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

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

January 1984

Prepared for
NATIONAL AERONAUTICS AND SPACE ADMINISTRATION
Lewis Research Center
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for
U.S. DEPARTMENT OF ENERGY
Morgantown Energy Technology Center
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Cleveland, Ohio 44115

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INTRODUCTION

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

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

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

The present report describes just the basic performance model of the fuel cell system, and the computer programs written for its analyses. Other reports are being prepared for the cost and optimization programs, which are hosted by the basic performance code, and for more detailed studies of subsystems such as the fuel cell stack, the fuel reformer, and the heat exchanger network optimization.
A listing of the steady state performance lumped model is included at the end of the report. It begins on page 81.

I. SYSTEM DESCRIPTION

As shown in Figure 1, methane which is circulated by compressor (C) is preheated by heat exchanger E-1 prior to mixing it with the super heated steam which receives its heat by passing through heat exchanger E-9. Before entering the reformer, the methane steam mixture is heated via heat exchangers E-2 and E-3. Inside the reformer, methane is catalytically reformed by reaction with excess steam to produce carbon monoxide, carbon dioxide, and the desired product, hydrogen. The effluent from the reformer is cooled by flowing through heat exchanger E-2 before it enters the high temperature shift converter S-1. The function of the high temperature shift converter is to increase the hydrogen concentration and to reduce the carbon monoxide concentration of the reformer gas effluent. The temperature of the effluent from the shift converter S-1 is then reduced by passing through heat exchangers E-1, E-9 and E-6 before entering the low temperature shift converter S-2. The low temperature shift converter further increases the hydrogen concentration by promoting the shift reaction at a lower operating temperature. The effluent from the low temperature shift converter then enters the fuel cell containing H2, CO, CH4, CO2 and H20. 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 PEM system
Before entering the burner, the mixture is preheated by the burner effluent via heat exchanger E-4. The spent fuel is then burned with whatever additional methane is needed to provide the thermal energy necessary for the reformer reaction.

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

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

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

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

2.1 Modeling of Fuel Processing Subsystem

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

2.1.1 Heat Exchanger

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

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

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

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

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

where:
- \( C_c \): capacity rate of fluid on cold side, \( M_{Ccpc}, J/s-K \)
- \( C_h \): capacity rate of fluid on hot side, \( M_{Cpc}, J/s-K \)
- \( C_{\max} \): 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, \( CO + H_2O = H_2 + CO_2 \) (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

\[
K_2 = \frac{P_{co} \cdot P_{H_2}}{P_{co} \cdot P_{H_2O}} = \frac{(F_{co_2} + x)(F_{H_2} + x)}{(F_{co} - x)(F_{H_2O} - x)}
\]

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

\[ \sum_{PS} n_j (\Delta h^0)_{fj} - \sum_{RS} n_i (\Delta h^0)_{fi} + \sum_{PS} n_j \int_{T_f}^{298} (C_p)_{pj} dT \]

\[ - \sum_{RS} n_i \int_{T_i}^{298} (C_p)_{pi} dT = 0 \]  

(2-1-6)

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

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

\[ \Delta P = 1878 \frac{(1-\varepsilon)G}{\varepsilon^3 \ dp \ g \ c \ \rho} \left( \frac{150(1-\varepsilon)\mu}{dp \ G} + 1.75 \right) h \]  

(2-1-7)

where \( \varepsilon \) : void fraction in bed

\( \mu \) : viscosity, Kg/m-s

\( dp \) : effective diameter of packing particle, m

\( G \) : superficial gas mass velocity, Kg/s-m

\( h \) : packed height, m

\( \rho \) : density, Kg/m^3

\( \Delta P \) : 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:

\[ \text{C}_n\text{H}_m + 2n\text{H}_2\text{O} = n\text{CO}_2 + (2n + m/2) \text{H}_2 \]

for naphtha and methane, and

\[ \text{CH}_3\text{OH} + \text{H}_2\text{O} = \text{CO}_2 + 3\text{H}_2 \]

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:

\[ \text{CH}_4 + \text{H}_2\text{O} = \text{CO} + 3\text{H}_2 \]  
(demethanation reaction)

and

\[ \text{CO} + \text{H}_2\text{O} = \text{CO}_2 + \text{H}_2 \]  
(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
\[ K_1 = \frac{p_{CO_2} p^3 H_2}{p_{CH_4} p_{H_2}O} = \frac{y_{CO_2} y^3 H_2}{y_{CH_4} y_{H_2}O} \] (demethanation)

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

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

\[ K_1 = \frac{(F_{CO} - x+y)(F_{H_2}^* + x+3y)}{(F_{CH_4}^* - y)(F_{H_2O} - x-y)(F_T + 2y)^2} \] (2-1-8)

and

\[ K_2 = \frac{(F_{CO_2}^* + x)(F_{H_2}^* + x+3y)}{(F_{CO}^* - x+y)(F_{H_2O}^* - x-y)} \] (2-1-9)

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

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

\[ Q_{B-R} = uA\Delta T_m = H_{out} - H_{in} \] (2-1-10)

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

\[ \Delta T_m = \frac{(T_{fc} - T_{iR}) - (T_a - T_{feR})}{\ln \frac{T_{fc} - T_{iR}}{T_a - T_{feR}}} \] (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,

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

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

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

\[
\frac{d}{dz} = \frac{-\gamma a e \beta}{c}
\]

(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
- \( e \beta \): 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

\[-ra' = ko e^{-EA/RT} p_{CH_4}\]

(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)

\[
\rho Ai V C_p \frac{dt}{dz} = (-\Delta H_1) \frac{dy}{dz} + (-\Delta H_2) \frac{dx}{dz} + h \xi d \xi (T_w - t) \quad (2-1-16)
\]

\[
\rho_0 \text{ Vo Ao Cpo} \frac{dt}{dz} = h \pi \xi (T - T_w) \quad (2-1-17)
\]

where \(\Delta H_1\): demethanation reaction enthalpy, J/g-mole CH₄

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

\(Ai\): inner tube cross area, m²
There is greater uncertainty in estimating the heat transfer coefficient at the wall of tube than the rate expression. The scatter in experimental data is very high (Refs. 2, 3, and 4). The situation will be even more complicated by considering the unequal stoichimetric reaction (Ref. 6). Due to Beek's recommendation (Ref. 7), the modified Thoenes-Kramers (Ref. 8) correlation should be used for sphere-like particles near the wall, which are used in the model:

\[ h_i(d_p/k_f) = 2.58(Re)^{1/3}(Pr)^{1/3} + 0.94 (Re)^{0.8}(Pr)^{0.4} \]  \hspace{1cm} (2-1-18)

where 
- \( d_p \): equivalent particle diameter, m
- \( k_f \): thermal conductivity, J/s-m-K
- \( Pr \): Prandtl number
- \( Re \): particle 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 depleted air, through the cathode exit. The overall reaction in the fuel cell power section is

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

(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:

\[ \text{NX}_\text{H}_2 = \text{NI}_\text{H}_2 - (\text{I}_{\text{mean}} \text{ A})/(n\text{F}) \]  

(2-2-2)

\[ \text{NX}_\text{O}_2 = \text{NI}_\text{O}_2 - (\text{I}_{\text{mean}} \text{ A})/(2n\text{F}) \]  

(2-2-3)

\[ \text{NX}_\text{H}_2\text{O} = \text{NI}_\text{H}_2\text{O} + (\text{I}_{\text{mean}} \text{ A})/(n\text{F}) \]  

(2-2-4)

where

- NX: exit flow rate of hydrogen, oxygen, or steam, g-mole/sec
- NI: inlet flow rate of hydrogen, oxygen, or steam, g-mole/sec
- I_{\text{mean}}: mean current density, A/cm²
- A: effective area of cell plate, cm²
- n: number of Faraday equivalents transferred
- F: Faraday constant
The energy balance for the fuel cell is
\[
- (Q + W_e) = \sum_{PF} n_j (\triangle h_{Fj}^o) - \sum_{rF} n_i (\triangle h_{Fi}^o)
\]
\[
+ \sum_{PF} n_j \int_{T_{FF}}^{T_{TF}} (Cp)_j \, dT - \sum_{rF} n_i \int_{T_{IF}}^{T_{IF}} (Cp)_i \, dT
\]

(2-2-5)

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

where:

\[
Q = N_p \, X_n \, Y_n \, Q_F \quad \text{(2-2-6)}
\]

and \(Q_F = (\frac{\Delta H_r}{n_F} - V) \, I \quad \text{(2-2-7)}
\]

where:

- \(Q\): total heat generated, J/sec
- \(Q_F\): heat generated per unit area of cell, J/sec cm\(^2\)
- \(N_p\): number of cells
- \(X_n\): width of cell plate, cm
- \(Y_n\): length of cell plate, cm
- \(I\): fuel cell current density, A/cm\(^2\)
- \(\Delta H_r\): heat of reaction, J/g-mole of H\(_2\)

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:

\[
E_0 = E_o(T) + \frac{RT}{nF} \ln \left( \frac{Y_{\text{H}_2}/P_{\text{O}_2}}{Y_{\text{H}_2\text{O}}} \right)
\]  
(2-2-9)

with \( P_{\text{t}} \): total pressure, atm

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

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

\( Y_{\text{H}_2} \): mean mole fraction of hydrogen at anode

\( Y_{\text{O}_2} \): mean mole fraction of oxygen at cathode

\( Y_{\text{H}_2\text{O}} \): mean mole fraction of water vapor at cathode

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

\[ n = na + nr + nd + n_{\text{co}} \]  
(2-2-10)

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

\( nr \): resistance polarization, volts

\( nd \): diffusion polarization, volts

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

and

\[
na = \frac{RT}{2F} \ln \left( \frac{i}{i_0(S)(A)(C)(L)(U)} \right)
\]  
(2-2-11)
with \( \alpha_0 \): transfer coefficient
\( i \): current density, mA/cm\(^2\)
\( i_0 \): exchange current density of cathode, mA/cm\(^2\)
\( \text{SA} \): specific catalyst surface area, cm\(^2\)/g
\( \text{CL} \): catalyst loading on cathode, g/cm\(^2\)
\( \text{CU} \): catalyst utilization factor

The exchange current is a function of the acid concentration, temperature, and partial pressure of the oxygen. The acid concentration is a function of the water vapor partial pressure which permits correlation of \( i_0 \) as a function of \( Y_2O \), \( Y_{H2O} \), and \( T \). An empirical fit is

\[
i_0 = 232.7 (P_{Y2O})^{0.8} (P_{YH2O})^{0.4377} \exp(-6652/T) \tag{2-2-12}
\]

The resistance polarization is

\[
nr = ir
\]

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

The expression of \( n_{co} \) was chosen to have strong temperature dependence, be directly proportional to \( Y_{co} \), and have a logarithmic dependence on \( i \), \( i_{ao} \), and catalyst effective area. The resulting expression (Ref. 9) is

\[
n_{co} = 0.0782P_{Yco} \exp \left[ 9190 \left( \frac{1}{T} - \frac{1}{450} \right) \right] \ln \frac{450}{\text{CLa} \ \text{SA} \ \text{CU} \ \text{iao}} \tag{2-2-13}
\]

where \( \text{CLa} \): anode catalyst loading, mg
\( \text{iao} \): 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):

$$\varepsilon_{FC} = \varepsilon_V \varepsilon_I \varepsilon_{TH} \varepsilon_H, \ldots$$

(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:

$$\varepsilon_V = \frac{V}{E}, \ldots$$

(2-2-15)

$$\varepsilon_I = \frac{I}{I_F}, \ldots$$

(2-2-16)

$$\varepsilon_{TH} = \frac{\Delta G_r}{\Delta H_C}, \ldots$$

(2-2-17)

$$\varepsilon_H = \frac{\Delta H_r}{\Delta H_C}, \ldots$$

(2-2-18)

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

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

3.1 Main Program

The main program performs the following functions:

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

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

These calculations are carried out for two cases. In the first case, the kinetic effect on the reformer performance is considered to be negligible. In this case, the main program carries out these calculations without calling subroutine (ENRE). In the second case, the kinetic effect on the reformer performance is taken into consideration. For this case, the main program calls subroutine (KREF) and bypasses subroutines (ENRE), (EQUK), (REF), and (SNAE).
Figure 3. PERFORMANCE MODEL
C. It creates a printout of the input data, the results of thermodynamic states of the gas streams, the system performance parameters, the output heat and electric energies.

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

The equations contained in the main program are given below:

1. Calculate inlet air flow rate in the burner:

\[
DNSS(33,2) = (1+EXT*0.01)*(DNSS(14,3)+DNSS(14,5))/2+CK*DNSS(14,1)
\]

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:

\[
T(22) = -B/(ALOG((DNSS(1,1)*SMRA-DNSS(21,6))/(DNSS(1,1)*SMRA-TKNSS(21))*POPS)-A)
\]

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

\[
AC = (-1.0148+SQRT(1.0148*2-4*0.056/108*(0.0472*108-WK))/2*0.0456/108)
\]

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

\[
DNSS(36,6) = QQT(5)/1/18/(355-TAT)
\]
<table>
<thead>
<tr>
<th>Nomenclature</th>
<th>Description</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: $\frac{AA3(1)+AA3(2)T+AA3(3)T^2+AA3(4)}{T^2}$</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., ft²</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/cm²</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>Enthalpy 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>
</tbody>
</table>

I : Gas number

I = 1  Fuel (methane, methanol, naphtha)
I = 2  Oxygen
I = 3  Carbon Monoxide
I = 4  Carbon Dioxide
I = 5  Hydrogen
I = 6  Water
I = 7  Nitrogen
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<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, (\text{lb-mole CH}_4/\text{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/lbm</td>
</tr>
<tr>
<td>SVW</td>
<td>Specific volume of water, ft³/lbm</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>Definition</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)</td>
<td>Heat capacity const. of gas I, Cal/g-mole–K of the form:</td>
</tr>
<tr>
<td>HCBS(I)</td>
<td></td>
</tr>
<tr>
<td>HCCS(I)</td>
<td></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>
Figure 4  Flow chart of executive program for simulating CSU's FAPC system steady state performance
Figure 4 continued
energy balance
fuel cell
CALL ENFU

Calculate AC output

E - 10
CALL CDPH

Mass balance
E - 7

Mixer
CALL DMIX

E - 5
CALL COND

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 contain 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

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

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 calculates 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

\[ WS = GAG \times 1.987 \times TIN \times 1.8 \times \left( \frac{POUT}{PIN} \right)^{2 \times ((GAG-1)/GAG)-1}/(GAG-1) \]  

2. Calculate the compressor shaft work assuming isothermal conditions

\[ WS = 1.987 \times TIN \times 1.8 \times ALOG(POUT/PIN) \]

3. Calculate the compressor power requirements

\[ POW = WS \times TDNS/641400 \]
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 correction for latent heat

\[ QT = QT + ((1 - (THO / 647.1)) / (1 - 0.577)^{0.38} \times 9700 \times DNSH(6)) \] (3-2-9)

where Watson correction is given as,

\[ \frac{(h_{fg})_2}{(h_{fg})_1} = 1 - T_{r2}^{0.38} \] (3-2-10)

where \( h_{fgi} \): molar heat of vaporization at condition \( i \)

\( T_{ri} \): reduced temperature at condition \( i \).

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

1. Calculate the roots of a given nonlinear function:

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

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

2. Calculate the outlet pressure

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

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, thermodynamic efficiency, heating value efficiency, and fuel cell efficiency. The flow chart for ENFU appears in Figure 10. Subroutine ENFU contains the Equations (2-2-5) to (2-2-18).

