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

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

January 1984

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NATIONAL AERONAUTICS AND SPACE ADMINISTRATION
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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.

1. 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 H2, CO, CH4, CO2 and H2O. 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 CSU designed PEMC 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.

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

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

\[
Q_T = E C_{min} (T_{hi} - T_{ci}) \quad (2-1-3)
\]

\[
E = \frac{1 - e^{-\left(1 - \frac{C_{min}}{C_{max}}\right) e^{-\frac{UA}{C_{min}} (1 - \frac{C_{min}}{C_{max}})}}}{1 - (\frac{C_{min}}{C_{max}}) e^{-\frac{UA}{C_{min}} (1 - \frac{C_{min}}{C_{max}})}} \quad (2-1-4)
\]

where

- \(C_{c}\): capacity rate of fluid on cold side, \(McC_{pc}\), J/s-K
- \(C_{h}\): capacity rate of fluid on hot side, \(MhC_{pc}\), J/s-K
- \(C_{max}\): maximum capacity rate, J/s-K
- \(C_{min}\): minimum capacity rate, J/s-K
- \(C_{pc}\): specific heat of cold side fluid, J/g-K
- \(C_{ph}\): specific heat of hot side fluid, J/g-K
- \(E\): heat exchanger effectiveness
- \(M_{c}\): fluid mass flow rate on cold side, g/s
- \(M_{h}\): fluid mass flow rate on hot side, g/s
- \(Q_T\): total heat transfer rate across heat exchanger, J/s
- \(T_{ci}\): cold side inlet temperature, K
Tco: cold side outlet temperature, K
Thi: hot side inlet temperature, K
Tho: hot side outlet temperature, K
UA: overall heat transfer coefficient of exchanger, J/m²·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

\[
K_2 = \frac{P_{\text{CO}_2} P_{\text{H}_2}}{P_{\text{CO}} P_{\text{H}_2\text{O}}} = \frac{(F_{\text{CO}_2} + x)(F_{\text{H}_2} + x)}{(F_{\text{CO}} - x)(F_{\text{H}_2\text{O}} - x)}
\]

(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

\[ \sum_{PS} n_j (\Delta h^0_f)j - \sum_{RS} n_i (\Delta h^0_f)i + \sum_{PS} n_j \left( \frac{T_f}{298} \right) (Cp)_j dT \]
\[ - \sum_{RS} n_i \left( \frac{T_i}{298} \right) (Cp)_i dT = 0 \]  

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 iteractively.

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):

\[ \Delta P = 1878 \left( \frac{1-\epsilon}{\epsilon} \right) G \left( \frac{150(1-\epsilon) \mu}{\text{dp} G} + 1.75 \right) h \]

where \( \epsilon \): void fraction in bed
\( \mu \): viscosity, Kg/m-s
\( \text{dp} \): effective diameter of packing particle, m
\( G \): superficial gas mass velocity, Kg/s-m
\( h \): packed height, m
\( \rho \): density, Kg/m³
\( \Delta P \): 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:

$$C_nH_m + 2nH_2O = nCO_2 + (2n + m/2) H_2$$

for naphtha and methane, and

$$CH_3OH + H_2O = CO_2 + 3H_2$$

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:

$$CH_4 + H_2O = CO + 3H_2$$  \hspace{1cm} \text{(demethanation reaction)}

and

$$CO + H_2O = CO_2 + H_2$$  \hspace{1cm} \text{(water shift reaction)}.

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
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:

\[
K_1 = \frac{p_{CO_2} p_3 H_2}{p_{CH_4} p_{H_2} O} = \frac{y_{CO_2} y^3 H_2}{y_{CH_4} y_{H_2} O} \quad \text{(demethanation)}
\]

\[
K_2 = \frac{p_{CO_2} p H_2}{p_{CO} p_{H_2} O} = \frac{y_{CO_2} y H_2}{y_{CO} y_{H_2} O} \quad \text{(water shift)}
\]

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

\[
Q_{B-R} = U A \Delta T_m = H_{out} - H_{IN} \quad (2-1-10)
\]

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,

\[
UA\Delta T_m = \sum_{PR} m_j (\Delta h_f^0)_j - \sum_{PR} m_i (\Delta h_f^0)_i + \sum_{PR} m_j \int_{298}^{T_{fR}} (Cp)_j \, dT
\]

\[
- \sum_{rR} m_k \int_{298}^{T_{rR}} (Cp)_i \, dT, \quad \ldots \quad (2-1-12)
\]

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.
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

\[
\text{CH}_4 + 2\text{H}_2\text{O} = \text{CO}_2 + 4\text{H}_2 \quad (2-1-13)
\]

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

\[ V \frac{dc}{dz} = -\frac{\gamma a}{e} \]  

(2-1-14)

where:
- \( V \): average velocity of fluid through the bed, m/s
- \( c \): g-mole of \( CH_4 \) per m\(^3\) fluid
- \( ra' \): reaction rate, g-mole of \( CH_4 \)/s-kg catalyst
- \( eB \): density of catalyst, kg/m\(^3\) 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

\[-ra' = K_0 e^{-EA/RT} P_{CH_4} \]  

(2-1-15)

in Arrhenius form,

where:
- \( K_0 \): 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)

\[
\rho A_i V C_p \frac{dT}{dz} = (-\Delta H_1) \frac{dy}{dz} + (-\Delta H_2) \frac{dx}{dz} + h_i \frac{d \xi}{d \xi} (T_w - T) \tag{2-1-16}
\]

\[
\rho_0 V_0 A_0 C_{po} \frac{dT}{dz} = h \sigma \sigma_0 (T - T_w) \tag{2-1-17}
\]

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\(^2\)
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 stoichiometric 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:

$$h_i(dp/k_f) = 2.58(Re)^{1/3}(Pr)^{1/3} + 0.94(Re)^{0.8}(Pr)^{0.4} \quad (2-1-18)$$

where $dp$: equivalent particle diameter, m

$k_f$: thermal conductivity, J/s-m-K

$Pr$: Prandtl number

$Re$: partial 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 energy at the anode. The anode input contains CH4, H2O, H2, CO and CO2. In this analysis, it is assumed that a fixed percentage of hydrogen is consumed at the anode, and the H2O being formed exits the fuel cell, with the depletea air, through the cathode exit. The overall reaction in the fuel cell power section is

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

(2-2-1)

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:

\[ \text{N}_X = \text{N}_I - \frac{(\text{Imean A})}{(n \mathcal{F})} \]  

(2-2-2)

\[ \text{N}_X = \text{N}_I - \frac{(\text{Imean A})}{(2n \mathcal{F})} \]  

(2-2-3)

\[ \text{N}_X = \text{N}_I + \frac{(\text{Imean A})}{(n \mathcal{F})} \]  

(2-2-4)

where

- \text{NX}: exit flow rate of hydrogen, oxygen, or steam, g-mole/sec
- \text{NI}: inlet flow rate of hydrogen, oxygen, or steam, g-mole/sec
- \text{Imean}: mean current density, A/cm²
- \text{A}: effective area of cell plate, cm²
- \text{n}: number of Faraday equivalents transferred
- \mathcal{F}: Faraday constant
The energy balance for the fuel cell is

\[- (Q + W_e) = \sum_{PF} n_j \left( \Delta h_f^0 \right)_j - \sum_{rF} n_i \left( \Delta h_f^0 \right)_i \]

\[+ \sum_{PF} n_j \int_{T_f}^{T_fF} (Cp)_j dT - \sum_{rF} n_i \int_{T_i}^{T_iF} (Cp)_i dT \]

(2-2-5)

where the subscripts PF, rF represent the products and reactants in the fuel cell, respectively. TFF is the final temperature of the products and TIF is the initial temperature of the reactants in the fuel cell. The nj and ni are the species flow rates of the products and reactants, respectively. The terms Q and W are the rates of heat and the electrical energy generation by the fuel cell, respectively. Q is proportional to the specific heat generation QF where:

\[Q = N_p X_n Y_n Q_F \]

(2-2-6)

and \[Q_F = \left( \frac{\Delta H_r}{n_F} - V \right) I \]

(2-2-7)

where:

- Q: total heat generated, J/sec
- QF: heat generated per unit area of cell, J/sec cm²
- Np: number of cells
- Xn: width of cell plate, cm
- Yn: length of cell plate, cm
- I: fuel cell current density, A/cm²
- \(\Delta H_r\): heat of reaction, J/g-mole of H₂

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:
\( V = E - n \)  

(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:

\[
E = E_0 + \frac{RT}{nF} \ln \frac{Y_{H_2}/P_{O_2}}{Y_{H_2}O_{2}}
\]

(2-2-9)

with \( P_t \): total pressure, atm  
\( E_0(T) \): standard E.M.F. of cell at temperature \( T \), volts  
\( E_0(T) = 1.261 - 0.00025 \ T, \ T, \ K \) (Ref. 9)

\( Y_{H_2} \): mean mole fraction of hydrogen at anode  
\( Y_{O_2} \): mean mole fraction of oxygen at cathode  
\( Y_{H_2}O \): mean mole fraction of water vapor at cathode

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

\[
n = n_a + n_r + n_d + n_{co}
\]

(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

\[
n_a = \frac{RT}{Z_{O_2}F} \ln \frac{i}{i_0(SA)(CL)(CU)}
\]

(2-2-11)
with $\alpha_0$: transfer coefficient

$i$: current density, mA/cm$^2$

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

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

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

$CU$: catalyst utilization factor

The exchange current is a function of the acid concentration, temperature, and partial pressure of the oxygen. The acid concentration is a function of the water vapor partial pressure which permits correlation of $io$ as a function of $YO_2$, $YH_2O$, and $T$. An empirical fit is

$$io = 232.7 (PtYO_2)^{0.8} (PtYH_2O)^{0.4377} \exp\left(-6652/T\right)$$  \hspace{1cm} (2-2-12)

The resistance polarization is

$$nr = ir$$

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

The expression of $nco$ was chosen to have strong temperature dependence, be directly proportional to $Yco$, and have a logarithmic dependence on $i$, $iao$, and catalyst effective area. The resulting expression (Ref. 9) is

$$nco = 0.0782PtYco \exp\left(9190 \left(\frac{1}{T} - \frac{1}{450}\right)\right) \ln \frac{i}{CLA \cdot SA \cdot CU \cdot iao}$$  \hspace{1cm} (2-2-13)

where $CLA$: anode catalyst loading, mg

$iao$: anode exchange current, mA/cm$^2$

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, $\varepsilon_{FC}$, can be written as (Ref. 10):

$$\varepsilon_{FC} = \varepsilon_V \varepsilon_I \varepsilon_{TH} \varepsilon_H, \cdots$$  \hspace{1cm} (2-2-14)

where the voltage efficiency $\varepsilon_V$, the current efficiency $\varepsilon_I$, the thermo-dynamic efficiency $\varepsilon_{TH}$, and the heating value efficiency $\varepsilon_H$, are defined as follows:

$$\varepsilon_V = \frac{V}{E}, \cdots$$  \hspace{1cm} (2-2-15)

$$\varepsilon_I = \frac{I}{I_F}, \cdots$$  \hspace{1cm} (2-2-16)

$$\varepsilon_{TH} = \frac{\Delta G_r}{\Delta H_r}, \cdots$$  \hspace{1cm} (2-2-17)

$$\varepsilon_H = \frac{\Delta H_r}{\Delta H_C}, \cdots$$  \hspace{1cm} (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, $\Delta H_r$ 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:
   \[
   \text{DNSS}(33,2) = (1 + \text{EXT} \times 0.01) \times \frac{\text{DNSS}(14,3) + \text{DNSS}(14,5)}{2} + \text{CK} \times \text{DNSS}(14,1)
   \]
   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:
   \[
   T(22) = -\frac{A}{\log\left(\frac{\text{DNSS}(1,1) \times \text{SMRA} - \text{DNSS}(21,6)}{\text{DNSS}(1,1) \times \text{SMRA} - \text{TKNSS}(21)}\right) - B} - A
   \]
   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
   \[
   AC = \frac{-1.0148 + \sqrt{1.0148^2 - 4 \times 0.056/108 \times (0.0472 \times 108 - WK))}}{2 \times 0.0456/108}
   \]

4. Calculate the flow rate of cooling water used in condenser
   \[
   \text{DNSS}(36,6) = \frac{\text{QQT}(5)/18}{(355 - \text{TAT})}
   \]
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>Constant for calculating saturated condition of water, atm</td>
</tr>
<tr>
<td>AA1</td>
<td>Thermal conductivity coeff. of gas I, Btu/hr-ft-R</td>
</tr>
<tr>
<td>AA2</td>
<td>Viscosity coeff of gas I, lbm/ft-hr</td>
</tr>
<tr>
<td>AA3</td>
<td>Specific heat capacity coeff. of gas I. Btu/R-lb-mole of the form:</td>
</tr>
<tr>
<td></td>
<td>$\frac{AA3(1)+AA3(2)*T+AA3(3)*T^2+AA3(4)}{T^2}$</td>
</tr>
<tr>
<td>AHLU</td>
<td>Mole fraction of available hydrogen</td>
</tr>
<tr>
<td>AHRN</td>
<td>Percent free gas space</td>
</tr>
<tr>
<td>AIRL</td>
<td>Length of air channel, ft</td>
</tr>
<tr>
<td>APPD</td>
<td>Total surface area of packing Acc. to the basis and oper. temp., ft^2</td>
</tr>
<tr>
<td>ATMP</td>
<td>Outlet temperature of gases, K</td>
</tr>
<tr>
<td>B</td>
<td>Constant for calculating saturated condition of water, atm-K</td>
</tr>
<tr>
<td>BPNA</td>
<td>Boiling point of naphtha, C</td>
</tr>
<tr>
<td>BSPAC</td>
<td>Baffle space, ft</td>
</tr>
<tr>
<td>CD</td>
<td>Current density, A/cm^2</td>
</tr>
<tr>
<td>CLENH</td>
<td>Length of tube in heat exchanger, ft</td>
</tr>
<tr>
<td>CLEPD</td>
<td>Length of shift converter (JK=1), reformer (JK-2 for methanol and naphtha), ft</td>
</tr>
<tr>
<td>CLH</td>
<td>Clearance in heat exchanger, ft</td>
</tr>
<tr>
<td>CN</td>
<td>U*A/CMIN in heat exchanger</td>
</tr>
<tr>
<td>DG</td>
<td>Standard free energy change, Cal/g-mole</td>
</tr>
<tr>
<td>DHIN</td>
<td>Enthalphy change due to temperature change of inlet fluid, Cal/g-mole</td>
</tr>
<tr>
<td>DHO</td>
<td>Integration constant to calculate H</td>
</tr>
<tr>
<td>DP</td>
<td>Catalyst pellet diameter, ft</td>
</tr>
</tbody>
</table>
TABLE 1

MAIN PROGRAM NOMENCLATURE (cont'd)

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>DPD</td>
<td>Diameter of shift converter (JK=1), reformer (JK=2 for methanol and naphtha), ft</td>
</tr>
<tr>
<td>DSHO</td>
<td>Cathode inlet water of fuel cell, g-mole/hr</td>
</tr>
<tr>
<td>DSN</td>
<td>Cathode inlet nitrogen of fuel cell, g-mole/hr</td>
</tr>
<tr>
<td>DSO</td>
<td>Cathode inlet oxygen of fuel cell, g-mole/hr</td>
</tr>
<tr>
<td>DTH</td>
<td>Fraction of Delta T over inlet gas film in the heat exchanger</td>
</tr>
<tr>
<td>DX1</td>
<td>Outside diameter of reformer center tube, ft</td>
</tr>
<tr>
<td>DX2</td>
<td>Inside diameter of outside reformer tube, ft</td>
</tr>
<tr>
<td>DX3</td>
<td>Outside diameter of outside reformer tube, ft</td>
</tr>
<tr>
<td>DZZ</td>
<td>Increment height of finite difference model in the reformer, ft</td>
</tr>
<tr>
<td>EA</td>
<td>Activation energy for Arrhenius expression, Cal/g-mole CH4</td>
</tr>
<tr>
<td>EPS</td>
<td>Reactor void fraction</td>
</tr>
<tr>
<td>ERR</td>
<td>Convergence criteria</td>
</tr>
<tr>
<td>EXA</td>
<td>Fraction of extra air in fuel cell</td>
</tr>
<tr>
<td>EXT</td>
<td>Fraction of extra air in burner</td>
</tr>
<tr>
<td>FCO</td>
<td>Mole fraction of co contain</td>
</tr>
<tr>
<td>FLOAR</td>
<td>Flow area in heat exchanger, ft²</td>
</tr>
<tr>
<td>FULE</td>
<td>Length of fuel channel, ft</td>
</tr>
<tr>
<td>HNA</td>
<td>Specific heat of naphtha, Btu/lbm-R</td>
</tr>
<tr>
<td>I</td>
<td>Gas number</td>
</tr>
<tr>
<td></td>
<td>I = 1 Fuel (methane, methanol, naphtha)</td>
</tr>
<tr>
<td></td>
<td>I = 2 Oxygen</td>
</tr>
<tr>
<td></td>
<td>I = 3 Carbon Monoxide</td>
</tr>
<tr>
<td></td>
<td>I = 4 Carbon Dioxide</td>
</tr>
<tr>
<td></td>
<td>I = 5 Hydrogen</td>
</tr>
<tr>
<td></td>
<td>I = 6 Water</td>
</tr>
<tr>
<td></td>
<td>I = 7 Nitrogen</td>
</tr>
<tr>
<td>Nomenclature</td>
<td>Description</td>
</tr>
<tr>
<td>--------------</td>
<td>-------------</td>
</tr>
<tr>
<td>ISSH</td>
<td>ID of shell in heat exchanger, ft</td>
</tr>
<tr>
<td>IDTH</td>
<td>ID of tube in heat exchanger, ft</td>
</tr>
<tr>
<td>IFUEL</td>
<td>Fuel Type</td>
</tr>
<tr>
<td></td>
<td>1 = Methane CH4</td>
</tr>
<tr>
<td></td>
<td>2 = Methanol CH3OH</td>
</tr>
<tr>
<td></td>
<td>3 = Naphtha C7H16</td>
</tr>
<tr>
<td>IDNO</td>
<td>Number of trial-and-error loops</td>
</tr>
<tr>
<td>IHUI</td>
<td>Stoichiometric number</td>
</tr>
<tr>
<td>IP</td>
<td>Index of operation condition in the reformer and shift converters</td>
</tr>
<tr>
<td></td>
<td>IP = 1  Adiabatic Operation</td>
</tr>
<tr>
<td></td>
<td>IP = 2  Isothermal Operation</td>
</tr>
<tr>
<td>KO</td>
<td>Frequency factor for Arrhenius expression, lb-mole CH4/lb cata.-hr-atm</td>
</tr>
<tr>
<td>NN</td>
<td>Stream number of exit of shift converter</td>
</tr>
<tr>
<td>NOR</td>
<td>Scale factor in the model of reformer</td>
</tr>
<tr>
<td>NPFU</td>
<td>Number of cell plates in the fuel cell stacks</td>
</tr>
<tr>
<td>NPH</td>
<td>Number of tube passes</td>
</tr>
<tr>
<td>NRH</td>
<td>Number of rows for tubes</td>
</tr>
<tr>
<td>NTAA</td>
<td>Number of air flow channel in one cell plate</td>
</tr>
<tr>
<td>NTAF</td>
<td>Number of fuel flow channel in one cell plate</td>
</tr>
<tr>
<td>NTPD</td>
<td>Number of tubes in shift converter (JK=1), Reformer (JK=2 for methanol and naphtha)</td>
</tr>
<tr>
<td>ODTH</td>
<td>OD of tube, ft</td>
</tr>
<tr>
<td>OU</td>
<td>O2 utilization</td>
</tr>
<tr>
<td>PAT</td>
<td>Ambient pressure, atm</td>
</tr>
<tr>
<td>Symbol</td>
<td>Description</td>
</tr>
<tr>
<td>---------</td>
<td>----------------------------------------------------------------------------</td>
</tr>
<tr>
<td>PIN</td>
<td>Inlet pressure, atm</td>
</tr>
<tr>
<td>PINFU</td>
<td>Inlet pressure of fuel cell stacks, atm</td>
</tr>
<tr>
<td>PITCH</td>
<td>Pitch of heat exchanger, ft</td>
</tr>
<tr>
<td>POP</td>
<td>Operation pressure, atm</td>
</tr>
<tr>
<td>POUT</td>
<td>Outlet pressure, atm</td>
</tr>
<tr>
<td>PL</td>
<td>Platinum catalyst loading, mgPT/CM²</td>
</tr>
<tr>
<td>RHOB</td>
<td>Bulk density of cata., lbs/ft³</td>
</tr>
<tr>
<td>S</td>
<td>Side length of an assumed square flow duct for combustion gas, ft</td>
</tr>
<tr>
<td>SITS2</td>
<td>Ratio of total inside-tube cross-sectional area per pass to header cross-sectional area per pass</td>
</tr>
<tr>
<td>SK</td>
<td>Equilibrium constant</td>
</tr>
<tr>
<td>SKI</td>
<td>Equilibrium constant with pressure different from 1 atm</td>
</tr>
<tr>
<td>SMRA</td>
<td>Steam/fuel ratio</td>
</tr>
<tr>
<td>SURFC</td>
<td>Surface per line, ft</td>
</tr>
<tr>
<td>SV(1)</td>
<td>Specific volume of fuel 1, ft³/1bm</td>
</tr>
<tr>
<td>SVW</td>
<td>Specific volume of water, ft³/1bm</td>
</tr>
<tr>
<td>TACOA</td>
<td>Inlet air temperature of fuel cell stack, K</td>
</tr>
<tr>
<td>TACOF</td>
<td>Inlet fuel temperature of fuel cell stack, K</td>
</tr>
<tr>
<td>TAT</td>
<td>Ambient temperature, K</td>
</tr>
<tr>
<td>TC</td>
<td>Critical temperature, K</td>
</tr>
<tr>
<td>TCAS</td>
<td>Total heat capacity constant A</td>
</tr>
<tr>
<td>TCBS</td>
<td>Total heat capacity constant B</td>
</tr>
<tr>
<td>TCCS</td>
<td>Total heat capacity constant C</td>
</tr>
<tr>
<td>Symbol</td>
<td>Description</td>
</tr>
<tr>
<td>--------</td>
<td>-------------</td>
</tr>
<tr>
<td>TDNS</td>
<td>Total amount of material, g-mole</td>
</tr>
<tr>
<td>TIN</td>
<td>Inlet fluid temperature, K</td>
</tr>
<tr>
<td>TOP</td>
<td>Operation temperature, K</td>
</tr>
<tr>
<td>TOVO</td>
<td>Total volume of inlet flow, m³</td>
</tr>
<tr>
<td>TOUT</td>
<td>Outlet temperature, K</td>
</tr>
<tr>
<td>VHNA</td>
<td>Vaporized heat of naphtha, Cal/g-mole</td>
</tr>
<tr>
<td>WAT</td>
<td>Relative humidity of air, g water/g air</td>
</tr>
<tr>
<td>WIDAA</td>
<td>Width of square air channel in the fuel cell stack, ft</td>
</tr>
<tr>
<td>WIDAF</td>
<td>Width of square fuel channel in the fuel cell stack, ft</td>
</tr>
<tr>
<td>X</td>
<td>Necessary amount of oxygen in cathode, g-mole/hr</td>
</tr>
<tr>
<td>ZH</td>
<td>Reformer length, ft</td>
</tr>
<tr>
<td>DINSC(I)</td>
<td>Inlet amount of gas I, g-mole</td>
</tr>
<tr>
<td>DNS(I)</td>
<td>Inlet (outlet) amount of gas I, g-mole</td>
</tr>
<tr>
<td>HA(J)</td>
<td>Surface area of heat exchanger J, m²</td>
</tr>
<tr>
<td>HCAS(I), HCBS(I), HCCS(I)</td>
<td>Heat capacity const. of gas I, Cal/g-mole-K of the form: ( HCAS + HCBS \cdot T + HCCS \cdot T^2 )</td>
</tr>
<tr>
<td>HS(I)</td>
<td>Heat of formation of gas I at 298 K, 1 atm, Cal/g-mole</td>
</tr>
<tr>
<td>NNS(I)</td>
<td>Stoichiometric coefficient of gas I</td>
</tr>
<tr>
<td>WM(I)</td>
<td>Molecular weight of gas I, g/g-mole</td>
</tr>
<tr>
<td>DNSS(I,J)</td>
<td>Flow rate of gas J in stream I, g-mole/hr</td>
</tr>
</tbody>
</table>
Formulate call.
For the simulation of fuel cell performance, we proceed as follows:

