F8.3)
116 WRITE(*,*)
117 WRITE(*,*)
Appendix 4 - program listing

```
571 1137 WRITE(*,*)' Input new monolith vertical face dimension.'
572 WRITE(*,*)' Value must be >=10mm and <=1000mm.'
573 READ(*,*) MFDV
574 IF ((MFDV.LT.10.0).OR.(MFDV.GT.1000.0)) GOTO 1137
575 102 WRITE(*,*)
576 WRITE(*,*)
577 WRITE(*,*)' Current monolith channel total'
578 WRITE(*,1077) MCST
579 1077 FORMAT(' wall thickness (mm) = ',F8.3)
580 WRITE(*,*)
581 WRITE(*,*)
582 WRITE(*,*)' Input the monolith channel total wall'
583 WRITE(*,*)' thickness(mm). (Including active layer)'
584 READ(*,*) MCST
585 IF (MCST.LE.0.0) GO TO 102
586 IF ((MCST.GE.MFDH).OR.(MCST.GE.MFDV)) THEN
587 WRITE(*,*)' Wall thickness must be less than the monolith'
588 WRITE(*,*)' face dimension! Right? Let us start over.'
589 GOTO 101
590 ENDIF
591 MCST = MCST / 2.0
592 103 WRITE(*,*)
593 WRITE(*,*)' Current square channel'
594 WRITE(*,1078) MCW
595 1078 FORMAT(' opening dimension (mm) = ',F8.3)
596 WRITE(*,*)
597 WRITE(*,*)' Input new monolith square'
598 WRITE(*,*)' channel opening dimension (mm).'
599 READ(*,*) MCW
600 IF (MCW.LE.0.0) GO TO 103
601 IF ((MCW.GE.MFDH).OR.(MCW.GE.MFDV)) THEN
602 WRITE(*,*)' Channel opening must be less than the monolith'
603 WRITE(*,*)' face dimension! Right? Let us start over.'
604 GOTO 101
605 ENDIF
606 MCH = MCW
607 104 WRITE(*,*)
608 WRITE(*,*)' Current active layer thickness'
609 WRITE(*,1079) MCWT
610 1079 FORMAT(' thickness (mm) = ',F8.3)
611 WRITE(*,*)
612 WRITE(*,*)
613 WRITE(*,*)' Input monolith channel active layer'
614 WRITE(*,*)' thickness (mm). Active layer cannot'
615 WRITE(*,1080) MCST*2.00
616 1080 FORMAT(' be greater than ',F8.3,' (mm),')
617 WRITE(*,*)'(1/2 total wall thickness)'
618 READ(*,*) MCWT
619 IF ((MCWT.LE.0.0).OR.(MCWT.GT.MCST)) GO TO 104
620 WRITE(*,*)
621 WRITE(*,*)
622 C Perform monolith parameter calculations
623 8900 CHWP = 2 * ( MCW + MCH )
624 CHSTV = CHWP / ( MCW * MCH )
625 NOCHH = (MFDH / (MCH+2*MCST))
626 NOCHV = (MFDV / (MCW+2*MCST))
627 CHHD = 4.0*(MCW*MCH)/CHWP
```
I

628       NOCHM = NOCHV * NOCHH
629       GO TO 100
630 C Input Gas composition
631 C Define Mole fractions of species Y(i)
632 C The index of Y(i) correspond to the species.
633 C Species: 1=He, 2=Ar, 3=CO2, 4=CO, 5=O2, 6=N2.
634 110 Write(*,*)' Input section for gas composition:'
635 WRITE(*,*)
636 Write(*,*)' The mixture can consist of only the following'
637 Write(*,*)' species: He, Ar, CO2, CO, O2, N2. All mole ':
638 Write(*,*)' fractions must be greater than zero. The sum'
639 WRITE(*,*)' of the mole fractions must be =1'
640 WRITE(*,*)' Current mole fractions: '
641 WRITE(*,3231) Y(1),Y(2),Y(3)
642 WRITE(*,3232) Y(4),Y(5),Y(6)
643 3231 FORMAT( ' He = ',F6.4, ' Ar = ',F6.4, ' CO2 = ',F6.4)
644 3232 FORMAT( ' CO = ',F6.4, ' O2 = ',F6.4, ' N2 = ',F6.4)
645 WRITE(*,*)
646 Write(*,*)' Input gas mole fraction for He'
647 Read(*,*) Y(1)
648 If (Y(1) .EQ.0.0) Y(1)=1E-7
649 Write(*,*)' Input gas mole fraction for Ar'
650 Read(*,*) Y(2)
651 If (Y(2) .EQ.0.0) Y(2)=1E-7
652 Write(*,*)' Input gas mole fraction for CO2'
653 Read(*,*) Y(3)
654 If (Y(3) .EQ.0.0) Y(3)=1E-7
655 WRITE(*,*)
656 Write(*,*)' Input gas mole fraction for O2'
657 WRITE(*,*)
658 Write(*,*)' Gas mole fraction for CO will be set to twice that'
659 Write(*,*)' of O2. This is because CO and O2 are presumed to'
660 Write(*,*)' be produced from the dissociation of CO2. '
661 Write(*,*)' Therefore, the stoichiometric 2:1 ratio applies.'
662 Write(*,*)' Also, the mole fraction of O2 is limited to a '
663 Write(*,*)' maximum of 0.03 (3.0%). Typically a CO2 lasers '
664 Write(*,*)' output is degraded at a O2 mole fraction of 0.01'
665 Write(*,*)' (1.0%).'
666 Read(*,*) Y(5)
667 IF (Y(5).LE.0.0) THEN
668 Write(*,*)' There must be O2 to convert !!!', BEEP,BEEP
669 Write(*,*)' Put in a mole fraction > 0'
670 GOTO 110
671 ENDIF
672 IF (Y(5).LT.1E-7) THEN
673 WRITE(*,*)' Awful low O2 concentration. The problem is'
674 Write(*,*)' no problem! Put in a mole fraction >= 1E-7'
675 Write(*,*) BEEP,BEEP
676 GOTO 110
677 ENDIF
678 IF (Y(5).GT.0.0300001) THEN
679 Write(*,*)' Awful high O2 concentration. The laser'
680 Write(*,*)' may explode! Shut it off immediately'
681 Write(*,*) BEEP,BEEP
682 Write(*,*)' Put in a mole fraction <= 0.03 '
683 GOTO 110
684 ENDIF
Y(4) = 2.0*Y(5)
O2ZER = Y(5)*100
Y(6) = 1.0 - Y(5) - Y(4) - Y(3) - Y(2) - Y(1)
IF ((Y(6).LT.0.0).OR.(Y(6).GT.1.0)) GOTO 110
IF ((Y(6).LT.1E-7).AND.(Y(6).GE.0)) Y(6) = 1E-7
WRITE(*,*)
C Check if restrictions are met. If not, force user to reinput values
DO 112 I=1,5
   IF ((Y(I).LT.0).OR.(Y(I).GT.1.0)) THEN
      WRITE(*,*) BEEP, BEEP
      WRITE(*,*)' Invalid mole fractions. Try again.'
      WRITE(*,*)' Restrictions are not met. Read below'
      WRITE(*,*)
      GOTO 110
   ENDIF
112 Continue
WRITE(*,2323) Y(6)
2323 FORMAT(' The gas mole fraction for N2 = ',F6.4)
Y10 = Y(1)
Y20 = Y(2)
Y30 = Y(3)
Y40 = Y(4)
Y50 = Y(5)
Y60 = Y(6)
WRITE(*,*)
WRITE(*,*)
WRITE(*,*) => Hit Return when Finished Viewing <=
WRITE(*,*)
READ(*,621) S
WRITE(*,*)
GO TO 100
C Input Inlet gas flowrate
120 WRITE(*,*)
121 WRITE(*,*)' Current inlet volumetric'
122 WRITE(*,1081) MVELZ
123 1081 FORMAT(' flowrate = ',F8.3, ' (l/s).')
124 WRITE(*,*)
125 WRITE(*,*)' Input monolith inlet volumetric flowrate.'
126 WRITE(*,*) MVELZ
127 IF (MVELZ.LE.0.0) GO TO 120
128 GO TO 100
C Input Inlet gas temperature
130 WRITE(*,*)
131 WRITE(*,*)' Current inlet gas '
132 WRITE(*,1082) TZERO
133 1082 FORMAT(' temperature = ',F8.3, ' (K),')
134 WRITE(*,*)
135 WRITE(*,*)' Input monolith inlet gas temperature.'
136 WRITE(*,*)' Temperature must be >200K and <700K.'
137 READ(*,*) TZERO
138 IF ((TZERO.EQ.0).OR.(TZERO.LT.200)) GO TO 130
139 IF (TZERO.GT.700) GO TO 130
140 GOTO 100
C Input Inlet Gas Pressure
140 WRITE(*,*)
141 PZERO = PZERO*101.325
WRITE(*,*)' Current inlet gas '
WRITE(*,1083) PZERO
1083 FORMAT(' pressure = ',F8.3,' (kPa)')
WRITE(*,*)
WRITE(*,*)' Inlet gas pressure must be between'
WRITE(*,*)' 0.1 and 350 kPa'
WRITE(*,*)' Input new inlet gas pressure.'
READ(*,*) PZERO
IF ((PZERO.LT.0.1) .OR. (PZERO.GT.350.0)) GOTO 140
C convert pressure back to atm.
PZERO=PZERO/101.325
GOTO 100
C Input catalyst activation energy
150 WRITE(*,*)
WRITE(*,1084) ENGACT
1084 FORMAT(' Current activation energy = ',F11.3,' (J/mol),')
WRITE(*,*)' Maximum activation energy (J/mol) = 300000'
WRITE(*,*)
READ(*,*) ENGACT
IF ((ENGACT.LE.0.0) .OR. (ENGACT.GT.300000)) GOTO 150
GO TO 100
C Input catalyst reaction rate constant
160 WRITE(*,*)
WRITE(*,1085) AREF
1085 FORMAT(' constant [at 298 K] = ',F11.3,' (mm^3/gcat-s),')
WRITE(*,*)
WRITE(*,*)' Input new catalyst reaction'
WRITE(*,*)' rate constant at 298 K (mm^3/gcat-s)'
WRITE(*,*)' Rate must be greater than zero'
READ(*,*) AREF
IF (AREF.LE.0.0) GOTO 160
GO TO 100
C Input catalyst active layer density
170 WRITE(*,*)
WRITE(*,1086) DENCAT
1086 FORMAT(' active layer = ',E10.4,' (g/mm^3),')
WRITE(*,*)
WRITE(*,*)' Input density of catalyst active layer (g/mm^3)'
WRITE(*,*)' Density must be greater than zero'
READ(*,*) DENCAT
IF (DENCAT.LE.0.0) GOTO 170
WRITE(*,*)
GOTO 100
C Input micro/macropore radii and void-fractions
180 WRITE(*,*)
WRITE(*,1087) RMICRO
1087 FORMAT(' radius = ',F9.4,' (nm),')
WRITE(*,*)' Input new average micropore radius (nm)'
WRITE(*,*)' Micro radius must be greater than zero'
READ(*,*) RMICRO
WRITE(*,*)
WRITE(*,1088) RMACRO
Appendix 4 - program listing

