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Manual of Phosphoric Acid Fuel Cell Stack Three-Dimensional Model and Computer Program

Cheng-yi Lu and Kalil A. Alkasab
Cleveland State University

May 1984

Prepared for
NATIONAL AERONAUTICS AND SPACE ADMINISTRATION
Lewis Research Center
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U.S. DEPARTMENT OF ENERGY
Morgantown Energy Technology Center
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Morgantown, West Virginia 26505
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INTRODUCTION

In the fuel cell power section, air, in excess of the stoichiometric mixture, enters the cathode side of the cell, and effluents from the low temperature shift converter enter at the anode. The anode input contains CH₄, H₂O, H₂, CO and CO₂. In this analysis, it is assumed that a fixed percentage of hydrogen is consumed at the anode, and the H₂O being formed exits the fuel cell, with the depleted air, through the cathode exit. The overall reaction in the fuel cell power section is,

\[ \text{H}_2 + \frac{1}{2} \text{O}_2 = \text{H}_2\text{O} \]

Two distinct mathematical models of fuel cells have been developed with computer programs for performing the necessary calculations. The first was a "lumped parameter" model; the second was a three-dimensional detailed model of the stack.

The simplified lumped model, described in the previous report, is an "input–output" model developed for the system trade-off studies (Ref. 1).

The detailed distributed model is a finite-difference model of the operation of the fuel cell which was used to calculate the effects of the cell and module design on performance. It calculates the current density distribution in the cells as a function of the local reactant compositions, local temperatures, catalyst utilization factors, etc. Since these are interdependent (e.g., the local temperature depends on the local current density), the computations are highly iterative and require considerably more computer capacity and time than the lumped model. An associated computer program will be used to compare an alternative design of cooling scheme in the stack.
I. LUMPED MODEL AND VOLTAGE—CURRENT CHARACTERISTIC

1.1 Mass and Energy Balances for Lumped Model

The lumped model provides a rapid (in terms of computation time) means of calculating the fuel cell module output characteristics (voltage, current, and heat generation rate) in terms of the inputs from the fuel processing subsystem and the gross fuel cell design parameters such as catalyst loading.

The mass balances of hydrogen, oxygen and water are as follows:

\[ \text{NX}_\text{H}_2 = \text{NI}_\text{H}_2 - \frac{(\text{Imean A})}{(n_f)} \] (1-1)
\[ \text{NX}_\text{O}_2 = \text{NI}_\text{O}_2 - \frac{(\text{Imean A})}{(2n_f)} \] (1-2)
\[ \text{NX}_\text{H}_2\text{O} = \text{NI}_\text{H}_2\text{O} + \frac{(\text{Imean A})}{(n_f)} \] (1-3)

where \( \text{NX} \): exit flow rate of hydrogen, oxygen, or steam, g—mole/sec
\( \text{NI} \): inlet flow rate of hydrogen, oxygen, or steam, g—mole/sec
\( \text{Imean} \): mean current density, A/cm²
\( A \): effective area of cell plate, cm²
\( n \): number of Faraday equivalents transferred
\( f \): Faraday constant

The energy balance for the fuel cell is:

\[ -(Q + W_e) = \sum_{PF} n_j \left( \Delta h_f^g \right) - \sum_{RF} n_i \left( \Delta h_f^g \right) + \sum_{PF} n_j \int_{298}^{T_F} \left( C_p \right)_j \, dT - \sum_{RF} n_i \int_{T_iF}^{298} \left( C_p \right)_i \, dT \] (1-4)

where the subscripts \( \text{PF}, rF \) represent the products and reactants in the fuel cell, respectively. \( T_F \) is the final temperature of the products and \( T_iF \) is the initial temperature of the reactants in the fuel cell. The \( n_j \) and \( n_i \) are
the species flow rates of the products and reactants, respectively. The terms $Q$ and $W$ are the rates of heat and the electrical energy generation by the fuel cell, respectively. $Q$ is proportional to the specific heat generation $Q_F$

where:

\[
Q = N_p \times N \times Q_f \\
\text{and } Q_f = \left(\frac{\Delta H_r}{I} + V\right) I
\]

where $Q$: total heat generated, J/sec

$Q_f$: heat generated per unit area of cell, J/sec cm$^2$

$N_p$: number of cells

$Xn$: width of cell plate, cm

$Yn$: length of cell plate, cm

$I$: fuel cell current density, A/cm$^2$

$\Delta H_r$: heat of reaction, J/g-mole of $H_2$

1.2 Voltage-Current Characteristics

Because of the irreversibility, the voltage $V$ for a working fuel cell is the difference between the open circuit voltage and the cell polarization terms:

\[
V = E - \eta
\]

where $E$: Nernst potential (reversible open circuit E.M.F.)

$\eta$: overpotential or polarization

The reversible cell potential, $E$ is given by the Nernst equation:
\[ E_0 = E(T) + \frac{RT}{nF} \ln \frac{YH_2\sqrt{PtYO_2}}{YH_2O} \]  

(1-8)

with \( Pt \): total pressure, atm

\( E_0(T) \): standard E.M.F. of cell at temperature \( T \), volts

\[ E_0(T) = 1.261 - 0.00025 T, \text{ } T, \text{ } K \text{ (Ref. 2)} \]

\( YH_2 \): mean mole fraction of hydrogen at anode

\( YO_2 \): mean mole fraction of oxygen at cathode

\( YH_2O \): mean mole fraction of water vapor at cathode

The polarization term \( \eta \) consists of four components,

\[ \eta = \eta_a + \eta_r + \eta_d + \eta_{co} \]  

(1-9)

where \( \eta_a \): activation polarization at cathode, volts

\( \eta_r \): resistance polarization, volts

\( \eta_d \): diffusion polarization, volts

\( \eta_{co} \): activation polarization at anode due to CO poisoning of catalyst, volts

and

\[ \eta_a = \frac{RT}{\pi \sigma Z F} \ln \left( \frac{i}{i_0} \right) \text{ (SA)(CL)(CU)} \]  

(1-10)

with \( \sigma \): transfer coefficient

\( i \): current density, mA/cm²

\( i_0 \): exchange current density of cathode, mA/cm²

\( SA \): specific catalyst surface area, cm²/g

\( CL \): catalyst loading on cathode, g/cm²

\( CU \): catalyst utilization factor
The exchange current is a function of the acid concentration, temperature, and partial pressure of the oxygen. The acid concentration is a function of the water vapor partial pressure which permits correlation of \( i_0 \) as a function of \( Y_{O2}, Y_{H2O}, \) and \( T \). An empirical fit is

\[
i_0 = 232.7 \ (Pty_{O2})^{0.8} \ (Pty_{H2O})^{0.4377} \exp \left( \frac{-6652}{T} \right)
\]

(1-11)

The resistance polarization is

\[
n_r = ir
\]

where \( r \): specific cell resistance, ohm-cm\(^2\).

The expression of \( n_{co} \) was chosen to have strong temperature dependence, be directly proportional to \( Y_{co} \), and have a logarithmic dependence on \( i \), \( i_{ao} \), and catalyst effective area. The resulting expression (Ref. 2) is

\[
n_{co} = 0.0782PtY_{co} \exp \left[ 9190 \left( \frac{1}{T} - \frac{1}{450} \right) \right] \ln \frac{i}{C_{La} \cdot S \cdot A \cdot C_{U} \cdot i_{ao}}
\]

(1-12)

where \( C_{La} \): anode catalyst loading, g/cm\(^2\)

\( i_{ao} \): anode exchange current, mA/cm\(^2\)

Diffusion polarization has been neglected here because it is significant only at very high current densities.

In the associated computer code, Subroutine VI, calculates cell voltage as a function of the current density or alternatively solves the nonlinear equation to evaluate current density as a function of the cell voltage.
II. CURRENT DENSITY DISTRIBUTION

In the fuel cell module, the combined modeling of temperature and current distribution is an absolute condition for reliable scaling-up of the results obtained with small cells, and for predictive models starting from elementary porous-electrode representations.

This subsection describes the calculation of the current density distribution over a cell plate on which the air and fuel flows are at right angles. The procedure divides a cell plate into "grids" which are small enough so that variations in fuel and oxidant composition and temperature are negligible. Then by means of calculation of the boundary conditions for each "grid" and iteration, a solution will be obtained that satisfies the input specifications (e.g., average current density, fuel and air utilization, and reactant flow rates). A diagram of the "grid" is shown in Figure 1.

The overall method is to first specify a desired average current density $i$ for the whole plate and then determine the corresponding voltage $V$ for the plate. This voltage will be determined such that it produces unique local current densities over the plate whose average value approximates $i$ within a specified tolerance. A trial-and-error procedure is used to estimate the local current density and overall voltage. The model basically applies the same voltage-current equation used in the lumped model (described in Chapter 1) to each grid section of the cell.
Figure 1 Finite Difference Model Definition of Current Density Distribution on Cell Plate
Mathematic Formulation

Exit flow of hydrogen from grid \((i,j)\)

\[ NX H_2(i,j) = NI H_2(i,j) - (I(i,j)A)/(nA) \quad (2-1) \]

Exit flow of oxygen from grid \((i,j)\)

\[ NX O_2(i,j) = NI O_2(i,j) - (I(i,j)A)/(2nA) \quad (2-2) \]

Exit flow of water from grid \((i,j)\)

\[ NX H_2O(i,j) = NI H_2O(i,j) + (I(i,j)A)/(nA) \quad (2-3) \]

where

- \(NX H_2, O_2, H_2O(i,j)\): hydrogen (oxygen or water) portion flow rate at exit of grid \((i,j)\), g-mole/sec.
- \(NI H_2, O_2, H_2O(i,j)\): hydrogen (oxygen or water) portion flow rate at inlet side of grid \((i,j)\), g-mole/sec.
- \(I(i,j)\): current density of grid \((i,j)\), A/cm²
- \(A\): area of grid, cm²

The flow charge of executive program (CUPRO) for calculating current density distribution is shown in Figure 2.
Figure 2 Flow Chart of CUPRO

(1): M=1 yields voltage
(2): M=2 yields C.D.
III. THERMAL ANALYSIS AND TEMPERATURE DISTRIBUTION

The electrical energy production in phosphoric acid fuel cells is accompanied by approximately equal amounts of heat energy generation. Removal of this heat can be accomplished by a suitable flow of input gases or by using separate cooling plates.