1. Assume composition 1 of 13\(^{*}\).
5. Mixer call.
7. Calculate compositions of 2, 3, 4, 5.

* Stream number (refer to Figure 1)

Figure 4 Flow chart of executive program for simulating CSU's FAPC 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 contains in BURN for methane input fuel are:

1. Calculate the amount of oxygen reacted:
   \[ X = 0.5 \times DNS(3) + 0.5 \times DNS(5) + 2 \times DNS(1) \]  \( (3-2-1) \)

2. Calculate the amount of carbon dioxide produced
   \[ XY = DNS(3) + DNS(1) \]  \( (3-2-2) \)

3. Calculate the amount of water produced
   \[ Y + DNS(5) + 2 \times DNS(1) \]  \( (3-2-3) \)

4. Calculate the exit composition
   \[ DNS(1) = 0 \]
   \[ DNS(3) = 0 \]
   \[ DNS(5) = 0 \]
   \[ DNS(2) = DNS(2) - X \]
   \[ DNS(4) = DNS(4) + XY \]
   \[ DNS(6) = DNS(6) + Y \]
Calculate the amount of oxygen reacted under different fuel input

Calculate the amount of carbon dioxide and water produced

Calculate the exit composition

RETURN

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

\[ QT = \left( \frac{(1-TC1)}{(1-0.577)} \right)^{0.38} \times 9700 \times DNSC(6) + (TCB-TC1) \times 1 \times 18 \times DNSC(6). \]  

(3-2-4)

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

\[ TCB = \frac{B}{A-ALOG(P)} \]

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

\[ WS = GAG \times 1.987 \times TIN \times 1.8 \times \left( \frac{P_{OUT}}{PIN} \right)^{\frac{(GAG-1)}{(GAG-1)}} \]  

(3-2-5)

2. Calculate the compressor shaft work assuming isothermal conditions

\[ WS = 1.987 \times TIN \times 1.8 \times ALOG(P_{OUT}/PIN) \]  

(3-2-6)

3. Calculate the compressor power requirements

\[ POW = WS \times TDNS / 641400 \]  

(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)

\[ QT = QT + DNSH(I) \times (HCAS(I) \times (THI - THO) + HCBS(I) \times (THI^{2} - THO^{2}) + HCCS(I) \times (THI^{3} - THO^{3}). \]  

\[ (3-2-8) \]

2. Calculate the condenser heat transfer capacity with the Watson

\[ QT = QT + ((1 - (THO/647.1)) / (1 - 0.577)^{0.38} \times 9700 \times DNSH(6)) \] 

\[ (3-2-9) \]

where Watson correction is given as,

\[ \frac{(h_{fg})_2}{(h_{fg})_1} = \frac{1 - T_{r}^{2}}{1 - T_{r}^{2}} \times 0.38 \] 

\[ (3-2-10) \]

where \( h_{fg} \): 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:

\[ XT = (XA(NR) \times YV - YA(NR) \times XV) / (XA(NR) - XV + YV - YA(NR)) \] 

\[ (3-2-11) \]

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.
Calculate the mean temperature of hot side

Calculate the heat capacity rate of hot side

Calculate the heat duty in the condenser

RETURN

Figure 8 Flow Chart of COND
Calculate the total thermal constant

Assume the initial guess of outlet temperature

Calculate the energy balance to obtain outlet temperature

Test for convergence
CALL CONV

Calculate the composition and pressure of outlet stream

RETURN

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

\[
T_{\text{OUTC}} = (T_{\text{CAS1}} T_{\text{IN1}} + T_{\text{CAS2}} (T_{\text{IN2}} - T_{\text{OUT}}) + T_{\text{CBS1}} / 2 \cdot (T_{\text{IN1}}^2 - T_{\text{OUT}}^2) + T_{\text{CBS2}} / 2 \cdot (T_{\text{IN2}}^2 - T_{\text{OUT}}^2) + T_{\text{CCS1}} \cdot (T_{\text{IN1}}^3 - T_{\text{OUT}}^3) / 3 + T_{\text{CCS2}} \cdot (T_{\text{IN2}}^3 - T_{\text{OUT}}^3) / 3) / T_{\text{CAS1}}
\]  

2. Calculate the outlet pressure

\[
P_{\text{OUT}} = (T_{\text{DNS1}} T_{\text{DNS2}}) / (T_{\text{DNS1}} T_{\text{IN1}} / P_{\text{IN1}} T_{\text{DNS2}} T_{\text{IN2}} / P_{\text{IN2}}) * T_{\text{OUT}}
\]  

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, thermo-dynamic 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
Calculate the molar fraction of hydrogen
Calculate the operating voltage of one cell
Calculate the open-circuit potential
Calculate the free energy change
Calculate the voltage and current efficiency
Calculate the electrical work
Calculate the thermodynamic efficiency
Calculate the heating value and total fuel cell efficiency

Figure 10 Flow Chart of ENFU
Calculate the material balance of fuel cell stack
CALL FUCE

Calculate the outlet composition

Assume the outlet temperature

Calculate the energy balance for obtaining outlet temperature

Test for convergence
CALL CONV

YES

Calculate the rejected heat

RETURN

NO

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

\[
d \ln K = \frac{\Delta H^0}{RT^2} dT
\]  

(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,

\[
\ln K = \frac{-DHO}{RT} + \frac{\Delta a}{R} \ln(T) + \frac{\Delta b}{2R} T + \frac{\Delta \gamma}{6R} T^2 + AI
\]  

(3-2-15)

where \( \Delta b \) 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:
Calculate the material balance of reformer (for methanol and naphtha) CALL REF

Calculate the outlet composition

Calculate the enthalpy change with temperature

Calculate the enthalpy change of reaction

Calculate the total capacity constant

Calculate the energy balance for obtaining outlet temperature

Test for convergence CALL CONV

RETURN

Figure 11: Flow Chart of ENRE
Calculate the material balance of shift converter
CALL PDSH

Calculate the outlet composition

Calculate the enthalpy change with temperature

Calculate the enthalphy change of reaction

Calculate the total capacity constant

Calculate the outlet temperature

Test for convergence
CALL CONV

RETURN

Figure 12 Flow Chart of ENSH
Figure 13 Flow Chart of EQUK
1. Calculate heat capacity constants
   
   \[ \text{TCAS} = \text{TCAS} + \text{NNS}(I) \times \text{HCAS}(I) \]
   \[ \text{TCBS} = \text{TCBS} + \text{NNS}(I) \times \text{HCBS}(I) \]
   \[ \text{TCCS} = \text{TCCS} + \text{NNS}(I) \times \text{HCCS}(I) \]  
   (3-2-16)

2. Calculate enthalpy of reaction change
   
   \[ \text{DH} = \text{DH} + \text{NNS}(I) \times \text{HS}(I) \]  
   (3-2-17)

3. Calculate free energy of reaction
   
   \[ \text{DG} = \text{DG} + \text{NNS}(I) \times \text{GS}(I) \]  
   (3-2-18)

4. Calculate constant DHO
   
   \[ \text{DHO} = \text{DH} - \text{TCAS} \times \text{TST} - \text{TCBS} \times \text{TST}^2/2 - \text{TCCS} \times \text{TST}^3/3 \] 
   (3-2-19)

5. Calculate constant A1
   
   \[ \text{A1} = \frac{(\text{DHO} - \text{DG} - \text{TCAS} \times \text{TST} \times \text{ALOG(TST)} - \text{TCBS}/2 \times \text{TST}^2 - \text{TCCS}/6 \times \text{TST}^3)}{\text{TST}/\text{R}} \] 
   (3-2-20)

6. Calculate equilibrium constant
   
   \[ \text{SK} = \exp(-\text{DHO}/\text{R} \times \text{TOP} + \text{TCAS}/\text{R} \times \text{ALOG(TOP)} + \text{TCBS}/2 \times \text{TOP}/\text{R} + \text{TCCS}/6 \times \text{TOP}^2/\text{R} + \text{AI}) \] 
   (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
   \[ DH = DH + DNS(I) \cdot HS(I) - DINS(I) \cdot HS(I) \]  
   \[ DH = DH + DNS(I) \cdot HS(I) \]  

2. Calculate the sensible enthalpy change
   \[ DH = DH + DINS(I) \cdot (HCAS(I) \cdot (298 - TIN) + HCBS(I) / 2 \cdot ((298)^2 - TIN^2) + hCCS(I) / 3 \cdot ((298)^3 - TIN^3)) \]  

3. Calculate total heat capacity constants
   \[ TCAS = TCAS + DNS(I) \cdot HCAS(I) \]  
   \[ TCBS = TCBS + DNS(I) \cdot HCBS(I) \]  
   \[ TCCS = TCCS + DNS(I) \cdot HCCS(I) \]  

4. Calculate the adiabatic FLAME temperature
   \[ TFC = (-DH - TCBS / 2 \cdot ((TF)^2 - (298)^2) - TCCS / 3 \cdot ((TF)^3 - (298)^3)) / TCAS + 298 \]  

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
Calculate the material balance of burner
CALL BURN

Calculate the enthalpy change of reaction

Calculate the enthalpy change with temperature

Calculate the total heat capacity constant

Calculate the energy balance for obtaining the outlet temperature

NO

Test for convergence
CALL CONV

YES

RETURN

Figure 14 Flow Chart of FLAME
Calculate $H_2$ consumption

Calculate cathode inlet molar rate

Calculate anode and cathode outlet molar rate

RETURN

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

\[ NT = \frac{HA}{0.3048^2/NP/CLEN/SURFC} \]  

(3-2-26)

2. Calculate number of baffles

\[ NB = CLEN/BSPAC \]  

(3-2-27)

3. Calculate free area between baffles

\[ FAREA = \frac{IDS/(ODT+CL)*CL*BSPAC}{ODT+CL} \]  

(3-2-28)

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

\[ XT = \frac{PITCH}{ODT} \]  

(3-2-29)

5. Calculate friction factor

\[ FPRI = SBO*(ODT*GS/AMUI)^{-0.15} \]  

(3-2-30)

6. Calculate pressure drop

\[ DP = B0*2*FPRT*NRT*GS^2/32.174/3600^2/RHO/2116.2 \]  

(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).
Calculate the number of tubes and baffles

Calculate FAREA, BO,XT

Calculate shell side mean molecular weight, viscosity, and density then mass flow rate

Calculate shell side friction then pressure drop

Calculate tube side mean molecular weight, density, conductivity, and heat transfer coefficient then mass flow rate

Calculate viscosity at bulk and inside tube wall temperature

Calculate tube side Reynolds number then friction

Calculate constants and pressure drop of tube side

RETURN

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

\[
POW = SVW \times 144 \times 0.05051 \times 0.0000001 \times WM(6) \times 14.7 \times (POUT - PIN) \times DNS(6) / 1453.6
\]

(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 $f_2(x_1, x_2) = 0$:

$$\begin{align*}
x_1' &= x_1 \text{ old} + \Delta x_1 \\
x_2' &= x_2 \text{ old} + \Delta x_2
\end{align*} \quad \text{(3-2-33)}$$

where

$$\Delta x_1 = \frac{f_2 \frac{\partial f_1}{\partial x_2} - f_1 \frac{\partial f_2}{\partial x_2}}{D} \quad \text{(3-2-34)}$$

and

$$\Delta x_2 = \frac{f_1 \frac{\partial f_2}{\partial x_1} - f_2 \frac{\partial f_1}{\partial x_1}}{D}$$

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

$$X_W = \frac{(TDNS-DNS(6))/(DK-1)}{\text{(3-2-35)}}$$
Calculate equilibrium constants of $\gamma_{xn 1}$ and $\gamma_{n 2}$
CALL EQUK

Change the equilibrium constants to molar fraction basis

Solve the material balance equations
CALL SNAE

Calculate the outlet composition

RETURN

Figure 17: Flow Chart of Subroutine REF
where $X_W$: amount of water in liquid phase

$D_K$: equilibrium constant of liquid-vapor system, which equals to $(P_{SAT}/P_{OP})$

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 discussion 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

\[ X_1(i+1) = X_1(i) = \frac{e_B}{U_0} \frac{P \Delta Z}{C_0} K_0 - \frac{E}{R[T_A(i+1)+460]} X_{M\text{COMP}}(i,1) \]

2. Water Gas Shift Equilibrium

\[ X_2 = \frac{-B - B^2 - 4CA}{2A} \]

with

\[ A = [K_2(i+1)-1][F_3+X_1(i+1) F_1]^2 \]
\[ B = [F_3+X_1(i+1) F_1][2X_1(i+1) F_1 K_2(i+1)-F_2 K_2(i+1)-F_4 K_2(i+1)-5X_1(i+1) F_1-F_3-F_5] \]
\[ C = K_2(i+1) F_4-2K_2(i+1) F_2 X_1(i+1) F_1-[F_3+X_1(i+1)] [F_5+4X_1(i+1) F_1] \]

3. Reforming Gas Energy Balance

\[ T_C(i+1) = \frac{T_H(i+1)}{AM} [AM-MH \ CH] + \frac{T_H(i)}{AM} [AM+MH \ CH] - T_C(i) \]

with

\[ AM = (U_1 \pi D_2 \Delta Z)/2 \]

4. Combustion Gas Energy Balance

\[ T_H(i+1) = T_H(i) \frac{AN+2(\Sigma FACP)}{AN} - T_C(i) \frac{2(\Sigma FACP)}{AN} - \frac{AL}{AN} \]

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

\[ AL = F_1 (-DH_1)[X_1(i+1)-X_1(i)]+[F_3+X_1(i+1) F_1](-DH_2)[X_2(i+1)-X_2(i)] \]

\[ AN = \frac{MH \ CH(\Sigma FACP)}{AM} - \Sigma FACP+MH \ CH \]

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

<table>
<thead>
<tr>
<th>Component</th>
<th>Compound</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>CH₄</td>
</tr>
<tr>
<td>2</td>
<td>CO</td>
</tr>
<tr>
<td>3</td>
<td>CO₂</td>
</tr>
<tr>
<td>4</td>
<td>H₂O</td>
</tr>
<tr>
<td>5</td>
<td>H₂</td>
</tr>
<tr>
<td>6</td>
<td>N₂</td>
</tr>
<tr>
<td>7</td>
<td>O₂</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Variable</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>FL for J = 0 to 7</td>
<td>Total reformer gas feed flow rate and component feed flow rates for components 1 through 7 (molar basis)</td>
</tr>
<tr>
<td>MH</td>
<td>Total combustion gas flow rate (molar basis)</td>
</tr>
<tr>
<td>CGCOM for J = 1 to 7</td>
<td>Combustion gas component flow rates for components 1 to 7 (molar basis)</td>
</tr>
<tr>
<td>K₁</td>
<td>Equilibrium constant for demethanation reaction</td>
</tr>
<tr>
<td>K₂</td>
<td>Equilibrium constant for water shift reaction</td>
</tr>
<tr>
<td>K₀</td>
<td>Frequency factor for Arrhenius expression $k + k₀ \exp(-Eₐₑₓ/(R·T))$</td>
</tr>
<tr>
<td>WM</td>
<td>Molecular weight</td>
</tr>
<tr>
<td>EA</td>
<td>Activation energy for demethanation reaction</td>
</tr>
<tr>
<td>RHOB</td>
<td>Catalyst bulk density</td>
</tr>
<tr>
<td>EPS</td>
<td>Reactor void volume</td>
</tr>
<tr>
<td>D₁</td>
<td>Reformer center tube outside diameter</td>
</tr>
<tr>
<td>D₂</td>
<td>Reformer outer tube inside diameter</td>
</tr>
<tr>
<td>D₃</td>
<td>Reformer outer tube outside diameter</td>
</tr>
<tr>
<td>S</td>
<td>Characteristic dimension of the combustion gas flow duct (geometry is square)</td>
</tr>
<tr>
<td>DP</td>
<td>Catalyst particle diameter</td>
</tr>
<tr>
<td>P</td>
<td>Pressure</td>
</tr>
</tbody>
</table>
TABLE 3
NOMENCLATURE OF VARIABLES AND FUNCTIONS IN SUBROUTINE KREF
(cont'd)

<table>
<thead>
<tr>
<th>Variable</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>TCO</td>
<td>Reformer gas feed temperature</td>
</tr>
<tr>
<td>THZ</td>
<td>Combustion gas feed temperature</td>
</tr>
<tr>
<td>Z</td>
<td>Length of reformer tube</td>
</tr>
<tr>
<td>X1(I)</td>
<td>Kinetic conversion by demethanation reaction in Increment I</td>
</tr>
<tr>
<td>XE2(I)</td>
<td>Actual conversion by water shift reaction in Increment I</td>
</tr>
<tr>
<td>CO</td>
<td>Initial methane concentration in reformer gas</td>
</tr>
<tr>
<td>UO</td>
<td>Initial reformer gas linear velocity</td>
</tr>
<tr>
<td>T</td>
<td>Temperature</td>
</tr>
<tr>
<td>TK2</td>
<td>Equilibrium constant for demethanation reaction at temperature T</td>
</tr>
<tr>
<td>TX2</td>
<td>Equilibrium conversion for water shift reaction at temperature T</td>
</tr>
<tr>
<td>TDH1</td>
<td>Heat of reaction for demethanation reaction at temperature T</td>
</tr>
<tr>
<td>TDH2</td>
<td>Heat of reaction for water shift reaction at temperature T</td>
</tr>
<tr>
<td>X2</td>
<td>Equilibrium conversion for water shift reaction</td>
</tr>
<tr>
<td>DH1</td>
<td>Heat of reaction for demethanation reaction</td>
</tr>
<tr>
<td>DH2</td>
<td>Heat of reaction for water shift reaction</td>
</tr>
<tr>
<td>TF</td>
<td>Total moles of reformer gas</td>
</tr>
<tr>
<td>TVIS</td>
<td>Viscosity at temperature T</td>
</tr>
<tr>
<td>VIS</td>
<td>Viscosity</td>
</tr>
<tr>
<td>THC</td>
<td>Thermal conductivity</td>
</tr>
<tr>
<td>Variable</td>
<td>Definition</td>
</tr>
<tr>
<td>-----------</td>
<td>---------------------------------------------------------------------------</td>
</tr>
<tr>
<td>TTHC</td>
<td>Thermal conductivity at temperature T</td>
</tr>
<tr>
<td>HI</td>
<td>Inside heat transfer coefficient for the reformer outer tube</td>
</tr>
<tr>
<td>THI</td>
<td>Same as HI evaluated at temperature T</td>
</tr>
<tr>
<td>HO</td>
<td>Outside heat transfer coefficient for the reformer gas outer tube</td>
</tr>
<tr>
<td>THO</td>
<td>HO evaluated at temperature T</td>
</tr>
<tr>
<td>UI</td>
<td>Overall heat transfer coefficient for reformer outer tube</td>
</tr>
<tr>
<td>TUI</td>
<td>UI evaluated at temperature T</td>
</tr>
<tr>
<td>FCP</td>
<td>Reformer gas heat capacity</td>
</tr>
<tr>
<td>TFCP</td>
<td>Reformer gas heat capacity at temperature T</td>
</tr>
<tr>
<td>THO</td>
<td>Combustion gas outlet temperature</td>
</tr>
<tr>
<td>DZZ</td>
<td>Incremental length</td>
</tr>
<tr>
<td>TA(I)</td>
<td>Average temperature in Increment I</td>
</tr>
<tr>
<td>I</td>
<td>Increment counter</td>
</tr>
<tr>
<td>TAK1</td>
<td>K1 evaluated at TA(I, K)</td>
</tr>
<tr>
<td>TAK2</td>
<td>K2 evaluated at TA(I, K)</td>
</tr>
<tr>
<td>TAX2</td>
<td>Conversion X2 for water shift reaction assuming total system equilibrium</td>
</tr>
<tr>
<td>XF</td>
<td>Total number of moles in the reformer gas</td>
</tr>
<tr>
<td>XUI</td>
<td>Overall heat transfer in Increment I</td>
</tr>
<tr>
<td>XCOMP(I, J)</td>
<td>Moles of component J in Increment I</td>
</tr>
<tr>
<td>COM(J)</td>
<td>Feed moles of component J</td>
</tr>
</tbody>
</table>
TABLE 3
NOMENCLATURE OF VARIABLES AND FUNCTIONS IN SUBROUTINE KREF
(cont'd)