I. Subroutine ENRE: This subroutine is used to calculate the energy balance of reformer in lumped model. This model was based on the assumption that all chemical reactions reach equilibrium at the input temperature (isothermal operation) or the average temperature (adiabatic operation). Then
Figure 10 Flow Chart of ENFU
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

Calculate the rejected heat

RETURN

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

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

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

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

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 enthalphy 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 enthalphy change with temperature

Calculate the enthalphy change of reaction

Calculate the total capacity constant

Calculate the outlet temperature

Test for convergence
CALL CONV

YES

RETURN

Figure 12 Flow Chart of ENSH
Figure 13 Flow Chart of EQUK
1. Calculate heat capacity constants

\[ \text{TCAS} = \text{TCAS} + \text{NNS}(I) \cdot \text{HCAS}(I) \]
\[ \text{TCBS} = \text{TCBS} + \text{NNS}(I) \cdot \text{HCB}(I) \]
\[ \text{TCCS} = \text{TCCS} + \text{NNS}(I) \cdot \text{HC}(I) \]  \hspace{1cm} (3-2-16)

2. Calculate enthalpy of reaction change

\[ \text{DH} = \text{DH} + \text{NNS}(I) \cdot \text{HS}(I) \]  \hspace{1cm} (3-2-17)

3. Calculate free energy of reaction

\[ \text{DG} = \text{DG} + \text{NNS}(I) \cdot \text{GS}(I) \]  \hspace{1cm} (3-2-18)

4. Calculate constant DHO

\[ \text{DHO} = \text{DH} - \text{TCAS} \cdot \text{TST} - \text{TCBS} \cdot \text{TST}^2/2 - \text{TCCS} \cdot \text{TST}^3/3 \]  \hspace{1cm} (3-2-19)

5. Calculate constant AI

\[ \text{AI} = \left( \text{DHO} - \text{DG} - \text{TCAS} \cdot \text{TST} \cdot \text{ALOG}(\text{TST}) - \text{TCBS}/2 \cdot \text{TST}^2 - \text{TCCS}/6 \cdot \text{TST}^3 \right) / \text{TST} / \text{R} \]  \hspace{1cm} (3-2-20)

6. Calculate equilibrium constant

\[ \text{SK} = \exp\left( -\text{DHO} / \text{R} / \text{TOP} + \text{TCAS} / \text{R} \cdot \text{ALOG}(\text{TOP}) + \text{TCBS} / 2 \cdot \text{TOP} / \text{R} + \text{TCCS} / 6 \cdot \text{R} \cdot \text{TOP}^2 / \text{AI} \right) \]  \hspace{1cm} (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
   \[ DH = DH + DNS(I) \cdot HS(I) - DINS(I) \cdot HS(I) \]  
   \[ (3-2-22) \]

2. Calculate the sensible enthalpy change
   \[ DH = DH + DNS(I) \cdot HCAS(I) \cdot ((298 - TIN) + HCBS(I) / 2 \cdot ((298)^2 - TIN^2) + HCCS(I) / 3 \cdot ((298)^3 - TIN^3)) \]  
   \[ (3-2-23) \]

3. Calculate total heat capacity constants
   \[ TCAS = TCAS + DNS(I) \cdot HCAS(I) \]  
   \[ (3-2-24) \]
   \[ TCBS = TCBS + DNS(I) \cdot HCBS(I) \]
   \[ TCCS = TCCS + DNS(I) \cdot HCCS(I) \]

4. Calculate the adiabatic FLAME temperature
   \[ TFC = \left( \frac{-DH - TCBS / 2 \cdot ((TF)^2 - (298)^2) - TCCS / 3 \cdot ((TF)^3 - (298)^3)}{TCAS + 298} \right) \]  
   \[ (3-2-25) \]

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

N. Subroutine HEPD: This subroutine calculates the pressure drop in the heat exchangers used in the fuel cell power plants. It was assumed that BWG14
Calculate the material balance of burner
CALL BURN

Calculate the enthalphy change of reaction

Calculate the enthalphy change with temperature

Calculate the total heat capacity constant

Calculate the energy balance for obtaining the outlet temperature

Test for convergence
CALL CONV

RETURN
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
   \[ NT = \frac{HA}{0.3048^2/NP/CLEN/SURFC} \]  \hspace{1cm} (3-2-26)

2. Calculate number of baffles
   \[ NB = CLEN/BSPAC \]  \hspace{1cm} (3-2-27)

3. Calculate free area between baffles
   \[ FAREA = IDS/(ODT+CL)*CL*BSPAC \]  \hspace{1cm} (3-2-28)

4. Calculate ratio of pitch, transverse to flow, to tube diameter
   \[ XT = \frac{PITCH}{ODT} \]  \hspace{1cm} (3-2-29)

5. Calculate friction factor
   \[ FPRI = SBO*(ODT*GS/AMUI)^{(-0.15)} \]  \hspace{1cm} (3-2-30)

6. Calculate pressure drop
   \[ DP = B0*2*FPRT*NR*GS**2/32.174/3600**2/RHO/2116.2 \]  \hspace{1cm} (3-2-31)

0. Subroutine HEXC: This subroutine calculates the energy analysis in the parallel, counter and crossflow heat exchangers. From the assumption described in Section 2.1.1, the counter mode will be the only option used for heat exchangers in the system. Mathematical model was shown in the Equations (2-1-1) to (2-1-4).
Figure 16 Flow Chart of HEPD
P. Subroutine PDFU: This subroutine calculates the pressure drops in the fuel channels and air channels. Dimensions of the fuel-cell stack are based on Westinghouse Stock No. 522. The mean pressure drop is evaluated by taking average of calculations based on inlet and outlet gas compositions.

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

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

1. Calculate the power required to pump water

\[
P OW = SVW \times 144.5 \times 0.05051 \times 0.0000001 \times WM(6) \times 14.7 \times (POUT-PIN) \times DNS(6) / 453.6
\]

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

\[
\begin{align*}
X_1^\text{NEW} &= X_1^\text{old} + \Delta X_1 \\
X_2^\text{NEW} &= X_2^\text{old} + \Delta X_2
\end{align*}
\]

(3-2-33)

where

\[
\begin{align*}
\Delta X_1 &= \frac{f_2 \frac{\partial f_1}{\partial x_2} - f_1 \frac{\partial f_2}{\partial x_2}}{D} \\
\Delta X_2 &= \frac{f_1 \frac{\partial f_2}{\partial x_1} - f_2 \frac{\partial f_1}{\partial x_1}}{D}
\end{align*}
\]

(3-2-34)

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

\[
\frac{\partial f_1}{\partial x_1} \frac{\partial f_2}{\partial x_2} - \frac{\partial f_1}{\partial x_2} \frac{\partial f_2}{\partial x_1}
\]

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

\[
X_W = \frac{(TDNS-DNS(6))/(DK-1)}{}
\]

(3-2-35)
Calculate equilibrium constants of $y_{xn\ 1}$ and $y_{xn\ 2}$
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 XW: amount of water in liquid phase
DK: equilibrium constant of liquid-vapor system, which equals to (PSAT/POP)

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

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

3.3 Subroutine KREF

The mathematical model developed in Section 2.1.3.2 was used to develop a Fortran computer code, which consists of an executive program (KREF), three subroutines and eleven functions. Finite difference method will be applied to solve these simultaneous differential equations (Equations (2-1-14) to (2-1-17)), with the inlet conditions as the boundary conditions. The definition of finite difference section is expressed in Figure 18 and the summary of the basic difference equations is shown in Table 2, where the nomenclature of
variables and functions in the program is listed in Table 3. Figure 19 shows the flow chart of this program.

KREF is similar to REPENT developed by Westinghouse (80-9E6-PAMEC-RI). A more detailed 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

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

2. Water Gas Shift Equilibrium

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

with

\[ A = [K_2(i+1)-1][F_3+X_1(i+1) F_1]^2 \]

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

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

3. Reforming Gas Energy Balance

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

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>
<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>

**Variable** | **Definition** |
--- | --- |
FL for J = 0 to 7 | Total reformer gas feed flow rate and component feed flow rates for components 1 through 7 (molar basis) |
MH | Total combustion gas flow rate (molar basis) |
CGCOM for J = 1 to 7 | Combustion gas component flow rates for components 1 to 7 (molar basis) |
K₁ | Equilibrium constant for demethanation reaction |
K₂ | Equilibrium constant for water shift reaction |
K₀ | Frequency factor for Arrhenius expression \( k + k₀ \exp(-E_{act}/RT) \) |
WM | Molecular weight |
EA | Activation energy for demethanation reaction |
RHOB | Catalyst bulk density |
EPS | Reactor void volume |
D₁ | Reformer center tube outside diameter |
D₂ | Reformer outer tube inside diameter |
D₃ | Reformer outer tube outside diameter |
S | Characteristic dimension of the combustion gas flow duct (geometry is square) |
DP | Catalyst particle diameter |
P | Pressure |
<table>
<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>
</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>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>
<tr>
<td>Variable</td>
<td>Definition</td>
</tr>
<tr>
<td>--------------</td>
<td>---------------------------------------------------------</td>
</tr>
<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>Interactive 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 (COND) 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 (REPD) 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</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>443</td>
<td>K</td>
<td></td>
<td>Operating temperature in fuel cell stack</td>
</tr>
<tr>
<td>OPFC</td>
<td>UT</td>
<td>0.8</td>
<td></td>
<td>mA/cm²</td>
<td>Utilization of H2 in stack</td>
</tr>
<tr>
<td>OPFC</td>
<td>CD</td>
<td>325</td>
<td>mA/cm²</td>
<td></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 (\text{CH}_4)/lb cata-hr-atm</td>
<td></td>
<td>Outside diameter of reforming tube</td>
</tr>
<tr>
<td>REPEN</td>
<td>EA</td>
<td>20000</td>
<td>Cal/g-mole CH(_4)</td>
<td></td>
<td>Rate constant of demethanation reaction</td>
</tr>
<tr>
<td>REPEN</td>
<td>RHOB</td>
<td>80</td>
<td>lb/ft(^3)</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>m(^{2})-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>Buffle space</td>
</tr>
<tr>
<td>HEPDC</td>
<td>ODTX</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>DTH</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>SAMPLE 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>ft(^2)</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>1</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>(\Omega \cdot \text{cm})</td>
<td></td>
<td>Cell resistance at 450° K</td>
</tr>
<tr>
<td>CATAI</td>
<td>SA</td>
<td>400</td>
<td>cm(^2)/mg</td>
<td></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>mg/cm(^2)</td>
<td></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>g-equivalent</td>
<td></td>
<td>Number of Faraday equivalents transferred</td>
</tr>
<tr>
<td>CATAI</td>
<td>FCONST</td>
<td>96500</td>
<td>C/g-equivalent</td>
<td></td>
<td>Faraday constant</td>
</tr>
<tr>
<td>CATAI</td>
<td>DKC</td>
<td>240000</td>
<td>A/atm</td>
<td></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.
&TOPFC TTOPFC=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=1.04E+04,EA=2000.,RH0B=80.
, EPS=0.487,S=0.25,DP=0.00328,DZZ=0.25,
&END
&HEATX CN=1.3,U=48825.1,HA(7)=0.2,HA(10)=0.2,
&END
&HEPDC NPH=2,NRH=5,BSPAC=1.,0DTH=.0625,PITCH=.0833,CLH=.0208,IDS=.833,
, IDTH=.04667,FLOAR=.001716,SURFC=.1466,CLENH=2.,S1TS2=.9,DTH=0.7,
&END
&PDSH DPD=1.18,0.,AHRN=0.66,0.,APPD=69.,0.,CLEP=5.91,0.,
NTPD=1.0.
&END
&PDFUH NTAF=140,FULE=1.42,WIDAF=.009744,NPFU=3365,
NTAA=40,AIRL=1.,WIDAA=.00515
&END
&CATAI SRO=.44,SA=400.,CU=.15,CL=.75,ALFA=.5,SN=2.,FCONST=96500.,
DKC=2.4E5,
&END

Figure 20 Sample Input Data
Figure 21 Sample Computer Run
NTPD= 1.0
#END
#PDFUH
NTAF= 140
FUE= 1.419999
WIDAF= 0.97440E-02
HPU= 3565
NTIA= 40
AIRL= 1.0
WIDAA= 0.5149998E-02
#END
#CATAI
SRO= 0.440
SA= 400.0
CU= 0.150
CL= 0.750
ALFA= 0.50
SN= 2.0
FCNST= 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: 4.90 ATM OUTLET PRESSURE: 4.72 ATM
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: 4.72 ATM
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: 4.72 ATM
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: 4.42 ATM

THE FRACTION OF CO IN THE FEED IS 0.00029

THE FUEL CELL IS OPERATING UNDER THESE CONDITIONS
THE OPERATING TEMPERATURE: 443.00 K
THE OPERATING PRESSURE: 4.79 ATM
THE OPEN CIRCUIT POTENTIAL: 1.171 V
THE OPERATING POTENTIAL: 0.658 V
THE CURRENT DENSITY: 0.325 A/CM²
THE CATALYST LOADING: 0.750 PT/CM²
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 03 KW
THE TOTAL HEAT RELEASE IS 0.53266E 08 CAL

THE AC OUTPUT IS 113.77 KW

Figure 21 continued
<table>
<thead>
<tr>
<th></th>
<th>E-1</th>
<th>E-2</th>
<th>E-3</th>
<th>E-4</th>
<th>E-5</th>
<th>E-6</th>
<th>E-7</th>
<th>E-8</th>
<th>E-9</th>
<th>E-10</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>THE DUTY OF HEAT EXCHANGER (CAL.)</strong> 0 MEANS NO THIS NO. HEAT EXCHANGER</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>0.45316E 07</td>
<td>0.99787E 07</td>
<td>0.14123E 08</td>
<td>0.33156E 08</td>
<td>0.10910E 09</td>
<td>0.10777E 08</td>
<td>0.53266E 08</td>
<td>0.00000</td>
<td>0.51060E 07</td>
<td>0.37070E 08</td>
</tr>
<tr>
<td><strong>THE SURFACE AREA OF HEAT EXCHANGER (M²X2)</strong> 0 MEANS NO THIS NO. HEAT EXCHANGER</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>0.38308E 00</td>
<td>0.13341E 01</td>
<td>0.14964E 01</td>
<td>0.22603E 01</td>
<td>0.21182E 02</td>
<td>0.14996E 01</td>
<td>0.20000E 00</td>
<td>0.00000</td>
<td>0.82420E 00</td>
<td>0.20000E 00</td>
</tr>
<tr>
<td><strong>THE EFFICIENCY OF HEAT EXCHANGER (0 MEANS NO THIS NO. HEAT EXCHANGER OR IS CONDENSER)</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>0.68881E 00</td>
<td>0.59346E 00</td>
<td>0.63181E 00</td>
<td>0.57412E 00</td>
<td>0.00000</td>
<td>0.00000</td>
<td>0.00000</td>
<td>0.00000</td>
<td>0.64153E 00</td>
<td>0.00000</td>
</tr>
<tr>
<td><strong>THE POWER OF AIR COMPRESSOR:</strong></td>
<td>64.04HP</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>THE POWER OF METHANE COMPRESSOR:</strong></td>
<td>3.80HP</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>THE POWER OF PUMP:</strong></td>
<td>0.00146HP</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

