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# Phosphoric Acid Fuel Cell Power Plant System Performance Model and Computer Program

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January 1984

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Lewis Research Center  
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for  
U.S. DEPARTMENT OF ENERGY  
Morgantown Energy Technology Center

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## INTRODUCTION

This report has been prepared by Cleveland State University for NASA Lewis Research Center to record the work done and to serve as documentation of the computer programs prepared under contract NCC3-17.

Under support contract C-44219-D, energy, mass, and electrochemical analysis in the reformer, the shift converter, and the fuel cell module were combined to develop a mathematical model for the performance of the phosphoric acid fuel cell system which is depicted in Figure 1.

The primary objective of the work performed under contract NCC3-17 was to derive the mathematical model and the associated digital computer program for optimizing cost and electric energy output of the phosphoric acid fuel cell system. To achieve this objective, all equations relating to system performance which were derived under the previous contract, were integrated into a computer program that determines electric output, heat generation rate, and the effects on system performance of such parameters as operating pressure and temperature, reformer heat transfer area, and hydrogen fractional utilization. In addition, the mathematical and associated digital computer models were derived for the power processor, system components and operation costs, and optimization of fuel usage and cost of electric energy output.

The present report describes just the basic performance model of the fuel cell system, and the computer programs written for its analyses. Other reports are being prepared for the cost and optimization programs, which are hosted by the basic performance code, and for more detailed studies of subsystems such as the fuel cell stack, the fuel reformer, and the heat exchanger network optimization.

A listing of the steady state performance lumped model is included at the end of the report. It begins on page 81.

## I. SYSTEM DESCRIPTION

As shown in Figure 1, methane which is circulated by compressor (C) is preheated by heat exchanger E-1 prior to mixing it with the super heated steam which receives its heat by passing through heat exchanger E-9. Before entering the reformer, the methane steam mixture is heated via heat exchangers E-2 and E-3. Inside the reformer, methane is catalytically reformed by reaction with excess steam to produce carbon monoxide, carbon dioxide, and the desired product, hydrogen. The effluent from the reformer is cooled by flowing through heat exchanger E-2 before it enters the high temperature shift converter S-1. The function of the high temperature shift converter is to increase the hydrogen concentration and to reduce the carbon monoxide concentration of the reformer gas effluent. The temperature of the effluent from the shift converter S-1 is then reduced by passing through heat exchangers E-1, E-9 and E-6 before entering the low temperature shift converter S-2. The low temperature shift converter further increases the hydrogen concentration by promoting the shift reaction at a lower operating temperature. The effluent from the low temperature shift converter then enters the fuel cell containing H<sub>2</sub>, CO, CH<sub>4</sub>, CO<sub>2</sub> and H<sub>2</sub>O. The fuel cell converts inputs of hydrogen and oxygen to DC power, water and heat. Oxygen is delivered to the fuel cell by air compressor A, which also provides air to the reformer burner. The spent fuel from the fuel cell anode goes to the burner after mixing with air supplied by compressor A.



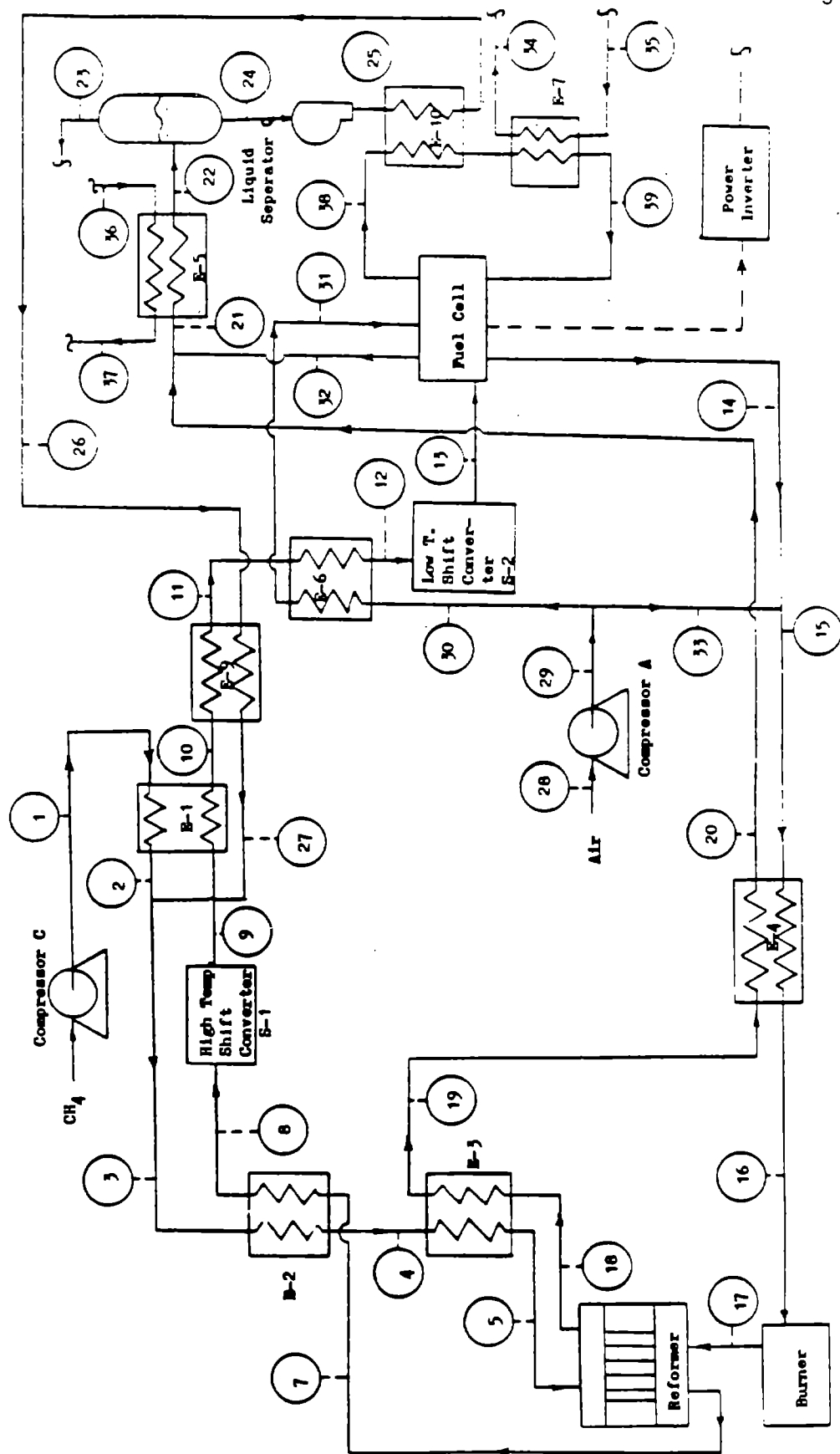


Figure 1 Flow diagram of GSU designed PAFC system

Before entering the burner, the mixture is preheated by the burner effluent via heat exchanger E-4. The spent fuel is then burned with whatever additional methane is needed to provide the thermal energy necessary for the reformer reaction.

Heat generated in the fuel cell is removed by heat exchangers E-7 and E-10. Heat from heat exchanger E-7 can then be utilized in industrial heat processing or space heating and cooling, while exchanger E-10 is used to preheat the water supplied by liquid separator Q to provide the necessary steam needed for the reforming process. The effluents from the burner and fuel cell cathode will have their water removed and separated by condenser E-5 and liquid separator Q before allowing them to be exhausted to the atmosphere.

## II. PERFORMANCE MATHEMATICAL MODEL

The mathematical model developed provides the basis for determining fuel cell voltage, current, and heat generation rate in terms of such parameters as flow rate, fuel composition, operating temperature, operating pressure, reformer heat transfer parameters, and steam-methane ratio.

In the derivation of the mathematical model, several simplifying assumptions were made. These assumptions include: one-dimensional, steady state flow of all gas streams, ideal gas behavior of all gas components, and a "lumped parameter" fuel cell stack model.

The following subsection will consider the derivation of mass and energy balance equations for the gases and the description of the governing equations for the system output characteristics (voltage, current, and heat generation).

### 2.1 Modeling of Fuel Processing Subsystem

Production of hydrogen, which is the major function of the fuel processing subsystem, occurs by reaction of the fuel with steam. The major components in this subsystem are the reformer, the high temperature shift converter, the low temperature shift converter, and several heat exchangers.

#### 2.1.1 Heat Exchanger

A zero capacitance sensible heat exchanger is modeled in the double-pipe counter mode.

For the counter mode, given the hot and cold side inlet temperature and flow rates, the effectiveness is calculated for a given fixed value of the overall heat transfer coefficient. The mathematical description which follows is covered in detail in Ref. 1.

$$T_{ho} = T_{hi} - E \left( \frac{C_{min}}{C_h} \right) (T_{hi} - T_{ci}) \quad (2-1-1)$$

$$T_{co} = E \left( \frac{C_{min}}{C_c} \right) (T_{hi} - T_{ci}) + T_{ci} \quad (2-1-2)$$

$$Q_T = EC_{min} (T_{hi} - T_{ci}) \quad (2-1-3)$$

$$E = \frac{1 - e^{-\frac{UA}{C_{min}} (1 - C_{min}/C_{max})}}{1 - (C_{min}/C_{max}) e^{-\frac{UA}{C_{min}} (1 - C_{min}/C_{max})}} \quad (2-1-4)$$

- where Cc: capacity rate of fluid on cold side, McCpc, J/s-K  
 Ch: capacity rate of fluid on hot side, MhCpc, J/s-K  
 Cmax: maximum capacity rate, J/s-K  
 Cmin: minimum capacity rate, J/s-K  
 Cpc: specific heat of cold side fluid, J/g-K  
 Cph: specific heat of hot side fluid, J/g-K  
 E: heat exchanger effectiveness  
 Mc: fluid mass flow rate on cold side, g/s  
 Mh: fluid mass flow rate on hot side, g/s  
 QT: total heat transfer rate across heat exchanger, J/s  
 Tci: cold side inlet temperature, K

- T<sub>co</sub>: cold side outlet temperature, K  
 T<sub>hi</sub>: hot side inlet temperature, K  
 T<sub>ho</sub>: hot side outlet temperature, K  
 UA: overall heat transfer coefficient of exchanger, J/m<sup>2</sup>-s-K

### 2.1.2 Shift Converters

The function of both types of shift converters (high temperature and low temperature) is to further increase the hydrogen concentration and to reduce the carbon monoxide concentration of the reformer gas effluent. The equation,  $\text{CO} + \text{H}_2\text{O} = \text{H}_2 + \text{CO}_2$  (water shift reaction), dominates the material changes in the shift converters. The methanol input fuel does not need to pass through shift converters because the carbon monoxide level is low.

In the lumped model, the water shift reaction is assumed to be at equilibrium at the input temperature (isothermal operation) or the average temperature (adiabatic operation). The material balance is

$$K_2 = \frac{P_{\text{CO}_2} P_{\text{H}_2}}{P_{\text{CO}} P_{\text{H}_2\text{O}}} = \frac{(F_{\text{CO}_2} + x)(F_{\text{H}_2} + x)}{(F_{\text{CO}} - x)(F_{\text{H}_2\text{O}} - x)} \quad (2-1-5)$$

- where  $K_2$ : equilibrium constant of shift reaction at ADT  
 P: partial pressure of component, atm  
 F: inlet molar flow rate of component, g-mole/s  
 x: reacted amount rate, g-mole/s

Equation 2-1-5 can be solved for x. Newton's method was used in the computer program.

The energy balance equation for the gases in the shift converter includes the reaction and sensible enthalpies. For adiabatic the process in the shift converter

$$\sum_{PS} n_j (\Delta h^{0f})_j - \sum_{RS} n_i (\Delta h^{0f})_i + \sum_{PS} n_j \int_{298}^{T_f} (C_p)_j dT - \sum_{RS} n_i \int_{298}^{T_i} (C_p)_i dT = 0 \quad (2-1-6)$$

where the subscripts PS, RS correspond to the products and reactants in the shift converter, respectively.  $T_f$  and  $T_i$  are the final and initial temperatures of the gases, respectively. The only unknown in the equation,  $T_f$ , is determined iteratively.

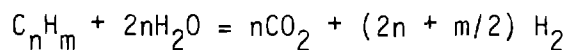
The Ergun equation, which estimates pressure drop caused by the flow of gas through dry packings, is used to determine the pressure drop in shift converter and reformer. The equation is (Ref. 2):

$$\Delta P = 1878 \frac{(1-\epsilon)G}{\epsilon^3 dp g_c \rho} \left( \frac{150(1-\epsilon)\mu}{dp G} + 1.75 \right) h \quad (2-1-7)$$

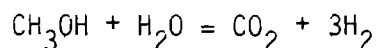
- where  $\epsilon$  : void fraction in bed  
 $\mu$  : viscosity, Kg/m-s  
 $dp$ : effective diameter of packing particle, m  
 $G$ : superficial gas mass velocity, Kg/s-m  
 $h$ : packed height, m  
 $\rho$  : density, Kg/m<sup>3</sup>  
 $\Delta P$ : pressure drop, atm

### 2.1.3 Reformer

The key component in the fuel processing subsystem is the reformer which catalytically reforms methane (methanol or naphtha) by reaction with excess steam to produce carbon monoxide, carbon dioxide, and the desired product, hydrogen. The overall reactions are:

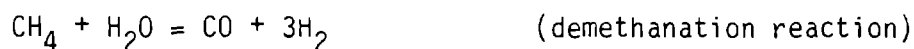


for naphtha and methane, and



for methanol. For simplicity, methane will be the only input fuel in the following discussions.

Two reactions are assumed to be the principle reforming reactions in the methane-reformer, they are:



and



Reference 11 lists all of the possible reactions and discusses the minimum steam to carbon ratio (S/C) required to avoid carbon formation.

#### 2.1.3.1 Lumped Model

In the lumped model both of the reactions, demethanation and shift reaction, were assumed to be at equilibrium by utilizing the respective ADT's of each. The equilibrium constants were determined from the temperature. The equilibrium expression are

$$K_1 = \frac{P_{CO_2} P_{H_2}^3}{P_{CH_4} P_{H_2O}} = \frac{Y_{CO_2} Y_{H_2}^3}{Y_{CH_4} Y_{H_2O}} \quad (\text{demethanation})$$

$$K_2 = \frac{P_{CO_2} P_{H_2}}{P_{CO} P_{H_2O}} = \frac{Y_{CO_2} Y_{H_2}}{Y_{CO} Y_{H_2O}} \quad (\text{water shift})$$

where  $K_1$  and  $K_2$  are the equilibrium constants of demethanation and water shift reaction, respectively. Expressing the mole fractions as the individual molar flows divided by the total molar flows yields:

$$K_1 = \frac{(F_{CO} - x + y)(F_{H_2} + x + 3y)^3 p^2}{(F_{CH_4} - y)(F_{H_2O} - x - y)(F_T + 2y)^2} \quad (2-1-8)$$

and

$$K_2 = \frac{(F_{CO_2} + x)(F_{H_2} + x + 3y)}{(F_{CO} - x + y)(F_{H_2O} - x - y)} \quad (2-1-9)$$

where  $y$  is the conversion amount rate in the demethanation reaction and  $F$  is the total inlet flow rate. Equations (2-1-8) and (2-1-9) can be solved for  $x$  and  $y$ . Newton's method was used in the computer program.

The quantities involved in the energy balance will be the sensible enthalpies of the gases, the reaction enthalpies of the gases, and the heat transferred from the combustion gases to the reformer gases,  $Q_{B-R}$ . The value of  $Q_{B-R}$  can be determined from

$$Q_{B-R} = UA\Delta T_m = H_{out} - H_{in} \quad (2-1-10)$$

where,  $\Delta T_m$  is the log mean temperature defined as

$$\Delta T_m = \frac{(T_{fc} - T_{iR}) - (T_a - T_{fR})}{\ln \frac{T_{fc} - T_{iR}}{T_a - T_{fR}}} \quad (2-1-11)$$



where,  $T_{fc}$  is the temperature of the combustion gases after leaving the reformer;  $T_{IR}$  and  $T_{fR}$  are the temperatures of the reformer gases before entering and after leaving the reformer;  $A$  is the heat transfer area; and  $U$  is a modified form of a heat transfer coefficient.

Thus, from the first law of thermodynamics and equation (2-1-11), the energy balance for the reformer gases can be written as,

$$U A \Delta T_m = \sum_{PR} m_j (\Delta h_f^\circ)_j - \sum_{PR} m_i (\Delta h_f^\circ)_i + \sum_{PR} m_j \int_{298}^{T_{fR}} (C_p)_j dT - \sum_{rR} m_k \int_{298}^{T_{iR}} (C_p)_i dT, \dots \quad (2-1-12)$$

where the subscripts PR and rR stand for products and reactants in the reformer, respectively.

### 2.1.3.2 Distributed Model

Kinetical analysis was used for simulation of the performance of the reformer. The reformer is basically a nonadiabatic, nonisothermal catalytic reactor that is heated on the shell side by combustion gases from burner. Methane will be the only input fuel considered in this model. Figure 2 shows its simplified scheme.

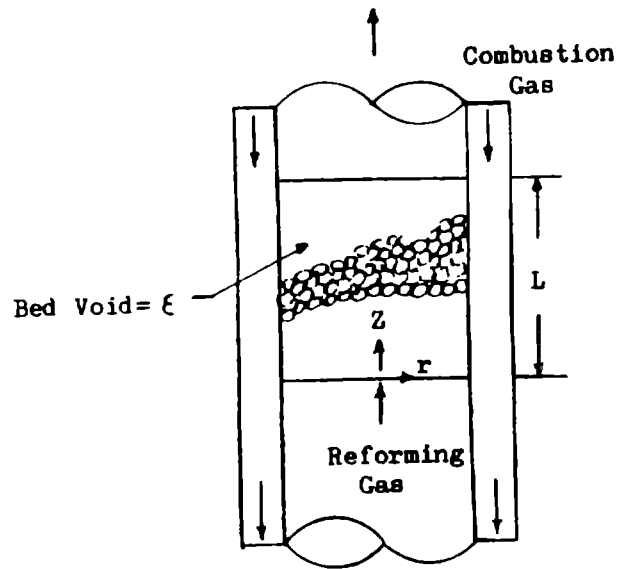


Figure 2 Simplified Reformer Diagram

In driving the mathematical model, the following assumptions were made:

1. The demethanation reaction is assumed to be kinetically controlled and, hence, occurs at a finite rate, while the water gas shift reaction is assumed to be equilibrium controlled. The demethanation reaction used in this model is slightly modified with linear combinations of the original demethanation reaction and shift reaction, which results in



In the equilibrium calculations, the demethanation reaction choice causes no changes in the final results. However, the kinetic consideration will cause the final results to vary slightly with the reaction choice.

2. Axial dispersion and radial gradient are negligible – plug flow condition. Generally, if the ratio of the length of the reactor to the catalyst's diameter is greater than 100, the axial dispersion effect is negligible.

3. A uniform temperature exists throughout each catalyst particle, and this temperature is the same as the gas temperature in that section of catalyst bed.

4. The kinetic expression represents a global rate, and, therefore, neglects reactivity differences found between the inside and outside of the catalyst particles.

5. Entrance effects are negligible.

6. Heat transfer by radiation is negligible.

7. Since tubular reactors inside a furnace are used commercially, it will be assumed that distribution of the gas to various parallel tubes is uniform and, hence, a single tube is sufficient for the purpose of theoretical investigations.

8. Ideal gas behavior is assumed.

9. The outside shell wall is adiabatic.

A more detailed discussion of assumptions 3 and 4 is provided in Ref. 11 by examination of the "internal" and "external" effectiveness factors of commercial catalysts used in the reformer.

Mass Balance: From the generalized continuity and the assumptions, the kinetic mass balance is

$$V \frac{dc}{dz} = -\frac{\gamma a' \epsilon_B}{\epsilon} \quad (2-1-14)$$

where V: average velocity of fluid through the bed, m/s  
 c: g-mole of CH<sub>4</sub> per m<sup>3</sup> fluid  
 ra': reaction rate, g-mole of CH<sub>4</sub>/s-kg catalyst  
 ε<sub>B</sub>: density of catalyst, kg/m<sup>3</sup> bed

Various kinetic expressions for the reforming of methane with steam have been proposed which could provide the rate equation (Refs. 3, 4, and 5). The simplest form among the proposed expressions is the first order rate expression, which is

$$-ra' = K_0 e^{-EA/RT} P_{CH_4} \quad (2-1-15)$$

in Arrhenius form,

where K<sub>0</sub>: Arrhenius frequency factor, g-mole/s-kg cat - atm  
 EA: activation energy, J/g-mole  
 R: gas constant  
 T: temperature, K

Unfortunately, little agreement can be found for the values of the kinetic parameters, some values may be three orders of magnitude different from others. The data from Ref. 5, using a commercial catalyst (Gindler G-56B), is used in this model.

The water gas shift reaction is assumed to be at equilibrium. The conversion quantity is based upon the carbon dioxide mass balance. Thus, when coupled with the demethanation reaction, the water gas shift reaction proceeds in reverse; therefore, the shift conversion is always negative. Using these two reaction schemes, all of the molar flows anywhere in the reformer can be written in terms of the feed quantities and the conversions of the two reactions.

Energy Balance: Two energy balances are required for the system: one for the reformer gases and one for the combustion gases. The reformer gas balance includes its own sensible heat change, reaction enthalpies, and heat transfer from the hotter combustion gases. The combustion gas balance involves sensible heat change and heat transfer. This translates quantitatively into equations (2-1-16) and (2-1-17)

$$\rho A_i V C_p \frac{dt}{dz} = (-\Delta H_1) \frac{dy}{dz} + (-\Delta H_2) \frac{dx}{dz} + h_i \chi d_i (T_w - t) \quad (2-1-16)$$

$$\rho_o V_o A_o C_{p_o} \frac{dt}{dz} = h_o \chi a_o (T - T_w) \quad (2-1-17)$$

where  $\Delta H_1$ : demethanation reaction enthalpy, J/g-mole  $CH_4$

$\Delta H_2$ : water shift reaction enthalpy, J/g-mole CO

$A_i$ : inner tube cross area,  $m^2$

$h_i$ : wall heat transfer coefficient of tube side,  $J/s-m^2-K$   
 $T_w$ : wall temperature, K  
 $d_i$ : inner tube diameter, m  
 $T$ : combustion gas temperature, K  
 $d_o$ : outer tube diameter, m  
 subscript o refers to the combustion gas side

There is greater uncertainty in estimating the heat transfer coefficient at the wall of tube than the rate expression. The scatter in experimental data is very high (Refs. 2, 3, and 4). The situation will be even more complicated by considering the unequal stoichimetric reaction (Ref. 6). Due to Beek's recommendation (Ref. 7), the modified Thoenes-Kramers (Ref. 8) correlation should be used for sphere-like particles near the wall, which are used in the model:

$$h_i(d_p/k_f) = 2.58(Re)^{1/3}(Pr)^{1/3} + .094 (Re)^{0.8}(Pr)^{0.4} \quad (2-1-18)$$

where  $d_p$ : equivalent particle diameter, m  
 $k_f$ : thermal conductivity,  $J/s-m-K$   
 $Pr$ : Prandtl number  
 $Re$ : partical Reynolds number

Differential equations, (2-1-5), (2-1-14), (2-1-16), and (2-1-17), were solved simultaneously with the inlet conditions as the boundary conditions. The Ergun equation (2-1-7) is used to evaluate the pressure drop.

## 2.2 Modeling of Fuel Cell Stack Subsystem

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 energy at the anode. The anode input contains CH<sub>4</sub>, H<sub>2</sub>O, H<sub>2</sub>, CO and CO<sub>2</sub>. In this analysis, it is assumed that a fixed percentage of hydrogen is consumed at the anode, and the H<sub>2</sub>O being formed exits the fuel cell, with the depleted air, through the cathode exit. The overall reaction in the fuel cell power section is



### 2.2.1 Mass and Energy Balances

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:

$$NX_{\text{H}_2} = NI_{\text{H}_2} - (I_{\text{mean}} A)/(n\mathcal{F}) \quad (2-2-2)$$

$$NX_{\text{O}_2} = NI_{\text{O}_2} - (I_{\text{mean}} A)/(2n\mathcal{F}) \quad (2-2-3)$$

$$NX_{\text{H}_2\text{O}} = NI_{\text{H}_2\text{O}} + (I_{\text{mean}} A)/(n\mathcal{F}) \quad (2-2-4)$$

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

I<sub>mean</sub>: mean current density, A/cm<sup>2</sup>

A: effective area of cell plate, cm<sup>2</sup>

n: number of Faraday equivalents transferred

$\mathcal{F}$ : Faraday constant

The energy balance for the fuel cell is

$$\begin{aligned}
 - (Q+W_e) = & \sum_{PF} n_j (\Delta h_f^\circ)_j - \sum_{rF} n_i (\Delta h_f^\circ)_i \\
 & + \sum_{PF} n_j \int_{298}^{T_{fF}} (C_p)_j dT - \sum_{rF} n_i \int_{T_{iF}}^{298} (C_p)_i dT
 \end{aligned} \tag{2-2-5}$$

where the subscripts PF, rF represent the products and reactants in the fuel cell, respectively.  $T_{fF}$  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:

$$Q = N_p X_n Y_n Q_F \tag{2-2-6}$$

$$\text{and } Q_F = \left( \frac{\Delta H_r}{n_F} - V \right) I \tag{2-2-7}$$

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

$Q_F$ : heat generated per unit area of cell, J/sec  $\text{cm}^2$

$N_p$ : number of cells

$X_n$ : width of cell plate, cm

$Y_n$ : length of cell plate, cm

$I$ : fuel cell current density,  $\text{A}/\text{cm}^2$

$\Delta H_r$ : heat of reaction, J/g-mole of  $\text{H}_2$

### 2.2.2 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:



$$V = E - n \quad (2-2-8)$$

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

n: overpotential or polarization

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

$$E_o = E(T) + \frac{RT}{nF} \ln \frac{Y_{H_2} \sqrt{PtY_{O_2}}}{Y_{H_2O}} \quad (2-2-9)$$

with Pt: total pressure, atm

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

$$E_o(T) = 1.261 - 0.00025 T, T, K \text{ (Ref. 9)}$$

$Y_{H_2}$ : mean mole fraction of hydrogen at anode

$Y_{O_2}$ : mean mole fraction of oxygen at cathode

$Y_{H_2O}$ : mean mole fraction of water vapor at cathode

The polarization term n consists of four components,

$$n = n_a + n_r + n_d + n_{co} \quad (2-2-10)$$

where  $n_a$ : activation polarization at cathode, volts

$n_r$ : resistance polarization, volts

$n_d$ : diffusion polarization, volts

$n_{co}$ : activation polarization at anode due to co poisoning of catalyst, volts

and

$$n_a = \frac{RT}{\alpha_o Z F} \ln \frac{i}{(i_o)(SA)(CL)(CU)} \quad (2-2-11)$$

with  $\alpha_0$ : transfer coefficient  
 $i$ : current density, mA/cm<sup>2</sup>  
 $i_0$ : exchange current density of cathode, mA/cm<sup>2</sup>  
 $SA$ : specific catalyst surface area, cm<sup>2</sup>/g  
 $CL$ : catalyst loading on cathode, g/cm<sup>2</sup>  
 $CU$ : 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  $Y_{O_2}$ ,  $Y_{H_2O}$ , and  $T$ . An empirical fit is

$$i_0 = 232.7 (PtY_{O_2})^{0.8} (PtY_{H_2O})^{0.4377} \exp(-6652/T) \quad (2-2-12)$$

The resistance polarization is

$$\eta_r = ir$$

where  $r$ : specific cell resistance, ohm-cm<sup>2</sup>.

The expression of  $\eta_{co}$  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. 9) is

$$\eta_{co} = 0.0782PtY_{co} \exp \left[ 9190 \left( \frac{1}{T} - \frac{1}{450} \right) \right] \ln \frac{i}{CL_a SA CU i_{ao}} \quad (2-2-13)$$

where  $CL_a$ : anode catalyst loading, mg

$i_{ao}$ : anode exchange current, mA/cm<sup>2</sup>

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

### 2.2.3 Stack Efficiency

The efficiency of the fuel cell to convert chemical energy to electrical energy,  $\epsilon_{FC}$ , can be written as (Ref. 10):

$$\epsilon_{FC} = \epsilon_V \epsilon_I \epsilon_{TH} \epsilon_H, \dots \quad (2-2-14)$$

where the voltage efficiency  $\epsilon_V$ , the current efficiency  $\epsilon_I$ , the thermodynamic efficiency  $\epsilon_{TH}$ , and the heating value efficiency  $\epsilon_H$ , are defined as follows:

$$\epsilon_V = \frac{V}{E}, \dots \quad (2-2-15)$$

$$\epsilon_I = \frac{I}{I_F}, \dots \quad (2-2-16)$$

$$\epsilon_{TH} = \frac{\Delta G_r}{\Delta H_r}, \dots \quad (2-2-17)$$

$$\epsilon_H = \frac{\Delta H_r}{\Delta H_C}, \dots \quad (2-2-18)$$

where  $V$  and  $I$  are the operating voltage and current, respectively,  $E$  is the fuel cell equilibrium potential,  $I_F$  is the amount of current produced by a reaction,  $\Delta G_r$  is Gibb's free energy change,  $\Delta H_C$  is lower heat of combustion of fuel cell feed, and  $\Delta h_r$  is the enthalpy change at fuel cell conditions of  $H_2 + \frac{1}{2} O_2 \rightarrow H_2O$ .

### III. PERFORMANCE COMPUTER MODEL

Figure 3 represents the overall computer program hierarchy. The main program establishes the link between subroutine (KREF), for the kinetic model of the reformer, and the following subroutines which determine the system performance and the mass and energy balance at various locations: BURN, CDPH, COMP, CON, CONV, DIVID, DMIX, ENFU, ENRE, ENSH, EQUK, FLAME, FUCE, HEPD, HEXC, PDFU, PDSH, PUMP, PUP, REF, SNAE, SEPAR, and SHIFT.

#### 3.1 Main Program

The main program performs the following functions:

A. It reads the following input data: the thermophysical properties of methane, methanol, naphtha, water, oxygen, hydrogen, carbon monoxide, carbon dioxide, and nitrogen; data related to various components of the fuel cell power plant.

B. For a given fuel, i.e., methane, methanol or naphtha, it carries out an iterative procedure to determine the thermodynamic state of the gas streams at various locations in the system, and to calculate the system efficiency and electric and heat energies output and other performance parameters.

These calculations are carried out for two cases. In the first case, the kinetic effect on the reformer performance is considered to be negligible. In this case, the main program carries out these calculations without calling subroutine (ENRE). In the second case, the kinetic effect on the reformer performance is taken into consideration. For this case, the main program calls subroutine (KREF) and bypasses subroutines (ENRE), (EQUK), (REF), and (SNAE).

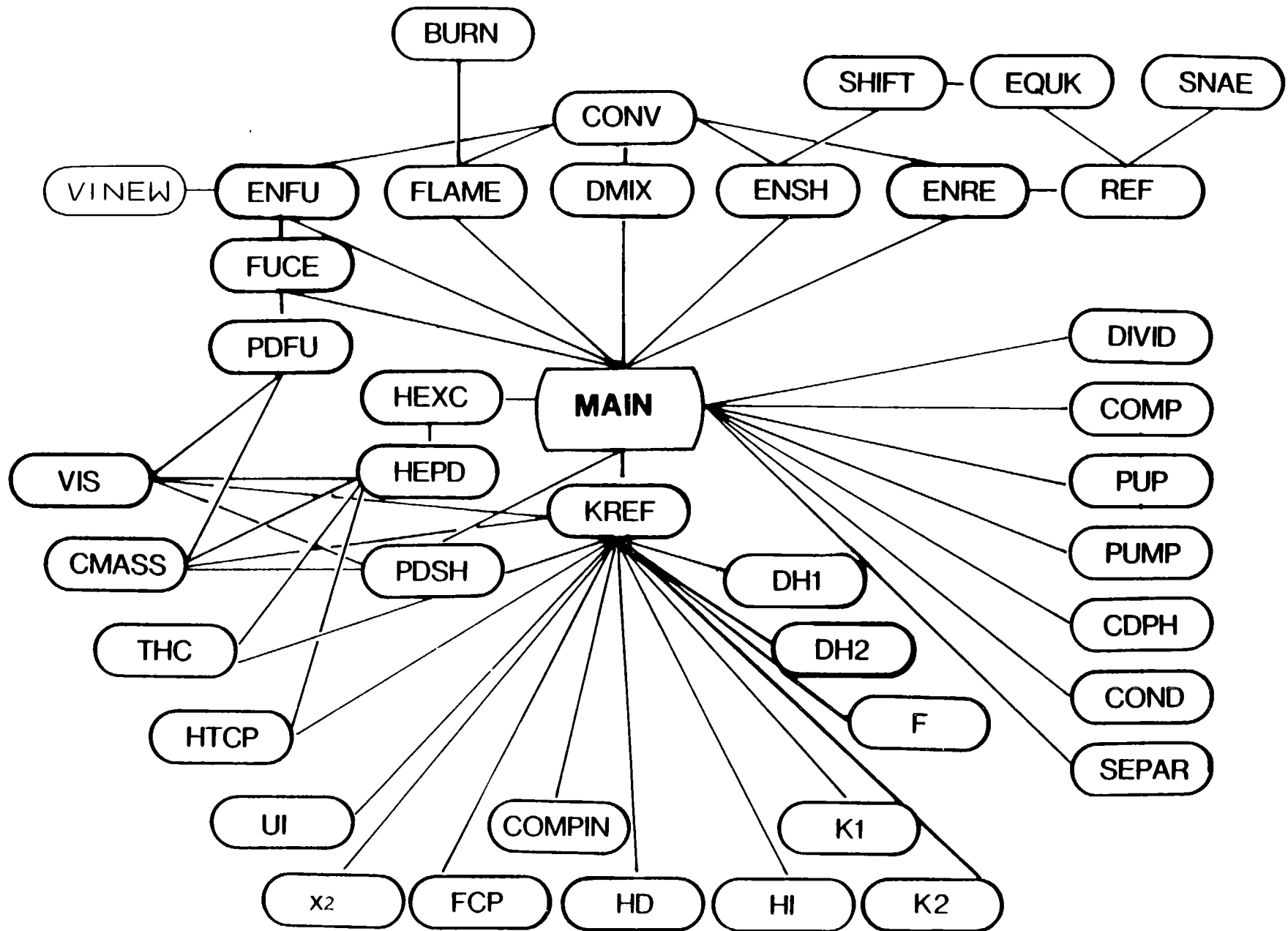


Figure 3. PERFORMANCE MODEL

C. It creates a printout of the input data, the results of thermodynamic states of the gas streams, the system performance parameters, the output heat and electric energies.

The nomenclature for the main program is shown in Table 1, and the flow chart appears in Figure 4.

