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

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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 CH_4, H_2O, H_2, CO and CO_2. In this analysis, it is assumed that a fixed percentage of hydrogen is consumed at the anode, and the H_2O being formed exits the fuel cell, with the depleted air, through the cathode exit. The overall reaction in the fuel cell power section is,

$$H_2 + 1/2\ O_2 = H_2O$$

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:

$$NX_{H2} = NI_{H2} - (\text{Imean } A)/(n\mathcal{F}) \quad (1\text{-}1)$$

$$NX_{O2} = NI_{O2} - (\text{Imean } A)/(2n\mathcal{F}) \quad (1\text{-}2)$$

$$NX_{H2O} = NI_{H2O} + (\text{Imean } A)/(n\mathcal{F}) \quad (1\text{-}3)$$

where NX: exit flow rate of hydrogen, oxygen, or steam, g-mole/sec

NI: inlet flow rate of hydrogen, oxygen, or steam, g-mole/sec

Imean: mean current density, A/cm^2

A: effective area of cell plate, cm^2

n: number of Faraday equivalents transferred

$\mathcal{F}$: Faraday constant

The energy balance for the fuel cell is

$$-(Q + W_e) = \sum_{PF} n_j (\Delta h_f^\circ)_j - \sum_{rF} n_i (\Delta h_f^\circ)_i + \sum_{PF} n_j \int_{298}^{T_{fF}} (Cp)_j \, dT - \sum_{rF} n_i \int_{T_{iF}}^{298} (Cp)_i \, dT \quad (1\text{-}4)$$

where the subscripts PF, rF represent the products and reactants in the fuel cell, respectively. TfF is the final temperature of the products and TiF is the initial temperature of the reactants in the fuel cell. The nj and ni 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:

$$Q = N_p \, Xn \, Yn \, Q_F \qquad (1\text{-}5)$$

$$\text{and } Q_F = \left(\frac{\Delta Hr}{[illegible]} - V\right) I \qquad (1\text{-}6)$$

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

ΔHr: 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:

$$V = E - \eta \qquad (1\text{-}7)$$

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

η: overpotential or polarization

The reversible cell potential, E is given by the Nernst equation:

$$E_o = E\,(T) + \frac{RT}{nF}\ln\frac{YH_2\sqrt{PtYO_2}}{YH_2O} \qquad (1\text{-}8)$$

with Pt: total pressure, atm

$E_o(T)$: standard E.M.F. of cell at temperature T, volts

$$E_o(T) = 1.261 - 0.00025\,T,\ T,\ K \text{ (Ref. 2)}$$

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 η consists of four components,

$$\eta = \eta a + \eta r + \eta d + \eta co \qquad (1\text{-}9)$$

where ηa: activation polarization at cathode, volts

ηr: resistance polarization, volts

ηd: diffusion polarization, volts

ηco: activation polarization at anode due to CO poisoning of catalyst, volts

and

$$\eta a = \frac{RT}{\alpha o ZF}\ln\frac{i}{(io)(SA)(CL)(CU)} \qquad (1\text{-}10)$$

with αo: transfer coefficient

i: current density, mA/cm^2

io: exchange current density of cathode, mA/cm^2

SA: specific catalyst surface area, cm^2/g

CL: catalyst loading on cathode, g/cm^2

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 correlaion of io as a function of YO2, YH2O, and T. An empirical fit is

$$io = 232.7\ (PtYO2)^{0.8}\ (PtYH2O)^{0.4377}\ \exp\ (-6652/T) \qquad (1\text{-}11)$$

The resistance polarization is

$$\eta r = ir$$

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

The expression of ηco was chosen to have strong temperature dependence, be directly proportional to Yco, and have a logarithmic dependence on i, iao, and catalyst effective area. The resulting expression (Ref. 2) is

$$\eta co = 0.0782PtYco\ \exp\left[9190\ \left(\frac{1}{T} - \frac{1}{450}\right)\right] \ln \frac{i}{CLa\ SA\ CU\ iao} \qquad (1\text{-}12)$$

where CLa: anode catalyst loading, g/cm^2

iao: 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.

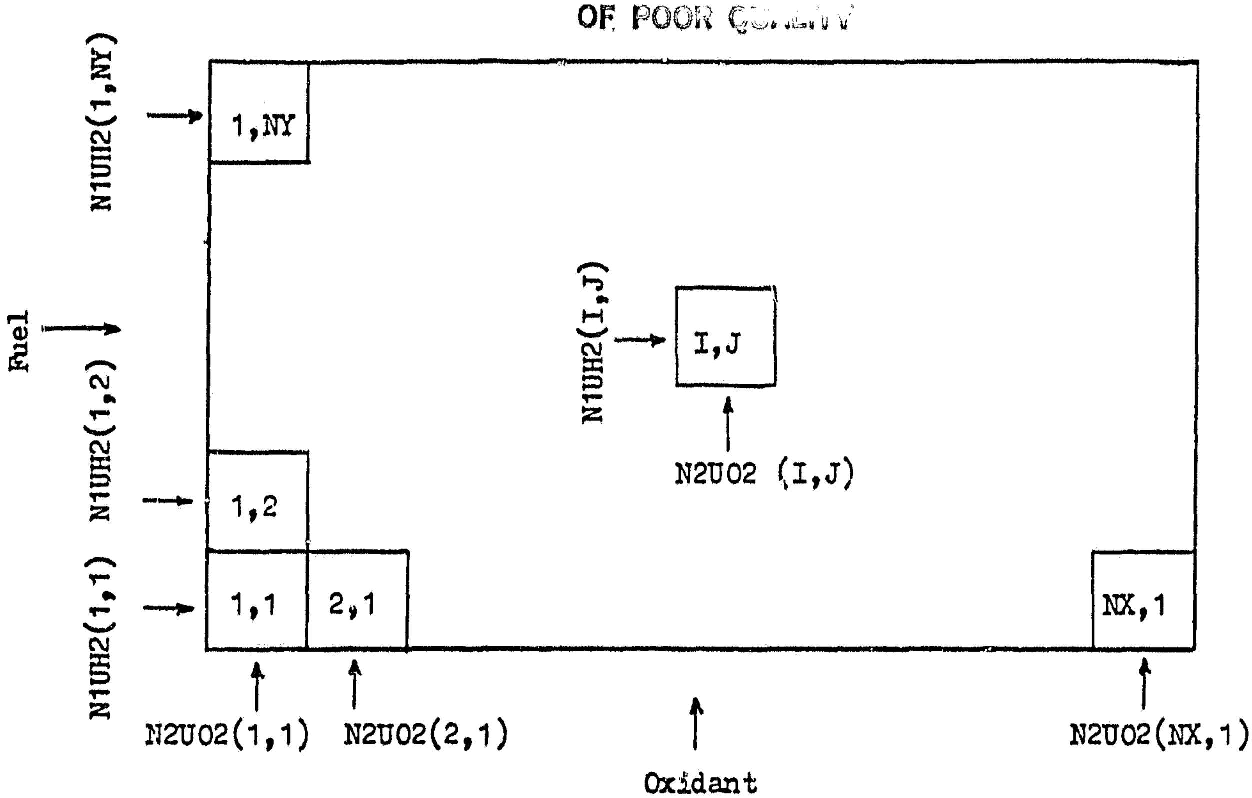

Figure 1 Finite Difference Model Definition of Current Density Distribution on Cell Plate

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Mathematic Formulation

Exit flow of hydrogen from gird (i,j)

$$NX\ H_2(i,j) = NI\ H_2(i,j) - (I(i,j)A)/(n\mathcal{F}) \quad (2-1)$$

Exit flow of oxygen from gid (i,j)

$$NX\ O_2(i,j) = NI\ O_2(i,j) - (I(i,j)A)/(2n\mathcal{F}) \quad (2-2)$$

Exit flow of water from grid (i,j)

$$NX\ H_2O(i,j) = NI\ H_2O(i,j) + (I(i,j)A)/(n\mathcal{F}) \quad (2-3)$$

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/cm^2
A	:	area of grid, cm^2

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

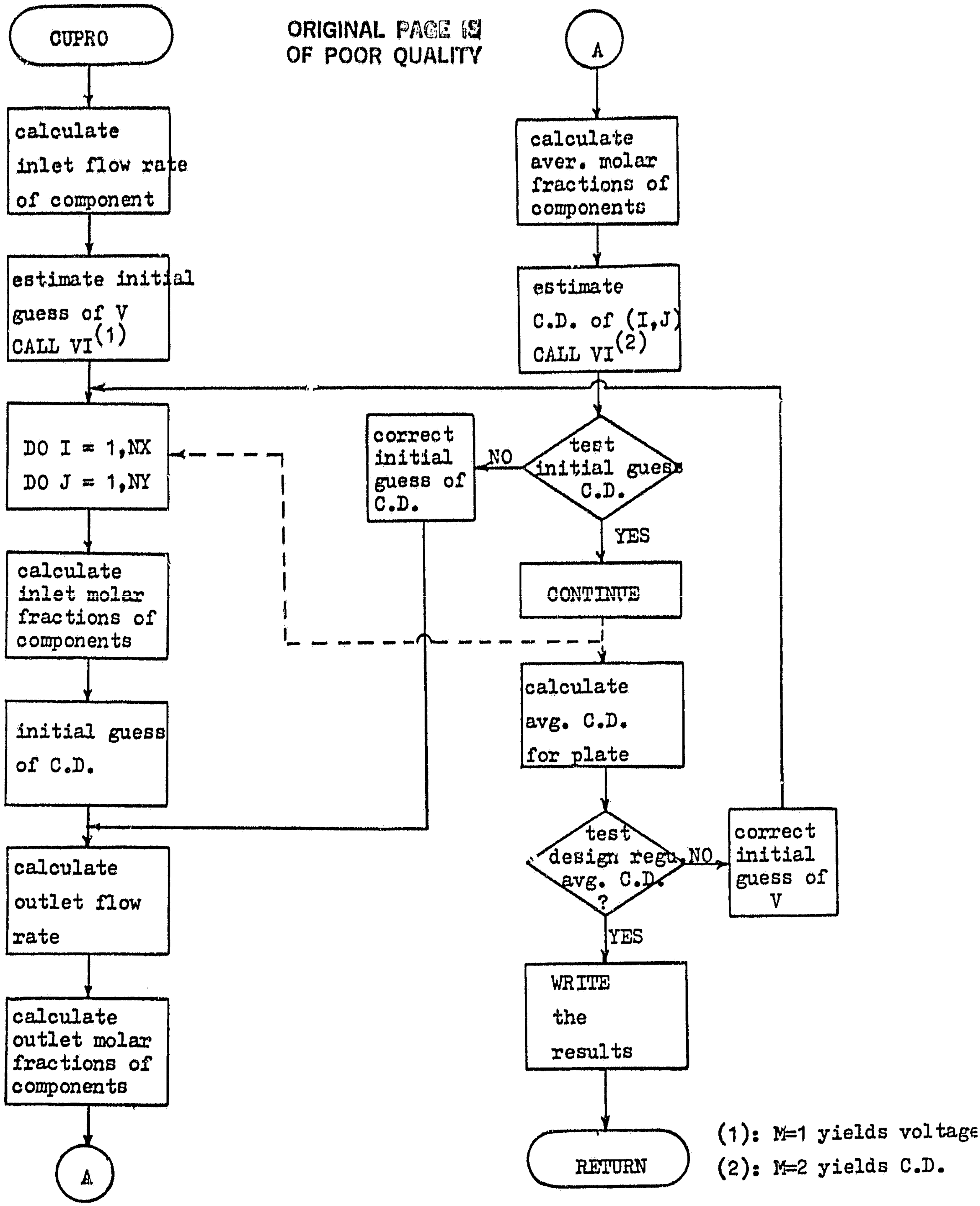

Figure 2 Flow Chart of CUPRO

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 oxident have been presented in Chapter 2. There are four energy balance equations for the cell plate, cooling plate, process air, and coolant.