The work reported in this section is directed towards estimating the steady state temperature profiles in practical phosphoric acid fuel cell stacks. The fuel cell stack considered in this section is composed of cell plates on which the air (oxygen) and fuel (hydrogen) flows are at right angles. A cooling plate is placed between individual groups of cells at a regular interval. Symmetry in the stacking direction occurs at the middle of a cooling plate and midway between cooling plates.

3.1 Previous Work

Estimation of the temperature profiles in an operating cell is important for the estimation of the power density distribution, thermal stability, and cooling requirements. Only a limited amount of information on this subject has been reported in the past. Baker and coworkers recognized this need and have performed a comprehensive study of steady state heat transfer in electrochemical systems (Refs. 3, 4, 5). They studied various cases involving one dimensional analysis of a single adiabatic fuel cell and a three dimensional analysis of a multicell stack.

A single fuel cell with no lateral heat transfer and no conduction of heat through the cell in the direction perpendicular to the gas flow was considered
(Ref. 4). Heat transfer by conduction in the direction of the gas flow was considered negligible in comparison to the heat transfer by convection, and analytical expressions for the electrolyte, fuel, and air temperature profiles were derived.

For the three-dimensional analysis of the stack, it was assumed that all of the walls except for the wall from which the air enters were maintained at a constant temperature. The rate of heat generation per unit volume of the stack was assumed constant. An analytical solution for the temperature profile was developed, assuming that the electrolyte and gas temperatures were not very different.

Another paper (Ref. 5) considered various limiting and special cases to determine the maximum temperature of a stack. Two-dimensional heat transfer analysis was carried out in the case of a thick stack where heat transfer in the direction of stacking was neglected. In the case of thin stacks, three-dimensional heat transfer was considered with each wall at a different temperature. Infinite series solutions were developed for both thick and thin stacks. The authors estimated the maximum stack temperature for the constant wall temperature case. An approximate formula to predict the effect of conductivities, size, and current density on the maximum stack temperature was developed. A generalized analysis, which can incorporate the effect of finite resistance to heat transfer at the wall, the effect of cold or hot feeds, or nonuniform heat generation, was also carried out using the method of Green's function.
3.2 Temperature Distribution

The temperature distribution for the module was developed from the temperature distributions within representative slices or strips within a set of cell and cooling plate cells. The analysis includes conduction within bipolar plates, conduction between plates, the separate cooling effects of the process air and the coolant (basically air is considered as the coolant), and the temperature change of air flows along their respective channels. The distribution of the heat generation is determined from the current density distribution.

The model assumes that (1) the temperature gradients in the direction of the fuel flow are small. This assumption is justified since the major temperature gradients are in the air flow direction and since the heat capacity of the fuel stream is only a few percent of the heat capacity of the air stream; (2) the edge of the cell is operating adiabatically; (3) a half set of cell plates between cooling plates is analyzed, which includes one half cooling plate and two and a half cell plates. Thus, because of the symmetry, all of the stack behaves similarly. The geometry of a representative slice (Lx x Ly x Lz) through the stack is shown in Figure 3.

Mathematical Formulation

The material balances of the fuel and the oxidant have been presented in Chapter 2. There are four energy balance equations for the cell plate, cooling plate, process air, and coolant.
cell on process air side in air flow direction

\[ t \left( K_y \frac{\partial^2 T}{\partial y^2} + K_x \frac{\partial T}{\partial x} \right) x + t - K_x \frac{\partial T}{\partial x} x - \frac{C_p m_p}{P_p} \frac{\partial T_p}{\partial y} = -(V^* - V) I \]  
\hspace{1cm} (3-1)

cooling plate in coolant direction

\[ t' \left( K_y \frac{\partial^2 T}{\partial y^2} + 2K_x \frac{\partial T}{\partial x} \right) x + t'/2 - \frac{C_c m_c}{P_c} \frac{\partial T_c}{\partial y} = 0 \]  
\hspace{1cm} (3-2)

process air side

\[ \frac{d}{d y} \frac{T_p}{T_p} = \frac{h_p S_p}{m_p C_p} (T - T_p) \]  
\hspace{1cm} (3-3)

coolant side

\[ \frac{d}{d y} \frac{T_c}{T_c} = \frac{h_c S_c}{m_c C_c} (T - T_c) \]  
\hspace{1cm} (3-4)

Boundary conditions

- \( x = 0 \) \( \frac{\partial T}{\partial x} = 0 \) symmetric condition
- \( y = 0 \) \( \frac{\partial T}{\partial y} = 0 \) adiabatic assumption
- \( x = L_x \) \( \frac{\partial T}{\partial x} = 0 \) symmetric condition
- \( y = L_y \) \( \frac{\partial T}{\partial y} = 0 \) adiabatic assumption
- \( y = 0 \) \( T_p = T_p \), inlet
- \( y = 0 \) \( T_c = T_c \), inlet

where

- \( m \) = mass flow rate, Kg/hr-channel
- \( C \) = heat capacity, J/Kg-K
- \( K_y \) = effective thermal conductivity of cell in flow direction, J/hr-m-K
- \( K_x \) = effective thermal conductivity of cell on stacking direction, J/hr-m-K
- \( t \) = thickness of cell including fuel and air channel, m
- \( x_1 \) = effective conduction distance from plate to upper cell plate, m
- \( x_2 \) = effective conduction distance from plate to lower cell plate, m
\[ P = \text{pitch of channel, m} \]
\[ x_1' = \text{effective conduction distance from cooling plate to upper cell plate, m} \]
\[ L_x, L_y = \text{height and length of one slice, respectively, m} \]
\[ V^* = \Delta H/ZF, V \]
\[ t' = \text{thickness of cooling plate, m} \]
\[ h = \text{heat transfer coefficient, J/hr-m}^2K \]
\[ S = \text{perimeter of the channel, m} \]

Subscript:
\[ p = \text{process air} \]
\[ c = \text{cooling air} \]

These simultaneous ordinary differential equations and corresponding boundary conditions were solved by the finite-difference method. The final difference equations are in next subsection.

**Finite-Difference Model**

The energy balance on an internal element \( j (2 < j < N-1) \) for bipolar plate \( i (2 < i < N) \) can now be written as (see Figure 3)

\[
\begin{align*}
- \frac{(K_y t)}{\Delta y^2} T_{i,j-1} + & \left(2 \frac{K_y t}{\Delta y^2} + \frac{K_x}{X_1} + \frac{K_x}{X_2} \right) T_{i,j} \\
- \frac{(K_y t)}{\Delta y^2} T_{i,j-1} + & \left(\frac{K_x}{X_1} T_{i-1,j} - \frac{K_x}{X_2} T_{i+1,j} \right) + \\
+ \left(\frac{M_p C_p}{P_p \Delta y} \right) (T_{pi,j} - T_{pi,j-1}) = & (V^*-V) I_{i,j}
\end{align*}
\]  

The energy balance on an internal element \( j (2 < j < N-1) \) of the cooling plate \( i=1 \) can be written as
The energy balance on interior element \( j \) \((2 \leq j \leq N-1)\) of the symmetric plate \( i = N/2 \) is

\[
- \left( \frac{K_y t_i'}{\Delta Y^2} \right) T_{i, j-1} + \left( 2 \frac{K_y t_i'}{\Delta Y^2} + 2 \frac{K_x}{X_i} \right) T_{i, j} - \left( \frac{K_y t_i'}{\Delta Y^2} \right) T_{i, j+1} - \left( 2 \frac{K_x}{X_i} \right) T_{i, j+2}
\]

\[
+ \left( \frac{M_c C_c}{P_c \Delta Y} \right) (T_{i+1, j} - T_{i, j}) = 0
\]  

(3-6)

The energy balance on element \( j = 1 \) are obtained as above, except for: the values of \( T_{i, 0} \) are replaced by \( T_{i, 1} \); the values of \( T_{p, 0} \) are replaced by \( T_{p0} \), which is the inlet process air temperature; and \( T_{c0} \) is replaced by \( T_{c0} \), the inlet cooling air temperature. The energy balances on elements \( j = N \) are obtained from the above with \( T_{i, j+1} \) replaced by \( T_{i, N} \).
For the process air flow, one can set up \( N \times N \) equations of the form

\[
TP_{i,j} = TP_{i,j-1} + (T_{i,j} - TP_{i,j-1}) (1-e^{-\dot{\phi}_{pi,j}}) \quad (3-8)
\]

where

\[
\dot{\phi}_{pi,j} = \frac{h_{i,j}SP}{M_p CP} \Delta Y \quad (3-9)
\]

For the cooling air flow, one obtains \( N \) equations of the form

\[
TC_j = TC_{j-1} + (T_{1,j} - TC_{j-1})(1-e^{-\dot{\phi}_{cj}}) \quad (3-10)
\]

where

\[
\dot{\phi}_{cj} = \frac{h_{cj}Sc}{Mc CC} \Delta Y \quad (3-11)
\]

Thus, the total number of temperature equations matches the number of unknown temperatures and the set can be solved using the Gaussian elimination method with calculated or input values of cell voltages, current densities, mass flow, heat generation and heat transfer coefficients. Each resulting temperature distribution is used to recalculate the current density distribution until convergence is reached. The relationship between voltage and current and the calculation of heat generation have been presented in Chapter 1.