799 1088 Format(' radius = ',F9.4,' (nm)',)
800 WRITE(*,*)' Input new average macropore radius (nm)'
801 WRITE(*,*)' Macro radius must be greater than zero'
802 READ(*,*) RMACRO
803 WRITE(*,*)
804 IF ((RMICRO.LE.0.0).OR.(RMACRO.LE.0.0)) GO TO 180
805 IF (RMICRO.GT.RMACRO) THEN
806 WRITE(*,*)' Hey Dude, What's the deal?'
807 WRITE(*,*)' You just entered macropore radius which is'
808 WRITE(*,*)' smaller than the micropore radius!! '
809 WRITE(*,*)' Try again, big guy !!!'
810 WRITE(*,*)
811 GOTO 180
812 ENDIF
813 190 WRITE(*,1089) EMICRO
814 WRITE(*,1090) EMACRO
815 1089 Format(' Current void-fraction as micropores ', F6.3)
816 1090 Format(' Current void-fraction as macropores ', F6.3)
817 WRITE(*,*)
818 WRITE(*,*)' The sum of micro and macropore void-fractions'
819 WRITE(*,*)' must be less than one (1) ' 
820 WRITE(*,*)' Void fractions must be >=0 and <=1'
821 WRITE(*,*)
822 WRITE(*,*)' Input void-fraction as micropores'
823 READ(*,*) EMICRO
824 WRITE(*,*)' Input void-fraction as macropores'
825 READ(*,*) EMACRO
826 WRITE(*,*)
827 IF((EMICRO.LT.0.0).OR.(EMACRO.LT.0.0)) THEN
828 WRITE(*,*)' You can't have a negative void fraction'
829 WRITE(*,*)
830 WRITE(*,*)
831 GOTO 190
832 ENDIF
833 IF (EMICRO+EMACRO.GT.1.0) THEN
834 WRITE(*,*)' The sum of micro and macropore void'
835 WRITE(*,*)' fractions must be less than one (1) '
836 WRITE(*,*)
837 GOTO 190
838 ENDIF
839 WRITE(*,*)
840 GOTO 100
841 C Input thermal operation: adiabatic or isothermal
842 200 IF (SSS.EQ.'I') THEN
843 WRITE(*,*)' Current operation is isothermal'
844 ELSE
845 WRITE(*,*)' Current operation is adiabatic'
846 END IF
847 WRITE(*,*)
848 WRITE(*,*)'Isothermal (I) or Adiabatic (A) operation?'
849 WRITE(*,*)'Type the letter I or the letter A. HIT RETURN'
850 READ(*,621) SSS
851 IF (SSS.EQ.'I') SSS = 'I'
852 IF (SSS.EQ.'A') SSS = 'A'
853 IF ((SSS.NE.'I').AND.(SSS.NE.'A')) GOTO 200
854 GO TO 100
855 C Input output profile type: full or summary
WRITE(*,*)' Full concentration and temperature profile (P) or'
WRITE(*,*)' Summary (S)?'
WRITE(*,*)' Type the letter P or the letter S. HIT RETURN.'
READ(*,621) SSSI
IF (SSSI.EQ.'P') SSSI = 'P'
IF (SSSI.EQ.'S') SSSI = 'S'
IF ((SSSI.NE.'P').AND.( SSSI.NE.'S')) GO TO 210
GO TO 100
C Input computation loop completion criteria
WRITE(*,*)' Integration can be stopped by either specifying'
WRITE(*,*)' an amount of O2 conversion (O), or by specifying'
WRITE(*,*)' a monolith length (L)'
WRITE(*,*)
IF (SSS2 .EQ. 'O') THEN
WRITE(*,*)' Currently, Integration will be stopped'
WRITE(*,*)' by specifying an amount of O2 conversion (O).'
ELSE
WRITE(*,*)' Currently, Integration will be stopped'
WRITE(*,*)' by specifying a monolith length (L).'
END IF
WRITE(*,*)' Type the letter O or the letter L. HIT RETURN.'
READ(*,621) SSSS
IF (SSS2.EQ.'0') SSSS2 = '0'
IF (SSS2.EQ.'L') SSSS2 = 'L'
IF ((SSS2.NE.'0').AND.( SSSS2.NE.'L')) GO TO 220
IF (SSS2.EQ.'0') THEN
WRITE(*,*)
WRITE(*,*)' Current % oxygen conversion = ',F8.3
END IF
WRITE(*,*)' Input desired % oxygen conversion'
WRITE(*,*)' between 0 and 100%.'
READ(*,*) CONV
IF ((CONV.GT.100.0) .OR. (CONV.LT.0)) GOTO 225
ENDIF
IF (SSS2.EQ.'L') THEN
WRITE(*,*)
WRITE(*,1091) MONOL
1091 FORMAT(' Current desired monolith length = ',F8.3,' (mm)')
WRITE(*,*)
WRITE(*,*)' Input desired monolith length (5-4000mm)'
WRITE(*,*)
READ(*,*) MONOL
IF (MONOL.LT.5.0) GOTO 227
IF (MONOL.GT.4000.0) GOTO 227
ENDIF
GO TO 100
C Input computation loop(integration) step size ***
WRITE(*,*)
WRITE(*,1093) CDI
1093 FORMAT(' Current computation display interval ', F6.3,' (mm)')
WRITE(*,*)' Minimum computation display interval = 0.001 mm.'
WRITE(*,*)' Maximum computation display interval = 100 mm.'
WRITE(*,*)' Values > 1 will be rounded to the nearest integer.'
WRITE(*,*)' Input desired computation display interval (mm).' 
WRITE(*,*)
WRITE(*,*) READ(*,*) CDI
IF (CDI.GT.100) GOTO 230
IF (CDI.GT.1.0) CDI=INT(CDI)
IF (CDI.LT.0.0009999) GOTO 230
WRITE(*,*)
WRITE(*,*) GO TO 100
C END of parameter input section
C Save present operating parameters to file
11000 WRITE(*,*)
C Give user option to save current operating parameters.
WRITE(*,*) WRITE(*,*)' Would you like to save the current operating' 
WRITE(*,*)' parameters to a New(N) or Existing(E) file?' 
WRITE(*,*)
READ(*,621) CH1
IF((CH1.NE.'E').AND.(CH1.NE.'e').AND.(CH1.NE.'N') 
* .AND. (CH1.NE.'n')) GOTO 11000
IF ((CH1.EQ.'E').OR.(CH1.EQ.'e')) THEN
WRITE(*,*)
WRITE(*,*)' What`s the name of the EXISTING' 
WRITE(*,*)' parameter file to be opened?' 
READ(*,621) FILNAM
OPEN( UNIT=24, FILE=FILNAM, STATUS='OLD')
ELSE
WRITE(*,*)
WRITE(*,*)' What`s the name of the NEW' 
WRITE(*,*)' parameter file to be opened?' 
READ(*,621) FILNAM
OPEN( UNIT=24, FILE=FILNAM, STATUS='NEW')
ENDIF
C Write default parameters to parameter file.
WRITE(24,*),MFDH
WRITE(24,*),MFDV
WRITE(24,*),MCST
WRITE(24,*),MCW
WRITE(24,*),MCR
WRITE(24,*),MCRT
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,*),FZERO
WRITE(24,622),SSS
WRITE(24,622),SSS1
WRITE(24,622),SSS2
WRITE(24,*),CONV
WRITE(24,*),MONOL
WRITE(24,*),ENACK
Appendix 4 - program listing

