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

Kalil A. Alkasab and Cheng-yi Lu
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Prepared for
NATIONAL AERONAUTICS AND SPACE ADMINISTRATION
Lewis Research Center
Cleveland, Ohio
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for
U.S. DEPARTMENT OF ENERGY
Morgantown Energy Technology Center

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Morgantown, West Virginia 26505
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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 optmization 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 excangers E-1, E-9 and E-6 before entering the low temperature shift converter S-2. The low temperature shift converter further increases the hydrogen concentration by promoting the shift reaction at a lower operating temperature. The effluent from the low temperature shift converter then enters the fuel cell containing H_2, CO, CH_4, CO_2 and H_2O. 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.

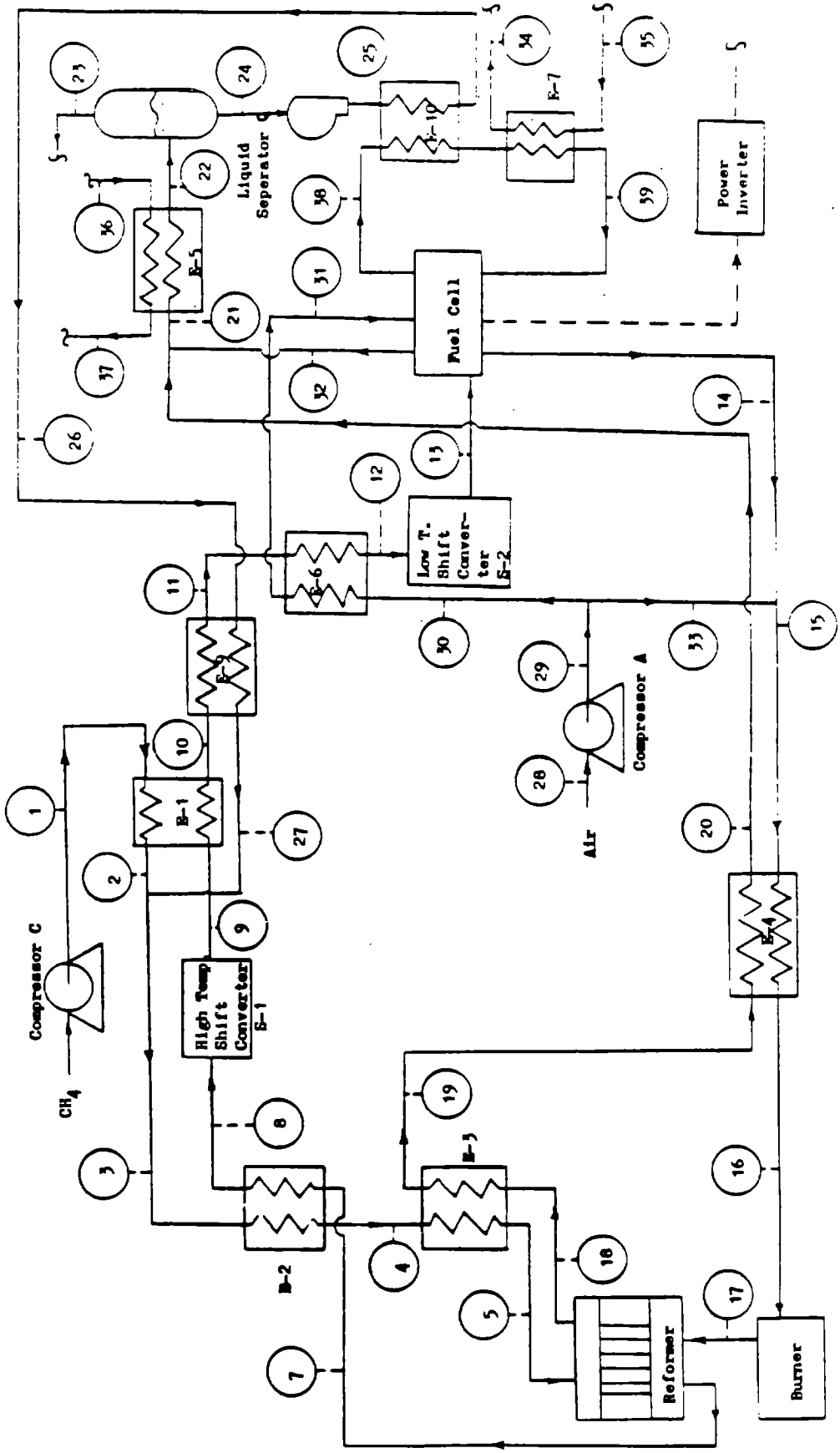


Figure 1 Flow diagram of CSU designed PAFC system

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

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

II. PERFORMANCE MATHEMATICAL MODEL

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

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

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

2.1 Modeling of Fuel Processing Subsystem

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

2.1.1 Heat Exchanger

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

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

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

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

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

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

where Cc: capacity rate of fluid on cold side, McCpc, J/s-K

Ch: capacity rate of fluid on hot side, MhCpc, J/s-K

Cmax: maximum capacity rate, J/s-K

Cmin: minimum capacity rate, J/s-K

Cpc: specific heat of cold side fluid, J/g-K

Cph: specific heat of hot side fluid, J/g-K

E: heat exchanger effectiveness

Mc: fluid mass flow rate on cold side, g/s

Mh: fluid mass flow rate on hot side, g/s

Q_T: total heat transfer rate across heat exchanger, J/s

Tci: 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/m^2-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