**Heat Transfer Coefficients**

An empirical equation (Ref. 6) for the Nusselt number for fully developed laminar flow in a rectangular channel is:

\[
N_u = 3.61 + 4.63 (1-\alpha)^{3.2} \quad (3-12)
\]

where \( \alpha = a/b \); \( a \) is the smaller side of rectangular channel and \( b \) is the larger side of the channel.
Near the inlet of a channel, the heat transfer coefficient is larger than the fully developed value due to development of the laminar boundary layer. If \( R \) is the ratio of the average Nusselt number for the region 0 to \( x \) to the fully developed Nusselt number, then (Ref. 7)

\[
R = 1 + \frac{0.0183 \, \text{Gz}}{1 + 0.04 \, \text{Gz}^{2/3}}
\]  

(3-13)

where Gz: Graetz number = Re Pr \( (D_H/x) \)
Re: Reynolds number based on \( D_H \)
Pr: Prandtl number of gas
\( D_H \): Hydraulic diameter, m

For turbulent flow, the average Nusselt number over the region 0 to \( x \) is described as (Ref. 8)

\[
\text{Nu}_t = 0.116 \, [\text{Re}^{2/3} - 125] \, \text{Pr}^{1/3} \left[ 1 + \left( \frac{D}{x} \right)^{2/3} \right]
\]  

(3-14)

The flow chart of the executive program (MAIN program) for calculating the temperature distribution in the stack is shown in Figure 4.
Figure 4 Flow Chart for Calculation of Temperature Distribution in Cell Stack
IV. COMPUTER CODE

4.1 Program Description

The computer code contains one executive program (MAIN program) and eleven subroutines. The mathematical model and algorithm used in MAIN program was shown in Chapter 3. Table 1 lists the nomenclature of the program.

All of the subroutines are listed in Table 2 associated with their specified functions. Among these, Subroutines VI and CUPRO have been described in Chapters 1 and 2, respectively. Subroutine DRAWE, which execute the contour drawing package, will not be used except running the program on IBM 370 of NASA Lewis Research Center. The rest of listed subroutines are used to estimate the properties of the process fluids or for I/O usage.

The whole program listing is shown in the end of this manual.

4.2 Program Operation

The program input only consists of a set of NAMELIST data in a specified order. The first NAMELIST set is called DIMEN and contains the dimensions of cell and cooling plates, number of cell plates between two cooling plates, number of cell plates between two cooling plates, number of air and fuel channels and utilization, pressure, number of finite difference sections, and input temperature on anode and cathode sides. The order of input data inside one NAMELIST need not be fixed.
TABLE 1

PROGRAM NOMENCLATURE

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>AL</td>
<td>aspect ratios of process air</td>
</tr>
<tr>
<td>AL1(I)</td>
<td>aspect ratios of cooling channel in different sections (treed form)</td>
</tr>
<tr>
<td>ALFA</td>
<td>transfer coefficient</td>
</tr>
<tr>
<td>AMUC</td>
<td>viscosity; lb/hr-ft</td>
</tr>
<tr>
<td>AMMA</td>
<td>molecular weight of process air; lb/lb-mole</td>
</tr>
<tr>
<td>AMMC</td>
<td>molecular weight of cooling air; lb/lb-mole</td>
</tr>
<tr>
<td>CL</td>
<td>catalyst loading; mg/cm²</td>
</tr>
<tr>
<td>CU</td>
<td>catalyst utilization</td>
</tr>
<tr>
<td>CM(I)</td>
<td>mole fraction of component I in cooling air</td>
</tr>
<tr>
<td>CMC(I)</td>
<td>mole fraction of component I in process air</td>
</tr>
<tr>
<td>CPC</td>
<td>heat capacity; Btu/lb-mole-R</td>
</tr>
<tr>
<td>DNSA(I)</td>
<td>moles of component I in process air; lb-mole</td>
</tr>
<tr>
<td>DNSC(I)</td>
<td>moles of component I in cooling air; lb-mole</td>
</tr>
<tr>
<td>DX</td>
<td>length of x-division; ft</td>
</tr>
<tr>
<td>FCONST</td>
<td>Faraday constant; 96500 coul./g-equivalent</td>
</tr>
<tr>
<td>G(I,J)</td>
<td>coefficient of simultaneous linear equations</td>
</tr>
<tr>
<td>GZ(I)</td>
<td>Graetz number of different sections in cooling channels</td>
</tr>
<tr>
<td>GZA</td>
<td>Graetz number in process air</td>
</tr>
<tr>
<td>H(I,J,K)</td>
<td>heat transfer coefficient of plate I x-division J y-division K of process air; Btu/ft²-hr-R</td>
</tr>
<tr>
<td>H2</td>
<td>required hydrogen; g-mole/hr-stack</td>
</tr>
<tr>
<td>HC(I)</td>
<td>heat transfer coefficient of division I in cooling channel</td>
</tr>
<tr>
<td>HH</td>
<td>required hydrogen; g-mole/sec-plate</td>
</tr>
<tr>
<td>PPRO(I,J,K)</td>
<td>current density of plate I x-division J y-division K; A/cm²</td>
</tr>
<tr>
<td>KX</td>
<td>effective thermal conductivity in stacking direction; Btu/hr-ft-R</td>
</tr>
<tr>
<td>KY</td>
<td>effective thermal conductivity in flow direction; Btu/hr-ft-R</td>
</tr>
<tr>
<td>MA</td>
<td>mass flow rate of process air; lb/hr-channel</td>
</tr>
<tr>
<td>MAC(I)</td>
<td>mass flow rate of cooling air in section I; lb/hr-channel</td>
</tr>
<tr>
<td>NC</td>
<td>number of stoich air in cooling channel</td>
</tr>
<tr>
<td>NCA</td>
<td>number of process air channels</td>
</tr>
<tr>
<td>GCC</td>
<td>number of cooling channels</td>
</tr>
<tr>
<td>NK</td>
<td>number of plates between cooling plate</td>
</tr>
<tr>
<td>NP</td>
<td>number of plates in a stack</td>
</tr>
<tr>
<td>NX</td>
<td>number of divisions in x direction</td>
</tr>
<tr>
<td>NY</td>
<td>number of divisions in y direction</td>
</tr>
<tr>
<td>O2</td>
<td>required oxygen; g-moles/hr-stack</td>
</tr>
<tr>
<td>QO</td>
<td>required oxygen; g-moles/sec-plate</td>
</tr>
<tr>
<td>HC</td>
<td>pitch of cooling channel; ft</td>
</tr>
<tr>
<td>PHI(I,J)</td>
<td>dimensionless group of plate I division J in process air</td>
</tr>
<tr>
<td>PH2(I)</td>
<td>dimensionless group of division I in cooling air</td>
</tr>
<tr>
<td>POP</td>
<td>inlet gas pressure; atm</td>
</tr>
<tr>
<td>PP</td>
<td>pitch of process air; ft</td>
</tr>
<tr>
<td>PR</td>
<td>Prandtl number of gas</td>
</tr>
<tr>
<td>QW(I,J)</td>
<td>heat generation rate of division J plate I; Btu/hr</td>
</tr>
</tbody>
</table>
TABLE 1 (cont'd)

PROGRAM NOMENCLATURE

R(I): ratio of average Nusselt number for region 0 to x to the fully developed Nusselt number of division I in cooling channel
RA: ratio of average Nusselt number for region 0 to x to the fully developed Nusselt number of division I in process channel
RE(I): Reynolds number of division I in cooling channel
SA: catalyst surface area; cm^2/mg
SRO: cell resistance at 450 K; Ohm-cm^2
T: thickness of cell including process channels; ft
T1: thickness of cooling plate; ft
TAIN: inlet temperature of process air; R
TKA: inlet temperature of process air; K
TCIN: inlet temperature of cooling air; R
TCK: inlet temperature of cooling air; K
TDNSC: total moles in cooling channel; g-mole/hr-division
TDH2(I,J): flow rate of hydrogen in fuel channel at division J plate I; g-mole/sec
TDH2O(I,J): flow rate of water in process air channel at division J plate I; g-mole/sec
TD02(I,J): flow rate of oxygen in process air channel at division J plate I; g-mole/sec
TD1(I,J): total flow rate in fuel channel; g-mole/sec
TD2(I,J): total flow rate in process air channel; g-mole/sec
TFA: inlet temperature of process air; F
TFC: inlet temperature of cooling air; F
TAK: thermal conductivity of process air; Btu/hr-ft-R
TCK: thermal conductivity of cooling air; Btu/hr-ft-R
TKAA: average temperature of process air; K
TKCC: average temperature of cooling air; K
TKF: inlet temperature of fuel; K
TRR(I): average operating temperature of plate I; R
TUN: Nusselt number
UTA: utilization of air
UTH: utilization of fuel
WA: hydraulic diameter of process air channel; ft
WAD: depth of process air channel; ft
WAW: width of process air channel; ft
WC: hydraulic diameter of cooling channel; ft
WCD: depth of cooling channel; ft
WCW: width of cooling channel; ft
WE: thickness of cell; ft
WFH: depth of fuel channel; ft
WFH: width of fuel channel; ft
WP: thickness between two cooling plate; ft
X(I): solution of simultaneous equations
XAMP: amp/plate
XDNSCO: designed current density; amp/cm^2

22
TABLE 1 (cont'd)

PROGRAM NOMENCLATURE

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
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<tr>
<td>XN:</td>
<td>length of cell in x-direction; ft</td>
</tr>
<tr>
<td>XOO(J,K)</td>
<td>same as PPRU(I,J,K) in each plate; A/cm^2</td>
</tr>
<tr>
<td>Y1:</td>
<td>effective conduction distance from cell plate to cooling plate; ft</td>
</tr>
<tr>
<td>Y2:</td>
<td>effective conduction distance from cell plate to another cell plate; ft</td>
</tr>
<tr>
<td>Y1CH4:</td>
<td>mole fraction of CH4 in fuel</td>
</tr>
<tr>
<td>Y1CO:</td>
<td>mole fraction of CO in fuel</td>
</tr>
<tr>
<td>Y1CO2:</td>
<td>mole fraction of CO2 in fuel</td>
</tr>
<tr>
<td>Y1H2:</td>
<td>mole fraction of H2 in fuel</td>
</tr>
<tr>
<td>Y1H2O:</td>
<td>mole fraction of H2O in fuel</td>
</tr>
<tr>
<td>Y2H2O:</td>
<td>mole fraction of H2O in air</td>
</tr>
<tr>
<td>Y2N2:</td>
<td>mole fraction of N2 in air</td>
</tr>
<tr>
<td>Y2O2:</td>
<td>mole fraction of O2 in air</td>
</tr>
<tr>
<td>YN:</td>
<td>length of cell in y-direction; ft</td>
</tr>
<tr>
<td>Z:</td>
<td>number of Faraday equivalents transferred</td>
</tr>
</tbody>
</table>
### TABLE 2

**DEFINITIONS OF SUBROUTINES**

<table>
<thead>
<tr>
<th>Subroutines</th>
<th>DESCRIPTION</th>
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</table>
| DATAIN      | 1. input data reading  
              2. changing units  
              3. calculation of the constants used in MAIN program |
| DATAACA     | calculations of the properties and coefficients for cooling air |
| VI          | calculation of the relationship between voltage and current density for specified fuel cell plate |
| CUPRO       | estimation of the steady state current density distribution on the cell plate |
| GAUSS       | Gauss-Seide iteration used to solve simultaneous linear equations |
| CMASS       | calculation of the mass fraction of gas stream |
| CMOLE       | calculation of the mole $^n$-action of gas stream |
| HTCP        | estimation of the heat capacity of specified gas mixture |
| THC         | estimation of the thermal conductivity of specified gas mixture |
| VIS         | estimation of the viscosity of specified gas mixture |
| DRAWE       | execution of the contour drawing package |
The second set (ERR) only contains the convergence criterion for program trial-and-error procedure. The third NAMELIST set (CZ) specifies the kinetic data of the catalyst used in anode and cathode sides.