970 WRITE (24, *) AREF
971 WRITE (24, *) TZERO
972 WRITE (24, *) MWLZ
973 WRITE (24, *) FACTOR
974 WRITE (24, *) DX
975 WRITE (24, *) DENCAT
976 WRITE (24, *) EMICRO
977 WRITE (24, *) EMACRO
978 WRITE (24, *) RMICRO
979 WRITE (24, *) RMACRO
980 CLOSE (UNIT = 24)
981 GOTO 100
982 C COMPUTE GAS AVG. MOLECULAR WEIGHT AND DENSITY *
983 348 AMW = FXN4(Y)
984 R = 8.3144
985 DENGAS = AMW * (PZERO/9896.0) / R / TZERO
986 C Parameters needed for thermal cond. calcuation
987 C Read in viscosity (VISC) values into matrix. Units for
988 C VISC are centipoises. The values are read off a nomograph
990 C The first index of VISC corresponds to the species.
991 C Species: 1=He, 2=Ar, 3=CO2, 4=CO, 5=O2, 6=N2.
992 C The second index of VISC corresponds to the temperature.
993 C Temperature: 2=200K, 3=300K, 4=400K, 5=500K, 6=600K, 7=700K
994 DATA VISC (1,2), VISC (1,3), VISC (1,4), VISC (1,5), VISC (1,6), VISC (1,7)
995 +/- .014, .0188, .022, .027, .031, .034/
996 DATA VISC (2,2), VISC (2,3), VISC (2,4), VISC (2,5), VISC (2,6), VISC (2,7)
997 +/- .0164, .0223, .0278, .0327, .0376, .041/
998 DATA VISC (3,2), VISC (3,3), VISC (3,4), VISC (3,5), VISC (3,6), VISC (3,7)
999 +/- .0105, .0147, .019, .023, .027, .031/
1000 DATA VISC (4,2), VISC (4,3), VISC (4,4), VISC (4,5), VISC (4,6), VISC (4,7)
1001 +/- .0138, .018, .022, .0255, .029, .0325/
1002 DATA VISC (5,2), VISC (5,3), VISC (5,4), VISC (5,5), VISC (5,6), VISC (5,7)
1003 +/- .0155, .02, .0247, .0288, .0327, .0368/
1004 DATA VISC (6,2), VISC (6,3), VISC (6,4), VISC (6,5), VISC (6,6), VISC (6,7)
1005 +/- .013, .0175, .0218, .026, .029, .0332/
1006 MVFLO = MVFLZ
1007 C CONVERT MVFLO FROM liters/s TO mm^3/s
1008 MVFLO = MVFLO * 1.0E+06
1009 C COMPUTE MOLAR FLOWRATE OF GAS. (M/s)
1010 MOLFLO = MVFLO*DENGAS*AMW
1011 C COMPUTE CHANNEL FLOW RATE AND CHANNEL VELOCITY
1012 CHFLO = MVFLO / NOCHM
1013 CHVEL = CHFLO / (MCW * MCH)
1014 CONTINUE
1015
1016 C INITIALIZE PHYSICAL PROPERTIES PARAMETERS
1017 1041 HEATRX=5.64E+05
1018 TREF=298.0
1019 PRESS = PZERO
1020 TGX = TZERO
1021 TSX = TZERO
1022 CGX = 4.092E-08 * (O2ZERO/100.0) * (298.0/TGX) * (PRESS/1.0)
1023 FGX = CGX * CHFLO
1024 PZERO = FGX
1025 FGXEND = PZERO * (1.0 - CONV/100.0)
1026 S = CHAR(9)
Appendix 4 - program listing

1027 SS = CHAR(13)
1028 X = 0.0
1029 CMCWT = ((MCH + 2*MCWT) * (MCW + 2*MCWT) - (MCH*MCW)) / 2 / (MCH + MCW)
1030 CONSTA = 0.0
1031 DCGX = 0.0
1032 DFGX = 0.0
1033 ICNT = 0
1034 C Initialize variables for Runge Kutta Integration method
1035 XNEW(1) = FGX
1036 XNEW(2) = PZERO
1037 XNEW(3) = TZERO
1038 C********** START OF STEP SIZE CHECK LOOP **********
1039 1040 DO 800 P = 0, 2
1041 1042 DX = 1E-6
1043 DENGAS = AMW*(PRESS/9896.0)/R/TGX
1044 C COMPUTE MONOLITH FLOW RATE, CHANNEL FLOW RATE AND CHANNEL VELOCITY
1045 MVFLO = MOLFLO / (AMW * DENGAS)
1046 CHFLO = MVFLO / NOCHM
1047 CHGVEL = CHFLO / (MCW * MCH)
1048 C COMPUTE BULK DIFFUSIVITY
1049 DAB = FXN3(Y, TGX)
1050 C COMPUTE EFFECTIVE DIFFUSIVITY
1051 + TSX, EMACRO, EMICRO)
1052 C COMPUTE THERMAL CONDUCTIVITY
1053 T = TGX
1054 C COMPUTE VISCOSITY OF COMPONENT GASES AT TGX
1055 CALL VIS(TGX, VISC, VISCT)
1056 C COMPUTE THERMAL CONDUCTIVITY OF COMPONENT GASES AT TGX
1057 CALL TCON(TGX, TCONT)
1058 C COMPUTE VISCOSITY AND THERMAL CONDUCTIVITY OF MIXTURE
1059 CALL PROP(Y, TCONT, VISCT, VISCTC, K)
1060 C COMPUTE HEAT CAPACITY OF GAS MIXTURE AT TGX
1061 CPGAS = FXN2(Y, TGX)
1062 KC = 2.976 * DAB / CHHD
1063 H = 2.976 * K / CHHD
1064 A = AREF * DEXP (-ENGACT / R * (1 / TSX - 1 / TREF))
1065 THIELE = CMCWT * (A * DENCAT / DABEFF) ** 0.5
1066 N = DTANH (THIELE) / THIELE
1067 CONST1 = N*A*CMCWT*DENCAT
1068 CSX = CGX * (K) / (K*CST1)
1069 TSX = TGX * HEATR*CSX*CONST1/H
1070 C FIRST TIME THROUGH COMPUTE 'A' TO USE FOR TSX, CSX CALCULATION
1071 IF (FIRST.EQ.0) THEN
1072 A = AREF * DEXP (-ENGACT / R * (1 / TSX - 1 / TREF))
1073 THIELE = CMCWT * (A * DENCAT / DABEFF) ** 0.5
1074 N = DTANH (THIELE) / THIELE
1075 CONST1 = N*A*CMCWT*DENCAT
1076 CSX = CGX * (K) / (K+CST1)
1077 TSX = TGX * HEATR*CSX*CONST1/H
1078 IF (SSS.EQ.'I') TSX = TGX
1079 IF (P.EQ.0) THEN
1080 XZ = 0
1081 CONVXZ = 0.0
1082 CGXZ = CGX
1083 CSXZ = CSX

ORIGINAL PAGE IS OF POOR QUALITY
TSX=TSX
ENDIF
ENDIF
RE=1000.0*CHHD*CHVEL*DENERG/VISCTC
CONVX = 100.0* (CGXZ-CGX)*TGX/TZERO*PZERO/PRESS)/CGXZ
C Reset variables each time Runge Kutta Subroutine is called
X0 (1) = XNEW (1)
X0 (2) = XNEW (2)
X0 (3) = XNEW (3)
C Call Runge Kutta Subroutine:
CALL RK4 (DX, X, XO, XNEW)
C PARAMETER UPDATE
FGX = XNEW (1)
PRESS = XNEW (2)
IF (SSS.EQ. 'I') THEN
  TGX = TZERO
ELSE
  TGX = XNEW (3)
ENDIF
CGX = FGX/CHFLO
X = X + DX
Y (5) = Y50* (100.0-CONVX)/100.0
Y (4) = Y40-2* (Y50-Y (5) )
Y (3) = Y30+2* (Y50-Y (5) )
Y (1) = Y10
Y (2) = Y20
Y (6) = Y60
CONST7 = Y (1) + Y (2) + Y (3) + Y (4) + Y (5) + Y (6)
DO 33446 JJ = 1, 6
  Y (JJ) = Y (JJ) /CONST7
33446 CONTINUE
DO 8001 CONTINUE
C************** END OF STEP SIZE CHECK LOOP **************
C CALCULATE STEP SIZE AND DISPLAY FACTOR USING COMPUTATIONAL
C DISPLAY FACTOR AND CONVX CALCULATED IN STEP SIZE CHECK LOOP
DX=1E-6*0.04/CONVX
IF (DX GT 5) DX=5
IF (DX LT 0.1E-4) DX=0.1E-4
IF (CDI LT DX) DX=CDI
 FACTOR=ENT (CDI/DX)
IF (FACTOR GE 250) THEN
  CDI=CDI*250/FACTOR
  FACTOR=250
ENDIF
DX=CDI/FACTOR
C INITIALIZE PARAMETERS FOR MAIN COMPUTATIONAL LOOP
PRESS = PZERO
TGX = TZERO
TXS = TZERO
CGX = 4.092E-08 * (O2ZERO/100.0) * (298.0/TGX) * (PRESS/1.0)
FGX=CGX*CHFLO
FZERO=FGX
FGXEND=FZERO*(1.0-CONV/100.0)
CGXTMP=CGX
X=0.0