The equations contained in the main program are given below:

1. Calculate inlet air flow rate in the burner:

$$\text{DNSS}(33,2) = (1+\text{EXT}*0.01)*(\text{DNSS}(14,3)+\text{DNSS}(14,5))/2+\text{CK}*\text{DNSS}(14,1) \quad (3-1-1)$$

where CK = stoichiometric number of oxygen used to burn the fuel:

for methane, CK = 2

for methanol, CK = 1.5

for naphtha, CK = 15

2. Calculate the saturation pressure of water for a given temperature:

$$T(22) = -B/(\text{ALOG}((\text{DNSS}(1,1)*\text{SMRA}-\text{DNSS}(21,6))/(\text{DNSS}(1,1)*\text{SMRA}-\text{TKNSS}(21)))*\text{POPS})-A) \quad (3-1-2)$$

where A and B are constants which have the following values for water:

A = 13.954316, atm

B = 5204.9597, atm-K

3. Calculate the output AC power for a given DC power

$$\text{AC} = (-1.0148+\text{SQRT}(1.0148*2-4*0.056/108*(0.0472*108-\text{WK}))/2*0.0456/108) \quad (3-1-3)$$

4. Calculate the flow rate of cooling water used in condenser

$$\text{DNSS}(36,6) = \text{QQT}(5)/1/18/(355-\text{TAT}) \quad (3-1-4)$$

TABLE 1

MAIN PROGRAM NOMENCLATURE

A	: Constant for calculating saturated condition of water, atm
AA1	: Thermal conductivity coeff. of gas I, Btu/hr-ft-R
AA2	: Viscosity coeff of gas I, lbm/ft-hr
AA3	: Specific heat capacity coeff. of gas I. Btu/R-lb-mole of the form: $AA3(1)+AA3(2)*T+AA3(3)*T^2+AA3(4)/T^2$
AHLU	: Mole fraction of available hydrogen
AHRN	: Percent free gas space
AIRL	: Length of air channel, ft
APPD	: Total surface area of packing Acc. to the basis and oper. temp., ft <sup>2</sup>
ATMP	: Outlet temperature of gases, K
B	: Constant for calculating saturated condition of water, atm-K
BPNA	: Boiling point of naphtha, C
BSPAC	: Baffle space, ft
CD	: Current density, A/cm <sup>2</sup>
CLENH	: Length of tube in heat exchanger, ft
CLEPD	: Length of shift converter (JK=1), reformer (JK=2 for methanol and naphtha), ft
CLH	: Clearance in heat exchanger, ft
CN	: U*A/CMIN in heat exchanger
DG	: Standard free energy change, Cal/g-mole
DHIN	: Enthalpy change due to temperature change of inlet fluid, Cal/g-mole
DHO	: Integration constant to calculate H
DP	: Catalyst pellet diameter, ft

TABLE 1

MAIN PROGRAM NOMENCLATURE  
(cont'd)

DPD	:	Diameter of shift converter (JK=1), reformer (JK=2 for methanol and naphtha), ft
DSHO	:	Cathode inlet water of fuel cell, g-mole/hr
DSN	:	Cathode inlet nitrogen of fuel cell, g-mole/hr
DSO	:	Cathode inlet oxygen of fuel cell, g-mole/hr
DTH	:	Fraction of Delta T over inlet gas film in the heat exchanger
DX1	:	Outside diameter of reformer center tube, ft
DX2	:	Inside diameter of outside reformer tube, ft
DX3	:	Outside diameter of outside reformer tube, ft
DZZ	:	Increment height of finite difference model in the reformer, ft
EA	:	Activation energy for Arrhenius expression, Cal/g-mole CH <sub>4</sub>
EPS	:	Reactor void fraction
ERR	:	Convergence criteria
EXA	:	Fraction of extra air in fuel cell
EXT	:	Fraction of extra air in burner
FCO	:	Mole fraction of co contain
FLOAR	:	Flow area in heat exchanger, ft <sup>2</sup>
FULE	:	Length of fuel channel, ft
HNA	:	Specific heat of naphtha, Btu/lbm-R
I	:	Gas number
		I = 1 Fuel (methane, methanol, naphtha)
		I = 2 Oxygen
		I = 3 Carbon Monoxide
		I = 4 Carbon Dioxide
		I = 5 Hydrogen
		I = 6 Water
		I = 7 Nitrogen



TABLE 1

MAIN PROGRAM NOMENCLATURE  
(cont'd)

ISSH	:	ID of shell in heat exchanger, ft
IDTH	:	ID of tube in heat exchanger, ft
IFUEL	:	Fuel Type
		1 = Methane CH <sub>4</sub>
		2 = Methanol CH <sub>3</sub> OH
		3 = Naphtha C <sub>7</sub> H <sub>16</sub>
IDNO	:	Number of trial-and-error loops
IHUI	:	Stoichiometric number
IP	:	Index of operation condition in the reformer and shift converters
		IP = 1 Adiabatic Operation
		IP = 2 Isothermal Operation
KO	:	Frequency factor for Arrhenius expression, lb-mole CH <sub>4</sub> /lb cata.-hr-atm
NN	:	Stream number of exit of shift converter
NOR	:	Scale factor in the model of reformer
NPFU	:	Number of cell plates in the fuel cell stacks
NPH	:	Number of tube passes
NRH	:	Number of rows for tubes
NTAA	:	Number of air flow channel in one cell plate
NTAF	:	Number of fuel flow channel in one cell plate
NTPD	:	Number of tubes in shift converter (JK=1), Reformer (JK=2 for methanol and naphtha)
ODTH	:	OD of tube, ft
OU	:	O <sub>2</sub> utilization
PAT	:	Ambient pressure, atm

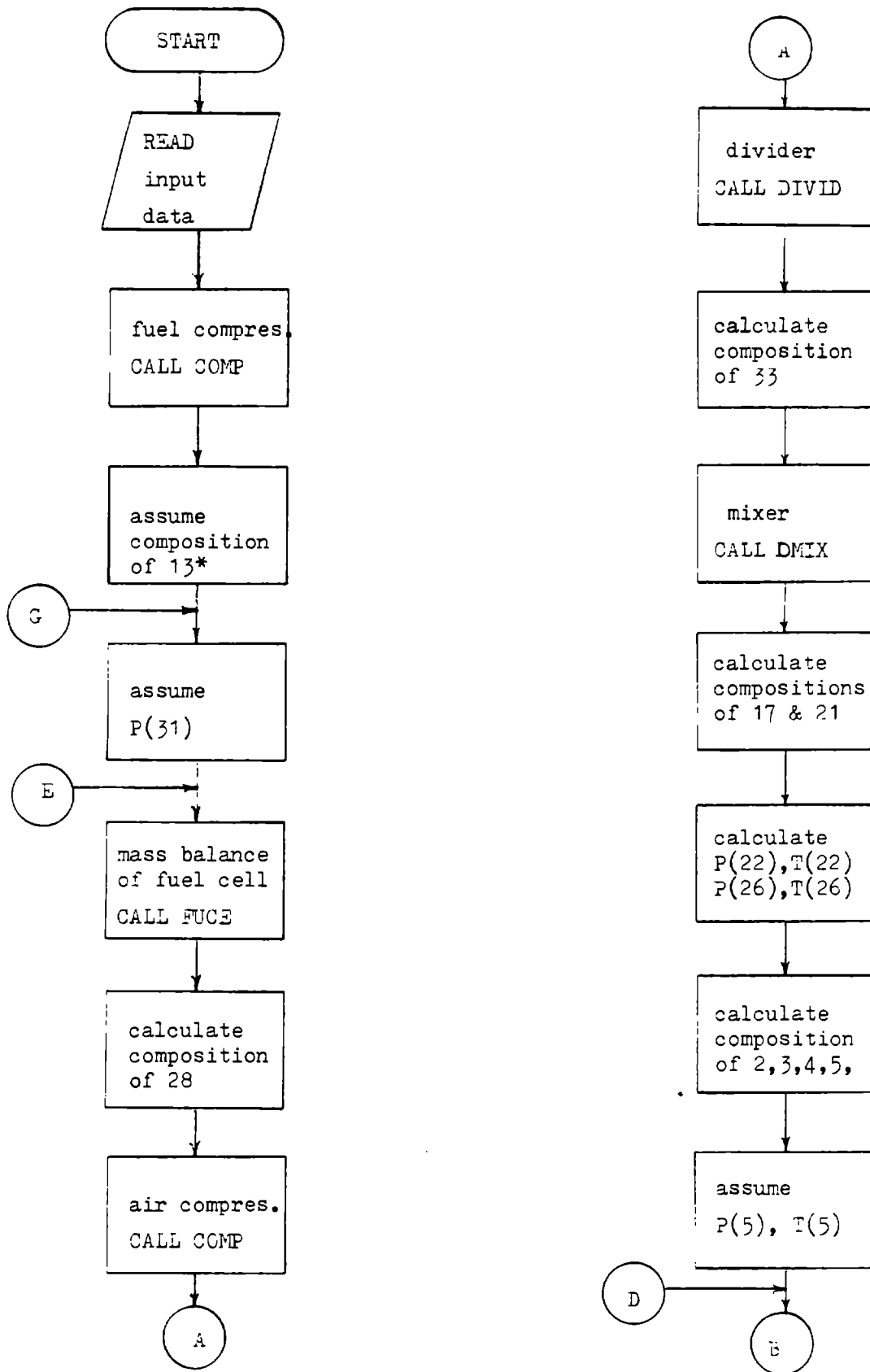
TABLE 1

MAIN PROGRAM NOMENCLATURE  
(cont'd)

PIN	: Inlet pressure, atm
PINFU	: Inlet pressure of fuel cell stacks, atm
PITCH	: Pitch of heat exchanger, ft
POP	: Operation pressure, atm
POUT	: Outlet pressure, atm
PL	: Platinum catalyst loading, mgPT/CM <sup>2</sup>
RHOB	: Bulk density of cata., lbs/ft <sup>3</sup>
S	: Side length of an assumed square flow duct for combustion gas, ft
SITS2	: Ratio of total inside-tube cross-sectional area per pass to header cross-sectional area per pass
SK	: Equilibrium constant
SKI	: Equilibrium constant with pressure different from 1 atm
SMRA	: Steam/fuel ratio
SURFC	: Surface per line, ft
SV(1)	: Specific volume of fuel 1, ft <sup>3</sup> /lbm
SVW	: Specific volume of water, ft <sup>3</sup> /lbm
TACOA	: Inlet air temperature of fuel cell stack, K
TACOF	: Inlet fuel temperature of fuel cell stack, K
TAT	: Ambient temperature, K
TC	: Critical temperature, K
TCAS	: Total heat capacity constant A
TCBS	: Total heat capacity constant B
TCCS	: Total heat capacity constant C

TABLE 1  
MAIN PROGRAM NOMENCLATURE  
 (cont'd)

TDNS	:	total amount of material, g-mole
TIN	:	Inlet fluid temperature, K
TOP	:	Operation temperature, K
TOVO	:	Total volume of inlet flow, m <sup>3</sup>
TOUT	:	Outlet temperature, K
VHNA	:	Vaporized heat of naphtha, Cal/g-mole
WAT	:	Relative humidity of air, g water/g air
WIDAA	:	Width of square air channel in the fuel cell stack, ft
WIDAF	:	Width of square fuel channel in the fuel cell stack, ft
X	:	Necessary amount of oxygen in cathode, g-mole/hr
ZH	:	Reformer length, ft
DINSC(I)	:	Inlet amount of gas I, g-mole
DNS(I)	:	Inlet (outlet) amount of gas I, g-mole
HA(J)	:	Surface area of heat exchanger J, m <sup>2</sup>
HCAS(I),		
HCBS(I),		
HCCS(I)	:	Heat capacity const. of gas I, Cal/g-mole-K of the form: $HCAS+HCBS*T+HCCS*T^2$
HS(I)	:	Heat of formation of gas I at 298 K, 1 atm, Cal/g-mole
NNS(I)	:	Stoichiometric coefficient of gas I
WM(I)	:	Molecular weight of gas I, g/g-mole
DNSS(I,J)	:	Flow rate of gas J in stream I, g-mole/hr



\* stream number (refer to Figure 1)  
 Figure 4 Flow chart of executive program for simulating CSU's PAFC system steady state performance

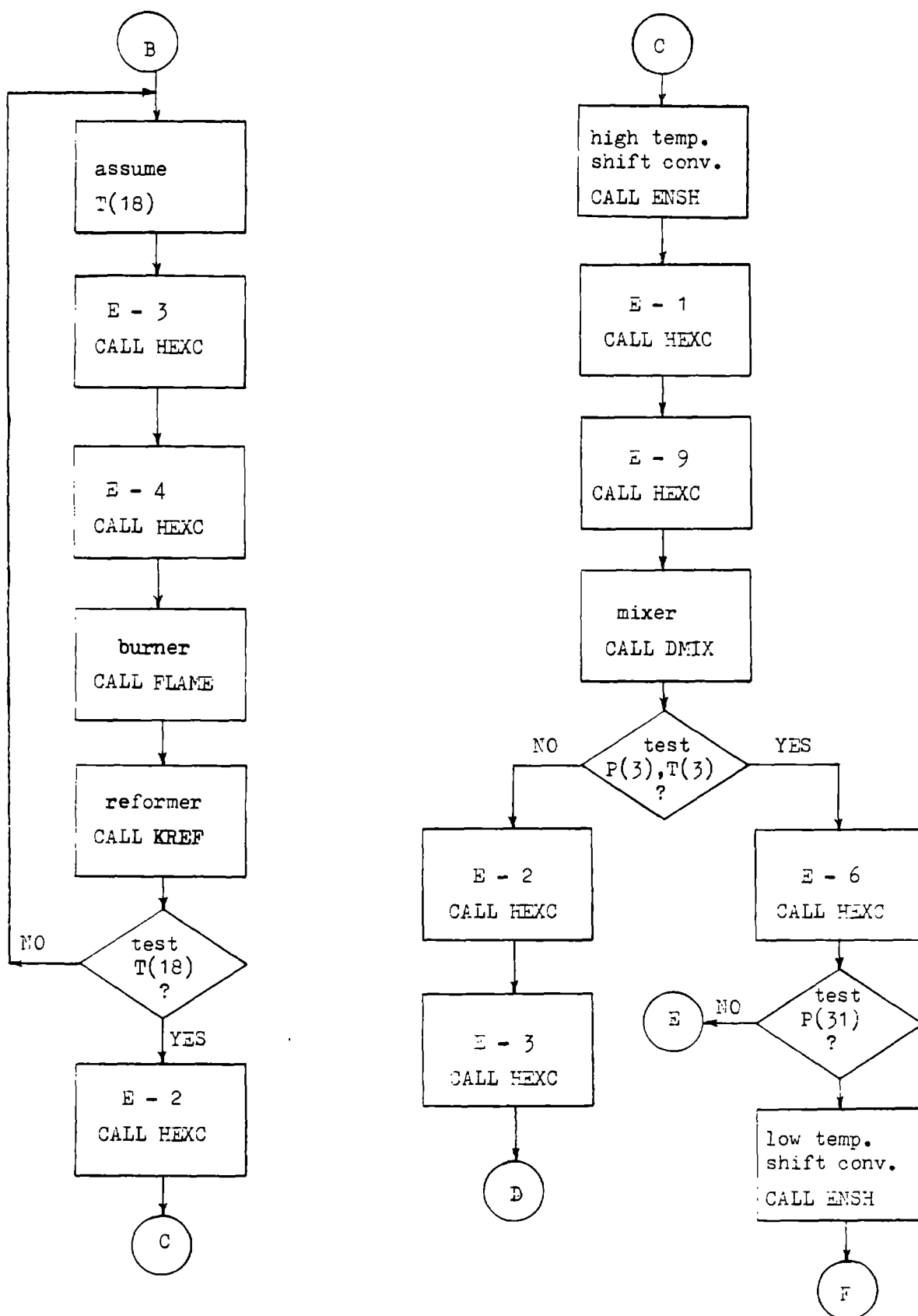


Figure 4 continued

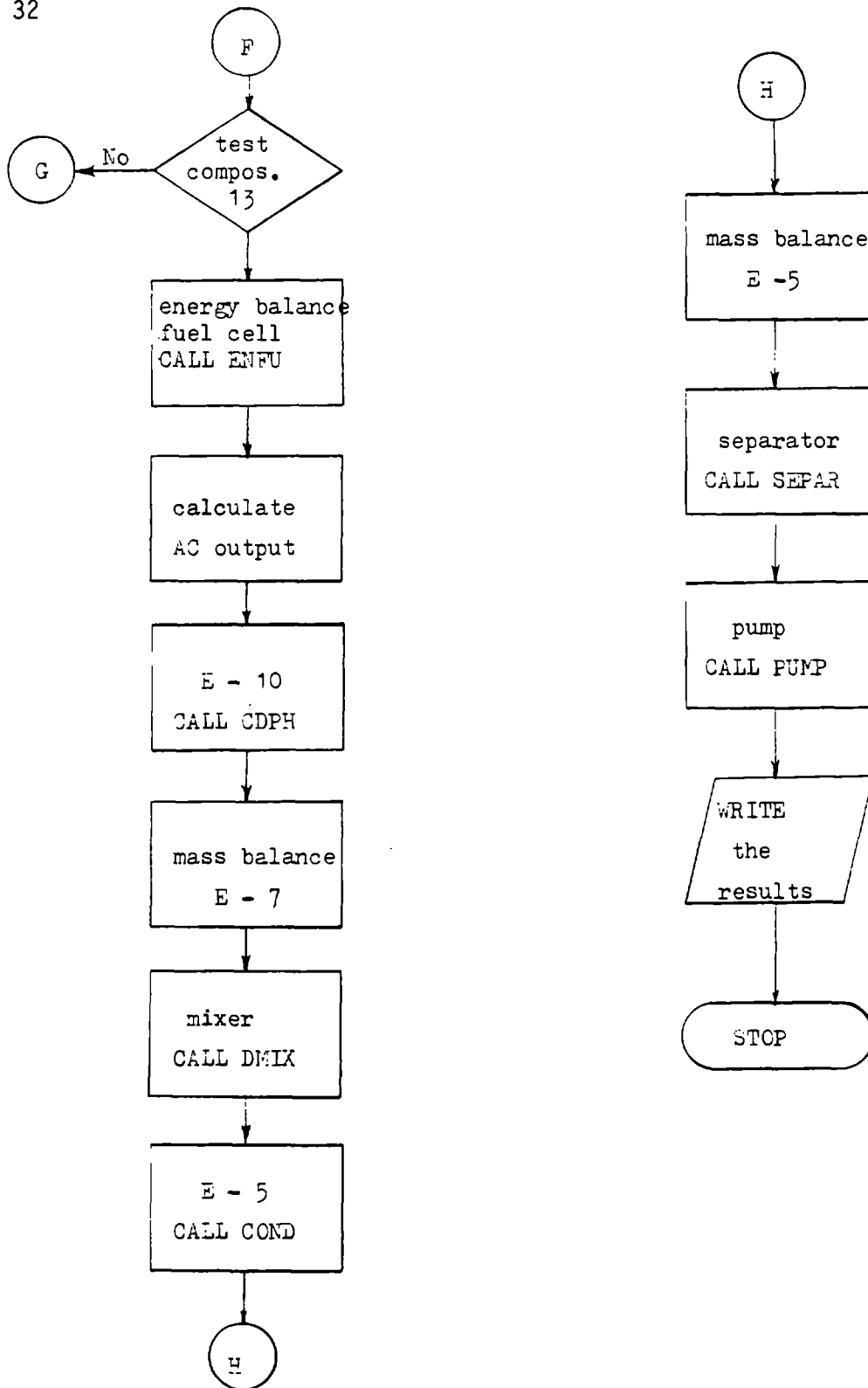


Figure 4 continued

### 3.2 Subroutines

BURN, CDPH, COMP, COND, CONV, DIVID, DMIX, ENFU, ENRE, ENSH, EQUK, FLAME, FUCE, HEPD, HEXC, PDFU, PDSH, PUMP, PUP, REF, SNAE, SEPAR, and SHIFT.

A. Subroutine BURN: This subroutine calculates the mass balance across the burner. It is assumed that combustion goes to completion and that the anode exhaust fuels the burner with 200 percent stoichiometric air. The illustrated equations contained in BURN for methane input fuel are:

1. Calculate the amount of oxygen reacted:

$$X = 0.5*DNS(3)+0.5*DNS(5)+2*DNS(1) \quad (3-2-1)$$

2. Calculate the amount of carbon dioxide produced

$$XY = DNS(3)+DNS(1) \quad (3-2-2)$$

3. Calculate the amount of water produced

$$Y = DNS(5)+2*DNS(1). \quad (3-2-3)$$

4. Calculate the exit composition

$$DNS(1) = 0$$

$$DNS(3) = 0$$

$$DNS(5) = 0$$

$$DNS(2) = DNS(2)-X$$

$$DNS(4) = DNS(4)+XY$$

$$DNS(6) = DNS(6)+Y$$

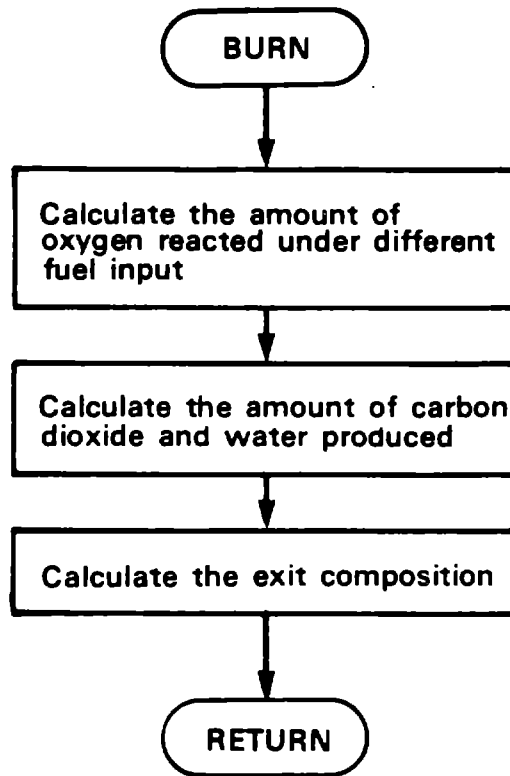


Figure 5 Flow Chart of BURN



B. Subroutine CDPH: This subroutine calculates the heat transfer rate in the evaporator E-10 and in the condenser E-7. The equations contained in CDPH are:

1. Calculate heat transfer rate in heat exchangers E-7 and E-10

$$QT = ((I-TC1)/(1-0.577))^{**}0.38*9700 \\ *DNSC(6)+(TCB-TC1)*1*18*DNSC(6). \quad (3-2-4)$$

2. Calculate the boiling temperature of water at a given pressure

$$TCB = B/(A-ALOG(P))$$

where A and B are constants referred to in Equation (3-1-2).

C. Subroutine COMP: This routine calculate the power requirement and shaft work for the fuel compressor. The equations contained in COMP are:

1. Calculate the compressor shaft work assuming adiabatic conditions

$$WS = GAG*1.987*TIN*1.8*\left(\frac{POUT}{PIN}\right)^{**}\left(\frac{GAG-1}{GAG}\right)-1/\left(GAG-1\right) \quad (3-2-5)$$

2. Calculate the compressor shaft work assuming isothermal conditions

$$WS = 1.987*TIN*1.8*ALOG(POUT/PIN) \quad (3-2-6)$$

3. Calculate the compressor power requirements

$$POW = WS*TDNS/641400 \quad (3-2-7)$$

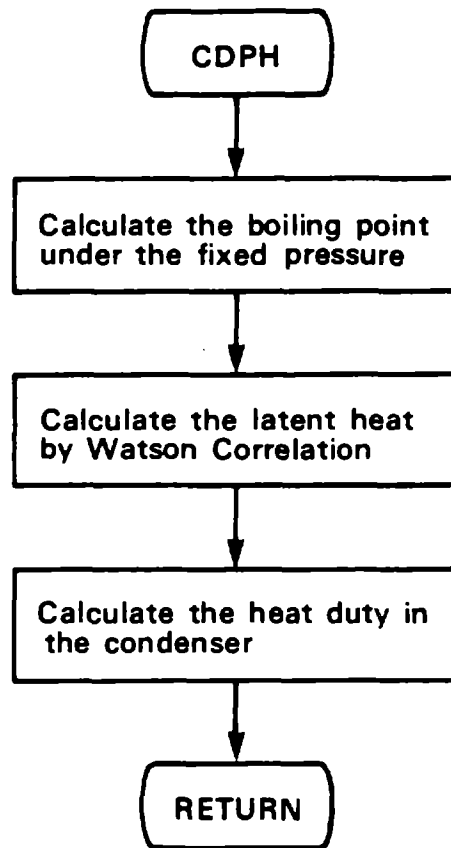


Figure 6 Flow Chart of CDPH

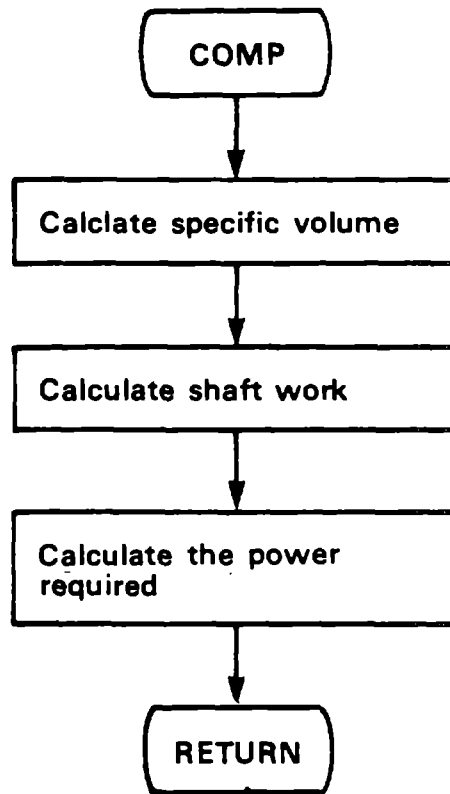


Figure 7 Flow Chart of COMP

D. Subroutine COND: This subroutine calculates the heat transfer duty in the condenser. The hot side stream is a gas mixture that contains steam.

COND contains the following equations:

1. Calculate the condenser heat transfer duty (sensible heat only)

$$QT = QT + DNSH(I) * (HCAS(I) * (THI - THO) + HCBS(I) * (THI^{**2} - THO^{**2}) + HCCS(I) * (THI^{**3} - THO^{**3})). \quad (3-2-8)$$

2. Calculate the condenser heat transfer capacity with the Watson correction for latent heat

$$QT = QT + ((1 - (THO/647.1)) / (1 - 0.577))^{**0.38} * 9700 * DNSH(6) \quad (3-2-9)$$

where Watson correction is given as,

$$\frac{(h_{fg})_2}{(h_{fg})_1} = \left( \frac{1 - T_{r2}}{1 - T_{r1}} \right)^{0.38} \quad (3-2-10)$$

where  $h_{fgi}$ : molar heat of vaporization at condition i

$T_{ri}$ : reduced temperature at condition i.

E. Subroutine CONV: This subroutine finds the roots of the nonlinear equation  $x=f(x)$  by the Wegstein iteration scheme which accelerates convergence to the roots provided  $f(x)$  has a continuous first derivative. CONV contains the following equation:

1. Calculate the roots of a given nonlinear function:

$$XT = (XA(NR) * YV - YA(NR) * XV) / (XA(NR) - XV + YV - YA(NR)) \quad (3-2-11)$$

F. Subroutine DIVID: This subroutine calculates the material balance around the divider with known divider factor. It is assumed that there is no temperature change in the streams and that specific enthalpy remains constant.

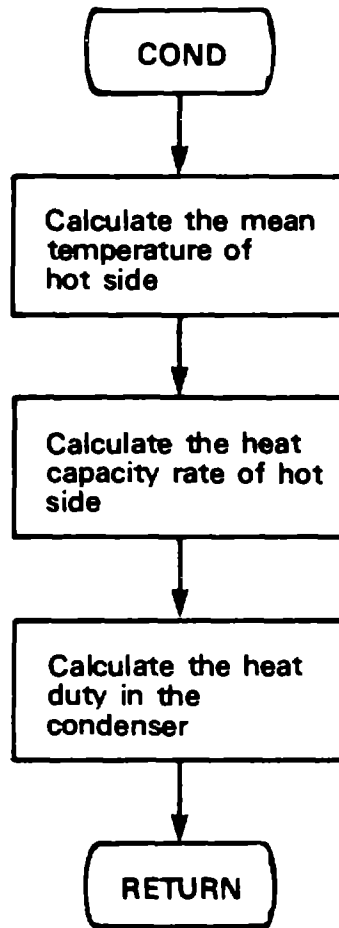


Figure 8 Flow Chart of COND

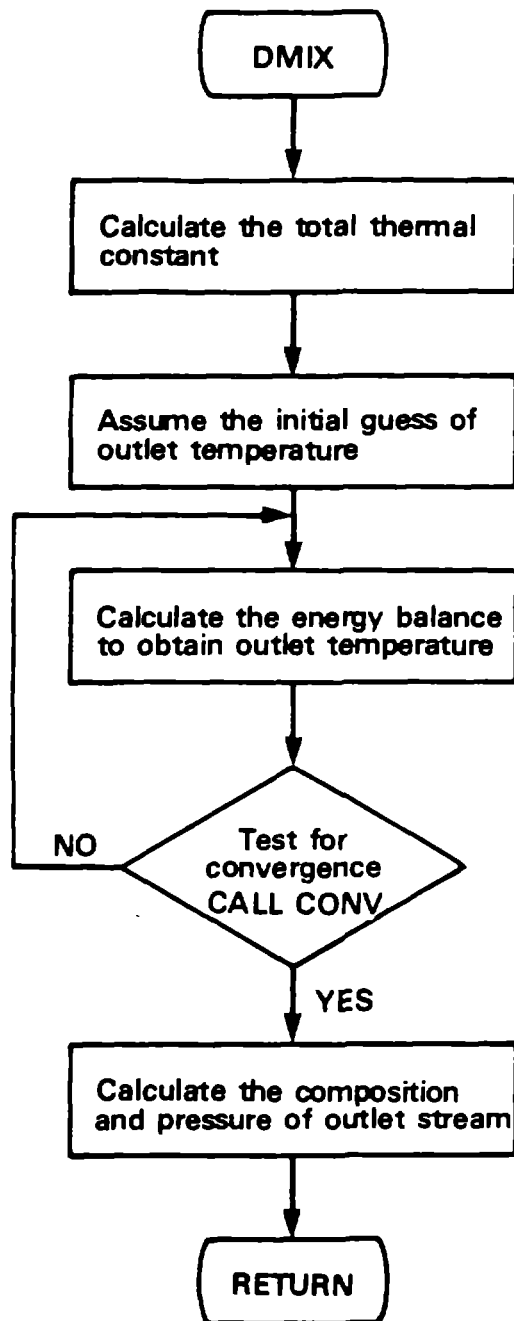


Figure 9 Flow Chart of DMIX

G. Subroutine DMIX: This subroutine calculates mass and energy balances around the mixer through which two streams combine to produce a single stream. The flow chart for DMIX is shown in Figure 8. DMIX contains the following equations:

1. Calculate the outlet temperature

$$\begin{aligned} TOUTC = & (TCAS1*TIN1+TCAS2*(TIN2-TOUT)+TCBS1/2.* \\ & (TIN1**2-TOUT**2)+TCBS2/2.*(TIN2**2-TOUT**2)+TCCS1* \\ & (TIN1**3-TOUT**3)/3.+TCCS2*(TIN2**3-TOUT**3)/3.)/TCAS1 \end{aligned} \quad (3-2-12)$$

2. Calculate the outlet pressure

$$POUT = (TDNS1+TDNS2)/(TDNS1*TINI/PINI+TDNS2*TIN2/PIN2)*TOUT \quad (3-2-13)$$

H. Subroutine ENFU: This subroutine uses mass and energy balances in the fuel cell to calculate the following performance parameters: operating voltage, open circuit voltage, free energy change at fuel cell operating conditions, heat of reaction for methane, heat of reaction for methanol, heat of reaction for naphtha, fuel cell outlet temperature and stream composition, electrical work produced, heat energy rejected, voltage efficiency, thermodynamic efficiency, heating value efficiency, and fuel cell efficiency. The flow chart for ENFU appears in Figure 10. Subroutine ENFU contains the Equations (2-2-5) to (2-2-18).

I. Subroutine ENRE: This subroutine is used to calculate the energy balance of reformer in lumped model. This model was based on the assumption that all chemical reactions reach equilibrium at the input temperature (isothermal operation) or the average temperature (adiabatic operation). Then

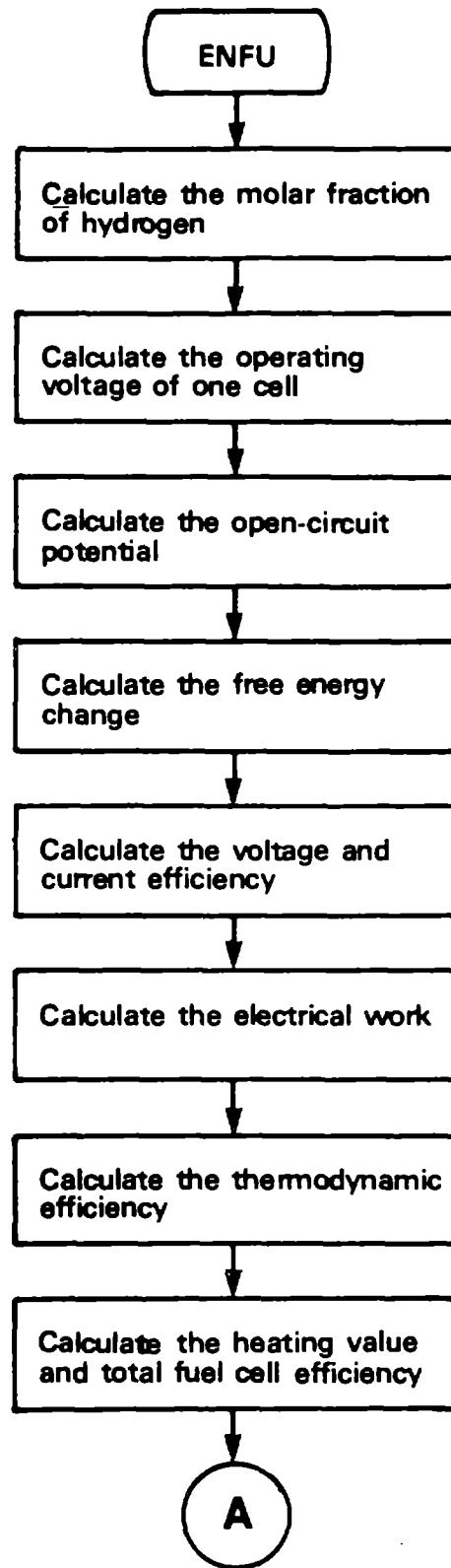


Figure 10 Flow Chart of ENFU



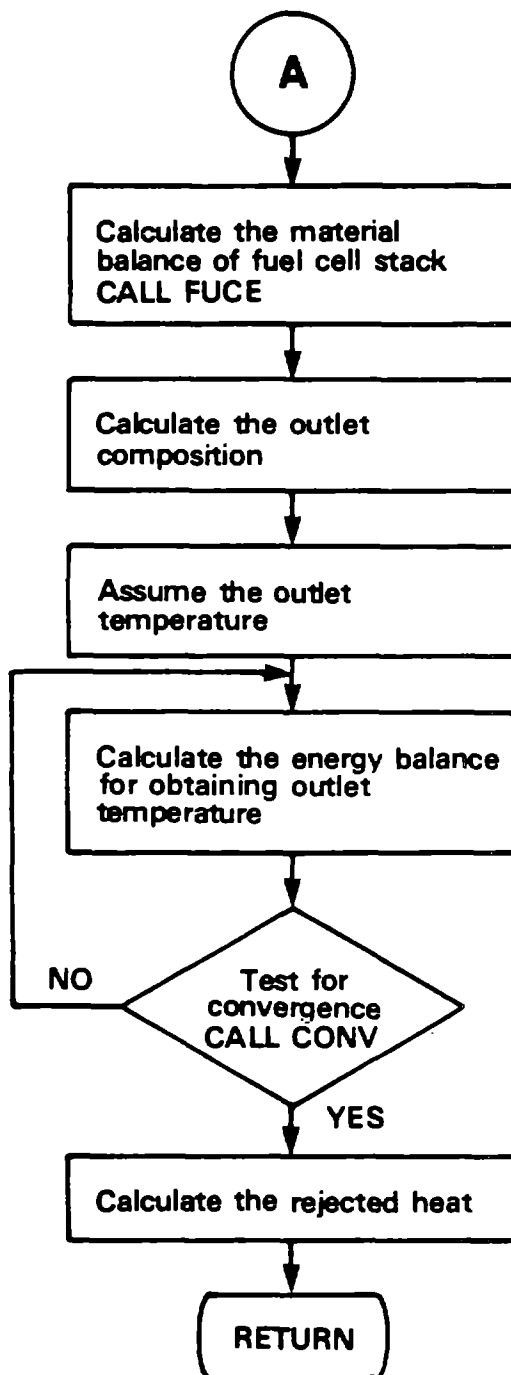


Figure 10 continued

the energy balance contains the sensible enthalpy change and the enthalpy change of reactions. The mathematical model was described in the Equations (2-1-10) to (2-1-12). The flow chart of ENRE is shown in Figure 11.

J. Subroutine ENSH: This subroutine is used to calculate the energy balance of shift converters (both high temperature converter and low temperature converter). Since methanol fuel does not need the shift converter, this subroutine will be skipped when input fuel is methanol. The mathematical model and flow chart of ENSH are shown in the Equation (2-1-6) and Figure 12, respectively.