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

<table>
<thead>
<tr>
<th>NAMELIST LIST</th>
<th>VARIABLE NAME</th>
<th>DIMENSION</th>
<th>SAMPLE VALUE</th>
<th>UNIT</th>
<th>DEFINITION</th>
</tr>
</thead>
<tbody>
<tr>
<td>OPFC</td>
<td>TOPFC</td>
<td></td>
<td>443</td>
<td>K</td>
<td>Operating temperature in fuel cell stack</td>
</tr>
<tr>
<td>OPFC</td>
<td>UT</td>
<td></td>
<td>0.8</td>
<td></td>
<td>Utilization of H2 in stack</td>
</tr>
<tr>
<td>OPFC</td>
<td>CD</td>
<td></td>
<td>325</td>
<td>mA/cm²</td>
<td>Designed current density</td>
</tr>
<tr>
<td>INIT</td>
<td>DNSM</td>
<td>1</td>
<td>1216.</td>
<td>g-mole/hr</td>
<td>Input mole flow rate of CH₄</td>
</tr>
<tr>
<td></td>
<td></td>
<td>2</td>
<td>0</td>
<td>g-mole/hr</td>
<td>Input mole flow rate of O₂</td>
</tr>
<tr>
<td></td>
<td></td>
<td>3</td>
<td>1.36</td>
<td>g-mole/hr</td>
<td>Input mole flow rate of CO</td>
</tr>
<tr>
<td></td>
<td></td>
<td>4</td>
<td>21.8</td>
<td>g-mole/hr</td>
<td>Input mole flow rate of CO₂</td>
</tr>
<tr>
<td></td>
<td></td>
<td>5</td>
<td>166.</td>
<td>g-mole/hr</td>
<td>Input mole flow rate of H₂</td>
</tr>
<tr>
<td></td>
<td></td>
<td>6</td>
<td>0</td>
<td>g-mole/hr</td>
<td>Input mole flow rate of H₂O</td>
</tr>
<tr>
<td></td>
<td></td>
<td>7</td>
<td>0</td>
<td>g-mole/hr</td>
<td>Input mole flow rate of N₂</td>
</tr>
<tr>
<td>INIT</td>
<td>TAT</td>
<td></td>
<td>298</td>
<td>K</td>
<td>Ambient temperature</td>
</tr>
<tr>
<td>INIT</td>
<td>PAT</td>
<td></td>
<td>1</td>
<td>atm</td>
<td>Ambient temperature</td>
</tr>
<tr>
<td>INIT</td>
<td>SMRA</td>
<td></td>
<td>3.0</td>
<td></td>
<td>Steam to carbon ratio</td>
</tr>
<tr>
<td>INIT</td>
<td>POPR</td>
<td></td>
<td>5.0</td>
<td>atm</td>
<td>Operating pressure of reformer</td>
</tr>
<tr>
<td>CONDT</td>
<td>IFUEL</td>
<td></td>
<td>1</td>
<td></td>
<td>= 1 Input fuel is methane</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>= 2 Input fuel is methanol</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>= 3 Input fuel is naphtha</td>
</tr>
<tr>
<td>CONDT</td>
<td>ERR</td>
<td></td>
<td>0.01</td>
<td></td>
<td>Criterion of convergence in system trial and error procedure</td>
</tr>
</tbody>
</table>
### TABLE 4 (cont'd)

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

**(SAMPLE RUN)**

<table>
<thead>
<tr>
<th>NAMELIST LIST</th>
<th>VARIABLE NAME</th>
<th>DIMENSION</th>
<th>SAMPLE VALUE</th>
<th>UNIT</th>
<th>DEFINITION</th>
</tr>
</thead>
<tbody>
<tr>
<td>CONDT</td>
<td>IP</td>
<td>2</td>
<td></td>
<td></td>
<td>= 1 adiabatic operation in shift converters</td>
</tr>
<tr>
<td>CONDT</td>
<td>I</td>
<td>7</td>
<td></td>
<td></td>
<td>= 2 isothermal operation in shift converters</td>
</tr>
<tr>
<td>CONDT</td>
<td>EXT</td>
<td>100</td>
<td></td>
<td></td>
<td>Number of components in whole system</td>
</tr>
<tr>
<td>CONDT</td>
<td>WAT</td>
<td>0.015</td>
<td>g water/g air</td>
<td></td>
<td>Extra percentage of needed air in burner</td>
</tr>
<tr>
<td>CONDT</td>
<td>EXA</td>
<td>100</td>
<td></td>
<td></td>
<td>Relative humidity of air</td>
</tr>
<tr>
<td>REPEN</td>
<td>ZH</td>
<td>6</td>
<td>ft</td>
<td></td>
<td>Extra percentage of air in fuel cell stack</td>
</tr>
<tr>
<td>REPEN</td>
<td>DX1</td>
<td>0</td>
<td>ft</td>
<td></td>
<td>Height of reformer</td>
</tr>
<tr>
<td>REPEN</td>
<td>DX2</td>
<td>0.15</td>
<td>ft</td>
<td></td>
<td>Outside diameter of regenerative tube</td>
</tr>
<tr>
<td>REPEN</td>
<td>DX3</td>
<td>0.1667</td>
<td>ft</td>
<td></td>
<td>Inside diameter of reforming tube</td>
</tr>
<tr>
<td>REPEN</td>
<td>KO</td>
<td>10400</td>
<td>lb-mole CH₄/</td>
<td>lb cata-hr-atm</td>
<td>Outside diameter of reforming tube</td>
</tr>
<tr>
<td>REPEN</td>
<td>EA</td>
<td>20000</td>
<td>Cal/g-mole CH₄</td>
<td></td>
<td>Rate constant of demethanation reaction</td>
</tr>
<tr>
<td>REPEN</td>
<td>RHOB</td>
<td>80</td>
<td>lb/ft³</td>
<td></td>
<td>Activity energy of demethanation reaction</td>
</tr>
<tr>
<td>REPEN</td>
<td>EPS</td>
<td>0.487</td>
<td></td>
<td></td>
<td>Density of packing in reformer</td>
</tr>
<tr>
<td>REPEN</td>
<td>S</td>
<td>0.25</td>
<td>ft</td>
<td></td>
<td>Void fraction in reformer</td>
</tr>
<tr>
<td>REPEN</td>
<td>DP</td>
<td>0.00328</td>
<td>ft</td>
<td></td>
<td>Width of combustion gas square duct</td>
</tr>
<tr>
<td>REPEN</td>
<td>DZZ</td>
<td>0.25</td>
<td>ft</td>
<td></td>
<td>Diameter of catalyst in reformer</td>
</tr>
<tr>
<td>HEATX</td>
<td>CN</td>
<td>1.3</td>
<td>m²-K</td>
<td></td>
<td>Height of finite-difference section</td>
</tr>
</tbody>
</table>

QxA/C min in heat exchanger
TABLE 4 (cont'd)

INPUT DATA FOR SIMULATION OF CSU PAFC SYSTEM STEADY STATE PERFORMANCE

(SAMPLE RUN)

<table>
<thead>
<tr>
<th>NAMELIST LIST</th>
<th>VARIABLE NAME</th>
<th>DIMENSION</th>
<th>SAMPLE VALUE</th>
<th>UNIT</th>
<th>DEFINITION</th>
</tr>
</thead>
<tbody>
<tr>
<td>HEATX</td>
<td>U</td>
<td></td>
<td>48825.1</td>
<td>cal/m²-hr-K</td>
<td>Overall heat transfer coefficient in heat exchanger</td>
</tr>
<tr>
<td>HEATX</td>
<td>HA</td>
<td>7</td>
<td>0.2</td>
<td>m²</td>
<td>Transfer area in E-7</td>
</tr>
<tr>
<td></td>
<td></td>
<td>10</td>
<td>0.2</td>
<td>m²</td>
<td>Transfer area in E-10</td>
</tr>
<tr>
<td>HEPDC</td>
<td>NPH</td>
<td></td>
<td>2</td>
<td></td>
<td>Number of tube passes</td>
</tr>
<tr>
<td>HEPDC</td>
<td>NRH</td>
<td></td>
<td>5</td>
<td></td>
<td>Number of tube rows</td>
</tr>
<tr>
<td>HEPDC</td>
<td>BASPC</td>
<td>1</td>
<td>ft</td>
<td></td>
<td>Baffle space</td>
</tr>
<tr>
<td>HEPDC</td>
<td>ODTH</td>
<td></td>
<td>0.0625</td>
<td>ft</td>
<td>O.D. of tube</td>
</tr>
<tr>
<td>HEPDC</td>
<td>PITCH</td>
<td></td>
<td>0.0833</td>
<td>ft</td>
<td>Pitch of heat exchanger</td>
</tr>
<tr>
<td>HEPDC</td>
<td>CLH</td>
<td></td>
<td>0.0208</td>
<td>ft</td>
<td>Clearance in heat exchanger</td>
</tr>
<tr>
<td>HEPDC</td>
<td>IDSH</td>
<td></td>
<td>0.833</td>
<td>ft</td>
<td>I.D. of shell</td>
</tr>
<tr>
<td>HEPDC</td>
<td>IDTH</td>
<td></td>
<td>0.04667</td>
<td>ft</td>
<td>I.D. of tube</td>
</tr>
<tr>
<td>HEPDC</td>
<td>FLOAR</td>
<td></td>
<td>0.001716</td>
<td>ft</td>
<td>Flow area in heat exchanger</td>
</tr>
<tr>
<td>HEPDC</td>
<td>SURFC</td>
<td></td>
<td>0.1466</td>
<td>ft</td>
<td>Surface area per line</td>
</tr>
<tr>
<td>HEPDC</td>
<td>CLENH</td>
<td>2</td>
<td>ft</td>
<td></td>
<td>Length of tube</td>
</tr>
<tr>
<td>HEPDC</td>
<td>SITSZ</td>
<td></td>
<td>0.5</td>
<td></td>
<td>Ratio of total inside tube cross-sectional area per pass to header cross-sectional area per pass</td>
</tr>
<tr>
<td>HEPDC</td>
<td>UTH</td>
<td></td>
<td>0.7</td>
<td></td>
<td>Fraction of ΔT over inlet gas film in heat exchanger</td>
</tr>
</tbody>
</table>
### TABLE 4 (cont'd)

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

*(SAMPLE RUN)*

<table>
<thead>
<tr>
<th>NAMELIST LIST</th>
<th>VARIABLE NAME</th>
<th>DIMENSION</th>
<th>VALUE</th>
<th>UNIT</th>
<th>DEFINITION</th>
</tr>
</thead>
<tbody>
<tr>
<td>PDSHH</td>
<td>DPD</td>
<td>1</td>
<td>1.18</td>
<td>ft</td>
<td>Diameter of shift converters</td>
</tr>
<tr>
<td>PDSHH</td>
<td>AHRN</td>
<td>1</td>
<td>0.66</td>
<td></td>
<td>Void fraction in shift converters</td>
</tr>
<tr>
<td>PDSHH</td>
<td>APPD</td>
<td>1</td>
<td>69</td>
<td>ft²</td>
<td>Total surface area of packing</td>
</tr>
<tr>
<td>PDSHH</td>
<td>CLEPD</td>
<td>1</td>
<td>5.91</td>
<td>ft</td>
<td>Length of shift converters</td>
</tr>
<tr>
<td>PDSHH</td>
<td>NTPD</td>
<td>1</td>
<td>1</td>
<td></td>
<td>Number of tubes in shift converters</td>
</tr>
<tr>
<td>PDFUH</td>
<td>NTAF</td>
<td></td>
<td>140</td>
<td></td>
<td>Number of fuel flow channels in stack</td>
</tr>
<tr>
<td>PDFUH</td>
<td>FULE</td>
<td></td>
<td>1.42</td>
<td>ft</td>
<td>Length of fuel channel</td>
</tr>
<tr>
<td>PDFUH</td>
<td>WIDAF</td>
<td></td>
<td>0.00974</td>
<td>ft</td>
<td>Width of square fuel channel</td>
</tr>
<tr>
<td>PDFUH</td>
<td>NPFU</td>
<td></td>
<td>3365</td>
<td></td>
<td>Number of cell plates</td>
</tr>
<tr>
<td>PDFUH</td>
<td>NTAA</td>
<td></td>
<td>40</td>
<td></td>
<td>Number of process air flow channels</td>
</tr>
<tr>
<td>PDFUH</td>
<td>AIRL</td>
<td>1</td>
<td></td>
<td>ft</td>
<td>Length of air channel</td>
</tr>
<tr>
<td>PDFUH</td>
<td>WIDAA</td>
<td></td>
<td>0.00515</td>
<td>ft</td>
<td>Width of square process air channel</td>
</tr>
<tr>
<td>CATAI</td>
<td>SRO</td>
<td>0.44</td>
<td></td>
<td>Ω-cm</td>
<td>Cell resistance at 450° K</td>
</tr>
<tr>
<td>CATAI</td>
<td>SA</td>
<td>400</td>
<td></td>
<td>cm²/mg</td>
<td>Surface area of catalyst</td>
</tr>
<tr>
<td>CATAI</td>
<td>CU</td>
<td>0.15</td>
<td></td>
<td></td>
<td>Utilization of catalyst</td>
</tr>
<tr>
<td>CATAI</td>
<td>CL</td>
<td>0.75</td>
<td></td>
<td>mg/cm²</td>
<td>Catalyst loading</td>
</tr>
<tr>
<td>CATAI</td>
<td>ALFA</td>
<td>0.50</td>
<td></td>
<td></td>
<td>Transfer coefficient</td>
</tr>
<tr>
<td>CATAI</td>
<td>SN</td>
<td>2</td>
<td></td>
<td>g-equivalent</td>
<td>Number of Faraday equivalents transferred</td>
</tr>
<tr>
<td>CATAI</td>
<td>FCONST</td>
<td>96500</td>
<td></td>
<td>C/g-equivalent</td>
<td>Faraday constant</td>
</tr>
<tr>
<td>CATAI</td>
<td>DKC</td>
<td>240000</td>
<td></td>
<td>A/atm</td>
<td>Constant to calculate limiting current density</td>
</tr>
</tbody>
</table>
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 oxidant 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 TOFC=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
&COND IFUEL=1,ERR=0.01,IP=2,1=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,DZ2=0.25,
&END
&HEATX CN=1.3,U=48825.1,HA(7)=0.2,HA(10)=0.2,
&END
&HEPDC NPH=2,MRH=5,BSPAC=1.,ODTH=.0625,PITCH=.0833,CLH=.0208,DISH=.833,
,IDTH=.04667,FLOAR=.001716,SURFC=.1466,CLENH=.125,SLTS2=0.5,DTH=0.7,
&END
&PDSH DPD=1.18,0.,AHRN=0.66.,0.,APPD=69.0.,CLEPD=5.91,0.,
NTPD=1.0,
&END
&PDFUH NATF=140,FLUE=1.42,WIDTH=.009744,NPFU=3365,
NTAA=40,AIRL=1.,WIDAA=.00515
&END
&CATAI SR0=.44,SA=400.,CN=.15,CL=.75,ALFA=.5,SN=2.,FCONST=96500.,
DKC=2.4E5,
&END

Figure 20 Sample Input Data
Figure 21 Sample Computer Run
NTPD= 1. 0
END
&PDFUH
NIAF= 140
FULE= 1.419999
WIDAF= 0.97440E-02
NPFU= 3565
NIAA= 40
ATJ= 1.0
WIDAA= 0.514996E-02
&END
&CATJA
SK0= 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 SEPARATOR 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 00
THE CURRENT EFFICIENCY IS 0.80000E 00
THE VOLTAGE EFFICIENCY IS 0.56251E 00
THE HEATING VALUE EFFICIENCY IS 0.90470E 00
THE FUEL CELL EFFICIENCY IS 0.3780
THE ELECTRICAL WORK IS 0.12601E 03KW
THE TOTAL HEAT RELEASE IS 0.53266E 08CAL

THE AC OUTPUT IS 113.77KW

Figure 21 continued
THE DUTY OF HEAT EXCHANGER (CAL.) (0 MEANS NO THIS NO. HEAT EXCHANGER)

E-1  E-2  E-3  E-4  E-5  E-6  E-7  E-8  E-9  E-10
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 (M²) (0 MEANS NO THIS NO. HEAT EXCHANGER)

E-1  E-2  E-3  E-4  E-5  E-6  E-7  E-8  E-9  E-10
0.38308E 00  0.13514E 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-1  E-2  E-3  E-4  E-5  E-6  E-7  E-8  E-9  E-10
0.68881E 00  0.59456E 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: 64.04 HP
THE POWER OF METHANE COMPRESSOR: 3.80 HP
THE POWER OF PUMP: 0.00146 HP