X0A=0.0

DCGX=0.0

DFGX=0.0

ICNT = 0

TNEW=TZERO

MVFL0=MVFLZ

Y(1)=Y10

Y(2)=Y20

Y(3)=Y30

Y(4)=Y40

Y(5)=Y50

Y(6)=Y60

C Initialize variables for Runge Kutta Integration method

XNEW(1) = FGX

XNEW(2) = PZERO

XNEW(3) = TZERO

JUMP = 0

ONCE = 0

1162 C*********** START OF MAIN COMPUTATIONAL LOOP **************

1163 1059 DO 8000 P=0,100000

1164 IF ((DCGX.GT.0.0).OR.(CGX.LT.0.0)) THEN

1165 WRITE(*,*)' Something is wrong, conversion is proceeding'

1166 WRITE(*,*)' in the wrong direction or the concentration'

1167 WRITE(*,*)' of O2 has dropped below zero.'

1168 WRITE(*,*)' Try a lower computation display increment.'

1169 WRITE(*,*)' Try a lower gas inlet temperature or flowrate.'

1170 WRITE(*,*)

1171 WRITE(*,*)' Change in conc of O2 per step(DCGX) = ',DCGX

1172 WRITE(*,*)' O2 concentration(CGX) = ',CGX

1173 WRITE(*,*)

1174 GOTO 17000

1175 ENDIF

1176 C Check to see if conversion has been reached.

1177 IF (SSS2.EQ.'O') THEN

1178 IF ((CONVX.GE.CONV) GOTO 9900

1179 ELSE

1180 IF (X.GT. MONOL) GOTO 9900

1181 ENDIF

1182 C COMPUTE GAS AVG. MOLECULAR WEIGHT AND DENSITY

1183 6250 AMX = FXN4(Y)

1184 DENGAS=AMX*(PRESS/9896.0)/R/TGX

1185 C COMPUTE MONOLITH FLOW RATE, CHANNEL FLOW RATE AND CHANNEL VELOCITY

1186 MVFL0 = MOLLFO / (AMX * DENGAS)

1187 CHFLO = MVFL0 / NOCHM

1188 CHGVEL = CHFLO / (MCW * MCH)

1189 C COMPUTE BULK DIFFUSIVITY OF O2

1190 DAB = FXN3(Y,TGX)

1191 C COMPUTE EFFECTIVE DIFFUSIVITY OF MIXTURE AT TSX

1192 DABEFF= FXN1(DAB,Y(5),PRESS,RMICRO,RMACRO,

1193 + TSX,EMACRO,EMICRO)