K. Subroutine EQUK: This subroutine calculates the equilibrium constants of the process gases in the demethanation and water shift reactions. The mathematical model for the equilibrium constant was based on the Van't Hoff equation

$$d \ln K = \frac{\Delta H^0}{RT^2} dT \quad (3-2-14)$$

This equation can be integrated after expressing  $\Delta H^0$  in terms of the specific heats of the stream gases to yield,

$$\ln K = \frac{-DHO}{RT} + \frac{\Delta\alpha}{R} \ln(T) + \frac{\Delta\beta}{2R} T + \frac{\Delta\gamma}{6R} T^2 + AI \quad (3-2-15)$$

where  $\Delta\beta$  and  $\Delta\gamma$  are total heat capacity constants in the specific reaction, DHO and AI are constants of integration which can be evaluated from the standard enthalpy and standard free energy change. The flow chart for EQUK appears in Figure 13. The equations contained in EQUK are:

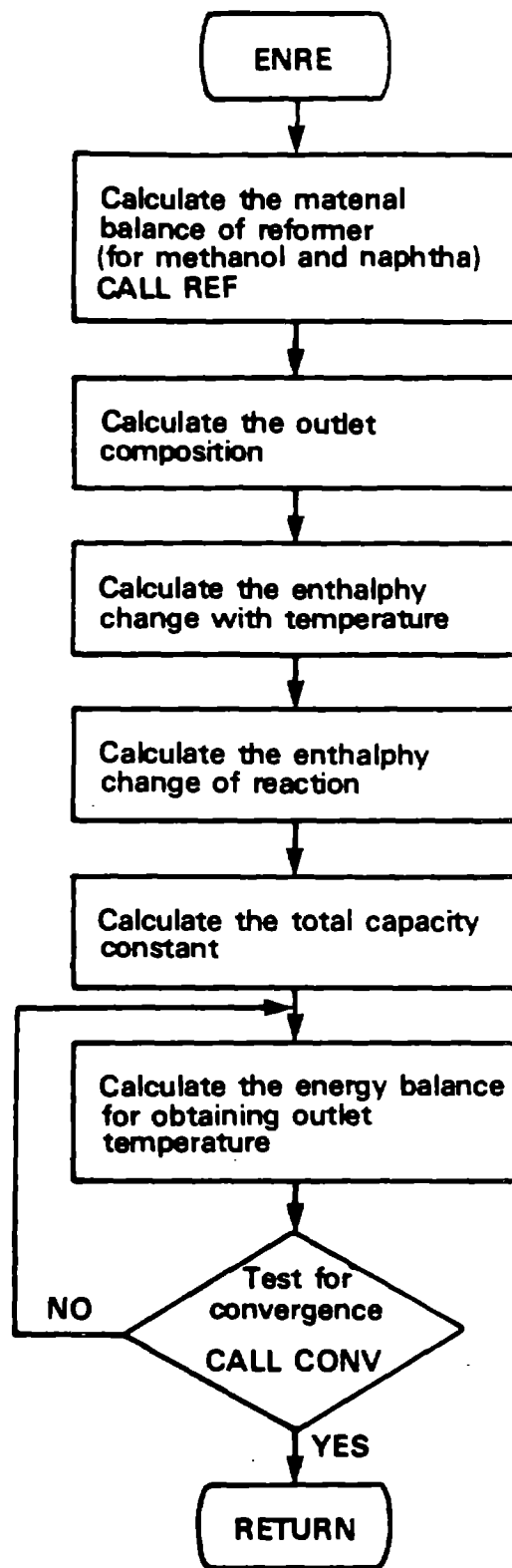


Figure 11 Flow Chart of ENRE

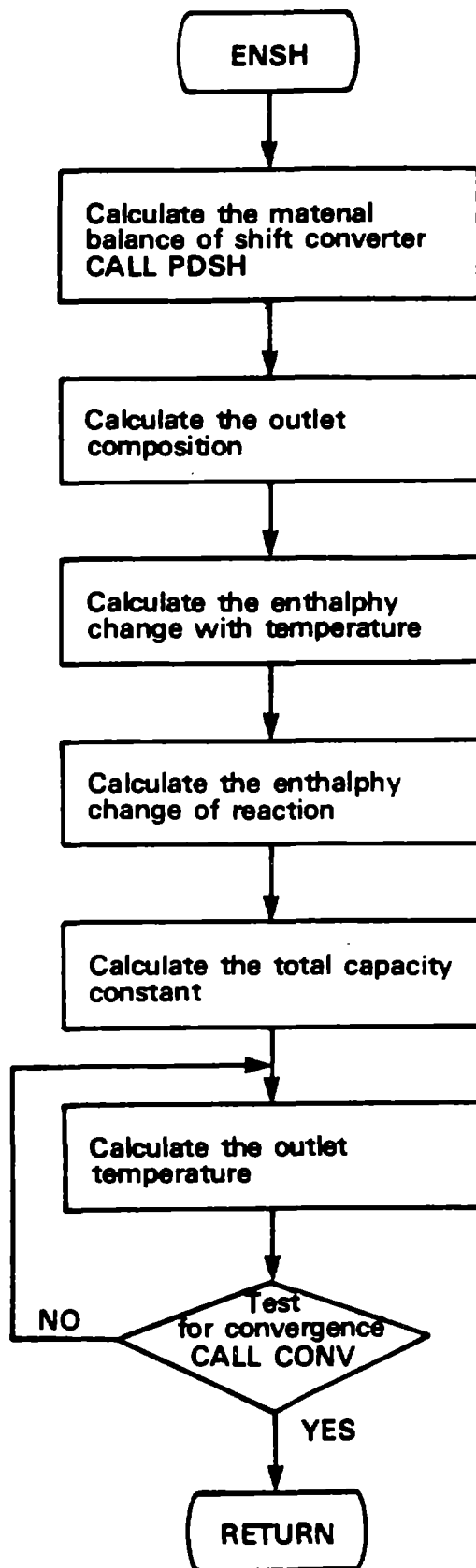


Figure 12 Flow Chart of ENSH

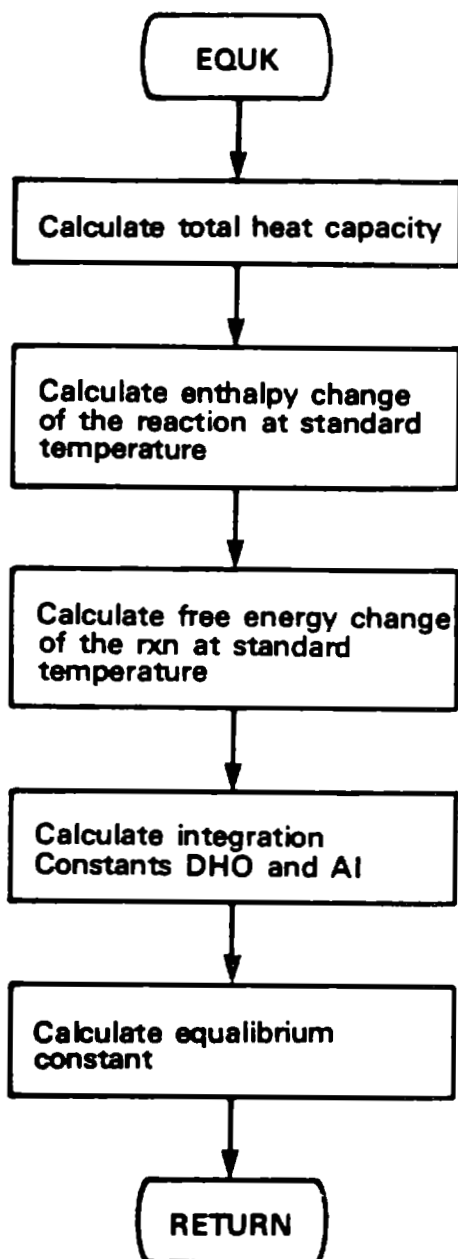


Figure 13 Flow Chart of EQUK

1. Calculate heat capacity constants

$$\begin{aligned} \text{TCAS} &= \text{TCAS} + \text{NNS}(\text{I}) * \text{HCAS}(\text{I}) \\ \text{TCBS} &= \text{TCBS} + \text{NNS}(\text{I}) * \text{HCBS}(\text{I}) \\ \text{TCCS} &= \text{TCCS} + \text{NNS}(\text{I}) * \text{HCCS}(\text{I}) \end{aligned} \quad (3-2-16)$$

2. Calculate enthalpy of reaction change

$$\text{DH} = \text{DH} + \text{NNS}(\text{I}) * \text{HS}(\text{I}) \quad (3-2-17)$$

3. Calculate free energy of reaction

$$\text{DG} = \text{DG} + \text{NNS}(\text{I}) * \text{GS}(\text{I}) \quad (3-2-18)$$

4. Calculate constant DHO

$$\text{DHO} = \text{DH} - \text{TCAS} * \text{TST} - \text{TCBS} * \text{TST}^2 / 2 - \text{TCCS} * \text{TST}^3 / 3 \quad (3-2-19)$$

5. Calculate constant AI

$$\begin{aligned} \text{AI} &= (\text{DHO} - \text{DG} - \text{TCAS} * \text{TST} * \text{ALOG}(\text{TST}) - \text{TCBS} / 2 * \text{TST}^2 \\ &\quad - \text{TCCS} / 6 * \text{TST}^3) / \text{TST} / \text{R} \end{aligned} \quad (3-2-20)$$

6. Calculate equilibrium constant

$$\begin{aligned} \text{SK} &= \text{EXP}(-\text{DHO} / \text{R} / \text{TOP} + \text{TCAS} / \text{R} * \text{ALOG}(\text{TOP}) + \text{TCBS} / 2 * \text{TOP} / \text{R} \\ &\quad + \text{TCCS} / 6 / \text{R} * \text{TOP}^2 + \text{AI}) \end{aligned} \quad (3-2-21)$$

L. Subroutine FLAME: This subroutine calculates the sensible enthalpy, the enthalpy change of reaction, and the maximum flame temperature in the burner. In the derivation of the mathematical model, it was assumed that the

combustion process goes to completion with negligible dissociation of the products and 200 percent stoichiometric air. The flow chart for FLAME appears in Figure 14. FLAME contains the following equations:

1. Calculate the enthalpy of reaction change at 298 K

$$DH = DH + DNS(I) * HS(I) - DINS(I) * HS(I) \quad (3-2-22)$$

2. Calculate the sensible enthalpy change

$$DH = DH + DINS(I) * (HCAS(I) * (298 - TIN) + HCBS(I) / 2 * ((298) ** 2 - TIN ** 2) + HCCS(I) / 3 * ((298) ** 3 - TIN ** 3)) \quad (3-2-23)$$

3. Calculate total heat capacity constants

$$TCAS = TCAS + DNS(I) * HCAS(I)$$

$$TCBS = TCBS + DNS(I) * HCBS(I) \quad (3-2-24)$$

$$TCCS = TCCS + DNS(I) * HCCS(I)$$

4. Calculate the adiabatic FLAME temperature

$$TFC = (-DH - TCBS / 2 * ((TF) ** 2 - (298) ** 2) - TCCS / 3 * ((TF) ** 3 - (298) ** 3)) / TCAS + 298 \quad (3-2-25)$$

M. Subroutine FUCE: This subroutine calculates the mass balance in the fuel cell stack, which is described in Equations (2-2-2) to (2-2-4). Flow chart of FUCE is shown in Figure 15.

N. Subroutine HEPD: This subroutine calculates the pressure drop in the heat exchangers used in the fuel cell power plants. It was assumed that BWG14

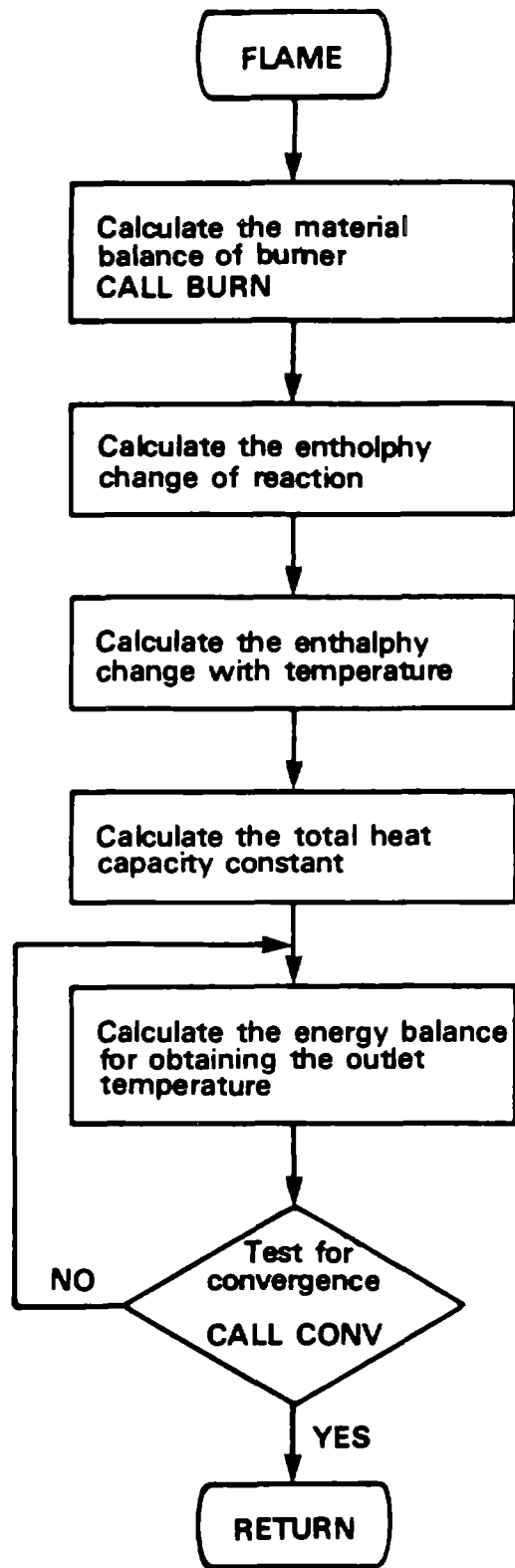


Figure 14 Flow Chart of FLAME



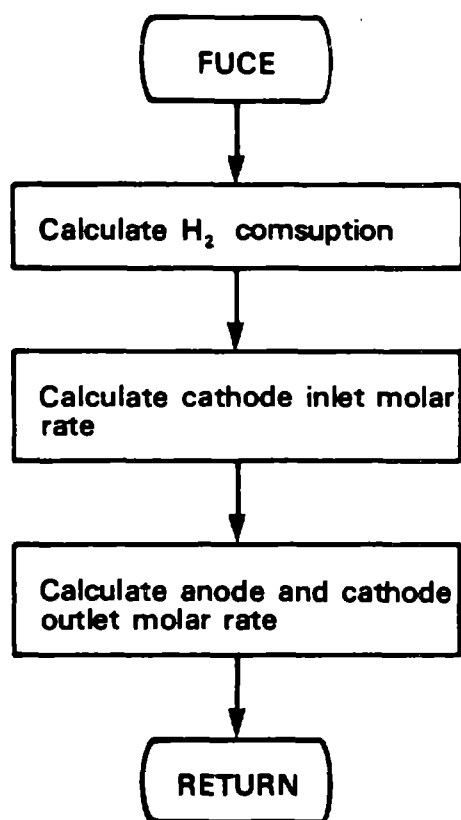


Figure 15 Flow Chart of FUCE

tubes with nominal size of 3/4 inch were used in the heat exchangers. The flow chart for HEPD appears in Figure 16. HEPD contains the following equations:

1. Calculate the number of tubes

$$NT = HA/0.3048^{**2}/NP/CLEN/SURFC \quad (3-2-26)$$

2. Calculate number of baffles

$$NB = CLEN/BSPAC \quad (3-2-27)$$

3. Calculate free area between baffles

$$FAREA = IDS/(ODT+CL)*CL*BSPAC \quad (3-2-28)$$

4. Calculate ratio of pitch, transverse to flow, to tube diameter

$$XT = PITCH/ODT \quad (3-2-29)$$

5. Calculate friction factor

$$FPRI = SBO*(ODT*GS/AMUI)^{**}(-0.15) \quad (3-2-30)$$

6. Calculate pressure drop

$$DP = BO*2*FPRT*NR*GS^{**2}/32.174/3600^{**2}/RHO/2116.2 \quad (3-2-31)$$

0. Subroutine HEXC: This subroutine calculates the energy analysis in the parallel, counter and crossflow heat exchangers. From the assumption described in Section 2.1.1, the counter mode will be the only option used for heat exchangers in the system. Mathematical model was shown in the Equations (2-1-1) to (2-1-4).

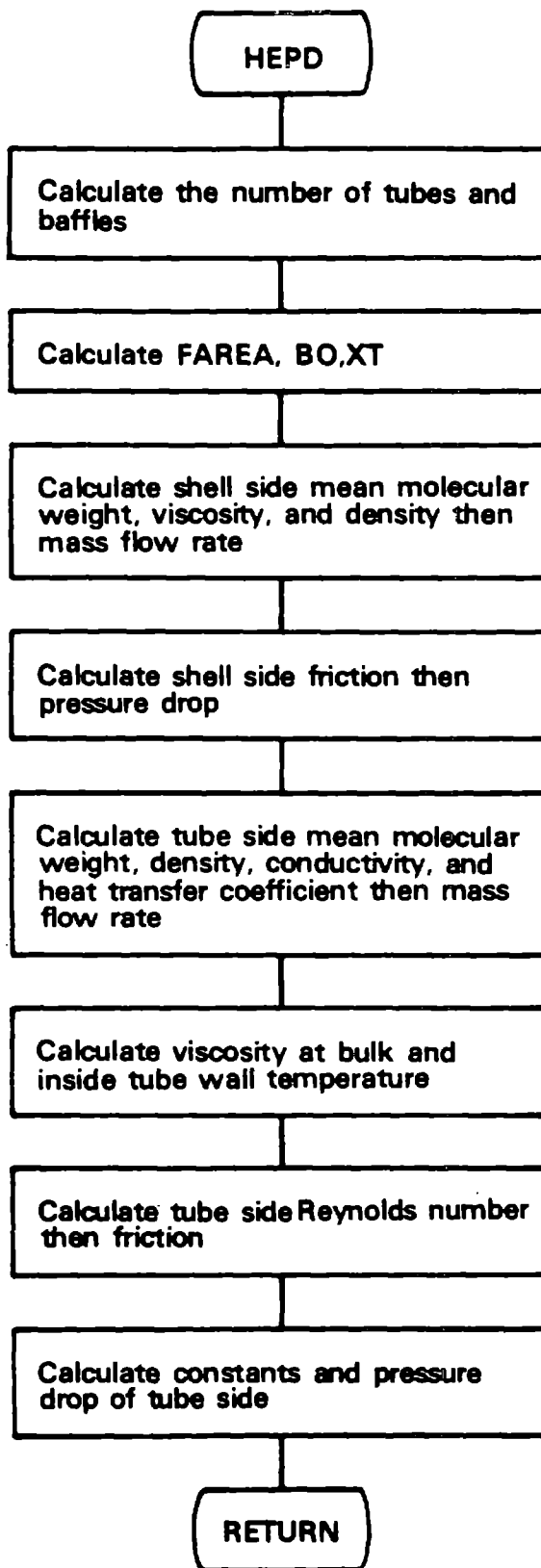


Figure 16 Flow Chart of HEPD

P. Subroutine PDFU: This subroutine calculates the pressure drops in the fuel channels and air channels. Dimensions of the fuel-cell stack are based on Westinghouse Stock No. 522. The mean pressure drop is evaluated by taking average of calculations based on inlet and outlet gas compositions.

Q. Subroutine PDSH: This subroutine calculates the pressure drop in the packed reactors which are reformer and shift converters in our system. Ergun equation stated in Equation (2-1-7) was used to calculate pressure drop of reacting fluid caused by flowing through the packings.

R. and S. Subroutines PUMP and PUP: Subroutine PUMP calculates the power required to pump water to a given pressure. PUP calculates the power required to pump naphtha or methanol to a given pressure. PUMP contains the following equation:

1. Calculate the power required to pump water

$$POW = SVW*144.*5.05051*0.0000001*WM(6)*14.7* \\ (POUT-PIN)*DNS(6)/453.6 \quad (3-2-32)$$

T. and U. Subroutines REF and SNAE: Material balance in the reformer at the equilibrium state (lumped model) is analyzed in subroutine REF. Subroutine SNAE solves two nonlinear algebraic equations generated in REF. These two subroutines were more likely for the system with methanol or naphtha input fuel, whereas the kinetic model (Section 2.1.3.2) was used for the system with methane input fuel.

The material balances for methanol or naphtha input fuel in the reformer are similar to the discussion in the Section 2.1.3.1, where methane input fuel was illustrated.

Newton-Raphson method for solution of nonlinear algebraic equations is used in SNAE repeatedly to approach the equilibrium conversions of two parallel reactions (demethanation and water shift reactions). The general description of Newton-Raphson method is as follows (Ref. 12), for two equations  $f_1(x_1, x_2) = 0$  and  $f_2(x_1, x_2) = 0$ :

$$\begin{aligned} X_1 \text{ NEW} &= X_1 \text{ old} + \Delta X_1 \\ X_2 \text{ NEW} &= X_2 \text{ old} + \Delta X_2 \end{aligned} \quad (3-2-33)$$

where

$$\begin{aligned} \Delta X_1 &= \frac{f_2 \frac{\partial f_1}{\partial x_2} - f_1 \frac{\partial f_2}{\partial x_2}}{D} \\ \Delta X_2 &= \frac{f_1 \frac{\partial f_2}{\partial x_1} - f_2 \frac{\partial f_1}{\partial x_1}}{D} \end{aligned} \quad (3-2-34)$$

and D is the determinant of coefficient matrix (the Jacobian), which equals to

$$\frac{\partial f_1}{\partial x_1} \frac{\partial f_2}{\partial x_2} - \frac{\partial f_1}{\partial x_2} \frac{\partial f_2}{\partial x_1}$$

V. Subroutine SEPAR: This subroutine calculates the outlet compositions in the liquid-vapor separator. The liquid-vapor equilibrium constant at given temperature is determined by Raoult's law which states

$$XW = (TDNS - DNS(6)) / (DK - 1) \quad (3-2-35)$$

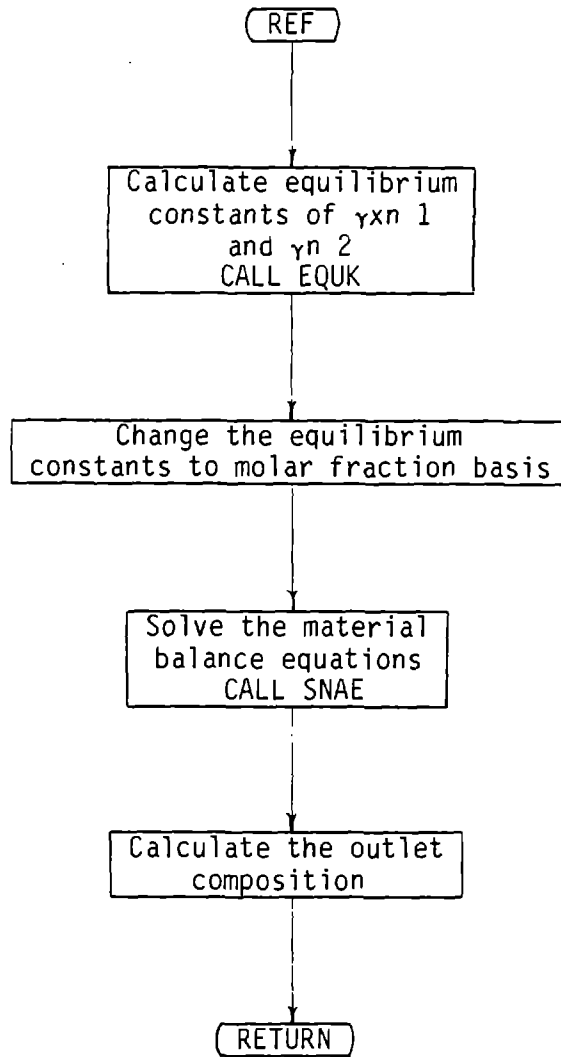


Figure 17: Flow Chart of Subroutine REF

where  $XW$ : amount of water in liquid phase  
DK: equilibrium constant of liquid-vapor system, which equals to  
( $PSAT/POP$ )

W. Subroutine SHIFT: SHIFT calculates the material balance in the shift converter. As discussed in Section 2.1.2, one reaction, water shift reaction, dominates the material change in the shift converter. The mathematical model described in the Equation (2-1-5) will be solved by Newton's method (Ref. 12) in this subroutine.

X. Subroutine VINEW: This subroutine calculates the characteristic of current density and operating voltage in the PAFC stack. The cell voltage can be expressed as an explicit function of reactions, products, and current density (Section 2.2.2), while the calculation of the current density involves a trial and error procedure. The mathematical model is shown in Equations (2-2-8) and (2-2-13).

### 3.3 Subroutine KREF

The mathematical model developed in Section 2.1.3.2 was used to develop a Fortran computer code, which consists of an executive program (KREF), three subroutines and eleven functions. Finite difference method will be applied to solve these simultaneous differential equations (Equations (2-1-14) to (2-1-17)), with the inlet conditions as the boundary conditions. The definition of finite difference section is expressed in Figure 18 and the summary of the basic difference equations is shown in Table 2, where the nomenclature of

variables and functions in the program is listed in Table 3. Figure 19 shows the flow chart of this program.

KREF is similar to REPENT developed by Westinghouse (80-9E6-PAMEC-RI). A more detailed discussin of the subroutines and functions is given in Ref. 3 and will not be repeated here.



TABLE 2

SUMMARY OF THE BASIC EQUATIONS  
USED IN THE KINETIC MODEL OF THE REFORMER

## 1. Demethanation Reaction Kinetic Mass Balance

$$X1(i+1) = X1(i) = \frac{e_B P \Delta Z}{U_o C_o} K_o^{-EA/R[TA(i+1)+460]} X_{MCOMP}(i,1)$$

## 2. Water Gas Shift Equilibrium

$$X2 = \frac{-B - \sqrt{B^2 - 4CA}}{2A}$$

with  $A = [K2(i+1)-1][F3+X1(i+1) F1]^2$

$$B = [F3+X1(i+1) F1][2X1(i+1) F1 K2(i+1)-F2 K2(i+1)-F4 K2(i+1)-5X1(i+1) F1-F3-F5]$$

$$C = K2(i+1) F2 F4 - 2K2(i+1) F2 X1(i+1) F1 - [F3+X1(i+1)] [F5+4X1(i+1) F1]$$

## 3. Reforming Gas Energy Balance

$$TC(i+1) = \frac{TH(i+1)}{AM} [AM-MH CH] + \frac{TH(i)}{AM} [AM+MH CH] - TC(i)$$

with  $AM = (UI \pi D2 \Delta Z)/2$

## 4. Combustion Gas Energy Balance

$$TH(i+1) = TH(i) \frac{AN+2(\Sigma FACP)}{AN} - TC(i) \frac{2(\Sigma FACP)}{AN} - \frac{AL}{AN}$$

where  $\Sigma FACP$ : sum of the component's heat capacity in the reforming gas

$$AL = F1 (-DH1)[X1(i+1)-X1(i)] + [F3+X1(i+1) F1](-DH2)[X2(i+1)-X2(i)]$$

$$\bar{AN} = \frac{MH CH(\Sigma FACP)}{AM} - \Sigma FACP + MH CH$$

## 5. Pressure Drop of Reforming Gas

$$P(i+1) = P(i) - \Delta P$$

where  $\Delta P$  can be calculated from Ergun equation (Equation (2-1-7)).

TABLE 3

NOMENCLATURE OF VARIABLES AND FUNCTIONS IN SUBROUTINE KREF

	<u>Component</u>	<u>Compound</u>
	1	CH <sub>4</sub>
	2	CO
	3	CO <sub>2</sub>
	4	H <sub>2</sub> O
	5	H <sub>2</sub>
	6	N <sub>2</sub>
	7	O <sub>2</sub>

<u>Variable</u>	<u>Definition</u>
FL for J = 0 to 7	Total reformer gas feed flow rate and component feed flow rates for components 1 through 7 (molar basis)
MH	Total combustion gas flow rate (molar basis)
CGCOM for J = 1 to 7	Combustion gas component flow rates for components 1 to 7 (molar basis)
K1	Equilibrium constant for demethanation reaction
K2	Equilibrium constant for water shift reaction
K0	Frequency factor for Arrhenius expression $k + k_0 \exp(-E_{act}/RT)$
WM	Molecular weight
EA	Activation energy for demethanation reaction
RHOB	Catalyst bulk density
EPS	Reactor void volume
D1	Reformer center tube outside diameter
D2	Reformer outer tube inside diameter
D3	Reformer outer tube outside diameter
S	Characteristic dimension of the combustion gas flow duct (geometry is square)
DP	Catalyst particle diameter
P	Pressure

TABLE 3  
NOMENCLATURE OF VARIABLES AND FUNCTIONS IN SUBROUTINE KREF  
 (cont'd)

<u>Variable</u>	<u>Definition</u>
TCO	Reformer gas feed temperature
THZ	Combustion gas feed temperature
Z	Length of reformer tube
X1(I)	Kinetic conversion by demethanation reaction in Increment I
XE2(I)	Actual conversion by water shift reaction in Increment I
CO	Initial methane concentration in reformer gas
UO	Initial reformer gas linear velocity
T	Temperature
TK2	Equilibrium constant for demethanation reaction at temperature T
TX2	Equilibrium conversion for water shift reaction at temperature T
TDH1	Heat of reaction for demethanation reaction at temperature T
TDH2	Heat of reaction for water shift reaction at temperature T
X2	Equilibrium conversion for water shift reaction
DH1	Heat of reaction for demethanation reaction
DH2	Heat of reaction for water shift reaction
TF	Total moles of reformer gas
TVIS	Viscosity at temperature T
VIS	Viscosity
THC	Thermal conductivity

TABLE 3

NOMENCLATURE OF VARIABLES AND FUNCTIONS IN SUBROUTINE KREF  
(cont'd)

<u>Variable</u>	<u>Definition</u>
TTHC	Thermal conductivity at temperature T
HI	Inside heat transfer coefficient for the reformer outer tube
THI	Same as HI evaluated at temperature T
HO	Outside heat transfer coefficient for the reformer gas outer tube
THO	HO evaluated at temperature T
UI	Overall heat transfer coefficient for reformer outer tube
TUI	UI evaluated at temperature T
FCP	Reformer gas heat capacity
TFCP	Reformer gas heat capacity at temperature T
THO	Combustion gas outlet temperature
DZZ	Incremental length
TA(I)	Average temperature in Increment I
I	Increment counter
TAK1	K1 evaluated at TA(I, K)
TAK2	K2 evaluated at TA(I, K)
TAX2	Conversion X2 for water shift reaction assuming total system equilibrium
XF	Total number of moles in the reformer gas
XUI	Overall heat transfer in Increment I
XCOMP(I, J)	Moles of component J in Increment I
COM(J)	Feed moles of component J

TABLE 3  
NOMENCLATURE OF VARIABLES AND FUNCTIONS IN SUBROUTINE KREF  
(cont'd)

<u>Variable</u>	<u>Definition</u>
XMCOMP(I, J)	Mole fraction components J, Increment I
TC(I)	Reformer gas temperature in Increment I
TH(I)	Combustion gas temperature in Increment I
TP(I)	Interactive variable for TC(I)
XDH1	Value of DH1 in Increment I
XDH2	Value of DH2 in Increment I
XVIS	Value of VIS in Increment I
XTHC	Value of THC in Increment I
XHI	Value of HI in Increment I
XCGVIS	Combustion gas viscosity in Increment I
XCGTHC	Combustion gas thermal conductivity in Increment I
XHO	Value of HO in Increment I
RE	Reynolds number
Error	Convergence criterion on methane conversion

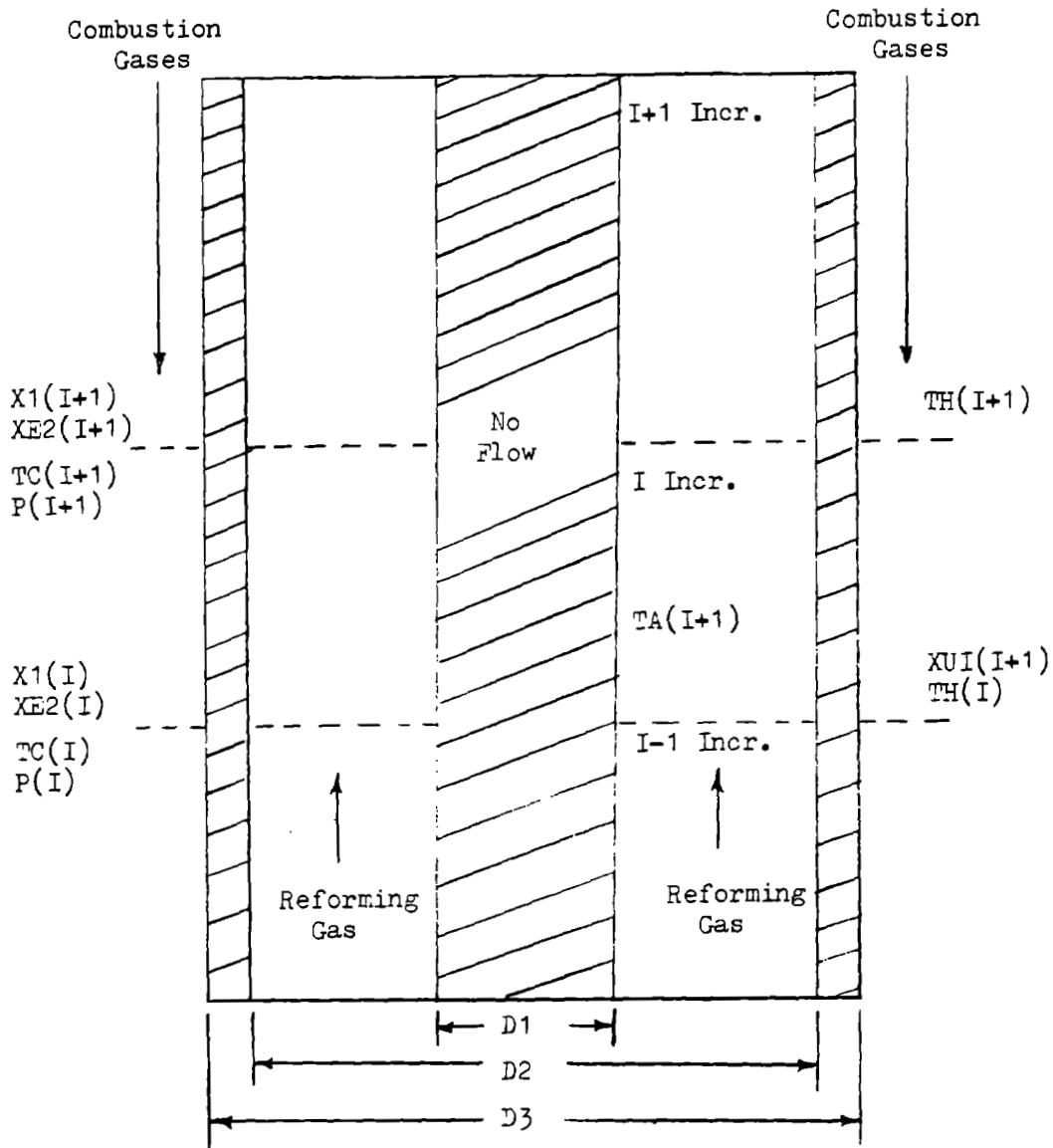


Figure 18 Single Tube Kinetic Reformer Model

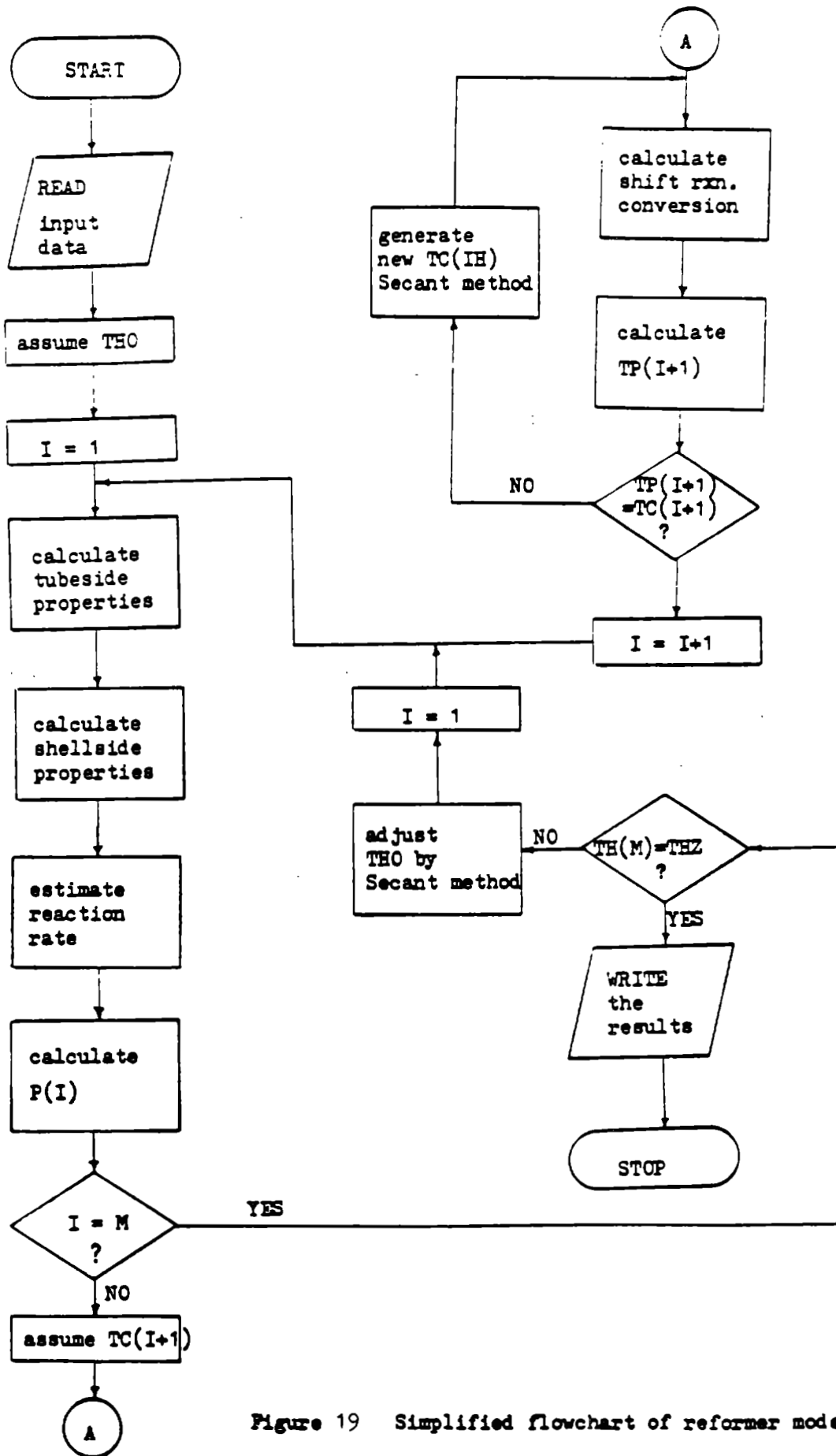


Figure 19 Simplified flowchart of reformer model

### 3.4 Program Operation

The program input only consists of a NAMELIST data deck which must be in a specified order. The first NAMELIST set is called OPFC and contains the three values of the operating conditions in the fuel cell stack. The order of input data inside one NAMELIST need not be fixed.

The second set (INIT) contains the 11 values of the amount of the input fuel and ambient temperature and pressure. The dimension orders in the variables for the properties of gas mixture are fixed, which are (1) methane, (2) oxygen, (3) carbon monoxide, (4) carbon dioxide, (5) hydrogen, (6) water, and (7) nitrogen.

The third set (CONDT) carries the information for the system operation, which includes the kind of input fuel, trial and error criterion, relative humidity, and extra percentage of needed air in the burner and the fuel cell stack.

The fourth set (REPEN) contains the information for the kinetic model of reformer. These are the dimensions of reformer and the catalyst kinetic data used in the reformer.

The fifth set (HEATX) contains the operating conditions for all the heat exchangers in the system and the transfer areas designed in the condenser and cooler.



The sixth, seventh, and eighth sets (HEPDC, PDSHH, and PDFUH) contain the dimensions of the heat exchanger, the shift converters, and the fuel cell stack, respectively. These data will be used to calculate the pressure drops in these three components.

The last NAMELIST set (CATAI) specifies the kinetic data of the catalyst used in the fuel cell stack.