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
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
AHUL: MOLE FRACTION OF AVAILABLE HYDROGEN
AMHN: 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.
B : CONSTANT FOR CAL. SATURATED CONDITION OF WATER
BNPA: BOILING POINT OF NAPHTHA, C
BPUL: OUTLET TEMP. OF GASES, K
BSPAC: BAFFLE SPACE, FT
CD: CURRENT DENSITY, AMP/CM**2
CL: CATALYST LOADING, MS/CM**2
CLEM: LENGTH OF TUBE IN HEAT EXCHANGER, FT
CLEFD: LENGTH OF SHIFT CONVERTER(JK=1), REFORMER(JK=2 FOR METHANOL and NAPHTHA), FT
CLH: CLEANER IN HEAT EXCHANGER, FT
CN: G/A/C/M IN HEAT EXCHANGER
CUN: CATALYST UTILIZATION
DG: STANDARD FREE ENERGY CHANGE, CAL/G-MOLE
DH: STANDARD ENTHALPY CHANGE AT REACTION, CAL/G-MOLE
DHIN: ENTHALPY CHANGE DUE TO TEMPERATURE CHANGE OF INLET FLUID
CAL/G-MOLE
DK: C: CONST. TO CALC. LIMITING CURRENT DENSITY
DLH: INTEGRATION CONSTANT IN CALCULATE H
DP: CATALYST PELLET DIAMETER, FT
DPD: DIA. OF SHIFT CONVERTER(JK=1), REFORMER(JK=2 FOR METHANOL AND NAPHTHA), FT
DSHO: CATHODE INLET WATER OF FUEL CELL, G-MOLE/HR.
DSN: CATHODE INLET NITROGEN OF FUEL CELL, G-MOLE/HR.
DSO: CATHODE INLET OXYGEN OF FUEL CELL, G-MOLE/HR.
DTH: FRACTION OF DELTA T OVER INLET GAS FILM IN THE HEAT EXCHANGER
DX1: OUTSIDE DIAMETER OF REFORMER CENTER TUBE, FT
DX2: INSIDE DIAMETER OF OUTSIDE REFORMER TUBE, FT
DX3: OUTSIDE DIAMETER OF OUTSIDE REFORMER TUBE, FT
DZZ: INCORRECT HEIGHT OF FINITE DIFFERENCE MODEL IN THE REFORMER,
EPS: REACTOR VOID FRACTION
ERR: CONVERGE CRITERIA
EXA: FRACTION OF EXTRA AIR IN FUEL CELL
EXT: FRACTION OF extra air in burner
FC: MOLE FRACTION OF CO CONTAIN
FCONS: FARADAY CONSTANT, 23061 CAL/VOLT-GM EQUIV.
FLOOR: FLOW AREA IN HEAT EXCHANGER, FT**2
FUEL: LENGTH OF FUEL CHANNEL, FT
FUEL: LENGTH OF FUEL CHANNEL, FT
FUX: FRACTION OF EXTRA AIR IN FUEL CELL
G: GAS NUMBER
I = 1 FUEL METHANE, METHANOL, NAPHTHA
I = 2 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>
</tr>
</thead>
<tbody>
<tr>
<td>0002220</td>
<td>I=3 CARBON MONOXIDE OR CARBON DIOXIDE( &quot; &quot; )</td>
</tr>
<tr>
<td>0002220</td>
<td>I=4 CARBON DIOXIDE OR WATER( &quot; &quot; )</td>
</tr>
<tr>
<td>0002240</td>
<td>I=5 HYDROGEN</td>
</tr>
<tr>
<td>0002260</td>
<td>I=6 WATER OR NITROGEN( &quot; &quot; )</td>
</tr>
<tr>
<td>0002280</td>
<td>I=7 NITROGEN OR OXYGEN( &quot; &quot; )</td>
</tr>
<tr>
<td>0002300</td>
<td>IDSH: ID OF SHELL IN HEAT EXCHANGER, FT</td>
</tr>
<tr>
<td>0002320</td>
<td>IDTH: ID OF TUBE IN HEAT EXCHANGER, FT</td>
</tr>
<tr>
<td>0002340</td>
<td>IFUEL: FUEL TYPE</td>
</tr>
<tr>
<td>0002360</td>
<td>1: METHANE CH4</td>
</tr>
<tr>
<td>0002380</td>
<td>2: METHANOL CH3OH</td>
</tr>
<tr>
<td>0002400</td>
<td>3: NAPHTHA C7H16</td>
</tr>
<tr>
<td>0002420</td>
<td>IDNO: NO. OF REDD</td>
</tr>
<tr>
<td>0002440</td>
<td>IMUI: STOICHIOMETRIC NUMBER</td>
</tr>
<tr>
<td>0002460</td>
<td>IP: INDEX OF OPERATION CONDITION IN THE REFORMER( NOT FOR METHANE)</td>
</tr>
<tr>
<td>0002480</td>
<td>ISHIFT: SHIFT CONVERTER</td>
</tr>
<tr>
<td>0002500</td>
<td>IP=1 ADIABATIC OPERATION</td>
</tr>
<tr>
<td>0002520</td>
<td>IP=2 ISOTHERMAL OPERATION</td>
</tr>
<tr>
<td>0002540</td>
<td>KO: FREQUENCY FACTOR FOR ARRHENIUS EXPRESSION, LB MOLE CH4/LB</td>
</tr>
<tr>
<td>0002560</td>
<td>CATA.-HR-ATM</td>
</tr>
<tr>
<td>0002580</td>
<td>NN: STREAM NUMBER OF EXIT OF SHIFT CONVERTER</td>
</tr>
<tr>
<td>0002600</td>
<td>NCR: SCALE UP FACTOR IN THE MODEL OF REFORMER</td>
</tr>
<tr>
<td>0002620</td>
<td>NPFU: NO. OF CELL PLATE IN THE FUEL CELL STACK</td>
</tr>
<tr>
<td>0002640</td>
<td>NPH: NO. OF TUBE PASSES</td>
</tr>
<tr>
<td>0002660</td>
<td>NSH: NO. OF ROHS FOR TUBES</td>
</tr>
<tr>
<td>0002680</td>
<td>NTAA: NO. OF AIR FLOW CHANNEL IN ONE CELL PLATE</td>
</tr>
<tr>
<td>0002700</td>
<td>NTAF: NO. OF FUEL FLOW CHANNEL IN ONE CELL PLATE</td>
</tr>
<tr>
<td>0002720</td>
<td>NTPD: NO. OF TUBES IN SHIFT CONVERTER(JK=1), REFORMER(JK=2 FOR METHANOL AND NAPHTHA)</td>
</tr>
<tr>
<td>0002750</td>
<td>OSTMH: CO OF TUBE, FT</td>
</tr>
<tr>
<td>0002760</td>
<td>CU: 02 UTILIZATION</td>
</tr>
<tr>
<td>0002800</td>
<td>PAT: AMBIENT PRESSURE, 1ATM</td>
</tr>
<tr>
<td>0002820</td>
<td>PIN: INLET PRESSURE, ATM</td>
</tr>
<tr>
<td>0002840</td>
<td>PINFU: INLET PRESSURE OF FUEL CELL STACK, ATM</td>
</tr>
<tr>
<td>0002860</td>
<td>PITCH: PITCH OF HEAT EXCHANGER, FT</td>
</tr>
<tr>
<td>0002880</td>
<td>POP: OPERATION PRESSURE, ATM</td>
</tr>
<tr>
<td>0002900</td>
<td>FOUT: OUTLET PRESSURE, ATM</td>
</tr>
<tr>
<td>0002920</td>
<td>ROHS: BULK DENSITY OF CATA., LBS/FT**3</td>
</tr>
<tr>
<td>0002940</td>
<td>S: SIDE LENGTH OF AN ASSUMED SQUARE FLOW DUCT FOR COMBUSTION GAS,</td>
</tr>
<tr>
<td>0002960</td>
<td>SITSD: RATIO OF TOTAL INSIDE-TUBE CROSS-SECTIONAL AREA PER PASS TO HEADER CROSS-SECTIONAL AREA PER PASS</td>
</tr>
<tr>
<td>0003000</td>
<td>SA: CATALYST SURFACE, CM**2/MS</td>
</tr>
<tr>
<td>0003020</td>
<td>SK: EQUILIBRIUM CONSTANT</td>
</tr>
<tr>
<td>0003040</td>
<td>SK1: EQUILIBRIUM CONSTANT WITH PRESSURE DIFFERENT FROM 1 ATM</td>
</tr>
<tr>
<td>0003060</td>
<td>SKA: STEAM/FUEL</td>
</tr>
<tr>
<td>0003080</td>
<td>SN: NUMBER OF FARADAY EQUIVALENTS TRANSFERED</td>
</tr>
<tr>
<td>0003100</td>
<td>SNO: CELL RESISTANCE AT 480 K, OHM-CM**2</td>
</tr>
<tr>
<td>0003120</td>
<td>SURFC: SURFACE PER LINE, FT</td>
</tr>
<tr>
<td>0003140</td>
<td>SV1(I): SPECIFIC VOLUME OF FUEL I, FT**3/LBM</td>
</tr>
<tr>
<td>0003160</td>
<td>SVW: SPECIFIC VOLUME OF WATER, FT**3/LBM</td>
</tr>
<tr>
<td>0003180</td>
<td>TACOA: INLET AIR TEMP. OF FUEL CELL STACK, K</td>
</tr>
<tr>
<td>0003200</td>
<td>TACOF: INLET FUEL TEMP. OF FUEL CELL STACK, K</td>
</tr>
<tr>
<td>0003220</td>
<td>TAT: AMBIENT TEMPERATURE, 298 K</td>
</tr>
<tr>
<td>0003240</td>
<td>TC: CRITICAL TEMPERATURE, K</td>
</tr>
<tr>
<td>0003260</td>
<td>TCAS: TOTAL HEAT CAPACITY CONSTANT A</td>
</tr>
</tbody>
</table>
000460 COMMON /CN1/ CN
000460 COMMON /NAPH/ HNA,BPNA,WNPA,VHNA
000460 COMMON /AM/ IM
000460 COMMON /HEPOT/ NPH,RRH,BSPAC,ODTH,PITCH,CLM,IDSH,IDTH,FLOAR,SURFC,-
0004440 ICLNH,SITSE,DTH
0004440 COMMON /PDESH/ DPD,AHRN,APPD,CLEPD,NTPD
0004440 COMMON /PDHUT/ HTHA,NTAA,FULE,AIRL,WIDAF,WIDAA,NPFE
0004440 COMMON /REP/ K0.KA,ANOB,EP5,DOZ
0004440 COMMON /SV/ SV,SVH
0004540 COMMON /HLHV1/ HLHV
0004540 COMMON /THCC/ AA1/VPFC/AA2/HTCPC/AA3
0004540 COMMON /CATA/ SRO,SA,CU,CL,ALFA,SN,FCONST,AREAF,DKC
000460 C
000460 DATA DNSS/273=0./
000460 C READ THE OPERATION CONDITION OF FUEL CELL
000460 READ (5,OPFC)
000460 WRITE (6,OPFC)
000470 C READ THE INLET AMOUNT AND CONDITION
000470 READ (5,INIT)
000470 WRITE (6,INIT)
000470 C READ OPERATION CONDITION
000470 READ (5,COND)
000470 WRITE (6,COND)
000480 C READ OPERATING COEFFICIENT IN THE REFORMER(METHANE FUEL ONLY)
000480 IF (IFUEL.EQ.1) READ (5,REPEN)
000480 IF (IFUEL.EQ.1) WRITE (6,REPEN)
000480 C READ CONDITION OF HEAT EXchanger
000490 READ (5,HEATX)
000490 WRITE (6,HEATX)
000490 C READ THE CONSTRUCTION OF HEAT EXCHANGER FOR CAL. PRESSURE DROP
000490 READ (5,HEFDC)
000490 WRITE (6,HEFDC)
000490 C READ CONFIGURATION COEFF. OF SHIFT CONVERTER FOR CAL. PRESSURE DROP
000500 READ (5,PESSH)
000500 WRITE (6,PESSH)
000500 C READ CONFIGURATION COEFF. OF FUEL CELL FOR CAL. PRESSURE DROP.
000500 READ (5,PDFUH)
000500 WRITE (6,PDFUH)
000500 C READ THE OPERATING TEMP. OF REFORMER FOR FUEL NAPHTHA AND METHANOL
000500 IF (IFUEL.NE.1) READ (5,TR)
000500 IF (IFUEL.NE.1) WRITE (6,TR)
000500 C READ CATALYST CONSTANTS
000500 READ (5,CATAI)
000500 WRITE (6,CATAI)
000500 C
000500 C CHANGE THE THERMAL DATA FOR DIFFERENT FUEL INPUT
000500 IF (IFUEL.EQ.2) GO TO 1
000500 IF (IFUEL.EQ.3) GO TO 2
000500 GO TO 3
000500 1 GS(1)=-38810.
000500 HSI(1)=-6050.
000500 HCAS(1)=4.394
000500 HCBS(1)=0.024274
HCCS(1)=-0.0000069
WM(1)=32.
HLMV(1)=-159258.
AA3(1,1)=4.394
AA3(2,1)=0.013466
AA3(3,1)=-2.1157E-06
AA3(4,1)=0.
AA1(1,1)=3.5E-05
AA1(2,1)=1.5E-02
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)=-0.000397
WH(1)=100.
HLMV(1)=1099580.
AA3(1,1)=7.488
AA3(2,1)=0.013467
AA3(3,1)=-1.0945E-05
AA3(4,1)=0.
AA2(1,1)=2.66E-02
AA2(2,1)=0.0157
AAl(1,1)=2.5E-05
AAl(2,1)=0.7E-02

GO TO 3

3 CONTINUE
IDNO=1

C FUEL INPUT COMPRESSOR(PUMP)***
PL1=PPOP*1.02

IF (IFUEL.EQ.1) CALL COMP (DNSH,TAT,TOUT,PAT,P(1),PDW,GAMM,I,IP)
IF (IFUEL.NE.1) CALL PUP (DNSH,TAT,TOUT,PAT,P(1),PDW,I,IFUEL)
DO 301 IA=1,I

DNSS(1,1)=DNSH(1,IA)
T(1)=TOUT

IF (IFUEL.EQ.1) CALL 13TH FLOW
DNSS(13,2)=0.
DNSS(13,7)=0.
DNSS(13,1)=0.147*DNSS(1,1)
DNSS(13,3)=0.0018*DNSS(1,1)+DNSS(1,3)
DNSS(13,4)=0.65*DNSS(1,1)+DNSS(1,4)
DNSS(13,5)=3.4*DNSS(1,1)+DNSS(1,5)
DNSS(13,6)=3.4*DNSS(1,1)+DNSS(1,6)

GO TO 6

4 DNSS(13,1)=0.000863487*DNSS(1,1)
DNSS(13,2)=0.01
DNSS(13,4)=0.999128*DNSS(1,1)
DNSS(13,5)=2.9974*DNSS(1,1)
DNSS(13,6)=0.60087*DNSS(1,1)
GO TO 6

5 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)=SRA*DNSS(1,1)-13.9645*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 (IDNO.GT.1) GO TO 8

8 P(31)=P(13)

DO 9 IB=1,I

9 DNS(IB)=DNS(13,IB)

C FUEL CELL MASS BALANCE***
C CALL FUCE(DNSS,TOPFC,POPFCT,DNSSAN,DNSCA,D50,D5N,D5H1,UT,IP,PINF,PINA-
1,FUEL)

10 DNS(14,IC)=DNSAN(14,IC)

DO 11 IC=1,I

11 DNS(28,ID)=DNS(28,ID)-1.0/GARH

DO 12 IE=1,I

12 DNSAI(IE)=DNS(28,IE)

C AIR COMPRESSOR***
13 DNS(29,18)=DNS(29,18)