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


Listing of the Steady State Performance Lumped Model

000020C  BLOCK DATA
000040CC
000060C  **** BLOCK DATA FOR CSU PROM FUEL CELL POWER PLANT PERFORMANCE
000080C  DIMENSION GS(7),HS(7),HCAS(7),HCBS(7),HCCS(7),WM(7),SV(3),
000100C  IHLMV(7),A1(2,7),A2(2,7),A3(4,7)
000120C  COMMON /ETHDA/ GS,HS,HCAS,HCBS,HCCS
000140C  COMMON /TC/ TC/CS/ A,B
000160C  COMMON /GAG/ GAG4,GAGA
000180C  COMMON /NH4+/NH4+,NH2+,VHNA
000200C  COMMON /RM/ WM
000220C  COMMON /SV/ SV,SW
000240C  COMMON /MLMV/ MLMV
000260C  COMMON /THCC/Al/HTPC/A2/HTPC/A3
000280C  STANDARD VALUE OF FREE ENERGY, ENTHALPHY AND HEAT CAPACITY CONSTANT
000300C  DATA GS/-1246.0,-32781.,-94259.,0.,-56435.,0./
000320C  DATA HS/-17659.0,-26416.,-94051.0,-57798.0/
000340C  DATA HCAS/3.381,6.148,6.214,6.947,7.256,6.524/
000360C  DATA HCBS/.018044,.001665,.001253,.001039,.001253/
000380C  DATA HCCS/-4.3E-06,-9.23E-07,-1.96E-07,-3.545E-06,4.81E-07,2.63E-07,1.E-09/
000400C  THE MOL. WEIGHT OF GASES
000420C  DATA KY/16.,32.,28.,40.12.,18.,28./
000440C  THE THERMAL DATA OF NAPHTHA
000460C  DATA HNA/0.68,103.4/,VHNA/7680./
000480C  THE CONST. FOR CAL. SATURATED PRESSURE (EXP(A-B/T))
000500C  DATA A,B/13.954316,5204.9597/
000520C  CRITICAL TEMPERATURE OF WATER
000540C  DATA TC/646.447/
000560C  INSERT RATIO OF HEAT CAPACITY
000580C  DATA GAG/1.3/,GAGA/1.4/
000600C  INSERT THE SPECIFIC VOLUME OF FUEL AND WATER
000620C  DATA SV/0.,.02034,.021/.SVW/.0162/
000640C  INSERT THE HEATING VALUE
000660C  DATA SV/0.,.02034,.021/.SVW/.0162/
000680C  INSERT THE HEATING VALUE
000700C  DATA HLHV/-191762.,0.,-67635.,0.,-57798.,0.,0./
000720C  INSERT THE SPECIFIC HEAT CAPACITIES, BTU/R-LB-MOLE
000740C  DATA A3/5.34,6.39E-03,0.0,.660,6.67E-04,0.0,.10,34,1.52E-03,0.0,
000760C  1.6,3342E+05,8.82,8.3E-05,4.135E-07,0.0,6.62,4.5E-04,0.0,.6,5,
000780C  25.56E-04,0.0,.6,732,8.36E-03,5.53E-09,0.0/
000800C  INSERT VISCOSITY, LBM/FT-HR
000820C  DATA A2/3.437SE-05,2.5861E-02,3.6185E-05,4.6688E-02,5.0368E-05,
000840C  13.3634E-02,5.221E-05,1.7532E-02,1.879E-05,2.312E-02,4.2316E-05,
000860C  24.672E-02,4.580E-05,5.5613E-02/
000880C  INSERT THERMAL CONDUCTIVITY, BTU/HR-FT-F
000900C  DATA A1/6.6539E-05,7.4614E-03,1.5349E-05,1.6581E-02,2.0651E-05,
000920C  11.1726E-02,2.64E-05,1.0705E-03,1.1998E-04,1.0128E-01,1.6774E-05,
000940C  21.918E-02,1.792E-05,1.67E-02/
000960C  END
000980C
001000C  **************************************************************************************************
001020C  THIS PROGRAM IS USING FORTRAN TO SIMULATE THE PHOSPHORIC ACID FUEL
001040C  CELL SYSTEM
001060C  **************************************************************************************************
001080C  DEFINITION:
A : CONSTANT FOR CAL. SATURATED CONDITION OF WATER
AA1: THERMAL CONDUCTIVITY COEFF. OF GAS I, BTU/HR-FT-F
AA2: VISCOSITY COEFF. OF GAS I, LB/FT-HR
AA3: SPECIFIC HEAT CAPACITY COEFF. OF GAS I, BTU/R-LB-ROLE
AHLU: MOLE FRACTION OF AVAILABLE HYDROGEN
AHLU: PERCENT FREE-GAS SPACE, FT
AIRL: LENGTH OF AIR CHANNEL, FT
ALFA: TRANSFER COEFF.
APFD: TOTAL SURFACE AREA OF PACKING ACC. TO THE BASIS AND OPER.
ATMP: OUTLET TEMP. OF GASES, K
BPNA: BOILING POINT OF NAPHTHA, C
BTA: TRANSFER COEFF.
BPSC: BAFFLE SPACE, FT
CM: CURRENT DENSITY, AMP/CM**2
CL: CATALYST LOADING, MS/CM**2
CLEF: LENGTH OF TUBE IN HEAT EXCHANGER, FT
CLEFD: LENGTH OF SHIFT CONVERTER(JK=1), REFORMER(JK=2 FOR METHANOL AND NAPHTHA), FT
CLH: CLEARED IN HEAT EXCHANGER, FT
CMN: CLEARANCE IN HEAT EXCHANGER
CPC: Catalyst Pellet Diameter, FT
DP: CATALYST PELLET DIAMETER, FT
DPA: DIA. OF SHIFT CONVERTER(JK=1), REFORMER(JK=2 FOR METHANOL AND NAPHTHA), FT
DSD: CATHODE INLET WATER OF FUEL CELL, G-MOLE/HR.
DSE: 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
DXI: OUTSIDE DIAMETER OF REFORMER CENTER TUBE, FT
DX2: INSIDE DIAMETER OF OUTSIDE REFORMER TUBE, FT
DX3: OUTSIDE DIAMETER OF OUTSIDE REFORMER TUBE, FT
DZ: INCREMENT HEIGHT OF FINITE DIFFERENCE MODEL IN THE REFORMER
FAC: ACTIVATION ENERGY FOR ARRHENIUS EXPRESSION, CAL/MOLE CM4
FRE: REACTOR VOID FRACTION
FRE: CONVERGE CRITERIA
EXA: FRACTION OF EXTRA AIR IN FUEL CELL
EEXT: FRACTION OF EXTRA AIR IN BURNER
EPC: MOLE FRACTION OF CO CONTAIN
FCONST: FARADAY CONSTANT, 96487 CAL/VOLT-GM EQUIV.
FLOOR: FLOW AREA IN HEAT EXCHANGER, FT**2
FUEL: 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 OR CARBON MONOXIDE (IN SUB. KREF AND RELATED SUBROUTINES)
<table>
<thead>
<tr>
<th>Code</th>
<th>Description</th>
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<tbody>
<tr>
<td>I=3</td>
<td>CARBON MONOXIDE OR CARBON DIOXIDE</td>
</tr>
<tr>
<td>I=4</td>
<td>CARBON DIOXIDE OR WATER</td>
</tr>
<tr>
<td>I=5</td>
<td>HYDROGEN</td>
</tr>
<tr>
<td>I=6</td>
<td>WATER OR NITROGEN</td>
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<tr>
<td>I=7</td>
<td>NITROGEN OR OXYGEN</td>
</tr>
<tr>
<td>IDSH</td>
<td>ID OF SHELL IN HEAT EXCHANGER, FT</td>
</tr>
<tr>
<td>IDTH</td>
<td>ID OF TUBE IN HEAT EXCHANGER, FT</td>
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<tr>
<td>IFUEL</td>
<td>FUEL TYPE</td>
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<tr>
<td>1</td>
<td>METHANE CH4</td>
</tr>
<tr>
<td>2</td>
<td>METHANOL CH3OH</td>
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<tr>
<td>3</td>
<td>NAPHTHA C7H16</td>
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<tr>
<td>IDNO</td>
<td>NO. OF REDD</td>
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<tr>
<td>IMUI</td>
<td>STOICHIOMETRIC NUMBER</td>
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<tr>
<td>IP</td>
<td>INDEX OF OPERATION CONDITION IN THE REFORMER (NOT FOR METHANE)</td>
</tr>
<tr>
<td>1</td>
<td>ADABATIC OPERATION</td>
</tr>
<tr>
<td>2</td>
<td>ISOHERMAL OPERATION</td>
</tr>
<tr>
<td>K0</td>
<td>FREQUENCY FACTOR FOR ARRHENIUS EXPRESSION, LB MOLE CH4/LB</td>
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<tr>
<td>CATA.</td>
<td>CATAL.-HR-ATM</td>
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<tr>
<td>NN</td>
<td>STREAM NUMBER OF EXIT OF SHIFT CONVERTER</td>
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<tr>
<td>NOR</td>
<td>SCALE UP FACTOR IN THE MODEL OF REFORMER</td>
</tr>
<tr>
<td>NPFU</td>
<td>NO. OF CELL PLATE IN THE FUEL CELL STACK</td>
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<tr>
<td>NPH</td>
<td>NO. OF TUBE PASSES</td>
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<tr>
<td>NSH</td>
<td>NO. OF RO:5 FOR TUBES</td>
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<tr>
<td>NTAA</td>
<td>NO. OF AIR FLOW CHANNEL IN ONE CELL PLATE</td>
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<tr>
<td>NTAF</td>
<td>NO. OF FUEL FLOW CHANNEL IN ONE CELL PLATE</td>
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<tr>
<td>NTPD</td>
<td>NO. OF TUBES IN SHIFT CONVERTER</td>
</tr>
<tr>
<td>NTH</td>
<td>NO. OF TUBES IN REFORMER (JK=2) FOR METHANOL AND NAPHTHA</td>
</tr>
<tr>
<td>OSTN</td>
<td>OD OF TUBE, FT</td>
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<tr>
<td>02UTL</td>
<td>O2 UTILIZATION</td>
</tr>
<tr>
<td>PAT</td>
<td>AMBIENT PRESSURE, 1ATM</td>
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<tr>
<td>PIN</td>
<td>INLET PRESSURE, ATM</td>
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<td>PINFU</td>
<td>INLET PRESSURE OF FUEL CELL STACK, ATM</td>
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<tr>
<td>PITCH</td>
<td>PITCH OF HEAT EXCHANGER, FT</td>
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<tr>
<td>POP</td>
<td>OPERATION PRESSURE, ATM</td>
</tr>
<tr>
<td>POUT</td>
<td>OUTLET PRESSURE, ATM</td>
</tr>
<tr>
<td>RHOB</td>
<td>BULK DENSITY OF CATA., LB/FT**3</td>
</tr>
<tr>
<td>S</td>
<td>SIDE LENGTH OF AN ASSUMED SQUARE FLOW DUCT FOR COMBUSTION GAS</td>
</tr>
<tr>
<td>SICS</td>
<td>RATIO OF TOTAL INSIDE-TUBE CROSS-SECTIONAL AREA PER PASS TO HEADER CROSS-SECTIONAL AREA PER PASS</td>
</tr>
<tr>
<td>SA</td>
<td>CATALYST SURFACE, CM**2/MG</td>
</tr>
<tr>
<td>SK</td>
<td>EQUILIBRUM CONSTANT</td>
</tr>
<tr>
<td>SK1</td>
<td>EQUILIBRUM CONSTANT WITH PRESSURE DIFFERENT FROM 1 ATN</td>
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<tr>
<td>SICE</td>
<td>STEAM/FUEL</td>
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<tr>
<td>SH</td>
<td>NUMBER OF FARADAY EQUIVALENTS TRANSFERED</td>
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<tr>
<td>SNO</td>
<td>CELL RESISTANCE AT 480 K, OHM-CM**2</td>
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<td>SURFC</td>
<td>SURFACE PER LINE, FT</td>
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<tr>
<td>SVF(I)</td>
<td>SPECIFIC VOLUME OF FUEL I, FT**3/LBM</td>
</tr>
<tr>
<td>SVW</td>
<td>SPECIFIC VOLUME OF WATER, FT**3/LBM</td>
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<tr>
<td>TACOA</td>
<td>INLET AIR TEMP. OF FUEL CELL STACK, K</td>
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<tr>
<td>TACOF</td>
<td>INLET FUEL TEMP. OF FUEL CELL STACK, K</td>
</tr>
<tr>
<td>TAT</td>
<td>AMBIENT TEMPERATURE, 298 K</td>
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<tr>
<td>TCAS</td>
<td>TOTAL HEAT CAPACITY CONSTANT A</td>
</tr>
</tbody>
</table>
TCBS: TOTAL HEAT CAPACITY CONSTANT B
TCCS: TOTAL HEAT CAPACITY CONSTANT C
TDNS: TOTAL AMOUNT OF MATERIAL, G-MOLE
TIN: INLET FLUID TEMPERATURE, K
TOP: OPERATION TEMPERATURE, K
TVO: TOTAL VOLUME OF INLET FLOW, M**3
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 : THE NECESSARY AMOUNT OF OXYGEN IN CATHODE, G-MOLE/HR.
ZH: REFORMER LENGTH, FT
DINSS(I): INLET AMOUNT OF GAS I, G-MOLE
DINSI(I): INLET (OUTLET) AMOUNT OF GAS I, G-MOLE
HAJ:I: SURFACE AREA OF HEAT EXCHANGER J
HCAS(I),HCBS(I),HCCS(I): HEAT CAPACITY CONST. OF GAS I, CAL/G-MOLE
HCAS(I),HCBS(I),HCCS(I): HEAT CAPACITY CONST. OF GAS I, CAL/G-MOLE
HS(1): HEAT OF FORMATION OF GAS I AT 298 K, J/MOL
NBS(I): STOICHIOMETRIC COEFFICIENT OF GAS I
WM(I): MOLECULAR WEIGHT OF GAS I, G/G-MOLE
DINSS(I,J): FLOW RATE OF GASJ IN STREAM I, G-MOLES/HR
REAL K0,IODS,IDOTh
DIMENSION GS(7), HS(7), HCAS(7), HCBS(7), HCCS(7), WM(7)
DIMENSION DNL(7), DNLV(7), HLNV(7)
DIMENSION DNSI(39,7), T(39), P(39), TDNSI(39)
DIMENSION DINSI(7), DNSI(7), DNS(7), DNSAN(7), DNSCA(7), D- 
HIS(I), DHC(I), DHF(7)
DIMENSION QSI(10), HA(10), EFF(10), NT(10)
DIMENSION DSS(7), DSSF(7)
DIMENSION DPSI(2), AMPSI(2), APPD(2), CLEPD(2), NTPD(2), SV(3)
DIMENSION AA(2,7), AA(2,7), AA(4,7)
NAMELIST /REPEI/ ZH,DX1,DX2,DX3,KO,EA,RHOB,EPS,S,DP,DZZ
NAMELIST /HEAT/ CH,U,HA
NAMELIST /TOPFC/ TOPFC,UT,CD
NAMELIST /INIT/ DSNM,TAT,PAT,SNMA,POPVR
NAMELIST /COST/ IFUEL,EPR,IP,I,EXT,WAT,EXA
NAMELIST /HEPFC/ NPH,NPH,BSAC,OTH,PITCH,CLH,IDOTh,IDTH,FLOAR,SURF- 
NAMELIST /CF/CLH,SC52,OTH
NAMELIST /PDPSH/ DPD,AMN,APPD,CLEPD,NTPD
NAMELIST /PFU/ NTF,ULE,WIDAF,NPFU,NTAA,AIRL,WIDAA
NAMELIST /TR/ TOPR
NAMELIST /CATAI/ SRO,SA,CU,CL,ALFA,SN,FCONST,DKC
NAMELIST /C/TC/G,CNSI/A,B/GAG,GAGM,GAGS
NAMELIST /COST/ I
NAMELIST /EXA/ EXA
NAMELIST /ETHA/ GS,HS,HCAS,HCBS,HCCS
NAMELIST /HUMI/ WAT
NAMELIST /EXT/ EXT
NAMELIST /XI/ U
NAMELIST /CONF/ E,ETH,El,Ev,EC,EFC
NAMELIST /HE/ HE
READ THE OPERATION CONDITION OF FUEL CELL

READ (5,OPFC)

WRITE (6,OPFC)

READ THE INLET AMOUNT AND CONDITION

READ (5,INIT)

WRITE (6,INIT)

READ OPERATION CONDITION

READ (5,COND1)

WRITE (6,COND1)

READ OPERATING COEFFICIENT IN THE REFORMER (METHANE FUEL ONLY)

IF (IFUEL.EQ.1) READ (5,REPEN)

WRITE (6,REPEN)

READ CONDITION OF HEAT EXCHANGER

READ (5,HEATX)

WRITE (6,HEATX)

READ THE CONSTRUCTION OF HEAT EXCHANGER FOR CAL. PRESSURE DROP

READ (5,HEFD)

WRITE (6,HEFD)

READ CONFIGURATION COEFF. OF SHIFT CONVERTER FOR CAL. PRESSURE DROP

READ (5,PDSH)

WRITE (6,PDSH)

READ CONFIGURATION COEFF. OF FUEL CELL FOR CAL. PRESSURE DROP

READ (5,PDFU)

WRITE (6,PDFU)

READ THE OPERATING TEMP. OF REFORMER FOR FUEL NAPHTHA AND METHANOL

IF (IFUEL.NE.1) READ (5,TR)

WRITE (6,TR)

READ CATALYST CONSTANTS

READ (5,CATAI)

WRITE (6,CATAI)

CHANGE THE THERMAL DATA FOR DIFFERENT FUEL INPUT

IF (IFUEL.EQ.2) GO TO 1

IF (IFUEL.EQ.3) GO TO 2

GO TO 3

1 GS(1)=-38810.

HS(1)=-46050.

HCAS(1)=4.394

HCBS(1)=0.024274
HCCS(1)=-0.0000069
WM(1)=32.
HLHV(1)=159.258.
AA3(1,1)=4.394
AA3(2,1)=0.013406
AA3(3,1)=-2.1157E-06
AA3(4,1)=0.
AA1(1,1)=3.5E-05
AA1(2,1)=1.5E-05
AA2(1,1)=1.8E-05
AA2(2,1)=0.0092
GO TO 3

2 GS(1)=6520.
HS(1)=42275.
HCAS(1)=7.094
HCBS(1)=0.123447
HCCS(1)=0.0000397
WM(1)=100.
HLHV(1)=1099580.
AA3(1,1)=7.488
AA3(2,1)=0.
AA3(3,1)=-1.0945E-05
AA3(4,1)=0.
AA1(1,1)=2.66E-05
AA1(2,1)=0.7E-02
GO TO 3

CONTINUE
IDNO=1
C FUEL INPUT COMPRESSOR(PUMP)***
P(1)=PDR=1.02
IF (IFUEL.EQ.1) CALL COMP (DNSM,TAT,TOUT,P(1),PDW,GAM,M,IP)
IF (IFUEL.NE.1) CALL PUP (DNSM,TAT,TOUT,P(1),PDW,M,IFUEL)
DO 301 IA=1,I

DNSS(1,IA)=DNSM(IA)
T(1)=TOUT
ASSUME THE COMP. OF 13TH FLOW
DNSS(13,2)=0.
DNSS(13,3)=0.
IF (IFUEL.EQ.2) GO TO 4
IF (IFUEL.EQ.3) GO TO 5
DNSS(13,1)=0.147*DNSS(1,1)
DNSS(13,3)=0.0018*DNSS(1,1)
DNSS(13,4)=0.63*DNSS(1,1)+DNSS(1,4)
DNSS(13,5)=3.4*DNSS(1,1)+DNSS(1,5)
DNSS(13,6)=SMRA*DNSS(1,1)-1.7*DNSS(1,1)
GO TO 6

DNSS(13,1)=0.00063487*DNSS(1,1)
DNSS(13,3)=0.01
DNSS(13,4)=0.99928*DNSS(1,1)
DNSS(13,5)=2.997*DNSS(1,1)
DNSS(13,6)=0.60087*DNSS(1,1)
GO TO 6
DNSS(13,1)=0.
DNSS(13, 3) = 0.0221 * DNSS(1, 1)

DNSS(13, 4) = 6.971 * DNSS(1, 1)

DNSS(13, 5) = 21.956 * DNSS(1, 1)

DNSS(13, 6) = SMRA * DNSS(1, 1) - 13.865 * DNSS(1, 1)

C ASSUME THE PRESSURE OF 13TH FLOW

6 P(13) = POPR * 0.958

C ASSUME THE PRESSURE OF 31ST FLOW

7 IF (IDNOGT.1) GO TO 8

P(31) = P(13)

T(31) = TAT

8 PINF = P(13)

PINA = P(31)

POPF = P(31)

DO 9 IB = 1, I

9 DNSS(IB) = DNSS(13, IB)

C FUEL CELL MASS BALANCE***

DO 80 IC = 1, I

CALL FUCE(DNS, TOPFC, POPFC, DNSAN, DNSCA, DSO, DSN, DSHO, UT, I, PINF, PINA - 1, IFUEL)

P(14) = PINF

P(32) = PINA

DO 10 IC = 1, I

10 DNSS(32, IC) = DNSS(14, IC)

T(32) = TOPFC

T(14) = TOPFC

IF (IFUEL.EQ.2) CK = 1.5

IF (IFUEL.EQ.1) CK = 2.

IF (IFUEL.EQ.3) CK = 15.

C CALL. THE DIVIDER FACTOR FOR THE ASSUMPTION OF DEFINED EXTRA AIR IN NER

DO 90 IC = 1, I

GARM = 1. / ((1. + EXT * 0.01) * ((DNSS(14, 3) + DNSS(14, 5)) / 2. + CK * DNSS(14, 1)) - 1) / DSO + 1.

DO 91 IC = 1, I

91 DNSS(28, IC) = DNSS(28, IC)

P(28) = PAT

DO 100 IC = 1, I

100 DNSS(29, IC) = DNSS(28, IC)

T(29) = TAT

P(29) = POPFC * 0.005

CALL CCMP (DNSAI(IE), T(28), TOUT, P(28), POUT, POA, GAGA, I, IP)

P(29) = POUT

DO 110 IC = 1, I

110 DNSS(33, IC) = DNSS(29, IC)

T(33) = TAT

C DIVIDER***

CALL DIVID (T(29), T(30), T(33), DNS, DNS1, DNS2, GARM, I)

DO 120 IC = 1, I

120 DNSS(33, IC) = DNSS(33, IC)
0007600  DNSS(30,1H)=DNSS(1H)
0007620  15 DNSS(31,1H)=DNSS(30,1H)
0007640  P(30)=P(29)
0007660  P(33)=P(29)
0007680  C CALL THE 33RD FLOW COMP. UNDER THESE ASSUMPTION:
0007700  (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  DNSS(II)=DNSS(33,II)
0007860  16 DNSS(14,1H)=DNSS(33,1H)
0007880  C MIXER**
0007900  CALL DMIX (DNSS1,DNSS2,DNSS,T(14),T(33),T(15),P(14),P(33),POUT)
0007920  P(15)=POUT
0007940  DO 17 IJ=1,I
0007960  DNSS(IJ)=DNSS(IJ)
0007980  DNSS(15,1J)=DNSS(15,1J)
0008000  17 DNSS(16,1J)=DNSS(15,1J)
0008020  C CALL. THE COMP. OF 17TH FLOW UNDER THE SAME ASSUMPTION AS BEFORE
0008040  IF (IFUEL.EQ.3) DNSS(17,4)=DNSS(15,3)+DNSS(15,4)+DNSS(15,1)
0008060  IF (IFUEL.EQ.3) DNSS(17,6)=DNSS(15,5)+DNSS(15,6)+2.*DNSS(15,1)
0008080  IF (IFUEL.EQ.3) DNSS(17,8)=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))-2.*DNSS(15,1)
0008120  DNSS(17,7)=DNSS(15,7)
0008140  DO 18 IK=1,I
0008160  DNSS(16,IK)=DNSS(17,IK)
0008180  DNSS(19,IK)=DNSS(18,IK)
0008200  DNSS(20,IK)=DNSS(19,IK)
0008220  16 CONTINUE
0008240  C CALL. 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 CALL. 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)=P(25)=1.0005
0008500  P(26)=P(25)
0008520  T(26)=B/A-ALOG(P(26))
0008540  DNSS(26,6)=DNSS(11,1)*SHMA
0008560  DO 21 IN=1,I
0008580  21 DNSS(25,IN)=DNSS(26,IN)
0008600  DO 22 IO=1,I
0008620  IF (IFUEL.EQ.2) DNSS(27,IO)=DNSS(26,IO)
0008640  22 DNSS(2,IO)=DNSS(1,IO)
0008660  DO 23 JN=1,I
0008600 IF (IFUEL.NE.2) DNSS(3,19)=DNSS(2,19)*DNSS(27,19)
0008600 IF (IFUEL.EQ.2) DNSS(3,19)=DNSS(2,19)*DNSS(26,19)
0008750 IF (IFUEL.NE.2) DNSS(4,19)=DNSS(3,19)
0008760 IF (IFUEL.EQ.2) DNSS(5,19)=DNSS(4,19)
0008700 23 CONTINUE
0008800 C ASSUME THE TEMP. AND PRESSURE OF 5TH FLOW
0008940 IF (ID[O.GT.1) GO TO 24
0008980 IF (IFUEL.EQ.1) T(51=1110.88
0008900 IF (IFUEL.EQ.2) T(51=661.59
0008920 IF (IFUEL.EQ.3) T(51=1052.00
0008940 24 CONTINUE
0009020 C DESIGN THE TUBE TO LET PRESSURE DROP THROUGH BURNER BE 6%
0009100 P(16)=P(15)*0.99
0009120 C DESIGN THE TUBE TO LET PRESSURE DROP THROUGH REFORMER TO BE 5%
0009140 P(18)=P(17)*0.95
0009160 25 CONTINUE
0009180 C E-3xxr
0009200 DO 26 IQ=1,I
0009220 DNSH(IQ)=DNSS(17,IQ)
0009240 26 CONTINUE
0009260 C E-4r*
0009280 605 GO TO 604
0009280 604 P(16)=P(15)
0009300 IF (ABS(P(16)-P(16))/P(15).LT.ERR) GO TO 605
EFF(4)=HE
QQT(4)=QT
C BURNER ENERGY BALANCE***
DO 20 INDEX=1,I
20 DNSR(INDEX)=DNSS(INDEX)
CALL FLAME (DNSR(T(16),T(17),I,FUEL))
DO 29 INDEX=1,I
29 DNSS(INDEX)=DNSR(INDEX)
IF (FUEL.NE.1) GO TO 33
C REFORMER(METHANE)***
NOR=DNSS(1,INDEX)/50.
DO 30 INDEX=1,I
30 DNSR(INDEX)=DNSS(INDEX)/453.6/NOR
IF (INDEX.NE.1) DNSF(INDEX)=DNSS(INDEX)/453.6/NOR
CALL KREF (DNSR,DNSF,INDEX,T(16),T(17),Z,FUEL)
TEST THE ASSUMPTION OF 16TH FLOW
IF (ABS((TTEST-T(16))/(TTEST+T(18))).LT.ERR) GO TO 31
T(16)=TTEST
GO TO 25
DO 31 INDEX=1,I
31 DNSH(INDEX)=DNSS(INDEX)
DI4SC(INDEX)=DNSS(INDEX)
PTEST=P(INDEX)
PS=P(INDEX)
CALL HEC (T(INDEX),DNSH,DNSC(INDEX),T(16),T(17),T(6),Z,FUEL)
TEST THE ASSUMPTION OF 18TH FLOW
IF ((ABS((TTEST-T(18))/(TTEST+T(18))).LT.ERR).AND.(ABS((PTEST-P(18)-
P(18)=P(18)+PTEST)/2.
GO TO 25
DO 35 INDEX=1,I
35 QQT(INDEX)=QT
T(INDEX)=TTEST
P(INDEX)=PTEST
DO 36 INDEX=1,I
36 DNSR(INDEX)=DNSS(INDEX)
C REFORMER(METHANE AND NAPHTHA)***
DO 37 INDEX=1,I
37 DNSI(INDEX)=DNSS(INDEX)
CALL ENRE (DNSI,INDEX,INDEX,T(16),T(17),INDEX,FUEL)
DO 38 INDEX=1,I
38 DNSN(INDEX)=DNSS(INDEX)
C CAL. PRESSURE DROP
=
CALL POSH(DNS,P(6),P(7),TOPR,2,IFUEL)

IF(IFUEL.EQ.2) GO TO 56

DO 40 IAA=1,7

DNSH(IAA)=DNSS(7,IAA)

DO 40 DNSC(IAA)=DNSS(3,IAA)

C E-2***

DO 40 PS=P(7)

IF(IFUEL.EQ.1) CALL HEXC(T(7),DNSH,DNSC,T(3),T(8),T(4),QT,1,HA(2),-

12,2,I,PT,PS,NT(2),IFUEL)

IF(IFUEL.EQ.3) CALL HEXC(T(7),DNSH,DNSC,T(3),T(9),T(4),QT,1,HA(2),-

12,2,I,PT,PS,NT(2),IFUEL)

P(3)=PT

IF(IFUEL.EQ.1) P(8)=PS

IF(IFUEL.EQ.3) P(9)=PS

EFF(2)=HE

QGT(2)=QG

DO 40 IBB=1,7

IF(IFUEL.EQ.1) DNSS(8,IBB)=DNSH(IBB)

IF(IFUEL.EQ.3) DNSS(9,IBB)=DNSH(IBB)

41 DNSS(4,IBB)=DNSS(IBB)

DO 40 IFUEL.EQ.3 GO TO 46

C HIGH TEMP. SHIFT CONVERTER***

TOPHS=T(8)

42 CONTINUE

POPS=P(8)

DO 40 ICC=1,7

DNS(ICC)=DNSS(8,ICC)

CALL ENSH(DNS,T(8),TOPH,POPS,I,IP,FUEL)

P(9)=POPHS

TM=T(9)+T(8)/2.