DIGA carries the information of coolant flow rate, the dimension of cooling channels, and the thermal conductivities along flow direction and stack direction.

The last NAMELIST set contains the inlet compositions of both anode and cathode sides.

All of the input variables are listed in Table 3, along with their units and numerical values in the sample run, which will be discussed in the next chapter.
TABLE 3

INPUT DATA FOR 3-D C.D. AND TEMPERATURE DISTRIBUTIONS (STEADY STATE)

<table>
<thead>
<tr>
<th>NAMELIST</th>
<th>VARIABLE</th>
<th>SAMPLE VALUE</th>
<th>UNIT</th>
<th>DEFINITION</th>
</tr>
</thead>
<tbody>
<tr>
<td>DIMEN XN</td>
<td>17</td>
<td>in</td>
<td></td>
<td>length of cell plate in x-direction</td>
</tr>
<tr>
<td>DIMEN YN</td>
<td>12</td>
<td>in</td>
<td></td>
<td>length of cell plate in y-direction</td>
</tr>
<tr>
<td>DIMEN DNSCO</td>
<td>0.325</td>
<td>A/cm²</td>
<td></td>
<td>designed current density</td>
</tr>
<tr>
<td>DIMEN UTA</td>
<td>0.5</td>
<td></td>
<td></td>
<td>utilization of O₂ in stack</td>
</tr>
<tr>
<td>DIMEN UTH</td>
<td>0.75</td>
<td></td>
<td></td>
<td>utilization of H₂ in stack</td>
</tr>
<tr>
<td>DIMEN POPC</td>
<td>3.4</td>
<td>atm</td>
<td></td>
<td>pressure of cooling air</td>
</tr>
<tr>
<td>DIMEN POP</td>
<td>3.4</td>
<td>atm</td>
<td></td>
<td>operating pressure in stack</td>
</tr>
<tr>
<td>DIMEN TKA</td>
<td>443</td>
<td>K</td>
<td></td>
<td>inlet temperature of process air</td>
</tr>
<tr>
<td>DIMEN WFD</td>
<td>0.00333</td>
<td>ft</td>
<td></td>
<td>depth of fuel channel</td>
</tr>
<tr>
<td>DIMEN WFW</td>
<td>0.01</td>
<td>ft</td>
<td></td>
<td>width of fuel channel</td>
</tr>
<tr>
<td>DIMEN NCC</td>
<td>30</td>
<td></td>
<td></td>
<td>number of cooling channels</td>
</tr>
<tr>
<td>DIMEN WE</td>
<td>0.00333</td>
<td>ft</td>
<td></td>
<td>thickness of cell (electrode and matrix)</td>
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<tr>
<td>DIMEN TKF</td>
<td>450</td>
<td>K</td>
<td></td>
<td>inlet temperature of fuel</td>
</tr>
<tr>
<td>DIMEN T</td>
<td>0.0108</td>
<td>ft</td>
<td></td>
<td>thickness of cell plate</td>
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<tr>
<td>DIMEN NK</td>
<td>5</td>
<td></td>
<td></td>
<td>number of plates between two cooling plates</td>
</tr>
<tr>
<td>DIMEN WAD</td>
<td>0.00333</td>
<td>ft</td>
<td></td>
<td>depth of process air channel</td>
</tr>
<tr>
<td>DIMEN WAW</td>
<td>0.01</td>
<td>ft</td>
<td></td>
<td>width of process air channel</td>
</tr>
<tr>
<td>DIMEN NP</td>
<td>23</td>
<td></td>
<td></td>
<td>number of cell plates</td>
</tr>
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<td>DIMEN NCA</td>
<td>80</td>
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<td>number of process air channels</td>
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<td>DIMEN NF</td>
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<td></td>
<td>number of fuel channels</td>
</tr>
<tr>
<td>DIMEN T1</td>
<td>0.02917</td>
<td>ft</td>
<td></td>
<td>thickness of cooling plate</td>
</tr>
<tr>
<td>DIMEN NX</td>
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<td></td>
<td>finite difference number in x-direction</td>
</tr>
<tr>
<td>DIMEN NY</td>
<td>12</td>
<td></td>
<td></td>
<td>finite difference number in y-direction</td>
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<tr>
<td>DIMEN TINGS</td>
<td>191</td>
<td>C</td>
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<td>initial guess of plate temperature</td>
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<td>ERR ER</td>
<td>0.01</td>
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<td></td>
<td>criterion for convergence</td>
</tr>
<tr>
<td>CZ CLCA</td>
<td>0.52</td>
<td>mg/cm²</td>
<td></td>
<td>catalyst loading on cathode side</td>
</tr>
<tr>
<td>CZ CLAN</td>
<td>0.34</td>
<td>mg/cm²</td>
<td></td>
<td>catalyst loading on anode side</td>
</tr>
<tr>
<td>CZ CU</td>
<td>0.15</td>
<td></td>
<td></td>
<td>utilization of catalyst</td>
</tr>
<tr>
<td>CZ SA</td>
<td>500</td>
<td>cm²/mg</td>
<td></td>
<td>surface area of catalyst</td>
</tr>
<tr>
<td>CZ SRO</td>
<td>0.44</td>
<td>-cm²</td>
<td></td>
<td>cell resistance at 450 K</td>
</tr>
<tr>
<td>CZ ALFA</td>
<td>0.5</td>
<td></td>
<td></td>
<td>transfer coefficient</td>
</tr>
<tr>
<td>CZ DKC</td>
<td>240000</td>
<td>A/atm</td>
<td></td>
<td>constant to calculate limiting current density</td>
</tr>
<tr>
<td>CZ R</td>
<td>J/(g·mol·K)</td>
<td>gas constant</td>
<td></td>
<td></td>
</tr>
<tr>
<td>FALA Z</td>
<td>g-equivalent</td>
<td>number of Faraday equivalents transferred</td>
<td></td>
<td></td>
</tr>
<tr>
<td>FALA FCONST</td>
<td>C-g/equivalent</td>
<td>Faraday constant</td>
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<td></td>
</tr>
<tr>
<td>DIGA NC</td>
<td></td>
<td>ratio of cooling air to air consumed in stack</td>
<td></td>
<td></td>
</tr>
<tr>
<td>DIGA KX</td>
<td>Btu/(ft·h·R)</td>
<td>effective thermal conductivity in stacking direction</td>
<td></td>
<td></td>
</tr>
<tr>
<td>DIGA KY</td>
<td>Btu/(ft·h·R)</td>
<td>effective thermal conductivity in flow direction</td>
<td></td>
<td></td>
</tr>
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<td>NAMELIST LIST</td>
<td>VARIABLE NAME</td>
<td>SAMPLE VALUE</td>
<td>UNIT</td>
<td>DEFINITION</td>
</tr>
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<td>---------------</td>
<td>--------------</td>
<td>------</td>
<td>------------</td>
</tr>
<tr>
<td>DIGA</td>
<td>TKC</td>
<td>K</td>
<td></td>
<td>inlet cooling air temperature</td>
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<td>WCW</td>
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<td>ft</td>
<td>width of cooling channel</td>
</tr>
<tr>
<td>DIGA</td>
<td>WCD</td>
<td>0.22</td>
<td>ft</td>
<td>depth of cooling channel</td>
</tr>
<tr>
<td>FUEL</td>
<td>Y1H₂</td>
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<td>mole fraction of H₂ in anode inlet</td>
</tr>
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<td>FUEL</td>
<td>Y1CO₂</td>
<td>0.24</td>
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<td>mole fraction of CO₂ in anode inlet</td>
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<td>mole fraction of CO in anode inlet</td>
</tr>
<tr>
<td>FUEL</td>
<td>Y1CH₄</td>
<td>0</td>
<td></td>
<td>mole fraction of CH₄ in anode inlet</td>
</tr>
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<td></td>
<td>mole fraction of H₂O in anode inlet</td>
</tr>
<tr>
<td>FUEL</td>
<td>Y1N₂</td>
<td>0</td>
<td></td>
<td>mole fraction of N₂ in anode inlet</td>
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<td>FUEL</td>
<td>Y2O₂</td>
<td>0.208</td>
<td></td>
<td>mole fraction of O₂ in cathode inlet</td>
</tr>
<tr>
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<td></td>
<td>mole fraction of N₂ in cathode inlet</td>
</tr>
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<td>HEATC</td>
<td>RHOP</td>
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<td>lbm/ft³</td>
<td>density of cell plate</td>
</tr>
<tr>
<td>HEATC</td>
<td>RHOc</td>
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<td>lbm/ft³</td>
<td>density of cooling plate</td>
</tr>
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<td>HEATC</td>
<td>CCP</td>
<td>0.25</td>
<td>Btu/(lbm-R)</td>
<td>heat capacity of cell plate</td>
</tr>
<tr>
<td>HEATC</td>
<td>CCC</td>
<td>0.201</td>
<td>Btu/(lbm-R)</td>
<td>heat capacity of cooling plate</td>
</tr>
</tbody>
</table>
V. SAMPLE PROBLEM

5.1 Sample Problem

The distribution of temperature and the accompanied current density profiles in the fuel cell stack with 17"x12" cell plate have been determined from the developed computer program. These distributions are shown in numbers at each corresponding grid. It is noted that the set of fuel cell stack considered is the symmetric part of cell plates between two cooling plates (Figure 3). The associated operating voltage of each considered cell plates is also shown in numbers.