C DIVIDER***
14 DNS(33,1H)=DNS(33,1H)
0007600 DNSS(30, IH) = DNSS(1H)
0007620 15 DNSS(31, IH) = DNSS(30, IH)
0007640 P(30) = P(29)
0007660 P(33) = P(29)
0007680 C CALL. THE 33RD FLOW COMP. UNDER THESE ASSUMPTION:
0007700 C (1). COMPLETE COMBUSTION
0007720 DNSS(33, 2) = (1. + EXT * 0.01) * (DNSS(14, 3) + DNSS(14, 5)) / 2. + CK * DNSS(14, 1) - 1
0007740 1
0007750 DNSS(33, 7) = DNSS(33, 2) * 3.76
0007770 DNSS(33, 6) = (DNSS(33, 2) + DNSS(33, 7)) * 28.8 * WAT / 18.
0007780 T(33) = TAT
0007800 DO 16 II = 1, I
0007820 DNSS(11, II) = DNSS(14, 11)
0007840 16 DNSS(15, II) = DNSS(33, II)
0007860 C MIXER**
0007880 CALL DMIX (DNS1, DNSS2, DNS5, T(14), T(33), T(15), I, P(14), P(33), POUT)
0007900 P(15) = POUT
0007920 DO 17 II = 1, I
0007940 DNSS(16, II) = DNSS(15, II)
0007960 17 DNSS(16, 1J) = DNSS(15, 1J)
0007980 C CALL. THE COMP. OF 17TH FLOW UNDER THE SAME ASSUMPTION AS BEFORE
0008000 C IF (IFUEL_NE.3) DNSS(17, 4) = DNSS(15, 3) + DNSS(15, 4) + DNSS(15, 1)
0008020 IF (IFUEL_EQ.3) DNSS(17, 4) = DNSS(15, 3) + DNSS(15, 4) + 7. * DNSS(15, 1)
0008040 IF (IFUEL_EQ.3) DNNS(17, 6) = DNSS(15, 6) + DNSS(15, 6) + 2. * DNSS(15, 1)
0008060 IF (IFUEL_EQ.3) DNSS(17, 6) = DNSS(15, 6) + DNSS(15, 6) + 6. * DNSS(15, 1)
0008080 DNSS(17, 2) = DNSS(15, 2) - 0.5 * (DNSS(15, 3) + DNNS(15, 5)) - CK * (DNSS(15, 1))
0008100 0008120 C CAL. THE TEMP. OF 21ST FLOW
0008140 DO 18 IK = 1, I
0008160 DNSS(18, IK) = DNSS(17, IK)
0008180 DO 19 IK = 1, I
0008200 DNSS(19, IK) = DNSS(18, IK)
0008220 DO 20 IK = 1, I
0008240 20 DNSS(20, IK) = DNSS(19, IK)
0008260 18 CONTINUE
0008280 19 DNSS(21, IL) = DNSS(20, IL) + DNSS(32, IL)
0008300 TDNSS(21) = 0.
0008320 DO 20 IM = 1, I
0008340 20 TDNSS(21) = TDNSS(21) + DNSS(21, IM)
0008360 C CAL. TEMP. OF 26TH FLOW
0008380 26 CONTINUE
0008400 C ASSUMPTION:
0008420 C (1). SATURATED PRESSURE IS ESTIMATED BY (EXP(A-B/T))
0008440 C (2). UNDER SATURATED CONDITION
0008460 C ASSUMPTION:
0008480 C ASSUME THE PRESSURE OF 26TH FLOW IS IDENTICAL TO 25TH FLOW (THE PRESS.
0008500 C DROP IS SMALL
0008520 P(25) = PPOP*1.0005
0008540 P(26) = P(25)
0008560 T(26) = B/A - ALOG(P(26))
0008580 DNSS(26, 6) = DNSS(11, 1) * SHRA
0008600 C DO 21 IN = 1, I
0008620 21 DNSS(25, IN) = DNSS(26, IN)
0008640 C DO 22 IO = 1, I
0008660 22 DNSS(27, IO) = DNSS(26, IO)
0008680 21 CONTINUE
0008700 22 CONTINUE
000860 IF (IFUEL.NE.2) DNSS(3,I9)=DNSS(2,I9)*DNSS(27,I9)
000870 IF (IFUEL.EQ.2) DNSS(3,I9)=DNSS(2,I9)*DNSS(26,I9)
0008720 IF (IFUEL.NE.2) DNSS(4,I9)=DNSS(3,I9)
0008740 IF (IFUEL.EQ.2) DNSS(4,I9)=DNSS(3,I9)
0008760 IF (IFUEL.NE.2) DNSS(5,I9)=DNSS(4,I9)
0008780 23 CONTINUE
0008800 C ASSUME THE TEMP. AND PRESSURE OF 5TH FLOW
0008820 IF (IDIO.GT.11) GO TO 24
0008840 IF (IFUEL.EQ.1) T(5)=1110.88
0008860 IF (IFUEL.EQ.2) T(5)=661.59
0008880 IF (IFUEL.EQ.3) T(5)=1052.
0008900 P(5)=PDR
0008920 24 CONTINUE
0008940 IF (IDIO.GT.11) GO TO 25
0008960 C ASSUME THE TEMP. OF 18TH FLOW
0008980 IF (IFUEL.EQ.1) T(18)=1222.
0009000 IF (IFUEL.EQ.2) T(18)=863.88
0009020 IF (IFUEL.EQ.3) T(18)=1398.94
0009040 C DESIGN THE TUBE TO LET PRESSURE DROP THROUGH BURNER BE 6%
0009060 25 CONTINUE
0009080 P(16)=P(15)*0.99
0009100 C DESIGN THE TUBE TO LET PRESSURE DROP THROUGH REFORMER TO BE 5%
0009120 P(18)=P(17)*0.95
0009140 26 CONTINUE
0009160 C -4**
0009180 DO 27 IR=1,I
0009200 DNSS(IR)=DNSS(19,IR)
0009220 DNSS(19)=DNSS(17,19)
0009240 27 CONTINUE
0009260 C E-***
0009280 PT=P(5)
0009300 PS=P(16)
0009320 IF (IFUEL.NE.2) CALL HEXC(T(18),DNSS,DNSC,T(4),T(19),T(5),QT,1,HA-
0009340 1(3),3,2,I,PT,PS,NT(3),IFUEL)
0009360 IF (IFUEL.EQ.2) CALL HEXC(T(18),DNSS,DNSC,T(3),T(19),T(5),QT,1,HA-
0009380 1(3),3,2,I,PT,PS,NT(3),IFUEL)
0009400 IF (IFUEL.NE.2) P(4)=PT
0009420 IF (IFUEL.EQ.2) P(3)=PT
0009440 P(20)=PS
0009460 P(16)=P(17)
0009480 605 P(16)=PT
0009500 P(20)=PS
DO 28 IS=1,I
   DNS(IS)=DNS(I6,IS)
   CALL FLAME (DNS,T(16),T(17),I,IFUEL)
28
DO 29 IT=1,I
   DNS(17,IT)=DNS(IT)
29
IF (IFUEL.NE.1) GO TO 33
C REFORMER(METHANE)***
000940 C     NOR=DNSS(1,1)/50.
000980 DO 30 IU=1,I
001000 DNSR(IU)=DNSS(5,1U)/653.6/NOR
001040 CALL KREF(DNSR,DNSF,DX1,DX2,DX3,P(5),T(5),T(17),Z,P(7),T(7))
30
C TEST THE ASSUMPTION OF 16TH FLOW
001080 C     IF (ABS(TTEST-T(18))/(TTEST+T(18)).LT.ERR) GO TO 31
001000 T(18)=TTEST
001040 GO TO 25
001060 DO 32 IV=1,I
001100 DNSH(IV)=DNSS(7,IV)
32
C CAL. PRESSURE DROP
001160 DNS(1,IV)=DNS(6,1V)
001200 CALL ENRE(DNS,TOPR,POPR,T(6),T(7),I,IFUEL)
001240 GO TO 25
001260 DO 35 IX=1,I
001300 DNSS(6,IX)=DNSS(16,IX)
35
C REFORMER(METHANOL AND NAPHTHA)***
001360 C     P(18)=(P(18)+PTEST)/2.
001400 GO TO 25
001460 P(18)=PTEST
001500 GO TO 39
001540 QQT(6)=QT
001580 T(18)=TTEST
001600 P(18)=PTEST
C CAL. PRESSURE DROP
001640 EFF(6)=HE
001680 DNS(6,IX)=DNSS(16,IX)
001700 C REFORMER(METHANOL AND NAPHTHA)***
001740 C     DO 37 IY=1,I
001780 DNS(6,1Y)=DNSS(6,1Y)
001820 CALL ENRE(DNS,TOPR,POPR,T(6),T(7),I,IFUEL)
001860 QQT(6)=QT
001900 T(18)=TTEST
001940 P(18)=PTEST
001980 EFF(6)=HE
002020 DNSS(6,IX)=DNSS(16,IX)
002060 DNSS(7,IX)=DNSS(16,IX)
002100 C CAL. PRESSURE DROP
002140
CALL P0SH(DNS,P(6),P(7),TOPR,2,IFUEL)
0010640 IF(IFUEL.EQ.2) GO TO 56
0010660 IF(IFUEL.EQ.1) CALL HEXC(T(7),DNSH,DNSC,T(3),T(8),T(4),QT,1,HA(2),-
0011020 12,1,PT,FS,NT(2),IFUEL)
0011040 IF(IFUEL.EQ.3) CALL HEXC(T(7),DNSH,DNSC,T(3),T(9),T(4),QT,1,HA(2),-
0011060 12,1,PT,FS,NT(2),IFUEL)
0011080 P(3)=PT
0011100 IF(IFUEL.EQ.1) P(8)=PS
0011120 IF(IFUEL.EQ.3) P(9)=PS
0011140 EFF(2)=HE
0011160 QGT(2)=QT
0011180 DO 41 IBB=1,1
0011200 IF(IFUEL.EQ.4) DNNS(8,IBB)=DNSH(IBB)
0011220 IF(IFUEL.EQ.3) DNNS(9,IBB)=DNSH(IBB)
0011240 41 DNNS(4,IBB)=DNSC(IBB)
0011260 IF(IFUEL.EQ.3) GO TO 46
0011280 C HIGH TEMP. SHIFT CONVERTER***
0011300 TOPHS=T(8)
0011320 42 CONTINUE
0011340 P0PHS=P(8)
0011360 DO 43 ICC=1,1
0011380 43 DNSH(ICC)=DNNS(8,ICC)
0011400 CALL ENSH(DNS,T(8),T(9),TOPHS,P0PHS,I,IP,FUEL)
0011420 P(9)=P0PHS
0011440 TM=(T(9)+T(8))/2.
0011460 IF((IP.EQ.2).OR.(ABS((TM-TOPHS)/(TM+TOPHS)),LT.ERR)) GO TO 44
0011480 TOPHS=TM
0011500 GO TO 42
0011520 44 CONTINUE
0011540 DO 45 IDD=1,1
0011560 45 DNSS(9,IDD)=DNNS(9)
0011580 46 CONTINUE
0011600 DO 47 IEE=1,1
0011620 DNSS(IEE)=DNSS(9,IEE)
0011640 47 DNSS(IEE)=DNSS(1,IEE)
0011660 IF(IFUEL.EQ.3) GO TO 48
0011680 C E-1(METHANE AND NAPHTHA)**
0011700 PT=P(1)
0011720 PS=P(9)
0011740 CALL HEXC(T(9),DNSH,DNSC,T(1),TH0,TCO,QT,1,HA(1),1,1,1,PT,PS,NT(1-
0011760 1),IFUEL)
0011780 P(10)=PS
0011800 P(2)=PT
0011820 EFF(1)=HE
0011840 QGT(1)=QT
0011860 T(2)=TCO
0011880 T(10)=TH0
0011900 GO TO 52
0011920
0011940
CONTINUE

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

TO 400

K FOR NAPHTHA FUEL

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

1)*VHNA+HCAS(1)\*(T(2)-T(1))+HCBS(1)\*(T(2)**2-T(1)**2)/2.+HCCS(1)\*(T-

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

ASSUME EFFICIENCY OF H-E 1 IS 0.7

EFF(1)=0.7

HA(1)=C rating\*(QQT(1)/EFF(1)\*\((T(9)-T(1)))/U

ASSUME AVERAGE TEMP. OF HOT SIDE

TAVG=T(9)-50.

CHH=0.

DO 50 IB=1,I

50 CHH=CHH+DNSS(9,IB)\*(HCAS(IB)+HCBS(IB)*TAVG+HCCS(IB)*TAVG**2)

T(10)=T(9)-QQT(1)/CHH

TEST THE ASSUMPTION OF AVERAGE TEMP.

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

10 TO 51

TAVG=(T(9)+T(10))/2.

GO TO 49

51 CONTINUE

ASSUME PRESSURE DROP IS NEGLECTABLE

P(2)=P(1)

P(10)=P(9)

DO 53 IFF=1,I

53 DO 55 IGG=1,I

55 CONTINUE

GO TO 60

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-

11,NT(9),IFUEL)

IS,NT(9),IFUEL)

P(1)=PS

P(27)=PT

EFF(9)=HE

QQT(9)=QT

DO 55 INH=1,I

DNSH(11,INH)=DNSH(INH)

DNSH(9,INH)=DNSC(INH)

DNSH(9,2,INH)=DNSS(9,2,INH)

DNSH(9,2,INH)=DNSS(9,2,INH)

55 CONTINUE

GO TO 60

E=1 METHANOL***

DO 56 III=1,I

56 DNSH(III)=DNSS(7,III)

DO 57 DNSC(III)=DNSS(1,III)

PT=P(1)

PS=P(7)
CALL HEXC (T(7),DNSH,DNSC,T(1),THO,TCO,GT,1,HA(1),1,1,1,PT,PS,NT(1-
001300 1),IFUEL)
001300 PTE=PS
001300 P(2)=PT
001300 EFF(1)=HE
001310 QTT(1)=QT
001310 DO 58 IJJ=1,I
001310 DNS(2,IJJ)=DNS(IJJ)
001310 T(2)=TCO
001310 T(13)=THO
001310 DNS(IJJ)=DNS(2,IJJ)
001320 DO 59 IJJ=1,I
001320 CONTINUE
001320 C MIXER**
001330 CALL OMIX (DNSH,DNSC,DNS,T(~),T(~),PTES~,I,P(~),P(~),PTEST)
001330 GO TO 61
001340 C TEST TEMP. OF 3RD FLOW
001340 IF ((ABS((TESTT-T(3))/TESTT+T(3)).LT.ERR).AND.((ABS((PTEST-P(3))/-
001350 1(PTEST+P(3))).LT.ERR)) GO TO 70
001340 IF (IFUEL.EQ.2) GO TO 66
001340 C E-2***
001340 DO 62 IKK=1,I
001340 DNS(3,IKK)=DNS(IKK)
001350 DNSH(IKK)=DNS(7,IKK)
001350 DNSC(IKK)=DNS(3,IKK)
001350 P(3)=(P(3)+PTEST)/2.
001350 T(3)=(TESTT+T(3))/2.
001350 P=P(3)
001360 PS=P(7)
001360 IF (IFUEL.EQ.3) GO TO 63
001360 CALL HEXC (T(7),DNSH,DNSC,T(3),T(8),T(4),GT,1,HA(2),2,1,1,PT,PS,NT-
001360 1(2),IFUEL)
001360 P(4)=PT
001370 P(8)=PS
001370 DO 64 ILL=1,I
001370 DNS(4,ILL)=DNSC(ILL)
001380 DNSH(ILL)=DNSH(18,ILL)
001390 DNSC(ILL)=DNS(4,ILL)
001390 PT=P(4)
001390 PS=P(18)
001390 CALL HEXC (T(10),DNSH,DNSC,T(4),T(19),T(5),GT,1,HA(3,3,1,1,PT,PS,-
001390 1NT(3),IFUEL)
001400 P(5)=PT
001400 P(19)=PS
001400 DO 66 IMM=1,I
001400 GO TO 66
001400 66
DNSS(3,IMM)=DNS(IMM)
DNSSH(IMM)=DNSS(18,IMM)

67 DNSC(IMM)=DNSS(3,IMM)
T(3)=T(3)+TESTT/2.
PT=P(18)
PS=(P(3)+PTEST)/2.
CALL HEXC(T(18),DNSH,DNSC,T(3),T(19),T(5),QT,1,HA(3),3,1,PT,PS,-
IMT(3),IFUEL)
P(19)=PT
P(5)=PS
EFF(3)=HE
QQT(3)=QT
DO 69 INN=1,1
DNSC(INN)=DNSS(INN)
IDNO=IDNO+1
GO TO 24

70 CONTINUE
IF (IFUEL.EQ.2) GO TO 77
DO 71 Ipp=1,I
DNSH(IPP)=DNSS(11,IPP)
DNSC(IPP)=DNSS(30,IPP)

C E-6***
PT=P(30)
PS=P(11)
CALL HEXC(T(11),DNSH,DNSC,T(30),T(12),T(31),QT,1,HA(6),6,1,PT,-
P(12)=PS
TEST=PT

C TEST THE PRESSURE OF 31ST FLOW
IF (ABS((PTEST-P(31))/(PTEST+P(31)))/LT.ERR) GO TO 72
GO TO 8

72 EFF(6)=HE
QQT(6)=QT
DO 73 IQQ=1,I
DNSH(IQQ)=DNSH(IQQ)
DNSC(IQQ)=DNSC(IQQ)

C LOW TEMP. SHEFT CONVERTER***
TOPLS=T(12)
POPLS=P(12)

C 74 CONTINUE
DO 75 IRR=1,I
DNSH(IIRR)=DNSH(12,IRR)
DNSC(IIRR)=DNSC(12,IRR)
CALL ENSH(DNSH,T(12),T(13),TOPLS,POPLS,I,IP,IFUEL)
TM=(T(12)+T(13))/2.
IF (((IP.EQ.2).OR.(ABS((TM-TOPLS)/(TM+TOPLS)).LT.ERR)) GO TO 76
TOPLS=TM