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cell on process air side in air flow direction

$$t\ Ky \frac{\partial^2 T}{\partial y^2} + Kx \frac{\partial T}{\partial x}\Big|_{x+t} - Kx \frac{\partial T}{\partial x}\Big|_{x} - \frac{C_p\ m_p}{Pp} \frac{\partial Tp}{\partial y} = -(V^*-V)I \qquad (3\text{-}1)$$

cooling plate in coolant direction

$$t'\ Ky \frac{\partial^2 T}{\partial y^2} + 2Kx\frac{\partial T}{\partial x}\Big|_{x+t'/2} - \frac{Cc\ m_c}{Pc} \frac{\partial Tc}{\partial y} = 0 \qquad (3\text{-}2)$$

process air side

$$\frac{d\ Tp}{d\ y} = \frac{hp\ Sp}{mp\ Cp}(T-Tp) \qquad (3\text{-}3)$$

coolant side

$$\frac{d\ Tc}{d\ y} = \frac{hc\ Sc}{mc\ Cc}(T-Tc) \qquad (3\text{-}4)$$

Boundary conditions

$x = 0$	$\partial T/\partial x = 0$	symmetric condition
$y = 0$	$\partial T/\partial y = 0$	adiabatic assumption
$x = Lx$	$\partial T/\partial x = 0$	symmetric condition
$y = Ly$	$\partial T/\partial y = 0$	adiabatic assumption
$y = 0$	$Tp = Tp$, inlet	
$y = 0$	$Tc = Tc$, inlet	

where m = mass flow rate, Kg/hr-channel

C = heat capacity, J/Kg-K

Ky = effective thermal conductivity of cell in flow direction, J/hr-m-K

Kx = effective thermal conductivity of cell on stacking direction, J/hr-m-K

t = thickness of cell including fuel and air channel, m

x1 = effective conduction distance from plate to upper cell plate, m

x2 = effective conduction distance from plate to lower cell plate, m

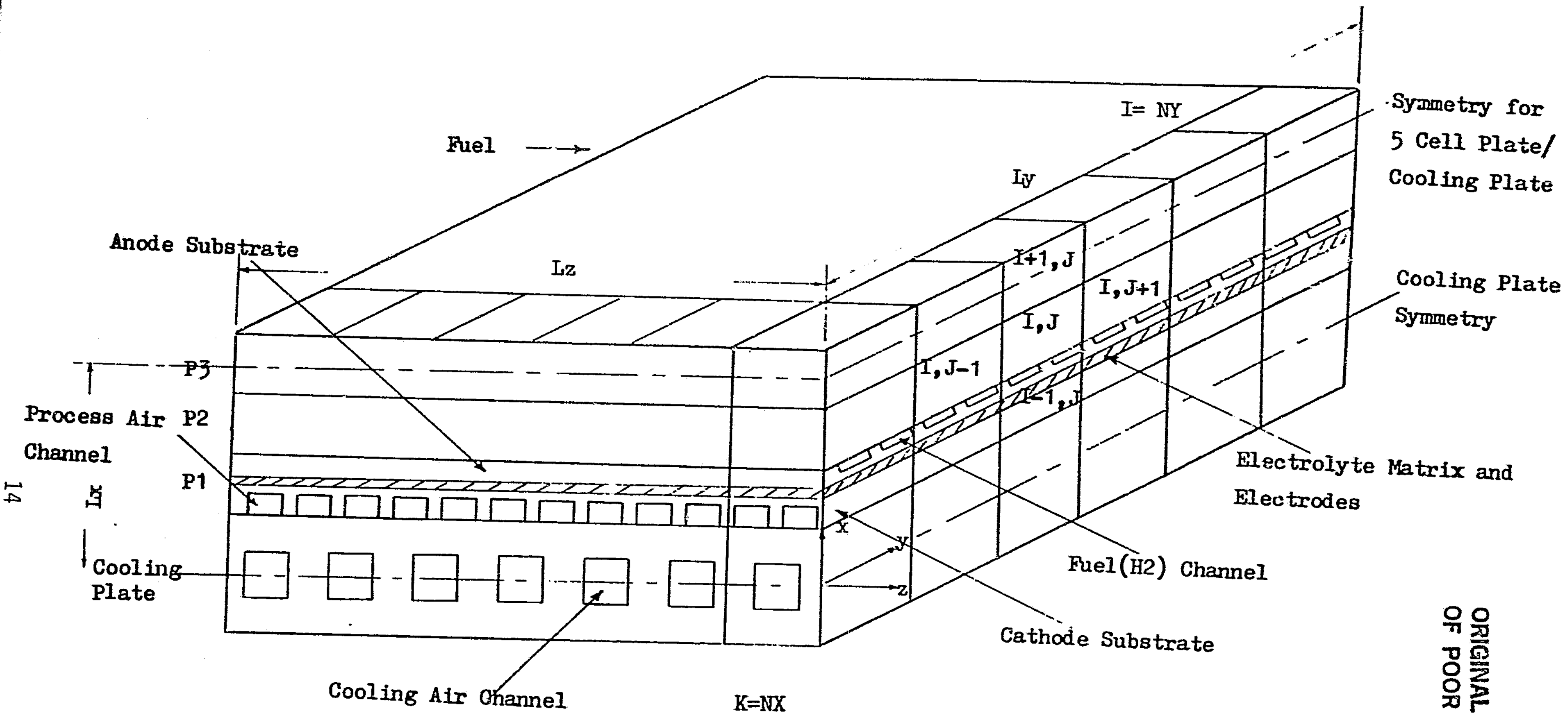

Figure 3 Geometry of a Strip of Element for the Thermal Analysis Model

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P = pitch of channel, m

xl' = effective conduction distance from cooling plate to upper cell plate, m

Lx, Ly = height and length of one slice, respectively, m

V* = ΔH/ZF, V

t' = thickness of cooling plate, m

h = heat transfer coefficient, J/hr-m^{2}K

S = perimeter of the channel, m

Subscription

p = process air

c = 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 ($2 \le j \le N-1$) for bipolar plate i ($2 \le i \le N1$) can now be written as (see Figure 3)

$$- \left(\frac{Ky\ t}{\Delta Y^2}\right) Ti,j-1 + \left(2 \frac{Ky\ t}{\Delta Y^2} + \frac{Kx}{X1} + \frac{Kx}{X2}\right) Ti,\ j$$

$$- \left(\frac{KY\ t}{\Delta Y^2}\right) Ti,y+1 - \left(\frac{Kx}{X1}\right) Ti-1,j - \left(\frac{Kx}{X2}\right) Ti+1,j \qquad (3\text{-}5)$$

$$+ \left(\frac{Mp\ Cp}{Pp\ \Delta Y}\right) (Tpi,j - Tpi,j-1) = (V^* - V)\ Ii,j$$

The energy balance on an internal element j ($2 \le j \le N-1$) of the cooling plate i=1 can be written as

$$- \left(\frac{Ky\ t'}{\Delta Y^2}\right) T1,\ j-1 + \left(2\ \frac{Ky\ t'}{\Delta Y^2} + 2\ \frac{Kx}{X1'}\right) T1,\ j$$

$$- \left(\frac{Ky\ t'}{\Delta Y^2}\right) T1,\ j+1 - \left(2\ \frac{Kx}{X1}\right) T2,\ j \qquad (3\text{-}6)$$

$$+ \left(\frac{Mc\ Cc}{Pc\ \Delta Y}\right) (TCj - TCj-1) = 0$$

The energy balance on interior element j ($2 \leq j \leq N-1$) of the symmetric plate i=N1 is

$$- \left(\frac{Ky\ t}{\Delta Y^2}\right) T_{N1,j-1} + \left(2\ \frac{Ky\ t}{\Delta Y^2} + \frac{\delta Kx}{X2}\right) T_{N1,j}$$

$$- \left(\frac{Ky\ t}{\Delta Y^2}\right) T_{N1,j+1} - \left(\frac{\delta Kx}{X2}\right) T_{N1-1,j} \qquad (3\text{-}7)$$

$$+ \left(\frac{Mp\ Cp}{Pp\ \Delta Y}\right) (Tp_{N1,j} - Tp_{N1,j-1}) = (V^* - V_{N1})\ I_{N1,j}$$

where δ = 2 for odd values of NK

δ = 1 for even values of NK

NK: the number of cell plates between two adjacent cooling plates

N1: 1 + NK/2 for even NK

1 + (NK+1)/2 for odd NK

The energy balance on elements j=1 are obtained as above, except for: the values of Ti,0 are replaced by Ti,1: the values of Tpi,0 are replaced by TP0, which is the inlet process air temperature; and TCo is replaced by TC0, the inlet cooling air temperature. The energy balances on elements j=N are obtained from the above with Ti,j+1 replaced by Ti,N.

For the process air flow, one can set up N1xN equations of the form

$$TP_{i,j} = TP_{i,j-1} + (T_{i,j} - TP_{i,j-1})\,(1-e^{-\phi_{pi,j}}) \qquad (3\text{-}8)$$

where

$$\phi_{pi,j} = \frac{h_{i,j}\ SP}{Mp\ Cp}\,\Delta Y \qquad (3\text{-}9)$$

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

$$TC_j = TC_{j-1} + (T_{1,j} - TC_{j-1})(1-e^{-\phi_{cj}}) \qquad (3\text{-}10)$$

where

$$\phi_{cj} = \frac{h_{cj} Sc}{Mc\ Cc}\,\Delta Y \qquad (3\text{-}11)$$

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 covergence 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:

$$Nuf = 3.61 + 4.63\,(1-\alpha)^{3.2} \qquad (3\text{-}12)$$

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)

$$R = 1 + \frac{0.0183\ Gz}{1+0.04\ Gz^{2/3}} \tag{3-13}$$

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)

$$Nu_t = 0.116\ [Re^{2/3} - 125]\ Pr^{1/3}\ [1 + (D/x)^{2/3}] \tag{3-14}$$

The flow chart of the executive program (MAIN program) for calculating the temperature distribution in the stack is shown in Figure 4.