The input data, which is discussed in the previous chapter, is displayed in Figure 5. Figure 6 contains the output generated by the sample data input, where the input data is reprinted first. Next, the operating voltage, the current density of each grid, and the temperature of each grid on the cell plate numbered from outmost plate to central plate are printed. The last piece of information printed is the average operating temperature, the operating pressure, and the DC outlet of the specified stack.

If the program was run on IBM 370 in NASA Lewis Research Center, the subroutine DRAWE can be called to draw the contours of different temperature levels. Figure 7 shows one of these drawings.

The CPU time depends quite on the trial-and-error procedure. The initial temperature guesses, the criteria of convergence, and the number of finite difference sections will determine the computation time. Usually, the CPU time to run this code on IBM 370 is about 1 minute.
V. SAMPLE PROBLEM

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&DIMEN
  XN=17.,
  YN=12.,
  XDMS=0.325,
  UTAM=0.5,
  UTBM=.75,
  POPC=3.4,
  POP=5.4,
  TK=443.,
  WFD=0.003333,
  WFN=0.01,
  NCC=30,
  WE=0.003333,
  TKF=450.,
  T=0.01833,
  NK=5,
  WAD=0.003333,
  WAN=0.01,
  NP=23,
  NCA=80,
  NF=55,
  T1=0.02917,
  NX=23,
  NY=12,
  TING=191.
&END
&ERR
  ER=0.01,
&END
&CZ
  CLCA=0.52,
  CLAN=0.34,
  CU=.15,
  SA=500.,
  SQ=0.44,
  ALFA=.5,DKC=240000.,R=8.314
&END
&FALA
  Z=2.,
  FCONST=96500.,
&END
&DGA
  NC=36.,
  KX=1.5,
  KY=30.,
  TKC=033.3,
  WCH=0.22,
  WCD=0.22.
&END
&FUEL
  Y1H2=0.76,
  Y1CO=0.24,
  Y1CO=0.,
  Y1CH4=0.,
**CELL PLATE**

THE VOLTAGE IS 0.5684 VOLT.

**CURRENT DENSITY (A/CM²)**

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<th>.3976</th>
<th>.3951</th>
<th>.3926</th>
<th>.3897</th>
<th>.3864</th>
<th>.3825</th>
<th>.3777</th>
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<th>.3277</th>
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**TEMPERATURE (C)**

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Figure 6 continued
### Cell Plate

**The Voltage is 0.5766 Volt.**

**Current Density (A/cm²)**

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*Figure 6 continued*
THE VOLTAGE IS 0.5792 VOLT.

**CURRENT DENSITY (A/CM²)**

| .3833 | .3859 | .3834 | .3806 | .3774 | .3736 | .3690 | .3635 | .3567 | .3480 | .3368 | .3217 |
| .3966 | .3940 | .3913 | .3882 | .3847 | .3805 | .3755 | .3694 | .3619 | .3524 | .3461 | .3254 |
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| .3795 | .3771 | .3745 | .3716 | .3683 | .3644 | .3598 | .3543 | .3477 | .3395 | .3292 | .3157 |
| .3630 | .3609 | .3586 | .3559 | .3530 | .3495 | .3455 | .3407 | .3350 | .3280 | .3193 | .3082 |
| .3466 | .3418 | .3398 | .3375 | .3349 | .3320 | .3286 | .3266 | .3198 | .3140 | .3070 | .2981 |
| .3292 | .3249 | .3214 | .3196 | .3177 | .3156 | .3132 | .3103 | .3071 | .3032 | .2986 | .2930 |
| .3026 | .3013 | .2999 | .2983 | .2966 | .2946 | .2923 | .2897 | .2866 | .2830 | .2786 | .2732 |
| .2845 | .2835 | .2823 | .2811 | .2796 | .2780 | .2762 | .2741 | .2716 | .2688 | .2653 | .2612 |
| .2712 | .2704 | .2694 | .2683 | .2671 | .2658 | .2643 | .2626 | .2606 | .2582 | .2555 | .2522 |
| .2662 | .2655 | .2646 | .2637 | .2626 | .2615 | .2601 | .2586 | .2568 | .2548 | .2524 | .2495 |

**TEMPERATURE (C)**

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THE AVERAGE OPERATING TEMPERATURE IS 0.46092E 03 K
THE OPERATING PRESSURE IS 3.40 ATM
THE FULL DC POWER OUTFIT IS 0.56544E 01 KW-DC

Figure 6 continued
5.2 Further Developments

Parametric Sensitivity and Cooling Scheme

The plate temperature is a function of the current density, the concentrations of hydrogen and oxygen, and the cooling effectiveness. In order to achieve the optimum design with respect to the temperature distribution, more studies of the parameters involved and the cooling scheme are necessary. The computer model discussed in the previous chapters is used to examine and compare these design parameters.

The examined parameters include dimension and size of cell plate, thermal conductivities in stack and flow directions, average current density, coolant flow rate and inlet temperature of process air.

There are three configurations of cooling channels considered, whose nomenclature and definitions are as follows:

1. Straight: the dimensions of cooling channel are fixed.
2. Branch: the cooling channel is branched along the coolant flow direction, one example is in Figure 8.
3. Varying Width: the width of cooling channel is different along the fuel flow direction.

After the cooling stream has become fully developed the heat transfer coefficient drop dramatically. The "branch" configuration was designed to prevent the formation of fully developed flow and to increase the flow rate (as the total crosssectional area is decreased). The "varying width" configuration will put more coolant on the larger heat generation side, but the heat transfer coefficient does not change.
Figure 8 One "branch" cooling channel

Width ratio \( W_1:W_2:W_3 = 1:0.5:0.25 \)

Section length \( L_1:L_2:L_3 = 5:3:2 \)
More detailed descriptions and results were shown in References 9, 10, and 11.

**Transient State**

In addition, load change is an important and frequent operation in the powerplant. Since the PAFC system can be subjected to sudden load changes and load ramping, an understanding of the effects of these transient conditions on the PAFC system's performance is essential for the optimal design and control of the system. The transient change of temperature distribution in the load ramping period was simulated by studying the dynamics of the fuel cell stack. The results were shown in References 10 and 11.
REFERENCES


C THIS PROGRAM ESTIMATE THE STEADY STATE CURRENT AND TEMPERATURE

REAL LE,LT,LEC,MA,NC

DIMENSION H(3,12,12),HC(12),YY(3,12),DNHA(7),
IZZ(12),PH1(3,12),PH2(12),GC(96,97),D1(3,12),TD2(3,12,12)

2,PRRO(3,12,12),QW(3,12),TD02(13,13),X(96),TD1(3,12,12)

3,TDH2O(13,13),AVG(4,12),TCCS,12,12),TT(12,12),TD2(13,13)

4,TTEM(12,12),DERI(3),XRAIO(13,12),TERM(4),TD1(13,13)

DIMENSION XXOO(12,12),WM(7),CA(7),CM(7),CMA(7)

1,VGUESS(3),XO2(3,12,12),XH2O(3,12,12),TR(3,12,12),TRR(3)

2,XH2(3,12,12),TDH2(13,13),TTDC(12,12)

COMMON/GUST/TINGS

COMMON/VOLCO/VGUESS,PPRO

COMMON/CATA/CLCA,CLAN,CU,SA,SR0,ALFA,DKC,R

COMMON/CONC/Y1H2,Y1CO2,Y1HO2,Y1CO,Y1CH4,Y1N2,Y2H2O,Y2O2,Y2N2

COMMON/TRANS/ TD02,TDH2O,TDH2,TD1,TD2

COMMON/CONPRO/TTD1,XH2,TTD2,XO2,XH2O,TTDC

COMMON/TRTR/TR

COMMON/CANNL/ NP,NC,NK,NCC,NCA,NX,NF,H1,N2

COMMON/PROP/ CPC,PC,CFA,PF,WCW,WCD,WAT,WAD,WFD

COMMON/PROP2/ HC,H

COMMON/SYTM/PFPC,POP

COMMON/CONST2/ AA,AA1,BB1,BB2,BB3,CC1,CC2,CC3,CC4

COMMON/CONST/ A,A1,B1,B2,B3,C1,C2,C3,C4,E

COMMON/CONST1/ TCIN,TAIN,DMCO,DMAIR,DFUEL,DC,DFL,DX,DS,DAREA

COMMON/CONT/ ER,SN,FCNST

COMMON/CONSTK/ K,K1,K2,K3,K4,K5,K6,K7,K8,K9,K10,K11,K12,K13,

1K14,K15,K16

COMMON/FULL/ PW,TFU,AREAF,CL,XDNF

COMMON/WMC/WM

COMMON/IDUG/ IDEBUG

DATA AVG/48X0. /

DATA TERM/40X0. /

DATA DERIV/3X0. /

C

IDECUBG=0

CALL DATAIN

CALL DATACRA(H2,O2)