C DO 76 CONTINUE
77 DO 78 ISS=1,I
IF (((IFUEL.NE.2).AND.(DNSH(ISS).LT.0.50).AND.(DNSC(ISS).LT.0.50)-
0.50)) GO TO 78
IF (((IFUEL.EQ.2).AND.(DNSH(ISS).LT.0.50).AND.(DNSC(ISS).LT.0.50)-
0.50))
IF ((IFUEL.NE.2).AND.(ABS((DNS11SS)-DNSS(13,ISS))/(DNS(ISS+DNSS(1-015200 13,ISS)))).LT.ERR)) GO TO 78
0015220 IF ((IFUEL.EQ.2).AND.(ABS((DNSH(ISS1-DNSS(~~IISS))/(DNSH(ISS)+DNSS-0015240 l(l3vISS))).LT.ERR)) GO TO 78
0015260 GO TO 79
0015280 78 CONTINUE
0015300 IF (IFUEL.EQ.2) POPLS-PTE
0015320 IF (ABS((POPLS-P(13))/(POPLS+P(13))).LT. ERR
0015340 GO TO 81
0015360 DO 80 ITT=1,1
0015380 IF (IFUEL.EQ.2) DNS(~~IITT)=(DNSS(13,ITT)+DNSS(IITT))/2.
0015400 IF (IFUEL.NE.2) DNS(~~IITT)=(DNSS(13,ITT)+DNSS(IITT))/2.
0015420 P(13)=(POPLS+P(13))/2.
0015440 GO TO 7
0015460 DO 82 IUU=1,1
0015480 IF (IFUEL.EQ.2) DNS(13pIUU)=DNSH(IUU)
0015500 IF (IFUEL.NE.2) DNS(13,IUU)=DNSH(IUU)
0015520 TDN13=0.
0015540 DO 83 IVV=1,1
0015560 DNS13=DNS13*DNSS(13,IW)
0015580 FD=DNSS(13,IVV)
0015600 FC=DNSS(13,IVV)
0015620 DNS(13,IVV)=DNS(13,IVV)
0015640 DNSC(13,IVV)=DNS(13,IVV)
0015660 C FUEL CELL ENERGY BALANCE***
0015680 AREAF=FUEL*AIRL*30.48**2
0015700 CD=CD/1000.
0015720 OU=1./(EXA*0.01+1.)
0015740 CALL ENFU(DNSAN,DNSCA,T(31),T(31),TOUT,POPFC,POPF,UT,1,I,QL, -
0015760 W1K,O,U,CD,CL,IFUEL
0015780 C QRT=QL
0015800 C CALCULATE THE OUTPUT OF AC POWER
0015820 AC=((-0.10146+SQRT(1.0146**2-4.*0.0456/108.*0.0472*108.-WK))) -
0015840 1/(2.*0.0456/108.)
0015860 DO 86 IYY=1,1
0015880 DNSC(IYY)=DNSH(25,IYY)
0015900 DO 87 IZZ=1,1
0015920 DNS1IZZ)=DNSH(20,IZZ)
0015940 DNS2(IZZ)=DNS(32,IZZ)
0015960 C MIXER***
0015980 CALL DMIX (DNS1,DNS2,DNS(T(31),T(31),TOUT,I,P(20),P(32),POUT)
0016000 P(21)=POUT
0016020 DO 88 II=1,1
0016040 DNSH(21,II)=DNS(II)
0016060 DNSH(21,II)=DNSH(21,II)
0016080 T(21)=TOUT
0016100 C ASSUME
0016120 P(22)=P(21)*1.001
0016140 60 T(22)=-6/(ALOG((DNSH(1,1)*SMRA-DNSS(21,6))/(DNSH(1,1)*SMRA- -
0016160 1/TONSS(21))*P(22))
0016180 C E-10***
0016200 T(25)=T(22)
0016220 CALL CDPH (QRT,T(25),T(26),DNSC,P(25),I,QL)
0016240 QQT(7)=QRT
0016260 C ASSUME HOT WATER IS FEEDING IN AT 3330K AND FEEDING OUT AT 355 K
0016280 DNSS(34,6)=QQT(7)/(355.0-333.0)/1.0/10.
0016300 DNSS(35,6)=DNSH(34,6)
0016320 T(34)=333.
0016340 T(35)=355.
0016360 P(34)=PAT
0016380 P(35)=PAT
0016400 C E-5***
0016420 CALL COND(T(21),T(22),DNSH,QT,HCH,I)
0016440 G1T(5)=QT
0016460 C ASSUME HOT WATER IS FEEDING IN AT TAT AND FEEDING OUT AT 3550K
0016480 DTL=((T(21)-355.0)-(T(22)-TAT))/ALOG((T(21)-355.0)/(T(22)-TAT))
0016500 T(36)=TAT
0016520 T(37)=355.
0016540 P(36)=PAT
0016560 P(37)=PAT
0016580 DNSS(36,6)=QQT(5)/1.0/(355.0-TAT)
0016600 DNSS(37,6)=DNSH(36,6)
0016620 C ASSUME E-5 IS THE TYPE OF COUNTERFLOW
0016640 HA(5)=QQT(5)/U/1.0/DTL
0016660 THM=(T(36)+T(37))/2.
0016680 TCM=(T(22)+T(21))/2.
0016700 CALL HEPD(DNSH,DNSH,THM,TCM,HA(5),P(21),P(36),5,DPJ,DP,NT,T(22),-)
0016720 IT(21).4)
0016740 P(22TE)=P(21)-DPJ
0016760 IF(ABS(P(22TE)-P(22))/(P(22TE)+P(22)).LT.ERR) GO TO 603
0016780 P(22)=(P(22)+P(22TE))/2.
0016800 GO TO 602
0016820 603 DO 89 IZ=1,I
0016840 DNSS(22,I2)=DNS(22)
0016860 89 DNSS(I2)=DNSH(22,I2)
0016880 C SEPARATOR***
0016900 POPSP=P(22)
0016920 CALL SEPAR(T(22),POPS,T(23),T(24),DNS,DNSL,DNSV,I)
0016940 DO 90 IZ=1,I
0016960 DNSS(24,IZ)=DNSL(IZ)
0016980 90 DNSS(23,IZ)=DNSV(IZ)
0017000 P(24)=POPS
0017020 P(23)=POPS
0017040 C PUMP***
0017060 DO 901 I4=1,I
0017080 901 DNSS(I4)=DNSH(24,I4)
0017100 CALL PUMP(DNS,T(24),T(25),P(24),P(25),POWS,I)
0017120 DO 92 IB=1,39
0017140 TDNS(IB)=0.
0017160 DO 91 IA=1,I
0017180 TDNS(IB)=TDNS(IB)+DNS(IB,IA)
0017200 91 CONTINUE
0017220 92 CONTINUE
0017240 C WRITE THE RESULT
0017260 IF(IFUEL.EQ.1) WRITE (6,108) SMRA
0017280 IF(IFUEL.EQ.2) WRITE (6,109) SMRA
0017300 IF(IFUEL.EQ.3) WRITE (6,110) SMRA
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)
0017360 IF (IFUEL.NE.2) WRITE (6,105) TOPHS,P(13),T(12),T(13)
0017380 WRITE (6,106) T(22),POPS
0017400 WRITE (6,108) FCO
0017420 WRITE (6,111) TOPFC,POPFC,E,VOP,CD,CL,UT,OU
0017440 WRITE (6,102) EFT,EI,ET,EC
0017460 WRITE (6,107) EFC
0017480 WRITE (6,108) WXpqRT
0017490 WRITE (6,111) AC
0017500 WRITE THE MATERIAL IN JTH FLOW
0017520 IF (IFUEL.EQ.1) WRITE (6,94)
0017530 IF (IFUEL.EQ.2) WRITE (6,95)
0017540 IF (IFUEL.EQ.3) WRITE (6,96)
0017540 IF (IFUEL.EQ.1) WRITE (6,93) (((J,(DNSS(J,IA),IA=1,10),T(1),P(J)),J=1,5),((II,(DNSS(II,IA),IA=1,10),T(1),P(II)),II=1,5)
0017540 2=7,37))
0017570 IF (IFUEL.EQ.3) WRITE (6,93) (((J,(DNSS(J,IA),IA=1,10),T(1),P(J)),J=1,5),((II,(DNSS(II,IA),IA=1,10),T(1),P(II)),II=1,5)
0017570 2=7,37))
0017580 WRITE THE EFFICIENCY OF HEAT EXCHANGER
0017590 WRITE (6,113)
0017590 WRITE (6,112)
0017590 WRITE (6,111)
0017590 WRITE (6,97)
0017590 WRITE (6,98) (QQT(IA),IA=1,10)
0017590 C WRITE SURFACE AREA OF HEAT EXCHANGER
0017590 WRITE (6,112)
0017590 WRITE (6,97)
0017590 WRITE (6,98) (HA(IA),IA=1,10)
0018000 C WRITE THE EFFICIENCY OF HEAT EXCHANGER
0018010 WRITE (6,113)
0018020 WRITE (6,97)
0018020 WRITE (6,98) (EFF(IA),IA=1,10)
0018030 IF (IFUEL.EQ.1) WRITE (6,114) POKA,POW,POWS
0018040 IF (IFUEL.EQ.2) WRITE (6,115) POKA,POW,POWS
0018050 IF (IFUEL.EQ.3) WRITE (6,116) POKA,POW,POWS
0018060 STOP
0018200 94 FORMAT (1X,'STREAM METHANE OXYGEN CAR. MONOXIDE CAR. DIOXIDE')
0018240 HYDROGEN WATER NITROGEN FLOW RATE TEMP.(K) PRE.(ATM)'
0018260 HYDROGEN WATER NITROGEN FLOW RATE TEMP.(K) PRE.(ATM)'
0018280 HYDROGEN WATER NITROGEN FLOW RATE TEMP.(K) PRE.(ATM)'
0018300 HYDROGEN WATER NITROGEN FLOW RATE TEMP.(K) PRE.(ATM)'
0018340 HYDROGEN WATER NITROGEN FLOW RATE TEMP.(K) PRE.(ATM)'
0018360 97 FORMAT (1X,'E-1 1 E-2 E-3 E-4 E-5 E-6 E-7 E-8 E-9 E-10')
0018380
The document contains formatted text that appears to be part of a computer program or algorithm, likely written in a programming language. The text includes various codes and mathematical expressions. The original context of the document is not clear from the text alone.
0020100 C***********************************************************************
0020200 C
0020300 C ASSUMPTION:
0020400 C
0020500 C (1) THE COMBUSTION IS COMPLETE
0020600 C X: THE AMOUNT OF O2 REACTED
0020700 C XY: THE AMOUNT OF CO2 PRODUCED
0020800 C Y: THE AMOUNT OF H2O PRODUCED
0020900 C IJ: 1 = METHANE AS INPUT GAS
0021000 C 2 = METHANOL AS INPUT GAS
0021100 C 3 = NAPHTHA AS INPUT GAS
0021200 C
0021300 DIMENSION DNS(I)
0021400 C
0021500 C CALCULATE THE NECESSARY AMOUNT OF O2
0021600 C IF(IJ.EQ.3) GO TO 4
0021700 IF(IJ.EQ.2) GO TO 2
0021800 X=1./2.*DNS(3)+1./2.*DNS(5)+2.*DNS(I)
0021900 GO TO 3
002200 2 X=.5*DNS(3)+.5*DNS(5)+1.5*DNS(I)
0022100 GO TO 3
0022200 4 X=0.5*DNS(3)+0.5*DNS(5)+15.*DNS(I)
0022300 XY=DNS(3)+7.*DNS(1)
0022400 Y=DNS(5)+8.*DNS(I)
0022500 GO TO 5
0022600 3 CONTINUE
0022700 XY=DNS(3)+DNS(I)
0022800 Y=DNS(5)+2.*DNS(I)
0022900 C CALCULATE THE EXIT COMPOSITION
002300 5 DNS(I)=0.
0023100 DNS(3)=0.
0023200 DNS(5)=0.
0023300 DNS(2)=DNS(2)-X
0023400 DNS(4)=DNS(4)+XY
0023500 DNS(6)=DNS(6)+Y
0023600 RETURN
0023700 C SUBROUTINE CDPH(QTI,TCI,TCO,DNSC,P,I,QT)
0023800 C THIS SUBROUTINE IS TO CAL. THE ENERGY ANALYSIS FOR E-7 AND E-10
0023900 C DEFINITION:
002400 C QTI: TOTAL HEAT TRANSFER FROM FUEL CELL
0024100 C TCB: BOILING POINT OF FIXED PRESSURE
0024200 C DIMENSION GS(7),HS(7),HCAS(7),HCBS(7),HCCS(7)
0024300 C DIMENSION DNSC(I)
0024400 C COMMON /ETHDA/ GS,HS,HCAS,HCBS,HCCS
0024500 C COMMON/TC/TC/CONS/AB
0024600 C COMMON/U/L/U
0024700 C ASSUME THE SATURATED PRESSURE IS EXP(A-B/T)
0024800 C TCB=B/(A-ALGS(P))
0024900 C ASSUME THE SATURATED STEAM OUTPUT
002500 C TCB=TCB
0025100 C ASSUME THE LATENT HEAT CAL. BY WATSON CORRELATION
0025200 TCI=TCB/TC
0025300 C ASSUME THE AVERAGE HEAT CAPACITY OF WATER IS 1 CAL/G-K
0025400 QT=((1.-TCI)/(1.-0.577))*0.38*9700.0*DNSC(6)+*(TCB-TCI)*1.8.
0025500 1*DNSC(6)
SUBROUTINE COMP(DNS,TIN,TOUT,PIN,POUT,PW,GAG,I,IP)
C*******************************************************************************
C THIS SUBROUTINE CALCULATES THE BALANCE OF COMPRRESSOR
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
DIMENSION DNS(I)
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.)/(GAG-1.)
RETURN
2 TOUT=TIN
K'S=1.987*TIN*ALOG(POUT/PIN)
RETURN
END
SUBROUTINE COND(THI,THO,DNSH,QT,CH,I)
C*******************************************************************************
C THIS SUBROUTINE ESTIMATES THE HEAT DUTY IN THE CONDENSER
C DEFINITION IS THE SAME AS HEXC
DIMENSION GS(7),HS(7),HCAS(7),HCBS(7),HCCS(7)
DIMENSION DNSH(I)
COMMON /ETHDA/ GS,HS,HCAS,HCBS,HCCS
COMMON /TC/TI
THM=(THI+THO)/2.
C THE MEAN TEMP. OF HOT SIDE
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)+HCBS(IA)*(THI-THO)+HCCS(IA)*(THI*THI-THO*THO) -
SUGROUTINE CONV(XV,YV,NR,NC)

C THIS SUBROUTINE USES WESSTEIN METHOD FOR ALGEBRAIC CONVERGENCE

C DEFINITION:

C XV: TRAIL VALUE
C YV: CALCULATED VALUE
C NR: CONVERGE INDEX
C NC: CONVERGE INDEX
C NC=1 CONVERGE
C NC=2 NONCONVERGE

DIMENSION XA(2),YA(2)

IF(ABS((XV-YV)/(XV+YV))<0.001) GO TO 2

XT=(XA(NR)*YV-YA(NR)*XV)/(XA(NR)-XV+YV-YA(NR))

XA(NR)=XV
YA(NR)=YV
XV=XT
RETURN

1 XA(NR)=XV
YA(NR)=YV
RETURN

NC=2
RETURN

2 X=XT
RETURN

ENDIF

SUGROUTINE DIVID(TIN,TOUT1,TOUT2,DNS1,DNS2,GARM,1)

C THIS SUBROUTINE CALCULATES THE BALANCE AROUND THE DIVIDER

D !SIS(DNS1(DNS1)=GARM*DNS1(DNS1)

1 CONTINUE

DO 2 IA=1,1

2 CONTINUE

TOUT=TIN
TOUT2=TIN
RETURN

ENDIF

SUGROUTINE DMIX(DNS1,DNS2,DNS,TIN1,TIN2,TOUT,1,PIN1,PIN2,POUT)

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

FRACTION OF AVAILABLE H2O

UT: FUEL UTILIZATION
VOP: ACTUAL FUEL CELL POTENTIAL
LE: ELECTRICAL WORK
HLHV(1): LOWER HEAT VALUE OF GAS 1
DIHEXIS(GS,HS,HCAS,HCBS,HCCS)
DIHEXIS(HLHV)

VOP:

CALL VIEW(1,VOP,CDO,TOP,POP,PPH2,PPO2,PPHO,PPCO)

CAL. FREE ENERGY CHANGE AT FUEL CELL CONDITION
\[ DGR = -2 \times 2.306 \times E^{AHLU \times TONS} \]

CAL. THE EFFICIENCY

\[ EV = VOP/E \]

CAL. THE ELECTRICAL WORK

\[ KE = -EV \times EI \]

CAL. THE THERMODYNAMIC EFFICIENCY

\[ DH = -5778.9 + DCAS(1) \times (TOP - 298.1) + HCBS(5) - HCBS(1) + 0.5 \times HCBS(2) \]

IF (TOP \geq 463)

\[ OH = -5818.6 \times AHLU \]

ETH = DGR / DH

IF (I,J \geq 1)

\[ DHC = FNAP(1) + (HCAS(4) + 2. \times HCAS(6) - HCAS(1) - 1.5 \times HCAS(2)) \]

IF (I,J \geq 2)

\[ DHC = FNAP(1) + HCAS(4) \]

IF (I,J \geq 3)

\[ DHC = FNAP(1) \]

DO 3 I,J = 1,I

CONTINUE

DO 4 I,J = 1,I

CONTINUE

CALL FUCE(DNSAI, TOP, DNSA, DNSC, DNS, DSO, DSN, DHSO, UT, I, PINF, PINA, IJ)

DO 2 I,J = 1,I

CONTINUE

CALL FUCE(DNSAI, TOP, DNSA, DNSC, DNS, DSO, DSN, DHSO, UT, I, PINF, PINA, IJ)

DO 2 I,J = 1,I

CONTINUE

CALL FUCE(DNSAI, TOP, DNSA, DNSC, DNS, DSO, DSN, DHSO, UT, I, PINF, PINA, IJ)
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 CONV(TOUT, TOUTC, 1, NC)
GO TO (8, 6), NC

C THE OUTLET TEMP.

IF(M.EQ.1) GO TO 7

CALL CONV(TOUT, TOUTC, 1, NC)

GO TO (8, 6), NC

C THE TOTAL HEAT REJECTED PER HR.

C CONTINUE

C 8 CONTINUE

C END

C SUBROUTINE ENRE(DNS, TOP, POP, TIN, TOUT, I, IP, IJ)

C DIMENSION GS(71), HS(7), HCAS(7), HCBS(7), HCCS(7)

C STORE THE INLET COMPOSITION

DO 1 IA = 1, I

DINS(IA) = DIAS(IA)

1 CONTINUE

C 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

C CALCULATE THE ENTHALPY CHANGE WITH TEMP. OF INLET GAS

DIN = 0.