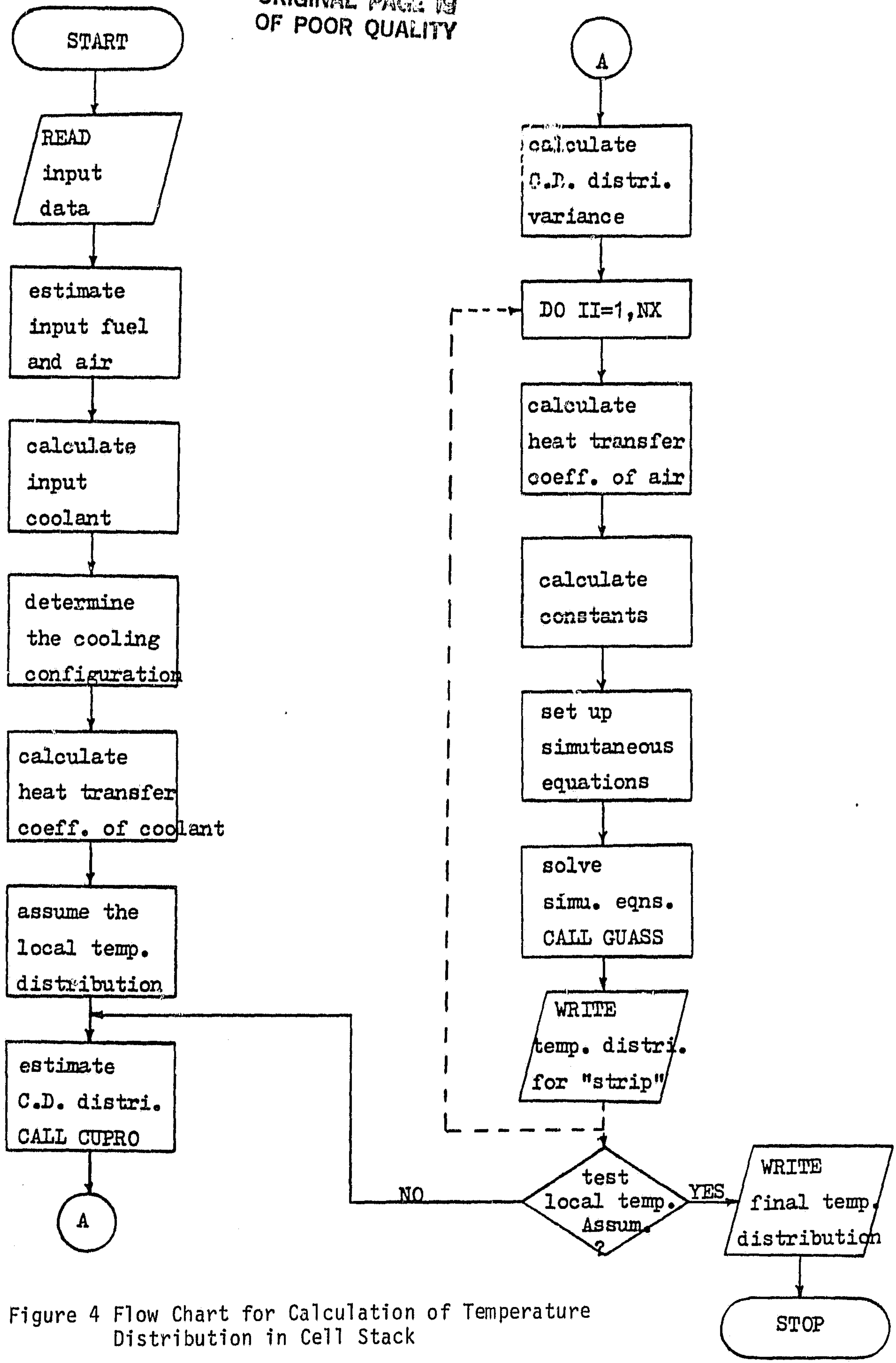

Figure 4 Flow Chart for Calculation of Temperature Distribution in Cell Stack

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

AL:	aspect ratios of process air
AL1(I):	aspect ratios of cooling channel in different sections (treed form)
ALFA:	transfer coefficient
AMUC:	viscosity; lb/hr-ft
AMWA:	molecular weight of process air; lb/lb-mole
AMWC:	molecular weight of cooling air; lb/lb-mole
CL:	catalyst loading; mg/cm^2
CU:	catalyst utilization
CM(I):	mole fraction of component I in cooling air
CMC(I):	mole fraction of component I in process air
CPC:	heat capacity; Btu/lb-mole-R
DNSA(I):	moles of component I in process air; lb-mole
DNSC(I):	moles of component I in cooling air; lb-mole
DX:	length of x-division; ft
FCONST:	Faraday constant; 96500 coul./g-equivalent
G(I,J):	coefficient of simultaneous linear equations
GZ(I):	Graetz number of different sections in cooling channels
GZA:	Graetz number in process air
H(I,J,K):	heat transfer coefficient of plate I x-division J y-division K of process air; Btu/ft^2-hr-R
H2:	required hydrogen; g-mole/hr-stack
HC(I):	heat transfer coefficient of division I in cooling channel
HH:	required hydrogen; g-mole/sec-plate
PPRO(I,J,K):	current density of plate I x-division J y-division K; A/cm^2
KX:	effective thermal conductivity in stacking direction; Btu/hr-ft-R
KY:	effective thermal conductivity in flow direction; Btu/hr-ft-R
MA:	mass flow rate of process air; lb/hr-channel
MAC(I):	mass flow rate of cooling air in section I; lb/hr-channel
NC:	number of stoich air in cooling channel
NCA:	number of process air channels
NCC:	number of cooling channels
NK:	number of plates between cooling plate
NP:	number of plates in a stack
NX:	number of divisions in x direction
NY:	number of divisions in y direction
O2:	required oxygen; g-moles/hr-stack
OO:	required oxygen; g-moles/sec-plate
PC:	pitch of cooling channel; ft
PH1(I,J):	dimensionless group of plate I division J in process air
PH2(I):	dimensionless group of division I in cooling air
POP:	inlet gas pressure; atm
PP:	pitch of process air; ft
PR:	Prandtl number of gas
QW(I,J):	heat generation rate of division J plate I; Btu/hr

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
TKC:	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
TDO2(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 temperture 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
WFD:	depth of fuel channel; ft
WFW:	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

TABLE 1 (cont'd)

PROGRAM NOMENCLATURE

XN:	length of cell in x-direction; ft
XXOO(J,K):	same as PPRO(I,J,K) in each plate; A/cm^2
Y1:	effective conduction distance from cell plate to cooling plate; ft
Y2:	effective conduction distance from cell plate to another cell plate; ft
$Y1CH_4$:	mole fraction of CH_4 in fuel
Y1CO:	mole fraction of CO in fuel
$Y1CO_2$:	mole fraction of CO_2 in fuel
$Y1H_2$:	mole fraction of H_2 in fuel
$Y1H_2O$:	mole fraction of H_2O in fuel
$Y2H_2O$:	mole fraction of H_2O in air
$Y2N_2$:	mole fraction of N_2 in air
$Y2O_2$:	mole fraction of O_2 in air
YN:	length of cell in y-direction; ft
Z:	number of Faraday equivalents transferred

TABLE 2

DEFINITIONS OF SUBROUTINES

Subroutines	DESCRIPTION
DATAIN	1. input data reading 2. changing units 3. calculation of the constants used in MAIN program
DATACA	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-Seidle iteration used to solve simultaneous linear equations
CMASS	calculation of the mass fraction of gas stream
CMOLE	calculation of the mole fraction 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 conductivites 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 thier units and numerical values in the sample run, which will be discussed in the next chapter.

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TABLE 3

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

NAMELIST LIST	VARIABLE NAME	SAMPLE VALUE	UNIT	DEFINITION
DIMEN	XN	17	in	length of cell plate in x-direction
DIMEN	YN	12	in	length of cell plate in y-direction
DIMEN	DNSCO	0.325	A/cm^2	designed current density
DIMEN	UTA	0.5		utilization of O_2 in stack
DIMEN	UTH	0.75		utilization of H_2 in stack
DIMEN	POPC	3.4	atm	pressure of cooling air
DIMEN	POP	3.4	atm	operating pressure in stack
DIMEN	TKA	443	K	inlet temperature of process air
DIMEN	WFD	0.00333	ft	depth of fuel channel
DIMEN	WFW	0.01	ft	width of fuel channel
DIMEN	NCC	30		number of cooling channels
DIMEN	WE	0.00333	ft	thickness of cell (electrode and matrix)
DIMEN	TKF	450	K	inlet temperature of fuel
DIMEN	T	0.0108	ft	thickness of cell plate
DIMEN	NK	5		number of plates between two cooling plates
DIMEN	WAD	0.00333	ft	depth of process air channel
DIMEN	WAW	0.01	ft	width of process air channel
DIMEN	NP	23		number of cell plates
DIMEN	NCA	80		number of process air channels
DIMEN	NF	55		number of fuel channels
DIMEN	T1	0.02917	ft	thickness of cooling plate
DIMEN	NX	12		finite difference number in x-direction
DIMEN	NY	12		finite difference number in y-direction
DIMEN	TINGS	191	C	initial guess of plate temperature
ERR	ER	0.01		criterion for convergence
CZ	CLCA	0.52	mg/cm^2	catalyst loading on cathode side
CZ	CLAN	0.34	mg/cm^2	catalyst loading on anode side
CZ	CU	0.15		utilization of catalyst
CZ	SA	500	cm^2/mg	surface area of catalyst
CZ	SRO	0.44	-cm^2	cell resistance at 450 K
CZ	ALFA	0.5		transfer coefficient
CZ	DKC	240000	A/atm	constant to calcuate limiting current density
CZ	R		J/(g-mol)(K)	gas constant
FALA	Z		g-equivalent	number of Faraday equivalents transferred
FALA	FCONST		C-g/equivalent	Faraday constant
DIGA	NC			ratio of cooling air to air consumed in stack
DIGA	KX		Btu/(ft-h-R)	effective thermal conductivity in stacking direction
DIGA	KY		Btu/(ft-h-R)	effective thermal conductivity in flow direction

TABLE 3 (cont'd)

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

NAMELIST LIST	VARIABLE NAME	SAMPLE VALUE	UNIT	DEFINITION
DIGA	TKC		K	inlet cooling air temperature
DIGA	WCW	0.22	ft	width of cooling channel
DIGA	WCD	0.22	ft	depth of cooling channel
FUEL	$Y1H_2$	0.76		mole fraction of H_2 in anode inlet
FUEL	$Y1CO_2$	0.24		mole fraction of CO_2 in anode inlet
FUEL	Y1CO	0		mole fraction of CO in anode inlet
FUEL	$Y1CH_4$	0		mole fraction of CH_4 in anode inlet
FUEL	$Y1H_2O$	0		mole fraction of H_2O in anode inlet
FUEL	$Y1N_2$	0		mole fraction of N_2 in anode inlet
FUEL	$Y2O_2$	0.208		mole fraction of O_2 in cathode inlet
FUEL	$Y2N_2$	0.782		mole fraction of N_2 in cathode inlet
FUEL	$Y2H_2O$	0.01		mole fraction of H_2O in cathode inlet
HEATC	RHOP	163	lbm/ft^3	density of cell plate
HEATC	RHOC	135	lbm/ft^3	density of cooling plate
HEATC	CCP	0.25	Btu/(lbm-R)	heat capacity of cell plate
HEATC	CCC	0.201	Btu/(lbm-R)	heat capacity of cooling plate

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.

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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.

```
&DIMEN
      XN=17.,
      YN=12.,
      XDNS0=.325,
      UTA=0.5,
      UTH=.75,
      POPC=3.4,
      POP=3.4,
      TKA=443.,
      WFD=0.003333,
      WFW=0.01,
      NCC=30,
      WE=0.0033333,
      TKF=450.,
      T=0.010833,
      NK=5,
      WAD=0.0033333,
      WAW=0.01,
      NP=23,
      NCA=80,
      NF=55,
      T1=0.02917,
      NX=12,
      NY=12,
      TINGS=191.
&END
&ERR
      ER=0.01,
&END
&CZ
      CLCA=0.52,
      CLAN=0.34,
      CU=.15,
      SA=500.,
      SRO=.44,
      ALFA=.5,DKC=240000.,R=8.314
&END
&FALA
      Z=2.,
      FCONST=96500.,
&END
&DIGA
      NC=36.,
      KX=1.5,
      KY=30.,
      TKC=403.3,
      WCW=0.22,
      WCD=0.22,
&END
&FUEL
      Y1H2=0.76,
      Y1CO2=0.24,
      Y1CO=0.,
      Y1CH4=0.,
```

Figure 5 Sample Input Data

```
     Y1H20=0.,
     Y1N2=0.,
     Y2O2=0.208,
     Y2N2=0.782
     Y2H20=0.01
&END
&HEATC RHOP=163.,RHOC=135.,CCP=0.25,CCC=0.201
&END
```

Figure 5 continued

```
&DIMEN
XN= 17.0
YN= 12.0
XDNS0= 0.3250
UTA= 0.50
UTH= 0.750
POPC= 3.40
POP= 3.40
TKA= 443.0
WFD= 0.33330E-02
WFW= 0.9999998E-02
NCC= 30
WE= 0.333330E-02
TKF= 450.0
T= 0.108330E-01
NK= 5
WAD= 0.333330E-02
WAW= 0.9999998E-02
NP= 23
NCA= 80
NF= 55
T1= 0.29170E-01
NX= 12
NY= 12
TINGS= 191.0
&END
&ERR
ER= 0.9999998E-02
&END
&CZ
CLCA= 0.520
CLAN= 0.340
CU= 0.150
SA= 500.0
SRO= 0.440
ALFA= 0.50
DKC= 240000.0
R= 8.313999
&END
&FALA
Z= 2.0
FCONST= 96500.0
&END
&DIGA
NC= 36.0
KX= 1.50
KY= 30.0
TKC= 403.2998
WCW= 0.220
WCD= 0.220
&END
&FUEL
Y1H2= 0.760
Y1CO2= 0.2399999
Y1CO= 0.0
Y1CH4= 0.0
Y1H2O= 0.0
Y1N2= 0.0
Y2O2= 0.2079999
```

Figure 6 Sample Computer Run

```
Y2N2= 0.7819999
Y2H20= 0.9999998E-02
&END
&HEATC
RHOP= 163.0
RHOC= 135.0
CCP= 0.250
CCC= 0.2010
&END
```

Figure 6 continued

```
*************
*AIR COOLING*
*************
```

Figure 6 continued

*** CELL PLATE *** 1

THE VOLTAGE IS 0.5684 VOLT.