TABLE 4

## INPUT DATA FOR SIMULATION OF CSU PAFC SYSTEM STEADY STATE PERFORMANCE

(SAMPLE RUN)

NAMLIST LIST	VARIABLE NAME	DIMENSION	SAMPLE VALUE	UNIT	DEFINITION
OPFC	TOPFC		443	K	Operating temperature in fuel cell stack
OPFC	UT		0.8		Utilization of H <sub>2</sub> in stack
OPFC	CD		325	mA/cm <sup>2</sup>	Designed current density
INIT	DNSM	1	1216.	g-mole/hr	Input mole flow rate of CH <sub>4</sub>
		2	0	g-mole/hr	Input mole flow rate of O <sub>2</sub>
		3	1.36	g-mole/hr	Input mole flow rate of CO
		4	21.8	g-mole/hr	Input mole flow rate of CO <sub>2</sub>
		5	166.	g-mole/hr	Input mole flow rate of H <sub>2</sub>
		6	0	g-mole/hr	Input mole flow rate of H <sub>2</sub> O
		7	0	g-mole/hr	Input mole flow rate of N <sub>2</sub>
INIT	TAT		298	K	Ambient temperature
INIT	PAT		1	atm	Ambient temperature
INIT	SMRA		3.0		Steam to carbon ratio
INIT	POPR		5.0	atm	Operating pressure of reformer
COND	IFUEL		1		= 1 Input fuel is methane
					= 2 Input fuel is methanol
					= 3 Input fuel is naphtha
COND	ERR		0.01		Criterion of convergence in system trial and error procedure

TABLE 4 (cont'd)

INPUT DATA FOR SIMULATION OF CSU PAFC SYSTEM STEADY STATE PERFORMANCE

(SAMPLE RUN)

NAMELIST LIST	VARIABLE NAME	DIMENSION	SAMPLE VALUE	UNIT	DEFINITION
CONDT	IP		2		= 1 adiabatic operation in shift converters = 2 isothermal operation in shift converters
CONDT	I		7		Number of components in whole system
CONDT	EXT		100		Extra percentage of needed air in burner
CONDT	WAT		0.015	g water/g air	Relative humidity of air
CONDT	EXA		100		Extra percentage of air in fuel cell stack
REPEN	ZH		6	ft	Height of reformer
REPEN	DX1		0	ft	Outside diameter of regenerative tube
REPEN	DX2		0.15	ft	Inside diameter of reforming tube
REPEN	DX3		0.1667	ft	Outside diameter of reforming tube
REPEN	KO		10400	lb-moleCH <sub>4</sub> / lb cata-hr-atm	Rate constant of demethanation reaction
REPEN	EA		20000	Cal/g-mole CH <sub>4</sub>	Activity energy of demethanation reaction
REPEN	RHOB		80	lb/ft <sup>3</sup>	Density of packing in reformer
REPEN	EPS		0.487		Void fraction in reformer
REPEN	S		0.25	ft	Width of combustion gas square duct
REPEN	DP		0.00328	ft	Diameter of catalyst in reformer
REPEN	DZZ		0.25	ft	Height of finite-difference section
HEATX	CN		1.3	m <sup>2</sup> -K	QxA/C min in heat exchanger

TABLE 4 (cont'd)

INPUT DATA FOR SIMULATION OF CSU PAFC SYSTEM STEADY STATE PERFORMANCE

(SAMPLE RUN)

NAMELIST LIST	VARIABLE NAME	DIMENSION	SAMPLE VALUE	UNIT	DEFINITION
HEATX	U		48825.1	cal/m <sup>2</sup> -hr-K	Overall heat transfer coefficient in heat exchanger
HEATX	HA	7	0.2	m <sup>2</sup>	Transfer area in E-7
		10	0.2	m <sup>2</sup>	Transfer area in E-10
HEPDC	NPH		2		Number of tube passes
HEPDC	NRH		5		Number of tube rows
HEPDC	BASPC		1	ft	Baffle space
HEPDC	ODTH		0.0625	ft	O.D. of tube
HEPDC	PITCH		0.0833	ft	Pitch of heat exchanger
HEPDC	CLH		0.0208	ft	Clearance in heat exchanger
HEPDC	IDSH		0.833	ft	I.D. of shell
HEPDC	IDTH		0.04667	ft	I.D. of tube
HEPDC	FLOAR		0.001716	ft	Flow area in heat exchanger
HEPDC	SURFC		0.1466	ft	Surface area per line
HEPDC	CLENH		2	ft	Length of tube
HEPDC	SITSZ		0.5		Ratio of total inside tube cross-sectional area per pass to header cross-sectional area per pass
HEPDC	DTH		0.7		Fraction of $\Delta T$ over inlet gas film in heat exchanger

TABLE 4 (cont'd)

INPUT DATA FOR SIMULATION OF CSU PAFC SYSTEM STEADY STATE PERFORMANCE

(SAMPLE RUN)

NAMELIST LIST	VARIABLE NAME	DIMENSION	SAMPLE VALUE	UNIT	DEFINITION
PDSHH	DPD	1	1.18	ft	Diameter of shift converters
PDSHH	AHRN	1	0.66		Void fraction in shift converters
PDSHH	APPD	1	69	ft <sup>2</sup>	Total surface area of packing
PDSHH	CLEPD	1	5.91	ft	Length of shift converters
PDSHH	NTPD	1	1		Number of tubes in shift converters
PDFUH	NTAF		140		Number of fuel flow channels in stack
PDFUH	FULE		1.42	ft	Length of fuel channel
PDFUH	WIDAF		0.00974	ft	Width of square fuel channel
PDFUH	NPFU		3365		Number of cell plates
PDFUH	NTAA		40		Number of process air flow channels
PDFUH	AIRL		1	ft	Length of air channel
PDFUH	WIDAA		0.00515	ft	Width of square process air channel
CATAI	SRO		0.44	$\Omega$ -cm	Cell resistance at 450° K
CATAI	SA		400	cm <sup>2</sup> /mg	Surface area of catalyst
CATAI	CU		0.15		Utilization of catalyst
CATAI	CL		0.75	mg/cm <sup>2</sup>	Catalyst loading
CATAI	ALFA		0.50		Transfer coefficient
CATAI	SN		2	g-equivalent	Number of Faraday equivalents transferred
CATAI	FCONST		96500	C/g-equivalent	Faraday constant
CATAI	DKC		240000	A/atm	Constant to calculate limiting current density

All of the input variables are listed in Table 4, along with their units and numerical values in the sample run, which will be discussed in the following section.

### 3.5 Sample Problem

The computer codes developed in previous sections were combined to simulate the PAFC system performance. The lumped model of each component was used to simulate the CSU design (Figure 1), except in the reformer where the distributed model was used for the methane input fuel.

This sample problem was to simulate the 110 kW AC PAFC system with methane input fuel. The input data, which is discussed in the previous section, is displayed in Figure 20. Figure 21 contains the output generated by the sample data input. First, the program reprints all of the input data. Next, the program prints out the operating conditions (temperature and pressure) of reformer, shift converters, and liquid separator. For the fuel cell stack, the printout will contain the operating temperature, operating pressure, open circuit potential, operating potential, current density, catalyst loading, fuel and oxident utilizations, the different kinds of efficiency, DC and AC electrical work, and heat released from the stack.

Next, the P-T-V (V as a flow rate) status of each stream numbered in Figure 1 will be listed on a new printout page. The last piece of information printed is the duty, transfer area, and efficiency of each heat exchanger numbered on flow diagram, and power spent in the air and fuel compressors and pump.

```
&OPFC TOPFC=443.,UT=0.8,CD=325.,
&END
&INIT DNSM=1216.,0.,1.360,21.8,166.,0.,0.,TAT=298.,PAT=1.,SMRA=3.,POPR=5.0
&END
&CONDT IFUEL=1,ERR=0.01,IP=2,I=7,EXT=100.,WAT=0.015,EXA=100.,
&END
&REPEN ZH=6.,DX1=0.,DX2=0.15,DX3=0.1667,K0=1.040E+04,EA=20000.,RHOB=80.
, EPS=0.487,S=0.25,DP=0.00328,DZZ=0.25,
&END
&HEATX CN=1.3,U=48825.1,HA(7)=0.2,HA(10)=0.2,
&END
&HEPDC NPH=2,NRH=5,BSPAC=1.,ODTH=.0625,PITCH=.0833,CLH=.0208,IDSH=.833,
IDTH=.04667,FLOAR=.001716,SURFC=.1466,CLENH=2.,SITS2=0.5,DTH=0.7,
&END
&PDSHH DPD=1.18,0.,AHRN=0.66,.0,APPD=69.,0.,CLEPD=5.91,0.,
NTPD=1,0,
&END
&PDFUH NTAF=140,FULE=1.42,WIDAF=.009744,NPFU=3365,
NTAA=40,AIRL=1.,WIDAA=.00515
&END
&CATAI SRO=.44,SA=400.,CU=.15,CL=.75,ALFA=.5,SN=2.,FCONST=96500.,
DKC=2.4E5,
&END
```

Figure 20 Sample Input Data

```

&OPFC
TOPFC= 443.0
UT= 0.80
CD= 325.0
&END
&INIT
DNMF= 1216.0, 0.0, 1.360, 21.79999, 166.0, 2*0.0
YAT= 298.0
PAT= 1.0
SMRA= 3.0
POPR= 5.0
&END
&CONDT
IFUEL= 1
ERR= 0.9999998E-02
IP= 2
I= 7
EXT= 100.0
WAT= 0.150E-01
EXA= 100.0
&END
&REPEN
ZH= 6.0
DX1= 0.0
DX2= 0.150
DX3= 0.1666999
KO= 10400.0
EA= 20000.0
RHOB= 80.0
EPS= 0.4870
S= 0.250
DP= 0.3280E-02
DZZ= 0.250
&END
&HEATX
CN= 1.299999
U= 48825.10
HA= 6*0.0, 0.20, 2*0.0, 0.20
&END
&HEPDC
NPH= 2
NRH= 5
BSPAC= 1.0
ODTH= 0.6250E-01
PITCH= 0.8329999E-01
CLH= 0.2080E-01
IDSH= 0.8329999
IDTH= 0.46670E-01
FLOOR= 0.17160E-02
SURFC= 0.1465999
CLENH= 2.0
SITS2= 0.50
DTH= 0.70
&END
&PDSHH
DPD= 1.179999, 0.0
AHRN= 0.660, 0.0
APPD= 69.0, 0.0
CLEPD= 5.910, 0.0

```

Figure 21 Sample Computer Run



NTPD= 1. 0  
&END  
&PDFUH  
NTAF= 140  
FULE= 1.419999  
WIDAF= 0.97440E-02  
NPFU= 3365  
NTAA= 40  
AIRL= 1.0  
WIDAA= 0.5149998E-02  
&END  
&CATAI  
SRO= 0.440  
SA= 400.0  
CU= 0.150  
CL= 0.750  
ALFA= 0.50  
SN= 2.0  
FCONST= 96500.0  
DKC= 240000.0  
&END

Figure 21 continued

THE STEAM/METHANE RATIO IN THE REFORMER IS 3.00

THE REFORMER IS OPERATING UNDER THESE CONDITIONS  
INLET PRESSURE 4.90ATM OUTLET PRESSURE 4.72ATM  
INLET TEMP. :1035.87 K OUTLET TEMP. : 920.63 K

THE HIGH TEMP. SHIFT CONVERTER IS OPERATING UNDER THESE CONDITIONS  
OPERATING TEMP.: 755.26 K  
OPERATING PRESSURE: 4.72ATM  
INLET TEMP.: 755.26 K  
OUTLET TEMP.: 755.26 K

THE LOW TEMP. SHIFT CONVERTER IS OPERATING UNDER THESE CONDITIONS  
OPERATING TEMP.: 399.68 K  
OPERATING PRESSURE: 4.72ATM  
INLET TEMP.: 399.68 K  
OUTLET TEMP.: 399.68 K

THE LIQUID SEPERATER IS OPERATING UNDER THESE CONDITIONS  
OPERATING TEMP.: 357.34 K  
OPERATING PRESSURE: 4.42ATM

THE FRACTION OF CO IN THE FEED IS 0.00029

THE FUEL CELL IS OPERATING UNDER THESE CONDITIONS  
THE OPERATING TEMPERATURE : 443.00K  
THE OPERATING PRESSURE: 4.79ATM  
THE OPEN CIRCUIT POTENTIAL: 1.171 V  
THE OPERATING POTENTIAL: 0.658 V  
THE CURRENT DENSITY: 0.325A/CM\*\*2  
THE CATALYST LOADING: 0.750PT/CM\*\*2  
THE FUEL UTILIZATION:0.800  
THE OXYGEN UTILIZATION:0.500  
THE ANODE SIDE INLET TEMP. IS 399.68 K  
THE CATHODE SIDE INLET TEMP. IS 386.41 K  
THE THERMODYNAMIC EFFICIENCY OF FUEL CELL IS 0.92847E 00THE CURRENT EFFICIENCY IS 0.80000E 00  
THE VOLTAGE EFFICIENCY IS 0.56251E 00THE HEATING VALUE EFFICIENCY IS 0.90470E 00  
THE FUEL CELL EFFICIENCY IS0.3780  
THE ELECTRICAL WORK IS 0.12601E 03KW  
THE TOTAL HEAT RELEASE IS 0.53266E 08CAL

THE AC OUTPUT IS 113.77KW

Figure 21 continued

STREAM	METHANE	OXYGEN	CAR. MONOXIDE	CAR. DIOXIDE	HYDROGEN	WATER	NITROGEN	FLOW RATE	TEMP. (K)	PRE. (ATM)
1	1216.00	0.00	1.36	21.80	166.00	0.00	0.00	1405.16	298.00	5.1000
2	1216.00	0.00	1.36	21.80	166.00	0.00	0.00	1405.16	612.96	5.0996
3	1216.00	0.00	1.36	21.80	166.00	3648.00	0.00	5053.16	588.38	4.8983
4	1216.00	0.00	1.36	21.80	166.00	3648.00	0.00	5053.16	784.59	4.8975
5	1216.00	0.00	1.36	21.80	166.00	3648.00	0.00	5053.16	1035.87	4.8965
7	141.97	0.00	531.09	566.10	3932.37	2029.68	0.00	7201.20	920.63	4.7243
8	141.97	0.00	531.09	566.10	3932.37	2029.68	0.00	7201.20	755.26	4.7242
9	141.97	0.00	312.87	784.31	4150.58	1811.46	0.00	7201.20	755.26	4.7242
10	141.97	0.00	312.87	784.31	4150.58	1811.46	0.00	7201.20	678.77	4.7241
11	141.97	0.00	312.87	784.31	4150.58	1811.46	0.00	7201.20	591.03	4.7240
12	141.97	0.00	312.87	784.31	4150.58	1811.46	0.00	7201.20	399.68	4.7239
13	141.97	0.00	2.09	1095.10	4461.37	1500.68	0.00	7201.20	399.68	4.7245
14	141.97	0.00	2.11	1095.06	892.25	1500.74	0.00	3632.13	443.00	4.7245
15	141.97	1462.25	2.11	1095.06	892.25	1667.78	5498.04	10759.47	353.52	4.7195
16	141.97	1462.25	2.11	1095.06	892.25	1667.78	5498.04	10759.47	744.09	4.7181
17	0.00	731.12	0.00	1239.15	0.00	2843.97	5498.04	10312.29	1575.99	4.4192
18	0.00	731.12	0.00	1239.15	0.00	2843.97	5498.04	10312.28	1182.31	4.1983
19	0.00	731.12	0.00	1239.15	0.00	2843.97	5498.04	10312.29	1033.81	4.1975
20	0.00	731.12	0.00	1239.15	0.00	2843.97	5498.04	10312.29	664.94	4.1970
21	0.00	2515.63	0.00	1239.15	0.00	6820.70	18917.51	29492.99	525.95	4.4154
22	0.00	2515.63	0.00	1239.15	0.00	6820.70	18917.51	29492.99	357.34	4.4198
23	0.00	2515.63	0.00	1239.15	0.00	3172.68	18917.51	25844.97	357.34	4.4198
24	0.00	0.00	0.00	0.00	0.00	3648.00	0.00	3648.00	357.34	5.0025
25	0.00	0.00	0.00	0.00	0.00	3648.00	0.00	3648.00	357.34	5.0025
26	0.00	0.00	0.00	0.00	0.00	3648.00	0.00	3648.00	421.65	5.0025
27	0.00	0.00	0.00	0.00	0.00	3648.00	0.00	3648.00	586.60	5.0018
28	0.00	5031.25	0.00	0.00	0.00	574.77	18917.50	24523.52	298.00	1.0000
29	0.00	5031.25	0.00	0.00	0.00	574.77	18917.50	24523.52	298.00	4.8139
30	0.00	3569.01	0.00	0.00	0.00	407.72	13419.46	17396.19	298.00	4.8139
31	0.00	3569.01	0.00	0.00	0.00	407.72	13419.46	17396.19	386.41	4.7900
32	0.00	1784.50	0.00	0.00	0.00	3976.73	13419.47	19180.70	443.00	4.7899
33	0.00	1462.25	0.00	0.00	0.00	167.05	5498.04	7127.34	298.00	4.8139
34	0.00	0.00	0.00	0.00	0.00	134510.94	0.00	134510.94	333.00	1.0000
35	0.00	0.00	0.00	0.00	0.00	134510.94	0.00	134510.94	355.00	1.0000
36	0.00	0.00	0.00	0.00	0.00	106332.44	0.00	106332.44	298.00	1.0000
37	0.00	0.00	0.00	0.00	0.00	106332.44	0.00	106332.44	355.00	1.0000

Figure 21 continued

THE DUTY OF HEAT EXCHANGER (CAL.) (0 MEANS NO THIS NO. HEAT EXCHANGER)										E-8	E-9	E-10
E-1	E-2	E-3	E-4	E-5	E-6	E-7						
0.45316E 07	0.99787E 07	0.14123E 08	0.33156E 08	0.10910E 09	0.10777E 08	0.53266E 08				0.00000	0.51060E 07	0.37070E 08
THE SURFACE AREA OF HEAT EXCHANGER (M**2) (0 MEANS NO THIS NO. HEAT EXCHANGER)										E-8	E-9	E-10
E-1	E-2	E-3	E-4	E-5	E-6	E-7						
0.38308E 00	0.13541E 01	0.14964E 01	0.22603E 01	0.21182E 02	0.14996E 01	0.20000E 00				0.00000	0.82420E 00	0.20000E 00
THE EFFICIENCY OF HEAT EXCHANGER (0 MEANS NO THIS NO. HEAT EXCHANGER OR IS CONDENSER)										E-8	E-9	E-10
E-1	E-2	E-3	E-4	E-5	E-6	E-7						
0.68881E 00	0.59056E 00	0.63181E 00	0.57412E 00	0.00000	0.65302E 00	0.00000				0.00000	0.64153E 00	0.00000
THE POWER OF AIR COMPRESSOR: 64.04HP												
THE POWER OF METHANE COMPRESSOR: 3.80HP												
THE POWER OF PUMP : 0.00146HP												

Figure 21 continued

### 3.6 Discussion

There has been much interest in the effect of alternate commercial fuels on the performance and costs of PAFC power plant. The computer program developed can allow for methanol or naphtha as input fuel. The system with methanol input fuel obtains the highest efficiency among the three fuels, where 40-45 percent of the PAFC stack compared to 35-40 percent of methane input fuel. More detailed discussion on this topic is presented in Ref. 14.

Since there are a lot of trial-and-error procedures in the program, the infeasible initial guesses will cause the calculations looping or overflowing.

For the naphtha input fuel, because of computation problem (overflow) in the subroutine SNAE, the conversion will be assumed in the reformer. The problem will be amended as required.

### 3.7 Further Developments

This PAFC system steady state simulation program can be modified to allow different flow diagram. For example, it has been used to simulate the Westinghouse 7.5 MW PAFC power plant (Ref. 13), and the results were shown in Ref. 11.

Further developments have been completed, which include 3-D temperature and current density distributions (distributed model) of fuel cell stack (Refs. 11, 15), kinetic model for regenerated-type reformer, distributed simulation of PAFC system steady state performance (Ref. 11), and the simulation of PAFC power plant system transient responses in the load changing period (Ref. 11).

REFERENCES

1. Kays, W.M. and London, A.L., "Compact Heat Exchangers", McGraw-Hill, New York, 1958.
2. Perry, J.H. (ed.), "Chemical Engineers' Handbook", 4th Ed., McGraw-Hill Book Company, New York, 1981.
3. Murray, A.P. and Snyder, T.S., "REPENT-Methane Reformer Kinetic Computer Model", Rept. of Westinghouse Corp. to NASA LeRC, DOE Contract DE-AC03-78ET11300, February 5, 1980.
4. Hyman, M.H., "Simulate Methane Reformer Reactions", Hydrocarbon Processing Vol. 47, No. 7, p. 131-137, July 1968.
5. Allen, D.W., Gerhard, E.R., and Likins, M.R., Jr., "Kinetics of the Methane-Steam Reaction", Ind. Eng. Chem., Process Des. Dev., Vol. 14, No. 3, p. 256-259, 1975.
6. Chao, R.E., Caban, R.A., and Irizarry, M.M., "Wall Heat Transfer to Chemical Reactors", Can. Chem. Eng., Vol. 51, p. 67, 1973.
7. Beek, J., "Design of Packed Catalytic Reactors", Adv. Chem. Eng., Vol. 3, p. 303, 1962.
8. Thoenes, D., Jr., and Kramers, H., "Mass Transfer from Spheres in Various Regular Packing to a Flowing Fluid", Chem. Eng. Sci., Vol. 8, p. 271, 1958.
9. Hoover, D.Q., "Cell and Stack Design Alternatives", First Qtly. Rept. of Westinghouse Corp. to NASA LeRC, Contract ET-78-C03-2031, January 1979.
10. Benjamin, T.G., Elias, H.C., and Marianowski, L.G., "Handbook of Fuel Cell Performance", Institute of Gas Technology, DOE Contract EC-77-C03-1545, Chicago, May 1980.
11. Lu, C.Y., "Transient Responses of Phosphoric Acid Fuel Cell Power Plant System", Ph.D. Dissertation, Cleveland State University, December 1983.
12. Franks, R.G.E., "Modeling and Simulation in Chemical Engineering", John Wiley & Sons, New York, p. 366, 1971.
13. Le, M.T., "A 75 MW Phosphoric Acid Fuel Cell System Concept with a Natural Gas Fueled Non-Integrated Fuel Processing Subsystem", DRM: 129, Westinghouse Electric Corp., March 23, 1982.
14. Alkasab, K.A., Presler, A.F., and Lu, C.Y., "Thermodynamic and Performance Model for Phosphoric Acid Fuel Cell System", Proceedings of Sixth IASTED International Symposium on ENERGY '83, San Francisco, May 16-18, 1983.
15. Alkasab, K.A., and Lu, C.Y., "Transient Effect of Changing the Electrical Load on the Performance of Phosphoric-Acid Fuel-Cell Power Plant", Proceedings of Eighth IASTED International Symposium on ENERGY '83, Orlando, November 9-11, 1983.

## Listing of the Steady State Performance Lumped Model

```

0000020C   BLOCK DATA
0000040CC
0000060 C*****BLOCK DATA FOR CSU PROGM FUEL CELL POWER PLANT PERFORMANCE
0000100C   DIMENSION GS(7),HS(7),HCAS(7),HCBS(7),HCCS(7),WM(7),SV(3),
0000120C   IHLHV(7),A1(2,7),A2(2,7),A3(4,7)
0000140C   COMMON /ETHDA/ GS,HS,HCAS,HCBS,HCCS
0000160C   COMMON /TC/ TC/CONS/ A,B
0000180C   COMMON /GAG/ GAG1,GAGA
0000200C   COMMON /NAPH/HNA,BPNA,WMNA,VHNA
0000220C   COMMON /WM/ WM
0000240C   COMMON/SV/ SV,SVW
0000260C   COMMON/HLHV1/ HLHV
0000280C   COMMON/THCC/A1/VIFC/A2/HTCPC/A3
0000300CC
0000320CC STANDARD VALUE OF FREE ENERGY, ENTHALPHY AND HEAT CAPACITY CONSTANT
0000340C   DATA GS/-12140.,0.,-32781.,-94259.,0.,-54635.,0./
0000360C   DATA HS/-17889.,0.,-26416.,-94051.,0.,-57798.,0./
0000380C   DATA HCAS/3.381,6.148,6.42,6.214,6.947,7.256,6.524/
0000400C   DATA HCBS/.018044,.003102,.001665,.010396,-.0002,.002298,.00125/
0000420C   DATA HCCS/-4.3E-06,-9.23E-07,-1.96E-07,-3.545E-06,4.81E-07,2.83E-07,1.E-09/
0000440CC THE MOL. WEIGHT OF GASES
0000460C   DATA WM/16.,32.,28.,40.,2.,18.,28./
0000480CC THE THERMAL DATA OF NAPHTHA
0000500C   DATA HNA/0.58/,BPNA/103.4/,VHNA/7680./
0000520CC THE CONST. FOR CAL. SATURATED PRESSURE (EXP(A-B/T))
0000540C   DATA A,B/13.954316,5204.9597/
0000560CC CRITICAL TEMPERATURE OF WATER
0000580C   DATA TC/646.447/
0000600CC INSERT RATIO OF HEAT CAPACITY
0000620C   DATA GAGM/1.3/,GAGA/1.4/
0000640CC INSERT THE SPECIFIC VOLUME OF FUEL AND WATER
0000660C   DATA SV/0.,.02034,.021/,SVW/.0162/
0000680CC INSERT THE HEATING VALUE
0000700C   DATA HLHV/-191762.,0.,-67636.,0.,-57798.,0.,0./
0000720CC INSERT THE SPECIFIC HEAT CAPACITIES, BTU/R-LB-MOLE
0000740C   DATA A3/5.34,6.39E-03,0.,0.,6.60,6.67E-04,0.,0.,10.34,1.52E-03,0.,
0000760C   1-6.33420E+05,8.22, 8.3E-05,4.136E-07,0.,6.62,4.5E-04,0.,0.,6.5,
0000780C   25.56E-04,0.,0.,6.732,8.36E-03,5.53E-09,0./
0000800CC INSERT VISCOSITY, LBM/FT-HR
0000820C   DATA A2/3.4373E-05,2.5861E-02,3.8185E-05,4.8688E-02,5.0368E-05,
0000840C   13.3634E-02,5.221E-05,1.7532E-02,1.8789E-05,2.312E-02,4.2318E-05,
0000860C   24.6721E-02,2.4580E-05,5.5613E-02/
0000880CC INSERT THERMAL CONDUCTIVITY, BTU/HR-FT-F
0000900C   DATA A1/6.6539E-05,7.4614E-03,1.5349E-05,1.6581E-02,2.0451E-05,
0000920C   11.1726E-02,4.046E-05,1.8785E-03,1.1899E-04,1.0126E-01,1.6774E-05,
0000940C   21.5182E-02,1.792E-05,1.67E-02/
0000960C   END
0000980 C
0001000 C   *****
0001020 C   THIS PROGRAM IS USING FORTRAN TO SIMULATE THE PHOSPHORIC ACID FUEL
0001040 C   CELL SYSTEM
0001060 C   *****
0001080 C
0001100 C   DEFINITION:

```

0001120 C A : CONSTANT FOR CAL. SATURATED CONDITION OF WATER  
 0001140 C AA1: THERMAL CONDUCTIVITY COEFF. OF GAS I, BTU/HR-FT-F  
 0001160 C AA2: VISCOSITY COEFF. OF GAS I, LBM/FT-HR  
 0001180 C AA3: SPECIFIC HEAT CAPACITY COEFF. OF GAS I, BTU/R-LB-MOLE  
 0001200 C OF THE FORM:AA3(1)+AA3(2)\*T+AA3(3)\*T\*\*2+AA3(4)/T\*\*2  
 0001220 C AHLU: MOLE FRACTION OF AVAILABLE HYDROGEN  
 0001240 C AHRN: PERCENT FREE-GAS SPACE  
 0001260 C AIRL: LENGTH OF AIR CHANNEL, FT  
 0001280 C ALFA: TRANSFER COEFF.  
 0001300 C APPD: TOTAL SURFACE AREA OF PACKING ACC. TO THE BASIS AND OPER.  
 0001320 C TEMPERATURE, FT\*\*2  
 0001340 C ATMP: OUTLET TEMP. OF GASES, K  
 0001360 C B : CONSTANT FOR CAL. SATURATED CONDITION OF WATER  
 0001380 C BPNA: BOILING POINT OF NAPHTHA, C  
 0001400 C BSPAC: BAFFLE SPACE, FT  
 0001420 C CD: CURRENT DENSITY,MAMP/CM\*\*2  
 0001440 C CL: CATALYST LOADING,MS/CM\*\*2  
 0001460 C CLENH: LENGTH OF TUBE IN HEAT EXCHANGER, FT  
 0001480 C CLEPD: LENGTH OF SHIFT CONVERTER(JK=1),REFORMER(JK=2 FOR METHANOL  
 0001500 C NAPHTHA), FT  
 0001520 C CLH: CLEARANCE IN HEAT EXCHANGER, FT  
 0001540 C CN: Q\*A/CHIN IN HEAT EXCHANGER  
 0001560 C CU: CATALYST UTILIZATION  
 0001580 C DG: STANDARD FREE ENERGY CHANGE,CAL/G-MOLE  
 0001600 C DH: STANDARD ENTHALPHY CHANGE AT REACTION,CAL/G-MOLE  
 0001620 C DHIN: ENTHALPHY CHANGE DUE TO TEMPERATURE CHANGE OF INLET FLUID  
 0001640 C CAL./G-MOLE  
 0001660 C DKC: CONST. TO CALC. LIMITING CURRENT DENSITY  
 0001680 C DHO: INTEGRATION CONSTANT IN CALCULATE H  
 0001700 C DP: CATALYST PELLET DIAMETER, FT  
 0001720 C DPD: DIA. OF SHIFT CONVERTER(JK=1),REFORMER(JK=2 FOR METHANOL AND  
 0001740 C NAPHTHA), FT  
 0001760 C DSHO: CATHODE INLET WATER OF FUEL CELL, G-MOLE/HR.  
 0001780 C DSN: CATHODE INLET NITROGEN OF FUEL CELL, G-MOLE/HR.  
 0001800 C DSO: CATHODE INLET OXYGEN OF FUEL CELL, G-MOLE/HR.  
 0001820 C DTH: FRACTION OF DELTA T OVER INLET GAS FILM IN THE HEAT EXCHANGER  
 0001840 C DX1: OUTSIDE DIAMETER OF REFORMER CENTER TUBE, FT  
 0001860 C DX2: INSIDE DIAMETER OF OUTSIDE REFORMER TUBE, FT  
 0001880 C DX3: OUTSIDE DIAMETER OF OUTSIDE REFORMER TUBE, FT  
 0001900 C DZZ: INCREMENT HEIGHT OF FINITE DIFFERENCE MODEL IN THE REFORMER,  
 0001920 C EA: ACTIVATION ENERGY FOR ARRHENIUS EXPRESSION, CAL/GMOLE CH4  
 0001940 C EPS: REACTOR VOID FRACTION  
 0001960 C ERR: CONVERGE CRITERIA  
 0001980 C EXA: FRACTION OF EXTRA AIR IN FUEL CELL  
 0002000 C EXT: FRACTION OF EXTRA AIR IN BURKER  
 0002020 C FCO: MOLE FRACTION OF CO CONTAIN  
 0002040 C FCCNST: FARADAY CONSTANT,23061 CAL/VOLT-GM EQUIV.  
 0002060 C FLOOR: FLOW AREA IN HEAT EXCHANGER, FT\*\*2  
 0002080 C FULE: LENGTH OF FUEL CHANNEL, FT  
 0002100 C HNA: SPECIFIC HEAT OF NAPHTHA, BTU/LBM-R  
 0002120 C I : GAS NUMBER  
 0002140 C I=1 FUEL(METHANE,METHANOL,NAPHTHA)  
 0002160 C I=2 OXYGEN OR CARBON MONOXIDE(IN SUB. KREF AND  
 0002180 C RELATED SUBROUTINES)



0002200 C I=3 CARBON MONOXIDE OR CARBON DIOXIDE( " )  
 0002220 C I=4 CARBON DIOXIDE OR WATER( " )  
 0002240 C I=5 HYDROGEN  
 0002260 C I=6 WATER OR NITROGEN( " )  
 0002280 C I=7 NITROGEN OR OXYGEN( " )  
 0002300 C IDSH: ID OF SHELL IN HEAT EXCHANGER, FT  
 0002320 C IDTH: ID OF TUBE IN HEAT EXCHANGER, FT  
 0002340 C IFUEL: FUEL TYPE  
 0002360 C 1: METHANE CH<sub>4</sub>  
 0002380 C 2: METHANOL CH<sub>3</sub>OH  
 0002400 C 3: NAPHTHA C<sub>7</sub>H<sub>16</sub>  
 0002420 C IDNO: NO. OF REDO  
 0002440 C IHUI: STOICHIOMETRIC NUMBER  
 0002460 C IP: INDEX OF OPERATION CONDITION IN THE REFORMER(NOT FOR METHANE)  
 0002480 C SHIFT CONVERTOR  
 0002500 C IP=1 ADIABATIC OPERATION  
 0002520 C IP=2 ISOTHERMAL OPERATION  
 0002540 C KO: FREQUENCY FACTOR FOR ARRHENIUS EXPRESSION, LB MOLE CH<sub>4</sub>/LB  
 0002560 C CATA.-HR-ATM  
 0002580 C NN: STREAM NU-MBER OF EXIT OF SHIFT CONVERTER  
 0002600 C NCR: SCALE UP FACTOR IN THE MODEL OF REFORMER  
 0002620 C NPFU: NO. OF CELL PLATE IN THE FUEL CELL STACK  
 0002640 C NPH: NO. OF TUBE PASSES  
 0002660 C NRH: NO. OF ROWS FOR TUBES  
 0002680 C NTAA: NO. OF AIR FLOW CHANNEL IN ONE CELL PLATE  
 0002700 C NTAF: NO. OF FUEL FLOW CHANNEL IN ONE CELL PLATE  
 0002720 C NTPD: NO. OF TUBES IN SHIFT CONVERTER(JK=1),REFORMER(JK=2 FOR  
 0002740 C METHANOL AND NAPHTHA)  
 0002760 C OOTH: OD OF TUBE, FT  
 0002780 C CU: O<sub>2</sub> UTILIZATION  
 0002800 C PAT: AMBIENT PRESSURE, 1ATM  
 0002820 C PIN: INLET PRESSURE, ATM  
 0002840 C PINFU: INLET PRESSURE OF FUEL CELL STACK, ATM  
 0002860 C PITCH: PITCH OF HEAT EXCHANGER, FT  
 0002880 C POP: OPERATION PRESSURE, ATM  
 0002900 C POUT: OUTLET PRESSURE, ATM  
 0002920 C RHOB: BULK DENSITY OF CATA., LBS/FT\*\*3  
 0002940 C S: SIDE LENGTH OF AN ASSUMED SQUARE FLOW DUCT FOR COMBUSTION GAS,  
 0002960 C SITS2: RATIO OF TOTAL INSIDE-TUBE CROSS-SECTIONAL AREA PER PASS TO  
 0002980 C HEADER CROSS-SECTIONAL AREA PER PASS  
 0003000 C SA: CATALYST SURFACE,CM\*\*2/MG  
 0003020 C SK: EQUALIBRIUM CONSTANT  
 0003040 C SK1: EQUALIBRIUM CONSTANT WITH PRESSURE DIFFERENT FROM 1 ATM  
 0003060 C SMRA: STEAM/FUEL  
 0003080 C SN: NUMBER OF FARADAY EQUIVALENTS TRANSFERED  
 0003100 C SRO: CELL RESISTANCE AT 480 K,OHM-CM\*\*2  
 0003120 C SURFC: SURFACE PER LINE, FT  
 0003140 C SV(I): SPECIFIC VOLUME OF FUEL I, FT\*\*3/LBM  
 0003160 C SVW: SPECIFIC VOLUME OF WATER, FT\*\*3/LEM  
 0003180 C TAOA: INLET AIR TEMP. OF FUEL CELL STACK, K  
 0003200 C TACOF: INLET FUEL TEMP. OF FUEL CELL STACK, K  
 0003220 C TAT: AMBIENT TEMPERATURE, 298 K  
 0003240 C TC: CRITICAL TEMPERATURE, K  
 0003260 C TCAS: TOTAL HEAT CAPACITY CONSTANT A

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0003290 C      TCBS: TOTAL HEAT CAPACITY CONSTANT B
0003300 C      TCCS: TOTAL HEAT CAPACITY CONSTANT C
0003320 C      TDNS: TOTAL AMOUNT OF MATERIAL, G-MOLE
0003340 C      TIN: INLET FLUID TEMPERATURE, K
0003350 C      TOP: OPERATION TEMPERATURE, K
0003380 C      TOVO: TOTAL VOLUME OF INLET FLOW, M**3
0003400 C      TOUT: OUTLET TEMPERATURE, K
0003420 C      VHNA: VAPORIZED HEAT OF NAFHTHA, CAL/G-MOLE
0003440 C      WAT: RELATIVE HUMIDITY OF AIR, G WATER/G AIR
0003460 C      WIDAA: WIDTH OF SQUARE AIR CHANNEL IN THE FUEL CELL STACK, FT
0003480 C      WIDAF: WIDTH OF SQUARE FUEL CHANNEL IN THE FUEL CELL STACK, FT
0003500 C      X : THE NECESSARY AMOUNT OF OXYGEN IN CATHODE, G-MOLE/HR.
0003520 C      ZH: REFORMER LENGTH, FT
0003540 C      DINS(I): INLET AMOUNT OF GAS I, G-MOLE
0003560 C      DNS(I): INLET (OUTLET) AMOUNT OF GAS I, G-MOLE
0003580 C      HA(J): SURFACE AREA OF HEAT EXCHANGER J
0003600 C      HCAS(I),HCBS(I),HCCS(I): HEAT CAPACITY CONST. OF GAS I, CAL/G-MOLE
0003620 C      OF THE FORM:HCAS+HCBS*T+HCCS*T**2
0003640 C      HS(I): HEAT OF FORMATION OF GAS I AT 298 K, IATM
0003660 C      NNS(I): STOICHIOMETRIC COEFFICIENT OF GAS I
0003680 C      WMI(I): MOLECULAR WEIGHT OF GAS I, G/G-MOLE
0003700 C      DNSS(I,J): FLOW RATE OF GASJ IN STREAM I, G-MOLES/HR
0003720 C
0003740      REAL K0,IDSH,IDTH
0003760      DIMENSION GS(7), HS(7), HCAS(7), HCBS(7), HCCS(7), WM(7)
0003780      DIMENSION DNSL(7), DNSV(7), HLHV(7)
0003800      DIMENSION DNSS(39,7), T(39), P(39), TDNSS(39)
0003820      DIMENSION DNS1(7), DNS2(7), DNS(7), DNSH(7), DNSAN(7), DNSCA(7), D-
0003840      INSAI(7), DNSC(7), DNSH(7)
0003860      DIMENSION QQT(10), HA(10), EFF(10), NT(10)
0003880      DIMENSION DNSR(7), DNSF(7)
0003900      DIMENSION DPD(2), AHRN(2), APPD(2), CLEPD(2), NTPD(2), SV(3)
0003920      DIMENSION AA1(2,7), AA2(2,7), AA3(4,7)
0003940      NAMELIST /REPEN/ ZH,DX1,DX2,DX3,K0,EA,RHOB,EPS,S,DP,DZZ
0003960      NAMELIST /HEATX/ CN,U,HA
0003980      NAMELIST /OPFC/ TOPFC,UT,CD
0004000      NAMELIST /INIT/ DNSM,TAT,PAT,SMRA,POPR
0004020      NAMELIST /COND/ IFUEL,ERR,IP,I,EXT,WAT,EXA
0004040      NAMELIST /HEPDC/ NPH,NRH,BSPAC,ODTH,PITCH,CLH,IDSH,IDTH,FLOAR,SURF-
0004060      IC,CLENH,SITS2,DTH
0004080      NAMELIST /POSHH/ DPD,AHRN,APPD,CLEPD,NTPD
0004100      NAMELIST /PDFUH/ NTAF,FULE,WIDAF,NPFU,NTAA,AIRL,WIDAA
0004120      NAMELIST /TR/ TOPR
0004140      NAMELIST /CATAI/ SRO,SA,CU,CL,ALFA,SN,FCONST,DKC
0004160 C
0004180      COMMON /TC/ TC/CONS/A,B/GAG/GAGM,GAGA
0004200      COMMON /CONST/ I
0004220      COMMON /EXA/ EXA
0004240      COMMON /ETHDA/ GS,HS,HCAS,HCBS,HCCS
0004260      COMMON /HUMI/ WAT
0004280      COMMON /EXT/ EXT
0004300      COMMON /UI/ U
0004320      COMMON /CONFC/ E,ETH,EI,EV,EC,EFC
0004340      COMMON /HE/ HE