DO 3 IA = 1, I

IF(IP.EQ.0) GO TO 3

3 CONTINUE

C CALCULATE THE ENTHALPY CHANGE OF REACTION

IF(IJ.EQ.1)

10H1 = (HS(3) + 3. * HS(5) - HS(1) - HS(6)) * X(1)

IF(IJ.EQ.2)

10H2 = (HS(4) + 3. * HS(5) - HS(1) - HS(6)) * X(1)

IF(IJ.EQ.3)

10H1 = (HS(3) + 15. * HS(5) - HS(1) - 7. * HS(6)) * X(1)

IF(IJ.EQ.2)

10H2 = (HS(4) + 10. * HS(5) - HS(1)) * X(2)

IF(IJ.EQ.3)

10H2 = (HS(4) + HS(5) - HS(3) - HS(6)) * X(2)

IF(IJ.EQ.0)

10H1 = (HS(3) + 9. * HS(5) - HS(1) - HS(6)) * X(1)
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)*HCB(IA)
TCCS=TCCS+DNS(IA)*HC(S(IA)
4 CONTINUE
C CALCULATE THE MAX. TEMP. OF OUTLET GAS
TOUT=TOP-500.
5 TOUT=(-DH-DNIN-TCBS/2.)*(TOUT)**2-(298.1)**2)-TCCS/3.*(TOUT)**3 -
1-(298.1)**3)/TCAS+298.
CALL CONV(TOUT,TOUTC,1,NC)
GO TO (6,5,NC
6 CONTINUE
RETURN
END
C**************************************************************
C THIS SUBROUTINE CALCULATES THE ENERGY BALANCE OF SHIFT CONVERTER
C**************************************************************
DIMENSION DNS(7),HS(7),HCAS(7),HCB(7),HCCS(7)
DIMENSION DNS(7),DNS(7)
COMMON/ETHDA/ 65,HS,HCAS,HCBS,HCCS
C STORE THE INITIAL COMPOSITION
DO 1 IA=1,I
1 DNS(IA)=DNS(IA)
CALL PDSH(DNS,PIN,POUT,TOP,1,1)
POP=(PIN+POUT)/2.
C CALCULATE THE OUTLET COMPOSITION
CALL SHIFT(DNS,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
DNIN=0.
DO 3 IA=1,I
IF(DNS(IA).EQ.0.) GO TO 3
DNIN=DNIN+DNS(IA)*(H(CAS(IA))*(298.-TIN)+HCBS(IA)/2.*((298.)**2 -
1*(TIN)**2)+HCCS(IA)/3.*((298.1)**3)-(TIN)**3))
3 CONTINUE
C CALCULATE THE ENTHALPY CHANGE OF REACTION
DNH=(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)*HCB(IA)
TCCS=TCCS+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

EUDP
SUSROUTINE EUPK(NNS,TOP,SK,II)

C THIS SUBROUTINE CALCULATES THE EQUILIBRIUM CONSTANT

C R: GAS CONSTANT; G=CAL/G-MOLE/K
C TST: STANDARD TEMPERATURE; K

DIMENSION GS(7),HS(7),HCAS(7),HCBS(7),HCCS(7)
DIMENSION NNS(I)
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,I
IF(NNS(IA).EQ.0) GO TO 1
TCAS=TCAS+NNS(IA)*HCAS(IA)
TCBS=TCBS+NNS(IA)*HCBS(IA)
TCCS=TCCS+NNS(IA)*HCCS(IA)
1 CONTINUE

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

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

C CAL. HEAT CONST.
DO=DH-TCAS*TST-TCBS*TST**2/2.-TCCS*TST**3/3.

C CAL. CONST. AI
AI=(DH=DG-TCAS*TST-ALOG(TST)-TCBS/2.*TST**2-TCCS/6.*TST**3)/TST/R

C CAL. EQU. CCNST.
SK=EXP(-DH/R/TOP+TCAS/R*ALOG(TOP)+TCBS/2.*TOP/R+TCCS/6./R*TOP**2 - 1)*AI
RETURN
SUBROUTINE FLAME(DNS,TIN,TF,I,IJ)

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

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 1 ATM

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

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

C CALCULATE THE EXIT FLUID
CALL BURN(DINS,I,IJ)

C CALCULATE THE EXIT TEMPERATURE
TF=TIN+500.

6 TF=(6-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
C THIS SUBROUTINE CALCULATES THE MASS BALANCE OF FUEL CELL
C
C X : CONSUMPTION OF H2 IN THE FUEL CELL UNDER UT UTILIZATION
C
C DIMENSION GS(7),HS(7),HCAS(7),HCDS(7),HCCS(7)
C
C COMMON /EXA/,EXA,
C COMMON /HUMI/,WAT
C
C THIS SUBROUTINE CALCULATES THE PRESSURE DROP IN THE HEAT EXCHANGER
C
C DIMENSION FLI(7),CL(7),CM(7),WM(7),FLJ(7),CMJ(7),CI(7)
C
C COMMON /HEPT/,NP,NR,BSPAC,ODT,PITCH,CL,IDS,IDL,FLOAR,SURFC
C
C THIS SUBROUTINE CALCULATES THE NUMBER OF BAFFLES
C
C NT= HA /0.3048**2/NP/CLEN/SURFC
C
C COMMON /HUMI/,WAT
C    FAREA = IDS/(ODT*CL1*CL#BSPACE)
C    RATIO OF PITCH TRANSVERSE TO FLOW TO TUBE DIA.
C    XT = PITCH/ODT
C    FLI(1) = DNSA(1)/453.6
C    FLI(2) = DNSA(3)/453.6
C    FLI(3) = DNSA(4)/453.6
C    FLI(4) = DNSA(5)/453.6
C    FLI(5) = DNSA(6)/453.6
C    FLI(6) = DNSA(7)/453.6
C    FLI(7) = DNSA(2)/453.6
C    FI = FLI(1) + FLI(2) + FLI(3) + FLI(4) + FLI(5) + FLI(6) + FLI(7)
C    DO 1 I = 1, 7
C    CM(1) = FLI(1)/FI
C    1 CONTINUE
C    A&W = CM(1)*WM(1) + CM(2)*WM(3) + CM(3)*WM(4) + CM(4)*WM(6) + CM(5)*WM(5)
C    1+CM(6)*WM(7) + CM(7)*WM(2)
C    TF = (TH - 273.16) * 1.8 + 32.
C    CALL CMASS(CFLI, FI)
C    ANUI = VIS(C, TF, FLI)
C    RHO = (A&W*PINS)/(0.7302*(TF*660.))
C 0076500 C CAL. SHELLSIDE MASS VELOCITY ACROSS TUBES
C    GS = FI*AKA/FAREA
C 0076810 C CAL. FRICTION FACTOR
C    FFPJ = SS0*(ODT*GS/AMUI)**1.051
C 0073300 C CAL. PRESSURE DROP OF SHELL SIDE FLOW
C    DP = B0*2.*FPRI*NR*GS**2/32.174/3600.*2/116.2
C 0079400 2 CONTINUE
C    CMJ(JJ) = FLI(JJ)/FJ
C    3 CONTINUE
C    A&W = CM(1)*WM(1) + CM(2)*WM(3) + CM(3)*WM(4) + CM(4)*WM(6) + CM(5)*WM(5)
C    1+CM(6)*WM(7) + CM(7)*WM(2)
C    DT = DTH + (THM - TCM)
C    TWF = (TH - 273.16)*1.8 + 32.
C    TCF = (TCM - 273.16)*1.8 + 32.
C    CALL CMASS(CJ, FLJ, FJ)
C    AMJ = VIS(CJ, TCF, FLJ)
0081500 AMU=VIS(CJ,TWF,IJ)
0081600 IF((AMU.LE.0.) OR (AMU.LE.0.)) GO TO 10
0081700 TKC=THC(CJ,TCF,IJ)
0081800 CP=HTC(CJ,TCF,IJ)
0081900 AROH=(AMU*PINT/(TCF+460.))
008200 GJ=AMU/FLOR/NT
0082100 REJ=AMU/NT
0082200 IF(REJ.LE.2100.)GO TO 4
0083000 SF=0.046/REJ**0.2
0083200 SF=16./REJ
0083400 CONTINUE
0083600 IF(SF2TS1.GT.0.7151)GO TO 6
0083700 CKC=0.4*(1.25-S2TS1)
0083800 CKC=0.75*(1.-S2TS1)
0083900 IF(REJ.GT.2100.)GO TO 8
0084000 PHI=1.11*AMU/AMU**0.25
0084100 PHI=1.11*AMU/AMU**0.25
0084200 BI=1.4*CKC/14./AMU**0.6667
0084300 DPJ: BI*2.*SF*GJ**2.*CLEN*NP/32.17/3600.*2/AROH/IDT/FH1/4./SF
0084400 WRITE(6,11)
0084500 FORMAT('THE TRYING TEMP. IS BELOW THE LIMIT OF CAL. VISCOSITY')
0084600 CONTINUE
0084700 RETURN
0084800 END
0085000 C**********************************************
0085200 C THIS SUBROUTINE IS TO CAL. THE ENERGY ANALYSIS FOR HEAT EXCHANGER
0085300 C*****************************************************************
0085400 C CC: CAPACITY RATE OF FLUID ON COLD SIDE ,DNSH*CPH
0085500 C CH: CAPACITY RATE OF FLUID ON HOT SIDE, DNSH*CPH
0085600 C CMAX: MAX. CAPACITY RATE
0085700 C CMIN: MIN. CAPACITY RATE
0085800 C CPC: SPECIFIC HEAT OF COLD SIDE FLUID
0085900 C CHPC: SPECIFIC HEAT OF HOT SIDE FLUID
0086000 C HE: HEAT EXCHANGER EFFECTIVENESS
0086100 C GT: TOTAL HEAT TRANSFER RATE ACROSS HEAT EXCHANGER
0086200 C GMAX: THE MAX. HEAT TRANSFER RATE ACROSS HEAT EXCHANGER
0086300 C TCI: COLD SIDE INLET TEMPERATURE
0086400 C TCO: COLD SIDE OUTLET TEMPERATURE
0086500 C THI: HOT SIDE INLET TEMPERATURE
0086600 C TDO: HOT SIDE OUTLET TEMPERATURE
0086700 C UA: OVERALL HEAT TRANSFER CCEFFICIENT OF EXCHANGER
0086800 C MOD: TYPE OF HEAT EXCHANGER
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006900 C MOD=1 COUNTERFLOW
007000 C MOD=2 CROSS FLOW
007100 C MOD=3 CONDENSER
007200 C THM: MEAN TEMP. OF HOT SIDE
007300 C TCM: MEAN TEMP. OF COLD SIDE
007400 C N: THE NUMBER OF HEAT EXCHANGER
007500 C M: THE INDEX OF INITIAL CONDITION
007600 C M=2 TEMP. OF BOTH SIDES ARE KNOWN
007700 C M=1 TEMP. OF HOT SIDE INLET AND COLD SIDE OUTLET ARE KNOWN
007800 DIMENSION GS(7),HS(7),HCAS(7),HCBS(7),HCCS(7)
007900 DIMENSION DNSH(7),DNSC(7)
008000 COMMON /ETHDA/ GS,HS,HCAS,HCBS,HCCS
008100 COMMON /UI/ U
008200 COMMON /CH/ CN
008300 COMMON /HE/ HE
008400 C ASSUME THE MEAN TEMP. AT COLD AND HOT SIDE
008500 IF(M.EQ.2) GO TO 1
008600 THM=(THI+10.+TCI)/2.
008700 TCM=(THI-10.+TCI)/2.
008800 GO TO 2
008900 1 THM=(THI+TCO-50.)/2.
009000 TCM=(TCO*2.-200.)/2.
009100 C CAL. CC AND CH
009200 2 CC=0.
009300 CH=0.
009400 DO 4 IA=1,I
009500 IF(DNSC(IA).EQ.0.) GO TO 3
009600 CC=CC+DNSC(IA)*HCAS(IA)*HCBS(IA)*TCM+HCCS(IA)*TCM**2)
009700 3 IF(DNSH(IA).EQ.0.) GO TO 4
009800 CH=CH+DNSH(IA)*HCAS(IA)*HCBS(IA)*THM+HCCS(IA)*THM**2)
009900 4 CONTINUE
010000 C CHOOSE THE CMAX ,CMIN.
010100 IF(CC.GT.CH) GO TO 5
010200 CMAX=CH
010300 CMIN=CC
010400 GO TO 6
010500 5 CMAX=CC
010600 CMIN=CH
010700 6 CONTINUE
010800 HA=CC/CMIN/U
010900 UA=HA/U
010000 C CAL. THE HEAT EXCHANGER EFFECTIVENESS
010100 IF(MOD.GE.2) GO TO 8
010200 IF(ABS(CMIN/CMAX).GE.0.01) GO TO 9
010300 HE=1.-EXP(-UA/CMIN)
010400 GO TO 12
010500 7 HE=1.-EXP((-UA/CMIN)*(1.-CHIN/CMAX))/(1.-CMIN/CMAX)*EXP((-UA -
010600 1/CMIN)*(1.-CMIN/CMAX))
010700 GO TO 12
010800 8 IF(MOD.GT.2) GO TO 11
010900 IF(ABS(CMIN/CMAX-1.).GE.0.01) GO TO 9
011000 HE=(UA/CMIN)/(UA/CMIN+1.)
011100 GO TO 12
011200 9 IF(ABS(CMIN/CMAX).GT.0.01) GO TO 10
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HE=1.-EXP(-UA/CMIN)
GO TO 12
10 IF(CMIN.EQ.CH) HE=1.-EXP((-CMAX/CMIN)*(1.-EXP(-UA/CMA))
11 IF(CMIN.EQ.CH) HE=(CMAX/CMIN)*(1.-EXP((-CHAX/CMAX)*(1.-EXP(-UA/CMA))
12 IF(M.EQ.2) GO TO 13
13 TCI=(HE*(CMIN/CC)*THI-TCO)/((HE*(CMIN/CC)-1.)
14 IF(ABS((THO+THI)/2.-THM).LT.(ABS((THO+THI)/2.)+TMM)M0.005) -
15 IF(ABS((TCO+TCI)/2.-TCC).LT.(ABS((TCO+TCI)/2.)+TMM)M0.005)) -
16 PT=PT+DPJ
17 CONTINUE
18 RETURN
19 END
20 SUBROUTINE PDFU(DNSA,DNSC,DNS,DNSO,DNSO,DP,ATMP,PIHF,PHIA,IJ)
21 C********************************************************************
22 C THIS SUBROUTINE CALCULATES PRESSURE DROP IN THE FUEL CELL STACK
23 C********************************************************************
24 REAL L(2),DP(4)
25 DIMENSION FLI(7),C(7),CHI(7),WM(7),DNSA(7),DNSC(7),DNS(7),DNSO(7)
26 DIMENSION NTA(2), WIDA(2),D(2)
27 COMMON/PDFUT/,NTA,L,WIDA,NN
28 COMMON /HM/WK
29 COMMON C8(19),WM
30 C********************************************************************
31 C BASIS: NO. 522 STACK
32 C********************************************************************
33 IT=1
34 DO 1 IA=1,7
35 DNSII(IA)=0.
36 DNSII(4)=DNSO
37 DNSII(6)=DNS
38 DNSII(7)=DNSO
39 JJ=1
40 C CAL. THE PRESSURE DROP OF FUEL SIDE
41 CALL HEFD(DNSA,DNSC,DNS,DNSO,DNSO,DP,ATMP,PIHF,PHIA,IJ)
0097400  D(I)=WIDA(I)
0097500  FLI(1)=DNS(I)/453.6
0097600  FLI(2)=DNS(3)/453.6
0097700  FLI(3)=DNS(4)/453.6
0097800  FLI(4)=DNS(6)/453.6
0097900  FLI(5)=DNS(5)/453.6
0098000  FLI(6)=DNS(7)/453.6
0098100  FLI(7)=DNS(2)/453.6
0098200  GO TO 3
0098300  2 FLI(1)=DNSA(1)/453.6
0098400  FLI(2)=DNSA(3)/453.6
0098500  FLI(3)=DNSA(4)/453.6
0098600  FLI(4)=DNSA(6)/453.6
0098700  FLI(5)=DNSA(5)/453.6
0098800  FLI(6)=DNSA(7)/453.6
0098900  FLI(7)=DNSA(2)/453.6
0099000  3 CONTINUE
0099100  TK=ATMP
0099200  FI=FLI(1)+FLI(2)+FLI(3)+FLI(4)+FLI(5)+FLI(6)+FLI(7)
0099300  DO 4 I=1,7
0099400  CM(I)=FLI(I)/FI
0099500  4 CONTINUE
0099600  AM=CM(1)+AM(1)+CM(2)+AM(2)+CM(3)+AM(3)+CM(4)+AM(4)+CM(5)+AM(5)
0099700  CM=CM(6)+CM(7)+AM(6)+AM(7)
0099800  G=FI*AM(1)/WIDA(IT)*2/NP/NTA(IT)
0099900  TF=(IT-273.16)*1.8+32.
0100000  CALL CMSS(C,FLI,FI)
0100100  AMUI=VISIC(TF,II)
0100200  RHO=(AMUI/PO1)/(0.7302*(TF+460.))
0100300  RE=D(II)*G/AMUI
0100400  CD(II)=5.72
0100500  FRIC=CD(II)/RE
0100600  DPI=100*FRIC*(G/PO1)**2/2.*0.5+0.6+FRIC*L(IT)/D(IT)*2116.2
0100700  L/3600.*2/32.174
0100800  JJ=JJ+1
0100900  IF(JJ.EQ.2) GO TO 2
0101000  IF(JJ.EQ.3) GO TO 5
0101100  IF(JJ.EQ.4) GO TO 6
0101200  IF(JJ.EQ.5) GO TO 8
0101300  1 CAL. THE PRESSURE DROP OF AIR SIDE
0101400  2 INSERT THE FLCH RATE OF EACH GAS
0101500  5 FLI(1)=DNSC(1)/453.6
0101600  FLI(2)=DNSC(3)/453.6
0101700  FLI(3)=DNSC(4)/453.6
0101800  FLI(4)=DNSC(6)/453.6
0101900  FLI(5)=DNSC(5)/453.6
0102000  FLI(6)=DNSC(7)/453.6
0102100  FLI(7)=DNSC(2)/453.6
0102200  IT=IT+1
0102300  D(I)=WIDA(2)
0102400  GO TO 3
0102500  6 DO 7 IA=1,7
0102600  7 FLI(IA)=DNS(IA)/453.6
0102700  GO TO 3
**SHIFT CONVERTER**

```plaintext
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,IJ)

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(CM/PDHT/ D,AHRN,AP,CLEN,NT
010400  CVISION /AP/ 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  FI=FLI(1)+FLI(2)+FLI(3)+FLI(4)+FLI(5)+FLI(6)+FLI(7)
010530  DO 1 I=1,7
010540  CI(I)=FLI(I)/FI
010550  1 CONTINUE
010560  AIM=CM(1)*WM(1)+CM(2)*WM(2)+CM(3)*WM(3)+CM(4)*WM(4)+CM(5)*WM(5)
010570  1+CM(6)*WM(6)+CM(7)*WM(7)
010580  G=FI*AVG(6./3.14159*O(JK)*2)
010590  CALL CMSSIC(C,FLI,F1)
010600  AMJ=VIS(C,TF,1J)
010610  RHO=AMJ*PIN/10.7302*(TF*40.1)
010620  DDEL=CLEN(JK)*1.-AHRN(JK))/AHRN(JK)**3/C**2/DP/4.18E+08
010630  1/ND=180.*1.-AHRN(JK))/AMJ/DP/9.175)/2116.2
010640  POUT=PIN-DEL
010650  RETURN
010660  END
010670  SUBROUTINE PUMP(DNS,TIN,TOUT,PIN,POUT,POW,I)

010680  C************************************************************************
010690  C THIS SUROUTINE 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),WM(7)
010740  COMMON/KM/ KM
010750  COMMON/SV/ SV
010760  TOUT=TIN
010770  C CAL. THE WORK
010780  C ASSUME AVERAGE SPECIFIC VOLUME OF WATER IS 0.0162 FT**3/LBM
010790  POW=5V*14.*5.05051*0.0000001*WM(6)*14.7*(POUT-PIN)*DNS(6)
010800  1/453.6
010810  RETURN
```
SUBROUTINE PUP(DNS,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=SV(IJ)*144.*5.05051*0.000001*WM(IJ)*14.7*(POUT-PIN)
1*DNS(I)/453.6
RETURN
END