CURRENT DENSITY(A/CM**2)

.3976	.3951	.3926	.3897	.3864	.3825	.3777	.3720	.3649	.3558	.3439	.3277
.4043	.4016	.3989	.3958	.3922	.3880	.3829	.3767	.3690	.3593	.3464	.3288
.4032	.4005	.3977	.3945	.3909	.3866	.3815	.3753	.3675	.3578	.3451	.3278
.3951	.3925	.3898	.3868	.3833	.3792	.3742	.3684	.3611	.3521	.3404	.3249
.3813	.3790	.3765	.3737	.3704	.3667	.3622	.3570	.3505	.3426	.3325	.3193
.3633	.3613	.3591	.3566	.3537	.3505	.3466	.3421	.3365	.3299	.3215	.3109
.3427	.3410	.3391	.3369	.3345	.3318	.3285	.3248	.3202	.3[illegible]48	.3081	.2997
.3209	.3195	.3179	.3161	.3141	.3118	.3092	.3062	.3025	.2982	.2930	.2866
.2994	.2982	.2969	.2955	.2939	.2921	.2900	.2876	.2847	.2814	.2773	.2725
.2796	.2787	.2776	.2765	.2752	.2738	.2721	.2703	.2680	.2655	.2624	.2587
.2634	.2626	.2618	.2609	.2598	.2587	.2574	.2559	.2541	.2522	.2498	.2469
.2542	.2536	.2529	.2521	.2512	.2503	.2492	.2479	.2465	.2448	.2429	.2405

TEMPERATURE(C)

212.	211.	211.	210.	209.	209.	208.	207.	206.	204.	202.	199.
210.	209.	209.	208.	208.	207.	206.	205.	204.	202.	200.	198.
207.	206.	206.	205.	205.	204.	203.	202.	201.	200.	198.	195.
202.	202.	202.	201.	201.	200.	199.	198.	197.	196.	194.	192.
197.	197.	196.	196.	196.	195.	194.	194.	193.	191.	190.	188.
191.	191.	191.	190.	190.	190.	189.	188.	187.	186.	185.	184.
185.	185.	185.	185.	184.	184.	183.	183.	182.	181.	180.	179.
179.	179.	179.	179.	178.	178.	177.	177.	176.	176.	175.	174.
173.	173.	173.	173.	172.	172.	172.	171.	171.	170.	170.	169.
168.	167.	167.	167.	167.	167.	166.	166.	166.	165.	165.	164.
163.	163.	163.	162.	162.	162.	162.	162.	161.	161.	161.	160.
160.	159.	159.	159.	159.	159.	159.	159.	158.	158.	158.	158.

Figure 6 continued

*** CELL PLATE *** 2

THE VOLTAGE IS 0.5766 VOLT.

CURRENT DENSITY(A/CM**2)

.3907	.3882	.3857	.3829	.3797	.3758	.3712	.3656	.3587	.3499	.3386	.3232
.3985	.3959	.3932	.3901	.3866	.3824	.3773	.3712	.3637	.3541	.3416	.3247
.3989	.3963	.3935	.3903	.3866	.3823	.3771	.3709	.3632	.3536	.3410	.3241
.3924	.3898	.3871	.3839	.3804	.3762	.3712	.3653	.3579	.3488	.3371	.3215
.3800	.3776	.3750	.3721	.3688	.3650	.3604	.3550	.3484	.3403	.3300	.3166
.3631	.3610	.3587	.3561	.3532	.3498	.3458	.3411	.3354	.3285	.3199	.3089
.3434	.3416	.3396	.3373	.3348	.3319	.3285	.3246	.3199	.3142	.3072	.2985
.3224	.3209	.3192	.3173	.3152	.3128	.3100	.3068	.3030	.2985	.2929	.2862
.3017	.3005	.2991	.2976	.2959	.2939	.2917	.2891	.2861	.2825	.2782	.2730
.2833	.2823	.2811	.2799	.2785	.2769	.2751	.2731	.2707	.2679	.2646	.2605
.2692	.2684	.2674	.2664	.2652	.2640	.2625	.2609	.2589	.2567	.2540	.2508
.2633	.2626	.2618	.2609	.2599	.2588	.2575	.2560	.2544	.2524	.2501	.2474

TEMPERATURE(C)

216.	215.	215.	214.	214.	213.	212.	211.	209.	208.	206.	203.
214.	214.	213.	213.	212.	211.	210.	209.	208.	206.	204.	201.
211.	211.	210.	210.	209.	208.	207.	206.	205.	204.	202.	199.
207.	206.	206.	205.	205.	204.	203.	202.	201.	200.	198.	196.
201.	201.	201.	200.	200.	199.	198.	198.	197.	195.	194.	192.
196.	195.	195.	195.	194.	194.	193.	192.	191.	190.	189.	187.
189.	189.	189.	189.	188.	188.	187.	187.	186.	185.	184.	182.
183.	183.	183.	182.	182.	182.	181.	181.	180.	179.	178.	177.
177.	177.	177.	176.	176.	176.	176.	175.	175.	174.	173.	172.
172.	171.	171.	171.	171.	171.	170.	170.	170.	169.	169.	168.
167.	167.	167.	167.	167.	166.	166.	166.	166.	165.	165.	164.
165.	164.	164.	164.	164.	164.	164.	164.	163.	163.	163.	162.

Figure 6 continued

*** CELL PLATE *** 3

THE VOLTAGE IS 0.5792 VOLT.

CURRENT DENSITY(A/CM**2)

.3883	.3859	.3834	.3806	.3774	.3736	.3690	.3635	.3567	.3480	.3368	.3217
.3966	.3940	.3913	.3882	.3847	.3805	.3755	.3694	.3619	.3524	.3401	.3234
.3975	.3948	.3920	.3889	.3852	.3809	.3757	.3695	.3618	.3522	.3397	.3229
.3914	.3889	.3861	.3830	.3794	.3752	.3702	.3642	.3569	.3477	.3360	.3205
.3795	.3771	.3745	.3716	.3683	.3644	.3598	.3543	.3477	.3395	.3292	.3157
.3630	.3609	.3586	.3559	.3530	.3495	.3455	.3407	.3350	.3280	.3193	.3082
.3436	.3418	.3398	.3375	.3349	.3320	.3286	.3246	.3198	.3140	.3070	.2981
.3229	.3214	.3196	.3177	.3156	.3132	.3103	.3071	.3032	.2986	.2930	.2861
.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)

217.	217.	216.	216.	215.	214.	213.	212.	211.	209.	207.	204.
216.	215.	214.	214.	213.	212.	212.	211.	209.	208.	205.	203.
212.	212.	211.	211.	210.	210.	209.	208.	206.	205.	203.	200.
208.	208.	207.	207.	206.	205.	205.	204.	202.	201.	199.	197.
203.	202.	202.	202.	201.	200.	200.	199.	198.	197.	195.	193.
197.	197.	196.	196.	195.	195.	194.	193.	193.	191.	190.	188.
191.	190.	190.	190.	189.	189.	188.	188.	187.	186.	185.	183.
184.	184.	184.	184.	183.	183.	182	182.	181.	181.	180.	178.
178.	178.	178.	178.	177.	177.	177.	176.	176.	175.	174.	174.
173.	173.	173.	172.	172.	172.	172.	171.	171.	170.	170.	169.
169.	168.	168.	168.	168.	168.	168.	167.	167.	167.	166.	166.
166.	166.	166.	166.	166.	166.	165.	165.	165.	165.	164.	164.