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0004360 COMMON /CN1/ CN
0004380 COMMON /NAPH/ HNA,BPNA,WMNA,VHNA
0004400 COMMON /WM/ WM
0004420 COMMON /HEPDT/ NPH,NRH,BSPAC,ODTH,PITCH,CLH,IDSH,IDTH,FLOAR,SURFC,-
0004440 1CLENH,SLTS2,DTH
0004460 COMMON /PDSHT/ DPD,AHRN,APPD,CLEPD,NTPD
0004480 COMMON /PJFUT/ NTAF,NTAA,FULE,AIRL,WIDAF,WIDAA,NPFU
0004500 COMMON /REP/ K0,EA,RHOB,EPS,DZZ
0004520 COMMON /SV/ SV,SVH
0004540 COMMON /HLHV1/ HLHV
0004560 COMMON /THCC/ AA1/VIPC/AA2/HTCPC/AA3
0004580 COMMON /CATAL/ SRO,SA,CU,CL,ALFA,SN,FCONST,AREAF,DKC
0004600 C
0004620 DATA DNSS/273*0./
0004640 C READ THE OPERATION CONDITION OF FUEL CELL
0004660 READ (5,OPFC)
0004680 WRITE (6,OPFC)
0004700 C READ THE INLET AMOUNT AND CONDITION
0004720 READ (5,INIT)
0004740 WRITE (6,INIT)
0004760 C READ OPERATION CONDITION
0004780 READ (5,CONDT)
0004800 WRITE (6,CONDT)
0004820 C READ OPERATING COEFFICIENT IN THE REFORMER(METHANE FUEL ONLY)
0004840 IF (IFUEL.EQ.1) READ (5,REPEN)
0004860 IF (IFUEL.EQ.1) WRITE (6,REPEN)
0004880 C READ CONDITION OF HEAT EXCHANGER
0004900 READ (5,HEATX)
0004920 WRITE (6,HEATX)
0004940 C READ THE CONSTRUCTION OF HEAT EXCHANGER FOR CAL. PRESSURE DROP
0004960 READ (5,HEFDC)
0004980 WRITE (6,HEFDC)
0005000 C READ CONFIGURATION COEFF. OF SHIFT CONVERTER FOR CAL. PRESSURE DRO
0005020 READ (5,PDSHH)
0005040 WRITE (6,PDSHH)
0005060 C READ CONFIGURATION COEFF. OF FUEL CELL FOR CAL. PRESSURE DROP
0005080 READ (5,PDFUH)
0005100 WRITE (6,PDFUH)
0005120 C READ THE OPERATING TEMP. OF REFORMER FOR FUEL NAPHTHA AND METHANOL
0005140 IF (IFUEL.NE.1) READ (5,TR)
0005160 IF (IFUEL.NE.1) WRITE (6,TR)
0005180 C READ CATALYST CONSTANTS
0005200 READ (5,CATAI)
0005220 WRITE(6,CATAI)
0005240 C
0005260 C
0005280 C CHANGE THE THERMAL DATA FOR DIFFERENT FUEL INPUT
0005300 IF (IFUEL.EQ.2) GO TO 1
0005320 IF (IFUEL.EQ.3) GO TO 2
0005340 GO TO 3
0005360 1 GS(1)=-38810.
0005380 HS(1)=-48050.
0005400 HCAS(1)=4.394
0005420 HCBS(1)=0.024274

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0005440      HCCS(1)=-0.0000069
0005460      WM(1)=32.
0005480      HLHV(1)=-159258.
0005500      AA3(1,1)=4.394
0005520      AA3(2,1)=0.013486
0005540      AA3(3,1)=-2.1157E-06
0005560      AA3(4,1)=0.
0005580      AA1(1,1)=3.E-05
0005600      AA1(2,1)=1.5E-02
0005620      AA2(1,1)=1.8E-05
0005640      AA2(2,1)=0.0092
0005660      GO TO 3
0005680      2 GS(1)=6520.
0005700      HS(1)=-42275.
0005720      HCAS(1)=7.094
0005740      HCBS(1)=0.123447
0005760      HCCS(1)=-0.0000387
0005780      WM(1)=100.
0005800      HLHV(1)=-1099580.
0005820      AA3(1,1)=7.488
0005840      AA3(2,1)=0.062467
0005860      AA3(3,1)=-1.0945E-05
0005880      AA3(4,1)=0.
0005900      AA2(1,1)=2.66E-05
0005920      AA2(2,1)=0.0157
0005940      AA1(1,1)=2.5E-05
0005960      AA1(2,1)=0.7E-02
0005980      3 CONTINUE
0006000      IDNO=1
0006020 C      FUEL INPUT COMPRESSOR(PUMP)***
0006040      P(1)=POPR*1.02
0006060      IF (IFUEL.EQ.1) CALL COMP (DNSM,TAT,TOUT,PAT,P(1),POWM,GAGM,I,IP)
0006080      IF (IFUEL.NE.1) CALL PUP (DNSM,TAT,TOUT,PAT,P(1),POWN,I,IFUEL)
0006100      DO 301 IA=1,I
0006120 301      DNSS(1,IA)=DNSM(IA)
0006140      T(1)=TOUT
0006160 C      ASSUME THE COMP. OF 13TH FLOW
0006180      DNSS(13,2)=0.
0006200      DNSS(13,7)=0.
0006220      IF (IFUEL.EQ.2) GO TO 4
0006240      IF (IFUEL.EQ.3) GO TO 5
0006260      DNSS(13,1)=0.147*DNSS(1,1)
0006280      DNSS(13,3)=0.0018*DNSS(1,1)+DNSS(1,3)
0006300      DNSS(13,4)=0.85*DNSS(1,1)+DNSS(1,4)
0006320      DNSS(13,5)=3.4*DNSS(1,1)+DNSS(1,5)
0006340      DNSS(13,6)=SMRA*DNSS(1,1)-1.7*DNSS(1,1)
0006360      GO TO 6
0006380      4 DNSS(13,1)=0.000863487*DNSS(1,1)
0006400      DNSS(13,3)=0.01
0006420      DNSS(13,4)=0.999128*DNSS(1,1)
0006440      DNSS(13,5)=2.9974*DNSS(1,1)
0006460      DNSS(13,6)=0.60087*DNSS(1,1)
0006480      GO TO 6
0006500      5 DNSS(13,1)=0.

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0006520      DNSS(13,3)=0.0221*DNSS(1,1)
0006540      DNSS(13,4)=6.971*DNSS(1,1)
0006560      DNSS(13,5)=21.956*DNSS(1,1)
0006580      DNSS(13,6)=SMRA*DNSS(1,1)-13.9645*DNSS(1,1)
0006600 C    ASSUME THE PRESSURE OF 13TH FLOW
0006620      6 P(13)=POPR*0.958
0006640 C    ASSUME THE PRESSURE OF 31ST FLOW
0006660      7 IF (IDNO.GT.1) GO TO 8
0006680      P(31)=P(13)
0006700      T(31)=TAT
0006720      8 PINF=P(13)
0006740      PINA=P(31)
0006760      POPFC=P(31)
0006780      DO 9 IB=1,I
0006800      9 DNS(IB)=DNSS(13,IB)
0006820 C    FUEL CELL MASS BALANCE***
0006840      CALL FUCE(DNS, TOPFC, POPFC, DNSAN, DNSCA, DSO, DSN, DSHO, UT, I, PINF, PINA -
0006860      1, IFUEL)
0006880      P(14)=PINF
0006900      P(32)=PINA
0006920      DO 10 IC=1,I
0006940      DNSS(32,IC)=DNSCA(IC)
0006960      10 DNSS(14,IC)=DNSAN(IC)
0006980      T(32)=TOPFC
0007000      T(14)=TOPFC
0007020      IF (IFUEL.EQ.2) CK=1.5
0007040      IF (IFUEL.EQ.1) CK=2.
0007060      IF (IFUEL.EQ.3) CK=15.
0007080 C    CAL. THE DIVIDER FACTOR FOR THE ASSUMPTION OF DEFINED EXTRA AIR IN
0007100 C    NER
0007120      GARM=1./(((1.+EXT*0.01)*((DNSS(14,3)+DNSS(14,5))/2.+CK*DNSS(14,1))-
0007140      1)/DSO+1.)
0007160      DO 11 ID=1,I
0007180      11 DNSS(28,ID)=0.
0007200      DNSS(28,2)=DSO/GARM
0007220      DNSS(28,6)=DSHO/GARM
0007240      DNSS(28,7)=DSN/GARM
0007260      P(28)=PAT
0007280      DO 12 IE=1,I
0007300      12 DNSAI(IE)=DNSS(28,IE)
0007320 C    AIR COMPRESSOR***
0007340      T(28)=TAT
0007360      POUT=POPFC*1.005
0007380      CALL COMP (DNSAI,T(28),TOUT,P(28),POUT,POWA,GAGA,I,IP)
0007400      P(29)=POUT
0007420      DO 13 I8=1,I
0007440      13 DNSS(29,I8)=DNSAI(I8)
0007460      DO 14 IG=1,I
0007480      14 DNS(IG)=DNSS(29,IG)
0007500      T(29)=TOUT
0007520 C    DIVIDER***
0007540      CALL DIVID (T(29),T(30),T(33),DNS,DNS1,DNS2,GARM,I)
0007560      DO 15 IH=1,I
0007580      DNSS(33,IH)=DNS2(IH)

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0007600      DNSS(30,IH)=DNS1(IH)
0007620      15 DNSS(31,IH)=DNSS(30,IH)
0007640      P(30)=P(29)
0007660      P(33)=P(29)
0007680 C     CAL. THE 33RD FLOW COMP. UNDER THESE ASSUMPTION:
0007700 C     (1). COMPLETE COMBUSTION
0007720      DNSS(33,2)=(1.+EXT*0.01)*((DNSS(14,3)+DNSS(14,5))/2.+CK*DNSS(14,1)-
0007740      1)
0007760      DNSS(33,7)=DNSS(33,2)*3.76
0007780      DNSS(33,6)=((DNSS(33,2)+DNSS(33,7))*28.8)*WAT/18.
0007800      T(33)=TAT
0007820      DO 16 II=1,I
0007840      DNS1(II)=DNSS(14,II)
0007860      16 DNS2(II)=DNSS(33,II)
0007880 C     MIXER***
0007900      CALL DMIX (DNS1,DNS2,DNS,T(14),T(33),T(15),I,P(14),P(33),POUT)
0007920      P(15)=POUT
0007940      DO 17 IJ=1,I
0007960      DNSS(15,IJ)=DNS(IJ)
0007980      17 DNSS(16,IJ)=DNSS(15,IJ)
0008000 C     CAL. THE COMP. OF 17TH FLOW UNDER THE SAME ASSUMPTION AS BEFORE
0008020      IF (IFUEL.NE.3) DNSS(17,4)=DNSS(15,3)+DNSS(15,4)+DNSS(15,1)
0008040      IF (IFUEL.NE.3) DNSS(17,4)=DNSS(15,3)+DNSS(15,4)+7.*DNSS(15,1)
0008060      IF (IFUEL.NE.3) DNSS(17,6)=DNSS(15,5)+DNSS(15,6)+2.*DNSS(15,1)
0008080      IF (IFUEL.NE.3) DNSS(17,6)=DNSS(15,5)+DNSS(15,6)+8.*DNSS(15,1)
0008100      DNSS(17,2)=DNSS(15,2)-0.5*(DNSS(15,3)+DNSS(15,5))-CK*(DNSS(15,1))
0008120      DNSS(17,7)=DNSS(15,7)
0008140      DO 18 IK=1,I
0008160      DNSS(18,IK)=DNSS(17,IK)
0008180      DNSS(19,IK)=DNSS(18,IK)
0008200      DNSS(20,IK)=DNSS(19,IK)
0008220      18 CONTINUE
0008240 C     CAL. THE COMP. OF 21ST FLOW
0008260      DO 19 IL=1,I
0008280      19 DNSS(21,IL)=DNSS(20,IL)+DNSS(32,IL)
0008300      TDNSS(21)=0.
0008320      DO 20 IM=1,I
0008340      20 TDNSS(21)=TDNSS(21)+DNSS(21,IM)
0008360 C     CAL. TEMP. OF 26TH FLOW
0008380 C     ASSUMPTION:
0008400 C     (1). SATURATED PRESSURE IS ESTIMATED BY (EXP(A-B/T))
0008420 C     (2). UNDER SATURATED CONDITION
0008440 C     ASSUME THE PRESSURE OF 26TH FLOW IS IDENTICAL TO 25TH FLOW (THE PRESS.
0008460 C     DROP IS SMALL)
0008480      P(25)=POPR*1.0005
0008500      P(26)=P(25)
0008520      T(26)=B/(A-ALOG(P(26)))
0008540      DNSS(26,6)=DNSS(1,1)*SMRA
0008560      DO 21 IN=1,I
0008580      21 DNSS(25,IN)=DNSS(26,IN)
0008600      DO 22 IO=1,I
0008620      IF (IFUEL.NE.2) DNSS(27,IO)=DNSS(26,IO)
0008640      22 DNSS(2,IO)=DNSS(1,IO)
0008660      DO 23 I9=1,I

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0008680     IF (IFUEL.NE.2) DNSS(3,I9)=DNSS(2,I9)+DNSS(27,I9)
0008700     IF (IFUEL.EQ.2) DNSS(3,I9)=DNSS(2,I9)+DNSS(26,I9)
0008720     IF (IFUEL.NE.2) DNSS(4,I9)=DNSS(3,I9)
0008740     IF (IFUEL.EQ.2) DNSS(5,I9)=DNSS(3,I9)
0008760     IF (IFUEL.NE.2) DNSS(5,I9)=DNSS(4,I9)
0008780     23 CONTINUE
0008800 C    ASSUME THE TEMP. AND PRESSURE OF 5TH FLOW
0008820     IF (IDNO.GT.1) GO TO 24
0008840     IF (IFUEL.EQ.1) T(5)=1110.88
0008860     IF (IFUEL.EQ.2) T(5)=661.59
0008880     IF (IFUEL.EQ.3) T(5)=1052.
0008900     P(5)=POPR
0008920     24 CONTINUE
0008940     IF (IDNO.GT.1) GO TO 25
0008960 C    ASSUME THE TEMP. OF 18TH FLOW
0008980     IF (IFUEL.EQ.1) T(18)=1222.
0009000     IF (IFUEL.EQ.2) T(18)=863.88
0009020     IF (IFUEL.EQ.3) T(18)=1398.94
0009040 C    ASSUME P(16)
0009060     P(16)=P(15)*0.99
0009080 C    DESIGN THE TUBE TO LET PRESSURE DROP THROUGH BURNER BE 6%
0009100     604 F(17)=P(16)*(1.-0.06)
0009120 C    ASSUME PRESSURE DROP OF COMBUSTIAN GAS THROUGH REFORMER TO BE 5%
0009140     P(18)=P(17)*0.95
0009160     25 CONTINUE
0009180 C    E-3***
0009200     DO 26 IQ=1,I
0009220     DNSH(IQ)=DNSS(17,IQ)
0009240     26 DNSC(IQ)=DNSS(5,IQ)
0009260     PT=P(5)
0009280     PS=P(18)
0009300     IF (IFUEL.NE.2) CALL HEXC (T(18),DNSH,DNDC,T(4),T(19),T(5),QT,1,HA-
0009320     1(3),3,2,I,PT,PS,NT(3),IFUEL)
0009340     IF (IFUEL.EQ.2) CALL HEXC (T(18),DNSH,DNDC,T(3),T(19),T(5),QT,1,HA-
0009360     1(3),3,2,I,PT,PS,NT(3),IFUEL)
0009380     IF (IFUEL.NE.2) P(4)=PT
0009400     IF (IFUEL.EQ.2) P(3)=PT
0009420     P(19)=PS
0009440     EFF(3)=HE
0009460     QQT(3)=QT
0009480 C    E-4***
0009500     DO 27 IR=1,I
0009520     DNSH(IR)=DNSS(19,IR)
0009540     DNDC(IR)=DNSS(15,IR)
0009560     27 CCNTINUE
0009580     PT=P(15)
0009600     PS=P(19)
0009620     CALL HEXC (T(19),DNSH,DNDC,T(15),T(20),T(16),QT,1,HA(4),4,1,I,PT,P-
0009640     1S,NT(4),IFUEL)
0009660     IF (ABS((PT-P(16))/(PT+P(16))).LT.ERR) GO TO 605
0009680     P(16)=(PT+P(16))/2.
0009700     GO TO 604
0009720     605 P(16)=PT
0009740     P(20)=PS

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0009760      EFF(4)=HE
0009780      QQT(4)=QT
0009800 C    BURNER ENERGY BALANCE***
0009820      DO 28 IS=1,I
0009840      28 DNS(IS)=DNSS(16,IS)
0009860      CALL FLAME (DNS,T(16),T(17),I,IFUEL)
0009880      DO 29 IT=1,I
0009900      29 DNSS(17,IT)=DNS(IT)
0009920      IF (IFUEL.NE.1) GO TO 33
0009940 C    REFORMER(METHANE)***
0009960      NOR=DNSS(1,1)/60.
0009980      DO 30 IU=1,I
0010000      DNSR(IU)=DNSS(5,IU)/453.6/NOR
0010020      30 DNSF(IU)=DNSS(17,IU)/453.6/NOR
0010040      CALL KREF(DNSR,DNSF,DX1,DX2,DX3,P(5),T(5),T(17),ZH,P(7),T(7) -
0010060      1,TTEST,S,DP,1)
0010080 C    TEST THE ASSUMPTION OF 18TH FLOW
0010100      IF (ABS((TTEST-T(18))/(TTEST+T(18))).LT.ERR) GO TO 31
0010120      T(18)=TTEST
0010140      GO TO 25
0010160      31 DO 32 IV=1,I
0010180      DNSS(7,IV)=DNSR(IV)*453.6*NOR
0010200      32 DNSS(18,IV)=DNSF(IV)*453.6*NOR
0010220      T(18)=TTEST
0010240      GO TO 39
0010260 C    E-8(METHANOL AND NAPHTHA)***
0010280      33 DO 34 IW=1,I
0010300      DNSH(IW)=DNSS(17,IW)
0010320      34 DNSC(IW)=DNSS(5,IW)
0010340      PTEST=P(17)
0010360      PS=P(5)
0010380      CALL HEXC (T(17),DNSH,DNSC,T(5),TTEST,T(6),QT,2,HA(8),8,1,I,PTEST,-
0010400      1FS,NT(8),IFUEL)
0010420 C    TEST THE ASSUMPTION OF 18TH FLOW
0010440      IF ((ABS((TTEST-T(18))/(TTEST+T(18))).LT.ERR).AND.(ABS((PTEST-P(18-
0010460      1))/(PTEST+P(18))).LT.ERR)) GO TO 35
0010480      T(18)=(TTEST+T(18))/2.
0010500      P(18)=(P(18)+PTEST)/2.
0010520      GO TO 25
0010540      35 QQT(8)=QT
0010560      T(18)=TTEST
0010580      P(18)=PTEST
0010600      P(6)=PS
0010620      EFF(8)=HE
0010640      DO 36 IX=1,I
0010660      DNSS(6,IX)=DNSC(IX)
0010680      36 DNSS(18,IX)=DNSH(IX)
0010700 C    REFORMER(METHANOL AND NAPHTHA)***
0010720      DO 37 IY=1,I
0010740      37 DNS(IY)=DNSS(6,IY)
0010760      CALL ENRE (DNS,TOPR,POPR,T(6),T(7),I,IP,IFUEL)
0010780      DO 38 IZ=1,I
0010800      38 DNSS(7,IZ)=DNS(IZ)
0010820 C    CAL. PRESSURE DROP

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0010840      CALL PDSH (DNS,P(6),P(7),TOPR,2,IFUEL)
0010860      IF (IFUEL.EQ.2) GO TO 56
0010880      39 DO 40 IAA=1,I
0010900          DNSH(IAA)=DNSS(7,IAA)
0010920      40 DNSC(IAA)=DNSS(3,IAA)
0010940      C      E-2***
0010960          PT=P(4)
0010980          PS=P(7)
0011000          IF(IFUEL.EQ.1) CALL HEXC(T(7),DNSH,DNSC,T(3),T(8),T(4),QT,1,HA(2),-
0011020      12,2,I,PT,PS,NT(2),IFUEL)
0011040          IF(IFUEL.EQ.3) CALL HEXC(T(7),DNSH,DNSC,T(3),T(9),T(4),QT,1,HA(2),-
0011060      12,2,I,PT,PS,NT(2),IFUEL)
0011080          P(3)=PT
0011100          IF (IFUEL.EQ.1) P(8)=PS
0011120          IF (IFUEL.EQ.3) P(9)=PS
0011140          EFF(2)=HE
0011160          QQT(2)=QT
0011180          DO 41 IBB=1,I
0011200          IF (IFUEL.EQ.1) DNSS(8,IBB)=DNSH(IBB)
0011220          IF (IFUEL.EQ.3) DNSS(9,IBB)=DNSH(IBB)
0011240      41 DNSS(4,IBB)=DNSC(IBB)
0011260          IF (IFUEL.EQ.3) GO TO 46
0011280      C      HIGH TEMP. SHIFT CONVERTER***
0011300          TOPHS=T(8)
0011320      42 CONTINUE
0011340          POPHS=P(8)
0011360          DO 43 ICC=1,I
0011380      43 DNS(ICC)=DNSS(8,ICC)
0011400          CALL ENSH (DNS,T(8),T(9),TOPHS,POPHS,I,IP,IFUEL)
0011420          P(9)=POPHS
0011440          TM=(T(9)+T(8))/2.
0011460          IF ((IP.EQ.2).OR.(ABS((TM-TOPHS)/(TM+TOPHS)).LT.ERR)) GO TO 44
0011480          TOPHS=TM
0011500          GO TO 42
0011520      44 CONTINUE
0011540          DO 45 IDD=1,I
0011560      45 DNSS(9,IDD)=DNS(IDD)
0011580      46 CONTINUE
0011600          DO 47 IEE=1,I
0011620          DNSH(IEE)=DNSS(9,IEE)
0011640      47 DNSC(IEE)=DNSS(1,IEE)
0011660          IF (IFUEL.EQ.3) GO TO 48
0011680      C      E-1(METHANE AND NAPHTHA)***
0011700          PT=P(1)
0011720          PS=P(9)
0011740          CALL HEXC (T(9),DNSH,DNSC,T(1),THO,TCO,QT,1,HA(1),1,1,I,PT,PS,NT(1-
0011760      1),IFUEL)
0011780          P(10)=PS
0011800          P(2)=PT
0011820          EFF(1)=HE
0011840          QQT(1)=QT
0011860          T(2)=TCO
0011880          T(10)=THO
0011900          GO TO 52

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0011920      48 CONTINUE
0011940 C    DESIGN THE HEAT EXCHANGER 1 TO VAPORIZE NAPHTHA AND RISE THE TEMP.
0011960 C    TO 400
0011980 C    K FOR NAPHTHA FUEL
0012000      T(2)=400.
0012020      QQT(1)=HNA*252./453.6*100.*1.8*DNSS(1,1)*(BPNA+273.-T(1))+DNSS(1,1-
0012040      1)*VHNA+HCAS(1)*(T(2)-T(1))+HCBS(1)*(T(2)**2-T(1)**2)/2.+HCCS(1)*(T-
0012060      2(2)**3-T(1)**3)/3.
0012080 C    ASSUME EFFICIENCY OF H-E 1 IS 0.7
0012100      EFF(1)=0.7
0012120      HA(1)=CN*QQT(1)/EFF(1)/(T(9)-T(1))/U
0012140 C    ASSUME AVERAGE TEMP. OF HOT SIDE
0012160      TAVG=T(9)-50.
0012180      49 CHH=0.
0012200      DO 50 IB=1,I
0012220      50 CHH=CHH+DNSS(9,IB)*(HCAS(IB)+HCBS(IB)*TAVG+HCCS(IB)*TAVG**2)
0012240      T(10)=T(9)-QQT(1)/CHH
0012260 C    TEST THE ASSUMPTION OF AVERAGE TEMP.
0012280      IF (ABS((T(10)+T(9))/2.-TAVG).LT.ABS((T(10)+T(9))/2.+TAVG)*0.001) -
0012300      IGO TO 51
0012320      TAVG=(T(9)+T(10))/2.
0012340      GO TO 49
0012360      51 CONTINUE
0012380 C    ASSUME PRESSURE DROP IS NEGLECTABLE
0012400      P(2)=P(1)
0012420      P(10)=P(9)
0012440      52 DO 53 IFF=1,I
0012460      IF (IFUEL.EQ.3) DNSS(10,IFF)=DNSS(9,IFF)
0012480      53 IF (IFUEL.EQ.1) DNSS(10,IFF)=DNSS(9,IFF)
0012500      DO 54 IGG=1,I
0012520      DNSH(IGG)=DNSS(10,IGG)
0012540      54 DNSC(IGG)=DNSS(26,IGG)
0012560 C    E-9***
0012580      PT=P(26)
0012600      PS=P(10)
0012620      CALL HEXC (T(10),DNSH,DNSC,T(26),T(11),T(27),QT,1,HA(9),9,1,I,PT,P-
0012640      1S,NT(9),IFUEL)
0012660      P(11)=PS
0012680      P(27)=PT
0012700      EFF(9)=HE
0012720      QQT(9)=QT
0012740      DO 55 IHH=1,I
0012760      DNSS(11,IHH)=DNSH(IHH)
0012780      DNSS(27,IHH)=DNSC(IHH)
0012800      DNS1(IHH)=DNSS(2,IHH)
0012820      DNS2(IHH)=DNSS(27,IHH)
0012840      55 CONTINUE
0012860      GO TO 60
0012880 C    E-1(METHANOL)***
0012900      56 DO 57 III=1,I
0012920      DNSH(III)=DNSS(7,III)
0012940      57 DNSC(III)=DNSS(1,III)
0012960      PT=P(1)
0012980      PS=P(7)

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0013000      CALL HEXC (T(7),DNSH,DNSC,T(1),THO,TCO,QT,1,HA(1),1,1,I,PT,PS,NT(1-
0013020      1),IFUEL)
0013040      PTE=PS
0013060      P(2)=PT
0013080      EFF(1)=HE
0013100      QQT(1)=QT
0013120      DO 58 IJJ=1,I
0013140      58 DNSS(2,IJJ)=DNSC(IJJ)
0013160      T(2)=TCO
0013180      T(13)=THO
0013200      DO 59 IJJ=1,I
0013220      DNS1(IJJ)=DNSS(2,IJJ)
0013240      DNS2(IJJ)=DNSS(26,IJJ)
0013260      59 CONTINUE
0013280 C     MIXER***
0013300      CALL DMIX (DNS1,DNS2,DNS,T(2),T(26),TESTT,I,P(2),P(26),PTEST)
0013320      GO TO 61
0013340      60 CALL DMIX (DNS1,DNS2,DNS,T(2),T(27),TESTT,I,P(2),P(27),PTEST)
0013360 C     TEST TEMP. OF 3RD FLOW
0013380      61 IF ((ABS((TESTT-T(3))/(TESTT+T(3))).LT.ERR).AND.(ABS((PTEST-P(3))/-
0013400      1(PTEST+P(3))).LT.ERR)) GO TO 70
0013420      IF (IFUEL.EQ.2) GO TO 66
0013440 C     E-2***
0013460      DO 62 IKK=1,I
0013480      DNSS(3,IKK)=DNS(IKK)
0013500      DNSH(IKK)=DNSS(7,IKK)
0013520      62 DNSC(IKK)=DNSS(3,IKK)
0013540      P(3)=(P(3)+PTEST)/2.
0013560      T(3)=(TESTT+T(3))/2.
0013580      PT=P(3)
0013600      PS=P(7)
0013620      IF (IFUEL.EQ.3) GO TO 63
0013640      CALL HEXC (T(7),DNSH,DNSC,T(3),T(8),T(4),QT,1,HA(2),2,1,I,PT,PS,NT-
0013660      1(2),IFUEL)
0013680      P(4)=PT
0013700      P(8)=PS
0013720      GO TO 64
0013740      63 CALL HEXC (T(7),DNSH,DNSC,T(3),T(9),T(4),QT,1,HA(2),2,1,I,PT,PS,NT-
0013760      1(2),IFUEL)
0013780      P(4)=PT
0013800      P(9)=PS
0013820 C     E-3***
0013840      64 DO 65 ILL=1,I
0013860      DNSS(4,ILL)=DNSC(ILL)
0013880      DNSH(ILL)=DNSS(18,ILL)
0013900      65 DNSC(ILL)=DNSS(4,ILL)
0013920      PT=P(4)
0013940      PS=P(18)
0013960      CALL HEXC (T(18),DNSH,DNSC,T(4),T(19),T(5),QT,1,HA(3),3,1,I,PT,PS,-
0013980      INT(3),IFUEL)
0014000      P(5)=PT
0014020      P(19)=PS
0014040      GO TO 68
0014060      66 DO 67 IMM=1,I

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0014080      DNSS(3,IMM)=DNS(IMM)
0014100      DNSH(IMM)=DNSS(18,IMM)
0014120      67 DNSC(IMM)=DNSS(3,IMM)
0014140      T(3)=(T(3)+TESTT)/2.
0014160      PT=P(18)
0014180      PS=(P(3)+PTEST)/2.
0014200      CALL HEXC (T(18),DNSH,DNSC,T(3),T(19),T(5),QT,1,HA(3),3,1,I,PT,PS,-
0014220      INT(3),IFUEL)
0014240      P(19)=PT
0014260      P(5)=PS
0014280      EFF(3)=HE
0014300      QQT(3)=QT
0014320      68 DO 69 INN=1,I
0014340      69 DNSS(5,INN)=DNSC(INN)
0014360      IDNO=IDNO+1
0014380      GO TO 24
0014400      70 CONTINUE
0014420      IF (IFUEL.EQ.2) GO TO 77
0014440      DO 71 IPP=1,I
0014460      DNSH(IPP)=DNSS(11,IPP)
0014480      71 DNSC(IPP)=DNSS(30,IPP)
0014500      C      E-6***
0014520      PT=P(30)
0014540      PS=P(11)
0014560      CALL HEXC (T(11),DNSH,DNSC,T(30),T(12),T(31),QT,1,HA(6),6,1,I,PT,P-
0014580      1S,NT(6),IFUEL)
0014600      P(12)=PS
0014620      PTEST=PT
0014640      C      TEST THE PRESSURE OF 31ST FLOW
0014660      IF (ABS((PTEST-P(31))/(PTEST+P(31))).LT.ERR) GO TO 72
0014680      P(31)=(PTEST+P(31))/2.
0014700      GO TO 8
0014720      72 EFF(6)=HE
0014740      QQT(6)=QT
0014760      DO 73 IQQ=1,I
0014780      DNSS(12,IQQ)=DNSH(IQQ)
0014800      73 DNSS(31,IQQ)=DNSC(IQQ)
0014820      C      LOW TEMP. SHIFT CONVERTER***
0014840      TOPLS=T(12)
0014860      POPLS=P(12)
0014880      74 CONTINUE
0014900      DO 75 IRR=1,I
0014920      75 DNS(IRR)=DNSS(12,IRR)
0014940      CALL ENSH (DNS,T(12),T(13),TOPLS,POPLS,I,IP,IFUEL)
0014960      TM=(T(12)+T(13))/2.
0014980      IF ((IP.EQ.2).OR.(ABS((TM-TOPLS)/(TM+TOPLS)).LT.ERR)) GO TO 76
0015000      TOPLS=TM
0015020      GO TO 74
0015040      76 CONTINUE
0015060      C      TEST THE ASSUMPTION OF 13TH FLOW
0015080      77 DO 78 ISS=1,I
0015100      IF ((IFUEL.NE.2).AND.(DNS(ISS).LT.0.50).AND.(DNSS(13,ISS).LT.0.50)-
0015120      1) GO TO 78
0015140      IF ((IFUEL.EQ.2).AND.(DNSH(ISS).LT.0.50).AND.(DNSS(13,ISS).LT.0.50-

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0015160      1)) GO TO 78
0015180      IF ((IFUEL.NE.2).AND.(ABS((DNS(ISS)-DNSS(13,ISS))/(DNS(ISS)+DNSS(1-
0015200      13,ISS))).LT.ERR)) GO TO 78
0015220      IF ((IFUEL.EQ.2).AND.(ABS((DNSH(ISS)-DNSS(13,ISS))/(DNSH(ISS)+DNSS-
0015240      1(13,ISS))).LT.ERR)) GO TO 78
0015260      GO TO 79
0015280      78 CONTINUE
0015300      IF (IFUEL.EQ.2) POPLS=PTE
0015320      IF (ABS((POPLS-P(13))/(POPLS+P(13))).LT.ERR) GO TO 81
0015340      79 DO 80 ITT=1,I
0015360      IF (IFUEL.EQ.2) DNSS(13,ITT)=(DNSS(13,ITT)+DNSH(ITT))/2.
0015380      80 IF (IFUEL.NE.2) DNSS(13,ITT)=(DNSS(13,ITT)+DNS(ITT))/2.
0015400      P(13)=(POPLS+P(13))/2.
0015420      GO TO 7
0015440      81 CONTINUE
0015460      DO 82 IUU=1,I
0015480      IF (IFUEL.EQ.2) DNSS(13,IUU)=DNSH(IUU)
0015500      82 IF (IFUEL.NE.2) DNSS(13,IUU)=DNS(IUU)
0015520      TDM13=0.
0015540      DO 83 IVV=1,I
0015560      83 TDM13=TDM13+DNSS(13,IVV)
0015580      FCO=DNSS(13,3)/TDM13
0015600      DO 84 IWW=1,I
0015620      DNSAN(IWW)=DNSS(13,IWW)
0015640      84 DNSCA(IWW)=DNSS(31,IWW)
0015660 C      FUEL CELL ENERGY BALANCE***
0015680      AREAF=FULE*AIRL*30.48**2
0015700      CD=CD/1000.
0015720      OU=1./(EXA*0.01+1.)
0015740      CALL ENFU(DNSAN,DNSCA,T(31),T(13),TOUT,TOFPC,POPFC,VOP,UT,1,I,QY, -
0015760      IWK,OU,CD,CL,IFUEL)
0015780      QRT=QY
0015800 C CALCULATE THE OUTPUT OF AC POWER
0015820      AC=( -1.0148+SQRT(1.0148**2-4.*0.0456/108.*(0.0472*108.-WK))) -
0015840      1/(2.*0.0456/108.)
0015860      DO 86 IYY=1,I
0015880      86 DNSC(IYY)=DNSS(25,IYY)
0015900      DO 87 IZZ=1,I
0015920      DNS1(IZZ)=DNSS(20,IZZ)
0015940      87 DNS2(IZZ)=DNSS(32,IZZ)
0015960 C      MIXER***
0015980      CALL DMIX (DNS1,DNS2,DNS,T(20),T(32),TOUT,I,P(20),P(32),POUT)
0016000      P(21)=POUT
0016020      DO 88 I1=1,I
0016040      DNSS(21,I1)=DNS(I1)
0016060      88 DNSH(I1)=DNSS(21,I1)
0016080      T(21)=TOUT
0016100 C ASSUME P(22)
0016120      P(22)=P(21)*1.001
0016140      602 T(22)=-B/(ALOG((DNSS(1,1)*SMRA-DNSS(21,6))/(DNSS(1,1)*SMRA- -
0016160      1TDNSS(21))*P(22))-A)
0016180 C      E-10***
0016200      T(25)=T(22)
0016220      CALL CDPH (QRT,T(25),T(26),DNSC,P(25),I,QQT(10))