SUBROUTINE REF(DNS,TOP,POP,XI,IJ)
C THIS SUBROUTINE IS TO CALCULATE THE MASS BALANCE OF REFORMER

DIMENSION NNS1(7),NNS2(7),DNS(7),SK1(I),X(2)

C CALCULATE THE EQU. CONSTANT OF REACTION 1

DO 1 IA=1,I
1 NNS1(I)=0
IF (IJ.EQ.3) GO TO 2
IF(IJ.EQ.2) NNS1(I)=1
IF (IJ.EQ.1) NNS1(I)=1
NNS1(1)=-1
NNS1(6)=-1
NNS1(5)=3
GO TO 5
2 NNS1(1)=-1
NNS1(6)=-7
NNS1(5)=7
NNS1(15)=15
3 CALL EQUK(NNS1,TOP,SK1)
IHUI=0
DO 4 IA=1,I
4 NNS2(IA)=0
IHUI=IHUI+NNS2(IA)
IHUI=IHUI+X1(IA)
SK1(I)=SK*POP**[(-IHUI)
1 C CALCULATE THE EQU. CONSTANT OF REACTION 2

DO 5 IA=1,I
5 NNS2(IA)=0
IF (IJ.EQ.2) GO TO 6
NNS2(4)=1
NNS2(5)=1
NNS2(6)=1
GO TO 7
6 NNS2(3)=1
7 CALL EQUK(NNS2,TOP,SK1)
IHUI=0
DO 8 IA=1,I
8 IHUI=IHUI+NNS2(IA)
SK1(I)=SK*POP**[(-IHUI)
0113600 C CALCULATE THE EXIT AMOUNT OF GAS I
0113700 C INITIAL CONDITION
0113800 IF (I,J,EQ.2) GO TO 10
0113900 IF (I,J,EQ.1) GO TO 9
0114000 C BECAUSE OF COMPUTATION PROBLEM (OVERFLOW) NAPHTHA INPUT FUEL USING THE
0114100 C REASONABLE ASSUMPTION OF CONVERSION
0114200 X(1)=0.999*DNS(1)
0114300 X(2)=2.9*DNS(1)
0114400 DNS(1)=DNS(1)-X(1)
0114500 DNS(3)=DNS(3)+7.*X(1)-X(2)
0114600 DNS(4)=DNS(4)+X(2)
0114700 DNS(5)=DNS(5)+X(2)-15.*X(1)
0114800 DNS(6)=DNS(6)-X(2)-7.*X(1)
0114900 GO TO 11
0115000 9 X(1)=0.8*DNS(1)
0115100 X(2)=0.35*DNS(1)
0115200 CALL SHADEX2,DNS,SK1,I,II)
0115300 DNS(1)=DNS(1)-X(1)
0115400 DNS(3)=DNS(3)-X(1)
0115500 DNS(4)=DNS(4)+X(2)
0115600 DNS(5)=DNS(5)-X(2)+3.*X(1)
0115700 DNS(6)=DNS(6)-X(2)-X(1)
0115800 GO TO 11
0115900 10 X(1)=0.96*DNS(1)
0116000 X(2)=0.04*DNS(1)
0116100 CALL SHADEX2,DNS,SK1,I,II)
0116200 DNS(1)=DNS(1)-X(1)
0116300 DNS(3)=DNS(3)-X(1)
0116400 DNS(4)=DNS(4)-X(1)
0116500 DNS(5)=DNS(5)-X(2)+3.*X(1)
0116600 DNS(6)=DNS(6)-X(1)
0116700 11 CONTINUE
0116800 RETURN
0116900 ENDSUBROUTINE SEPARATIONPOPOUT,TOUL,DNS,DNSL,DNSV,I)
0116960 C****************************************************************************************
0116900 C THIS SUBROUTINE IS TO CAL. THE MASS BALANCE AROUND THE LIQUID SEPARATOR
0116990 C****************************************************************************************
0117000 C ASSUMPTION:
0117020 C (1). ONLY WATER EXIST IN LIQUID PHASE
0117040 C PSAT: SATURATE PRESSURE AT T; EXP(A-B/T) FOR WATER
0117060 C DK: EQU. CONST. OF LIQUID-VAPOR
0117080 C XW: AMOUNT OF WATER IN LIQUID PHASE
0117100 DIMENSION DNS(2),DNSV(1),DNSL(1)
0117120 COMMON/PS,PS,T/CONS/A,B
0117140 C CAL. THE EQU. CONST. OF LIQUID-VAPOR
0117160 PSAT=EXP(A-B/TIN)
0117180 DK=PSAT/POP
0117200 C CAL. THE EQU. AMOUNT OF LIQUID-VAPOR WATER
0117220 DNS=0.
0117240 GO TO 11
0117260 DNS=DNS+DNS(1A)
0117280 1 CONTINUE
0117300 XW=(DNS*DK-DNS(6))/(DK-1.)
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C ALGEBRAIC EQUATIONS IN REFORMER

0118400  C DIMENSION XY(XX),DNSI(I),SK11(X)
0118420
0118440  F1(X,Y)=(D3+X-Y)*(D5+X+3.*Y)**3-SKA*(TDNS+2.*Y)**2*(D1-Y)*(D6-X-Y)
0118460  F2(X,Y)=(D4+X)*(D5+X+3.*Y)-SKB*(D6-X-Y)*(D3+X-Y).
0118480  F3(X,Y)=ID3+Y-X)**3-SKA*(TDNS+Z.*Y)**2*(D1-Y)
0118500  F4(X,Y)=-ID3+Y-X+*(D5+X+3.*Y)**2+SKA*(TDNS+2.*Y)
0118520  1Y)**2*(D1-Y)
0118540  DF1(X,Y)=(D5+X+3.*Y)**3+9.*(D3+X-Y)*(D5+X+3.*Y)**2-SKA*(-(TDNS+2.*Y)
0118560  1Y)**2*(D1-Y)+(TDNS+2.*Y)*(D1-Y)*(D6-X-Y)
0118580  2-Y)
0118600  DF2(X,Y)=(D5+X+3.*Y)**3+(D4+X)*SKB*((D3+X+Y)+(D6-X-Y))
0118620  DF3(X,Y)=ID3+Y-X)**3-SKA*(TDNS+Z.*Y)**2*(D1-Y)
0118640  DF4(X,Y)=(D5+X+3.*Y)**3+9.*(D4+X)**2-SKA*(TDNS+2.*Y)
0118660  1(Y)**2*(D1-Y)
0118680  DF5(X,Y)=(D5+X+3.*Y)**3+9.*(D4+X)**2-SKA*(TDNS+2.*Y)
0118700  1(Y)**2*(D1-Y)
0118720  DF6(X,Y)=(D5+X+3.*Y)**3+9.*(D4+X)**2-SKA*(TDNS+2.*Y)
0118740  1(Y)**2*(D1-Y)
0118760  DF7(X,Y)=(D5+X+3.*Y)**3+9.*(D4+X)**2-SKA*(TDNS+2.*Y)
0118780  1(Y)**2*(D1-Y)
0118800  DF8(X,Y)=(D5+X+3.*Y)**3+9.*(D4+X)**2-SKA*(TDNS+2.*Y)
0118820  1(Y)**2*(D1-Y)
0118840  DF9(X,Y)=(D5+X+3.*Y)**3+9.*(D4+X)**2-SKA*(TDNS+2.*Y)
0118860  1(Y)**2*(D1-Y)
0118880  DF10(X,Y)=(D5+X+3.*Y)**3+9.*(D4+X)**2-SKA*(TDNS+2.*Y)
0118900  1(Y)**2*(D1-Y)
0118920  DF11(X,Y)=(D5+X+3.*Y)**3+9.*(D4+X)**2-SKA*(TDNS+2.*Y)
0118940  1(Y)**2*(D1-Y)
0118960  DF12(X,Y)=(D5+X+3.*Y)**3+9.*(D4+X)**2-SKA*(TDNS+2.*Y)
0118980  1(Y)**2*(D1-Y)
0119000  DF13(X,Y)=(D5+X+3.*Y)**3+9.*(D4+X)**2-SKA*(TDNS+2.*Y)
0119020  1(Y)**2*(D1-Y)
0119040  DF14(X,Y)=(D5+X+3.*Y)**3+9.*(D4+X)**2-SKA*(TDNS+2.*Y)
0119060  1(Y)**2*(D1-Y)
0119080  DF15(X,Y)=(D5+X+3.*Y)**3+9.*(D4+X)**2-SKA*(TDNS+2.*Y)
0119100  1(Y)**2*(D1-Y)
0119120  DF16(X,Y)=(D5+X+3.*Y)**3+9.*(D4+X)**2-SKA*(TDNS+2.*Y)
0119140  1(Y)**2*(D1-Y)
0119160  DF17(X,Y)=(D5+X+3.*Y)**3+9.*(D4+X)**2-SKA*(TDNS+2.*Y)
0119180  1(Y)**2*(D1-Y)
0119200  C CALCULATE THE TOTAL AMOUNT
0119220  IF ((IJ.EQ.2).OR.(IJ.EQ.3)) GO TO 51
0119240  DO 5 IA=1,7
0119260  DO 5 IA=1,7
0119280  5 CONTINUE
0119300  51 TDNS=0.
0119320  DO 1 IA=1,3
0119340  TDNS=TDNS+DNSI(I)
0119360  1 CONTINUE
0119380  DO 1 IA=1,3
0119400  D1=DNSI(1)
0119420  D2=DNSI(2)
0119440  D3=DNSI(3)
0119460  D4=DNSI(4)
0119480  D5=DNSI(5)
D6 = DNS(6)
D7 = DNS(7)
SKA = SK1(1)
SKB = SK1(2)

IF (IJ.EQ.1) GO TO 61

IF (IJ.EQ.2) GO TO 62

X = XY(1)/1000.

DO 2 IA = 1, 500

D = DFX5(X, Y) * DFY6(X, Y) - DFX6(X, Y) * DFY5(X, Y)

DO 2 IA = 1, 500

DX = (F6(X, Y) * DFY5(X, Y) - F5(X, Y) * DFX6(X, Y)) / D

DY = (F5(X, Y) * DFX6(X, Y) - F6(X, Y) * DFX5(X, Y)) / D

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

2 CONTINUE

WRITE(6, 101)

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

RETURN

9

XY(1) = Y * 1000.

XY(2) = X * 1000.

61

DO 3 IA = 1, 500

D = DFX1(X, Y) * DFY2(X, Y) - DFX2(X, Y) * DFY1(X, Y)

DO 3 IA = 1, 500

DX = (F2(X, Y) * DFY1(X, Y) - F1(X, Y) * DFX2(X, Y)) / D

DY = (F1(X, Y) * DFX2(X, Y) - F2(X, Y) * DFX1(X, Y)) / D

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

3 CONTINUE

WRITE(6, 101)

RETURN

91

XY(1) = Y

XY(2) = X

RETURN

62

DO 4 IA = 1, 500

D = DFX3(X, Y) * DFY4(X, Y) - DFX4(X, Y) * DFY3(X, Y)

DO 4 IA = 1, 500

DX = (F4(X, Y) * DFY3(X, Y) - F3(X, Y) * DFX4(X, Y)) / D

DY = (F3(X, Y) * DFX4(X, Y) - F4(X, Y) * DFX3(X, Y)) / D

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

4 CONTINUE

WRITE(6, 101)

RETURN
SUBROUTINE VIEW (M,V,Z,TK,POP,PPH2,PPO2,PPH2O,PPCO,XO)
CD=SN/VTAL/SA,CU,CL,ALFA,SN,FCONST,AREAF,DXC
RETURN
R=8.314
ERR=0.005
CLA=CL
DA=D/ALFA
CDL=CL/AREAF*(PPO2*POP)
IF (M.EQ.2) GO TO 2
V=B-DA*ALOG(Z/C)-Z*SR-EX*ALOG(Z/Cl)-D*ALOG(CDL/(CDL-Z))
GO TO 6
Z=XO
CONTINUE
DO 5 I=1,50
AZ=Z*SR+DA*ALOG(Z/C)+V-B*EX*ALOG(Z/Cl)+D*ALOG(CDL/(CDL-Z))
GO TO 6
Z=Z+AZ
CONTINUE
IF (Z.LE.0.) GO TO 7
IF (ABS(DZ).LT.ERR) GO TO 6
CONTINUE
WRITE(6,201)
GO TO 6
ERR=ERR+0.001
GO TO 2
CONTINUE
RETURN
SUBROUTINE KREF(DNSR,DNSF,DX,DT,DP,TCO,THZ,Z,POUT,TCOUT)
THOUT,E1,DP1,IFUEL
REAL K0,THOB,THOB,THZ
COMMON/REP/ K0,EO,THOB,THOB,THZ
END
COMMON/ADDR/ D1,D2,D3,S,DP,P
COMMON /AM/ AM
COMMON /FCG/ F7,CG7
DIMENSION X1(50),TAX2(50),XE2(50),TC(50),
1TH(50),XI(50),TA(50),TAK1(50),TAK2(50),
2XF(50),XCOMP(50),71,XMCOMP(50,71),XI(50,71),
3XUL(50),TP(50),FL(7),C(7),AM(7),CM(7),CGCOMP(7),TCGC(7)
DIMENSION REN(50)
DIMENSION P(50)
DIMENSION DNSR(7),DNSF(7)
DATA EPOR/0.01/
DATA XCOMP/ 350*0.0.
IDBugs=0
D1=DX
D2=DX
D3=DX
DP=DP1
S=SI
P(1)=PK
F1=DNSR(1)
F2=DNSR(3)
F3=DNSR(4)
F4=DNSR(6)
F5=DNSR(5)
F6=DNSR(7)
F7=DNSR(2)
F0=F1+F2+F3+F4+F5+F6+F7
CG1=DNSF(1)
CG2=DNSF(3)
CG3=DNSF(4)
CG4=DNSF(6)
CG5=DNSF(5)
CG6=DNSF(7)
CG7=DNSF(2)
M=CG1+CG2+CG3+CG4+CG5+CG6+CG7
X1(1)=0.
XE2(1)=0.
TCO=(TCO-273.16)*9./5.+32.
THZ=(THZ-273.16)*9./5.+32.
KINS=0
CO=(Fl*(1.-X1(1)))*P(1)/(.7302*(F0+2.*X1(1)*Fl)*(TCO+460.))
U0=(4.*.7302*(F0+2.*X1(1)*Fl)*(TCO+460.))/(3.1415927*P(1))
K(2)=-EPS
C FIRST ASSUMPTION -- THO
TH=9.
AX=Z*RHOB*K0*P(1)*Fl*(2.*F0+X*X*(2.*F1-F0))/(2.*F0*(F0+2.*X*F1))
1U0=CO
T=-.90455*EA/ALOG(X/AX)-460.
TK2=K2(T)
TX2=X2(T,K2)
TDH1=DH1(T)
TDH2=DH2(T)
AY=F1*TDH1*X*(F3*X*F1)*TDH2*TX2
FL(1)=F1*(1.-X)
DO 122760 J=1,7
122760 XCOMP(1,J)=XCO(1)/XF(1)