1194 IF (MOD( CONSTA,4 ) .GT. 0.0 ) GO TO 6669

1195 T=TSX

1196 C COMPUTE VISCOSITY OF COMPONENT GASES AT TGX

1197 CALL VIS(TGX,VISC,VISCT)
C COMPUTE THERMAL CONDUCTIVITY OF COMPONENT GASES AT TGX
1199 CALL TCON(TGX,TCONT)
1200 C COMPUTE VISCOSITY AND THERMAL CONDUCTIVITY OF MIXTURE
1201 CALL PROP(Y,TCONT,VISCT,VISCTC,K)
1202 6666 CONTINUE
1203 C COMPUTE HEAT CAPACITY OF GAS MIXTURE AT TGX
1204 CGAS=FNX2(Y,TGX)
1205 C Limiting Nu and Sh numbers are 2.976. This is taken from page
1206 C 241 of Convective Heat Transfer by Burmeister, L. C., John
1207 C Wiley & Sons, (1983). This assumes a constant temperature
1208 C profile (Nu) or concentration profile (Sh).
1209 6669 KC = 2.976 * DAB / CHHD
1210 H = 2.976 * K / CHHD
1211 A = AREF * DEXP(-ENGACT/ R *(TREF-TSX)/TSX/TREF)
1212 THIELE = CMCWT * DSQRT( A * DENCAT / DABEFF)
1213 IF ( (THIELE.GT.100.0) .AND. (ONCE.NE.1) ) THEN
1214 WRITE(*,*) 'THIELE MODULUS IS > 100. SETTING THIELE=100'
1215 WRITE(*,*) 'TO PREVENT NUMERIC OVERFLOW ERROR'
1216 ONCE=1
1217 ENDIF
1218 IF ( (THIELE.GT.100.0) ) THIELE=100.0
1219 N = DTANH ( THIELE ) / THIELE
1220 CONST1= N*A*CMCWT*DENCAT
1221 CSX = CGX * ( KC ) / (KC+CONST1)
1222 TSX =TGX + HEATRX*CSX*CONST1/H
1223 IF (FIRST.EQ..TRUE.) THEN
1224 A = AREF*DEXP(-ENGACT/ R*(TREF-TSX)/TSX/TREF)
1225 THIELE = CMCWT * DSQRT( A * DENCAT / DABEFF)
1226 N = DTANH ( THIELE ) / THIELE
1227 CONST1= N*A*CMCWT*DENCAT
1228 CSX = CGX * ( KC ) / (KC+CONST1)
1229 TSX =TGX + HEATRX*CSX*CONST1/H
1230 IF (SSS.EQ.'I') TSX=TGX
1231 IF (P.EQ.0) THEN
1232 XZ=0
1233 CONVXZ=0.0
1234 CGXZ=CGX
1235 CSXZ=CSX
1236 TSXZ=TSX
1237 ENDIF
1238 ENDIF
1239 FE=1000.0*CHHD*CHGVEL*DENGAS/VISCTC
1240 CONYX = 100.0*(CGXZ-CGX*TSX) / TZERO*PZERO/PRESS) /CGXZ
1241 C HEADER OUTPUT SECTION
1242 C Print out Reynold's number the first time through the loop.
1243 C If First = .true. then print out reynold's number, else don't
1244 C worry about it. Also, print out header and results at position X=0
1245 IF (FIRST.EQ..TRUE.) THEN
1246 C Output of selectable parameter to data file
1247 CALL OUTPUT(1,MSMT,MTDF,MTDV,MCW,NOCHV,NOCHH,MCWT,
1248 + Y,MYFLZ,TZERO,PZERO,DENCAT,AREF,ENGACT,
1249 + EMIHRO,EMACRO,EMICO,EMACRO,SSS,SSS1,SSS2,
1250 + DABEFF,PRESS,Y,DX)
1251 FIRST=.FALSE.
1252 WRITE(*,*)
```
1255 WRITE (25,*)
1256 WRITE (*,9950)
1257 WRITE (25,9950)
1258 WRITE(*,9951)
1259 WRITE(25,9951)
1260 9950 FORMAT('Distance',1X,'%Conver',2X,'O2gas',4X,'O2wall',2X,
1261 +'O2center',3X,'Tgas',5X,'Twall',3X,'DPress')
1262 9951 FORMAT('mm',11X,'(mMOL/L)',1X,'(mMOL/L)',1X,'(mMOL/L)',
1263 +1X,'(Kelvin)',1X,'(Kelvin)',3X,'(kPa)')
1264 WRITE(*,*)
1265 WRITE(25,*)
1266 WRITE(*,10) XZ,CONVX,CGX*1E+09,CSX*1E+09,
1267 +(-CSX*1E+09/DCOSH(THIELE)),TZERO,TSXZ,(PZERO-PZERO)*101.325
1268 WRITE(25,20) XZ,S,CONVX,S,CGX*1E+09,S,CSX*1E+09,S,
1269 +(CSX*1E+09/DCOSH(THIELE)),S,TZERO,S,TSXZ,S,
1270 +(PZERO-PZERO)*101.325
1271 10 FORMAT(F8.3,1X,F8.4,1X,F7.4,1X,F7.4,1X,F7.4,1X,F7.4,1X,F7.4,5X,F7.3,1X,F8.3
1272 +,1X,E10.3)
1273 20 FORMAT(F8.3,A1,F8.4,A1,F7.4,A1,F7.4,A1,F7.4,A1,F7.3,A1,F8.3
1274 +,A1,E10.3)
1275 ELSE
1276 C COMPUTED VALUES OUTPUTTED TO SCREEN AND FILE AT DISPLAY INTERVAL
1277 C WRITE RESULTS TO SCREEN WHEN REMAINDER OF CONSTA/FACTOR > 0
1278 C ELSE, JUST CALCULATE VALUES AND DON'T PRINT THEM OUT.
1279 IF (MOD(CONSTA,FACTOR).GT.0.0) GOTO 7777
1280 IF (SSS1.EQ.'I') GOTO 7777
1281 IF (SSS.EQ. 'I') TSX=TGX
1282 WRITE(*,10) X,CONVX,CGX*1E+09,CSX*1E+09,
1283 +(CSX*1E+09/DCOSH(THIELE)),TGX,TSX,(PRESS-PZERO)*101.325
1284 WRITE(25,20) X,S,CONVX,S,CGX*1E+09,S,CSX*1E+09,S,
1285 +(CSX*1E+09/DCOSH(THIELE)),S,TGX,S,TSX,S,
1286 +(PRESS-PZERO)*101.325
1287 7777 ENDIF
1288 C Reset variables each time Runge Kutta Subroutine is called
1289 7888 X0(1) = XNEW(1)
1290 X0 (2) = XNEW(2)
1291 X0 (3) = XNEW(3)
1292 C Call Runge Kutta Subroutine:
1293 CALL RK4(DX,X,X0,XNEW)
1294 C PARAMETER UPDATE SECTION
1295 C VALUE OF THE PARAMETER UPDATE SECTION
1296 FGX = XNEW(1)
1297 PRESS = XNEW(2)
1298 IF (SSS.EQ. 'I') THEN
1299 TGX = TZERO
1300 ELSE
1301 TGX = XNEW(3)
1302 ENDIF
1303 CGX = FGX/CHFLO
1304 DCGX=CGX-CGSTMP
1305 X = X + DX
1306 CGXTMP=CGX
1307 Y(5) = Y50*(100.0-CONVX)/100.0
1308 Y(4) = Y40-2*(Y50-Y(5))
1309 Y(3) = Y30+2*(Y50-Y(5))
1310 Y(1) = Y10
1311 Y(2) = Y20
```
Y(6)=Y60
CONST7 = Y(1) + Y(2) + Y(3) + Y(4) + Y(5) + Y(6)
DO 33445 JJ=1,6
   Y(JJ)=Y(JJ)/CONST7
33445 CONTINUE
C ADAPTIVE STEP SIZE SECTION
IF (((-100.*DCGX/CGX.GT.0.08)) .AND. (JUMP.LT.1.)) THEN
   DX = DX/5.0
   FACTOR = FACTOR*5
   CONSTA=FACTOR-1
   WRITE(*,*) 'Reduced step size to ', DX, ' mm'
ENDIF
CONSTA=CONSTA + 1
C PARAMETER BOUNDARY CHECK
C Check to make sure that Temperature, Pressure, and Reynold's 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
IF (TGX.GT.700.0) THEN
   WRITE(*,*) 'Current Gas Temperature = ',TGX
   WRITE(*,*) 'Error:'
   WRITE(*,*) 'This value exceeds the allowable' maximum temperature of 700 K'
   WRITE(*,*) 'Lower the inlet gas temperature.'
   WRITE(*,*)
   WRITE(*,*) 'Hit Return When Finished Viewing'
   WRITE(*,*)
   READ(*,621) S
   WRITE(*,*)
   WRITE(*,*)
   GOTO 7564
ELSE IF (RE.GT.2300.0) THEN
   WRITE(*,*) 'Current Reynolds number = ',RE
   WRITE(*,*) 'Error:'
   WRITE(*,*) 'This value exceeds the maximum'
   WRITE(*,*) 'allowable Reynolds number of 2300.'
   WRITE(*,*) 'Reduce the inlet gas flowrate.'
   WRITE(*,*)
   WRITE(*,*)
   WRITE(*,*) 'Hit Return When Finished Viewing'
   WRITE(*,*)
   READ(*,621) S
   WRITE(*,*)
   WRITE(*,*)
   GOTO 7564
ELSE IF ((TGX.LT.200.0)) THEN
   WRITE(*,*)
   WRITE(*,*) 'Current Gas Temperature = ',TGX
   WRITE(*,*) 'Error:'
   WRITE(*,*) 'This value is less than the minimum'
   WRITE(*,*) 'allowable Temperature of 200 K.'
1369 WRITE(*,*),'Raise the inlet gas temperature.'
1370 WRITE(*,*)
1371 WRITE(*,*),'Hit Return When Finished Viewing'
1372 WRITE(*,*)
1373 READ(*,621) S
1374 WRITE(*,*)
1375 WRITE(*,*)
1376 GOTO 7564
1377 ELSE IF(PRESS*101.325.GT.350.0) THEN
1378 WRITE(*,*)
1379 WRITE(*,*),'Current Pressure= ',PRESS*101.325,' kPa'
1380 WRITE(*,*)
1381 WRITE(*,*),'Error:'
1382 WRITE(*,*),'This value exceeds the maximum '
1383 WRITE(*,*),'allowable Pressure of 350 kPa.'
1384 WRITE(*,*),'Reduce the inlet gas pressure.'
1385 WRITE(*,*)
1386 WRITE(*,*),'Hit Return When Finished Viewing'
1387 WRITE(*,*)
1388 READ(*,621) S
1389 WRITE(*,*)
1390 WRITE(*,*)
1391 GOTO 7564
1392 ELSE IF (PRESS*101.325.LT.0.1) THEN
1393 WRITE(*,*)
1394 WRITE(*,*),'Current Pressure= ',PRESS*101.325,' kPa'
1395 WRITE(*,*)
1396 WRITE(*,*),'Error:'
1397 WRITE(*,*),'This value is below the minimum '
1398 WRITE(*,*),'allowable Pressure of 0.1 kPa.'
1399 WRITE(*,*),'Raise the inlet gas pressure.'
1400 WRITE(*,*)
1401 WRITE(*,*),'Hit Return When Finished Viewing'
1402 WRITE(*,*)
1403 READ(*,621) S
1404 WRITE(*,*)
1405 WRITE(*,*)
1406 GOTO 7564

C***END OF MAIN COMPUTATION LOOP***

C OUTPUT OF FINAL PARAMETERS VALUES TO SCREEN AND FILE
1410 1411 1412 1413 1414 1415 1416 1417 1418 1419 1420 1421 1422 1423 1424 1425 16900 WRITE(25,*)
16950 CSX = CGX * ( KC ) / (KC+CONST1)
16970 TSX =TGX + HEATRX*CSX*CONST1/
16980 IF (SSS.EQ.'T') TSX=TGX
16990 CONVX = 100.0* (CGX2-CGX*TGX/TZEROPZERO/PRESS)/CGX2
17000 WRITE(*,10) X,CONVX,CGX*1E+09,CSX*1E+09,
17010 + (CGX2*1E09/DCOSH(THIELE)),TGX,TSX, (PRESS-PZERO)*101.325
17020 WRITE(25,20) X,S,CONVX,S,CGX*1E+09,S,CSX*1E+09,S,
17030 + (CSX*1E+09/DCOSH(THIELE)),S,TGX,TSX,S,
17040 + (PRESS-PZERO)*101.325
17050 WRITE(25,*)
RE=1000.0*CHHD*CHGVEL*DENGAS/VISCTC
CALL HEADER (1, RE, CPGAS, DENGAS, CHGVEL, N, DAB, + DABEFF, PRESS, Y, DX)
WRITE(*,*) BEEP, BEEP, BEEP
WRITE(*,*)  
CALL HEADER (1, RE, CPGAS, DENGAS, CHGVEL, N, DAB, + DABEFF, PRESS, Y, DX)
WRITE(*,*) BEEP, BEEP, BEEP
READ(*,621) S
C RESET OTHER PARAMETERS BACK TO ORIGINAL VALUES.
MVFLO=MVFLZ
Y (1)=Y10
Y (2)=Y20
Y (3)=Y30
Y (4)=Y40
Y (5)=Y50
Y (6)=Y60
GOTO 9001
99999 END
C********************************************************END OF MAIN PROGRAM********************************************

C********************************************************SUBROUTINE RK4 ********************************************************
C** Programmer: Seth Daniel Goldblum, UCSD, July 1988
C** Runge Kutta Subroutine to solve N differential
C** Equations simultaneously.
C** This subroutine relies on a main program to feed it
C** the following:
C** 1) The starting value of the independent variable, P
C** 2) The step size, DX
C** The subroutine returns the values of all dependent variables
C** at the evaluated point of the independent variable in an array
C** Xnew(N)
C** The subroutine requires and additional subroutine called func
C** which is declared external and contains the functions of all
C** derivatives to be evaluated simultaneously.
C** Identifiers:
C** X0 (N) array of N initial values of the functions
C** P initial value of the independent variable
C** F(N) array of N elements containing the values of
C** the functions evaluated at some point.
C** DX step size
C** XNEW(N) array of N values containing the values of
C** the dependent variables
C** KL (N) array of N values containing the values of KL
C** used in the Runge - Kutta method
C-* K2(N) array of N values containing the values of K2
C-* used in the Runge-Kutta method
C-* K3(N) array of N values containing the values of K3
C-* used in the Runge - Kutta method
C-* K4(N) array of N values containing the values of K4
C-* used in the Runge-Kutta method