IF(((IP.EQ.2).OR.(ABS((TM-TOPH)/(TM+TOPH)).LT.ERR)) GO TO 44

TOPHS=TM

DO TO 42

CONTINUE

DO 40 IOD=1,7

DNS(9,IOD)=DNSS(9,IOD)

CONTINUE

DO 40 IEE=1,7

DNS(IEE)=DNSS(9,IEE)

CONTINUE

DO 47 ID=1,7

DNSC(IEE)=DNSS(1,IEE)

IF(IFUEL.EQ.3) GO TO 48

C E-1(METHANE AND NAPHTHA)***

PT=P(1)

PS=P(9)

CALL HEXC(T(9),DNSH,DNSC,T(1),THO,TCO,QT,1,HA(1),1,1,I,PT,PS,NT(1-

1),IFUEL)

CONTINUE

P(10)=PS

P(2)=PT

EFF(1)=HE

QGT(1)=QG

TCO=TCO

THO=THO

GO TO 52
CONTINUE

DESIGN THE HEAT EXCHANGER 1 TO VAPORIZE NAPHTHA AND RISE THE TEMP.

K FOR NAPHTHA FUEL

T(2)=400.

QQT(1)=HNA*252./453.6*100.*1.8*DNSS(1,1)*(BPNA+273.-T(1))*DNSS(1,1-

1)*VH/HCAS(1)*(T(2)-T(1))+HCBS(1)*(T(2)**2-T(1)**2)/2.+HCSS(1)*(T-

2)**3-T(1)**3)/3.

ASSUME EFFICIENCY OF H-E 1 IS 0.7

EFF(1)=0.7

HA(1)=C=M=QQT(1)/EFF(1)/(T(9)-T(1))/U

ASSUME AVERAGE TEMP. OF HOT SIDE

TAVG=T(9)-50.

DMH=0.

DO 50 IB=1,I

CHH=CHH+DNSS(9,IB)*(HCAS(1IB)+HCBS(1IB)*TAVG+HCSS(1IB)*TAVG**2)

GO TO 49

TEST THE ASSUMPTION OF AVERAGE TEMP.

IF (ABS((T(10)+T(9))/2.-TAVG).LT.ABS((T(10)-T(9))/2.+TAVG)*0.001) -

1GO TO 51

GO TO 49

ASSUME PRESSURE DROP IS NEGLECTABLE

P(2)=P(1)

P(10)=P(9)

DO 53 IFF=1,I

DNSS(9,IFF)=DNSS(9,IFF)

IF (IFUEL.EQ.3) DNSS(10,IFF)=DNSS(9,IFF)

IFUEL.EQ.1) DNSS(10,IFF)=DNSS(10,IFF)

DO 54 IGG=1,I

DNSS(10,IFF)=DNSS(10,IFF)

DNSS(26,10)=DNSS(26,10)

E-9**

PT=P(26)

PS=P(10)

CALL HEXC(T(10),DNSH,DNSC,T(26),T(11),T(27),QT,1,HA(9),9,1,I,PT,P-

10640 1S,NT(9),IFUEL)

P(1)=PS

P(27)=PT

EFF(9)=HE

QQT(9)=QT

DO 55 INH=1,I

DNSS(11,INH)=DNSS(INH)

DNSS(12,INH)=DNSS(INH)

DNSS(26,INH)=DNSS(26,INH)

DNSS(18,INH)=DNSS(18,INH)

DNSS(19,INH)=DNSS(19,INH)

DO 55 CONTINUE

GO TO 60

E-1(METHANOL)**

DO 56 III=1,I

DNSS(III)=DNSS(7,III)

DNSS(III)=DNSS(1,III)

PT=P(1)

PS=P(7)
CALL HEXC (T(7),DNSH,DNSC,T(1),THO,TCQ,QT,1,HA(1),1,1,I,PT,PS,NT(1-)
1),IFUEL)

PTE=PS
P(2)=PT
EFF(1)=HE
QTT(1)=QT

DO 58 IJJ=1,I

DO 58 DNSS(2,IJJ)=DNSC(IJJ)

Ti(2)=TCO
Ti(13)=THO

DO 59 IJJ=1,I

DNS1(IJJ)=DNSS(2,IJJ)
DMS2(IJJ)=DNSS(26,IJJ)

CONTINUE

MIXER**%

CALL OMIX (DNS~~DNS~,DNS,T(~),T(~~)PTES~,I,P(~),P(~~),PTEST)
GO TO 61

60 CALL DMIX (DNS1,DNS2,DNS,T(2),T(26),TESTT,I,P(2),P(26),PTEST)

TEST TEMP. OF 3RD FLOW

DO 61 IF ((ABS((TESTT-T(3))/TESTT).LT.ERR).AND.(ABS((PTEST-P(3))/-

P(3)).LT.ERR)) GO TO 70

IF (IFUEL.EQ.2) GO TO 66

E-2**

DO 62 IKK=1*I

DNS3(IKK)=DNSS(3,IKK)

DNSH1(IKK)=DNSI(7,IKK)

DNSC(IKK)=DNSS(3,IKK)

P(3)=(P(3)+PTEST)/2.

T(3)=(TESTT+T(3))/2.

PT=P(3)
PS=P(7)

IF (IFUEL.EQ.3) GO TO 63

CALL HEXC (T(7),DNSH,DNSC,T(3),T(8),T(4),QT,1,HA(2),2,1,I,PT,PS,NT-

1,IFUEL)

P(4)=PT
P(8)=PS

GO TO 64

63 CALL HEXC (T(7),DNSH,DNSC,T(3),T(9),T(4),QT,1,HA(2),2,1,I,PT,PS,NT-

1,IFUEL)

P(4)=PT
P(9)=PS

E-3**

64 DO 65 ILL=1,I

DNSS(4,ILL)=DNSC(ILL)

DNSH(ILL)=DNSS(18,ILL)

DNS(ILL)=DNSS(4,ILL)

PT=P(4)
PS=P(18)

65 CALL HEXC (T(18),DNSH,DNSC,T(4),T(19),T(5),QT,1,HA(3),3,1,I,PT,PS,-

1,IFUEL)

P(5)=PT
P(19)=PS

GO TO 68

66 DO 67 IMM=1,I
00140600  DNSS(3,IMM)=DNS(IMM)
00141000  DNSS(IMM)=DNSS(18,IMM)
00141200  DNSS(18,IMM)=DNS(3,IMM)
00141400  T(3)=(T(3)+TEST)/2.
00141600  PT=P(18)
00141800  PS=(P(3)+PTEST)/2.
00142000  CALL HEXC(DNSH,DNSC,T(3),T(19),T(5),QT,1,HA(3),3,1,PT,PS,-
00142200  IM(3),IFUEL)
00142400  P(19)=P(19)
00142600  P(5)=PS
00142800  EFF(3)=HE
00143000  QT(3)=QT
00143200  DO 69 INN=1,I
00143400  DNSS(6,INN)=DNSC(INN)
00143600  IDNO=IDNO+1
00143800  GO TO 24
00144000  70 CONTINUE
00144200  IF (IFUEL.EQ.2) GO TO 77
00144400  DO 71 IPP=1,I
00144600  DNSH(IPP)=DNSS(11,IPP)
00144800  71 DNSC(IPP)=DNSS(30,IPP)
00145000  C  E-6***
00145200  PT=P(30)
00145400  PS=P(31)
00145600  CALL HEXC(T(11),DNSH,DNSC,T(30),T(12),T(31),QT,1,HA(6),6,1,IPP,-
00145800  15,NT(6),IFUEL)
00146000  P(12)=PS
00146200  PTEST=PT
00146400  C  TEST THE PRESSURE OF 31ST FLOW
00146600  IF (ABS((PTEST-P(31))/(PTEST+P(31)))/.LT.ERR) GO TO 72
00146800  P(31)=(PTEST+P(31))/2.
00147000  GO TO 8
00147200  72 EFF(6)=HE
00147400  QT(6)=QT
00147600  DO 73 IQQ=1,I
00147800  DNSS(12,IQQ)=DNSH(IQQ)
00148000  73 DNSC(31,IQQ)=DNSC(IQQ)
00148200  C  LOW TEMP. SHEFT CONVERTER***
00148400  TOPLS=T(12)
00148600  POPLS=P(12)
00148800  74 CONTINUE
00149000  DO 75 IRR=1,I
00149200  75 DNS(I RR)=DNSS(12,IRR)
00149400  CALL ENSH(DNS(12),T(13),TOPLS,POPLS,1,IP,IFUEL)
00149600  TM=(T(12)+T(13))/2.
00149800  IF ((IP.EQ.2).OR.(ABS((TM-TOPLS)/(TM+TOPLS)).LT.ERR)) GO TO 76
00150000  TOPLS=TM
00150200  GO TO 76
00150400  76 CONTINUE
00150600  C  TEST THE ASSUMPTION OF 13TH FLOW
00150800  DO 77 ISS=1,I
00151000  IF ((IFUEL.EQ.2).AND.(DNS(ISS).LT.0.50).AND.(DNSS(13,ISS).LT.0.50)-
00151200  1) GO TO 78
00151400  IF ((IFUEL.EQ.2).AND.(DNS(ISS).LT.0.50).AND.(DNSS(13,ISS).LT.0.50)-
0015160 1)) GO TO 78
0015180 IF ((IFUEL.NE.2).AND.(ABS((DNS(13,ISS)-DNS(13,ISS))/DNS(13,ISS)+DNS(13,ISS))).LT.ERR)) GO TO 78
0015200 IF ((IFUEL.EQ.2).AND.(ABS((DNSH(ISS-1(ISS)))/DNSH(ISS)+DNSH(ISS))).LT.ERR)) GO TO 78
0015220 GO TO 79
0015240 78 CONTINUE
0015260 IF (IFUEL.EQ.2) POPLS-PTE
0015280 IF (ABS((POPLS-P(13))/POPLS+P(13)+1.1)).LT.ERR) GO TO 81
0015300 79 DO 80 ITT=1
0015320 IF (IFUEL.EQ.2) DNSH(ISS-1(ISS))=DNSS(ISS-1(ISS)),ONSH(ISS-1(ISS)))/2.
0015340 80 IF (IFUEL.NE.2) DNSH(ISS-1(ISS))=DNSH(ISS-1(ISS)))/2.
0015360 P(13)=(POPLS+P(13))/2.
0015380 GO TO 7
0015400 81 CONTINUE
0015420 DO 82 IU=1
0015440 IF (IFUEL.EQ.2) DNSH(IU)=DNSH(IU)
0015460 82 IF (IFUEL.NE.2) DNSH(IU)=DNSH(IU)
0015480 TDN13=0.
0015500 DO 83 IVV=1
0015520 TDN13=TDN13+DNSS(IU)
0015540 83 TDN13=TDN13+DNSS(IU)
0015560 PCO=DNSS(IU)/TDN13
0015580 DO 84 ITT=1
0015600 DNSH(IU)=DNSS(IU)
0015620 84 DNSH(IU)=DNSS(IU)
0015640 C FUEL CELL ENERGY BALANCE***
0015660 AREAF=FUEL*AIRL*30.48**2
0015680 CD=CD/1000.
0015700 OU=1./(EXA*0.01+1.)
0015720 CENFU(DNNS,DNCCA,T(31),T(31),TOUT,TPF,POPFC,VPD,UT,1,I,Qt, -
0015740 Q=OU
0015760 C CALCULATE THE OUTPUT OF AC POWER
0015780 AC=(0.0146*SQRT(1.0146**2-4.*0.0456/108.*0.0472/108.-WK)) #
0015800 0.0146/108.*0.0456/108.
0015820 DO 86 IYY=1
0015840 DNSH(IYY)=DNSH(IYY)
0015860 86 DNSH(IYY)=DNSH(IYY)
0015880 DO 87 IZZ=1
0015900 DNSH(IZZ)=DNSH(IZZ)
0015920 87 DNSH(IZZ)=DNSH(IZZ)
0015940 C MIXER***
0015960 CALL DDMIX(DNS1,DNS2,DNS,T(32),TOUT,P(20),P(32),POUT)
0015980 P(21)=POUT
0015990 DO 88 II=1
0015810 DNSH(II)=DNSH(II)
0015830 88 DNSH(II)=DNSH(II)
0015850 TD(21)=TOUT
0015860 C ASSUME P(22)
0015880 P(22)=P(21)*1.001
0015900 602 T(22)=-8/(ALOG((DNSS(I,1),I)*SMRA-DNSS(21,6)/(DNSS(I,1),I)*SMRA- -
0015920 I+DNSS(21,1))=DNS(II)
0015940 E-10***
0015960 T(25)=T(22)
0015980 CALL CDPM (QRT,T(25),T(26),DNSC,P(25),I,GQT(10))
QQT(7) = QT

ASSUME HOT WATER IS FEEDING IN AT 3330K AND FEEDING OUT AT 355 K

DNS(34,6) = QQT(7) / (355. - 333.) / 1. / 18.

DNS(35,6) = DNS(34,6)

T(34) = 333.

T(35) = 355.

P(34) = PAT

P(35) = PAT

E-5***

CALL COND (T(21), T(22), DNSH, QT, HCH, I)

QQT(5) = QT

ASSUME HOT WATER IS FEEDING IN AT TAT AND FEEDING OUT AT 3550K

DTL = ((T(21) - 355.) - (T(22) - TAT)) / ALOG((T(21) - 355.) / (T(22) - TAT))

T(36) = TAT

T(37) = 355.

P(36) = PAT

P(37) = PAT

DNS(36,6) = QQT(5) / 1. / 18. / (355. - TAT)

DNS(37,6) = DNS(36,6)

ASSUME E-5 IS THE TYPE OF COUNTERFLOW

HA(5) = QQT(5) / U / 1. / DTL

THM = (T(36) + T(37)) / 2.

TCH = (T(22) + T(21)) / 2.

CALL HEPD(DNSH, DNSH, THM, TCH, HA(5), P(21), P(36), 5, DPJ, DP, NT, T(22),

T(21), 4)

P22TE = P(22) - DPJ

IF (ABS(P22TE - P(22)) / (P22TE + P(22))). LT. ERR) GO TO 603

P(22) = (P(22) + P22TE) / 2.

GO TO 602

DO 89 I2 = 1, I

DO 89I2 = DNSH(I2)

89

DNS(I2) = DNSH(I2)

SEP***

POPS = P(I2)

CALL SEPAR (T(I2), POPTS, T(I2), DNS, DNSL, DNSV, I)

DO 90 I2 = 1, I

DO 90I2 = DNS(I2)

90

DNS(I2) = DNSL(I2)

DNS(I2) = DNSV(I2)

R070000 P(24) = POPTS

R070200 P(23) = POPTS

PUMP***

R070000 DO 901 I4 = 1, I

R070800 DNS(I4) = DNS(I4)

R071000 CALL PUMP (DNS, T(I4), I4, P(I4), P(24), P(25), POWS, I)

R071200 DO 92 IB = 1, 39

R071400 TDNS(IB) = 0.

R071600 DO 91 IA = 1, I

R071800 TDNS(IB) = TDNS(IB) + DNS(IB, IA)

R072000 91 CONTINUE

R072200 92 CONTINUE

WRITE THE RESULT

R072400 IF (IFUEL.EQ.1) WRITE (6, 108) SMRA

R072600 IF (IFUEL.EQ.2) WRITE (6, 109) SMRA

R073000 IF (IFUEL.EQ.3) WRITE (6, 110) SMRA
WRITE (6,103) P(5),P(7),T(5),T(7)
0017360 IF (IFUEL.EQ.1) WRITE (6,104) TOPHS,P(8),T(8),T(9)
0017380 WRITE (6,105) T(22),POPS
0017400 WRITE (6,99) FCO
0017420 WRITE (6,118) TOPFC,POPFC,E,VOP,CD,CL,UT,OU
0017440 WRITE (6,103) T(81),T(121),T(131)
0017460 WRITE (6,107) EFC
0017480 WRITE (6,101) FCO
0017500 WRITE (6,117) AC
0017520 WRITE (6,119) AC
0017540 C WRITE THE MATERIAL IN JTH FLOW
0017560 10280 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=1,1),TDNSS(J),T(J-1),P(J)),J=1,5),((II,(DNSS(II,IA),IA=1,1),TDNSS(II),T(II),P(II)),II-1)
0017660 2=7,37))
0017700 IF (IFUEL.EQ.2) WRITE (6,93) ((J,(DNSS(J,IA),IA=1,1),TDNSS(J),T(J-1),P(J)),J=1,3),((II,(DNSS(II,IA),IA=1,1),TDNSS(II),T(II),P(II)),II-1)
0017740 2=5,7))
0017760 IF (IFUEL.EQ.3) WRITE (6,93) ((J,(DNSS(J,IA),IA=1,1),TDNSS(J),T(J-1),P(J)),J=1,7),((II,(DNSS(II,IA),IA=1,1),TDNSS(II),T(II),P(II)),II-1)
0017780 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,POXI,POWS
0018100 IF (IFUEL.EQ.2) WRITE (6,115) POWA,POXI,POWS
0018120 IF (IFUEL.EQ.3) WRITE (6,116) POWA,POXI,POWS
0018140 STOP
0018160 C
0018180 93 FORMAT (1X,2X,I2,2X,F8.2,1X,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')
The fraction of CO in the feed is F8.5/

The thermodynamic efficiency of the fuel cell is E13.5/
The current efficiency is E13.5/
The voltage efficiency is E13.5/
The heating value efficiency is E13.5/

The reformation is operating under these conditions '6X,'/
1. inlet pressure: F7.2, 'atm,'
2. inlet temp.: F7.2, 'k'/

The electric work is E13.5, 'kw,'/
The total heat released is E13.5, 'cal,'/
The anode side inlet temp. is F7.2, 'k'/
The cathode-
1 side inlet temp. is F7.2, 'k'/

The thermodynamic efficiency of the fuel cell is E13.5/
The operational efficiency is E13.5/
The voltage efficiency is E13.5/
The heat value efficiency is E13.5/

The electrical work is F10.2, 'hp,'/
The total heat released is F10.5, 'cal,'/
The reactor side inlet temp. is F7.2, 'k'/
The reactor side outlet temp. is F7.2, 'k'/

The operational temperature is F7.2, 'k'/
The operating pressure is F7.2, 'atm,'/
The open circuit potential is F8.3, 'v'/

3. the operational potential is F8.3, 'v,'/
4. the current density is F8.3, 'pa/cm2,'/

5. the fuel utilization is F5.3/
6. the oxygen utilization is F5.3/

This subroutine is to calculate the mass balance of burner.
**ASSUMPTION:**

1. THE COMBUSTION IS COMPLETE
2. THE AMOUNT OF O2 REACTED
3. THE AMOUNT OF CO2 PRODUCED
4. THE AMOUNT OF H2O PRODUCED

**IF:** IJ = 1

METHANE AS INPUT GAS

**IF:** IJ = 2

METHANOL AS INPUT GAS

**IF:** IJ = 3

NAPHTHA AS INPUT GAS

**CALCULATE THE NECESSARY AMOUNT OF O2**

**IF**(IJ.EQ.3) GO TO 4

**IF**(IJ.EQ.2) GO TO 2

**IF**(IJ.EQ.1) GO TO 3

**GO TO** 3

**GO TO** 2

**GO TO** 3

**GO TO** 4

**CALCULATE THE EXIT COMPOSITION**

**RETURN**

**END**

**SUBROUTINE** CDPH(QTI,TCI,TCO,DNSC,P,I,QTS)

**DEFINITION:**

**QTI:** TOTAL HEAT TRANSFER FROM FUEL CELL

**TCB:** BOILING POINT OF FIXED PRESSURE

**GS:** SATURATED, PRESSURE IS EXP(A-B/T)

**HCAS:** SATURATED STEAM OUTPUT

**CONS:** THE AVERAGE HEAT CAPACITY OF WATER IS 1 CAL/G-K

**RETURN**

**TCB =** B/(A-ALGS(P))
SUBROUTINE COMP(DNS,TIN,TOUT,PIN,POUT,GAG,I,IP)

C*******************************************************************************
C THIS SUBROUTINE CALCULATES THE BALANCE OF COMPRESSOR
C*******************************************************************************
C ASSUMPTION:
C 1) IDEAL GAS BEHAVIOR
C GAG: RATIO OF HEAT CAPACITY
C HS: SHIFT WORK
C PIN: POWER REQUIRED; HP
C V0: SPECIFIC VOLUME OF GAS AT APPLIED CONDITION; M**3/G-MOLE
C DIMENSION DNS(I)
C TDNS=0.
DO 1 IA=1,I
IF(DNS(IA).EQ.0.) GO TO 1
TDNS=TDNS+DNS(IA)
1 CONTINUE
IF(IP.EQ.2) GO TO 2
TOUT=TIN*POUT/PIN**((GAG-1.)/GAG)
WS=GAG*1.987*TIN*1.8*POUT/PIN**(GAG-1.)/GAG-1.1/GAG-1.2
FOW=WS*TDNS/641400.
RETURN
2 TOUT=TIN
k'S=1.987*TIN*1.8*ALOG(POUT/PIN)
FOW=WS*TDNS/641400.
RETURN
END