AREAF=XNYXK2.54X2

C INITIAL ASSUMPTION

DO 1 I=1,N2

1 CONTINUE

KING=0

2 TERM(J)=0.

DO 3 J=1,NX

10 CONTINUE

DO 3 J=1,NX

10 CONTINUE
DO 3 J=1,NX
DO 3 L=1,NY
3 TR(I,J,L)=(TR(I,J,L)+273.16)*1.8
C CALCULATE THE AVERAGE TEMPERATURE
DO 5 I=1,N2
SUM=0
DO 4 J=1,NX
DO 4 L=1,NY
4 SUM=SUM+TR(I,J,L)
TRC(I)=SUM/NX/NY
5 CONTINUE
C CALCULATE THE CURRENT DENSITY PROFILE
C LET THE UNIT BE G-MOLE/SEC/CELL
DO=02/NP/3600.
HH=H2/NP/3600.
NY1=NY+1
DO 6 IT=1,NY
DO 6 ITR=1,N1
6 AVGCITY,ITR)=0.
DO 11 IU=1,N2
IF(IDEBUG.EQ.1) WRITE(6,118) IU
CALL CUPRO(XXOO,TRR(IU),HH,DO,VGUESS(IU),NX,NY,DX,DY,IU)
SUM=0.
SQ2=0.
DO 7 IBM=1,NX
DO 7 ICM=1,NY
7 SUM=SUM+XXOO(IBM,ICM)
SUM=SUM/NX/NY
DO 8 IBM=1,NX
DO 8 ICM=1,NY
8 SQ2=SQ2+((XXOO(IBM,ICM)-AUG)**2
SQ2=SQRT(SQ2/(NX*NY-1))
DO 9 IJ=1,NX
DO 9 IV=1,NY
9 CONTINUE
PPRO(IU,IJ,IV)=XXOO(IJ,IV)
CONY=3600./453.6
DO 10 IS=1,NX
DO 10 IT=1,NY
10 CONTINUE