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0016240      QQT(7)=QRT
0016260 C    ASSUME HOT WATER IS FEEDING IN AT 333OK AND FEEDING OUT AT 355 K
0016280      DNSS(34,6)=QQT(7)/(355.-333.)/1./18.
0016300      DNSS(35,6)=DNSS(34,6)
0016320      T(34)=333.
0016340      T(35)=355.
0016360      P(34)=PAT
0016380      P(35)=PAT
0016400 C    E-5***
0016420      CALL COND (T(21),T(22),DNSH,QT,HCH,I)
0016440      QQT(5)=QT
0016460 C    ASSUME HOT WATER IS FEEDING IN AT TAT  AND FEEDING OUT AT 355OK
0016480      DTL=((T(21)-355.)-(T(22)-TAT))/ALOG((T(21)-355.)/(T(22)-TAT))
0016500      T(36)=TAT
0016520      T(37)=355.
0016540      P(36)=PAT
0016560      P(37)=PAT
0016580      DNSS(36,6)=QQT(5)/1./18./(355.-TAT)
0016600      DNSS(37,6)=DNSS(36,6)
0016620 C    ASSUME E-5 IS THE TYPE OF COUNTERFLOW
0016640      HA(5)=QQT(5)/U/1./DTL
0016660      THM=(T(36)+T(37))/2.
0016680      TCM=(T(22)+T(21))/2.
0016700      CALL HEPD(DNS,DNSH,THM,TCM,HA(5),P(21),P(36),5,DPJ,DP,NT,T(22),
0016720      1T(21),4)
0016740      P22TE=P(21)-DPJ
0016760      IF(ABS((P22TE-P(22))/(P22TE+P(22))).LT.ERR) GO TO 603
0016780      P(22)=(P(22)+P22TE)/2.
0016800      GO TO 602
0016820 603 DO 89 I2=1,I
0016840      DNSS(22,I2)=DNSH(I2)
0016860 89 DNS(I2)=DNSS(22,I2)
0016880 C    SEPARATER***
0016900      POPS=P(22)
0016920      CALL SEPAR (T(22),POPS,T(23),T(24),DNS,DNSL,DNSV,I)
0016940      DO 90 I3=1,I
0016960      DNSS(24,I3)=DNSL(I3)
0016980 90 DNSS(23,I3)=DNSV(I3)
0017000      P(24)=POPS
0017020      P(23)=POPS
0017040 C    PUMP***
0017060      DO 901 I4=1,I
0017080 901 DNS(I4)=DNSS(24,I4)
0017100      CALL PUMP (DNS,T(24),T(25),P(24),P(25),POWS,I)
0017120      DO 92 IB=1,39
0017140      TDNSS(IB)=0.
0017160      DO 91 IA=1,I
0017180      TDNSS(IB)=TDNSS(IB)+DNSS(IB,IA)
0017200 91 CONTINUE
0017220 92 CONTINUE
0017240 C    WRITE THE RESULT
0017260      IF (IFUEL.EQ.1) WRITE (6,108) SMRA
0017280      IF (IFUEL.EQ.2) WRITE (6,109) SMRA
0017300      IF (IFUEL.EQ.3) WRITE (6,110) SMRA

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0017320      WRITE (6,103) P(5),P(7),T(5),T(7)
0017340      IF (IFUEL.EQ.1) WRITE (6,104) TOPHS,P(8),T(8),T(9)
0017360      IF (IFUEL.NE.2) WRITE (6,105) TOPLS,P(13),T(12),T(13)
0017380      WRITE (6,106) T(22),POPS
0017400      WRITE (6,99) FCO
0017420      WRITE (6,118) TOPFC,POPFC,E,VOP,CD,CL,UT,OU
0017440      WRITE (6,102) T(13),T(31)
0017460      WRITE (6,100) ETH,EI,EV,EC
0017480      WRITE (6,107) EFC
0017500      WRITE (6,101) WK,QRT
0017520      WRITE (6,117) AC
0017540 C     WRITE THE MATERIAL IN JTH FLOW
0017560 18280 WRITE(6,119)
0017580      IF (IFUEL.EQ.1) WRITE (6,94)
0017600      IF (IFUEL.EQ.2) WRITE (6,95)
0017620      IF (IFUEL.EQ.3) WRITE (6,96)
0017640      IF (IFUEL.EQ.1) WRITE (6,93) (((J,(DNSS(J,IA),IA=1,I),TDNSS(J),T(J-
0017660      1),P(J)),J=1,5),((II,(DNSS(II,IA),IA=1,I),TDNSS(II),T(II),P(II)),II-
0017680      2=7,37))
0017700      IF (IFUEL.EQ.2) WRITE (6,93) (((J,(DNSS(J,IA),IA=1,I),TDNSS(J),T(J-
0017720      1),P(J)),J=1,3),((II,(DNSS(II,IA),IA=1,I),TDNSS(II),T(II),P(II)),II-
0017740      2=5,7))
0017760      IF (IFUEL.EQ.3) WRITE (6,93) (((J,(DNSS(J,IA),IA=1,I),TDNSS(J),T(J-
0017780      1),P(J)),J=1,7),((II,(DNSS(II,IA),IA=1,I),TDNSS(II),T(II),P(II)),II-
0017800      2=9,37))
0017820 C     WRITE DUTY OF HEAT EXCHANGER OR CONDENSER
0017840      WRITE(6,119)
0017860      WRITE (6,111)
0017880      WRITE (6,97)
0017900      WRITE (6,98) (QQT(IA),IA=1,10)
0017920 C     WRITE SURFACE AREA OF HEAT EXCHANGER
0017940      WRITE (6,112)
0017960      WRITE (6,97)
0017980      WRITE (6,98) (HA(IA),IA=1,10)
0018000 C     WRITE THE EFFICIENCY OF HEAT EXCHANGER
0018020      WRITE (6,113)
0018040      WRITE (6,97)
0018060      WRITE (6,98) (EFF(IA),IA=1,10)
0018080      IF (IFUEL.EQ.1) WRITE (6,114) POWA,POWM,POWS
0018100      IF (IFUEL.EQ.2) WRITE (6,115) POWA,POWN,POWS
0018120      IF (IFUEL.EQ.3) WRITE (6,116) POWA,POWN,POWS
0018140      STOP
0018160 C
0018180      93 FORMAT (1X,2X,I2,2X,F8.2,1X,F8.2,1X,3X,F8.2,6X,F8.2,5X,F8.2,F10.2,-
0018200      11X,F8.2,3X,F10.2,4X,F7.2,2X,F6.4)
0018220      94 FORMAT (1X,'STREAM METHANE OXYGEN CAR. MONOXIDE CAR. DIOXIDE -
0018240      1HYDROGEN WATER NITROGEN FLOW RATE TEMP.(K) PRE.(ATM)')
0018260      95 FORMAT (1X,'STREAM METHANOL OXYGEN CAR. MONOXIDE CAR. DIOXIDE -
0018280      1HYDROGEN WATER NITROGEN FLOW RATE TEMP.(K) PRE.(ATM)')
0018300      96 FORMAT (1X,'STREAM NAPHTHA OXYGEN CAR. MONOXIDE CAR. DIOXIDE -
0018320      1HYDROGEN WATER NITROGEN FLOW RATE TEMP.(K) PRE.(ATM)')
0018340      97 FORMAT (1X,' E- 1 E-2 E-3 E-4 -
0018360      1 E-5 E-6 E-7 E-8 E-9 -
0018380      2 E-10')

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0018400 98 FORMAT (1X,10(E12.5,1X)/)
0018420 99 FORMAT (1X,'THE FRACTION OF CO IN THE FEED IS',F8.5/)
0018440 100 FORMAT (1X,'THE THERMODYNAMIC EFFICIENCY OF FUEL CELL IS',E13.5,'T-
0018460 THE CURRENT EFFICIENCY IS',E13.5/' THE VOLTAGE EFFICIENCY IS',E13.5-
0018480 2,'THE HEATING VALUE EFFICIENCY IS',E13.5)
0018500 101 FORMAT (1X,'THE ELECTRICAL WORK IS',E13.5,'KW '/' THE TOTAL HEAT R-
0018520 1 RELEASE IS',E13.5,'CAL'//)
0018540 102 FORMAT (1X,'THE ANODE SIDE INLET TEMP. IS',F7.2,' K'/' THE CATHODE-
0018560 1 SIDE INLET TEMP. IS',F7.2,' K')
0018580 103 FORMAT (' THE REFORMER IS OPERATING UNDER THESE CONDITIONS ',6X,/'-
0018600 1 INLET PRESSURE',F7.2,'ATM',' OUTLET PRESSURE',F7.2,'ATM'/ ' -
0018620 2 INLET TEMP. :',F7.2,' K',' OUTLET TEMP. :',F7.2,' K'//)
0018640 104 FORMAT (' THE HIGH TEMP. SHIFT CONVERTER IS OPERATING UNDER THESE -
0018660 1 CONDITIONS ',6X,/ -
0018680 2 ' OPERATING TEMP.:',F7.2,' K'/' OPERATING PRESSURE:',F7.2,'ATM-
0018700 3'/' INLET TEMP.:',F7.2,' K'/' OUTLET TEMP.:',F7.2,' K'//)
0018720 105 FORMAT (1X,'THE LOW TEMP. SHIFT CONVERTER IS OPERATING UNDER THESE-
0018740 1 CONDITIONS ',6X,/ -
0018760 2 ' OPERATING TEMP.:',F7.2,' K'/' OPERATING PRESSURE:',F7.2,'ATM-
0018780 3'/' INLET TEMP.:',F7.2,' K'/' OUTLET TEMP.:',F7.2,' K'//)
0018800 106 FORMAT (' THE LIQUID SEPARATOR IS OPERATING UNDER THESE CONDITIONS-
0018820 1 ',6X,/' OPERATING TEMP.:',F7.2,' K'/' OPERATING PRESSURE:',F7.2,'-
0018840 2ATM'//)
0018860 107 FORMAT (1X,'THE FUEL CELL EFFICIENCY IS',F6.4)
0018880 108 FORMAT ('1',1X,'THE STEAM/METHANE RATIO IN THE REFORMER IS',F7.2/)
0018900 109 FORMAT ('1',' THE STEAM/METHANOL RATIO IN THE REFORMER IS',F7.2/)
0018920 110 FORMAT ('1',' THE STEAM/NAPHTHA RATIO IN THE REFORMER IS',F7.2/)
0018940 111 FORMAT (1X,'THE DUTY OF HEAT EXCHANGER (CAL.) (0 MEANS NO THIS NO.-
0018960 1 HEAT EXCHANGER)')
0018980 112 FORMAT (1X,'THE SURFACE AREA OF HEAT EXCHANGER (M**2) (0 MEANS NO -
0019000 1 THIS NO. HEAT EXCHANGER)')
0019020 113 FORMAT (1X,'THE EFFICIENCY OF HEAT EXCHANGER (0 MEANS NO THIS NO. -
0019040 1 HEAT EXCHANGER OR IS CONDENSER)')
0019060 114 FORMAT (1X,'THE POWER OF AIR COMPRESSOR:',F10.2,'HP'/1X,'THE POWER-
0019080 1 OF METHANE COMPRESSOR:',F10.2,'HP'/1X,'THE POWER OF PUMP :',F10.5-
0019100 2,'HP')
0019120 115 FORMAT (1X,'THE POWER OF AIR COMPRESSOR:',F10.2,'HP'/1X,'THE POWER-
0019140 1 OF METHANOL COMPRESSOR:',F10.5,'HP'/1X,'THE POWER OF PUMP :',F10.-
0019160 25,'HP')
0019180 116 FORMAT (1X,'THE POWER OF AIR COMPRESSOR:',F10.2,'HP'/1X,'THE POWER-
0019200 1 OF NAPHTHA PUMP:',F10.5,'HP'/1X,'THE POWER OF PUMP :',F10.5,'HP')
0019220 117 FORMAT (//1X,'THE AC OUTPUT IS ',F7.2,'KW'//)
0019240 118 FORMAT(' THE FUEL CELL IS OPERATING UNDER THESE CONDITIONS ',6X,/'-
0019260 1 THE OPERATING TEMPERATURE :',F7.2,'K'/' THE OPERATING PRESSURE:',-
0019280 2F5.2,'ATM'/' THE OPEN CIRCUIT POTENTIAL:',F8.3,' V' / -
0019300 3' THE OPERATING POTENTIAL:',F8.3,' V'/' THE CURRENT DENSITY:',F8.3-
0019320 4,'A/CM**2'/' THE CATALYST LOADING:',F8.3,'PT/CM**2' / -
0019340 5 ' THE FUEL UTILIZATION:',F5.3/ -
0019360 6' THE OXYGEN UTILIZATION:',F5.3)
0019380 119 FORMAT('1')
0019400 END
0019800 SUBROUTINE BURN(DNS,I,IJ)
0019900 C*****
0020000 C THIS SUBROUTINE IS TO CALCULATE THE MASS BALANCE OF BURNER

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0020100 C*****
0020200 C ASSUMPTION:
0020300 C      (1) THE COMBUSTION IS COMPLETE
0020400 C X : THE AMOUNT OF O2 REACTED
0020500 C XY : THE AMOUNT OF CO2 PRODUCED
0020600 C Y : THE AMOUNT OF H2O PRODUCED
0020700 C IJ: 1 =MATHANE AS INPUT GAS
0020800 C      2 =METHANOL AS INPUT GAS
0020900 C      3 =NAPHTHA AS INPUT GAS
0021000 C      DIMENSION DNS(I)
0021100 C CALCULATE THE NECESSARY AMOUNT OF O2
0021200 C      IF(IJ.EQ.3) GO TO 4
0021300 C      IF(IJ.EQ.2) GO TO 2
0021400 C      X=1./2.*DNS(3)+1./2.*DNS(5)+2.*DNS(1)
0021500 C      GO TO 3
0021600 C      2 X=-.5*DNS(3)+.5*DNS(5)+1.5*DNS(1)
0021700 C      GO TO 3
0021800 C      4 X=0.5*DNS(3)+0.5*DNS(5)+15.*DNS(1)
0021900 C      XY=DNS(3)+7.*DNS(1)
0022000 C      Y=DNS(5)+8.*DNS(1)
0022100 C      GO TO 5
0022200 C      3 CONTINUE
0022300 C      XY=DNS(3)+DNS(1)
0022400 C      Y=DNS(5)+2.*DNS(1)
0022500 C CALCULATE THE EXIT COMPOSITION
0022600 C      5 DNS(1)=0.
0022700 C      DNS(3)=0.
0022800 C      DNS(5)=0.
0022900 C      DNS(2)=DNS(2)-X
0023000 C      DNS(4)=DNS(4)+XY
0023100 C      DNS(6)=DNS(6)+Y
0023200 C      RETURN
0023300 C      END
0023400 C      SUBROUTINE CDPH(QTI,TCI,TCO,DNSC,P,I,QTS)
0023500 C*****
0023600 C THIS SUBROUTINE IS TO CAL. THE ENERGY ANALYSIS FOR E-7 AND E-10
0023700 C*****
0023900 C DEFINITION:
0024000 C QTI: TOTAL HEAT TRANSFER FROM FUEL CELL
0024100 C TCB: BOILING POINT OF FIXED PRESSURE
0024200 C      DIMENSION GS(7),HS(7),HCAS(7),HCBS(7),HCCS(7)
0024300 C      DIMENSION DNSC(I)
0024400 C      COMMON /ETHDA/ GS,HS,HCAS,HCBS,HCCS
0024500 C      COMMON/TC/TC/CONS/A,B
0024600 C      COMMON/UI/ U
0024700 C ASSUME THE SATURATED PRESSURE IS EXP(A-B/T)
0024800 C      TCB=B/(A-ALOG(P))
0024900 C ASSUME THE SATURATED STEAM OUTPUT
0025000 C      TCO=TCB
0025100 C ASSUME THE LATENT HEAT CAL. BY WATSON CORRELATION
0025200 C      TCI=TCB/TC
0025300 C ASSUME THE AVERAGE HEAT CAPACITY OF WATER IS 1 CAL/G-K
0025400 C      QT=((1.-TCI)/(1.-0.577))*0.38*9700.0*DNSC(6)+(TCB-TCI)*1.*18.
0025500 C      1*DNSC(6)

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0025600      IF(QT.GE.QTI) GO TO 1
0025700      QTI=QTI-QT
0025800      QTS=QT
0025900      GO TO 2
0026000      1 TCO=TCB
0026100      2 CONTINUE
0026200      RETURN
0026300      END
0026302      SUBROUTINE COMP(DNS,TIN,TOU,PIN,POU,POW,GAG,I,IP)
0026304 C*****
0026306 C THIS SUBROUTINE CALCULATES THE BALANCE OF COMPRESSOR
0026308 C*****
0026310 C ASSUMPTION:
0026312 C      (1). IDEAL GAS BEHAVIOR
0026314 C GAG: RATIO OF HEAT CAPACITY
0026316 C WS: SHIFT WORK
0026318 C POW: POWER REQUIRED; HP
0026320 C VO: SPECIFIC VOLUME OF GAS AT APPLIED CONDITION; M**3/G-MOLE
0026322      DIMENSION DNS(I)
0026324      TDNS=0.
0026326      DO 1 IA=1,I
0026328      IF(DNS(IA).EQ.0.) GO TO 1
0026330      TDNS=TDNS+DNS(IA)
0026332      1 CONTINUE
0026334      IF(IP.EQ.2) GO TO 2
0026336      TOUT=TIN*(POU/PIN)**((GAG-1.)/GAG)
0026338      WS=GAG*1.987*TIN*1.8*((POU/PIN)**((GAG-1.)/GAG)-1.)/(GAG-1.)
0026340      POW=WS*TDNS/641400.
0026342      RETURN
0026344      2 TOUT=TIN
0026346      WS=1.987*TIN*1.8*ALOG( POU/PIN)
0026348      POW=WS*TDNS/641400.
0026350      RETURN
0026352      END
0026400      SUBROUTINE COND(THI,THO,DNSH,QT,CH,I)
0026500 C*****
0026520 C THIS SUBROUTINE ESTIMATES THE HEAT DUTY IN THE CONDENSER
0026700 C*****
0026800 C DEFINITION IS THE SAME AS HEXC
0026900      DIMENSION GS(7),HS(7),HCAS(7),HCBS(7),HCCS(7)
0027000      DIMENSION DNSH(I)
0027100      COMMON /ETHDA/ GS,HS,HCAS,HCBS,HCCS
0027120      COMMON/TC/TC
0027200 C CAL. THE MEAN TEMP. OF HOT SIDE
0027300      THM=(THI+THO)/2.
0027400 C CAL. THE CAPACITY RATE OF FLUID OF HOT SIDE
0027500      CH=0.
0027600      DO 1 IA=1,I
0027700      IF(DNSH(IA).EQ.0.) GO TO 1
0027800      CH=CH+DNSH(IA)*(HCAS(IA)+HCBS(IA)*THM+HCCS(IA)*THM**2)
0027900      1 CONTINUE
0028000      QT=0.
0028100      DO 2 IA=1,I
0028200      QT=QT+DNSH(IA)*(HCAS(IA)*(THI-THO)+HCBS(IA)*(THI*THI-THO*THO)

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0028300      1+HCCS(IA)*(THI**3-THO**3))
0028400      2 CONTINUE
0028420      QTL=((1.-(THO/TC))/(1.-0.577))**0.38*9700.*DNSH(6)
0028440      QT=QT+QTL
0028500      RETURN
0028600      END
0028700      SUBROUTINE CONV(XV,YV,NR,NC)
0028800 C*****
0028820 C THIS SUBROUTINE USES WEGSTEIN METHOD FOR ALGEBRAIC CONVERGENCE
0029100 C*****
0029200 C DEFINITION:
0029300 C   XV: TRIAL VALUE
0029400 C   YV: CALCULATED VALUE
0029500 C   NC: CONVERGE INDEX
0029600 C       NC=1 CONVERGE
0029700 C       NC=2 NONCONVERGE
0029800      DIMENSION XA(2),YA(2)
0029900      IF(ABS((XV-YV)/(XV+YV)).LT.0.001) GO TO 2
0030000      IF(NC.LE.1) GO TO 1
0030100      XT=(XA(NR)*YV-YA(NR)*XV)/(XA(NR)-XV+YV-YA(NR))
0030200      XA(NR)=XV
0030300      YA(NR)=YV
0030400      XV=XT
0030500      RETURN
0030600      1 XA(NR)=XV
0030700      YA(NR)=YV
0030800      XV=YV
0030900      NC=2
0031000      RETURN
0031100      2 XV=YV
0031200      NC=1
0031300      RETURN
0031400      END
0031500      SUBROUTINE DIVID(TIN,TOUT1,TOUT2,DNS,DNS1,DNS2,GARM,I)
0031600 C*****
0031700 C THIS SUBROUTINE CALCULATES THE BALANCE AROUND THE DIVIDER
0031800 C*****
0031900 C GARM: DIVIDER FACTOR OF STREAM 32
0032000      DIMENSION DNS(I),DNS1(I),DNS2(I)
0032100 C CAL. THE OUTLET CONDITION
0032200      DO 1 IA=1,I
0032300      DNS1(IA)=GARM*DNS(IA)
0032400      1 CONTINUE
0032500      DO 2 IA=1,I
0032600      DNS2(IA)=(1.-GARM)*DNS(IA)
0032700      2 CONTINUE
0032800      TOUT1=TIN
0032900      TOUT2=TIN
0033000      RETURN
0033100      END
0033200      SUBROUTINE DMIX(DNS1,DNS2,DNS,TIN1,TIN2,TOUT,I,PIN1,PIN2,POUT)
0033300 C*****
0033400 C THIS SUBROUTINE CALCULATES THE BALANCE AROUND THE MIXER
0033500 C*****

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0033600      DIMENSION GS(7),HS(7),HCAS(7),HCBS(7),HCCS(7)
0033700      DIMENSION DNS1(I),DNS2(I),DNS(I)
0033800      COMMON /ETHDA/ GS,HS,HCAS,HCBS,HCCS
0033900 C CAL. THE TOTAL THERMAL CONST.
0034000      TCAS1=0.
0034100      TCBS1=0.
0034200      TCCS1=0.
0034300      TCAS2=0.
0034400      TCBS2=0.
0034500      TCCS2=0.
0034600      DO 1 IA=1,I
0034700      TCAS1=TCAS1+DNS1(IA)*HCAS(IA)
0034800      TCAS2=TCAS2+DNS2(IA)*HCAS(IA)
0034900      TCBS1=TCBS1+DNS1(IA)*HCBS(IA)
0035000      TCBS2=TCBS2+DNS2(IA)*HCBS(IA)
0035100      TCCS1=TCCS1+DNS1(IA)*HCCS(IA)
0035200      TCCS2=TCCS2+DNS2(IA)*HCCS(IA)
0035300      1 CONTINUE
0035400 C ASSUME THE INITIAL VALUE
0035500      TOUT=(TIN1+TIN2)/2.
0035600 C CAL. THE ENERGY BALANCE
0035700      2 TOUTC=(TCAS1*TIN1+TCAS2*(TIN2-TOUT)+TCBS1/2.*(TIN1**2-TOUT**2) -
0035800      1+TCBS2/2.*(TIN2**2-TOUT**2)+TCCS1*(TIN1**3-TOUT**3)/3.+TCCS2 -
0035900      2*(TIN2**3-TOUT**3)/3.)/TCAS1
0036000      CALL CONV(TOUT,TOUTC,1,NC)
0036100      GO TO (3,2),NC
0036200 C CAL. AND WRITE THE OUTLET COMPOSITION
0036300      3 DO 4 IA=1,I
0036400      DNS(IA)=DNS1(IA)+DNS2(IA)
0036500      4 CONTINUE
0036600      TDNS1=0.
0036700      TDNS2=0.
0036800      DO 5 IA=1,7
0036900      TDNS1=TDNS1+DNS1(IA)
0037000      TDNS2=TDNS2+DNS2(IA)
0037100      5 CONTINUE
0037200 C ASSUME PRESSURE DROP TO BE 3% AT MIXER
0037300      POUT=(TDNS1+TDNS2)/(TDNS1*TIN1/PIN1+TDNS2*TIN2/PIN2)*TOUT*0.97
0037400      RETURN
0037500      END
0037600      SUBROUTINE ENFU(DNSA,DNSC,TINC,TINA,TOUT,POP,VOF,UT,M,I,QT,WE,-
0037700      1OU,CD,PT,IJ)
0037800 C*****
0037900 C THIS SUBROUTINE IS TO CAL. ENERGY BALANCE OF FUEL CELL
0038000 C*****
0038100 C DEFINITION:
0038200 C DGR: FREE ENERGY CHANGE AT FUEL CELL CONDITION
0038300 C E: FUEL CELL EQU. POTENTIAL
0038400 C EC: HEATING VALUE EFFICIENCY
0038500 C EFC: FUEL CELL EFFICIENCY
0038600 C EI: CURRENT EFFICIENCY
0038700 C EO: FUEL CELL STANDARD EQU. POTENTIAL
0038800 C EV: VOLTAGE EFFICIENCY
0038900 C FCH4: FRACTION OF METHANE

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0039000 C FME: FRACTION OF METHANOL
0039100 C FNAP: FRACTION OF NAPHTHA
0039200 C M: INDEX OF OUTLET CONDITION
0039300 C M=1 OUTLET TEMP. IS FIXED TO TOPFC
0039400 C M=2 OUTLET TEMP. IS NOT FIXED
0039500 C PCO: MOL. FRACTION OF CO
0039600 C Q: TOTAL HEAT RELEASE PER HR.
0039700 C SIS: INTEGRATION CONST. IN CALCULATING S
0039800 C TAUHO: MOL. FRACTION OF AVAILABLE H2O
0039900 C UT: FUEL UTILIZATION
0040000 C VOP: ACTUAL FUEL CELL POTENTIAL
0040100 C WE: ELECTRICAL WORK
0040200 C HLHV(I): LOWER HEATING VALUE OF GAS I
0040300 DIMENSION GS(7),HS(7),HCAS(7),HCBS(7),HCCS(7)
0040400 DIMENSION HLHV(7),DNSA(7),DNOSC(7),DNS(7),DNSCI(7),DNSAO(7),
0040500 IDNSAI(7)
0040600 COMMON /ETHDA/ GS,HS,HCAS,HCBS,HCCS
0040700 COMMON/CONF/ E,ETH,EI,EV,EC,EFC
0040900 COMMON/HLHV1/ HLHV
0041000 C CAL. THE MOL. FRACTION OF AVAILABLE HYDROGEN
0041100 TDNS=0.
0041200 TDNSC=0.
0041300 DO 1 IA=1,I
0041400 IF(DNSA(IA).EQ.0.) GO TO 1
0041500 TDNS=TDNS+DNSA(IA)
0041600 IF(DNSC(IA).EQ.0.) GO TO 1
0041700 TDNSC=TDNSC+DNSC(IA)
0041800 1 CONTINUE
0041900 IF(IJ.EQ.1) FCH4=DNSA(1)/TDNS
0042000 IF(IJ.EQ.2) FME=DNSA(1)/TDNS
0042100 IF(IJ.EQ.3) FNAP=DNSA(1)/TDNS
0042200 AHLU=DNSA(5)/TDNS
0042300 TAUHO=DNSA(6)/TDNS
0042400 PCO=DNSA(3)/TDNS
0042500 PPH2=SQRT(DNSA(5)/TDNS*DNSA(5)*(1-UT)/(TDNS-DNSA(5)*UT))
0042600 PPCO=SQRT(DNSA(3)/TDNS*DNSA(3)/(TDNS-DNSA(5)*UT))
0042700 PPO2=SQRT(DNSC(2)/TDNSC*DNSC(2)*(1-OU)/(TDNSC+DNSC(2)*OU))
0042800 PPH2O=SQRT(DNSC(6)/TDNSC*DNSC(6)/(TDNSC+DNSC(2)*OU))
0042900 CALL VINEW(1,VOP,CD,POP,PPH2,PPO2,PPH2O,PPCO,
0043000 1X0)
0043100 C CAL. THE OPEN-CIRCUIT POTENTIAL
0043200 DHCAS=HCAS(6)-1./2.*HCAS(2)-HCAS(5)
0043300 DHCBS=HCBS(6)-1./2.*HCBS(2)-HCBS(5)
0043400 DHCCS=HCCS(6)-1./2.*HCCS(2)-HCCS(5)
0043500 DHO=HS(6)-1./2.*HS(2)-HS(5)-DHCAS*298.-1./2.*DHCBS*298.**2-1./3.*
0043600 1DHCCS*298.**3
0043700 SIS=DHO/298.+DHCAS-(GS(6)-1./2.*GS(2)-GS(5))/298.-DHCAS*ALOG(298.)-
0043800 1-DHCBS*298./2.-DHCCS*298.**2/6.
0043900 DG=DHO+(DHCAS-SIS)*TOP-DHCAS*ALOG(TOP)*TOP-DHCBS/2.*TOP**2
0044000 1-DHCCS/6.*TOP**3
0044100 IF(TOP.EQ.463.) DG=-52798.
0044200 EO=-DG/2./23060.
0044300 E=EO+1.987*TOP/2./23060.*ALOG(AHLU*0.21**0.5/TAUHO*POP**0.5)
0044400 C CAL. FREE ENERGY CHANGE AT FUEL CELL CONDITION

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0044500      DGR=-2.*23060.*E*AHLU*TDNS
0044600 C CAL. THE EFFICIENCY
0044700      EV=VOP/E
0044800      EI=UT
0044900 C CAL. THE ELECTRICAL WORK
0045000      WE=-EV*EI*DGR
0045100 C CAL. THE THERMODYNAMIC EFFICIENCY
0045200      DH=(-57798.+DHCAS*(TOP-298.)+DHCBS/2.*(TOP**2-298.**2)+DHCCS*
0045300      1(TOP**3-298.**3)/3.)*AHLU
0045400      IF(TOP.EQ.463) DH=-58186.*AHLU
0045500      ETH=DGR/DH/TDNS
0045600      IF (IJ.EQ.1)
0045700      1DHC=FCH4*(HLHV(1)+(HCAS(4)+2.*HCAS(6)-HCAS(1)-2.*HCAS(2))
0045800      1*(TOP-298.)+(HCBS(4)+2.*HCBS(6)-HCBS(1)-2.*HCBS(2))/2.
0045900      2*(TOP**2-298.**2)+(HCCS(4)+2.*HCCS(6)-HCCS(1)-2.*HCCS(2))/3.
0046000      3*(TOP**3-298.**3))
0046100      IF (IJ.EQ.2)
0046200      1DHC=FME*(HLHV(1)+(HCAS(4)+2.*HCAS(6)-HCAS(1)-1.5*HCAS(2))
0046300      1*(TOP-298.)+(HCBS(4)+2.*HCBS(6)-HCBS(1)-1.5*HCBS(2))/2.
0046400      2*(TOP**2-298.**2)+(HCCS(4)+2.*HCCS(6)-HCCS(1)-1.5*HCCS(2))/3.
0046500      3*(TOP**3-298.**3))
0046600      IF (IJ.EQ.3)
0046700      1DHC=FNAP*(HLHV(1)+(7.*HCAS(4)+8.*HCAS(6)-HCAS(1)-15.*HCAS(2))
0046800      2*(TOP-298.)
0046900      1+(8.*HCBS(6)+7.*HCBS(4)-HCBS(1)-15.*HCBS(2))* (TOP**2-298.**2)/2.
0047000      3+(8.*HCCS(6)+7.*HCCS(4)-HCCS(1)-15.*HCCS(2))/3.
0047100      3*(TOP**3-298.**3))
0047200      DHC=DHC+FCO*(HLHV(3)+(HCAS(4)-HCAS(3)-0.5*HCAS(2))
0047300      4*(TOP-298.)+(HCBS(4)-HCBS(3)-1./2.*HCBS(2))/2.
0047400      5*(TOP**2-298.**2)+(HCCS(4)-HCCS(3)-1./2.*HCCS(2))/3.*(TOP**3-298.
0047500      6**3))+AHLU*(HLHV(5)+(HCAS(6)-HCAS(5)-1./2.*HCAS(2))*(TOP-298.)
0047600      7+(HCBS(6)-HCBS(5)-1./2.*HCBS(2))/2.*(TOP**2-298.**2)+(HCCS(6)
0047700      8-HCCS(5)-1./2.*HCCS(2))/3.*(TOP**3-298.**3))
0047800      EC=DH/DHC
0047900      EFC=ETH*EV*EI*EC
0048000      DO 2 IA=1,I
0048100      DNSCI(IA)=DNSC(IA)
0048200      2 DNSAI(IA)=DNSA(IA)
0048300      CALL FUCE(DNSAI,TOP,POP,DNSA,DNSC,DSO,DSN,DSHO,UT,I,PINF,PINA,IJ)
0048400      DHIN=0.
0048500      DO 3 IA=1,I
0048600      DHIN=CHIN+DNSAI(IA)*(HCAS(IA)*(298.-TINA)+HCBS(IA)/2.*(298.**2
0048700      1-TINA**2)+HCCS(IA)/3.*(298.**3-TINA**3))+DNSCI(IA)*(HCAS(IA)*
0048800      2(298.-TINC)+HCBS(IA)/2.*(298.**2-TINC**2)+HCCS(IA)/3.*
0048900      3(298.**3-TINC**3))
0049000      3 CONTINUE
0049100      DH=-57973.*(DNSAI(5)-DNSA(5))
0049200 C CAL. THE OUTLET COMPOSITION
0049300      DO 4 IA=1,I
0049400      4 DNS(IA)=DNSA(IA)+DNSC(IA)
0049500      TCAS=0.
0049600      TCBS=0.
0049700      TCCS=0.
0049800      DO 5 IA=1,I

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0049900      TCAS=TCAS+DNS(IA)*HCAS(IA)
0050000      TCBS=TCBS+DNS(IA)*HCBS(IA)
0050100      TCCS=TCCS+DNS(IA)*HCCS(IA)
0050200      5 CONTINUE
0050300      TOUT=TOP
0050400      IF(M.EQ.1) GO TO 7
0050500 C CAL. THE OUTLET TEMP.
0050600      6 TOUTC=(-DHIN-DH-WE -TCBS/2.*((TOUT)**2-(298.)**2)-TCCS/3.      -
0050700      1*((TOUT)**3-(298.)**3))/TCAS+298.
0050800      CALL CONV(TOUT,TOUTC,1,NC)
0050900      GO TO (8,6),NC
0051000 C CAL. THE TOTAL HEAT REJECTED PER HR.
0051100      7 QT=-DHIN-DH-WE -TCAS*(TOUT-298.)-TCBS/2.*(TOUT**2-298.**2)      -
0051200      1-TCCS/3.*(TOUT**3-298.**3)
0051300      8 CONTINUE
0051400 C 1 KWHR=860076CAL
0051500      WE=WE/860076.
0051600      RETURN
0051700      END
0051800      SUBROUTINE ENRE(DNS, TOP, POP, TIN, TOUT, I, IP, IJ)
0051900 C*****
0052000 C THIS SUBROUTINE CALCULATES THE ENERGY BALANCE OF REFORMER
0052100 C*****
0052200      DIMENSION GS(7),HS(7),HCAS(7),HCBS(7),HCCS(7)
0052300      DIMENSION DNS(7),DINS(7),X(2)
0052400      COMMON/ETHDA/ GS,HS,HCAS,HCBS,HCCS
0052500 C STORE THE INLET COMPOSITION
0052600      DO 1 IA=1,I
0052700      DINS(IA)=DNS(IA)
0052800      1 CONTINUE
0052900 C CALCULATE THE OUTLET COMP.
0053000      CALL REF(DNS, TOP, POP, X, I, IJ)
0053100      IF(IP.EQ.1) GO TO 2
0053200      TOUT=TIN
0053300      GO TO 6
0053400      2 CONTINUE
0053500 C CALCULATE THE ENTHALPY CHANGE WITH TEMP. OF INLET GAS
0053600      DHIN=0.
0053700      DO 3 IA=1,I
0053800      IF(DINS(IA).EQ.0.) GO TO 3
0053900      DHIN=DHIN+DINS(IA)*(HCAS(IA)*(298.-TIN)+HCBS(IA)/2.*((298.)**2      -
0054000      1-TIN**2)+HCCS(IA)/3.*((298.)**3-(TIN)**3))
0054100      3 CONTINUE
0054200 C CALCULATE THE ENTHALPY CHANGE OF REACTION
0054300      IF (IJ.EQ.1)      -
0054400      1DH1=(HS(3)+3.*HS(5)-HS(1)-HS(6))*X(1)
0054500      IF (IJ.EQ.2)      -
0054600      1DH1=(HS(4)+3.*HS(5)-HS(1)-HS(6))*X(1)
0054700      IF (IJ.EQ.3)      -
0054800      1DH1=(7.*HS(3)+15.*HS(5)-HS(1)- 7.*HS(6))*X(1)
0054900      IF(IJ.EQ.2)      -
0055000      1DH2=(HS(3)+2.*HS(5)-HS(1))*X(2)
0055100      IF ((IJ.EQ.1).OR.(IJ.EQ.3))      -
0055200      1DH2=(HS(4)+HS(5)-HS(3)-HS(6))*X(2)

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0055300      DH=DH1+DH2
0055400 C CALCULATE THE TOTAL HEAT CAP. CONSTANT OF OUTLET GAS
0055500      TCAS=0.
0055600      TCBS=0.
0055700      TCCS=0.
0055800      DO 4 IA=1,I
0055900      IF(DNS(IA).EQ.0.) GO TO 4
0056000      TCAS=TCAS+DNS(IA)*HCAS(IA)
0056100      TCBS=TCBS+DNS(IA)*HCBS(IA)
0056200      TCCS=TCCS+DNS(IA)*HCCS(IA)
0056300      4 CONTINUE
0056400 C CALCULATE THE MAX. TEMP. OF OUTLET GAS
0056500      TOUT=TOP-500.
0056600      5 TOUTC=(-DH-DHIN-TCBS/2.*((TOUT)**2-(298.)**2)-TCCS/3.*((TOUT)**3 -
0056700      1-(298.)**3))/TCAS+298.
0056800      CALL CONV(TOUT,TOUTC,1,NC)
0056900      GO TO (6,5),NC
0057000      6 CONTINUE
0057100      RETURN
0057200      END
0057300      SUBROUTINE ENSH(DNS,TIN,TOUT,TOP,PIN,I,IP,IJ)
0057400 C*****
0057500 C THIS SUBROUTINE CALCULATES THE ENERGY BALANCE OF SHIFT CONVERTER
0057600 C*****
0057700      DIMENSION GS(7),HS(7),HCAS(7),HCBS(7),HCCS(7)
0057800      DIMENSION DNS(7),DINS(7)
0057900      COMMON/ETHDA/ GS,HS,HCAS,HCBS,HCCS
0058000 C STORE THE INITIAL COMPOSITION
0058100      DO 1 IA=1,I
0058200      1 DINS(IA)=DNS(IA)
0058300      CALL PDSH(DINS,PIN,POUT,TOP,1,IJ)
0058400      POP=(PIN+POUT)/2.
0058500 C CALCULATE THE OUTLET COMPOSITION
0058600      CALL SHIFT(DNS,POP,X,I)
0058700      IF(IP.EQ.1) GO TO 2
0058800      TOUT=TIN
0058900      GO TO 6
0059000      2 CONTINUE
0059100 C CALCULATE THE ENTHALPY CHANGE WITH TEMP. OF INLET GAS
0059200      DHIN=0.
0059300      DO 3 IA=1,I
0059400      IF(DNS(IA).EQ.0.) GO TO 3
0059500      DHIN=DHIN+DINS(IA)*(HCAS(IA)*(298.-TIN)+HCBS(IA)/2.*((298.)**2-
0059600      1(TIN)**2)+HCCS(IA)/3.*((298.)**3-(TIN)**3))
0059700      3 CONTINUE
0059800 C CALCULATE THE ENTHALPY CHANGE OF REACTION
0059900      DH=(HS(4)+HS(5)-HS(3)-HS(6))*X
0060000      TCAS=0.
0060100      TCBS=0.
0060200      TCCS=0.
0060300      DO 4 IA=1,I
0060400      IF(DNS(IA).EQ.0.) GO TO 4
0060500      TCAS=TCAS+DNS(IA)*HCAS(IA)
0060600      TCBS=TCBS+DNS(IA)*HCBS(IA)