SUBROUTINE COND(THI,THO,DNSH,QT,CH,1)
C*******************************************************************************
C THIS SUBROUTINE ESTIMATES THE HEAT DUTY IN THE CONDENSER
C DEFINITION IS THE SAME AS HEXC
C DIMENSION GS(7),HS(7),HCAS(7),HCBS(7),HCCS(7)
C DIMENSION DNSH(I)
C COMMON /ETHDA/ GS,HS,HCAS,HCBS,HCCS
C COMMON /TC/TC
C THM=(THI+THO)/2.
C QTZ=THE CAPACITY RATE OF FLUID OF HOT SIDE
C CH=0.
DO 1 IA=1,I
IF(DNSH(IA).EQ.0.) GO TO 1
CH=CH+DNSH(IA)*(HCAS(IA)+HCBS(IA))\(THM+HCCS(IA)*THM**2)
1 CONTINUE
QT=0.
DO 2 IA=1,I
QT=QT+DNSH(IA)*(HCAS(IA)*THI-THO)+HCBS(IA)*THI*THI-THO*THO)
0028300 1+HCCS(I)*(THI**3-TH0**3)
0028400 2 CONTINUE
0028420 QT=(1-(TH0/TH1))/(1-0.577)**0.38*9700.*DNSH(6)
0028440 QT=QT+QTL
0028500 RETURN
0028500 END
0028700 SUBROUTINE CONV(XV,YV,NC)
0028800 C******************************************************************************
0028900 C THIS SUBROUTINE USES WESSTEIN METHOD FOR ALGEBRAIC CONVERGENCE
002900 C******************************************************************************
0029100 C DEFINITION:
0029200 C XV: TRIAL VALUE
0029300 C YV: CALCULATED VALUE
0029400 C NC: CONVERGE INDEX
0029500 C NC=1 CONVERGE
0029600 C NC=2 NONCONVERGE
0029700 C
0029800 DIMENSION XA(1),YA(1)
0029900 IF(ABS((XV-YV)/(XV+YV)).LT.0.001) GO TO 2
0030000 IF(NC.LE.1) GO TO 1
0030100 XT=(X(NR)*YV-YA(NR1)*XV)/(X(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 NC=2
0030900 RETURN
0031000 2 XV+YV
0031100 NC=1
0031200 RETURN
0031300 ENDC
0031500 SUBROUTINE DIVIDE(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 DNS1(I),DNS1(1),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 ENDC
0033200 SUBROUTINE MIX(DNS1,DNS2,DNS,TIN1,TIN2,TOUT1,PIN1,PIN2,POUT)
0033300 C******************************************************************************
0033400 C THIS SUBROUTINE CALCULATES THE BALANCE AROUND THE MIXER
0033500 C******************************************************************************
SUBROUTINE ENFU(DNSA,DNSC,TINC,TINA,TOUT,UTOP,VOP,UT,M,I,QT,WE,---
1OU,CD,PT,IJ)

REAL TIN1,TIN2,PIN1,PIN2,TOUT,TDNS1,TDNS2,TOUTC
REAL TOUT=(TIN1+TIN2)/2.

C DIMENSION FOR TOTAL THERMAL CONST.
DIMENSION GS(7),HS(7),HCAS(7),HCBS(7),HCCS(7)

C COMMON /ETHDA/ GS,HS,HCAS,HCBS,HCCS
COMMON /ETHDA/ GS,HS,HCAS,HCBS,HCCS

C DIMENSION FOR TOTAL THERMAL CONST.
DIMENSION DNS1(I),DNS2(I),DNS(I)

C CAL. THE TOTAL THERMAL CONST.
TCAS1=0.
TCBS1=0.
TCCS1=0.
TCCS2=0.
DO 1 IA=1,I
1 TCAS1=TCAS1+DNS1(IA)*HCAS(IA)
TCAS2=TCAS2+DNS2(IA)*HCAS(IA)
TCBS1=TCBS1+DNS1(IA)*HCBS(IA)
TCBS2=TCBS2+DNS2(IA)*HCBS(IA)
TCCS1=TCCS1+DNS1(IA)*HCCS(IA)
TCCS2=TCCS2+DNS2(IA)*HCCS(IA)

C CONTINUE
1 CONTINUE
TCAS1=TCAS1+DNS1(IA)*HCAS(IA)
TCAS2=TCAS2+DNS2(IA)*HCAS(IA)
TCBS1=TCBS1+DNS1(IA)*HCBS(IA)
TCBS2=TCBS2+DNS2(IA)*HCBS(IA)
TCCS1=TCCS1+DNS1(IA)*HCCS(IA)
TCCS2=TCCS2+DNS2(IA)*HCCS(IA)

C DO 1 IA=1,I
1 CONTINUE
C TCAS1=TCAS1+DNS1(IA)*HCAS(IA)

C CAL. THE ENERGY BALANCE
2 TOUTC=(TCAS1*TIN1+TCAS2*(TIN2-TOUT)+TCBS1/2.*TIN1**2-TOUT**2)-
2*(TIN2**2-TOUT**2)+TCCS1*(TIN1**3-TOUT**3)/3./TCAS1

C CALL CONV(TOUT,TOUTC,1,NC)

C CAL. AND WRITE THE OUTLET COMPOSITION
3 DO 4 IA=1,I
4 DNS(IA)=DNS1(IA)+DNS2(IA)

C CAL. THE ENERGY BALANCE
5 TOUT=(TDNS1+TDNS2/(TDNS2*TIN1/PIN1+TDNS2*TIN2/PIN2)*TOUT*0.97

C RETURN

C THIS SUBROUTINE IS TO CAL. ENERGY BALANCE OF FUEL CELL

C DEFINITION:
C DGR: FREE ENERGY CHANGE AT FUEL CELL CONDITION
C EC: HEATING VALUE EFFICIENCY
C EFC: FUEL CELL EFFICIENCY
C EI: CURRENT EFFICIENCY
C EO: FUEL CELL STANDARD EQN. POTENTIAL
C EV: VOLTAGE EFFICIENCY
C FCH4: FRACTION OF METHANE
FME: FRACTION OF METHANOL
FNAP: FRACTION OF NAPHTHA
M: INDEX OF OUTLET CONDITION
Mc=1 OUTLET TEMP. IS FIXED TO TOPFC
M=2 OUTLET TEMP. IS NOT FIXED
PCO: MOL. FRACTION OF CO
FNAP: FRACTION OF NAPHTHA

M=1 OUTLET TEMP. IS FIXED TO TOPFC
M=2 OUTLET TEMP. IS NOT FIXED
PCO: MOL. FRACTION OF AVAILABLE H2O
PCO: MOL. FRACTION OF AVAILABLE H2O

WE: ELECTRICAL WORK

0040200 C M=1 OUTLET TEMP. IS FIXED TO TOPFC
0040300 C M=2 OUTLET TEMP. IS NOT FIXED
0040400 C PCO: MOL. FRACTION OF CO
0040500 C Q: TOTAL HEAT RELEASE PER HR.
0040600 C SIS: INTEGRATION CONST. IN CALCULATING S
0040700 C TAUHO: MOL. FRACTION OF AVAILABLE H2O
0040800 C VOP: ACTUAL FUEL CELL POTENTIAL
0040900 C LE: ELECTRICAL WORK

0041000 C CAL. THE MOL. FRACTION OF AVAILABLE HYDROGEN

0041100 TDNS=0.
0041200 TDNSC=0.
0041300 DD 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)

1 CONTINUE
0041900 IF(IJ.EQ.1) FCH4=DNSA(1)/TDNS
0042000 IF(IJ.EQ.2) FM=DNSA(1)/TDNS
0042100 IF(IJ.EQ.3) FNAP=DNSA(1)/TDNS
0042200 AML=DNSA(5)/TDNS
0042300 TAUHO=DNSA(1)/TDNS
0042400 PCO=DNSA(1)/TDNS
0042500 PPH2=SCRT(DNSA(5)*TDNS*DNSA(5)*/(1-U)/TDNS-DNSA(5)*UT))
0042600 PPH2O=SCRT(DNSC(6)/TDNSC*DNSC(6)/TDNSC*DNSC(6)*/(TDNSC+DNSC(6)*YOU))
0042700 PFD2=SCRT(DNSC(2)/TDNSC*DNSC(2)*/1-U/)/TDNSC+DNSC(2)*YOU))
0042800 PPH2O=SCRT(DNSC(6)/TDNSC*DNSC(6)/TDNSC+DNSC(2)*YOU))

0042900 CALL VIEW(1,VOP,CD,TOP,POP,PPH2,PPH2O,PCO,
0043000 1X0
0043100 C CAL. THE OPEN-CIRCUIT POTENTIAL

0043200 DCAS=HCAS(6-1.2.*HCAS(2)-HCAS(6))
0043300 DCBS=HCBS(6-1.2.*HCBS(2)-HCBS(6))
0043400 DHCCS=HCBS(6-2.*HCBS(2)-HCBS(6))
0043500 DHH2S(6-1.2.*HS(2)-HS(6))
0043600 DHCAS=HCAS(6-2.*HCAS(2)-HCAS(6))
0043700 DHCBS=HCBS(6-2.*HCBS(2)-HCBS(6))
0043800 DG=DH2S(6-2.*DHCBS(6-2.*DHCBS(6))
0043900 DG=DH2S(6-2.*DHCBS(6-2.*DHCBS(6))
0044000 1-DHCCS/6.*TOP**3
0044100 IF(TOP.EQ.463.1 DG=-52798.
0044200 EO=-Et/2./23060.*+ALOG(AHLU*0.21**O.5/TAUHO*POP**O.5l
0044300 IF(TOP.EQ.463.1 DG=-52798.
0044400 1-DHCCS/6.*TOP**3
0044500 IF(TOP.EQ.463.1 DG=-52798.
0044600 EO=-Et/2./23060.*+ALOG(AHLU*0.21**O.5/TAUHO*POP**O.5l

0044700 C CAL. FREE ENERGY CHANGE AT FUEL CELL CONDITION
TCAS = TCAS + DNS(IA) * HCAS(IA)
TCBS = TCBS + DNS(IA) * HCBS(IA)
TCCS = TCCS + DNS(IA) * HCCS(IA)

5 CONTINUE
TOUT = TOUT

IF(M.EQ.1) GO TO 7

CALL CINV(TOUT, TOUTC, 1, NC)
GO TO (8, 6, NC)

TCAL. THE TOTAL HEAT REJECTED PER HR.

7 DT = DMIN - DH - HE - TCAS*(TOUT - 298.) - TCBS/2.*((TOUT**2 - 298.**2) - TCCS/3.*((TOUT**3 - 298.**3)

C CONTINUE

CALL CC(C, TOUT, 1, NC)
RETURN

C THIS SUBROUTINE CALCULATES THE ENERGY BALANCE OF REFORMER

DIMENSION GS(7), HS(7), HCAS(7), HCBS(7), HCCS(7)

CALL ETHDA/GS, HS, HCAS, HCBS, HCCS

STORE THE INLET COMPOSITION

DO 1 IA = 1, I

DINS(IA) = DNS(IA)

1 CONTINUE

CALCULATE THE OUTLET COMP.

CALL REF(DNS, TOP, POP, X, I, IJ)

IF(IP.EQ.1) GO TO 2

TOUT = TIN

GO TO 6

2 CONTINUE

CALCULATE THE ENTHALPY CHANGE WITH TEMP. OF INLET GAS

DMIN = 0.

DO 3 IA = 1, I

IF(DINS(IA).EQ.0.) GO TO 3

DMIN = DMIN + DINS(IA) * (HCAS(IA) * ((298.-TIN)+HCBS(IA))/2.*((298.)**2 - 1-TIN**2)*HCCS(IA)/3.*((298.)**3 - (TIN)**3))

3 CONTINUE

CALCULATE THE ENTHALPY CHANGE OF REACTION

1DH1 = (HS(3)+2.*HS(5)-HS(1)) * X(2)

IF(IJ.EQ.3) 

1DH2 = (HS(1)+15.*HS(5)-HS(1)-7.*HS(6))*X(1)

IF(IJ.EQ.2) 

1DH3 = (HS(3)+2.*HS(5)-HS(1))*X(2)

IF(IJ.EQ.1, 07, IJ.EQ.3) 

1DH4 = (HS(4)+HS(5)-HS(3)-HS(6))*X(2)
DH=DH1+DH2
C CALCULATE THE TOTAL HEAT CAP. CONSTANT OF OUTLET GAS
TCAS=0.
TCBS=0.
TCCS=0.
DO 4 IA=1,I
   IF(DNS(IA).EQ.0.) GO TO 4
   TCAS=TCAS+DNS(IA)*HCAS(IA)
   TCBS=TCBS+DNS(IA)*HCBS(IA)
   TCCS=TCCS+DNS(IA)*HCCS(IA)
4 CONTINUE
C CALCULATE THE MAX. TEMP. OF OUTLET GAS
TCAS=0.
TCBS=0.
TCCS=0.
DO 5 IA=1,I
   IF(DNS(IA).EQ.0.) GO TO 5
   TOUT=(-DH-DHIN-TCBS/2.*((TOUT)**2*(298.)**2)-TCCS/3.*((TOUT)**3-1*(298.)**3))/TCAS+298.
   CALL CONV(TOUT,TOUTC,1,NC)
   GO TO (6,5,NC)
5 CONTINUE
RETURN
END
SUBROUTINE ENSH(DNS,TIN,TOUT,TOP,NC)
C***********+*************%********X*****Y**************~*****~***********
C THIS SUBROUTINE CALCULATES THE ENERGY BALANCE OF SHIFT CONVERTER
DIMS7:GS(7),HS(7),HCAS(7),HCBS(7),HCCS(7)
DINS7:DNS(7),DINS(7)
COMMON/ETHDA/ 6S,HS,HCAS,HCBS,HCCS
C STORE THE INITIAL COMPOSITION
DO 1 IA=1,I
   DINS(IA)=DNS(IA)
   CALL PDSH(DINS,PIN,POUT,TOP,1,I)
   POP=(PIN+POUT)/2.
1 CONTINUE
C CALCULATE THE OUTLET COMPOSITION
CALL SHIFT(DINS,TOP,POP,X,1)
IF(IP.EQ.1) GO TO 2
TOUT=TIN
GO TO 6
2 CONTINUE
C CALCULATE THE ENTHALPY CHANGE WITH TEMP. OF INLET GAS
DH=0.
DO 3 IA=1,I
   IF(DNS(IA).EQ.0.) GO TO 3
   DH=DN=+DNS(IA)*((HCAS(IA)*(298.-TIN)+HCBS(IA))/2.*((298.)**2-1*(TIN)**2)+HCCS(IA))/3.*((298.)**3-(TIN)**3))
3 CONTINUE
C CALCULATE THE ENTHALPY CHANGE OF REACTION
DH=+(HS(4)+HS(5)-HS(3)-HS(6))*X
TCAS=0.
TCBS=0.
TCCS=0.
DO 4 IA=1,I
   IF(DNS(IA).EQ.0.) GO TO 4
   TCAS=TCAS+DNS(IA)*HCAS(IA)
   TCBS=TCBS+DNS(IA)*HCBS(IA)
4 CONTINUE
TCCS=TCAS+DNS(IA)+HCCS(IA)

4 CONTINUE

C CALCULATE THE MAX. TEMPERATURE OF OUTLET GAS
TOUT=TOP+10.
5 TOUTC=(-DH-DHIN-TCBS/2.*(TOUT)**2-(298.)*2)-TCCS/3.*(TOUT)**3 -
1-(298.)*3)/TCAS+298.
CALL CONV(TOUT,TOUTC,1,NC)
GO TO (6,5,1,NC)
6 CONTINUE
RETURN

SUBROUTINE EQU(R,NS,TOP,SK,IA)
C THIS SUBROUTINE CALCULATES THE EQUILIBRUM CONSTANT
R: GAS CONSTANT: G-CAL/P-MOLE-K
TST: STANDARD TEMPERATURE; K

DIMENSION GS(71),HS(71),HCAS(71),HCBS(71),HCCS(71)
DIMENSION NS(IA)
COMMON /ETHDA/ GS,HS,HCAS,HCBS,HCCS
DATA R/1.987/
DATA TST/298./

C CAL. THE TOTAL HEAT CAPACITY CONSTANT
TCAS=0.
TCBS=0.
TCCS=0.
DO 1 IA=1,IA
IF(NS(IA).EQ.0) GO TO 1
TCAS=TCAS+NS(IA)*HCAS(IA)
TCBS=TCBS+NS(IA)*HCBS(IA)
TCCS=TCCS+NS(IA)*HCCS(IA)
1 CONTINUE

C CAL. HEAT CHANGE OF REACTION
DH=0.
DO 2 IA=1,IA
IF(NS(IA).EQ.0) GO TO 2
DH=DH+NS(IA)*HS(IA)
2 CONTINUE

C CAL. FREE ENERGY OF REACTION
DG=0.
DO 3 IA=1,IA
IF(NS(IA).EQ.0) GO TO 3
DG=DG+NS(IA)*GS(IA)
3 CONTINUE

C CAL. HEAT CONST.
AI=DH-NHEX/TCAS*TST**2-TCBS**2/TST**3/3.
C CAL. CONST. AI
1+AI
RETURN

END
SUBROUTINE FLAME(DNS,TIN,TF,I,IJ)

C THIS SUBROUTINE CALCULATES THE MAX. ADIABATIC FLAME TEMPERATURE
FOR 203% THEORETICAL AIR

C**+*+*Y%**************%******%***********************%*************
C THIS SUBROUTINE CALCULATES THE MAX. ADIABATIC FLAME TEMPERATURE
C***c**r**n*****x**u+****it*********+***************+*********~*x**x*****~*
C ASSUMPTION:
(1). THE COMBUSTION PROCESS GOES TO COMPLETION
(2). HEAT LOSSES ARE NEGligible
(3). NEGligible DISSOCIATION OF THE PRODUCTS OF COMBUSTION
(4). PRESSURE IS LOW AROUND 1ATM

TF: MAX. TEMPERATURE OF ADIABATIC FLAME

DIMENSION DS(7),HS(7),HCAS(7),HCBS(7),HCCS(7)
DIMENSION DNS(7),DNS(7)
COMMON/ETHDA/ GS,HS,HCAS,HCBS,HCCS
COMMON /EXT/EXT

C STORE THE INLET FLUID
DO 1 IA=1,I
DN(S(IA)=DNS(IA)
1 CONTINUE

C CALCULATE THE EXIT FLUID
CALL BURN(DNS,1,IJ)

C CALCULATE THE HEAT CHANGE OF REACTION AT 298 K
DH=0.
DO 2 IA=1,I
IF(DINS(IA).EQ.0.) GO TO 2
DH=DH+DNS(IA)*HS(IA)
2 CONTINUE

DO 3 IA=1,I
IF(DINS(IA).EQ.0.) GO TO 3
DH=DH+DNS(IA)*HS(IA)
3 CONTINUE

C CALCULATE THE ENTHALPY WITH TEMP. CHANGE
DO 4 IA=1,I
IF(DINS(IA).EQ.0.) GO TO 4
DH=DH+DNS(IA)*(HCAS(IA)*(298.-TIN)+HCBS(IA)/2.*((298.)**2-TIN**2)-
HCBS(IA)/3.*((298.)**3-TIN**3))
4 CONTINUE

C CALCULATE THE TOTAL HEAT CAPACITY CONSTANT
TCAS=0.
TCBS=0.
TCCS=0.
DO 5 IA=1,I
IF(DINS(IA).EQ.0.) GO TO 5
TCAS=TCAS+DNS(IA)*HCAS(IA)
TCBS=TCBS+DNS(IA)*HCBS(IA)
TCCS=TCCS+DNS(IA)*HCCS(IA)
5 CONTINUE