C CALCULATE THE MEAN FLOW RATE OF AIR SIDE (LB-MOLE/HR)
DO 38 IL=1,NX
DO 38 IU=1,N2
DO 38 J=1,NY
J2=J-1
DO 12 IA=1,7
12 DNSA(A)=0.
002200 IF(J.EQ.1) DNSA(4)=(XH20(IU,II,J)+DMAIR*Y2H20)/2.
002220 IF(J.EQ.1) DNSA(7)=(XO2(IU,II,J)+DMAIR*Y2O2)/2.
002240 IF(J.NE.1) DNSA(4)=(XH20(IU,II,J)+XH20(IU,II,J2))/2.
002260 IF(J.NE.1) DNSA(7)=(XO2(IU,II,J)+XO2(IU,II,J2))/2.
002280 DNSA(6)=D2/Y2O2*Y2N2/45.6/IN/HP
002300 TDNSA=DNSA(1)+DNSA(2)+DNSA(3)+DNSA(4)+DNSA(5)+DNSA(6)+DNSA(7)
002320 AMNA=0.
002340 DO 13 IB=1,7
002360 CMA(IB)=DNSA(IB)/TDNSA
002380 13 AMNA=AMNA+AMM(IB)\*CMA(IB)
002400 C ASSUME THE PROCESS AIR RISE 85. K AND LINEAR INCREASE
002420 TKAA=TAIN/1.8+85./NYKJ
002440 TFA=(TKAA-273.16)*1.8+32.
002460 CALL CMMS5(CA,DNSA,TDNSA)
002480 CALL CMOLE(CA,CM)
002500 CPA=HTCP(CM,TFA)
002520 TAK=THC(CM,TFA)
002540 MA=TDNSA*AMWA/NX/NCA
002560 IF(WAD.GT.WAW) AL=WAW/WAD
002580 IF(WAD.LE.WAW) AL=WAD/WAW
002600 IF(WAD.GT.WAW) WA=2.*WAW/(1.+AL)
002620 IF(WAD.LE.WAW) WA=2.*WAW/(1.+AL)
002640 GZA=CPA/AMWA+MA/(J*XJ)/TAK+6.*3.14159
002660 RA=1.+0.0183*GZA/(1.+0.04*GZA*GZA*6.67)
002680 IF(J.EQ.1).AND.(AL.NE.1.) HIU,II,J=(3.61*4.63*(1.-AL)*X3.2) -
002700 1KRA/WATK
002720 IF(J.EQ.1).AND.(AL.EQ.1.) HIU,II,J=3.61*RA/WATK
002740 IF(J.GT.1).AND.(AL.EQ.1.) HIU,II,J=(J*RA-J-1)*XRJ)X3.61+4.63 -
002760 1K(1.-AL)*X3.2)WATK
002780 IF(J.GT.1).AND.(AL.EQ.1.) HIU,II,J=(J*RA-J-1)*XRJ)X3.61/WATK
002800 RJA=RA
002820 PH(IU,J)=HIU,II,JX(WAW+WAD)*2. )DX/(TDNSA*NX/NCA)/CPA
002840 YY(IU,J)=-1.-EXP(-PHI(IU,J))
002860 DI(IU,J)=TDNSA*NX/NCA*CPA/DX/PP
002880 14 CONTINUE
002900 15 CONTINUE
002920 C CALCULATE THE VARIABLE OF TEMP. PROFILE
002940 DO 16 JA=1,NY
002960 PH2(JA)=HC(JA)*((WCH+WCD)*2.)DX/(DMCD*NX/NCC)/CPC
002980 16 ZZ(JA)=-1.-EXP(-PH2(JA))
003000 N=1+N*2
003020 NP1=N+1
003040 C SET UP THE SIMULATION EQUATIONS
003060 DO 17 IC=1,N
003080 DO 17 JC=1,NP1
003100 G(IC,JC)=0.
003120 17 CONTINUE
003140 G(1,1)=B3-A1
003160 G(1,2)=A1
003180 G(1,K)=-C4
003200 G(1,K2)=E
003220 JD=K2
003240 DO 18 ID=2,NY
G(1D,JD)=E
 JD=JD+1
 18  G(1D,JD)=E
  JD=NY
  DO 19 IE=K4,K5
  JE=JE+1
 1Z=(IE-N1*NY)-1/NY
  IF(1E=IE/NY)NY
  IF(1Y.EQ.0) IY=NY
  19  G(IE,JE)=YY(IZ,IY)
  JF=0
  DO 20 LF=K2,K6
  JF=JF+1
  IF(LF=NY)NY
  IF(X.EQ.0) IX=NY
  20  G(LF,JF)=ZI(X)
  JG=K6
  DO 21 IG=K4,K5
  IW=(IG-N1*NY)-1/NY
  IV=IG/NY
  IF(1V.EQ.0) IV=NY
  G(IG,JG)=YY(IW,IV)-1.
  21  G(IG,JG)=1.
  JH=K1
  DO 22 IH=K4,K7,NY
  JH=JH+NY
  22  G(IH,JH)=0.
  JJ=K2
  DO 23 IJ=K8,K6
  IU1=IJ-IJ/NY
  IU1=NY
  IF(IU1.EQ.0) IU1=NY
  G(IJ,JJ)=ZI(IU1)-1.
  23  G(IJ,JJ)=1.
  GK2,K2)=1.
  24  IF(IDEBUG.EQ.1) WRITE(6,901) A1
  901 FORMAT(* 1 -- A1='",E13.5)
  DO 26 IK=2,K9
  G(IK,JK)=A1
  JK=JK+1
  G(IK,JK)=B3
  JK=JK+1
  G(IK,JK)=A1
  JK=JK+K9
  G(IK,JK)=C4
  JK=JK
  24  CONTINUE
  IF(IDEBUG.EQ.1) WRITE(6,902) A1
  902 FORMAT(* 2 -- A1='",E13.5)
  G(NY,K9)=A1
  G(NY,NY)=B3-A1
  G(NY,K10)=C4
JR=IR+1
0005440   GCSR.JR)=D1(IS,IT)
0005460 28 CONTINUE
0005480   G(1,K2)=0.
0005500   DO 29 I1=1,H2
0005520   DO 29 J1=1,N.Y
0005540 29 QW(I1,J1)=[(56042.1+2.344*TR(I1,II,J1)/1.8-400.)]*0.184
0005560 1/(2.*FCONST)-VGUESS(I1)*PPDA(I1,II,J1)*50.48*2/1000.*
0005580 256.87*60.
0005600   DO 30 I2=1,N.Y
0005620   30 G(I2,NPl)=0.
0005640   DO 31 I3=K,K1
0005660   I4=(I3-1)/NY
0005680   I5=I3-I3/NY*NY
0005700   IF(I5.EQ.0) I5=NY
0005720   31 G(I3,NPl)=QW(I4,I5)
0005740   DO 32 I6=K,K3,NY
0005760   I7=(K-1-NY)/NY+1
0005780   32 G(I6,NPl)=G(I6,NPl)+D1(7,1)*TAIN
0005800   G(1,NPl)=G(1,NPl)+EMTCIN
0005820   I8=0
0005840   DO 33 I9=K4,K7,NY
0005860   18=I8+1
0005880   33 G(I9,NPl)=TAIN*(1.-YY(I8,1))
0005900   G(K2,NPl)=TAIN*(1.-ZZ(I))
0005920   CALL GAUSS(G,X,N,NPl)
0005940   DO 34 I10=1,N
0005960   34 X(I10)=X(I10)/1-273.16
0006000   IF(IDEBUG.EQ.1) WRITE(6,104)
0006020   IF(IDEBUG.EQ.1) WRITE(6,105) (X(I11),I11=1,K1)
0006040   IF(IDEBUG.EQ.1) WRITE(6,106) (X(I12),I12=K4,K5)
0006080   IF(IDEBUG.EQ.1) WRITE(6,108) (X(I13),I13=K2,K6)
0006100   DO 35 I14=1,N.Y
0006120   TTERM(II,II4)=X(I14)
0006140   TERM(I)=TERM(I)+X(I14)
0006160   I15=I14+NY
0006180   TERM(2)=TERM(2)+X(I15)
0006200   T(1,1,II4)=X(I15)
0006220   I16=I14+NY2
0006240   TERM(3)=TERM(3)+X(I16)
0006260   T(2,1,II4)=X(I16)
0006280   I17=I14+NY3
0006300   TERM(4)=TERM(4)+X(I17)
0006320   T(3,1,II4)=X(I17)
0006340   35 CONTINUE
0006360   DO 35 I18=1,N.Y
0006380   J16=K1+I18
0006400   I19=NY+I18
0006420   J19=K1+I19
0006440   I20=I19+NY
0006460   J20=K1+I20
0006480   I21=I20+NY
0006500 J21=K1+I21
0006520 Tten(I1,118)=X(J18)
0006540 Tten(I1,119)=X(J19)
0006560 Tten(I1,120)=X(J20)
0006580 36 Tten(I1,121)=X(J21)
0006600 N3=N1*N2
0006620 DO 37 I22=1,N3
6006640 I23=(I22-1)*NY+1
0006660 I24=I22-(I23-1)*NY
0006680 38 CONTINUE
0006700 DO 39 I00=1,4
0006720 39 Tرن(I00)=Tرن(I00)/NY/NX
0006740 Tرن(I)=Tرن(2)+Tرن(3)+Tرن(4))/3.
0006760 DO 40 IY=1,3
0006780 Tرن(IY)=Tرن(IY)/1.8-273.16
0006800 40 CONTINUE
0006820 DO 41 I=1,N2
0006840 DO 41 J=1,NX
0006860 DO 41 J=1,NY
0006880 TR(I,J)=TR(I,J)/1.8-273.16
0006900 DO 42 I=1,N2
0006920 DO 42 I=1,NX
0006940 DO 42 J=1,NY
0006960 IF(Abs(T(I,J)-TR(I,J))/TT(I,J)+TR(I,J)).GT.ER/5.) - 1G0 TO 43
0006980 1G0 TO 43
0007000 42 CONTINUE
0007020 43 KI=KING+1
0007040 IF(KING.GE.15) ER=ER*X2.
0007060 IF(KING.GE.15) ER=ER*X2.
0007080 IF(KING.GT.40) GO TO 55
0007100 DO 44 I=1,N2
0007120 DO 44 J=1,NX
0007140 DO 44 J=1,NY
0007160 TR(I,J,L)=(TT(I,J,L)+TR(I,J,L))/2.
0007180 44 CONTINUE
0007200 IF(debug.NE.1) GO TO 2
0007220 45 CONTINUE
0007240 WRITE(6,115) IG
0007260 WRITE(6,116) (TT(I,G,IG+1-J),I=1,NX),J=1,NY)
0007280 45 CONTINUE
0007300 WRITE(6,117)
0007320 46 CONTINUE
0007340 DO 48 IG=1,N2
0007360 DO 47 IG=1,N2
0007380 DO 48 J=1,NY
0007400 DO 48 IG=1,N2
0007420 DO 47 IG=1,N2
0007440 XRAI(I,G,IG)=(TT(I,G,IG)+273.16)/(TERM(I,G)+273.16)
0007460 47 DERIV(IG)=DERIV(IG)+(TT(I,G,IG)-TERM(I,G))*2
0007480 48 DERIV(IG)=SQR(DERIV(IG)/(NX*NY-1))
0007500 49 WRITE(6,103)
0007520 WRITE(6,115) IG
0007540 WRITE(6,115) IG
0007560 WRITE(6,115) IG
0084100  B2=2.*KYWT/DX**2+2.*KX/Y2
0084200  B3=2.*KYWT1/DX**2+2.*KX/Y1
0084300  C1=KX/Y1
0084400  C2=KX/Y2
0084500  C3=2.*KX/Y2
0084600  C4=2.*KX/Y1
0084700  DPL=RHOP*CC*(T-WFD-WAD)+0.5*(WFD+WAD)
0084800  DC=RHOC*CC*(T1-WCD/2.-WAD)+0.5*(WCD/2.+WAD)
0084900  AA=A*DPL
0085000  AA=A1/DPL
0085100  BB1=B1/DPL
0085200  BB2=B2/DPL
0085300  BB3=B3/DPL
0085400  CC1=C1/DPL
0085500  CC2=C2/DPL
0085600  CC3=C3/DPL
0085700  CC4=C4/DPL
0085800  K=NY+1
0085900  K1=NY+1
0086000  K2=K1+1
0086100  K3=NYK(N1-1)+1
0086200  K4=NYK(N1+1)+1
0086300  K5=NYK(N1+2)
0086400  K6=NYK(N1+1)
0086500  K7=NYK(2*N1-1)+1
0086600  K8=K1+2
0086700  K9=NY-1
0086800  K10=NY+2
0086900  K11=K1
0087000  K12=K10+1
0087100  K13=K12+1
0087200  K14=NYK(N1-1)
0087300  K15=K6-1
0087400  K16=K6+NY
0087500  RETURN
0087600  END
0087620  SUBROUTINE DATAACA(H2,02)
0087640  REAL MAC,NC
0087660  DIMENSION DNSC(7),GZ(12),R(12)
0087680  DIMENSION CM(7),WWM(7),CC(7),CM(7),DNSA(7),CMA(7),CA(7)
0087700  COMMON/FUE/C XDN50,UTH.UFA ,XN,YN
0087720  COMMON/CONC/ Y1H2,Y1C02,Y1H20,Y1CO,Y1CH4,Y1N2,Y2H20,Y202,Y2N2
0087740  COMMON/COUNT/ EP,SN,FCONST
0087760  COMMON/WMC/ WM
0087780  COMMON/CONPRE/ TTD1(3,12,12),XH2(3,12,12),TTD2(3,12,12),
0087800  1XO2(3,12,12),XH2O(3,12,12),TTDC(12,12)
0087820  COMMON/CONST/ TCIN,TAIN,DMCO,DMAIR,DFUEL,DC,DPL,DX,DY,DAREA
0087840  COMMON/CONST/ A,A1,B1,B2,B3,C1,C2,C3,C4,E
0087860  COMMON/PROP1/ CPC,PC,CPA,PP,PP,WCW,WCD,MAN,WAD,MFW,WF
0087880  COMMON/PROP2/ HC(12),H(3,12,12)
0087900  COMMON/CONST/ NP,NC,NK,NCC,NCA,NX,NY,NF,N1,N2
0087920  C = A.M. AMOUNT OF INPUT FUEL
0087940  XAMP=XDN50**XNYH2.54**X2
0087960  H2=XAMP/(SN+FCONST*UTh )*NP*3600.
DFUEL=H2/Y1H2/NP/NY/453.6
C CAL. AMOUNT OF INPUT 02
Q2=2XNP/(2.XNPFC=1X=UTA)XNPX3600.
C INSERT THE FLOW RATE OF COOLING SIDE (LB-MOLE/HR)
DO 1 IA=1,7
1 DNSC(IA)=0.
DNSC(1)=Q2/Y202XC=1XNKXUTA/NP)X2Y202/453.6
DNSC(6)=Q2/Y202XUTA=1X=KNKXNKXNP)X2Y202/453.6
DNSC(7)=Q2/Y202XUTA=1X=KNKXUTA/NP)X2Y202/453.6
DNSC(1)=DNSC(1)+DNSC(2)+DNSC(3)+DNSC(4)+DNSC(5)+DNSC(6)+DNSC(7)
AMWC=0.
DO 2 IA=1,7
CMC(IA)=DNSC(IA)/TDNSC
CMC(IA)=AMWC+WM(IA)MC(IA)
C ASSUME THE COOLING AIR RISE 45. K AND LINEAR INCREASE
DO 3 I=1,10
I2=I-1
TKCC=TCIN/1.8+45./NYX1
TFC=(TKCC-273.16)*1.8+32.
CALL CMASS(CC,DNSC,TDNSC)
CALL CMGLE(CC,CM)
TCK=THCCCM,TFC)
CPC=HTCP(CM,TFC)
MAC=TDNSC*AMWC/NC
AMUC=VIS(CM,TFC)
PR=CPC/AMUC*AMUC/TCK
IF(NDC.GT.WC) ALL=WCN/WCD
IF(NDC.LE.WC) ALL=WCD/WCN
IF(NDC.GT.WC) WC=2.*W-CN/(1.+ALL)
IF(NDC.LE.WC) WC=W-CN/(1.+ALL)
RE=MAC/AMUC
GZ(1)=CPC/AMUC*MAC/(IMDX)*TCKX6.+3.1459
R(I)=1.1.+0.003*GZ(1)/I.+0.004*GZ(1)*WX.007)
IF(RE.LT.2100.) AND.(ALL.NE.1.) TUN=3.61+4.63X(1.-ALL)
1)*3.2
IF(RE.GE.2100.) TUN=.116*(REX.667-125.)*PRX.333X(1.+)
2
1(NCX(1)MX.067)
IF(IEQ.1.) HCl=]/TUNXR(I)X/TCK/ WC
IF(GT.1.) HC1=]/(R(I)-R(I)-R(I))X/TUNX/TCK/ WC
3 CONTINUE
DRAIR=Q2/Y202/453.6/NP/NX
DMC0=TDNSC/NX
E=DMC(NX/NC/PX/DXPC
RETURN
END
SUBROUTINE VIX(M,V,Z,TK,PDP,PPH2,PP02,PPH20,PPCO,XO)
FZ=2XSR+DAALG(Z/C)+V-B+EXALOG(Z/C)+DAALOG(CDL/(CDL-Z))
DFZ=SR+DAZR+EX/2ZD/(CDL-Z)
D2FZ=-DAZK2-EX/2ZK2-1D/(CDL-Z)*XK2
GFZ=DAALOG(Z/C)+V-B+EXALOG(Z/C)+DAALOG(CDL/(CDL-Z))/-SR
COMMON/ZAT/C,CL/CLA/Cl/S,SRD/Al/F,DK/R
COMMON/FULLO/PW,TFU,AREAF,CF,XDNF
COMMON/CONT/ERR,SN,FCONST
0108200 2XDNS(12,12)
0108300 COMMON/FUCE/ XDNS0,TAH2,TAO2,XLENG,YLENG
0108400 COMMON/CATA/ CL,CLA,CU,SA,SRD,ALFA
0108500 COMMON/CONC/ Y1H2,Y1CO2,Y1H20,Y1CO,Y1CH4,Y1H2,Y2H20,Y2O2,Y2H2
0108600 COMMON/TRANS/ U2U02,U2H20,U1UH2,UIUTOT,U2UTOT
0108700 COMMON/SYTM/ POPC,POP
0108800 COMMON/TRIT/ TRR
0108900 COMMON/CONT/ERR,Z,FCONST
01089200 COMMON/IDUG/ IDEBUG
0109000 TKAVG=TR/1.8
0109100 LZ=1
0109200 S=1./TAO2
0109300 N2O2=02
0109400 N2TOT=N2O2/Y2O2
0109500 N2N2=N2TOT*Y2N2
0109600 N2H20=N2TOT*Y2H20
0109700 N1H2=H2
0109800 N1TOT=N1H2/Y1H2
0109900 N1CH4=N1TOT*Y1CH4
011000 N1CO2=N1TOT*Y1CO2
0110100 N1H20=N1TOT*Y1H20
0110200 N1CO=N1TOT*Y1CO
0110300 DO 1 I=1,NX
0110400 U2UTOT(I,1)=N2TOT/NX
0110500 U2U02(I,1)=N2O2/NX
0110600 1 U2UH20(I,1)=N2H20/NX
0110700 DO 2 J=1,NY
0110800 UIUTOT(I,J) =N1TOT/NY
0110900 2 UIUH2(I,J) =N1H2/NY
0111000 NICO=N1CO/NY
0111100 YBH2=SQR(T(Y1H2*(1.-TAH2)/(1.-Y1H2*TAH2)*Y1H2))
0111200 YB102=SQR(T(Y1CO*(Y1CO/(1.-Y1H2*TAH2))))
0111300 YB02=SQR(T(Y2O2*(Y2O2/(1.-TAO2)/(1.-Y2O2*TAO2)))/2)
0111500 XG=XDNS0
0111600 CALL V1(VGUESS,XG,TKAVG,POP,YBH2,YB02,YBH20,YBC0,XDNS0)
0111700 GO TO 4
0111800 3 VGUESS=VGUESS+0.001
0111900 IXD=1
0112000 4 MZ=1
0112100 5 CONTINUE
0112200 DO 14 I=1,NX
0112300 J2=I+1
0112400 DO 13 J=1,NY
0112500 J2=J+1
0112600 YHY=UIUH2(I,J)/UIUTOT(I,J)
0112700 YOX=U2U02(I,J)/U2UTOT(I,J)
0112800 YMA=U2UH20(I,J)/U2UTOT(I,J)
0112900 YCO=NICO/UIUTOT(I,J)
0113000 NZ=1
0113100 IF(I.EQ.1) GO TO 6
0113200 XDFRST=XDNS(I-1,J)
0113300 GO TO 8
0113400 6 XDFRST=XDNS0
0118900 IF(MZ.GT.40) ERR=0.002
0119000 IF(MZ.GT.60) GO TO 18
0119100 GO TO 5
0119120 16 IF(IDEBUG.NE.1) RETURN
0119200 WRITE(6,105) VGUESS
0119220 WRITE(6,109)
0119300 WRITE(6,106) ((XDNS(I,NY+1-J),I=1,NX),J=1,NY)
0119400 RETURN
0119500 17 WRITE(6,107) I,J
0119600 STOP
0119700 18 WRITE(6,108)
0119800 C
0119900 101 FORMAT(' WARNING ---- H2 IS USED UP --- INCREASE V GUESS')
0120000 102 FORMAT(' WARNING ---- H2 IS USED UP --- DECREASE C. D. GUESS')
0120100 103 FORMAT(' I=I2, J=J2, NZ=Z2, XD=DIS=, E13.5, XD=LAST=, E13.5 - 1)'
0120200 104 FORMAT('X.F7.6)
0120300 105 FORMAT(' THE VOLTAGE IS',F6.4,' VOLT.')/
0120400 106 FORMAT('X,F5.4,x)'
0120500 107 FORMAT(' XDNS LOOPING AT I=I2,2X,J=J2)
0120600 108 FORMAT(' VGUESS LOOPING')
0120700 109 FORMAT(' CURRENT DENSITY(A/CM**2)')
0120800 C
0120900 RETURN
0121000 END
0121020 SUBROUTINE GAUSS(A,X,N,NP1)
0121040 DIMENSION A(96,97),X(96)
0121060 NM=1=N1
0121080 DO 4 K=1,NM1
0121100 KNP=K+1
0121120 L=K
0121140 1 IF(AABS(A(K,K)).GT.ABS(A(L,K))) L=I
0121160 IF(L.EQ.K) GO TO 3
0121180 DO 2 J=K,NP1
0121200 TEMP=A(K,J)
0121220 A(K,J)=A(L,J)
0121240 2 A(L,J)=TEMP
0121260 DO 3 IA=K+1,NP1
0121280 TEMP=A(IA,K)
0121300 A(IA,K)=A(IA,J)
0121320 3 X(N)=A(N,NP1)/A(N,N)
0121340 I=N1
0121360 4 IF(I.EQ.1) GO TO 5
0121380 I=I+1
0121400 SUM=0.
0121420 DO 6 J=I1,NP1
0121440 SUM=SUM+A(I,J)*X(J)
0121460 6 X(I)=(A(I,NP1)-SUM)/A(I,I)
0121480 I=I-1
0121500 IF(I.GE.1) GO TO 5
0121520 RETURN
0121540 END
0121560 SUBROUTINE CMASS(C,FL,F)
DIMENSION C(7),WM(7),FL(7)