SUBROUTINE RK4(DX,P,XO,XNEW)
REAL*8 XO(3), P, F(3), DX, XNEW(3), K1(3), K2(3), K3(3), K4(3)

first approx.
CALL FUNC(P,XO,F)
DO 10 J=1,3
   K1(J)=DX*F(J)
   XNEW(J)=XO(J) + K1(J)/2.0
10 CONTINUE

second approx.
CALL FUNC(DX/2.0 + P, XNEW,F)
DO 20 J=1,3
   K2(J)=F(J)*DX
   XNEW(J)=XO(J) + K2(J)/2.0
20 CONTINUE

third approx.
CALL FUNC(DX/2.0 + P, XNEW,F)
DO 30 J=1,3
   K3(J)=F(J)*DX
   XNEW(J)=XO(J) + K3(J)
30 CONTINUE

fourth approx.
CALL FUNC(DX + P, XNEW,F)
DO 40 J=1,3
   K4(J)=F(J)*DX
   XNEW(J)=XO(J) + (K1(J) + 2*K2(J) +2*K3(J) +K4(J))/6.0
40 CONTINUE
RETURN
END

C**************************SUBROUTINE FUNC**************************

SUBROUTINE FUNC(P,XO,F)

This subroutine is used to store the functions used
in the runge-kutta method for solving them.
COMMON /ELK/ KC,CHSTV,MCH,MCW,CSX,CGX,CHFLO,CPGAS
COMMON /ELK2/ VISCTC,CHGVEL,CHHD,H,TSX,DENGAS
REAL*8 F(3),XO(3)
REAL*8 KC,CHSTV,MCH,MCW,CSX,CGX,CHFLO,CPGAS
REAL*8 VISCTC,CHGVEL,CHHD,H,TSX,DENGAS
FGX=XO(1)
TGX=XO(3)

F(1) is the differential equation describing the change
in molar flowrate of O2 (moles/s) for a change in length:
F(1) = -KC*CHSTV*MCH*MCW*(CGX-CSX)

F(2) is the differential equation describing the change
in Pressure for a change in length
F(2) = -32.0*(VISCTC/1000.0)*CHGVEL/CHHD/CHHD/101330.0

C-
C-* F(3) is the differential equation describing the change
C-* in temperature for a change in length.
C-*
F(3) = H*CHSTV*MCH*MCW/CHF'LO* (TSX-TGX) /
C-*
(DENGAS*CPGAS)
C-*
RETURN
END
1540
1541
1542 Subroutine LINES(K)
1543 Integer J,K
1544 DO 459 J=1,K
1545 WRITE(*,*)
459 CONTINUE
1546 Return
End
1547
1548 Subroutine HEADER(FLAG, RE, CPGAS, DENGAS, CHGVEL, N, DAB,
1549 + DABEFF, PRESS, Y, DX)
1550 Real*8 PRESS, RE, CPGAS, DENGAS, CHGVEL, N, DAB, DABEFF, Y(6), DX
1551 Integer FLAG
1552 If (FLAG.EQ.0) THEN
1553 Write(*,*), ' Initial values'
1554 Write(25,*), ' Initial values'
1555 ENDIF
1556 If (FLAG.EQ.1) THEN
1557 Write(*,*), ' Final values'
1558 Write(25,*), ' Final values'
1559 WRITE(*,*) Mole fractions: '
1560 WRITE(*,3233) Y(1),Y(2),Y(3)
1561 WRITE(*,3234) Y(4),Y(5),Y(6)
1562 WRITE(25,*), Mole fractions: '
1563 WRITE(25,3233) Y(1),Y(2),Y(3)
1564 WRITE(25,3234) Y(4),Y(5),Y(6)
1565 Format(' He = ',F6.4,' Ar = ',F6.4,' CO2 = ',F6.4)
1566 Format(' CO = ',F6.4,' O2 = ',F6.4,' N2 = ',F6.4)
1567 WRITE(*,6777) PRESS*101.325
1568 Write(25,6777) PRESS*101.325
1569 ENDIF
1570 Write(*,10), RE
1571 Format(' Reynolds number = ',F9.3)
1572 Write(*,20), CPGAS
1573 Format(' Gas Heat Capacity (J/K-g) = ',F9.3)
1574 WRITE(*,30) DENGAS*1000
1575 Format(' Gas Density (g/cm^3) = ',F10.7)
1576 WRITE(*,40) CHGVEL
1577 Format(' Gas Velocity (mm/s) = ',F9.3)
1578 WRITE(*,50) N
1579 Format(' Effectiveness factor = ',F9.5)
1580 Write(*,60) DAB/100.0
1581 Format(' Bulk Gas Diffusivity(cm^2/s) = ',F9.5)
1582 WRITE(*,70) DABEFF/100.0
Appendix 4 - program listing

1597 70 Format(' Effective Diffusivity(cm^2/s)= ',F9.6)
1598 WRITE(*,80) DX
1599 80 Format(' Step size(mm) = ',F9.6)
1600 WRITE(25,10) RE
1601 WRITE(25,20) CGAS
1602 WRITE(25,30) DENGAS*1000
1603 WRITE(25,40) CHGVEL
1604 WRITE(25,50) N
1605 WRITE(25,60) DAB/100
1606 WRITE(25,70) DABEFF/100
1607 WRITE(25,80) DX
1608 Return
1609 End

1610 Subroutine TCON (T, TCONT)
1611 Real*8 T, TCONT (6)
1612 C Compute thermal cond. (TCONT(i)) for a given species at temp. T
1613 C Units on TCON are mW/cm-K.
1614 C The index of TCONT(i) corresponds to the species.
1615 C Species: 1=He, 2=Ar, 3=CO2, 4=CO, 5=O2, 6=N2.
1616 C The following polynomial equations used to compute the
1617 C thermal conductivity of each species at temperature T
1618 C have been taken from page 515 of "Properties of Gases and Liquids"
1619 C 4th Ed. Reid, Prausnitz, & Sherwood
1620 TCONT(1) = (3.722E-2 + 3.896E-4*T - 7.450E-8*T**2 +
1621 1 1.290E-11*T**3)*10.0
1622 TCONT(2) = (2.714E-3 + 5.540E-5*T - 2.178E-8*T**2 +
1623 1 5.528E-12*T**3)*10.0
1624 TCONT(3) = (-7.215E-3 + 8.015E-5*T + 5.477E-9*T**2 -
1625 1 1.053E-11*T**3)*10.0
1626 TCONT(4) = (5.067E-4 + 9.125E-5*T - 3.524E-8*T**2 +
1627 1 8.199E-12*T**3)*10.0
1628 TCONT(5) = (-3.273E-4 + 9.966E-5*T - 3.743E-8*T**2 +
1629 1 9.732E-12*T**3)*10.0
1630 TCONT(6) = (3.919E-4 + 9.816E-5*T - 5.067E-8*T**2 +
1631 1 1.504E-11*T**3)*10.0
1632 Return
1633 End

1634 Subroutine PROP(Y, TCONT, VISCT, VISCTC, K)
1635 Real*8 AX(6,6), VISCTC, K, SUM, MW(6), Y(6), TCONT(6)
1636 Real*8 CONSTD, VISCT(6), LAMBDA, CONSTF
1637 Integer I, J
1638 C Read in molecular weights MW(I) into array.
1639 C The index of MW correspond to the species.
1640 C Species: 1=He, 2=Ar, 3=CO2, 4=CO, 5=O2, 6=N2.
1641 DATA MW(1), MW(2), MW(3), MW(4), MW(5), MW(6)
1642 + / 4.0026, 39.948, 44.01, 28.0105, 31.9988, 28.0134/
1643 C Compute parameter matrix AX(i,j)
1644 C The indexes of AX(i,j) correspond to the species.
1645 C Species: 1=He, 2=Ar, 3=CO2, 4=CO, 5=O2, 6=N2.
The AX(i, j) matrix is defined on p. 531 of "Properties of Gases and Liquids", 4th ed., Reid, Prausnitz, & Sherwood. Both the bulk gas thermal conductivity and the bulk gas viscosity can be computed using the AX(6, 6) matrix.

```fortran
VISCTC = 0.0
LAMBMX=0.0
DO 551 I =1,6
    SUM = 0.0
    DO 651 J = 1,6
       IF (I.EQ.J) THEN
          AX(I,J)=1.0
       ELSE
          CONSTE = MW(I)/MW(J)
          CONSTD = VISCT(I)/(CONSTE*VISCT(J))
          AX(I,J) = (1+CONSTD*CONSTE**0.25)**2/
                     DSQRT(8.0*(1.0+CONSTE))
       END IF
    SUM = SUM + Y(I)*AX(I,J)
CONTINUE
CONSTF = Y(1)/SUM
LAMBMX = LAMBMX + CONSTF*TCONT(I)
VISCTC = VISCTC + CONSTF*VISCT(I)
CONTINUE
K = LAMBMX/10000.0
RETURN
END
```