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122760 THO=TC0+250.
122760 IF( THO.LT.TC0
122760 THO=TC0+250.
122760 IF( THO.LT.TC0
122760 THO=TC0+250.
013800 70 TA(I+1)=(TC(I)+TC(I+1))/2.
013820 TA(I+1)=K1(TA(I+1))
013840 TAK2(TA(I)+K2(TA(I+1))
013860 B1=DZZ*RHOB*K0*PI(I)/(U0*C0)
013880 B2=EXP(-.9045*EA/(TA(I+1)+.460.))
013900 X1(I+1)=X1(I)+B1*B2*XMCMP(I+1)
013920 X2(I+1)=X2(I)+X3(I+1), TAK2(I+1)
013940 XDH1=-DH1(TA(I))
013960 XDH2=-DH2(TA(I+1))
013980 AL2=FL(I+1)-AL1
014000 AL2=AL1+AL2
014020 FL(I)=F1+FL(I)+X1(I+1)
014040 FL(I+1)=F2+X2(I+1)+X3(I+1)+F1
014060 FL(I+1)=F3+X1(I+1)*F1+X2(I+1)*(F3+X1(I+1)*F1)
014080 FL(I+1)=F4+X3(I+1)*F1+X1(I+1)*(F3+X1(I+1)*F1)
014100 FL(I+1)=F5+X4(I+1)*F1+X1(I+1)*(F3+X1(I+1)*F1)
014120 FL(I+1)=F6
014140 FL(I+1)=F7
014160 XF(I+1)=FL(I+1)
014180 CALL CMASSIC,FL, XF(I+1)
014200 DO 10 J=1,7
014220 XCOMP(I+1,J)=FL(I+1)
014240 XCOMP(I+1,J)=XCOMP(I+1,J)/XF(I+1)
014260 XCI(I+1, J)=C(I)
014280 CONTINUE
014300 XF(IS)=VIS(TA(I),1,IFUEL)
014320 XTHC=THC(TC(I),1,IFUEL)
014340 V=CM(I)*F1+CM(I)*F2+CM(I)*F3+CM(I)*F4+CM(I)*F5+CM(I)*F6+CM(I)*F7
014360 V=(1./4.3145827*(D2-D1)/1.75)*OGE2/2116.8
014380 RH=ZA*P(I)/RO
014400 DELP=(1.-EPS1)*EPS1/G1P*V**2/DP/4.18*08/RHO*(1.75)*XVIS/DP
014420 V=1.75*OGE2/2116.8
014440 P(I+1)=P(I)-DELP
014460 XHI=HI(XF(I+1),XTHC)
014480 XCVS=VIS(XGTC,TH(I),1,IFUEL)
014500 XCGT=THC(TGTC,TH(I),1,IFUEL)
014520 XGHTCP=HTCP(TGTC,TH(I))
014540 XGHTCP=HTCP(TGTC,TH(I))
014560 XGHTCP=HTCP(TGTC,TH(I))
014580 XGHTCP=HTCP(TGTC,TH(I))
014600 XGHTCP=HTCP(TGTC,TH(I))
014620 XGHTCP=HTCP(TGTC,TH(I))
014640 XGHTCP=HTCP(TGTC,TH(I))
014660 XGHTCP=HTCP(TGTC,TH(I))
014680 AN=TH+XGHTCP/XFCP/AM-XFCP+MH+XGHTCP
014700 TH(I)=TH(I)+AN+Z.XFCP/AN+XFCP/TC(I)+AN-AL/AN
014720 TH(I)=TH(I)+AN+Z.XFCP/AN+XFCP/TC(I)+AN-AL/AN
014740 C TEST SECOND ASSUMPTION
014760 EE=ABS(TP(I+1)-TC(I+1))/TC(I+1)
014780 IF(EE.LE.ERROR) GO TO 71
014800 1KWRITE(6,2020) TP(I+1),TC(I+1),EE
014820 20 FORMAT(EE,1PE15.7,5X,'TC=',E15.7,5X,'EE=',E15.7)
014840 IF(EE.LE.ERROR) GO TO 71
014860 IF(KICG.LE.15) TC(I+1)=TC(I+1)+TP(I+1))/2.
TC2=TC(I+1)

EETC2=TH(I+1)*(AM-MH*XGHTCP1)/AM+TH(I)*(AM+MH*XGHTCP1)/AM -

ITC(I)=TC2

IF(KING.LE.15) GO TO 97

IF(EETC1.EQ.EETC2) TC3=(TC2*(EETC2-EETC1))/(TC2-TC1)

IF(EETC1.NE.EETC2) TC3=(TC2+TP(I+1))/2

TC(I+1)=TC3

97 KING=KING+1

TC1=TC2

EETC1=EETC2

IF(KING.GE.40) GO TO 959

GO TO 70

IF(KIEG.LE.151 

GO TO 97

IF(EETC1.NE.EETC2) 

TC3=TC2-(EETC2/(EETC2-EETC1))*(TC2-TC1)

IF(EETC1.EQ.EETC2) 

TC3=(TC2+TP(I+1))/2

IC=IC+1

GO TO 73

73 N=IC+1

C TEST FIRST ASSUMPTION

AB=ABS((TH(I+1)-THZ)/THZ)

THO2=THO

THZ2=TH(N)

THO3=TH0+THZ2

THO3=(THO2-THO)/(THZ-THZ2)*THO2

IDEA=2

THZ1=TH(N)

TH01=THO

THO=THO3

IF(TH0.LT.TCO) TH0=THO

IF(IHOPE.EQ.51 

GO TO 975

GO TO 75

74 CONTINUE

IF(K.EQ.1) \n
GO TO 954

954 CONTINUE

WRITE(6,976) THO

976 FORMAT(1H1,'***INSUFFICIENT COMB. GAS HEAT CAPACITY*'/

1'I'OHO=',F17.3,'THIS IS LESS THAN TCO'/*RAISE THZ AND/OR COMB. -

2GAS FLOW RATES*')

GO TO 954

958 FORMAT(1H1,'LOOPING ON TC FOR ',I4,'ITERATIONS IN INCRM',I4)

954 CONTINUE

TCO=(TCO-32.1*5./9.+273.16

THZ=(THZ-32.1*5./9.+273.16

DNST(1)=XCOMP(N,1)
0125960  DNSR(3)=XCOMP(N,2)
0125980  DNSR(4)=XCOMP(N,3)
0126000  DNSR(5)=XCOMP(N,5)
0126020  DNSR(6)=XCOMP(N,4)
0126040  DNSR(7)=XCOMP(N,6)
0126060  RETURN
0126080  END
0163100  SUBROUTINE CMASSIC(FL,F)
0163200  DIMENSION C(7),WM(7),FL(7)
0163300  COMMON /WM/ WM
0163400  WM(0)=FL(1)*WM(1)+FL(2)*WM(3)+FL(4)*WM(4)+FL(6)*WM(5)+-F
0163500  IF(6)*WM(7)+FL(7)*WM(2))/F
0163600  C(1)=FL(1)*WM(1)/(F*WM)
0163700  C(2)=FL(2)*WM(3)/(F*WM)
0163800  C(3)=FL(3)*WM(4)/(F*WM)
0163900  C(4)=FL(4)*WM(6)/(F*WM)
0164000  C(5)=FL(5)*WM(5)/(F*WM)
0164100  C(6)=FL(6)*WM(7)/(F*WM)
0164200  C(7)=FL(7)*WM(2)/(F*WM)
0164300  RETURN
0164400  END
0164500  SUBROUTINE COMPIN(COM,X1,X2)
0164600  REAL HM
0164700  COMMON F0,F1,F2,F3,F4,F5,F6,MH,CG1,CG2,CG3,CG4,CG5,CG6
0164800  COMMON/ADDRE/ D1,D2,D3,D6,P
0164900  COMMON /FCG/F7,CG7
0165000  DIMENSION COM(7)
0165100  DO 8 J=1,7
0165200  IF(J.EQ.1) COM(J)=F1*(1.-X1)
0165300  IF(J.EQ.2) COM(J)=F2-X2*(F3+X1*F1)
0165400  IF(J.EQ.3) COM(J)=F3+X1*F2+X2*(F3+X1*F1)
0165500  IF(J.EQ.4) COM(J)=F4-2.*X1*F1-X2*(F3+X1*F1)
0165600  IF(J.EQ.5) COM(J)=F5+4.*X1*F1+X2*(F3+X1*F1)
0165700  IF(J.EQ.6) COM(J)=F6
0165800  IF(J.EQ.7) COM(J)=F7
0165900  END
0166000  RETURN
0166100  END
0166200  FUNCTION DH1(T)
0166300  DH1=-2.7285E-03*(T**2+12.698*T+7.002E+04*
0166400  RETURN
0166500  END
0166600  FUNCTION DH2(T)
0166700  DH2=2.3280*T-18111.4
0166800  RETURN
0166900  END
0167000  FUNCTION F(X1)
0167100  REAL HM
0167200  COMMON F0,F1,F2,F3,F4,F5,F6,MH,CG1,CG2,CG3,CG4,CG5,CG6
0167300  COMMON/ADDRE/ D1,D2,D3,D6,P
0167400  COMMON /FCG/F7,CG7
0167500  F=F0+2.*X1*F1
0167600  RETURN
0167700  END
FUNCTION FCP(TP, CO1)

DIMENSION CO1(7)

DATA A/5.34, 0.76E-03, 0., 0.66, 0.67E-04, 0., 0., 10.34, 1.52E-03, 0., 0.66, 0.732, 0.36E-03, 0.53E-09, 0.60/

TP = TP + 460.

FCP = FCP + CO1(I)*TP*10./TP + A(I) + TP**2 + A(4, I)/TP**2

END

FUNCTION HI(VIS, THC)

REAL KH

DIMENSION KM(7)

COMMON FO, F1, F2, F3, F4, F5, F6, MH, CG1, CG2, CG3, CG4, CG5, CG6

COMMON/ADDRE/ D1, D2, D3, S, DP, P

COMMON/WM/ WM

COMMON /FCG/F7, CG7

HI = 0.

V = (WM(1) + F1 + WM(3) + WM(4) + F3 + WM(6) + F4 + WM(5) + F5 + WM(7) + F6

1 + WM(2) + F7)

GHM = (V*4./((3.1415927*D2**2 - D1**2)**.5))

HID = (.813*GHM*DP/VIS)**.9*EXP(-6.*DP/(D2-D1))

HI = (HID + THC)/(D2-D1)

RETURN

END

FUNCTION HO(VIS, THC, HTCP, Z, T, RE)

REAL MH

DIMENSION WM(7)

COMMON FO, F1, F2, F3, F4, F5, F6, MH, CG1, CG2, CG3, CG4, CG5, CG6

COMMON/ADDRE/ D1, D2, D3, S, DP, P

COMMON /FCG/F7, CG7

COMMON/WM/ WM

A1 = (CG1**2 - WM(1) + CG2**2 - WM(3) + CG3**2 - WM(4) + CG4**2 - WM(6) + CG5**2 - WM(5) + CG6**2 - WM(7)

1 + CG7**2)

H0 = 0.

G = (3.1415927*D3**2)/4.

DE = A1*(G - S**2 - 3.1415927*D3**2 + G - S**2 - 1.531415927*D3 + 4.*S)

RE = (HTCP + VIS)/THC + AMW

PR = HTCP + VIS)

RH = (AM**2P)/(0.7302*(T460.))

GR = (Z**31) + (RH + 2100.)*10E6*100.)/(VIS**2)

IF(RE.GE.10000.) GO TO 300

IF(RE.LE.2100.) GO TO 200

C 2100<RE<10000

HO21 = (1. + THC/DE)*SQRT(PR) + (DE/Z)**.4*(S/D3)**.8

1*GR**.05

HO10 = (1.02*THC/DE)/(10000.*.8)**(PR**.333)/(S/D3)**.53

SLOPE = HO10*HO21)/(10000. - 2100.)

HO = HO*HO1 + SLOPE*(RE-2100.)

RETURN

C 2100<RE<10000

HO = (1. - THC/DE)*SLOPE*(PR) + (DE/Z)**.4*(S/D3)**.8

RETURN

END
REElTNE \( R \geq 10000 \)

\[ Ha = (0.02 \times THC/DE) \times (R^{0.81} \times PR^{0.33} \times (S/D)^{0.53}) \]

RETURN

**FUNCTION**

\[ HTCP(CM, T) \]

**DIMENSION** \( CM(7), C(7), A(4, 7), P(7) \)

\[ 1-6.33\times 10^{-2} \times 6.22, 8.3E-05 \times 4.136E-07, 6.6E-04 \times 6.65, 4.5E-04 \times 6.55 \]

\[ 25.5E-04, 0 \times 4.4, 10.2E-09 \times 0 \times 16.2E-04, 6.3E-03, 5.5E-09 \times 0 \times 6.3342E+05, 8.22 \times 8.3E-05, 14.136E-07, 0 \times 6.6 \times 4.5E-04, 0 \times 6.55 \]

\[ TK = CM(1)/WM(1) + CM(2)/WM(2) + CM(3)/WM(3) + CM(4)/WM(4) + CM(5)/WM(5) \]

\[ TP = T + 460. \]

\[ K1 = EXP(B) \]

\[ K2 = EXP(B) \]

**FUNCTION**

\[ THC(C, T, I, J) \]

**DIMENSION** \( C(7), A(2, 7) \)

**RETURN**

\[ R = 0.005 \]
0176100 THMET=4.659E-03*T+6.248
0176200 U1=1./(1.5*DI/D3*H0!) + ((D3-D2)*D2)/(THMET*D1+R)
0176300 RETURN
0176400 END
0176500 FUNCTION VIS(C,T,II)
0176600 DIMENSION A(2,7),C(7)
0176700 COMMON/VIFC/A
0176800 VIS=0
0176900 5 DO 4 I=1,7
0177000 VIS=VIS+*(A(I,1)*T+A(2,I))
0177100 4 CONTINUE
0177200 RETURN
0177300 END
0177400 FUNCTION X2(X,K2)
0177500 REAL K2
0177600 REAL K2
0177900 COMMON F0,F1,F2,F3,F4,F5,F6,MH,CG1,CG2,CG3,CG4,CG5,CG6
0178200 COMMON/ADDR/E D1,D2,D3,P,P
0178500 COMMON /FCG/F7,C7
0178800 A=(X2-1.)*((F3*X)*F1)*2
0179000 B=(F3*X*F1)*(2.*X*F1-K2-K2+K2*K2-F2-K2-X*F1-F1-F1-F5)
0179200 C=X2*F2*F4-2.*F1*X*K2*X-(F3*X*F1)*X(F5+4.*F1*X)
0179400 X2=-(-SQRT(B**2-4.*A*C))/2.*A
0179500 RETURN
0179600 END
0179700 &DPFC T0PFC=443.,UT=0.8,CD=325.,
0179800 &END
0179900 &INIT DNSM=1216.,0.,1.360,21.8,166.,0.,0.,TAT=298.,PAT=1.,SMA=3.,POPR=5.0
0180000 &END
0180100 &CEN T IFUEL=1,ERR=0.01,IP=2,7,EXT=100.,WAT=0.015,EXA=100.,
0180200 &END
0180300 &REFEN ZH=6.,DX1=0.,DX2=0.15,DX3=0.167,K0=1.040E+04,EA=20000.,RHOB=80.
0180400 ,EPS=0.463,S=0.25,DP=0.00328,0.ZZ=0.25,
0180500 &END
0180600 &HEATC CN=1.3,UA=482.51,HA(7)=0.2,HA(10)=0.2,
0180700 &END
0180800 &FDSH NPH=2,NRH=5,ESPAC=1.,ODTH=.0625,PITCH=.0833,CLH=.0208,IDS=0.833.
0180900 &END
0181000 &IDTH= .04667,FLOOR=.01716,SURFC=.1466,CLENH=2.,S1S2=0.5,ODTH=0.7,
0181100 &END
0181200 &FOREF DP=69.,0.0,APPD=69.,0.0,CLEPD=5.91,0.
0181300 &END
0181400 &TFDUE TNP=1.0,
0181500 &END
0181600 &FDFUH NTAF=140,FUE=1.42,WIDA=.009744,NPFU=3365.
0181700 &END
0181800 &NTPA=40,AIRL=1.,WIDA=0.0515
0181900 &END
0182000 &CATAI SRO=.44,SA=400.,CU=.15,CL=.75,ALFA=.5,SN=2.,FCNST=96500.,
0182100 &END
0182200 &END
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