C CALCULATE THE MAX. TEMPERATURE
TC=TI N+500.
6 TFC=(-DH-TCBS/2.*((TF)**2-(298.)**2)-TCCS/3.*((TF)**3-(298.)**3))-
1/TCAS+298.
CALL CONV(TF,TFC,1,NC)
GO TO (7,6),NC
7 CONTINUE
0071500        RETURN
0071600        END
0071700        SUBROUTINE FCU(DNS,TOP,POP,DNSA,DNSC,DSO,DSN,DSHO,UT,I,PINF,PINA,-
0071800         IJ)
0071900        C***********************************************************************
0072000 C THIS SUBROUTINE CALCULATES THE MASS BALANCE OF FUEL CELL
0072100       ********************************************************************
0072200 C X : CONSUMPTION OF H2 IN THE FUEL CELL UNDER UT UTILIZATION
0072300       DIMENSION GS(7),HS(7),HCAS(7),HCCS(7)
0072400       DIMENSION DNS(7),DNSA(7),DNSC(7),DNS(7)
0072500       COMMON /EXA/ EXA
0072600       COMMON /HUM/ WAT
0072700       X=UT*DNS(7)
0072800       C THIS SUBROUTINE CALCULATES THE HASS BALANCE OF FUEL CELL
0072900       H2
0073000       DO 1 IA=1,7
0073100       DNSA(IA)=DNS(IA)
0073200       CONTINUE
0073300       DNSA(5)=DNS(5)-X
0073400       DO 2 IA=1,5
0073500       DNSC(IA)=DNSC(IA)-DNSA(IA)
0073600       CONTINUE
0073700       DNSC(2)=EXA/100.*(1./2.*X-DNS(2))
0073800       DNSC(6)=DNS+X
0073900       DNSC(7)=DNS
0074000       CALL PFDU(DNSA,DNSC,DNS,DSO,DSN,DSHO,POP,UT,PINF,PINA,IJ)
0074100       RETURN
0074200       C CAL. AND WRITE THE INLET COMPOSITION OF AIR
0074300       DO 2 IA=1,7
0074400       DNSA(IA)=DNS(IA)
0074500       CONTINUE
0074600       DNSA(5)=DNS(5)-X
0074700       DO 3 IA=1,5
0074800       DNSC(IA)=DNSC(IA)-DNSA(IA)
0074900       CONTINUE
007500       DNSC(2)=EXA/100.*(1./2.*X-DNS(2))
007510       DNSC(6)=DNS+X
0075200       DNSC(7)=DNS
0075300       CALL PFDU(DNSA,DNSC,DNS,DSO,DSN,DSHO,POP,UT,PINF,PINA,IJ)
0075400       RETURN
0075500        END
0075600        SUBROUTINE HEP(DNSA,DNSC,THM,TCM,HA,PINT,PINS,N,DPJ,DP,NT,TG,TC-
0075700         IJ)
0075800       REJ=REYNOLDS NUMBER OF TUBE SIDE
0075900       GS= SHELL SIDE MASS VELOCITY
0076000       FPZ= FRICTION FACTOR
0076100       REAL IDT,IDS,DNSA(7),DNSC(7)
0076200       DIMENSION FLI(7),CM(7),CM(7),CM(7),CM(7),CM(7),CM(7)
0076300       COMMON /KMP/ IM
0076400       COMMON /HEPT/ NP,HR,BSPAC,ODT,PITCH,CL,IDS,IDT,FLOAR,SURFC
0076500       1,CLEN,SITZ2,DTH
0076600       C***********************************************************************
0076700       C HEAT EXCHANGER BASIS: 3/4 IN TUBE OD AND B:\G 14
0076800       C***********************************************************************
0076900       NT= HA /0.3048*2/NP/CLEN/SURFC
0077000       NCAL. NO. OF BAFFLES
0077100       NS=CLEN/BSPAC
0077200       C CAL. FREE AREA BETWEEN BAFFLES
0076100 C FAREA = IDS/(ODT + CL*CL*BSPACE)
0076200 C CAL. CORRECTION FACTOR
0076300 B0 = 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 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 A*W = CM(1)*W(1) + CM(2)*W(2) + CM(3)*W(3) + CM(4)*W(4) + CM(5)*W(5) + CM(6)*W(6) + CM(7)*W(7)
0078100 1*CM(6)*W(7) + CM(7)*W(8)
0078200 TF = (THM - 273.16)*1.8 + 32.
0078300 CALL CMASS(CF, FLI, FI)
0078400 AMU = VIS(CF, TF, IJ)
0078500 RHO = (A*W*PINS)/(0.7302*(TF+60.))
0078600 C CAL. SHELL SIDE MASS VELOCITY ACROSS TUBES
0078700 GS = FI*AMU/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 FPI = SBO*(ODT*GS/AMU)**(-0.15)
0079200 C CAL. PRESSURE DROP OF SHELL SIDE FLOW
0079300 DP = B0*2.*FPI*NMR*GS**2/32.174/3600.***2/RMD/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 J = 1, 7
0080500 CMJ(J) = FLJ(J)/FJ
0080600 3 CONTINUE
0080700 A*W = CM(J)*W(1) + CM(J)*W(2) + CM(J)*W(3) + CM(J)*W(4) + CM(J)*W(5) + CM(J)*W(6) + CM(J)*W(7) + CM(J)*W(8)
0080800 1 + CM(J)*W(7) + CM(J)*W(8)
0080900 DT = DTH*(THM-TCM)
0081000 TW = DT+TCM
0081100 TKF = (TW-273.16)*1.8 + 32.
0081200 TCF = (TCF-273.16)*1.8 + 32.
0081300 CALL CMASS(CF, FLJ, FJ)
0081400 AMU = VIS(CF, TCF, IJ)
AMJ=VIS(CJ,TF,IJ)
AMW=VIS(CJ,TF,IJ)
IF((AMUJ.LE.0.1).OR.(AMMW.LE.0.)) GO TO 10
THC=THC(CJ,TF,IJ)
CP=HTCP(CJ,TF,IJ)
AROH=(AMW*PINT/(0.7302*(TCF+460.))
GJ=AM/J/FLOAR/N
REJ=REJ/J/AM
IF(REJ.LE.2100.)GO TO 4
SF=0.046/REJ**0.2
IF(SF.LT.0.15)GO TO 5
SF=16./REJ
CONTINUE
IF(SF2.GT.0.715)GO TO 6
CKC=0.4*(1.25-S2TS1)
6
CKC=0.75*(1.-S2TS1)
CONTINUE
7
CKI=(1.-S2TS1)**2+CKC+0.5*(NP-1.)/NP
8
BI=1.*CKI*IDT*PHI4./SF/CLEN
CONTINUE
9
BI=1.+0.51*CKI**NP*(TH-TCM)/(AMUJ/AMW)**0.28/(TCO-TCI)
10
1/(CP*AMUJ/TKC/AMJ)**0.6667
CONTINUE
11
FORMAT(‘THE TRYING TEMP. IS BELOW THE LIMIT OF CAL. VISCOSITY’)!
CONTINUE
RETURN
END
SUBROUTINE HEXC(THI,DNSH,DNSC,TCI,THO,TCO,QT,MOD,HA,N,M,I,PT,PS,NT)
C*****************************************************************************
C THIS SUBROUTINE IS TO CAL. THE ENERGY ANALYSIS FOR HEAT EXCHANGER
C*****************************************************************************
CC: CAPACITY RATE OF FLUID ON COLD SIDE ,DNSC*CPH
CN: CAPACITY RATE OF FLUID ON HOT SIDE, DNSH*CPH
CMAX: MAX. CAPACITY RATE
CMIN: MIN. CAPACITY RATE
CPC: SPECIFIC HEAT OF COLD SIDE FLUID
CPH: SPECIFIC HEAT OF HOT SIDE FLUID
CH: HEAT EXCHANGER EFFECTIVENESS
GT: TOTAL HEAT TRANSFER RATE ACROSS HEAT EXCHANGER
QMAX: THE MAX. HEAT TRANSFER RATE ACROSS HEAT EXCHANGER
TC: COLD SIDE INLET TEMPERATURE
TCO: COLD SIDE OUTLET TEMPERATURE
THI: HOT SIDE INLET TEMPERATURE
THO: HOT SIDE OUTLET TEMPERATURE
UA: OVERALL HEAT TRANSFER COEFFICIENT OF EXCHANGER
MOD: TYPE OF HEAT EXCHANGER
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 C THM=(THH*10.+TCI)/2.
0087900 C TCM=(THH-10.*TCI)/2.
0088000 C IF(M.EQ.2) GO TO 1.
0088100 C IF(DN=1) GO TO 3.
0088200 C CC=0.
0088300 C CH=0.
0088400 C PHASE II
0088500 C THM=(THH*10.+TCI)/2.
0088600 C TCM=(THH-10.*TCI)/2.
0088700 C GO TO 2.
0088800 C THM=(THH+TCO-50.)/2.
0088900 C TCM=(TCO*2-200.)/2.
0089000 C CC=0.
0089100 C PHASE III
0089200 C CC=0.
0089300 C CH=0.
0089400 DO 4 IA=1,N
0089500 C IF(DN=1) GO TO 3.
0089600 C CC=CC+DN=1*HCAS(IA)*HCBSt IA)*THH+HCCSt IA)*THM**2.
0089700 C CH=CH+DN=1*HCAS(IA)+HCBSt IA)*THM.*THM**2.
0089800 C CONTINUE
0089900 C CHOOSE THE CMAX, CMIN.
0090000 C IF(CC.GT.CH) GO TO 5.
0090100 C CMAX=CH.
0090200 C MIN=CC.
0090300 C CH=CC.
0090400 C GO TO 6.
0090500 C CMAX=CC.
0090600 C MIN=CH.
0090700 C GO TO 6.
0090800 C HA=CN/CHIN/U.
0090900 C UA=HA*U.
0091000 C CAL. THE HEAT EXCHANGER EFFECTIVENESS.
0091100 C IF(MOD.GE.2) GO TO 8.
0091200 C IF((CMIN/CMA)=GT.0.01) GO TO 7.
0091300 C HE=1.-EXP(-UA/CHIN).
0091400 C GO TO 12.
0091500 C HE=(1.-EXP(-UA/CHIN)/(1.-(CHIN/CMA)*EXP((-UA-
0091600 C 1./CHIN)+(1.-(CHIN/CMA)))).
0091700 C GO TO 12.
0091800 C IF(MOD.GT.2) GO TO 11.
0091900 C IF(CHIN/CMA=GT.0.01) GO TO 9.
0092000 C HE=(UA/CHIN)/UA/CHIN+1.)
0092100 C GO TO 12.
0092200 C IF((CMIN/CMA).GT.0.01) GO TO 10.
HE = 1. - EXP(-UA/CHIN)
HE = 1. - EXP((-CMAX/CHIN)*(1. - EXP(-UA/CMAX)))
IF(CHAX.EQ.CH)
HE = 1. - EXP((1-CMAX/CHAX)*(1. - EXP(-UA/CMAX)))
IF(CMIN.EQ.CH)
HE = (CMAX/CHIN)*I
1. - EXP((-CMIN/CHAX)*I)
IF(-EXP(-UA/CHIN))
   GO TO 12
11
   IF(AO.EQ.(THO+THI)/2.) LT. (ABS((THO+THI)/2. + THM)*0.005)
   GO TO 13
   IF(AO.EQ.(TCO+TCI)/2.- TCM). LT. (ABS((TCO+TCI)/2. - TCM)*0.005))
   GO TO 15
   THM = (THO+THI)/2.
   TCM = (TCO+TCI)/2.
   CALL HEFD(DNSA,DNSC,DNS,DNS,DSO,DSN,DPJ,DP,NT,TCO,TCI,IJ)
   IF(M.EQ.2) GO TO 16
   PT = PT-DPJ
   PS = PS-DP
   GO TO 17
   PT = PT+DPJ
   PS = PS-DP
   CONTINUE
   RETURN
SUBROUTINE PDFU(DNSA,DNSC,DNS,DNS,DNS,DNS,DPJ,DP,NT,TCO,TCI,IJ)
DIMENSION FLI(7),C(7),CM(7),KD(7),DNSA(7),DNSC(7),DNS(7),DNS(7)
DIMENSION NTA(2), WIDA(2),D(2)
COMMON/PD/FUT/NTA,L,WIDA,NP
COMMON /WM/ WM
C******************************************************************************
C THIS SUBROUTINE CALCULATES PRESSURE DROP IN THE FUEL CELL STACK
C******************************************************************************
I=1
DO 1 IA=1,7
1 DNSI(IA)=0.
DIMENSION L(2),D(4)
COMMON/PD/FUT/NTA,L,WIDA,NP
COMMON /WM/ WM
C******************************************************************************
C BASIS: NO. 522 STACK
C******************************************************************************
IT=1
DO 1 IA=1,7
1 DNSI(IA)=0.
DIMENSION L(2),D(4)
COMMON/PD/FUT/NTA,L,WIDA,NP
COMMON /WM/ WM
C******************************************************************************
C CAL. THE PRESSURE DROP OF FUEL SIDE
C******************************************************************************
D(1)=WIDA(1)
FLI(1)=DNS(1)/453.6
FLI(2)=DNS(3)/453.6
FLI(3)=DNS(4)/453.6
FLI(4)=DNS(6)/453.6
FLI(5)=DNS(5)/453.6
FLI(6)=DNS(7)/453.6
FLI(7)=DNS(2)/453.6
GO TO 3
2 FLI(1)=DNSA(1)/453.6
FLI(2)=DNSA(3)/453.6
FLI(3)=DNSA(4)/453.6
FLI(4)=DNSA(6)/453.6
FLI(5)=DNSA(5)/453.6
FLI(6)=DNSA(7)/453.6
FLI(7)=DNSA(2)/453.6
3 CONTINUE
TK=ATMP
FI=FLI(1)+FLI(2)+FLI(3)+FLI(4)+FLI(5)+FLI(6)+FLI(7)
DO 4 I=1,7
CM(I)=FLI(I)/FI
4 CONTINUE
AM=CM(1)+CM(2)+CM(3)+CM(4)+CM(5)+CM(6)+CM(7)
1*CM(6)+CM(7)*CM(2)
G=FLI*AM/WM(I)/2/NP/NTA(I)
TF=(FX-273.16)/1.8+32.
CALL CMSS(C,FLI,F)
AMUI=VISIC(TF,IT)
RHO=AMUI/POP/(7.302*(TF+460.1))
RE=D(IT)*G/AMUI
CD=S57.2
FRIC=CONS/RE
D(J)=RHO*(G/PHO)**2/2.*(0.5+1.+0.6*FRIC*L(IT)/D(IT))/21.62
JJ=JJ+1
100 IF(JJ.EQ.2) GO TO 2
101 IF(JJ.EQ.3) GO TO 5
102 IF(JJ.EQ.4) GO TO 6
103 IF(JJ.EQ.5) GO TO 8
C CAL. THE PRESSURE DROP OF AIR SIDE
C INSERT THE FLCH RATE OF EACH GAS
5 FLI(1)=DNSC(1)/453.6
FLI(2)=DNSC(3)/453.6
FLI(3)=DNSC(4)/453.6
FLI(4)=DNSC(6)/453.6
FLI(5)=DNSC(5)/453.6
FLI(6)=DNSC(7)/453.6
FLI(7)=DNSC(2)/453.6
IT=IT+1
6 DO 7 IA=1,7
7 FLII(IA)=DNSII(IA)/453.6
GO TO 3
010280 & CONTINUE
010290 PINF=PINF-(DP(1)+DP(2))/2.
010300 PINA=PINA-(DP(3)+DP(4))/2.
010310 RETURN
010320 END
010330 SUBROUTINE POSH(DNS,PIN,POUT,TK,JK,IK)
010340 C******************************************************************************
010350 C THIS SUBROUTINE CALCULATES PRESSURE DROP IN THE SHIFT CONVERTER
010360 C******************************************************************************
010370 DIMENSION D(2),AHRN(2),AP(2),CLEN(2),NT(2)
010380 DIMENSION FLI(7),C(7),CM(7),KM(7),DNS(7)
010390 C/DON/PDSHT/ D,AHRN,AP,CLEN,NT
010400 C/DON/ KM
010410 C JK=1 SHIFT CONVERTER
010420 C JK=2 REFORMER FOR METHANOL AND NAPHTHA FUEL
010430 TF=TK-273.16)*1.8+32.
010440 DP=6.*(1.-AHRN(JK))/AP(JK)
010450 FLI(1)=DNS(1)/453.6/NT(JK)
010460 FLI(2)=DNS(3)/453.6/NT(JK)
010470 FLI(3)=DNS(4)/453.6/NT(JK)
010480 FLI(4)=DNS(6)/453.6/NT(JK)
010490 FLI(5)=DNS(5)/453.6/NT(JK)
010500 FLI(6)=DNS(7)/453.6/NT(JK)
010510 FLI(7)=DNS(2)/453.6/NT(JK)
010520 F1=FLI(1)+FLI(2)+FLI(3)+FLI(4)+FLI(5)+FLI(6)+FLI(7)
010530 DO 1 I=1,7
010540 CM(I)=FLI(I)/F1
010550 1 CONTINUE
010560 AM=CHM(1)/CM(1)/CM(2)/CM(3)/CM(4)/CM(5)/CM(6)/CM(7)/CM(8)
010570 CM(1)=CM(2)/CM(7)/CM(9)
010580 G=F1/AM**4./(3.14159*0(IK)**2)
010590 CALL CMASS(C,FLI,F1)
010600 AMJ=VIS(C,TF,TK)
010610 IDH=(AMJ*PIN)/10.7302*(TF+460.1)
010620 DEMP=CLEN(JK)/1.-AHRN(JK)/1./AP(JK)**3/3.*DP/4.18E+08
010630 1/RH0=1.07*(1.-AHRN(JK))/AMJ/0.0162/453.6/DNS(6)
010640 POUT=PIN-DELP
010650 RETURN
010660 END
010670 SUBROUTINE PUMP(DNS,TIN,TOUT,PIN,POUT,POW,I)
010680 C******************************************************************************
010690 C THIS SUBROUTINE IS TO CAL. THE BALANCE OF PUMP FOR WATER
010700 C******************************************************************************
010710 C ASSUMPTION AND DEFINITION IS THE SAME AS COMP.
010720 DIMENSION DNS(7)
010730 DIMENSION SV(3),CM(7)
010740 COMMON/WM/ WM
010750 COMMON/SV/ SV
010760 TOUT=DLTIM
010770 C CAL. THE WORK
010780 C ASSUME AVERAGE SPECIFIC VOLUME OF WATER IS 0.0162 FT**3/LBM
010790 POW=5*4.14*5.05051*0.0000001*AKM(6)*14.7*(POUT-PIN)*DNS(6)
010800 1/453.6
010810 RETURN
SUBROUTINE PUP(DT1S~TIN~TOUT,PIN~POUT,POW~I~IJ)

C THIS SUBROUTINE CALCULATES POWER NEEDED IN THE FUEL PUMP

DIMENSION DNS(7),WM(7),SV(3)

COMMON/SV/ SV,SVW

COMMON/WM/ WM

TOUT=TIN

POW=5V(1J)*144.*5.05051*0.0000001*WM(IJ)*14.7*(POUT-PIN)

I*DNS(1)/453.6

RETURN

END

SUBROUTINE REF(DNS,TOP,POP,X1,I,J)

C THIS SUBROUTINE IS TO CALCULATE THE MASS BALANCE OF REFORMER

DIMENSION NNS1(7),NNS2(7),DNS(7),SK1(2),Xi(2)

C CALCULATE THE EQU. CONSTANT OF REACTION 1

DO 1 IA=1,I

1 NNS1(IA)=0

IF (IJ.EQ.3) GO TO 2

IF (IJ.EQ.1) NNS1(1)=1

IF (IJ.EQ.2) NNS1(4)=1

NNS1(1)=-1

NNS1(6)=-1

NNS1(5)=3

GO TO 3

2 NNS1(1)=-1

NNS1(6)=-7

NNS1(3)=7

NNS1(5)=15

3 CALL EQUK(NNS1,TOP,SK,I)

IHUI=0

4 IHUI=IHUI+NNS1(IA)

IHUI=IHUI+TOP

IHUI=IHUI-NNS1(IA)

5 CALL EQUK(NNS2,TOP,SK,I)

6 NNS2(IA)=0

IF (IJ.EQ.2) GO TO 6

NNS2(4)=1

NNS2(5)=1

NNS2(1)=1

GO TO 7

6 NNS2(3)=1

7 CALL EQUK(NNS2,TOP,SK,I)

IHUI=0

8 IHUI=IHUI+NNS2(IA)

SK1(2)=SK*POP**(-IHUI)
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) NAPTHA INPUT FUEL USING THE
0114100 C REASONABLE ASSUMPTION OF CC:CONVERSION
0114200 X(1)=0.999*DNS(I)
0114300 X(2)=2.9*DNS(I)
0114400 DNS(I)=DNS(I)-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(I)
0115100 X(2)=0.35*DNS(I)
0115200 CALL SHAE(X,2,DNS,S(K,I),IJ)
0115300 DNS(I)=DNS(I)-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(I)
0116000 X(2)=0.04*DNS(I)
0116100 CALL SHAE(X,2,DNS,S(K,I),IJ)
0116200 DNS(I)=DNS(I)-X(1)-X(2)
0116300 DNS(3)=DNS(3)-X(1)
0116400 DNS(4)=DNS(4)+X(2)
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
0117000 SUBROUTINE SEPAR(TIN,POTV,TOUTL,DNS,DNSL,DNSV,I)
0117100 C******************************************************************************
0117200 C THIS SUBROUTINE IS TO CAL. THE MASS BALANCE AROUND THE LIQUID SEPARATOR
0117300 C******************************************************************************
0117400 C ASSUMPTION:
0117500 C (1). ONLY WATER EXIST IN LIQUID PHASE
0117600 C PSAT: SATURATE PRESSURE AT T; EXP(A-B/T) FOR WATER
0117700 C DK: EQUI. CONST. OF LIQUID-VAPOR
0117800 C XW: AMOUNT OF WATER IN LIQUID PHASE
0117900 C DSTEP: AMOUNT OF WATER IN LIQUID PHASE
0118000 C DIMENSION DNS(I),DNSV(I),DNSL(I)
0118100 COMMON /PS,PS,T/CONS/,A,B
0118200 C CAL. THE EQUI. CONST. OF LIQUID-VAPOR
0118300 PSAT=EXP(A-B/TIN)
0118400 DK=PSAT/POP
0118500 C CAL. THE EQUI. AMOUNT OF LIQUID-VAPOR WATER
0118600 TDNS=0.
0118700 GO 1 IA=1,I
0118800 TDNS=TDNS+DNS(I)
0118900 1 CONTINUE
011900 C W=(TDNS*DK-DNS(6))/(DK-1.)
C THIS SUBROUTINE IS CALCULATE THE MASS BALANCE OF SHIFT CONVERTER
C ASSUMPTION:
C (1). ONLY ONE REACTION (CO+H2O->H2+CO2) DOMINATE

C DIMENSION NNS(7),DNS(7)
C F(X)=(D4+X)*(D5+X)-SK*(D3-X)*(D6-X)
C DF(X)=(D4+X)+(D5+X)+SK*[(D3-X)+(D6-X)]
C NEWTON-RAPHSON METHOD TO SOLVE NONLINEAR ALGEBRAIC EQUATION
C CALL EDK(NNS,TOPISKII)
C THIS SUBROUTINE IS USING NEWTON-RAPHSON ITERATION TO SOLVE TWO NONLINE.
C ALGEBRAIC EQUATIONS IN REFORMER

DIMENSION XY(XX),DNS(I),SK1(IX)

F1(X,Y) = (D3+Y+X)**3-SKA*(TDNS+2.*Y)**2/(D1-Y)*(D6-X-Y)

F2(X,Y) = (D4+X)*(D5+X**3.)*SKB*(D6-X-Y)*(D3+Y)**2


DF2(X,Y) = (D3+Y)**3+9.*SKA*(TDNS+2.*Y)**2/1.1E08

F3(X,Y) = (D4+X)*(D5+X**3.)*SKB*(D6-X-Y)*(D3+Y)**2/(D1-Y)

DF3(X,Y) = 3.*(D5+X**2.*Y)**2/(D1-Y)**2+(D3+Y-X)**7-SKA/1.1E08

F4(X,Y) = (D3+Y-X)**7/1.1E08

DF4(X,Y) = (D3+Y-X)**6/1.1E08

F5(X,Y) = (D3+Y-X)**6/1.1E08

DF5(X,Y) = 4.*(D4+X)**15/1.1E08

F6(X,Y) = (D3+Y-X)**6/1.1E08

DF6(X,Y) = 4.*(D4+X)**15/1.1E08

D1=DNS(1)

D2=DNS(2)

D3=DNS(3)

D4=DNS(4)

D5=DNS(5)
D6 = DNS(6)
D7 = DNS(7)
SKA = SKL(1)
SKB = SKL(2)

IF (IA.EQ.1) GO TO 61
IF (IA.EQ.2) GO TO 62

X = XY(1)/1000.