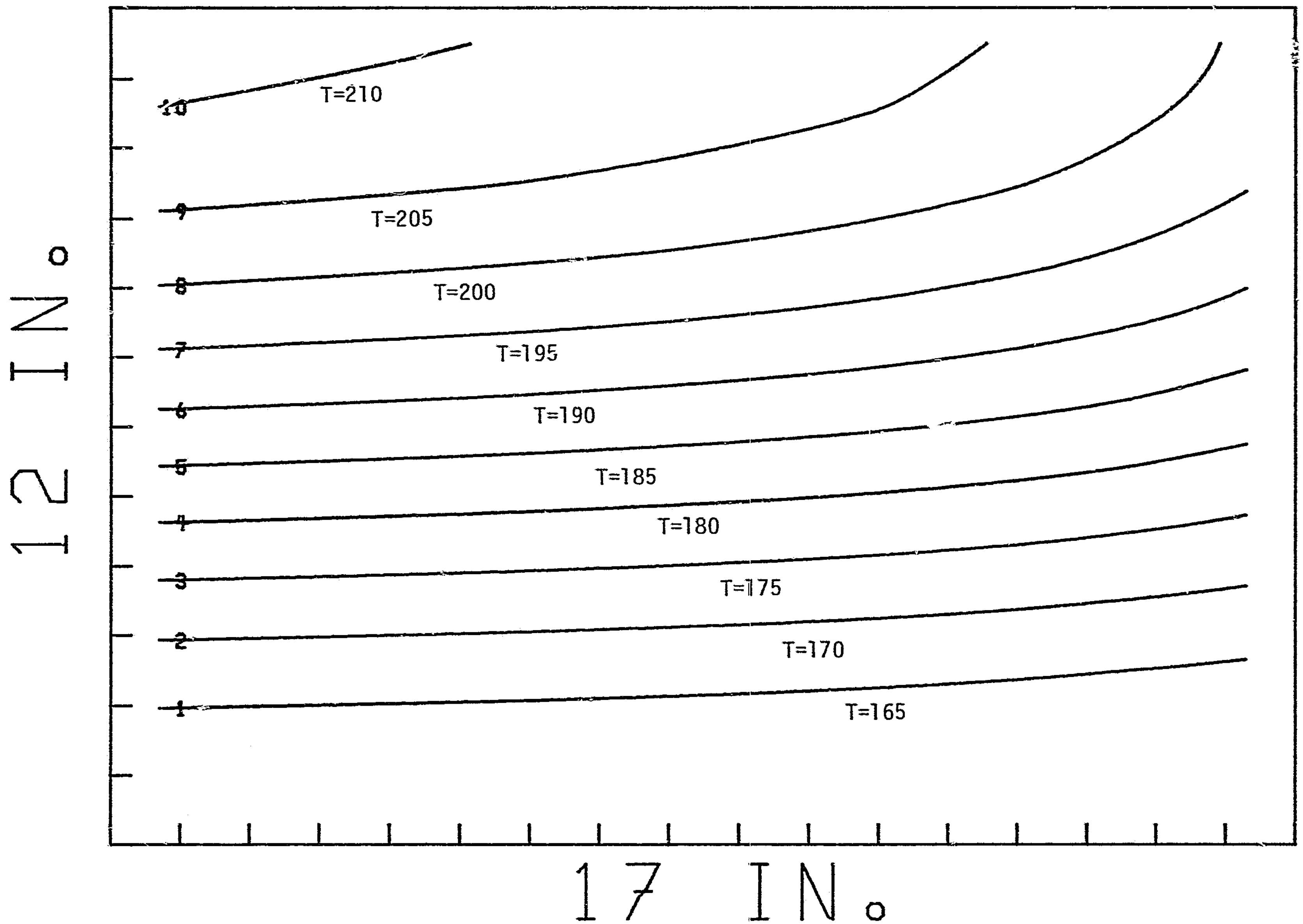
Figure 6 continued

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

Figure 6 continued

Figure 7

TEMPERATURE DISTRIBUTION ON CELL PLATE



5.2 Further Developments

Parametric Sensitivity and Cooling Scheme

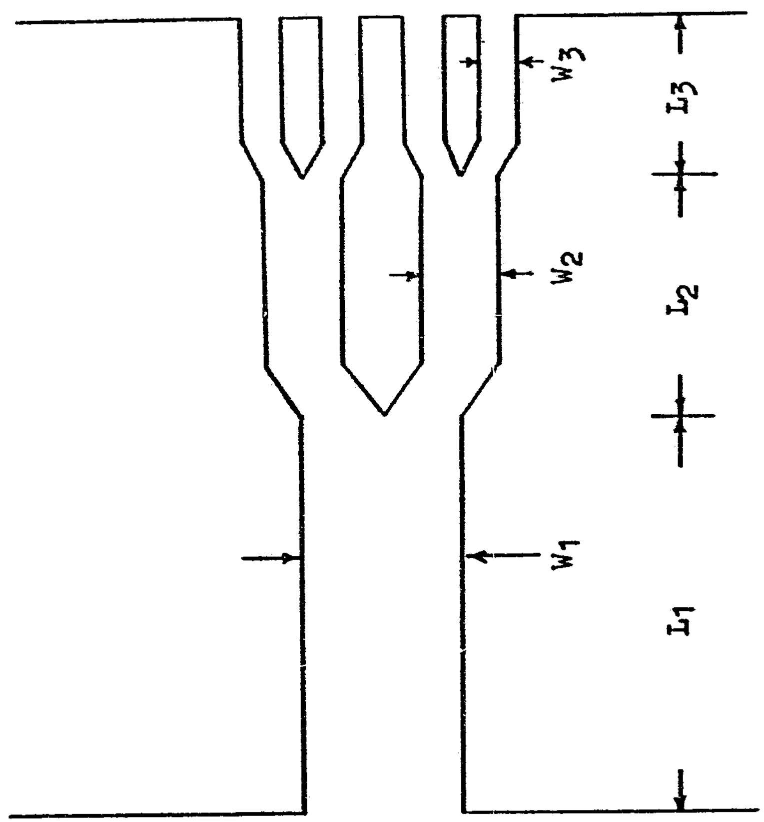
The plate temperature is a function of the current density, the concentrations of hydrogen and oxygen, and the cooling effectiveness. In order to achieve the optimum design with respect to the temperature distribution, more studies of the parameters involved and the cooling scheme are necessary. The 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 crossectional 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.



Width ratio $W_1:W_2:W_3 = 1:0.5:0.25$

Section length $L_1:L_2:L_3 = 5:3:2$
ratio

Figure 8 One "Branch" cooling channel

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.

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PROGRAM LISTING

ORIGINAL PAGE IS
OF POOR QUALITY

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C****************************************************************************
C THIS PROGRAM ESTIMATE THE STEADY STATE CURRENT AND TEMPERATURE
C DISTRIBUTIONS IN THE FUEL CELL STACK
C****************************************************************************
      REAL LE,LT,LEC,MA,NC
      DIMENSION H(3,12,12),HC(12),YY(3,12),DNSA(7),
     1ZZ(12),PH1(3,12),PH2(12),G(96,97),D1(3,12),TTD2(3,12,12)
     2,PPRO(3,12,12),QW(3,12),TDO2(13,13),X(96),TTD1(3,12,12)
     3,TDH2O(13,13),AVG(4,12),TT(3,12,12),TTEN(12,12),TD2(13,13)
     4,TTEM(12,12),DERIV(3),XRATIO(3,12,12),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/FUCE/ XDNSO,UTH,UTA,XN,YN
      COMMON/GUST/ TINGS
      COMMON/VOLCO/ VGUESS,PPRO
      COMMON/CATA/ CLCA,CLAN,CU,SA,SRO,ALFA,DKC,R
      COMMON/CONC/ Y1H2,Y1CO2,Y1H2O,Y1CO,Y1CH4,Y1N2,Y2H2O,Y2O2,Y2N2
      COMMON/TRANSS/ TDO2,TDH2O,TDH2,TD1,TD2
      COMMON/CONPRO/ TTD1,XH2,TTD2,XO2,XH2O,TTDC
      COMMON/TRTT/ TR
      COMMON/CANNL/ NP,NC,NK,NCC,NCA,NX,NY,NF,N1,N2
      COMMON/PROP1/ CPC,PC,CPA,PP,PF,WCW,WCD,WAW,WAD,WFW,WFD
      COMMON/PROP2/ HC,H
      COMMON/SYTTM/ POPC,POP
      COMMON/CONST2/ AA,AA1,BB1,BB2,BB3,CC1,CC2,CC3,CC4
      COMMON/CONST3/ A,A1,B1,B2,B3,C1,C2,C3,C4,E
      COMMON/CONST1/ TCIN,TAIN,DMCO,DMAIR,DFUEL,DC,DPL,DX,DY,DAREA
      COMMON/CONT/ ER,SN,FCONST
      COMMON/CONSTK/ K,K1,K2,K3,K4,K5,K6,K7,K8,K9,K10,K11,K12,K13,
     1K14,K15,K16
      COMMON/FULLO/ PW,TFU,AREAF,CX,XDNF
      COMMON/WMC/ WM
      COMMON/IDUG/ IDEBUG
      DATA AVG/48*0./
      DATA TERM/4*0./
      DATA DERIV/3*0./
C
      IDEBUG=0
      CALL DATAIN
      CALL DATACA(H2,O2)
      AREAF=XN*YN*2.54**2
C INITIAL ASSUMPTION
      DO 1 I=1,N2
      DO 1 L=1,NY
      DO 1 J=1,NX
      TR(I,J,L)=TINGS
    1 CONTINUE
      KING=0
    2 TERM(1)=0.
      TERM(2)=0.
      TERM(3)=0.
      TERM(4)=0.
      DO 3 I=1,N2
```

```
      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)
      TRR(I)=SUM/NX/NY
    5 CONTINUE
C CALCULATE THE CURRENT DENSITY PROFILE
C LET THE UNIT BE G-MOLE/SEC/CELL
      OO=O2/NP/3600.
      HH=H2/3600./NP
      NY1=NY+1
      DO 6 ITR=1,NY
      DO 6 ITY=1,N1
    6 AVG(ITY,ITR)=0.
      DO 11 IU=1,N2
      IF(IDEBUG.EQ.1) WRITE(6,118) IU
      CALL CUPRO(XXOO,TRR(IU),HH,OO,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)
      AUG=SUM/NX/NY
      DO 8 IBN=1,NX
      DO 8 ICN=1,NY
    8 SQ2=SQ2+(XXOO(IBN,ICN)-AUG)**2
      SQ2=SQRT(SQ2/(NX*NY-1))
      IF(IDEBUG.EQ.1) WRITE(6,101) SQ2
      DO 9 IJ=1,NX
      DO 9 IV=1,NY
      PPRO(IU,IJ,IV)=XXOO(IJ,IV)
    9 CONTINUE
      CONY=3600./453.6
      DO 10 IS=1,NX
      DO 10 IT=1,NY
      IV1=IT+1
      IJ1=IS+1
      TTD2(IU,IS,IT)=TD2(IS,IV1)*CONY
      TTD1(IU,IS,IT)=TD1(IJ1,IT)*CONY
      XH2(IU,IS,IT)=TDH2(IJ1,IT)*CONY
      XO2(IU,IS,IT)=TDO2(IS,IV1)*CONY
   10 XH2O(IU,IS,IT)=TDH2O(IS,IV1)*CONY
   11 CONTINUE
C CAL.   THE MEAN FLOW RATE OF AIR SIDE (LB-MOLE/HR)
      DO 38 II=1,NX
      DO 15 IU=1,N2
      DO 14 J=1,NY
      J2=J-1
      DO 12 IA=1,7
```

```
   12 DNSA(IA)=0.
      IF(J.EQ.1) DNSA(4)=(XH2O(IU,II,J)+DMAIR*Y2H2O)/2.
      IF(J.EQ.1) DNSA(7)=(XO2(IU,II,J)+DMAIR*Y2O2)/2.
      IF(J.NE.1) DNSA(4)=(XH2O(IU,II,J)+XH2O(IU,II,J2))/2.
      IF(J.NE.1) DNSA(7)=(XO2(IU,II,J)+XO2(IU,II,J2))/2.
      DNSA(6)=O2/Y2O2*Y2N2/453.6/NX/NP
      TDNSA=DNSA(1)+DNSA(2)+DNSA(3)+DNSA(4)+DNSA(5)+DNSA(6)+DNSA(7)
      AMWA=0.
      DO 13 IB=1,7
      CMA(IB)=DNSA(IB)/TDNSA
   13 AMWA=AMWA+WM(IB)*CMA(IB)
C ASSUME THE PROCESS AIR RISE 85. K AND LINEAR INCREASE
      TKAA=TAIN/1.8+85./NY*J
      TFA=(TKAA-273.16)*1.8+32.
      CALL CMASS(CA,DNSA,TDNSA)
      CALL CMOLE(CA,CM)
      CPA=HTCP(CM,TFA)
      TAK=THC(CM,TFA)
      MA=TDNSA*AMWA*NX/NCA
      IF(WAD.GT.WAW) AL=WAW/WAD
      IF(WAD.LE.WAW) AL=WAD/WAW
      IF(WAD.GT.WAW) WA=2.*WAW/(1.+AL)
      IF(WAD.LE.WAW) WA=2.*WAD/(1.+AL)
      GZA=CPA/AMWA*MA/(J*DX)/TAK*4./3.14159
      RA=1.+.0183*GZA  /(1.+.04*GZA**.667)
      IF((J.EQ.1).AND.(AL.NE.1.)) H(IU,II,J)=(3.61+4.63*(1.-AL)**3.2)   -
     1*RA/WA*TAK
      IF((J.EQ.1).AND.(AL.EQ.1.)) H(IU,II,J)=3.61*RA/WA*TAK
      IF((J.GT.1).AND.(AL.NE.1.)) H(IU,II,J)=(J*RA-(J-1)*RJ)*(3.61+4.63 -
     1*(1.-AL)**3.2)/WA*TAK
      IF((J.GT.1).AND.(AL.EQ.1.)) H(IU,II,J)=(J*RA-(J-1)*RJ)*3.61/WA*TAK
      RJ=RA
      PH1(IU,J)=H(IU,II,J)*((WAW+WAD)*2. )*DX/(TDNSA*NX/NCA)/CPA
      YY(IU,J)=1.-EXP(-PH1(IU,J))
      D1(IU,J)=TDNSA*NX/NCA*CPA/DX/PP
   14 CONTINUE
   15 CONTINUE
C CALCULATE THE VARIABLE OF TEMP. PROFILE
      DO 16 JA=1,NY
      PH2(JA)=HC(JA)*((WCW+WCD)*2.)*DX/(DMCO*NX/NCC)/CPC
   16 ZZ(JA)=1.-EXP(-PH2(JA))
      N=N1*NY*2
      NP1=N+1
C SET UP THE SIMUTANIANCE EQUATIONS
      DO 17 IC=1,N
      DO 17 JC=1,NP1
      G(IC,JC)=0.
   17 CONTINUE
      G(1,1)=B3-A1
      G(1,2)=-A1
      G(1,K)= -C4
      G(1,K2)=E
      JD=K2
      DO 18 ID=2,NY
```