Subroutine VIS(T,VISC,VISCT)
```fortran
Real*8 T,VISC(6,2:7),VISCT(6),CONST5
Integer I
Compute viscosity (VISCT(i)) for a given species at temp. T
Units on VISCT are centipoises.
The index of VISC corresponds to the species.
Species: 1=He, 2=Ar, 3=CO2, 4=CO, 5=O2, 6=N2.
CONST5 is a temporary value holding constant
DO 2223 I=1,6
   CONST5=VISC(I,INT(1+T/100.0)) - VISC(I,INT(T/100.0))
   CONST5=CONST5*(T/100.0-INT(T/100.0))
   VISCT(I)=VISCT(I,INT(T/100.0)) + CONST5
CONTINUE
RETURN
END
```

Subroutine OUTPUT(FLAG,MCST,MPDH,MPDV,MCW,NOCHV,NOCHH,MCWT,
```fortran
+ Y,MVFLZ,TZERO,PZERO,DENCAT,AREF,ENGACT,
+ EMICRO,EMACRO,RCMICRO,RMACRO,SSS,SSS1,SSS2,
+ CONV,MONOL,DX,CDI)
Integer FLAG
Real*8 MCST,MPDH,MPDV,MCW,NOCHV,NOCHH,MCWT
Real*8 Y(6),MVFLZ,TZERO,PZERO,DENCAT,AREF,ENGACT
```

```
C**************************************************************************
C** SUBROUTINE VIS *******************************************************
C**************************************************************************

Subroutine VIS(T,VISC,VISCT)
Real*8 T,VISC(6,2:7),VISCT(6),CONST5
Integer I
Compute viscosity (VISCT(i)) for a given species at temp. T
Units on VISCT are centipoises.
The index of VISC corresponds to the species.
Species: 1=He, 2=Ar, 3=CO2, 4=CO, 5=O2, 6=N2.
CONST5 is a temporary value holding constant
DO 2223 I=1,6
   CONST5=VISC(I,INT(1+T/100.0)) - VISC(I,INT(T/100.0))
   CONST5=CONST5*(T/100.0-INT(T/100.0))
   VISCT(I)=VISCT(I,INT(T/100.0)) + CONST5
CONTINUE
RETURN
END

Subroutine OUTPUT(FLAG,MCST,MPDH,MPDV,MCW,NOCHV,NOCHH,MCWT,
   + Y,MVFLZ,TZERO,PZERO,DENCAT,AREF,ENGACT,
   + EMICRO,EMACRO,RCMICRO,RMACRO,SSS,SSS1,SSS2,
   + CONV,MONOL,DX,CDI)
Integer FLAG
Real*8 MCST,MPDH,MPDV,MCW,NOCHV,NOCHH,MCWT
Real*8 Y(6),MVFLZ,TZERO,PZERO,DENCAT,AREF,ENGACT
```

```
C**************************************************************************
C** SUBROUTINE OUTPUT *****************************************************
C**************************************************************************

Subroutine OUTPUT(FLAG,MCST,MPDH,MPDV,MCW,NOCHV,NOCHH,MCWT,
   + Y,MVFLZ,TZERO,PZERO,DENCAT,AREF,ENGACT,
   + EMICRO,EMACRO,RCMICRO,RMACRO,SSS,SSS1,SSS2,
   + CONV,MONOL,DX,CDI)
Integer FLAG
Real*8 MCST,MPDH,MPDV,MCW,NOCHV,NOCHH,MCWT
Real*8 Y(6),MVFLZ,TZERO,PZERO,DENCAT,AREF,ENGACT
```
Program Listing 31