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0060700      TCCS=TCCS+DNS(IA)*HCCS(IA)
0060800      4 CONTINUE
0060900 C CALCULATE THE MAX. TEMPERATURE OF OUTLET GAS
0061000      TOUT=TOP+10.
0061100      5 TOUTC=(-DH-DHIN-TCBS/2.*((TOUT)**2-(298.)**2)-TCCS/3.*((TOUT)**3 -
0061200      1-(298.)**3))/TCAS+298.
0061300      CALL CONV(TOUT,TOUTC,1,NC)
0061400      GO TO (6,5),NC
0061500      6 CONTINUE
0061600      RETURN
0061700      END
0061800      SUBROUTINE EQUK(NNS, TOP, SK, I)
0061900 C*****
0062000 C THIS SUBROUTINE CALCULATES THE EQUALIBRIUM CONSTANT
0062100 C*****
0062200 C      R: GAS CONSTANT;G-CAL/G-MOLE-K
0062300 C      TST: STANDARD TEMPERATURE; K
0062400 C
0062500      DIMENSION GS(7),HS(7),HCAS(7),HCBS(7),HCCS(7)
0062600      DIMENSION NNS(I)
0062700      COMMON /ETHDA/ GS,HS,HCAS,HCBS,HCCS
0062800      DATA R/1.987/
0062900      DATA TST/298./
0063000 C CAL. THE TOTAL HEAT CAPACITY CONSTANT
0063100      TCAS=0.
0063200      TCBS=0.
0063300      TCCS=0.
0063400      DO 1 IA=1,I
0063500      IF(NNS(IA).EQ.0) GO TO 1
0063600      TCAS=TCAS+NNS(IA)*HCAS(IA)
0063700      TCBS=TCBS+NNS(IA)*HCBS(IA)
0063800      TCCS=TCCS+NNS(IA)*HCCS(IA)
0063900      1 CONTINUE
0064000 C CAL. HEAT CHANGE OF REACTION
0064100      DH=0.
0064200      DO 2 IA=1,I
0064300      IF(NNS(IA).EQ.0) GO TO 2
0064400      DH=DH+NNS(IA)*HS(IA)
0064500      2 CONTINUE
0064600 C CAL. FREE ENERGY OF REACTION
0064700      DG=0.
0064800      DO 3 IA=1,I
0064900      IF(NNS(IA).EQ.0) GO TO 3
0065000      DG=DG+NNS(IA)*GS(IA)
0065100      3 CONTINUE
0065200 C CAL. HEAT CONST.
0065300      DHQ=DH-TCAS*TST-TCBS*TST**2/2.-TCCS*TST**3/3.
0065400 C CAL. CONST. AI
0065500      AI=(DHQ-DG-TCAS*TST*ALOG(TST)-TCBS/2.*TST**2-TCCS/6.*TST**3)/TST/R
0065600 C CAL. EQU. CONST.
0065700      SK=EXP(-DHQ/R/TOP+TCAS/R*ALOG(TOP)+TCBS/2.*TOP/R+TCCS/6./R*TOP**2 -
0065800      1+AI)
0065900      RETURN
0066000      END

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0066100      SUBROUTINE FLAME(DNS,TIN,TF,I,IJ)
0066200 C*****
0066300 C THIS SUBROUTINE CALCULATES THE MAX. ADIABATIC FLAME TEMPERATURE
0066400 C FOR 200% THEORETICAL AIR
0066500 C*****
0066600 C ASSUMPTION:
0066700 C      (1). THE COMBUSTION PROCESS GOES TO COMPLETION
0066800 C      (2). HEAT LOSSES ARE NEGLIGIBLE
0066900 C      (3). NEGLIGIBLE DISSOCIATION OF THE PRODUCTS OF COMBUSTION
0067000 C      (4). PRESSURE IS LOW AROUND 1ATM
0067100 C TF: MAX. TEMPERATURE OF ADIABATIC FLAME
0067200      DIMENSION GS(7),HS(7),HCAS(7),HCBS(7),HCCS(7)
0067300      DIMENSION DNS(7),DINS(7)
0067400      COMMON/ETHDA/ GS,HS,HCAS,HCBS,HCCS
0067500      COMMON /EXT/EXT
0067600 C STORE THE INLET FLUID
0067700      DO 1 IA=1,I
0067800      DINS(IA)=DNS(IA)
0067900      1 CONTINUE
0068000 C CALCULATE THE EXIT FLUID
0068100      CALL BURN(DNS,I,IJ)
0068200 C CALCULATE THE HEAT CHANGE OF REACTION AT 298 K
0068300      DH=0.
0068400      DO 2 IA=1,I
0068500      IF(DNS(IA).EQ.0.) GO TO 2
0068600      DH=DH+DNS(IA)*HS(IA)
0068700      2 CONTINUE
0068800      DO 3 IA=1,I
0068900      IF(DINS(IA).EQ.0.) GO TO 3
0069000      DH=DH-DINS(IA)*HS(IA)
0069100      3 CONTINUE
0069200 C CALCULATE THE ENTHALPY WITH TEMP. CHANGE
0069300      DO 4 IA=1,I
0069400      IF(DINS(IA).EQ.0.) GO TO 4
0069500      DH=DH+DINS(IA)*(HCAS(IA)*(298.-TIN)+HCBS(IA)/2.*((298.)**2-TIN**2)-
0069600      1+HCCS(IA)/3.*((298.)**3-TIN**3))
0069700      4 CONTINUE
0069800 C CALCULATE THE TOTAL HEAT CAPACITY CONSTANT
0069900      TCAS=0.
0070000      TCBS=0.
0070100      TCCS=0.
0070200      DO 5 IA=1,I
0070300      IF(DNS(IA).EQ.0.) GO TO 5
0070400      TCAS=TCAS+DNS(IA)*HCAS(IA)
0070500      TCBS=TCBS+DINS(IA)*HCBS(IA)
0070600      TCCS=TCCS+DINS(IA)*HCCS(IA)
0070700      5 CONTINUE
0070800 C CALCULATE THE MAX. TEMPERATURE
0070900      TF=TIN+500.
0071000      6 TFC=(-DH-TCBS/2.*((TF)**2-(298.)**2)-TCCS/3.*((TF)**3-(298.)**3)) -
0071100      1/TCAS+298.
0071200      CALL CONV(TF,TFC,1,NC)
0071300      GO TO (7,6),NC
0071400      7 CONTINUE

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0071500     RETURN
0071600     END
0071700     SUBROUTINE FUCE(DNS, TOP, POP, DNSA, DNSC, DSO, DSN, DSHO, UT, I, PINF, PINA, -
0071800     IJJ)
0071900 C*****
0072000 C THIS SUBROUTINE CALCULATES THE MASS BALANCE OF FUEL CELL
0072100 C*****
0072200 C X : CONSUMPTION OF H2 IN THE FUEL CELL UNDER UT UTILIZATION
0072300     DIMENSION GS(7), HS(7), HCAS(7), HCBS(7), HCCS(7)
0072400     DIMENSION DNS(7), DNSA(7), DNSC(7), NNS(7)
0072500     COMMON /EXA/ EXA
0072600     COMMON /HUMI/ WAT
0072700     X=UT*DNS(5)
0072800 C CAL. AND WRITE THE INLET COMPOSITION OF AIR
0072900     1 DSO=(1.+EXA/100.)*(1./2.*X-DNS(2))
0073000     DSN=DSO*3.76
0073100     DSHO=((DSO+DSN)*26.8)*WAT/18.
0073200 C CAL. AND WRITE THE OUTLET COMPOSITION
0073300     DO 2 IA=1,I
0073400     DNSA(IA)=DNS(IA)
0073500     2 CONTINUE
0073600     DNSA(5)=DNS(5)-X
0073700     DO 3 IA=1,I
0073800     DNSC(IA)=0.
0073900     3 CONTINUE
0074000     DNSC(2)=EXA/100.*(1./2.*X-DNS(2))
0074100     DNSC(6)=DSHO+X
0074200     DNSC(7)=DSN
0074300     CALL PDFU(DNSA, DNSC, DNS, DSO, DSN, DSHO, POP, TOP, PINF, PINA, IJ)
0074400     RETURN
0074500     END
0074600     SUBROUTINE HEPD(DNSA, DNSC, THM, TCM, HA, PINT, PINS, N, DPJ, DP, NT, TCO, TCI-
0074700     1, IJ)
0074710 C*****
0074740 C THIS SUBROUTINE CALCULATES PRESSURE DROP IN THE HEAT EXCHANGER
0074760 C*****
0074765 C DP : PRESSURE DROP ON THE SHELL SIDE
0074770 C DPJ : PRESSURE DROP ON THE TUBE SIDE
0074775 C REJ : REYNOLDS NUMBER OF TUBE SIDE
0074780 C GS : SHELL SIDE MASS VELOCITY
0074785 C FPRI : FRICTION FACTOR
0074800     REAL IDT, IDS, DNSA(7), DNSC(7)
0074900     DIMENSION FLI(7), C(7), CH(7), WM(7), FLJ(7), CMJ(7), CJ(7)
0075000     COMMON /WM/ WM
0075100     COMMON /HEPDT/ NP, NR, BSPAC, ODT, PITCH, CL, IDS, IDT, FLOOR, SURFC
0075200     1, CLEN, SITS2, DTH
0075300 C*****
0075400 C HEAT EXCHANGER BASIS: 3/4 IN TUBE OD AND BWG 14
0075500 C*****
0075600 C CALCULATE NO. OF TUBES
0075700     NT= HA /0.3048**2/NP/CLEN/SURFC
0075800 C CAL. NO. OF BAFFLES
0075900     NB=CLEN/BSPAC
0076000 C CAL. FREE AREA BETWEEN BAFFLES

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0076100      FAREA=IDS/(ODT+CL)*CL*BSPAC
0076200 C CAL. CORRECTION FACTOR
0076300      BO=NS+1.
0076400 C CAL. RATIO OF PITCH TRANSVERSE TO FLOW TO TUBE DIA.
0076500      XT=PITCH/ODT
0076600      IF (IJ.GT.3) GO TO 2
0076700 C INSERT FLOW RATE OF EACH GAS
0076800 C SHELLSIDE CALCULATIONS
0076900      FLI(1)=DNSA(1)/453.6
0077000      FLI(2)=DNSA(3)/453.6
0077100      FLI(3)=DNSA(4)/453.6
0077200      FLI(4)=DNSA(6)/453.6
0077300      FLI(5)=DNSA(5)/453.6
0077400      FLI(6)=DNSA(7)/453.6
0077500      FLI(7)=DNSA(2)/453.6
0077600      FI=FLI(1)+FLI(2)+FLI(3)+FLI(4)+FLI(5)+FLI(6)+FLI(7)
0077700      DO 1 I=1,7
0077800      CM(I)=FLI(I)/FI
0077900      1 CONTINUE
0078000      AMW=CM(1)*WM(1)+CM(2)*WM(3)+CM(3)*WM(4)+CM(4)*WM(6)+CM(5)*WM(5) -
0078100      1+CM(6)*WM(7)+CM(7)*WM(2)
0078200      TF=(THM -273.16)*1.8+32.
0078300      CALL CMASS(C,FLI,FI)
0078400      AMUI=VIS(C,TF,IJ)
0078500      RHO=(AMW*PINS)/(0.7302*(TF+460.))
0078600 C CAL. SHELL SIDE MASS VELOCITY ACROSS TUBES
0078700      GS=FI*AMW/FAREA
0078800 C CAL. CONST. SBO (FOR STAGGERED TUBES)
0078900      SBO=0.23+0.11/(XT-1.)*1.08
0079000 C CAL. FRICTION FACTOR
0079100      FPRI=SBO*(ODT*GS/AMUI)**(-0.15)
0079200 C CAL. PRESSURE DROP OF SHELL SIDE FLOW
0079300      DP= BO*2.*FPRI*NR*GS**2/32.174/3600.**2/RHO/2116.2
0079400      2 CONTINUE
0079500 C TUBESIDE CALCULATIONS
0079600      FLJ(1)=DNSC(1)/453.6
0079700      FLJ(2)=DNSC(3)/453.6
0079800      FLJ(3)=DNSC(4)/453.6
0079900      FLJ(4)=DNSC(6)/453.6
0080000      FLJ(5)=DNSC(5)/453.6
0080100      FLJ(6)=DNSC(7)/453.6
0080200      FLJ(7)=DNSC(2)/453.6
0080300      FJ=FLJ(1)+FLJ(2)+FLJ(3)+FLJ(4)+FLJ(5)+FLJ(6)+FLJ(7)
0080400      DO 3 JJ=1,7
0080500      CMJ(JJ)=FLJ(JJ)/FJ
0080600      3 CONTINUE
0080700      AMJ=CMJ(1)*WM(1)+CMJ(2)*WM(3)+CMJ(3)*WM(4)+CMJ(4)*WM(6) -
0080800      1+CMJ(5)*WM(5)+CMJ(6)*WM(7)+CMJ(7)*WM(2)
0080900      DT=DTH*(THM-TCM)
0081000      TW=DT+TCM
0081100      TW=(TW-273.16)*1.8+32.
0081200      TCF=(TCM-273.16)*1.8+32.
0081300      CALL CMASS(CJ,FLJ,FJ)
0081400      AMUJ=VIS(CJ,TCF,IJ)

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0081500      AMUW=VIS(CJ,TWF,IJ)
0081600      IF((AMUJ.LE.0.).OR.(AMUW.LE.0.)) GO TO 10
0081700      TKC=THC(CJ,TCF,IJ)
0081800      CP=HTCP(CJ,TCF,IJ)
0081900      AROH=(AWM*PINT)/(0.7302*(TCF+460.))
0082000      GJ=FJ*AHM /FLOOR/NT
0082100      REJ=GJ*IDT/AMUJ
0082200      IF(REJ.LE.2100.)GO TO 4
0082300      SF=0.046/REJ**0.2
0082400      GO TO 5
0082500      4 SF=16./REJ
0082600      5 CONTINUE
0082700      IF(S1TS2.GT.0.715) GO TO 6
0082800      CKC=0.4*(1.25-S2TS1)
0082900      GO TO 7
0083000      6 CKC=0.75*(1.-S2TS1)
0083100      7 CCNTINUE
0083200      CK1=(1.-S2TS1)**2+CKC+0.5*(NP-1.)/NP
0083300      IF(REJ.GT.2100.) GO TO 8
0083400      PHI=1.1*(AMUJ/AMUW)**0.25
0083500      BI=1.+CK1*IDT*PHI/4./SF/CLEN
0083600      GO TO 9
0083700      8 PHI=1.02*(AMUJ/AMUW)**0.14
0083800      BI=1.+0.51*CK1*NP*(TW -TCM)*(AMUJ/AMUW)**0.28/(TCO-TCI)
0083900      1/(CP*AMUJ/TKC/AWM )**0.6667
0084000 C CAL. TUBESIDE DP
0084100      9 DPJ= BI*2.*SF*GJ**2*CLEN*NP/32.17/3600.**2/AROH/IDT/PHI/2116.2
0084200      GO TO 12
0084300      10 DPJ=0.
0084400      WRITE(6,11)
0084500      11 FORMAT('THE TRYING TEMP. IS BELOW THE LIMIT OF CAL. VISCOSITY')
0084600      12 CONTINUE
0084700      RETURN
0084800      END
0084900      SUBROUTINE HEXC(THI,DNSH,DNSC,TCI,THO,TCO,QT,MOD,HA,N,M,I,PT,PS,NT-
0085000      1,IJ)
0085100 C*****
0085200 C THIS SUBROUTINE IS TO CAL. THE ENERGY ANALYSIS FOR HAET EXCHANGER
0085300 C*****
0085400 C CC: CAPACITY RATE OF FLUID ON COLD SIDE ,DNSC*CPC
0085500 C CH: CAPACITY RATE OF FLUID ON HOT SIDE, DNSH*CPH
0085600 C CMAX: MAX. CAPACITY RATE
0085700 C CMIN: MIN. CAPACITY RATE
0085800 C CPC: SPECIFIC HEAT OF COLD SIDE FLUID
0085900 C CPH: SPECIFIC HEAT OF HOT SIDE FLUID
0086000 C HE: HEAT EXCHANGER EFFECTIVENESS
0086100 C QT: TOTAL HEAT TRANSFER RATE ACROSS HEAT EXCHANGER
0086200 C QMAX: THE MAX. HEAT TRANSFER RATE ACROSS HEAT EXCHANGER
0086300 C TCI: COLD SIDE INLET TEMPERATURE
0086400 C TCO: COLD SIDE OUTLET TEMPERATURE
0086500 C THI: HOT SIDE INLET TEMPERATURE
0086600 C THO: HOT SIDE OUTLET TEMPERATURE
0086700 C UA: OVERALL HEAT TRANSFER CCEFFICIENT OF EXCHANGER
0086800 C MOD: TYPE OF HEAT EXCHANGER

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0086900 C      MOD=1 COUNTERFLOW
0087000 C      MOD=2 CROSS FLOW
0087100 C      MOD=3 CONDENSER
0087200 C      THM: MEAN TEMP. OF HOT SIDE
0087300 C      TCM: MEAN TEMP. OF COLD SIDE
0087400 C      N: THE NUMBER OF HEAT EXCHANGER
0087500 C      M: THE INDEX OF INITIAL CONDITION
0087600 C      M=1 TEMP. OF BOTH SIDES ARE KNOWN
0087700 C      M=2 TEMP. OF HOT SIDE INLET AND COLD SIDE OUTLET ARE KNOWN
0087800      DIMENSION GS(7),HS(7),HCAS(7),HCBS(7),HCCS(7)
0087900      DIMENSION DNSH(7),DNSC(7)
0088000      COMMON /ETHDA/ GS,HS,HCAS,HCBS,HCCS
0088100      COMMON/UL/ U
0088200      COMMON/CH1/ CN
0088300      COMMON/HE/ HE
0088400 C ASSUME THE MEAN TEMP. AT COLD AND HOT SIDE
0088500      IF(M.EQ.2) GO TO 1
0088600      THM=(THI+10.+TCI)/2.
0088700      TCM=(THI-10.+TCI)/2.
0088800      GO TO 2
0088900      1 THM=(THI+TCO-50.)/2.
0089000      TCM=(TCO*2.-200.)/2.
0089100 C CAL. CC AND CH
0089200      2 CC=0.
0089300      CH=0.
0089400      DO 4 IA=1,I
0089500      IF(DNSC(IA).EQ.0.) GO TO 3
0089600      CC=CC+DNSC(IA)*(HCAS(IA)+HCBS(IA)*TCM+HCCS(IA)*TCM**2)
0089700      3 IF(DNSH(IA).EQ.0.) GO TO 4
0089800      CH=CH+DNSH(IA)*(HCAS(IA)+HCBS(IA)*THM+HCCS(IA)*THM**2)
0089900      4 CONTINUE
0090000 C CHOOSE THE CMAX. ,CMIN.
0090100      IF(CC.GT.CH) GO TO 5
0090200      CMAX=CH
0090300      CMIN=CC
0090400      GO TO 6
0090500      5 CMAX=CC
0090600      CMIN=CH
0090700      6 CONTINUE
0090800      HA=CN*CMIN/U
0090900      UA=HA*U
0091000 C CAL. THE HEAT EXCHANGER EFFECTIVENESS
0091100      IF(MOD.GE.2) GO TO 8
0091200      IF((CMIN/CMAX).GT.0.01) GO TO 7
0091300      HE=1.-EXP(-UA/CMIN)
0091400      GO TO 12
0091500      7 HE=(1.-EXP((-UA/CMIN)*(1.-CMIN/CMAX)))/(1.-((CMIN/CMAX)*EXP((-UA
0091600      1/CMIN)*(1.-CMIN/CMAX)))
0091700      GO TO 12
0091800      8 IF(MOD.GT.2) GO TO 11
0091900      IF(ABS(CMIN/CMAX-1.).GE.0.01) GO TO 9
0092000      HE=(UA/CMIN)/(UA/CMIN+1.)
0092100      GO TO 12
0092200      9 IF((CMIN/CMAX).GT.0.01) GO TO 10

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0092300      HE=1.-EXP(-UA/CMIN)
0092400      GO TO 12
0092500      10 IF(CMAX.EQ.CH) HE=1.-EXP((-CMAX/CMIN)*(1.-EXP(-UA/CMAX)))
0092600      IF(CMIN.EQ.CH) HE=(CMAX/CMIN)*(1.-EXP((-CMIN/CMAX)*(1.-EXP(-UA/
0092700      LCMIN))))
0092800      GO TO 12
0092900      11 HE=1.-EXP(-UA/CMIN)
0093000 C CAL. THE OUTLET CONDITION AND TOTAL HEAT TRANSFER RATE
0093100      12 IF(M.EQ.2) GO TO 13
0093200      THO=THI-HE*(CMIN/CH)*(THI-TCI)
0093300      TCO=HE*(CMIN/CC)*(THI-TCI)+TCI
0093400      QT=HE*CMIN*(THI-TCI)
0093500      GO TO 14
0093600      13 TCI=(HE*(CMIN/CC)*THI-TCO)/(HE*(CMIN/CC)-1.)
0093700      THO=THI-HE*(CMIN/CH)*(THI-TCI)
0093800      QT=HE*CMIN*(THI-TCI)
0093900      14 IF((ABS((THO+THI)/2.-THM).LT.(ABS((THO+THI)/2.+THM)*0.005)
0094000      1).AND.(ABS((TCO+TCI)/2.-TCM).LT.(ABS((TCO+TCI)/2.+TCM)*0.005)))
0094100      2 GO TO 15
0094200      THM=(THO+THI)/2.
0094300      TCM=(TCO+TCI)/2.
0094400      GO TO 2
0094500      15 THM=(THO+THI)/2.
0094600      TCM=(TCO+TCI)/2.
0094700      CALL HEPD(DNSH,DNSC,THM,TCM,HA,PT,PS,N,DPJ,DP,NT,TCO,TCI,I,J)
0094800      IF(M.EQ.2) GO TO 16
0094900      PT=PT-DPJ
0095000      PS=PS-DP
0095100      GO TO 17
0095200      16 PT=PT+DPJ
0095300      PS=PS-DP
0095400      17 CONTINUE
0095500      RETURN
0095600      END
0095700      SUBROUTINE PDFU(DNSA,DNSC,DNS,DSO,DSN,DSHO,POP,ATMP,PINF,PINA,IJ)
0095710 C*****
0095720 C THIS SUBROUTINE CALCULATES PRESSURE DROP IN THE FUEL CELL STACK
0095730 C*****
0095800      REAL L(2),DP(4)
0095900      DIMENSION FLI(7),C(7),CM(7),WM(7),DNSA(7),DNSC(7),DNS(7),DNSI(7)
0096000      DIMENSION NTA(2), WIDA(2),D(2)
0096100      COMMON/PDFUT/ NTA,L,WIDA,NP
0096200      COMMON /WM/ WM
0096300 C*****
0096400 C BASIS: NO. 522 STACK
0096500 C*****
0096600      IT=1
0096700      DO 1 IA=1,7
0096800      1 DNSI(IA)=0.
0096900      DNSI(4)=DSHO
0097000      DNSI(6)=DSN
0097100      DNSI(7)=DSO
0097200 C CAL. THE PRESSURE DROP OF FUEL SIDE
0097300      JJ=1

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0097400      D(1)=WIDA(1)
0097500      FLI(1)=DNS(1)/453.6
0097600      FLI(2)=DNS(3)/453.6
0097700      FLI(3)=DNS(4) /453.6
0097800      FLI(4)=DNS(6) /453.6
0097900      FLI(5)=DNS(5) /453.6
0098000      FLI(6)=DNS(7)/453.6
0098100      FLI(7)=DNS(2)/453.6
0098200      GO TO 3
0098300      2 FLI(1)=DNSA(1)/453.6
0098400      FLI(2)=DNSA(3)/453.6
0098500      FLI(3)=DNSA(4)/453.6
0098600      FLI(4)=DNSA(6)/453.6
0098700      FLI(5)=DNSA(5)/453.6
0098800      FLI(6)=DNSA(7)/453.6
0098900      FLI(7)=DNSA(2)/453.6
0099000      3 CONTINUE
0099100      TK=ATMP
0099200      FI=FLI(1)+FLI(2)+FLI(3)+FLI(4)+FLI(5)+FLI(6)+FLI(7)
0099300      DO 4 I=1,7
0099400      CM(I)=FLI(I)/FI
0099500      4 CONTINUE
0099600      AMW=CM(1)*WM(1)+CM(2)*WM(3)+CM(3)*WM(4)+CM(4)*WM(6)+CM(5)*WM(5) -
0099700      1+CM(6)*WM(7)+CM(7)*WM(2)
0099800      G=FI*AMW/WIDA(IT)**2/NP/NTA(IT)
0099900      TF=(TK-273.16)*1.8+32.
0100000      CALL CMASS(C,FLI,FI)
0100100      AMUI=VIS(C,TF,IJ)
0100200      RHO=(AMW*POP)/(0.7302*(TF+460.))
0100300      RE=D(IT)*G/AMUI
0100400      CONS=57.2
0100500      FRIC=CONS/RE
0100600      DP(JJ)=RHO*(G/RHO)**2/2.*(0.5+1.+0.6+FRIC*L(IT)/D(IT))/2116.2 -
0100700      1/3600.**2/32.174
0100800      JJ=JJ+1
0100900      IF(JJ.EQ.2) GO TO 2
0101000      IF(JJ.EQ.3) GO TO 5
0101100      IF(JJ.EQ.4) GO TO 6
0101200      IF(JJ.EQ.5) GO TO 8
0101300 C CAL. THE PRESSURE DROP OF AIR SIDE
0101400 C INSERT THE FLOW RATE OF EACH GAS
0101500      5 FLI(1)=DNSC(1)/453.6
0101600      FLI(2)=DNSC(3)/453.6
0101700      FLI(3)=DNSC(4)/453.6
0101800      FLI(4)=DNSC(6)/453.6
0101900      FLI(5)=DNSC(5)/453.6
0102000      FLI(6)=DNSC(7)/453.6
0102100      FLI(7)=DNSC(2)/453.6
0102200      IT=IT+1
0102300      D(2)=WIDA(2)
0102400      GO TO 3
0102500      6 DO 7 IA=1,7
0102600      7 FLI(IA)=DNSI(IA)/453.6
0102700      GO TO 3

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0102800      8 CONTINUE
0102900      PINF=PINF-(DP(1)+DP(2))/2.
0103000      PINA=PINA-(DP(3)+DP(4))/2.
0103100      RETURN
0103200      END
0103300      SUBROUTINE POSH(DNS,PIN,POUT,TK,JK,IJ)
0103400 C*****
0103500 C THIS SUBROUTINE CALCULATES PRESSURE DROP IN THE SHIFT CONVERTER
0103600 C*****
0103700      DIMENSION D(2),AHRN(2),AP(2),CLEN(2),NT(2)
0103800      DIMENSION FLI(7),C(7),CM(7),WM(7),DNS(7)
0103900      COMMON/PDSHT/ D,AHRN,AP,CLEN,NT
0104000      COMMON /WM/ WM
0104100 C JK=1 SHIFT CONVERTER
0104200 C JK=2 REFORMER FOR METHANOL AND NAPHTHA FUEL
0104300      TF=(TK-273.16)*1.8+32.
0104400      DP=6.*(1.-AHRN(JK))/AP(JK)
0104500      FLI(1)=DNS(1)/453.6/NT(JK)
0104600      FLI(2)=DNS(3)/453.6/NT(JK)
0104700      FLI(3)=DNS(4)/453.6/NT(JK)
0104800      FLI(4)=DNS(6)/453.6/NT(JK)
0104900      FLI(5)=DNS(5)/453.6/NT(JK)
0105000      FLI(6)=DNS(7)/453.6/NT(JK)
0105100      FLI(7)=DNS(2)/453.6/NT(JK)
0105200      FI=FLI(1)+FLI(2)+FLI(3)+FLI(4)+FLI(5)+FLI(6)+FLI(7)
0105300      DO 1 I=1,7
0105400      CM(I)=FLI(I)/FI
0105500      1 CONTINUE
0105600      AMW=CM(1)*WM(1)+CM(2)*WM(3)+CM(3)*WM(4)+CM(4)*WM(6)+CM(5)*WM(5) -
0105700      1+CM(6)*WM(7)+CM(7)*WM(2)
0105800      G=FI*AMW*4./((3.14159*D(JK)**2)
0105900      CALL CMASS(C,FLI,FI)
0106000      AMUI=VIS(C,TF,IJ)
0106100      RHO=(AMW*PIN)/(0.7302*(TF+460.))
0106200      DELP=CLEN(JK)*(1.-AHRN(JK))/AHRN(JK)**3*G**2/DP/4.18E+08 -
0106300      1/RHO*(150.*(1.-AHRN(JK))*AMUI/DP/G+1.75)/2116.2
0106400      POUT=PIN-DELP
0106500      RETURN
0106600      END
0106700      SUBROUTINE PUMP(DNS,TIN,TOUT,PIN,POUT,POW,I)
0106800 C*****
0106900 C THIS SUBROUTINE IS TO CAL. THE BALANCE OF PUMP FOR WATER
0107000 C*****
0107100 C ASSUMPTION AND DEFINITION IS THE SAME AS COMPR
0107200      DIMENSION DNS(7)
0107300      DIMENSION SV(3),WM(7)
0107400      COMMON/WM/ WM
0107500      COMMON/SV/ SV,SVW
0107600      TOUT=TIN
0107700 C CAL. THE WCRK
0107800 C ASSUME AVERAGE SPECIFIC VOLUME OF WATER IS 0.0162 FT**3/LBM
0107900      POW=SVW*144.*5.05051*0.000001*WM(6)*14.7*(POUT-PIN)*DNS(6) -
0108000      1/453.6
0108100      RETURN

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0108200      END
0108300      SUBROUTINE PUP(DNS,TIN,TOUT,PIN,POUT,POW,I,IJ)
0108400 C*****
0108500 C THIS SUBROUTINE CALCULATES POWER NEEDED IN THE FUEL PUMP
0108600 C*****
0108700      DIMENSION DNS(7),WM(7),SV(3)
0108800      COMMON/SV/ SV,SVW
0108900      COMMON/WM/ WM
0109000      TOUT=TIN
0109100      POW=SV(IJ)*144.*5.05051*0.0000001*WM(IJ)*14.7*(POUT-PIN)
0109200      1*DNS(1)/453.6
0109300      RETURN
0109400      END
0109500      SUBROUTINE REF(DNS,POP,POP,X,I,IJ)
0109600 C*****
0109700 C THIS SUBROUTINE IS TO CALCULATE THE MASS BALANCE OF REFORMER
0109800 C*****
0109900      DIMENSION NNS1(7),NNS2(7),DNS(7),SK1(2),X(2)
0110000 C CALCULATE THE EQU. CONSTANT OF REACTION 1
0110100      DO 1 IA=1,I
0110200      1 NNS1(IA)=0
0110300      IF (IJ.EQ.3) GO TO 2
0110400      IF (IJ.EQ.1) NNS1(3)=1
0110500      IF (IJ.EQ.2) NNS1(4)=1
0110600      NNS1(1)=-1
0110700      NNS1(6)=-1
0110800      NNS1(5)=3
0110900      GO TO 3
0111000      2 NNS1(1)=-1
0111100      NNS1(6)=-7
0111200      NNS1(3)=7
0111300      NNS1(5)=15
0111400      3 CALL EQUK(NNS1,POP,SK,I)
0111500      IHUI=0
0111600      DO 4 IA=1,I
0111700      4 IHUI=IHUI+NNS1(IA)
0111800      SK1(1)=SK*POP**(-IHUI)
0111900 C CALCULATE THE EQU. CONSTANT OF REACTION 2
0112000      DO 5 IA=1,I
0112100      5 NNS2(IA)=0
0112200      IF (IJ.EQ.2) GO TO 6
0112300      NNS2(4)=1
0112400      NNS2(5)=1
0112500      NNS2(3)=-1
0112600      NNS2(6)=-1
0112700      GO TO 7
0112800      6 NNS2(3)=1
0112900      NNS2(5)=2
0113000      NNS2(1)=-1
0113100      7 CALL EQUK(NNS2,POP,SK,I)
0113200      IHUI=0
0113300      DO 8 IA=1,I
0113400      8 IHUI=IHUI+NNS2(IA)
0113500      SK1(2)=SK*POP**(-IHUI)

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0113600 C CALCULATE THE EXIT AMOUNT OF GAS I
0113700 C INITIAL CONDITION
0113800     IF (IJ.EQ.2) GO TO 10
0113900     IF (IJ.EQ.1) GO TO 9
0114000 C BECAUSE OF COMPUTATION PROBLEM(OVERFLOW) NAPHTHA INPUT FUEL USING THE
0114100 C REASONABLE ASSUMPTION OF CONVERSION
0114200     X(1)=0.999*DNS(1)
0114300     X(2)=2.9*DNS(1)
0114400     DNS(1)=DNS(1)-X(1)
0114500     DNS(3)=DNS(3)+7.*X(1)-X(2)
0114600     DNS(4)=DNS(4)+X(2)
0114700     DNS(5)=DNS(5)+X(2)+15.*X(1)
0114800     DNS(6)=DNS(6)-X(2)-7.*X(1)
0114900     GO TO 11
0115000 9 X(1)=0.8*DNS(1)
0115100     X(2)=0.35*DNS(1)
0115200     CALL SNAE(X,2,DNS,SK1,I,IJ)
0115300     DNS(1)=DNS(1)-X(1)
0115400     DNS(3)=DNS(3)+X(1)-X(2)
0115500     DNS(4)=DNS(4)+X(2)
0115600     DNS(5)=DNS(5)+X(2)+3.*X(1)
0115700     DNS(6)=DNS(6)-X(2)-X(1)
0115800     GO TO 11
0115900 10 X(1)=0.96*DNS(1)
0116000     X(2)=0.04*DNS(1)
0116100     CALL SNAE(X,2,DNS,SK1,I,IJ)
0116200     DNS(1)=DNS(1)-X(1)-X(2)
0116300     DNS(3)=DNS(3)+X(2)
0116400     DNS(4)=DNS(4)+X(1)
0116500     DNS(5)=DNS(5)+2.*X(2)+3.*X(1)
0116600     DNS(6)=DNS(6)-X(1)
0116700 11 CONTINUE
0116800     RETURN
0116900     END
0116920     SUBROUTINE SEPAR(TIN,POP,TOUTV,TOUTL,DNS,DNSL,DNSV,I)
0116940 C*****
0116960 C THIS SUBROUTINE IS TO CAL. THE MASS BALANCE AROUND THE LIQUID SEPARATO
0116980 C*****
0117000 C ASSUMPTION:
0117020 C     (1). ONLY WATER EXIST IN LIQUID PHASE
0117040 C PSAT: SATURATE PRESSURE AT T; EXP(A-B/T) FOR WATER
0117060 C DK: EQU. CONST. OF LIQEID-VAPOR
0117080 C XW: AMOUNT OF WATER IN LIQUID PHASE
0117100     DIMENSION DNS(I),DNSV(I),DNSL(I)
0117120     COMMON /PS/ PS,TC/CONS/ A,B
0117140 C CAL. THE EQU. CONST. OF LIQUID-VAPOR
0117160     PSAT=EXP(A-B/TIN)
0117180     DK=PSAT/POP
0117200 C CAL. THE EQU. AMOUNT OF LIQUID-VAPOR WATER
0117220     TDNS=0.
0117240     DO 1 IA=1,I
0117260     TDNS=TDNS+DNS(IA)
0117280 1 CONTINUE
0117300     XW=(TDNS*DK-DNS(6))/(DK-1.)