```
      G(ID,JD)=-E
      JD=JD+1
   18 G(ID,JD)=E
      JE=NY
      DO 19 IE=K4,K5
      JE=JE+1
      IZ=(IE-N1*NY-1)/NY
      IY=IE-IE/NY*NY
      IF(IY.EQ.0) IY=NY
   19 G(IE,JE)=-YY(IZ,IY)
      JF=0
      DO 20 LF=K2,K6
      JF=JF+1
      IX=LF-LF/NY*NY
      IF(IX.EQ.0) IX=NY
   20 G(LF,JF)=-ZZ(IX)
      JG=K6
      DO 21 IG=K4,K5
      IW=(IG-N1*NY-1)/NY
      IV=IG-IG/NY*NY
      IF(IV.EQ.0) IV=NY
      G(IG,JG)=YY(IW,IV)-1.
      JG=JG+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*NY
      IF(IU1.EQ.0) IU1=NY
      G(IJ,JJ)=ZZ(IU1)-1.
      JJ=JJ+1
   23 G(IJ,JJ)=1.
      G(K2,K2)=1.
      JK=1
      IF(IDEBUG.EQ.1) WRITE(6,901) A1
  901 FORMAT(' 1 -- A1=',E13.5)
      DO 24 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=IK
   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
```

```
      G(K,1)= -C1
      G(K,K)=  B1-A
      G(K,K11)=-A
      G(K,K12)=-C2
      JM=2
      DO 25 IL=K11,K10
      G(IL,JM)=-C1
      JL=JM+K9
      G(IL,JL)=-A
      JL=JL+1
      G(IL,JL)=B1
      JL=JL+1
      G(IL,JL)=-A
      JL=JL+K9
      G(IL,JL)=-C2
   25 JM=JM+1
      G(K10,K10)=B1-A
      G(K10,K12)=0.
      G(K12,K)=-C2
      G(K12,K12)=B2-A
      G(K12,K13)=-A
      G(K12,K3)=-C2
      JN=K11
      DO 26 IO=K13,K14
      G(IO,JN)=-C2
      JO=JN+K9
      G(IO,JO)=-A
      JO=JO+1
      G(IO,JO)=B2
      JO=JO+1
      G(IO,JO)=-A
      JO=JO+K9
      G(IO,JO)=-C2
   26 JN=JN+1
      G(K14,K14)=B2-A
      G(K14,K3)=0.
      JP=K12
      DO 27 IQ=K3,K1
      G(IQ,JP)=-C3
      JQ=JP+K9
      G(IQ,JQ)=-A
      JQ=JQ+1
      G(IQ,JQ)=B2
      JQ=JQ+1
      G(IQ,JQ)=-A
   27 JP=JP+1
      G(K3,K14)=0.
      G(K3,K3)=B2-A
      G(K1,K1)=B2-A
      JR=K6
      DO 28 IR=K,K1
      IS=(IR-NY-1)/NY+1
      IT=(IR-NY-1)-(IR-NY-1)/NY*NY+1
      IF((IR-1).NE.(IR-1)/NY*NY) G(IR,JR)=-D1(IS,IT)
```

```
      JR=JR+1
      G(IR,JR)=D1(IS,IT)
   28 CONTINUE
      G(K1,K2)=0.
      DO 29 I1=1,N2
      DO 29 J1=1,NY
   29 QW(I1,J1)=((58042.1+2.344*(TR(I1,II,J1)/1.8-400.))*4.184
     1/(2.*FCONST)-VGUESS(I1))*PPRO(I1,II,J1) *30.48**2/1000.*
     256.87*60.
      DO 30 I2=1,NY
   30 G(I2,NP1)=0.
      DO 31 I3=K,K1
      I4=(I3-1)/NY
      I5=I3-I3/NY*NY
      IF(I5.EQ.0) I5=NY
   31 G(I3,NP1)=QW(I4,I5)
      DO 32 I6=K,K3,NY
      I7=(K-1-NY)/NY+1
   32 G(I6,NP1)=G(I6,NP1)+D1(I7,1)*TAIN
      G(1,NP1)=G(1,NP1)+ E*TCIN
      I8=0
      DO 33 I9=K4,K7,NY
      I8=I8+1
   33 G(I9,NP1)=TAIN*(1.-YY(I8,1))
      G(K2,NP1)=TCIN*(1.-ZZ(1))
      CALL GAUSS(G,X,N,NP1)
      DO 34 I10=1,N
   34 X(I10)=X(I10)/1.8-273.16
      IF(IDEBUG.EQ.1) WRITE(6,104)
      IF(IDEBUG.EQ.1) WRITE(6,105) (X(I11),I11=1,K1)
      IF(IDEBUG.EQ.1) WRITE(6,106)
      IF(IDEBUG.EQ.1) WRITE(6,107) (X(I12),I12=K4,K5)
      IF(IDEBUG.EQ.1) WRITE(6,108)
      IF(IDEBUG.EQ.1) WRITE(6,109) (X(I13),I13=K2,K6)
      DO 35 I14=1,NY
      TTEM(II,I14)=X(I14)
      TERM(1)=TERM(1)+X(I14)
      I15=I14+NY
      TERM(2)=TERM(2)+X(I15)
      TT(1,II,I14)=X(I15)
      I16=I14+NY*2
      TERM(3)=TERM(3)+X(I16)
      TT(2,II,I14)=X(I16)
      I17=I14+NY*3
      TERM(4)=TERM(4)+X(I17)
      TT(3,II,I14)=X(I17)
   35 CONTINUE
      DO 36 I18=1,NY
      J18=K1+I18
      I19=NY+I18
      J19=K1+I19
      I20=I19+NY
      J20=K1+I20
      I21=I20+NY
```

```
      J21=K1+I21
      TTEN(II,I18)=X(J18)
      TTEN(II,I19)=X(J19)
      TTEN(II,I20)=X(J20)
   36 TTEN(II,I21)=X(J21)
      N3=N1*NY
      DO 37 I22=1,N3
      I23=(I22-1)/NY+1
      I24=I22-(I23-1)*NY
   37 AVG(I23,I24)=X(I22)/NX+AVG(I23,I24)
   38 CONTINUE
      DO 39 I00=1,4
   39 TERM(I00)=TERM(I00)/NY/NX
      TTR=(TERM(2)+TERM(3)+TERM(4))/3.
      DO 40 IY=1,3
      TRR(IY)=TRR(IY)/1.8-273.16
   40 CONTINUE
      DO 41 L=1,N2
      DO 41 I=1,NX
      DO 41 J=1,NY
   41 TR(L,I,J)=TR(L,I,J)/1.8-273.16
      DO 42 L=1,N2
      DO 42 I=1,NX
      DO 42 J=1,NY
      IF(ABS(TT(L,I,J)-TR(L,I,J))/(TT(L,I,J)+TR(L,I,J)).GT.ER/5. )
     1GO TO 43
   42 CONTINUE
      GO TO 46
   43 KING=KING+1
      IF(KING.GE.15) ER=ER*2.
      IF(KING.GE.15) ER=ER*2.
      IF(KING.GT.40) GO TO 55
      DO 44 I=1,N2
      DO 44 J=1,NX
      DO 44 L=1,NY
      TR(I,J,L)=(TT(I,J,L)+TR(I,J,L))/2.
   44 CONTINUE
      IF(IDEBUG.NE.1) GO TO 2
      DO 45 IG=1,N2
      WRITE(6,115) IG
      WRITE(6,116) ((TT(IG,I,NY+1-J),I=1,NX),J=1,NY)
   45 CONTINUE
      WRITE(6,117)
      GO TO 2
   46 CONTINUE
      DO 48 IG=1,N2
      DO 47 I=1,NX
      DO 47 J=1,NY
      XRATIO(IG,I,J)=(TT(IG,I,J)+273.16)/(TERM(IG+1)+273.16)
   47 DERIV(IG)=DERIV(IG)+(TT(IG,I,J)-TERM(IG+1))**2
   48 DERIV(IG)=SQRT(DERIV(IG)/(NX*NY-1))
      WRITE(6,103)
      DO 49 IG=1,N2
      WRITE(6,115) IG
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      WRITE(6,110) VGUESS(IG)
      WRITE(6,112)
      WRITE(6,111) ((PPRO(IG,I,NY+1-J),I=1,NX),J=1,NY)
      WRITE(6,113)
      WRITE(6,116) ((TT(IG,I,NY+1-J),I=1,NX),J=1,NY)
   49 CONTINUE
      TFU=(TERM(2)+TERM(3)+TERM(4))/3.+273.16
      PW=XDNF*(VGUESS(1)+VGUESS(2)+VGUESS(3))/3.*AREAF/1000.*NP
      WRITE(6,121) TFU,POP,PW
      GO TO 50
C IF RUN AT NASA LEWIS RESEARCH CENTER
C     DO 56 I=1,NX
C     DO 56 J=1,NY
C  56 TX(I,J)=TT(1,J,I)
C     CALL DRAWE(TX)
   55 WRITE(6,120) KING
   50 CONTINUE
C
  101 FORMAT(/1X,'THE ESTIMATED STANDARD DEVIATION OF CURRENT DENSITY ' -
     1,E13.5/)
  103 FORMAT('1',///////'     *************'/'     *AIR COOLING*'/'      -
     1*************'//)
  104 FORMAT(1X,'FUEL CELL TEMPERATURE PROFILE')
  105 FORMAT(1X,12F5.0/1X,12F5.0/1X,12F5.0/1X,12F5.0/)
  106 FORMAT(1X,'PROCESS AIR TEMPERATURE PROFILE')
  107 FORMAT(1X,12F5.0/1X,12F5.0/1X,12F5.0/)
  108 FORMAT(1X,'COOLING AIR TEMPERATURE PROFILE')
  109 FORMAT(1X,12F5.0/)
  110 FORMAT(/' THE VOLTAGE IS ',F6.4,' VOLT.'/)
  111 FORMAT((1X,12(F5.4,1X)))
  112 FORMAT(' CURRENT DENSITY(A/CM**2)'/)
  113 FORMAT(/' TEMPERATURE(C)'/)
  115 FORMAT('1',' *** CELL PLATE *** ',I2)
  116 FORMAT(1X,12F5.0)
  117 FORMAT('1')
  118 FORMAT(//' CELL PLATE',I3)
  120 FORMAT(' TEMPERATURE CALCULATION LOOPING KING=',I3)
  121 FORMAT('1',' THE AVERAGE OPERATING TEMPERATURE IS',E13.5,' K'/    -
     1' THE OPERATING PRESSURE IS',F5.2,' ATM'/                         -
     2' THE FULL DC POWER OUTLET IS',E13.5,' KW-DC')
C
      STOP
      END
      SUBROUTINE DATAIN
      REAL KY,KX,NC
      NAMELIST/DIMEN/ XN,YN,XDNS0,UTA,UTH,POPC,POP,TKA,WFD,WFW,NCC,WE   -
     1,TKF,T,NK,WAD,WAW,NP,NCA,NF,T1,NX,NY,TINGS
      NAMELIST/CZ/ CLCA,CLAN,CU,SA,SRO,ALFA,DKC,R
      NAMELIST/FALA/ Z,FCONST
      NAMELIST/DIGA/ NC,KX,KY,TKC,WCW,WCD
      NAMELIST/FUEL/ Y1H2,Y1CO2,Y1CO,Y1CH4,Y1H2O,Y1N2,Y2O2,Y2N2,Y2H2O
      NAMELIST/ERR/ ER
      NAMELIST/HEATC/ RHOP,RHOC,CCP,CCC
      COMMON/FUCE/ XDNS0,UTH,UTA,XN,YN
```