Appendix 4

1711 Real*8 EMICRO, EMACRO, RMICRO, RMACRO
1712 Character*1 SSS, SSSI, SSS2, S
1713 Real*8 CONV, MONOL, DX, CDI
1714 C Flag=0 => Output parameters to screen for review
1715 C Flag=1 => Output parameters to file LDATA
1716 IF (FLAG.EQ.1) GOTO 40000
1717 WRITE(*,6000)
1718 6000 FORMAT(20X,'SELECTABLE PARAMETER SUMMARY')
1719 WRITE(*,*)'Monolith Dimensions (mm):
1720 WRITE(*,6001) MCST, MFDC, MFNV
1721 6001 FORMAT('Support wall thickness: ',F6.2,3X,'Face dimension: ',
1722 2F7.2, 'x', F7.2)
1723 WRITE(*,6002) MCW, NOCHV, NOCHH
1724 6002 FORMAT('Channel inner dimension: ',F6.2,3X,'Face channels',
1725 2': ',F6.2,'x',F6.2)
1726 WRITE(*,6003) MCWT, 100*(MCW**2/(MCST*2+MCW)**2)
1727 6003 FORMAT('Active layer thickness: ',F6.2,4X,'% monol volume',
1728 'on: ',F6.1)
1729 WRITE(*,*)
1730 WRITE(*,*)'Monolith inlet parameters:
1731 WRITE(*,6006) Y(3), Y(4), Y(5), Y(6), Y(1), Y(2)
1732 6006 FORMAT('Gas Composition (mole fraction): CO2: ',F6.4,2X,
1733 2'CO: ',F6.4,2X,'O2: ',F6.4,2X,'He: ',F6.4,2X,
1734 3'Ar: ',F6.4)
1735 WRITE(*,6007) MVFLZ, TZERO, PZERO*101.325
1736 6007 FORMAT('Gas Flowrate (liters/s): ',F7.3,
1737 2Gas Temperature (K): ',F7.3)
1738 WRITE(*,*)
1739 WRITE(*,*)'Catalyst Properties:
1740 WRITE(*,6008) DENCAT
1741 6008 FORMAT('Catalyst Density (g/mm^3): ',E10.3)
1742 WRITE(*,6009) AREF
1743 6009 FORMAT('Reaction rate constant at 298K(mm^3/gcat-s): ',F8.2)
1744 WRITE(*,6010) ENGACT
1745 6010 FORMAT('Activation energy (J/mol): ',F10.2)
1746 WRITE(*,6004) EMICRO, EMACRO
1747 6004 FORMAT('Void-fraction as micropores: ',F4.2,
1748 2'Void-fraction as macropores: ',F4.2)
1749 WRITE(*,6005) RMICRO, RMACRO
1750 6005 FORMAT('Avg. micropore radius (nm): ',E7.2,
1751 2'Avg. macropore radius (nm): ',E7.2)
1752 WRITE(*,*)'Computational loop parameters:
1753 IF (SSS.EQ.'A') WRITE(*,6011)
1754 6011 FORMAT('Thermal Operation (adiabatic/isothermal): Adiabatic')
1755 IF (SSS.EQ.'I') WRITE(*,6012)
1756 6012 FORMAT('Thermal Operation (adiabatic/isothermal): Isothermal')
1757 WRITE(*,*)
1758 WRITE(*,*)'Output file (Full Profile/Summary):
1759 IF (SSS1.EQ.'S') WRITE(*,6013)
1760 6013 FORMAT('Output file (Full Profile/Summary): Summary')
1761 IF (SSS1.EQ.'P') WRITE(*,6014)
1762 6014 FORMAT('Output file (Full Profile/Summary): Full Profile')
1763 IF (SSS2.EQ.'O') WRITE(*,6015) CONV
1764 6015 FORMAT('Termination on (O2 conversion/Length): ',
1765 2'O2 conversion. %: ',F7.3)
1766 IF (SSS2.EQ.'L') WRITE(*,6016) MONOL
1767 6016 FORMAT('Termination on (O2 conversion/Length): ',
1768 2'Length. Length (mm): ', F7.3)
IF (SSI.EQ.'P') WRITE(*,6017) DX,CDI
1769 6017 FORMAT(' Computation loop step size (mm): ',F7.4)
1770 2   ' Display every ',F6.2,' mm')
1771 IF (SSI.EQ.'S') WRITE(*,6018) DX
1772 6018 FORMAT(' Computation loop step size (mm): ',F7.4)
1773 WRITE('(*,*')
1774 WRITE('(*,6019')
1775 6019 FORMAT(15X,' => Hit Return When Finished Viewing <=')
1776 621 FORMAT(A)
1777 READ(*,621) S
1778 WRITE('(*,*')
1779 WRITE('(*,*')
1780 GOTO 80000
1781 40000 WRITE('(*,*')
1782 WRITE(25,*)
1783 WRITE(25,6000)
1784 WRITE(25,*)' Monolith Dimensions (mm): '
1785 WRITE(25,6001) MCST, MFDH, MFDV
1786 WRITE(25,6002) MCW, NOCHV, NOCHH
1787 WRITE(25,6003) MCWT, 100*(MCW**2/(MCST*2+MCW)**2)
1788 WRITE(25,*)
1789 WRITE(25,*)' Monolith inlet parameters: '
1790 WRITE(25,6006) Y(3), Y(4), Y(5), Y(6), Y(1), Y(2)
1791 WRITE(25,6007) MVFLZ, TZERO, PZERO*101.325
1792 WRITE(25,*)
1793 WRITE(25,*)' Catalyst Properties: '
1794 WRITE(25,6008) DENCAT
1795 WRITE(25,6009) AREF
1796 WRITE(25,6010) ENGACT
1797 WRITE(25,6004) EMICRO, EMACRO
1798 WRITE(25,6005) RMICRO, RMACRO
1799 IF (SSI.EQ.'A') WRITE(25,6011)
1800 IF (SSI.EQ.'I') WRITE(25,6012)
1801 WRITE(25,*)
1802 WRITE(25,*)' Computational loop parameters: '
1803 IF (SSI.EQ.'S') WRITE(25,6013)
1804 IF (SSI.EQ.'P') WRITE(25,6014)
1805 IF (SSI.EQ.'O') WRITE(25,6015) CONV
1806 IF (SSI.EQ.'L') WRITE(25,6016) MONOL
1807 IF (SSI.EQ.'P') WRITE(25,6017) DX, CDI
1808 IF (SSI.EQ.'S') WRITE(25,6018) DX
1809 WRITE(25,*)
1810 WRITE('(*,*')
1811 80000 RETURN
1812 END
1813
1814
1815
1816 C************** FUNCTION FXN1  **************
1817 FUNCTION FXN1(TDAB, Y5, PRESS, RMICRO, RMACRO,
1818 + TSX, EMACRO, EMICRO)
1819 REAL*8 TDAB, Y5, PRESS, RMICRO, RMACRO
1820 REAL*8 TSX, EMACRO, EMICRO, DMICR, DMACR
1821 REAL*8 DMACRO, DMICRO
1822 C Effective diffusivity is computed using the micro-macro
1823 C pore model of Wakao and Smith as described on pages 170-
1824 C 171 of Chemical Reactor Analysis and Design by Froment
and Bishoff

```
1825 C
1826 TDAB=(1-Y5)/TDAB/PRESS
1827 DVMICR =171482.0*RMICRO/1E+7*DSQT(TSX)
1828 DMACR =171482.0*RMACRO/1E+7*DSQT(TSX)
1829 DMICR =1.0/(1.0/ TDAB + 1.0/DVMICR)
1830 DMACR =1.0/(1.0/ TDAB + 1.0/DMACR)
1831 FXN1 = EMACRO**2*DMACR + (EMICRO**2*DMICR* (1.0 +
1832                  * 3.0*EMACRO))/(1.0 - EMACRO)
1833 RETURN
1834 END
1835
1836 C****************** FUNCTION FXN2 ********************
1837 C Function computes heat capacity of gas mixture using
1838 C data from the JANAF tables.
1839 C MW, CP, Y indexes 1=He, 2=Ar, 3=CO2, 4=CO, 5=O2, 6=N2
1840 Real*8 Y (6), TGX, CP (6), MW (6)
1841 C Read in molecular weights MW(I) into array.
1842 DATA MW (1), MW(2), MW (3), MW (4), MW (5), MW (6)
1843 + / 4.0026, 39.948, 44.01, 28.0105, 31.9988, 28.0134 /
1844 CP (1) = 20.786
1845 CP (2) = 20.786
1846 CP (3) = 20.712+6.2501E-02*TGX-1.186E-5*TGX*TGX
1847 + -5.5737E-08*TGX*TGX*TGX + 4.1875E-11*TGX*TGX*TGX*TGX
1848 CP (4) = 28.777 + 5.5297E-03*TGX -3.1851E-5*TGX*TGX
1849 + +7.0946E-08*TGX*TGX*TGX -4.2501E-11*TGX*TGX*TGX
1850 CP (5) = 31.033 - 2.0261E-02*TGX +6.3410E-05*TGX*TGX
1851 CP (6) = 28.567 + 7.3978E-03*TGX -3.5831E-05*TGX*TGX
1852 + +6.9415E-08*TGX*TGX*TGX -3.8499E-11*TGX*TGX*TGX
1853 FXN2 = Y (1) * CP (1) / MW (1) + Y (2) * CP (2) / MW (2) +
1854 + Y (3) * CP (3) / MW (3) + Y (4) * CP (4) / MW (4) +
1855 + Y (5) * CP (5) / MW (5) + Y (6) * CP (6) / MW (6)
1856 RETURN
1857 END
1858
1859 C******************FUNCTION FXN3**************
1860 C Function FXN3(Y,TGX)
1861 Real*8 Y (6), D (6), TGX, CONST
1862 C Compute diffusivity of O2 in gas mixture
1863 C Read in binary diffusivity coefficients D(I) into array.
1864 C The index of D correspond to the species in which O2 is diffusing
1865 C Note: There is no D(5) defined. These are reference values at
1866 C 298K, 1 atm, units(mm^2/s)
1867 C Species: 1=He, 2=Ar, 3=CO2, 4=CO, 6=N2.
1868 DATA D(1), D(2), D(3), D(4), D(6)
1869 + / 72.9, 21.2, 16.4, 15.6, 22.5 /
1870 CONST=0.0
1871 DO 8451 I = 1, 6
1872 IF (I.EQ.5) GO TO 8451
1873 CONST= Y (I) / (D (I) * (TGX/298.0)**1.5) + CONST
1874 8451 CONTINUE
1875 FXN3=CONST
```

```
1825 C
1826 TDAB=(1-Y5)/TDAB/PRESS
1827 DVMICR =171482.0*RMICRO/1E+7*DSQT(TSX)
1828 DMACR =171482.0*RMACRO/1E+7*DSQT(TSX)
1829 DMICR =1.0/(1.0/ TDAB + 1.0/DVMICR)
1830 DMACR =1.0/(1.0/ TDAB + 1.0/DMACR)
1831 FXN1 = EMACRO**2*DMACR + (EMICRO**2*DMICR* (1.0 +
1832                  * 3.0*EMACRO))/(1.0 - EMACRO)
1833 RETURN
1834 END
1835
1836 C****************** FUNCTION FXN2 ********************
1837 C Function computes heat capacity of gas mixture using data
1838 C from the JANAF tables.
1839 C MW, CP, Y indexes 1=He, 2=Ar, 3=CO2, 4=CO, 5=O2, 6=N2
1840 Real*8 Y (6), TGX, CP (6), MW (6)
1841 C Read in molecular weights MW(I) into array.
1842 DATA MW (1), MW(2), MW (3), MW (4), MW (5), MW (6)
1843 + / 4.0026, 39.948, 44.01, 28.0105, 31.9988, 28.0134 /
1844 CP (1) = 20.786
1845 CP (2) = 20.786
1846 CP (3) = 20.712+6.2501E-02*TGX-1.186E-5*TGX*TGX
1847 + -5.5737E-08*TGX*TGX*TGX + 4.1875E-11*TGX*TGX*TGX*TGX
1848 CP (4) = 28.777 + 5.5297E-03*TGX -3.1851E-5*TGX*TGX
1849 + +7.0946E-08*TGX*TGX*TGX -4.2501E-11*TGX*TGX*TGX
1850 CP (5) = 31.033 - 2.0261E-02*TGX +6.3410E-05*TGX*TGX
1851 CP (6) = 28.567 + 7.3978E-03*TGX -3.5831E-05*TGX*TGX
1852 + +6.9415E-08*TGX*TGX*TGX -3.8499E-11*TGX*TGX*TGX
1853 FXN2 = Y (1) * CP (1) / MW (1) + Y (2) * CP (2) / MW (2) +
1854 + Y (3) * CP (3) / MW (3) + Y (4) * CP (4) / MW (4) +
1855 + Y (5) * CP (5) / MW (5) + Y (6) * CP (6) / MW (6)
1856 RETURN
1857 END
1858
1859 C******************FUNCTION FXN3**************
1860 C Function FXN3(Y,TGX)
1861 Real*8 Y (6), D (6), TGX, CONST
1862 C Compute diffusivity of O2 in gas mixture
1863 C Read in binary diffusivity coefficients D(I) into array.
1864 C The index of D correspond to the species in which O2 is diffusing
1865 C Note: There is no D(5) defined. These are reference values at
1866 C 298K, 1 atm, units(mm^2/s)
1867 C Species: 1=He, 2=Ar, 3=CO2, 4=CO, 6=N2.
1868 DATA D(1), D(2), D(3), D(4), D(6)
1869 + / 72.9, 21.2, 16.4, 15.6, 22.5 /
1870 CONST=0.0
1871 DO 8451 I = 1, 6
1872 IF (I.EQ.5) GO TO 8451
1873 CONST= Y (I) / (D (I) * (TGX/298.0)**1.5) + CONST
1874 8451 CONTINUE
1875 FXN3=CONST
```
RETURN
END

FUNCTION FXN4******FUNCTION FXN4**************

Function FXN4(Y)

Real*8 MW(6),Y(6),CONST

C Compute gas average molecular weight

C MW, Y indexes 1=He, 2=Ar, 3=CO2, 4=CO, 5=O2, 6=N2

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/

CONST=0.0

DO 355 I=1,6

CONST=MW(I)*Y(I)+CONST

CONTINUE

FXN4=CONST

RETURN

END

END OF LISTING

**************************************************************************