COMMON /WMC/ WM

WM=(FL(1)*WM(1)+FL(2)*WM(2)+FL(3)*WM(3)+WM(4)*FL(4)+FL(5)*WM(5))

IF(L(6)*WM(6)+L(7)*WM(7))/F

DO 1 I=1,7

1 C(I)=FL(I)*WM(I)/(F*WM)

RETURN

END

SUBROUTINE CMOLE(C,CM)

DIMENSION C(7),CM(7),WM(7)

COMMON /WMC/ WM

TC=C(1)/WM(1)+C(2)/WM(2)+C(3)/WM(3)+C(4)/WM(4)+C(5)/WM(5)+C(6)

DO 1 WM(6)+C(7)/WM(7)

RETURN

END

FUNCTION HTPC(CM,T)

DIMENSION CM(7),A(4,7),WM(7)

COMMON /WMC/ WM

COMMON/HTPC/ A

TP=T+460.

HTP=T.

DO 1 I=1,7

HTP=HTP+CM(I)*(A(1,1)+A(2,1)*TP+A(3,1)*TP**2+A(4,1)/(TP**2))

1 CONTINUE

RETURN

END

FUNCTION THC(C,I)

DIMENSION C(7),A(2,7),WM(7),SC(7),AJ(7,7),AI(7),AI(2,7)

COMMON/THCC/ A

COMMON/WMC/ WM

COMMON/SU/ SC

COMMON/VIC/ A1

DO 1 I=1,7

1 AI(I)=0.

THC=0.

T1=(T+460.)/1.8

DO 4 I=1,7

IF(C(I).EQ.0.) GO TO 4

DO 3 J=1,7

IF(C(J).EQ.0.) GO TO 3

IF(C(J).EQ.1.) A(J,I)=1.

IF(C(J).EQ.0.) AI(I,J)=1.

IF(C(J).EQ.1.) GO TO 2

IF(C(J).EQ.0.) AI(I,J)=0.75*(AI(I,J)+SUC(I)/AI(I,J))

A(J,I)=0.25*(AI(I,J)+SUC(I)*AI(I,J))

WM(I)=WM(I)**0.75*(1.+SUC(I)/AI(I,J))

1 AI(I,J)=0.25*(AI(I,J)+SUC(I)*AI(I,J))

2*WM(I)**0.75*(1.+SUC(I)/AI(I,J))

AI(I,J)=0.25*(AI(I,J)+SUC(I)*AI(I,J))

THC=THC*(A(I,J)*AI(I,J)*(1.+SUC(I)/AI(I,J)))

CONTINUE

RETURN
0159900  END
0160000  FUNCTION VIS(C,T)
0160100  DIMENSION A(2,7),C(7),WM(7),AI(7),AJ(7,7)
0160200  COMMON/VIP/ A
0160300  COMMON/WM/C WM
0160400  DO I=1,7
0160500   A(I)=0.
0160600   VIS=0.
0160700   DO 4 I=1,7
0160800   IF(C(I).EQ.0.) GO TO 4
0160900   DO 3 J=1,7
0161000   IF(C(J).EQ.0.) GO TO 3
0161100   IF(J.EQ.1) AJ(I,J)=1.
0161200   IF(J.EQ.1) GO TO 2
0161300   AJ(I,J)=(1.+((A(I,J)**2.)/(1.+WM(I)/WM(J))))**0.5*WM(J)/
0161400   WM(I))**2.5**2/(3.*WM(I)/WM(J))**0.5)
0161500  2 A(I)=A(I)+AJ(I,J)*C(J)
0161600  3 CONTINUE
0161700  VIS=VIS+(A(1,1)**2+2.)/(1.+C(I)**4AI(I))
0161800  4 CONTINUE
0161900  RETURN
0162000  END
0162100  SUBROUTINE DRAWE(T)
0162200  INTEGER DA(4)
0162300  REAL NC
0162400  DIMENSION T(12,12),X(12,12),Y(12,12),FL(5),IFLG(7),CORNER(8)
0162500  DIMENSION XII(2),YII(2),PII(10)
0162520  DIMENSION XI(3),WAR(11),IVARS(11),Y1(3)
0162600  COMMON/F ace/ XD50,UTH,UTA,XN,YN
0162700  COMMON/C ANHL/ NP,NC,NK,NCC,NCX,HX,NY,NF,N1,N2
0162800  DATA DA/-1.2,0,
0162820  DATA XI/0.,17.,17./
0162840  DATA YI/12.,12.,0,
0162900  DATA XII/ 17.,'IN. ',/.
0163000  DATA YII/ 12.,'IN. ',/
0163100  DATA PII/'TEMP', 'ERAT', 'URE ', 'DIST', 'RIBU', 'TION',
0163200  1, 'ON ', 'CELL', 'PLA', 'TE ' /
0163300  NFC=10
0163400  DO 1 I=1,NX
0163500  DO 1 J=1,NY
0163600  X(I,J)=XH/NX*(J-1)+XH/NX/2.
0163700  1 Y(I,J)=YN/NY*(I-1)+YN/NY/2.
0163800  DO 2 L=1,NFC
0163900  2 FL(L)=LM5.+160.
0164000  IFLGC(1)=NY
0164100  IFLG(2)=NX
0164200  IFLG(3)=NFC
0164300  IFLG(4)=0
0164400  IFLG(5)=0
0164500  IFLG(6)=0
0164600  IFLG(7)=0
0164700  CORNER(1)=0.
0164800  CORNER(2)=17.
0164900  CORNER(3)=0.