DO 2 IA = 1, 500

DX = FX1(X,Y)*F2(X,Y) - FX2(X,Y)*F1(X,Y)
DY = FY1(X,Y)*FY2(X,Y) - FY3(X,Y)*FY4(X,Y)

X = X + DX
Y = Y + DY

AX = ABS(DX)
AY = ABS(DY)

IF (AX.LT.0.001 .AND. AY.LT.0.001) GO TO 9

CONTINUE

WRITE(6, 101)

101 FORMAT(1X, 'SOLVE THE EQUATION FAIL AFTER 500 ITERATIONS')

RETURN

9

XY(1) = Y * 1000.
XY(2) = X * 1000.

DO 3 IA = 1, 500

DX = FX1(X,Y)*F3(X,Y) - FX3(X,Y)*F1(X,Y)
DY = FY1(X,Y)*FY3(X,Y) - FY1(X,Y)*FY3(X,Y)

X = X + DX
Y = Y + DY

AX = ABS(DX)
AY = ABS(DY)

IF (AX.LT.0.001 .AND. AY.LT.0.001) GO TO 91

RETURN

91

XY(1) = Y
XY(2) = X

RETURN

DO 4 IA = 1, 500

DX = FX1(X,Y)*F4(X,Y) - FX4(X,Y)*F1(X,Y)
DY = FY1(X,Y)*FY4(X,Y) - FY1(X,Y)*FY4(X,Y)

X = X + DX
Y = Y + DY

AX = ABS(DX)
AY = ABS(DY)

IF (AX.LT.0.001 .AND. AY.LT.0.001) GO TO 92

RETURN

4 CONTINUE

WRITE(6, 101)

RETURN
SUBROUTINE VIEW (M,V,Z,TK,POP,PPM2,PPO2,PPH2O,PPCO,X0)

CD=M/2/SA+CL+ALFA,SN,FCOH,AREAF,DXC

RETURN

END

SUBROUTINE KREFIDNSR(DNSF,DXIDY,DQ,PX,TCO,THZ,Z,PO,TOUT,TDOUT)

LTHOUT,E1,DPI,FUEL

REAL K0,HM,K1,K2

COMMON/F K0,EA,RHOB,EPS,DZ
0121640 COMMON /ADDRE/ D1,D2,D3,DP,P
0121660 COMMON /WM/ WM
0121660 COMMON /FCG/ F7,CG
0121700 DIMENSION XI( 50),TA( 50),XE( 50),TC( 50),
0121720 TH( 50),XI( 50),TA( 50),TAK1( 50),TAK2( 50),
0121740 XCF( 50),XCOMP( 50,7),XMC( 50,7),XCI( 50,7),
0121760 XUNI( 50),TP( 50),FL( 7),C( 7),WM( 7),CM( 7),CG( 7),CGCOMP( 7),TCGC( 7)
0121780 DIMENSION REN( 50)
0121800 DIMENSION P( 50)
0121820 DIMENSION DNSR( 7),DNSF( 7)
0121840 DATA EPSF/0.01/
0121860 DATA XCOMP/ 350*0./
0121880 IDBUGS=0
0121900 D1=DX
0121920 D2=DY
0121940 D3=D0
0121960 DP=DP1
0121980 S=81
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 MI=CG1+CG2+CG3+CG4+CG5+CG6+CG7
0122340 XI1(1)=0.
0122360 XE2(1)=0.
0122380 TCO=(TCO-273.16)*9./5.+32.
0122400 THZ=(THZ-273.161*9./5.+32.
0122420 KINS=0
0122440 CO=(Fl*(1.-XI1(1)))*P(1)/(.7302*(F0+2.*XI1(1)*F1)*(TCO+460.))
0122460 U0=(4.*.7302*(F0+2.*XI1(1)*F1)*(TCO+460.))/(3.1415927*P(1))
0122480 1/(D2**2-D1**2)*EPS1
0122500 C FIRST ASSUHPTION -- THO
0122520 X=.9
0122540 AX=Z*RHOB*K0*P(1)*F1*(2.*F0+X*(2.*F1-F0))/(2.*F0*(F0+2.*X*F1)
0122560 U0=CD)
0122580 T=-.9045*EA/ALOG(X/AX)-460.
0122600 TK2=K2(T)
0122620 TX2=X2(T,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)
FL(2)=F2-TX2*(F3*X*F1)
FL(3)=F5+X*F1+TX2*(F3*X*F1)
FL(4)=F4-2.*X*F1-TX2*(F3*X*F1)
FL(5)=F5+4.*X*F1+TX2*(F3*X*F1)
FL(6)=F6
FL(7)=F7
TF=FX(X)
CALL CMS[C,FL,TF]
TVIS=VIS(C,T,IFUE)
TTHC=THC(C,T,IFUE)
THI=HI(TVIS,TTHC)
CGCOMP(1)=CG1
CGCOMP(2)=CG2
CGCOMP(3)=CG3
CGCOMP(4)=CG4
CGCOMP(5)=CG5
CGCOMP(6)=CG6
CGCOMP(7)=CG7
CALL CMS(TCCG,CGCOMP,PM)
CGVIS=VIS(TCCG,T,F)
CGTHC=THC(TCCG,T,F)
CGTCP=TCP(TCCG,T,F)
TH0=0.0(CGVIS,CGTHC,CGTCP,Z,THZ,RE)
THI=HI(TH0,TH0,TH0)
Z=3.1415927*TH0+ZD/2.
CALL CMS(COM,COM,11,1,2)
TFCP=TCP(T,COM)
AW=(A+MCTCP*TCPF/PZ+A+MCTCP*TCPF/TCPF)/(A+MCTCP*TCPF/TCPF)
TH0=(A+Z+ZTCP*TCPF/A+Z+ZTCP*TCPF)/(A+Z+ZTCP*TCPF)
IF(TH0.LT.TCG) TH0=TCG+250.
IDEA=1
IHPE=1
75 I=1
75 I=1
TAK(1)=0.
75 I=1
75 I=1
75 I=1
75 I=1
75 I=1
75 I=1
75 I=1
75 I=1
75 I=1
DO 79 J=1,7
79 CONTINUE
DO 80 J=1,7
80 CONTINUE
DO 81 J=1,7
81 CONTINUE
DO 82 J=1,7
82 CONTINUE
DO 83 J=1,7
83 CONTINUE
C SECOND ASSUMPTION --TC(I+1)
72 TC(I+1)=TC(I)
72 TC(I+1)=TC(I)
\begin{verbatim}
0123600 70 TAI+1=(TC(I)+TC(I+1))/2.
0123620 TAI+1=K1(TAI+1))
0123640 TAI+1=K2(TAI+1))
0123660 B1=DDZ*RHOB*KQ*XPI(I)/(U0+C0)
0123680 B2=EXP(-.9045*A/(TA(I+1)+460.))
0123900 X1(I+1)=X1(I+1)+B1*B2*XMCMP(I+1)
0123920 X2(I+1)=X2(I+1)+TA(I+1)
0123940 XDH1=2-M1(TAI+1)
0123960 XDH2=2-M2(TAI+1)
0123980 AL1=F1*XDH1*(X1(I+1)-X1(I)
0124000 AL2=(F3*X1(I+1)+F1)*XDM2*(XE2(I+1)-XE2(I))
0124020 AL2=AL1+AL2
0124040 FL1=F1*(1.-X1(I+1))
0124060 FL2=X2(I+1)*F3*X1(I+1)*F1
0124080 FL1=F1*F3*X1(I+1)*F1*XE2(I+1)*F1
0124100 FL1=F4-F2.*X1(I+1)*F1-2.*X1(I+1)*F1
0124120 FL1=F4-F2.*X1(I+1)*F1-2.*X1(I+1)*F1
0124140 FL1=F6
0124160 FL7=F7
0124180 XF(I+1)=F1*(1.-X1(I+)
0124200 CALL CLASSIC,FL,XF(I+1)
0124220 DO 10 J=1,7
0124240 XCOMP(I+1,J)=FL(J)
0124260 XMCMP(I+1,J)=XCOMP(I+1,J)/XF(I+1)
0124280 XCI(I+1,J)=C(J)
0124300 CONTINUE
0124320 XVIS=VIS(C,TA(I+1),IFUEL)
0124340 XTHC=THC(C,TA(I+1),IFUEL)
0124360 V=CM1(I)*F1+CM3(I)*F3+CM5(I)*F5+CM7(I)*F6+CM9(I)*F7
0124380 S=(1.41527*FD2*FD12)/FD2
0124400 AM1=F0
0124420 RHO=AM1/P(I+/1)/0.7302*(T460.))
0124440 DELP=(1.-EPS3)/EPS3*3.+GMW*2/DP*4.18E+08/RHO*150.*(1.-EPS)*XVIS/DP-
0124460 1/GMV+1.75*DDZ/2116.6
0124480 P(I+/1)=P(I+1)-DELP
0124500 XH(I+1)=XVIS/XTMC
0124520 XCGVIS=VIS(TGC,TH(I+1),IFUEL)
0124540 XCGTHC=THC(TGC,TH(I+1),IFUEL)
0124560 XGHTCP=HTC(TGC,TH(I))
0124580 XH0=HO(XCVS,THCG,TH(I)+RE)
0124600 REN(I+1)=RE
0124620 XUI(I+1)=UI(XH,TH(I)+TA(I+1))
0124640 AM1=(3.41527*XUI(I+1)*DDZ/2.)
0124660 XFCP=FCP(TA(I),FL)
0124680 AN=(SN+XHTCP+XFCP)/AM-XFCP+MH*XGHTCP
0124700 TH(I+1)=TH(I)+AN/2.*XFCP*TC(I)+AN-2.*XFCP*TC(I)+AN-2.*XFCP*TC(I)
0124720 TP(I+1)=TH(I+1)+AM-2.*XHTCP/AM+TH(I)+AM-2.*XHTCP/AM+TH(I)+AM-2.*XHTCP/AM-TC(I)
0124740 C TEST SECOND ASSUMPTION
0124760 C TEST SECOND ASSUMPTION
0124780 EE=ABS(TP(I+1)-TC(I+1))/TC(I+1)
0124800 IF(EE.LE.ERROR) GO TO 71
0124820 IF(KEV.LE.ERROR) GO TO 71
0124840 IF(KEV.LE.ERROR) GO TO 71
0124860 IF(KEV.LE.ERROR) GO TO 71
0124880 IF(KEV.LE.ERROR) GO TO 71
\end{verbatim}
0124880  TC2=TC(I+1)
0124900  EETC2=TH(I+1)*(AM-MH*XGHTCP)/AM+TH(I)*(AM+MH*XGHTCP)/AM -
0124920  ITC(I)=TC2
0124940  IF(KING.LE.15) GO TO 97
0124960  IF(EETCI.NE.EETC2) TC3=TC2-(EETC2/(EETC2-EETCI))*(TC2-TC1)
0124980  IF(EETCI.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=1
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)-THI)/THZ)
0125340  IF(AB.LE.0.001) GO TO 74
0125360  THO2=THO
0125380  THZ2=TH(N)
0125400  IF(IDEA.LT.2) THO3=THO+THZ2
0125420  IF(IDEA.EQ.2) THO3=(THO+THO2)/(THZ1-THZ2)+THO2
0125440  IDEA=2
0125460  THZ1=TH(N)
0125480  THO1=THO
0125500  THO=THO3
0125520  IF(THO.LT.TCO) IHOP=IHOP+1
0125540  IF(THO.LT.TCO) THO=THO+50.
0125560  IF(IHOP.EQ.5) GO TO 975
0125580  GO TO 75
0125600  74 CONTINUE
0125620  IF(K.EQ.1) L=N
0125640  GO TO 954
0125660  95 CONTINUE
0125680  WRITE(6,976) THO
0125700  976 FORMAT(1H1,'***INSUFFICIENT COMB. GAS HEAT CAPACITY'/ -
0125720  1'OTHO='F17.3,'THIS IS LESS THAN TCO'/ORAISE THZ AND/OR COMB. -
0125740  2GAS FLOW RATES'
0125760  GO TO 954
0125780  958 WRITE(6,958) KING,
0125800  958 FORMAT(1H1,'+LOOPING ON TC FOR ',I4,'ITERATIONS IN INCRM',I4)
0125820  956 CONTINUE
0125840  TCO=(TCO-32.)*5./9.+273.16
0125860  THZ=(THZ-32.)*5./9.+273.16
0125880  FCUT=P(N)
0125900  TCGUT=(TC(N)+32.)*5./9.+273.16
0125920  THOUT=(TH(1)+32.)*5./9.+273.16
0125940  DNR(1)=XCOMP(N,1)
0125960   DNGR(3)=XCOMP(N,2)
0125980   DNGR(4)=XCOMP(N,3)
0126000   DNGR(5)=XCOMP(N,5)
0126020   DNGR(6)=XCOMP(N,4)
0126040   DNGR(7)=XCOMP(N,6)
0126060   RETURN
0126080   END
0163100   SUBROUTINE CMASI(C,FL,F)
0163200   DIMENSION C(7),WM(7),FL(7)
0163300   COMMON /WM/ WM
0163400   IF (1)=FL(1)*WM(1)/(F*WM)
0163500   IF (2)=FL(2)*WM(2)/(F*WM)
0163600   IF (3)=FL(3)*WM(3)/(F*WM)
0163700   IF (4)=FL(4)*WM(4)/(F*WM)
0163800   IF (5)=FL(5)*WM(5)/(F*WM)
0163900   IF (6)=FL(6)*WM(6)/(F*WM)
0164000   IF (7)=FL(7)*WM(7)/(F*WM)
0164100   RETURN
0164200   END
0164400   END
0164500   SUBROUTINE CMASIN(XM,X)
0164600   REAL XM
0164700   COMMON F0,F1,F2,F3,F4,F5,F6,M0,C01,C02,C03,C04,C05,C06
0164800   COMMON ADDRE/D0,D1,D2,D3,D4,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.-XM)
0165300   IF (J.EQ.2) COM(J)=F2-F3*XM
0165400   IF (J.EQ.3) COM(J)=F3+XM*F1
0165500   IF (J.EQ.4) COM(J)=F4-2.*XM*F1
0165600   IF (J.EQ.5) COM(J)=F5+4.*XM*F1
0165700   IF (J.EQ.6) COM(J)=F6
0165800   IF (J.EQ.7) COM(J)=F7
0165900   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(X)
0167100   REAL XM
0167200   COMMON F0,F1,F2,F3,F4,F5,F6,M0,C01,C02,C03,C04,C05,C06
0167300   COMMON ADDRE/D0,D1,D2,D3,D4,P
0167400   COMMON /FCG/F7,CG7
0167500   F=F0*2.*XM*F1
0167600   RETURN
0167700   END
0167800 FUNCTION FCP(T,C)
0167900 DIMENSION COM(7),A(4,7)
0168000 DATA A/5.34,6.39E-03,0.,0.6,6.67E-04,0.,0.10,34,1.52E-03,0.,-
0168100 1.6342E05,8.5,8.3E-05,4.136E-07,0.,6.62,4.5E-04,0.,0.,6.5,-
0168200 85.5,6E-04,0.,0.6,732,8.36E-03,5.53E-09,0.0/
0168300 T=P+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 KH
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,D4,P
0169500 COMMON/WM/ WM
0169600 COMMON /FCG/F7,C7
0169700 HI=0.
0169800 V=(W(1)*F1+W(2)*F2+W(4)*F3+W(6)*F4+W(5)*F5+W(7)*F6
0169900 1+MH(I)/F7)
0170000 GMV=(1.941/(3.1415927*D2**2.-D1**2.))
0170100 HIDI=.813*(GMV*P/VIS)**.9*EXP(-6.*D6/(D2-D1))
0170200 HI=(HIDI+THC)/(D2-D1)
0170300 RETURN
0170400 END
0170500 FUNCTION HO(VIS,THC,HTCP,ZTR,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,D4,P
0171000 COMMON /FCG/F7,C7
0171100 COMMON/WM/ WM
0171200 HO=(CG1*M1*CG2*WM(3)+CG3*WM(4)+CG4*WM(5)+CG5*WM(6)+CG6*WM(7)-
0171300 1+CG7*WM(2))'MH
0171400 HO=0.
0171500 G=FM*(1**2-(-3.1415927*D3**2)/4.)
0171600 DE=4.*G*(1**2-3.1415927*D3**2/4.)/(3.1415927*D3**2+4.*G)
0171700 RE=HTCP*VIS/THC*WM
0171800 PR=HTCP*VIS/THC*WM
0171900 RH0=(AM*P)/(0.7302*(T460.))
0172000 GR=(Z**3)*(RHO**2)*4.18E8*100./(VIS**2)
0172100 IF(RE<GE.10000.) GO TO 300
0172200 IF(RE<GE.10000.) GO TO 300
0172300 C 2100. RE=10000.
0172400 HO21=(1.*THC/DE)**(2100.*.45)*SQRT(PR)*(DE/Z)**.4*(S/D3)**.8-
0172500 1**0.05
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
017300 C RE=2100
0173100 200 HO=(1.02*THC/DE)*(RE**.45)*SQRT(PR)*(DE/Z)**.4*(S/D3)**.8
FUNCTION HTCP(CM,T)
DIMENSION CM(7),C(7),A(4,7),W(7)
DATA A/5.346.39E-03,0.0,0.6.60.6.67E-04,0.0,0.10.34,1.52E-03,0.0,
1.6.3342E+05,8.3E-05,4.136E-07,0.6.65,4.35E-04,0.0,0.6.5,
25.56E-04,0.0,0.6.732,8.36E-03,5.53E-09,0.0/
DATA W/16.04,44.0,2,8,12,8,32./
TC=CM(1)/W(1)+CM(2)/W(2)+CM(3)/W(3)+CM(4)/W(4)+CM(5)/W(5) -
1+CM(6)/W(6)+CM(7)/W(7)
C(1)=CM(1)/W(1)/TC
C(2)=CM(2)/W(2)/TC
C(3)=CM(3)/W(3)/TC
C(4)=CM(4)/W(4)/TC
C(5)=CM(5)/W(5)/TC
C(6)=CM(6)/W(6)/TC
C(7)=CM(7)/W(7)/TC
TP=T+460.
RETURN
END

FUNCTION THC(C,T,I,J)
DIMENSION C(7),A(2,7)
COMA=F/THC/ A
THC=0.
DO 5 I=1,7
THC=THC+C(I)*A(1,I)*T+A(2,I)
5 CONTINUE
RETURN
END

FUNCTION UI(HI,HO,T)
REAL HI,HO
CXXO:4/ADDRE/ D1,D2,D3,S,DP,P
CXXE:i F7,C7
DLM=(03-02/ALOG/(03/02)
R=0.005

RETURN
END
THMET = 4.659E-03 * T + 6.248
UI = 1. / (THMET + D2 / (D3 * D2))
RETURN
END
FUNCTION VIS(C,T,I)
DIMENSION A(2,7), C(7)
CDMICH/VIFC/ A
VIS = 0.
5 DO 4 I = 1, 7
VIS = VIS + A(I, T) * A(2, I)
CONTINUE
RETURN
END
FUNCTION X2(X,K)
REAL RH, K2
COGN: ADDрене/ D1, D2, D3, DP, P
CONE/ FCG, F7
AZ(K2 - 1.) * (F3 + X*F1) ** 2
A = (X2-1.) * (F3 + X*F1)**2
B = (F3 + X*F1)*2. * (X - F2 - K2*F4 - 5.*X*F1 - F3 - F5)
C = K2*F2*F4 - 2.*F1*F2*K2*X - (F3 + X*F1)*F5 + 4.*F1*X
X2 = (-B - SQRT(B**2 - 4.*A*C)) / (2.*A)
RETURN
END
DO 100700 TOPFC = 443., UT = 0.8, CD = 325.,
100800 &END
DO 100900 IFUEL = 1., ERR = 0.01, IP = 7, EXT = 100., WAT = 0.015, EXA = 100.,
101000 &END
IF(AND(X2.LT.-1., OR. X2.GT.0.), X2 = (-B - SQRT(B**2 - 4.*A*C)) / (2.*A)
101200 RETURN
101300 END
DO 101000 &DPFC TOPFC = 443., UT = 0.8, CD = 325.,
101100 &END
DO 101200 &HEATX CN = 1.3, U = 48825.1, HA(7) = 0.2, HA(10) = 0.2,
101300 &END
DO 101400 &HEATX CN = 1.3, U = 48825.1, HA(7) = 0.2, HA(10) = 0.2,
101500 &END
DO 101600 &HEATX CN = 1.3, U = 48825.1, HA(7) = 0.2, HA(10) = 0.2,
101700 &END
DO 101800 &HEATX CN = 1.3, U = 48825.1, HA(7) = 0.2, HA(10) = 0.2,
101900 &END
DO 102000 &HEATX CN = 1.3, U = 48825.1, HA(7) = 0.2, HA(10) = 0.2,
102100 &END
DO 102200 &HEATX CN = 1.3, U = 48825.1, HA(7) = 0.2, HA(10) = 0.2,
102300 &END
DO 102400 &HEATX CN = 1.3, U = 48825.1, HA(7) = 0.2, HA(10) = 0.2,
102500 &END
DO 102600 &HEATX CN = 1.3, U = 48825.1, HA(7) = 0.2, HA(10) = 0.2,
102700 &END
DO 102800 &HEATX CN = 1.3, U = 48825.1, HA(7) = 0.2, HA(10) = 0.2,
**Title and Subtitle**
Phosphoric Acid Fuel Cell Power System Performance Model and Computer Program

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**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.

**Key Words**
Phosphoric acid fuel cell, Reformer, Shift converter, Lumped model, Distributed kinetic model

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