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0117320      DO 2 IA=1,I
0117340      DNSL(IA)=0.
0117360      2 CONTINUE
0117380      DNSL(6)=XW
0117400      DO 3 IA=1,I
0117420      DNSV(IA)=DNS(IA)
0117440      3 CONTINUE
0117460      DNSV(6)=DNS(6)-DNSL(6)
0117480      TOUTL=TIN
0117500      TOUTV=TIN
0117520      RETURN
0117540      END
0117560      SUBROUTINE SHIFT(DNS, TOP, POP, X, I)
0117580 C*****
0117600 C THIS SUBROUTINE IS CALCULATE THE MASS BALANCE OF SHIFT CONVERTER
0117620 C*****
0117640 C ASSUMPTION:
0117660 C      (1). ONLY ONE REACTION (CO+H2O_H2+CO2) DOMINATE
0117680      DIMENSION MNS(7),DNS(7)
0117700      F(X)=(D4+X)*(D5+X)-SK*(D3-X)*(D6-X)
0117720      DF(X)=(D4+X)+(D5+X)+SK*((D3-X)+(D6-X))
0117740      D1=DNS(1)
0117760      D2=DNS(2)
0117780      D3=DNS(3)
0117800      D4=DNS(4)
0117820      D5=DNS(5)
0117840      D6=DNS(6)
0117860      D7=DNS(7)
0117880 C CALCULATE EQUALIBRIUM CONSTANT
0117900      DO 1 IA=1,I
0117920      1 MNS(IA)=0
0117940      MNS(4)=1
0117960      MNS(5)=1
0117980      MNS(3)=-1
0118000      MNS(6)=-1
0118020      CALL EQUK(MNS, TOP, SK, I)
0118040 C NEWTON-RAPHSON METHOD TO SOLVE NONLINEAR ALGEBRAIC EQUATION
0118060      X=0.5*DNS(3)
0118080      DO 2 IA=1,500
0118100      DX=ABS(F(X)/DF(X))
0118120      X=X-F(X)/DF(X)
0118140      IF(DX.LT.0.01) GO TO 3
0118160      2 CONTINUE
0118180      3 CONTINUE
0118200 C CALCULATE THE EXIT AMOUNT OF GAS I
0118220      DNS(4)=DNS(4)+X
0118240      DNS(5)=DNS(5)+X
0118260      DNS(3)=DNS(3)-X
0118280      DNS(6)=DNS(6)-X
0118300      RETURN
0118320      END
0118340      SUBROUTINE SNAE(XY, IX, DNS, SK1, I, IJ)
0118360 C*****
0118380 C THIS SUBROUTINE IS USING NEWTON-RAPHSON ITERATION TO SOLVE TWO NONLINE

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0118400 C ALGEBRAIC EQUATIONS IN REFORMER
0118420 C*****
0118440 DIMENSION XY(IX),DNS(I),SK1(IX)
0118460 F1(X,Y)=(D3+Y-X)*(D5+X+3.*Y)**3-SKA*(TDNS+2.*Y)**2*(D1-Y)*(D6-X-Y)
0118480 F2(X,Y)=(D4+X)*(D5+X+3.*Y)-SKB*(D6-X-Y)*(D3-X+Y)
0118500 DFX1(X,Y)=- (D5+X+3.*Y)**3+3.*(D3+Y-X)*(D5+X+3.*Y)**2+SKA*(TDNS+2.-
0118520 1*Y)**2*(D1-Y)
0118540 DFY1(X,Y)=(D5+X+3.*Y)**3+9.*(D3+Y-X)*(D5+X+3.*Y)**2-SKA*(-(TDNS+2.-
0118560 1*Y)**2*(D1-Y)-(TDNS+2.*Y)**2*(D6-X-Y)+4.*(TDNS+2.*Y)*(D1-Y)*(D6-X-
0118580 2-Y))
0118600 DFX2(X,Y)=(D5+X+3.*Y)+(D4+X)+SKB*((D3-X+Y)+(D6-X-Y))
0118620 DFY2(X,Y)=3.*(D4+X)-SKB*((D6-X-Y)-(D3-X+Y))
0118640 F3(X,Y)=(D4+X)*(D5+3.*X+2.*Y)**3-SKA*(TDNS+2.*X+2.*Y)**2*(D1-X-Y -
0118660 1)*(D6-X)
0118680 F4(X,Y)=(D3+Y)*(D5+3.*X+2.*Y)**2-SKB*(TDNS+2.*X+2.*Y)*(D1-X-Y)
0118700 DFX3(X,Y)=(D5+3.*X+2.*Y)**3+9.*(D5+3.*X+2.*Y)**2*(D4+X)-2.*SKA -
0118720 1*(TDNS+2.*X+2.*Y)*(D1-X-Y)*(D6-X)*2.+SKA*(TDNS+2.*X+2.*Y) -
0118740 2**2*(D6-X)+SKA*(TDNS+2.*X+2.*Y)**2*(D1-X-Y)
0118760 DFY3(X,Y)=(D4+X)*6.*(D5+3.*X+2.*Y)**2-4.*SKA*(TDNS+2.*X+2.*Y)* -
0118780 1*(D1-X-Y)*(D6-X)+SKA*(TDNS+2.*X+2.*Y)**2*(D6-X)
0118800 DFX4(X,Y)=(D3+Y)*6.*(D5+3.*X+2.*Y)+SKB*(TDNS+2.*X+2.*Y) -
0118820 1-2.*SKB*(D1-X-Y)
0118840 DFY4(X,Y)=4.*(D5+3.*X+2.*Y)*(D3+Y)+(D5+3.*X+2.*Y)**2+SKB -
0118860 1*(TDNS+2.*X+2.*Y)-2.*SKB*(D1-X-Y)
0118880 F5(X,Y)=((D3+7.*Y-X)**7/10000.*(D5+X+15.*Y)**15-SKA/10000. -
0118900 1*(TDNS+14.*Y)**14 -
0118920 1*(D1-Y)*(D6-X-7.*Y)/10000.)/1.E10
0118940 F6(X,Y)=(D4+X)*(D5+X+15.*Y)-SKB*(D6-X-7.*Y)*(D3+7.*Y-X)
0118960 DFX5(X,Y)=- (D5+X+15.*Y)**15/10000.*7.*(D3+7.*Y-X)**6/100. -
0118980 1*(D3+7.*Y-X)**7/10000.*15.*(D5+X+15.*Y)**14/100.+SKA/1000000.* -
0119000 4*(TDNS+
0119020 214.*Y)**14*(D1-Y))/1.E08
0119040 DFY5(X,Y)=(7.*(D3+7.*Y-X)**6/10000.*7.*(D5+X+15.*Y)**15 -
0119060 1+15./10000.*(D5+X+15.*Y)**14 -
0119080 1*15.*(D3+7.*Y-X)**7+SKA/10000.*(TDNS+14.*Y)**14*(D6-X-7.*Y)-SKA -
0119100 2/10000.*14.*(
0119120 2TDNS+14.*Y)**13*14.*(D1-Y)*(D6-X-7.*Y)-SKA/10000.*(TDNS+14.*Y)**14-
0119140 4*(D1-Y)*(-7.))/1.E10
0119160 DFX6(X,Y)=(D5+X+15.*Y)+(D4+X)+SKB*((D3+7.*Y-X)+(D6-X-7.*Y))
0119180 DFY6(X,Y)=15.*(D4+X)-7.*SKB*((D6-X-7.*Y)-(D3+7.*Y-X))
0119200 C CAL. THE TOTAL AMOUNT
0119220 IF ((IJ.EQ.2).OR.(IJ.EQ.3)) GO TO 51
0119240 DO 5 IA=1,7
0119260 DNS(IA)=DNS(IA)/1000.
0119280 5 CONTINUE
0119300 51 TDNS=0.
0119320 DO 1 IA=1,I
0119340 TDNS=TDNS+DNS(IA)
0119360 1 CONTINUE
0119380 D1=DNS(1)
0119400 D2=DNS(2)
0119420 D3=DNS(3)
0119440 D4=DNS(4)
0119460 D5=DNS(5)

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0119480      D6=DNS(6)
0119500      D7=DNS(7)
0119520      SKA=SK1(1)
0119540      SKB=SK1(2)
0119560      IF (IJ.EQ.1) GO TO 61
0119580      IF (IJ.EQ.2) GO TO 62
0119600      X=XY(2)/1000.
0119620      Y=XY(1)/1000.
0119640      DO 2 IA=1,500
0119660      D=DFX5(X,Y)*DFY6(X,Y)-DFX6(X,Y)*DFY5(X,Y)
0119680      DX=(F6(X,Y)*DFY5(X,Y)-F5(X,Y)*DFY6(X,Y))/D
0119700      DY=(F5(X,Y)*DFX6(X,Y)-F6(X,Y)*DFX5(X,Y))/D
0119720      X=X+DX
0119740      Y=Y+DY
0119760      AX=ABS(DX)
0119780      AY=ABS(DY)
0119800      IF((AX.LT.0.001).AND.(AY.LT.0.001)) GO TO 9
0119820      2 CONTINUE
0119840      WRITE(6,101)
0119860      101 FORMAT(1X,'SOLVE THE EQU. EQUATION FAIL AFTER 500 ITERATIONS')
0119880      RETURN
0119900      9 XY(1)=Y*1000.
0119920      XY(2)=X*1000.
0119940      61 X=XY(2)
0119960      Y=XY(1)
0119980      DO 3 IA=1,500
0120000      D=DFX1(X,Y)*DFY2(X,Y)-DFX2(X,Y)*DFY1(X,Y)
0120020      DX=(F2(X,Y)*DFY1(X,Y)-F1(X,Y)*DFY2(X,Y))/D
0120040      DY=(F1(X,Y)*DFX2(X,Y)-F2(X,Y)*DFX1(X,Y))/D
0120060      X=X+DX
0120080      Y=Y+DY
0120100      AX=ABS(DX)
0120120      AY=ABS(DY)
0120140      IF((AX.LT.0.001).AND.(AY.LT.0.001)) GO TO 91
0120160      3 CONTINUE
0120180      WRITE(6,101)
0120200      RETURN
0120220      91 XY(1)=Y
0120240      XY(2)=X
0120260      RETURN
0120280      62 X=XY(1)
0120300      Y=XY(2)
0120320      DO 4 IA=1,500
0120340      D=DFX3(X,Y)*DFY4(X,Y)-DFX4(X,Y)*DFY3(X,Y)
0120360      DX=(F4(X,Y)*DFY3(X,Y)-F3(X,Y)*DFY4(X,Y))/D
0120380      DY=(F3(X,Y)*DFX4(X,Y)-F4(X,Y)*DFX3(X,Y))/D
0120400      X=X+DX
0120420      Y=Y+DY
0120440      AX=ABS(DX)
0120460      AY=ABS(DY)
0120480      IF((AX.LT.0.001).AND.(AY.LT.0.001)) GO TO 92
0120500      4 CONTINUE
0120520      WRITE(6,101)
0120540      RETURN

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0120560 92 XY(1)=X
0120580 XY(2)=Y
0120600 RETURN
0120620 END
0120640 SUBROUTINE VINEW (M,V,Z,TK,POP,PPH2,PP02,PPH20,PPCO,X0)
0120660 COMMON/CATAL/SRO,SA,CU,CL,ALFA,SN,FCONST,AREAF,DKC
0120680 1 R=8.314
0120700 ERR=0.005
0120720 CLA=CL
0120740 EZ=1.261-.00025*TK
0120760 SR=SRO*EXP(3650.*(1./TK-1./450.))
0120780 SIO=.2327*(PP02*POP)**.8*(PPH20*POP)**.4377*EXP(-6652./TK)
0120800 C=SIO*SA*CU*CL
0120820 EX=11.85*.0066*PPCO*POP*EXP(9190.*(1./TK-1./450.))
0120840 A=ALOG(PPH2/PPH20*(PP02*POP)**0.5)
0120860 C1=CLA*SA*CU*.000053
0120880 D=R*TK/SN/FCONST
0120900 B=EZ+D*A
0120920 DA=D/ALFA
0120940 CDL=C/KC/AREAF*(PPO2*POP)
0120960 IF (M.EQ.2) GO TO 2
0120980 V=B-DA*ALOG(Z/C)-Z*SR-EX*ALOG(Z/C1)-D*ALOG(CDL/(CDL-Z))
0121000 GO TO 6
0121020 2 Z=X0
0121040 3 CONTINUE
0121060 DO 5 I=1,50
0121080 FZ=Z*SR+DA*ALOG(Z/C)+V-B+EX*ALOG(Z/C1)+D*ALOG(CDL/(CDL-Z))
0121100 DFZ=S?+DA/Z+EX/Z+D/(CDL-Z)
0121120 DZ=FZ/DFZ
0121140 Z=Z-DZ
0121160 4 IF (Z.LE.0.) GO TO 7
0121180 IF (ABS(DZ).LT.ERR) GO TO 6
0121200 5 CONTINUE
0121220 7 Z=X0
0121240 DO 8 I=1,50
0121260 GFZ=(DA*ALOG(Z/C)+V-B+EX*ALOG(Z/C1)+D*ALOG(CDL/(CDL-Z)))/(-SR)
0121280 GZ=Z
0121300 Z=GFZ
0121320 IF (Z.LE.0.) GO TO 19
0121340 IF (ABS((GZ-Z)/(Z+GZ)).LT.ERR) GO TO 6
0121360 8 CONTINUE
0121380 WRITE(6,201)
0121400 201 FORMAT(1X,'CURRENT DENSITY LOOPING')
0121420 GO TO 6
0121440 19 ERR=ERR+0.001
0121460 GO TO 2
0121480 6 CONTINUE
0121500 RETURN
0121520 END
0121540 SUBROUTINE KREF(DNSR,DNSF,DX,DY,DQ,PX,TCO,THZ,Z,POUT,TCOUT
0121560 1,THOUT,S1,DP1,IFUEL)
0121580 REAL K0,MH,K1,K2
0121600 COMMON F0,F1,F2,F3,F4,F5,F6,MH,CG1,CG2,CG3,CG4,CG5,CG6
0121620 COMMON/REP/ K0,EA,RHOB,EPS,DZZ

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0121640      COMMON/ADDRE/ D1,D2,D3,S,DP,P
0121660      COMMON /WM/ WM
0121680      COMMON /FCG/ F7,CG7
0121700      DIMENSION X1( 50),TAX2( 50),XE2( 50),TC( 50),
0121720      1TH( 50),XE( 50),TA(50),TAK1( 50),TAK2( 50),
0121740      2XF( 50),XCOMP( 50,7),XMCOMP( 50,7),XC( 50,7),
0121760      3XU1( 50),TP( 50),FL(7),C(7),WM(7),COM(7),CGCOMP(7),TCGC(7)
0121780      DIMENSION REN( 50)
0121800      DIMENSION P( 50)
0121820      DIMENSION DNSR(7),DNSF(7)
0121840      DATA ERROR/0.01/
0121860      DATA XCOMP/ 350*0./
0121880      IDEBUG=0
0121900      D1=DX
0121920      D2=DY
0121940      D3=DQ
0121960      DP=DP1
0121980      S=S1
0122000      P(1)=PX
0122020      F1=DNSR(1)
0122040      F2=DNSR(3)
0122060      F3=DNSR(4)
0122080      F4=DNSR(6)
0122100      F5=DNSR(5)
0122120      F6=DNSR(7)
0122140      F7=DNSR(2)
0122160      F0=F1+F2+F3+F4+F5+F6+F7
0122180      CG1=DNSF(1)
0122200      CG2=DNSF(3)
0122220      CG3=DNSF(4)
0122240      CG4=DNSF(6)
0122260      CG5=DNSF(5)
0122280      CG6=DNSF(7)
0122300      CG7=DNSF(2)
0122320      MH=CG1+CG2+CG3+CG4+CG5+CG6+CG7
0122340      X1(1)=0.
0122360      XE2(1)=0.
0122380      TCO=(TCO-273.16)*9./5.+32.
0122400      THZ=(THZ-273.16)*9./5.+32.
0122420      KING=0
0122440      C0=(F1*(1.-X1(1))*P(1))/(.7302*(F0+2.*X1(1)*F1)*(TCO+460.))
0122460      U0=(4.*.7302*(F0+2.*X1(1)*F1)*(TCO+460.))/(3.1415927*P(1)
0122480      1*(D2**2-D1**2)*EPS)
0122500 C FIRST ASSUMPTION -- TH0
0122520      X=.9
0122540      AX=Z*RHOB*K0*P(1)*F1*(2.*F0+X*(2.*F1-F0))/(2.*F0*(F0+2.*X*F1)*
0122560      IU0*C0)
0122580      T=-.9045*EA/ALOG(X/AX)-460.
0122600      TK2=K2(T)
0122620      TX2=X2(X,TK2)
0122640      TDH1=-DH1(T)
0122660      TDH2=-DH2(T)
0122680      AY=F1*TDH1*X+(F3+X*F1)*TDH2*TX2
0122700      FL(1)=F1*(1.-X)

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0122720      FL(2)=F2-TX2*(F3+X*F1)
0122740      FL(3)=F3+X*F1+TX2*(F3+X *F1)
0122760      FL(4)=F4-2.*X*F1-TX2*(F3+X *F1)
0122780      FL(5)=F5+4.*X*F1+TX2*(F3+X *F1)
0122800      FL(6)=F6
0122820      FL(7)=F7
0122840      TF=F(X)
0122860      CALL CHASS(C,FL,TF)
0122880      TVIS=VIS(C,T,IFUEL)
0122900      TTHC=THC(C,T,IFUEL)
0122920      THI=HI(TVIS,TTHC)
0122940      CGCOMP(1)=CG1
0122960      CGCOMP(2)=CG2
0122980      CGCOMP(3)=CG3
0123000      CGCOMP(4)=CG4
0123020      CGCOMP(5)=CG5
0123040      CGCOMP(6)=CG6
0123060      CGCOMP(7)=CG7
0123080      CALL CHASS(TCGC,CGCOMP,MH)
0123100      CGVIS=VIS(TCGC,THZ,IFUEL)
0123120      CGTHC=THC(TCGC,THZ,IFUEL)
0123140      CGHTCP=HTCP(TCGC,THZ)
0123160      THO=HO(CGVIS,CGTHC,CGHTCP,Z,THZ,RE)
0123180      TUI=UI(THI,THO,T)
0123200      AZ=3.1415927*TUI*Z*D2/2.
0123220      CALL COMPIN(COM,X1(1),XE2(1))
0123240      TFCP=FCP(T,COM)
0123260      AW=(MH*CGHTCP*TFCP)/AZ+MH*CGHTCP-TFCP
0123280      THO=(AW*THZ+2.*TFCP*TCO+AY)/(AW+2.*TFCP)
0123300      IF(THO.LT.TCO) THO=TCO+250.
0123320      IDEA=1
0123340      IHOPE=1
0123360      75 I=1
0123380      TAK1(1)=0.
0123400      TAK2(1)=0.
0123420      XU1(1)=0.
0123440      TA(1)=TCO
0123460      TAX2(1)=0.
0123480      XF(1)=F0+2.*F1*X1(1)
0123500      DO 80 J=1,7
0123520      XCOMP(1,J)=COM(J)
0123540      XMCOMP(1,J)=XCOMP(1,J)/XF(1)
0123560      80 CONTINUE
0123580      WM=1=0.
0123600      DO 81 J=1,7
0123620      WMM1=WMM1+(XCOMP(1,J)*WM(J))/XF(1)
0123640      81 CONTINUE
0123660      DO 82 J=1,7
0123680      XC(1,J)=(XCOMP(1,J)*WM(J))/(XF(1)*WMM1)
0123700      82 CONTINUE
0123720      TC(1)=TCO
0123740      TH(1)=THO
0123760 C SECOND ASSUMPTION --TC(I+1)
0123780      72 TC(I+1)=TC(I)

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0123800 70 TA(I+1)=(TC(I)+TC(I+1))/2.
0123820 TAK1(I+1)=K1(TA(I+1))
0123340 TAK2(I+1)=K2(TA(I+1))
0123860 B1=DZZ*RHOB*K0*P(I)/(U0*C0)
0123880 B2=EXP(-.9045*EA/(TA(I+1)+460.))
0123900 X1(I+1)=X1(I)+B1*B2*XMCOMP(I,1)
0123920 XE2(I+1)=X2(X1(I+1),TAK2(I+1))
0123940 XDH1=-DH1(TA(I+1))
0123960 XDH2=-DH2(TA(I+1))
0123980 AL1=F1*XDH1*(X1(I+1)-X1(I))
0124000 AL2=(F3+X1(I+1)*F1)*XDH2*(XE2(I+1)-XE2(I))
0124020 AL=AL1+AL2
0124040 FL(1)=F1*(1.-X1(I+1))
0124060 FL(2)=F2-XE2(I+1)*(F3+X1(I+1)*F1)
0124080 FL(3)=F3+X1(I+1)*F1+XE2(I+1)*(F3+X1(I+1)*F1)
0124100 FL(4)=F4-2.*X1(I+1)*F1-XE2(I+1)*(F3+X1(I+1)*F1)
0124120 FL(5)=F5+4.*X1(I+1)*F1+XE2(I+1)*(F3+X1(I+1)*F1)
0124140 FL(6)=F6
0124160 FL(7)=F7
0124180 XF(I+1)=F(X1(I+1))
0124200 CALL CMASS(C,FL,XF(I+1))
0124220 DO 10 J=1,7
0124240 XCOMP(I+1,J)=FL(J)
0124260 XMCOMP(I+1,J)=XCOMP(I+1,J)/XF(I+1)
0124280 XC(I+1,J)=C(J)
0124300 10 CONTINUE
0124320 XVIS=VIS(C,TA(I+1),IFUEL)
0124340 XTHC=THC(C,TA(I+1),IFUEL)
0124360 V=WM(1)*F1+WM(3)*F2+WM(4)*F3+WM(6)*F4+WM(5)*F5+WM(7)*F6+WM(2)*F7
0124380 GMV=(V*4.)/(3.1415927*(D2**2-D1**2))
0124400 AMV=V/F0
0124420 RHO=(AMV*P(I))/(0.7302*(T+460.))
0124440 DELP=(1.-EPS)/EPS**3*GMV**2/DP/4.18E+08/RHO*(150.*(1.-EPS)*XVIS/DP-
0124460 1/GMV+1.75)*DZZ/2116.8
0124480 P(I+1)=P(I)-DELP
0124500 XHI=HI(XVIS,XTHC)
0124520 XCGVIS=VIS(TCGC,TH(I),IFUEL)
0124540 XCGTHC=THC(TCGC,TH(I),IFUEL)
0124560 XGHTCP=HTCP(TCGC,TH(I))
0124580 XHO=HO(XCGVIS,XCGTHC,XGHTCP,Z,TH(I),RE)
0124600 REN(I+1)=RE
0124620 XU1(I+1)=UI(XHI,XHO,TA(I+1))
0124640 AM=(3.1415927*XU1(I+1)*DZZ*02)/2.
0124660 XFCP=FCP(TA(I),FL)
0124680 AN=(MH*XGHTCP*XFCP)/AM-XFCP+MH*XGHTCP
0124700 TH(I+1)=TH(I)*(AN+2.*XFCP)/AN-2.*XFCP*TC(I)/AN-AL/AN
0124720 TP(I+1)=TH(I+1)*(AM-MH*XGHTCP)/AM+TH(I)*(AM+MH*XGHTCP)/AM-TC(I)
0124740 C TEST SECOND ASSUMPTION
0124760 EE=ABS((TP(I+1)-TC(I+1))/TC(I+1))
0124780 IF(IDEBUG.NE.0)
0124800 1WRITE(6,2020) TP(I+1),TC(I+1),EE
0124820 2020 FORMAT('OTP=',1PE15.7,5X,'TC=',E15.7,5X,'EE=',E15.7)
0124840 IF(EE.LE.ERROR) GO TO 71
0124860 IF(KING.LE.15) TC(I+1)=(TC(I+1)+TP(I+1))/2.

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0124880      TC2=TC(I+1)
0124900      EETC2=TH(I+1)*(AM-MH*XGHTCP)/AM+TH(I)*(AM+MH*XGHTCP)/AM- -
0124920      1TC(I)-TC2
0124940      IF(KING.LE.15) GO TO 97
0124960      IF(EETC1.NE.EETC2) TC3=TC2-(EETC2/(EETC2-EETC1))*(TC2-TC1)
0124980      IF(EETC1.EQ.EETC2) TC3=(TC2+TP(I+1))/2
0125000      TC(I+1)=TC3
0125020      97 KING=KING+1
0125040      TC1=TC2
0125060      EETC1=EETC2
0125080      IF(KING.GE.40) GO TO 959
0125100      GO TO 70
0125120      71 CONTINUE
0125140      TC(I+1)=TP(I+1)
0125160      AA=I
0125180      AAA=AA*DZZ
0125200      IF(AAA.GE.Z) GO TO 73
0125220      I=I+1
0125240      KING=0
0125260      GO TO 72
0125280      73 N=I+1
0125300      C TEST FIRST ASSUMPTION
0125320      AB=ABS((TH(I+1)-THZ)/THZ)
0125340      IF(AB.LE.0.001) GO TO 74
0125360      THO2=THO
0125380      THZ2=TH(N)
0125400      IF(IDEA.LT.2) THO3=THO+THZ-THZ2
0125420      IF(IDEA.EQ.2) THO3=(THO1-THO2)/(THZ1-THZ2)*(THZ-THZ2)+THO2
0125440      IDEA=2
0125460      THZ1=TH(N)
0125480      THO1=THO
0125500      THO=THO3
0125520      IF(THO.LT.TCO) IHOPE=IHOPE+1
0125540      IF(THO.LT.TCO) THO=TCO+50.
0125560      IF(IHOPE.EQ.5) GO TO 975
0125580      GO TO 75
0125600      74 CONTINUE
0125620      IF(K.EQ.1) L=N
0125640      GO TO 954
0125660      975 CONTINUE
0125680      WRITE(6,976) THO
0125700      976 FORMAT(1H1,'***INSUFFICIENT COMB. GAS HEAT CAPACITY' / -
0125720      1'0THO=',F17.3,'THIS IS LESS THAN TCO'/'ORAISE THZ AND/OR COMB. -
0125740      2GAS FLOW RATES')
0125760      GO TO 954
0125780      959 WRITE(6,958) KING,I
0125800      958 FORMAT(1H1,'LOOPING ON TC FOR ',I4,'ITERATIONS IN INCRM',I4)
0125820      954 CONTINUE
0125840      TCO=(TCO-32.)*5./9.+273.16
0125860      THZ=(THZ-32.)*5./9.+273.16
0125880      PCUT=P(N)
0125900      TCCUT=(TC(N)-32.)*5./9.+273.16
0125920      THOUT=(TH(1)-32.)*5./9.+273.16
0125940      DNSR(1)=XCOMP(N,1)

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0125960      DNSR(3)=XCOMP(N,2)
0125980      DNSR(4)=XCOMP(N,3)
0126000      DNSR(5)=XCOMP(N,5)
0126020      DNSR(6)=XCOMP(N,4)
0126040      DNSR(7)=XCOMP(N,6)
0126060      RETURN
0126080      END
0163100      SUBROUTINE CMASS(C,FL,F)
0163200      DIMENSION C(7),WM(7),FL(7)
0163300      COMMON /WM/ WM
0163400      WMM=(FL(1)*WM(1)+FL(2)*WM(3)+FL(3)*WM(4)+WM(6)*FL(4)+FL(5)*WM(5)+ -
0163500      IFL(6)*WM(7)+FL(7)*WM(2))/F
0163600      C(1)=FL(1)*WM(1)/(F*WMM)
0163700      C(2)=FL(2)*WM(3)/(F*WMM)
0163800      C(3)=FL(3)*WM(4)/(F*WMM)
0163900      C(4)=FL(4)*WM(6)/(F*WMM)
0164000      C(5)=FL(5)*WM(5)/(F*WMM)
0164100      C(6)=FL(6)*WM(7)/(F*WMM)
0164200      C(7)=FL(7)*WM(2)/(F*WMM)
0164300      RETURN
0164400      END
0164500      SUBROUTINE COMPIN(COM,X1,X2)
0164600      REAL MH
0164700      COMMON F0,F1,F2,F3,F4,F5,F6,MH,CG1,CG2,CG3,CG4,CG5,CG6
0164800      COMMON/ADDRE/ D1,D2,D3,S,DP,P
0164900      COMMON /FCG/F7,CG7
0165000      DIMENSION COM(7)
0165100      DO 8 J=1,7
0165200      IF(J.EQ.1) COM(J)=F1*(1.-X1)
0165300      IF(J.EQ.2) COM(J)=F2-X2*(F3+X1*F1)
0165400      IF(J.EQ.3) COM(J)=F3+X1*F1+X2*(F3+X1*F1)
0165500      IF(J.EQ.4) COM(J)=F4-2.*X1*F1-X2*(F3+X1*F1)
0165600      IF(J.EQ.5) COM(J)=F5+4.*X1*F1+X2*(F3+X1*F1)
0165700      IF(J.EQ.6) COM(J)=F6
0165800      IF(J.EQ.7) COM(J)=F7
0165900      8 CONTINUE
0166000      RETURN
0166100      END
0166200      FUNCTION DH1(T)
0166300      DH1=-2.7285E-03*(T**2)+12.698*T+7.002E+04
0166400      RETURN
0166500      END
0166600      FUNCTION DH2(T)
0166700      DH2=2.3280*T-18111.4
0166800      RETURN
0166900      END
0167000      FUNCTION F(X1)
0167100      REAL MH
0167200      COMMON F0,F1,F2,F3,F4,F5,F6,MH,CG1,CG2,CG3,CG4,CG5,CG6
0167300      COMMON/ADDRE/ D1,D2,D3,S,DP,P
0167400      COMMON /FCG/F7,CG7
0167500      F=F0+2.*X1*F1
0167600      RETURN
0167700      END

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0167800      FUNCTION FCP(T,COM)
0167900      DIMENSION COM(7),A(4,7)
0168000      DATA A/5.34,6.39E-03,0.,0.,6.60,6.67E-04,0.,0.,10.34,1.52E-03,0., -
0168100      1-6.33420E+05,8.22, 8.3E-05,4.136E-07,0.,6.62,4.5E-04,0.,0.,6.5, -
0168200      25.56E-04,0.,0.,6.732,8.36E-03,5.53E-09,0.0/
0168300      TP=T+460.
0168400      FCP=0.
0168500      DO 9 I=1,7
0168600      FCP=FCP+COM(I)*(A(1,I)+A(2,I)*TP+A(3,I)*TP**2+A(4,I)/(TP**2))
0168700 9 CONTINUE
0168800      RETURN
0168900      END
0169000      FUNCTION HI(VIS,THC)
0169100      REAL MH
0169200      DIMENSION WM(7)
0169300      COMMON F0,F1,F2,F3,F4,F5,F6,MH,CG1,CG2,CG3,CG4,CG5,CG6
0169400      COMMON/ADDRE/ D1,D2,D3,S,DP,P
0169500      COMMON/WM/ WM
0169600      COMMON /FCG/F7,CG7
0169700      HI=0.
0169800      V=(WM(1)*F1+WM(3)*F2+WM(4)*F3+WM(6)*F4+WM(5)*F5+WM(7)*F6 -
0169900      1+WM(2)*F7)
0170000      GMV=(V*4.)/(3.1415927*(D2**2.-D1**2.))
0170100      HID=(.813*(GMV*DP/VIS)**.9)*EXP(-6.*DP/(D2-D1))
0170200      HI=(HID*THC)/(D2-D1)
0170300      RETURN
0170400      END
0170500      FUNCTION HO(VIS,THC,HTCP,Z,T,RE)
0170600      REAL MH
0170700      DIMENSION WM(7)
0170800      COMMON F0,F1,F2,F3,F4,F5,F6,MH,CG1,CG2,CG3,CG4,CG5,CG6
0170900      COMMON/ADDRE/ D1,D2,D3,S,DP,P
0171000      COMMON /FCG/F7,CG7
0171100      COMMON/WM/ WM
0171200      AMW=(CG1*WM(1)+CG2*WM(3)+CG3*WM(4)+CG4*WM(6)+CG5*WM(5)+CG6*WM(7) -
0171300      1+CG7*WM(2))/MH
0171400      HO=0.
0171500      G=MH/(S**2-(3.1415927*D3**2)/4.)
0171600      DE=4.*(S**2-3.1415927*D3**2./4.)/(3.1415927*D3+4.*S)
0171700      RE=(DE*G*AMW)/VIS
0171800      PR=(HTCP*VIS)/(THC*AMW)
0171900      RHO=(AMW*P)/(0.7302*(T+460.))
0172000      GR=(Z**3)*(RHO**2)*4.18E08*100./(VIS**2)
0172100      IF(RE.GE.10000.) GO TO 300
0172200      IF(RE.LE.2100.) GO TO 200
0172300 C      2100<RE<10000
0172400      HO21=(1.*THC/DE)*(2100.**.45)*SQRT(PR)*(DE/Z)**.4*(S/D3)**.8 -
0172500      1*GR**.05
0172600      HO10=(.02*THC/DE)*(10000.**.8)*(PR**.333)*(S/D3)**.53
0172700      SLOPE=(HO10-HO21)/(10000.-2100.)
0172800      HO=HO21+SLOPE*(RE-2100.)
0172900      RETURN
0173000 C      RE<=2100
0173100 200 HO=(1.02*THC/DE)*(RE**.45)*SQRT(PR)*(DE/Z)**.4*(S/D3)**.8 -

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0173200      1*GR** .05
0173300      RETURN
0173400 C      RE >= 10000
0173500      300 HO = (.02*THC/DE)*(RE**.8)*(PR**.333)*(S/D3)**.53
0173600      RETURN
0173700      END
0173720C     FUNCTION HTCP(CM,T)
0173740C     DIMENSION CM(7),C(7),A(4,7),WM(7)
0173760C     DATA A/5.34,6.39E-03,0.,0.,6.60,6.67E-04,0.,0.,10.34,1.52E-03,0.,
0173780C     1-6.3342E+05,8.22, 8.3E-05,4.136E-07,0.,6.62,4.5E-04,0.,0.,6.5,
0173800C     25.56E-04,0.,0.,6.732,8.36E-03,5.53E-09,0./
0173820C     DATA WM/16.,28.,44.,18.,2.,28.,32./
0173840C     TC=CM(1)/WM(1)+CM(2)/WM(2)+CM(3)/WM(3)+CM(4)/WM(4)+CM(5)/WM(5)
0173860C     1+CM(6)/WM(6)+CM(7)/WM(7)
0173880C     C(1)=CM(1)/WM(1)/TC
0173900C     C(2)=CM(2)/WM(2)/TC
0173920C     C(3)=CM(3)/WM(3)/TC
0173940C     C(4)=CM(4)/WM(4)/TC
0173960C     C(5)=CM(5)/WM(5)/TC
0173980C     C(6)=CM(6)/WM(6)/TC
0174000C     C(7)=CM(7)/WM(7)/TC
0174020C     TP=T+460.
0174040C     HTCP=0.
0174060C     DO 1 I=1,7
0174080C     1 HTCP=HTCP+C(I)*(A(1,I)+A(2,I)*TP+A(3,I)*TP**2+A(4,I)/TP**2)
0174100C     RETURN
0174120C     END
0175400     REAL FUNCTION K1(T)
0175500     TP=T+460.
0175600     B=-8.7153E+08/(TP**3)+5.2409E+06/(TP**2.)-4.6299E+04/TP+27.849
0175700     K1=EXP(B)
0175800     RETURN
0175900     END
0176000     REAL FUNCTION K2(T)
0176100     TP=T+460.
0176200     B=-9.0283E+08/(TP**3)+3.5603E+06/(TP**2)+4.3662E+03/TP-3.0526
0176300     K2=EXP(B)
0176400     RETURN
0176500     END
0176600     FUNCTION THC(C,T,IJ)
0176700     DIMENSION C(7),A(2,7)
0176800     COMMON/THCC/ A
0176900     THC=0.
0177000     DO 5 I=1,7
0177100     THC=THC+C(I)*(A(1,I)*T+A(2,I))
0177200     5 CONTINUE
0177300     RETURN
0177400     END
0177500     FUNCTION UI(HI,HO,T)
0177600     REAL MH
0177700     COMMON/ADDRE/ D1,D2,D3,S,DP,P
0177800     COMMON /FCG/F7,CG7
0177900     DLM=(D3-D2)/ALOG(D3/D2)
0178000     R=0.005

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0178100      THMET=4.659E-03*T+6.248
0178200      UI=1./(1./HI+D2/(D3*HO)+((D3-D2)*D2)/(THMET*DLM)+R)
0178300      RETURN
0178400      END
0178500      FUNCTION VIS(C,T,IJ)
0178600      DIMENSION A(2,7),C(7)
0178700      COMMON/VIPC/ A
0178800      VIS=0.
0178900      5 DO 4 I=1,7
0179000      VIS=VIS+C(I)*(A(1,I)*T+A(2,I))
0179100      4 CONTINUE
0179200      RETURN
0179300      END
0179400      FUNCTION X2(X,K2)
0179500      REAL MH
0179600      REAL K2
0179700      COMMON F0,F1,F2,F3,F4,F5,F6,MH,CG1,CG2,CG3,CG4,CG5,CG6
0179800      COMMON/ADDRE/ D1,D2,D3,S,DP,P
0179900      COMMON /FCG/F7,CG7
0180000      A=(K2-1.)*(F3+X*F1)**2
0180100      B=(F3+X*F1)*(2.*X*F1*K2-K2*F2-K2*F4-5.*X*F1-F3-F5)
0180200      C=K2*F2*F4-2.*F1*F2*K2*X-(F3+X*F1)*(F5+4.*F1*X)
0180300      X2=(-B-SQRT(B**2-4.*A*C))/(2.*A)
0180400      IF(X2.LT.-1..OR.X2.GT.0.) X2=(-B+SQRT(B**2-4.*A*C))/(2.*A)
0180500      RETURN
0180600      END
0180700      &OPFC TOPFC=443.,UT=0.8,CD=325.,
0180800      &END
0180900      &INIT DNSM=1216.,0.,1.360,21.8,166.,0.,0.,TAT=298.,PAT=1.,SMRA=3.,POPR=5.0
0181000      &END
0181100      &CCNDT IFUEL=1,ERR=0.01,IP=2,I=7,EXT=100.,WAT=0.015,EXA=100.,
0181200      &END
0181300      &REFEN ZH=6.,DX1=0.,DX2=0.15,DX3=0.1667,K0=1.040E+04,EA=20000.,RHOB=80.
0181400      ,EPS=0.487,S=0.25,DP=0.00328,DZZ=0.25,
0181500      &END
0181600      &HEATX CN=1.3,U=48825.1,HA(7)=0.2,HA(10)=0.2,
0181700      &END
0181800      &HEPDC NPH=2,NRH=5,BSPAC=1.,ODTH=.0625,PITCH=.0833,CLH=.0208,IDSH=.833,
0181900      IDTH=.04667,FLOAR=.001716,SURFC=.1466,CLENH=2.,SLTS2=0.5,DTH=0.7,
0182000      &END
0182100      &FDSHH DPD=1.18,0.,AHRN=0.66.,0,APPD=69.,0.,CLEPD=5.91,0.,
0182200      NTPD=1,0,
0182300      &END
0182400      &PDFUH NTA=140,FULE=1.42,WIDAF=.009744,NPFU=3365,
0182500      NTAA=40,AIRL=1.,WIDAA=.00515
0182600      &END
0182700      &CATAI SRO=.44,SA=400.,CU=.15,CL=.75,ALFA=.5,SN=2.,FCONST=96500.,
0182800      DKC=2.4E5,
0182900      &END

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16. Abstract A FORTRAN computer program has been developed for analyzing the performance of phosphoric acid fuel cell power plant systems. Energy mass and electrochemical analysis in the reformer, the shaft converters, the heat exchangers, and the fuel cell stack were combined to develop a mathematical model for the power plant for both atmospheric and pressurized conditions, and for several commercial fuels.					
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