```
      COMMON/GUST/ TINGS
      COMMON/CATA/ CLCA,CLAN,CU,SA,SRO,ALFA,DKC,R
      COMMON/CONC/ Y1H2,Y1CO2,Y1H2O,Y1CO,Y1CH4,Y1N2,Y2H2O,Y2O2,Y2N2
      COMMON/CANNL/ NP,NC,NK,NCC,NCA,NX,NY,NF,N1,N2
      COMMON/PROP1/ CPC,PC,CPA,PP,PF,WCW,WCD,WAW,WAD,WFW,WFD
      COMMON/SYTTM/ POPC,POP
      COMMON/FULLO/ PW,TFU,AREAF,CX,XDNF
      COMMON/CONST2/ AA,AA1,BB1,BB2,BB3,CC1,CC2,CC3,CC4
      COMMON/CONST3/ A,A1,B1,B2,B3,C1,C2,C3,C4,E
      COMMON/CONST1/ TCIN,TAIN,DMCO,DMAIR,DFUEL,DC,DPL,DX,DY,DAREA
      COMMON/CONT/ ER,Z,FCONST
      COMMON/CONSTK/ K,K1,K2,K3,K4,K5,K6,K7,K8,K9,K10,K11,K12,K13,
     1K14,K15,K16
C
      READ(5,DIMEN)
      WRITE(6,DIMEN)
      DX= YN/NY/12.
      DY=XN/NX/12.
      DAREA=DX*DY
      TAIN=TKA*1.8
      XDNF=XDNS0
C
      READ(5,ERR)
      WRITE(6,ERR)
C
      READ(5,CZ)
      WRITE(6,CZ)
C
      READ(5,FALA)
      WRITE(6,FALA)
C
      READ(5,DIGA)
      WRITE(6,DIGA)
      TCIN=TKC*1.8
C
      READ(5,FUEL)
      WRITE(6,FUEL)
C
      READ(5,HEATC)
      WRITE(6,HEATC)
C
      WCW=WCW/12.
      WCD=WCD/12.
      PP=XN /12./NCA
      PC=XN/12./NCC
      PF=YN/12./NF
      Y1=(T1+T)/2.
      Y2=T
      IF(NK/2*2.EQ.NK) N1=1+NK/2
      IF(NK/2*2.NE.NK) N1=1+(NK+1)/2
      N2=N1-1
      A=KY*T/DX**2
      A1=KY*T1/DX**2
      B1=2.*KY*T/DX**2+KX/Y1+KX/Y2
```

```
      B2=2.*KY*T/DX**2+2.*KX/Y2
      B3=2.*KY*T1/DX**2+2.*KX/Y1
      C1=KX/Y1
      C2=KX/Y2
      C3=2.*KX/Y2
      C4=2.*KX/Y1
      DPL=RHOP*CCP*((T-WFD-WAD)+0.5*(WFD+WAD))
      DC=RHOC*CCC*((T1-WCD/2.-WAD)+0.5*(WCD/2.+WAD))
      AA=A/DPL
      AA1=A1/DC
      BB1=B1/DPL
      BB2=B2/DPL
      BB3=B3/DC
      CC1=C1/DPL
      CC2=C2/DPL
      CC3=C3/DPL
      CC4=C4/DC
      K=NY+1
      K1=NY*N1
      K2=K1+1
      K3=NY*(N1-1)+1
      K4=NY*(N1+1)+1
      K5=NY*N1*2
      K6=NY*(N1+1)
      K7=NY*(2*N1-1)+1
      K8=K1+2
      K9=NY-1
      K10=NY*2
      K11=K+1
      K12=K10+1
      K13=K12+1
      K14=NY*(N1-1)
      K15=K6-1
      K16=K6+NY
      RETURN
      END
      SUBROUTINE DATACA(H2,O2)
      REAL MAC,NC
      DIMENSION DNSC(7),GZ(12),R(12)
      DIMENSION CMC(7),WM(7),CC(7),CM(7),DNSA(7),CMA(7),CA(7)
      COMMON/FUCE/ XDNS0,UTH,UTA ,XN,YN
      COMMON/CONC/ Y1H2,Y1CO2,Y1H2O,Y1CO,Y1CH4,Y1N2,Y2H2O,Y2O2,Y2N2
      COMMON/CONT/ ER,SN,FCONST
      COMMON/WMC/ WM
      COMMON/CONPRO/ TTD1(3,12,12),XH2(3,12,12),TTD2(3,12,12),
     1XO2(3,12,12),XH2O(3,12,12),TTDC(12,12)
      COMMON/CONST1/ TCIN,TAIN,DMCO,DMAIR,DFUEL,DC,DPL,DX,DY,DAREA
      COMMON/CONST3/ A,A1,B1,B2,B3,C1,C2,C3,C4,E
      COMMON/PROP1/ CPC,PC,CPA,PP,PF,WCW,WCD,WAW,WAD,WFW,WFD
      COMMON/PROP2/ HC(12),H(3,12,12)
      COMMON/CANNL/ NP,NC,NK,NCC,NCA,NX,NY,NF,N1,N2
C CAL. AMOUNT OF INPUT FUEL
      XAMP=XDNS0*XN*YN*2.54**2
      H2=XAMP/(SN*FCONST*UTH )*NP*3600.
```

```
      DFUEL=H2/Y1H2/NP/NY/453.6
C CAL. AMOUNT OF INPUT O2
      O2=XAMP/(2.*SN*FCONST*UTA)*NP*3600.
C INSERT THE FLOW RATE OF COOLING SIDE  (LB-MOLE/HR)
      DO 1 IA=1,7
    1 DNSC(IA)=0.
      DNSC(4)=(O2/Y2O2*NC*NK*UTA/NP)*Y2H2O/453.6
      DNSC(6)=(O2/Y2O2*UTA*NC*NK/NP)*Y2N2/453.6
      DNSC(7)=(O2/Y2O2*UTA*NC*NK/NP)*Y2O2/453.6
      TDNSC=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
    2 AMWC=AMWC+WM(IA)*CMC(IA)
C ASSUME THE COOLING AIR RISE 45.  K AND LINEAR INCREASE
      DO 3 I=1,NY
      I2=I-1
      TKCC=TCIN/1.8+45./NY*I
      TFC=(TKCC-273.16)*1.8+32.
      CALL CMASS(CC,DNSC,TDNSC)
      CALL CMOLE(CC,CM)
      TCK=THC(CM,TFC)
      CPC=HTCP(CM,TFC)
      MAC= TDNSC*AMWC/NCC
      AMUC=VIS(CM,TFC)
      PR=CPC/AMWC*AMUC/TCK
      IF(WCD.GT.WCW) AL1=WCW/WCD
      IF(WCD.LE.WCW) AL1=WCD/WCW
      IF(WCD.GT.WCW) WC=2.*WCW/(1.+AL1)
      IF(WCD.LE.WCW) WC=2.*WCD/(1.+AL1)
      RE=MAC/WC/AMUC
      GZ(I)=CPC/AMWC*MAC/(I*DX)/TCK*4./3.14159
      R(I)=1.+.0183*GZ(I)/(1.+.04*GZ(I)**.667)
      IF((RE.LT.2100.).AND.(AL1.NE.1.))TUN=3.61+4.63*(1.-AL1
     1)**3.2
      IF((RE.LT.2100.).AND.(AL1.EQ.1.)) TUN=3.61
      IF(RE.GE.2100.) TUN=.116*(RE**.667-125.)*PR**.333*(1.+
     1(WC/(I*DX))**.667)
      IF(I.EQ.1) HC(I)=TUN*R(I)*TCK/ WC
      IF(I.GT.1) HC(I)=(I*R(I)-(I-1)*R(I2))*TUN*TCK/ WC
    3 CONTINUE
      DMAIR=O2/Y2O2/453.6/NP/NX
      DMCO=TDNSC/NX
      E=DMCO*NX/NCC/PC/DX*CPC
      RETURN
      END
      SUBROUTINE VI(M,V,Z,TK,POP,PPH2,PPO2,PPH2O,PPCO,XO)
      F(Z)=Z*SR+DA*ALOG(Z/C)+V-B+EX*ALOG(Z/C1)+D*ALOG(CDL/(CDL-Z))
      DF(Z)=SR+DA/Z+EX/Z+D/(CDL-Z)
      D2F(Z)=-DA/Z**2 -EX/Z**2+D/(CDL-Z)**2
      GF(Z)=(DA*ALOG(Z/C)+V-B+EX*ALOG(Z/C1)+D*ALOG(CDL/(CDL-Z)))/(-SR)
      COMMON/CATA/ CL,CLA,CU,SA,SRO,ALFA,DKC,R
      COMMON/FULLO/ PW,TFU,AREAF,CX,XDNF
      COMMON/CONT/ ERR,SN,FCONST
```

```
      ER=0.001
      ICAL=0
      EZ=1.2605-0.00025*TK
      SR=SRO*EXP(3650.*(1./TK-1./450.))
      SIO=0.2327*(PPO2*POP)**0.8*(PPH2O*POP)**0.4377*EXP(-6652./TK)
      C=SIO*SA*CU*CL
      EX=11.85*0.0066*PPCO*POP*EXP(9190.*(1./TK-1./450.))
      A=ALOG(PPH2/PPH2O*SQRT(PPO2*POP))
      C1=CLA*SA*CU*.000053
      D=R*TK/SN/FCONST
      B=EZ+D*A
      DA=D/ALFA
      CDL=DKC/AREAF*(PPO2*POP)
      IF(M.EQ.2) GO TO 1
      V=B-DA*ALOG(Z/C)-Z*SR-EX*ALOG(Z/C1)-D*ALOG(CDL/(CDL-Z))
      GO TO 8
    1 Z=X0
    2 CONTINUE
      DO 4 I=1,100
      DZ=F(Z)/DF(Z)
      Z=Z-DZ
    3 IF(Z.LE.0.) ICAL=ICAL+1
      IF(ICAL.GT.20) GO TO 9
      IF(Z.LE.0.) GO TO 5
      IF(ABS(DZ).LT.ER) GO TO 8
    4 CONTINUE
    5 WRITE(6,101)
      Z=X0
      DO 6 I=1,100
      GZ=Z
      Z=GF(Z)
      IF(Z.LE.0.) ICAL=ICAL+1
      IF(ICAL.GT.20) GO TO 9
      IF(Z.LE.0.) GO TO 7
      IF(ABS((GZ-Z)/(Z+GZ)).LT.ER) GO TO 8
    6 CONTINUE
      WRITE(6,102) ER
    7 ER=ER+0.001
      Z=X0*(1.+ICAL*0.02)
      GO TO 1
    8 CONTINUE
      RETURN
    9 WRITE(6,103)
C
  101 FORMAT(' 1ST METHOD CAN NOT GET THE RESULT')
  102 FORMAT(' 2ND METHOD CAN NOT GET RESULT --- INCREASE ER',E13.5)
  103 FORMAT(' CHECK INPUT DATA -- I VALUE CAN NOT SOLVE FROM KNOWN V')
C
      STOP
      END
      SUBROUTINE CUPRO(XDNS,TR,H2,O2,VGUESS,NX,NY,DDX,DDY,IU)
      REAL N1TOT,N2TOT,N2O2,N2H2O,N2N2,N1H2,N1CO2,N1CO,N1H2O,LAMDA,N1CH4
      DIMENSION U1UTOT(13,13),U1UH2(13,13),                             -
     1TRR(3,12,12),U2UTOT(13,13),U2UO2(13,13),U2UH2O(13,13),            -
```

```
     2XDNS(12,12)
      COMMON/FUCE/ XDNS0,TAH2,TAO2,XLENG,YLENG
      COMMON/CATA/ CL,CLA,CU,SA,SRO,ALFA
      COMMON/CONC/ Y1H2,Y1CO2,Y1H2O,Y1CO,Y1CH4,Y1N2,Y2H2O,Y2O2,Y2N2
      COMMON/TRANSS/ U2UO2,U2UH2O,U1UH2,U1UTOT,U2UTOT
      COMMON/SYTTM/ POPC,POP
      COMMON/TRTT/ TRR
      COMMON/CONT/ERR,Z,FCONST
      COMMON/IDUG/ IDEBUG
      TKAVG=TR/1.8
      LZ=1
      S=1./TAO2
      N2O2=O2
      N2TOT=N2O2/Y2O2
      N2N2=N2TOT*Y2N2
      N2H2O=N2TOT*Y2H2O
      N1H2=H2
      N1TOT=N1H2/Y1H2
      N1CH4=N1TOT*Y1CH4
      N1CO2=N1TOT*Y1CO2
      N1H2O=N1TOT*Y1H2O
      N1CO=N1TOT*Y1CO
      DO 1 I=1,NX
      U2UTOT(I,1)=N2TOT/NX
      U2UO2(I,1)=N2O2/NX
    1 U2UH2O(I,1)=N2H2O/NX
      DO 2 J=1,NY
      U1UTOT(1,J)   =N1TOT/NY
    2 U1UH2(1,J)   =N1H2/NY
      N1CO=N1CO/NY
      YBH2=SQRT(Y1H2*(1.-TAH2)/(1.-Y1H2*TAH2)*Y1H2)
      YBCO=SQRT(Y1CO*(Y1CO/(1.-Y1H2*TAH2)))
      YBO2=SQRT(Y2O2*(Y2O2*(1.-TAO2)/(1.+Y2O2*TAO2)))
      YBH2O=(Y2H2O+((Y2H2O+2.*Y2O2*TAO2)/(1.+Y2O2*TAO2)))/2.
      X0=XDNS0
      CALL VI(1,VGUESS,X0,TKAVG,POP,YBH2,YBO2,YBH2O,YBCO,XDNS0)
      GO TO 4
    3 VGUESS=VGUESS+0.001
      IXD=1
    4 MZ=1
    5 CONTINUE
      DO 14 I=1,NX
      I2=I+1
      DO 13 J=1,NY
      J2=J+1
      YHY=U1UH2(I,J)/U1UTOT(I,J)
      YOX=U2UO2(I,J)/U2UTOT(I,J)
      YWA=U2UH2O(I,J)/U2UTOT(I,J)
      YCO=N1CO/U1UTOT(I,J)
      NZ=1
      IF(I.EQ.1) GO TO 6
      XDFRST=XDNS(I-1,J)
      GO TO 8
    6 XDFRST=XDNS0
```

```
      GO TO 8
    7 XDFRST=XDFRST-0.001
      IXD=IXD+1
      IF(IXD.GT.100) WRITE(6,101)
      IF(IXD.GT.100) GO TO 3
    8 CONTINUE
      AREA=DDX*DDY*30.48**2
      U1UH2(I2,J) =U1UH2(I,J)-(XDFRST*AREA)/(Z*FCONST)
      U1UTOT(I2,J) =U1UTOT(I,J)-(U1UH2(I,J)-U1UH2(I2,J) )
      U2UO2(I,J2) =U2UO2(I,J)-(XDFRST*AREA)/(2.*Z*FCONST)
      U2UH2O(I,J2) =U2UH2O(I,J)+(XDFRST*AREA)/(Z*FCONST)
      U2UTOT(I,J2) =U2UTOT(I,J)+(U2UO2(I,J)-U2UO2(I,J2) )
      YXHY=U1UH2(I2,J) /U1UTOT(I2,J)
      YXCO=N1CO/U1UTOT(I2,J)
      YXOX=U2UO2(I,J2) /U2UTOT(I,J2)
      YXWA=U2UH2O(I,J2) /U2UTOT(I,J2)
      IF(YXHY.LT.0.) WRITE(6,102)
      IF(YXHY.LT.0.) GO TO 7
      YBHY=SQRT(YXHY*YHY)
      YBOX=SQRT(YXOX*YOX)
      YBWA=(YXWA+YWA)/2.
      YBCO=SQRT(YXCO*YCO)
      TK=TRR(IU,I,J)/1.8
      CALL VI(2,VGUESS,XDLAST,TK,POP,YBHY,YBOX,YBWA,YBCO,XDNS0)
      IF(ABS((XDLAST-XDFRST)/(XDLAST+XDFRST)).LT.ERR/10.) GO TO 12
      IF(NZ.GT.40) GO TO 17
      XD2=XDFRST
      IF(NZ.GT.30) GO TO 10
      EXD2=XDLAST-XD2
      IF(NZ.LE.15) XDFRST=(XDLAST+XDFRST)/2.
      IF(NZ.LE.15) GO TO 9
      IF(EXD1.NE.EXD2) XD3=XD2-(EXD2/(EXD2-EXD1))*(XD2-XD1)
      IF(EXD1.EQ.EXD2) XD3=(XD2+XDLAST)/2.
      XDFRST=XD3
    9 NZ=NZ+1
      XD1=XD2
      EXD1=EXD2
      GO TO 11
   10 XDFRST=XDLAST
      NZ=NZ+1
   11 IF(NZ.GT.10) WRITE(6,103) I,J,NZ,XD2,XDLAST
      GO TO 8
   12 XDNS(I,J)=XDLAST
   13 CONTINUE
   14 CONTINUE
      XDNST=0.
      DO 15 I=1,NX
      DO 15 J=1,NY
   15 XDNST=XDNST+XDNS(I,J)
      XDNSAV=XDNST/NX/NY
C     WRITE(6,104) XDNSAV
      IF (ABS((XDNSAV-XDNS0)/(XDNSAV+XDNS0)).LT.ERR/10.) GO TO 16
      VGUESS=VGUESS+(XDNSAV-XDNS0)*(SR0+0.038/XDNSAV)
      MZ=MZ+1
```

```
      IF(MZ.GT.40) ERR=0.002
      IF(MZ.GT.60) GO TO 18
      GO TO 5
   16 IF(IDEBUG.NE.1) RETURN
      WRITE(6,105) VGUESS
      WRITE(6,109)
      WRITE(6,106) ((XDNS(I,NY+1-J),I=1,NX),J=1,NY)
      RETURN
   17 WRITE(6,107) I,J
      STOP
   18 WRITE(6,108)
C
  101 FORMAT(' WARNING ---- H2 IS USED UP --- INCREASE V      GUESS')
  102 FORMAT(' WARNING ---- H2 IS USED UP --- DECREASE C. D. GUESS')
  103 FORMAT(' I=',I2,'J=',I2,'NZ=',I2,'XDFRST=',E13.5,'XDLAST=',E13.5  -
     1)
  104 FORMAT(1X,F7.6)
  105 FORMAT(/' THE VOLTAGE IS',F6.4,' VOLT.'/)
  106 FORMAT((1X,12(F5.4,1X)))
  107 FORMAT(' XDNS LOOPING AT I=',I2,2X,'J=',I2)
  108 FORMAT(' VGUESS LOOPING')
  109 FORMAT(' CURRENT DENSITY(A/CM**2)'/)
C
      RETURN
      END
      SUBROUTINE GAUSS(A,X,N,NP1)
      DIMENSION A(96,97),X(96)
      NM1=N-1
      DO 4 K=1,NM1
      KP1=K+1
      L=K
      DO 1 I=KP1,N
    1 IF(ABS(A(I,K)).GT.ABS(A(L,K))) L=I
      IF(L.EQ.K) GO TO 3
      DO 2 J=K,NP1
      TEMP=A(K,J)
      A(K,J)=A(L,J)
    2 A(L,J)=TEMP
    3 DO 4 IA=KP1,N
      FACTOR=A(IA,K)/A(K,K)
      DO 4 JA=KP1,NP1
    4 A(IA,JA)=A(IA,JA)-FACTOR*A(K,JA)
      X(N)=A(N,NP1)/A(N,N)
      I=NM1
    5 IP1=I+1
      SUM=0.
      DO 6 J=IP1,N
    6 SUM=SUM+A(I,J)*X(J)
      X(I)=(A(I,NP1)-SUM)/A(I,I)
      I=I-1
      IF(I.GE.1) GO TO 5
      RETURN
      END
      SUBROUTINE CMASS(C,FL,F)
```

```
      DIMENSION C(7),WM(7),FL(7)
      COMMON /WMC/ WM
      WMM=(FL(1)*WM(1)+FL(2)*WM(2)+FL(3)*WM(3)+WM(4)*FL(4)+FL(5)*WM(5)+
     1FL(6)*WM(6)+FL(7)*WM(7))/F
      DO 1 I=1,7
    1 C(I)=FL(I)*WM(I)/(F*WMM)
      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)
     1/WM(6)+C(7)/WM(7)
      DO 1 I=1,7
    1 CM(I)=C(I)/WM(I)/TC
      RETURN
      END
      FUNCTION HTCP(CM,T)
      DIMENSION CM(7),A(4,7),WM(7)
      COMMON /WMC/ WM
      COMMON/HTCPC/ A
      TP=T+460.
      HTCP=0.
      DO 1 I=1,7
      HTCP=HTCP+CM(I)*(A(1,I)+A(2,I)*TP+A(3,I)*(TP**2)+A(4,I)/(TP**2))
    1 CONTINUE
      RETURN
      END
      FUNCTION THC(C,T)
      DIMENSION C(7),A(2,7),WM(7),SUC(7),AJ(7,7),AI(7),A1(2,7)
      COMMON/THCC/ A
      COMMON/WMC/ WM
      COMMON/SU/ SUC
      COMMON/VIPC/ 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(J.EQ.I) AJ(I,J)=1.
      IF(J.EQ.I) GO TO 2
      IF(I.NE.4.AND.J.NE.4) SM=SQRT(SUC(I)*SUC(J))
      IF(I.EQ.4.OR.J.EQ.4) SM=0.733*SQRT(SUC(I)*SUC(J))
      AJ(I,J)=0.25*(1.+((A1(1,I)*T+A1(2,I))/(A1(1,J)*T+A1(2,J))
     1*(WM(J)/WM(I))**0.75*(1.+SUC(I)/T1)/(1.+SUC(J)/T1))**0.5
     2)**2*(1.+SM/T1)/(1.+SUC(I)/T1)
    2 AI(I)=AI(I)+AJ(I,J)*C(J)
    3 CONTINUE
      THC=THC+(A(1,I)*T+A(2,I))/(1./C(I)*AI(I))
    4 CONTINUE
      RETURN
```

```
      END
      FUNCTION VIS(C,T)
      DIMENSION A(2,7),C(7),WM(7),AI(7),AJ(7,7)
      COMMON/VIPC/ A
      COMMON/WMC/ WM
      DO 1 I=1,7
    1 AI(I)=0.
      VIS=0.
      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(J.EQ.I) AJ(I,J)=1.
      IF(J.EQ.I) GO TO 2
      AJ(I,J)=(1.+((A(1,I)*T+A(2,I))/(A(1,J)*T+A(2,J)))**0.5*(WM(J)/
     1WM(I))**0.25)**2/(8.**0.5*(1.+WM(I)/WM(J))**0.5)
    2 AI(I)=AI(I)+AJ(I,J)*C(J)
    3 CONTINUE
      VIS=VIS+(A(1,I)*T+A(2,I))/(1./C(I)*AI(I))
    4 CONTINUE
      RETURN
      END
      SUBROUTINE DRAWE(T)
      INTEGER DA(4)
      REAL NC
      DIMENSION T(12,12),X(12,12),Y(12,12),FL(5),IFLG(7),CORNER(8)
      DIMENSION XTIT(2),YTIT(2),PTIT(10)
      DIMENSION X1(3),VAR(11),IVARS(11),Y1(3)
      COMMON/FUCE/ XDNS0,UTH,UTA,XN,YN
      COMMON/CANNL/ NP,NC,NK,NCC,NCA,NX,NY,NF,N1,N2
      DATA DA/-1,2,0,0/
      DATA X1/0.,17.,17./
      DATA Y1/12.,12.,0./
      DATA XTIT/' 17 ','IN. '/
      DATA YTIT/' 12 ','IN. '/
      DATA PTIT/'TEMP','ERAT','URE ','DIST','RIBU','TION',
     1' ON ','CELL',' PLA','TE  '/
      NFC=10
      DO 1 I=1,NX
      DO 1 J=1,NY
      X(I,J)=XN/NX*(J-1)+XN/NX/2.
    1 Y(I,J)=YN/NY*(I-1)+YN/NY/2.
      DO 2 L=1,NFC
    2 FL(L)=L*5.+160.
      IFLG(1)=NY
      IFLG(2)=NX
      IFLG(3)=NFC
      IFLG(4)=0
      IFLG(5)=0
      IFLG(6)=0
      IFLG(7)=0
      CORNER(1)=0.
      CORNER(2)=17.
      CORNER(3)=0.
```