$$K_2 = \frac{Pco_2\ PH_2}{Pco\ PH_2O} = \frac{(Fco_2 + x)(FH_2 + x)}{(Fco - x)(FH_2O - x)} \qquad (2\text{-}1\text{-}5)$$

where K_2: equilibrium constant of shift reaction at ADT

P: partial pressure of component, atm

F: inlet molar flow rate of component, g-mole/s

x: reacted amount rate, g-mole/s

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

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

$$\sum_{PS} nj\ (\Delta h^{o}f)j - \sum_{RS} ni\ (\Delta h^{o}f)i + \sum_{PS} nj \int_{298}^{Tf} (Cp)j\ dT - \sum_{RS} ni \int_{298}^{T_i} (Cp)i\ dT = 0 \qquad (2\text{-}1\text{-}6)$$

where the subscripts PS, RS correspond to the products and reactants in the shift converter, respectively. Tf and Ti are the final and intial temperatures of the gases, respectively. The only unknown in the equation, Tf, is determined iteractively.

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

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

where ϵ : void fraction in bed

μ : viscosity, Kg/m-s

dp: effective diameter of packing particle, m

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

h: packed height, m

ρ : density, Kg/m^3

ΔP: pressure drop, atm

2.1.3 Reformer

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

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

for naphtha and methane, and

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

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

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

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

and

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

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

2.1.3.1 Lumped Model

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

$$K_1 = \frac{P_{co_2} P^3_{H_2}}{P_{CH_4} P_{H_2O}} = \frac{Y_{co_2} Y^3_{H_2}}{Y_{CH_4} Y_{H_2O}} \qquad \text{(demethanation)}$$

$$K_2 = \frac{P_{co_2} P_{H_2}}{P_{co} P_{H_2O}} = \frac{Y_{co_2} Y_{H_2}}{Y_{co} Y_{H_2O}} \qquad \text{(water shift)}$$

where K1 and K2 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:

$$K_1 = \frac{(F_{co}-x+y)(F_{H2}+x+3y)^3 P^2}{(F_{CH4}-y)(F_{H2O}-x-y)(F_T+2y)^2} \qquad (2\text{-}1\text{-}8)$$

and

$$K_2 = \frac{(Fco_2 +x)(F_{H2}+x+3y)}{(Fco-x+y)(F_{H2O}-x-y)} \qquad (2\text{-}1\text{-}9)$$

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 quantitites 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

$$Q_{B-R} = UA\Delta T_m = Hout - HIN \qquad (2\text{-}1\text{-}10)$$

where, ΔT_m is the log mean temperature defined as

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

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

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

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

$$- \sum_{rR} m_K \int_{298}^{T_{iR}} (Cp)_i \, dT, \ \ldots \qquad (2\text{-}1\text{-}12)$$

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

2.1.3.2 Distributed Model

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

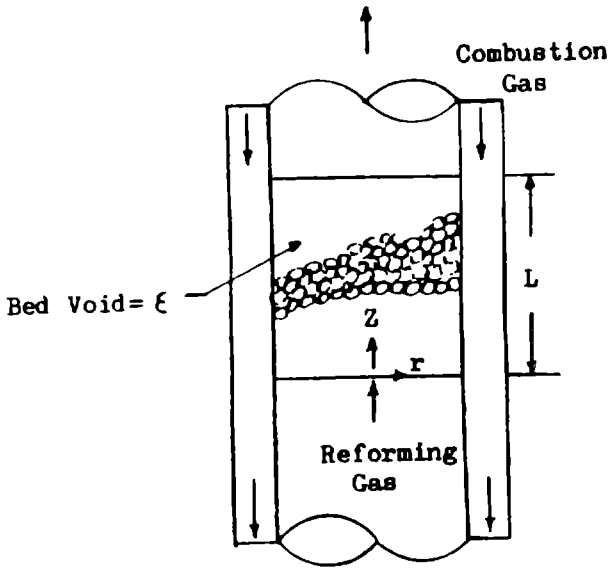


Figure 2 Simplified Reformer Diagram

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

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

$$CH4 + 2H2O = CO2 + 4H2 \qquad (2\text{-}1\text{-}13)$$

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

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

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

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

5. Entrance effects are negligible.

6. Heat transfer by radiation is negligible.

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

8. Ideal gas behavior is assumed.

9. The outside shell wall is adiabatic.

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

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

$$V \frac{dc}{dz} = -\frac{\gamma a' e_B}{\epsilon} \qquad (2\text{-}1\text{-}14)$$

where V: average velocity of fluid through the bed, m/s

c: g-mole of CH_4 per m^3 fluid

ra': raction rate, g-mole of CH_4/s-kg catalyst

e_B: 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

$$-ra' = Ko\ e^{-EA/RT}\ P_{CH4} \qquad (2\text{-}1\text{-}15)$$

in Arrhenius form,

where K_o: 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)

$$\rho Ai V\, Cp \frac{dt}{dz} = (-\Delta H_1) \frac{dy}{dz} + (-\Delta H_2) \frac{dx}{dz} + hi\pi di\,(Tw-t) \qquad (2\text{-}1\text{-}16)$$

$$\rho o\, Vo\, Ao\, Cpo \frac{dt}{dz} = ho\pi ao\,(T-Tw) \qquad (2\text{-}1\text{-}17)$$

where ΔH_1: demethanation reaction enthalpy, J/g-mole CH_4

ΔH_2: water shift reaction enthalpy, J/g-mole CO

Ai: inner tube cross area, m^2

hi: wall heat transfer coefficient of tube side, $J/s\text{-}m^2\text{-}K$

Tw: wall temperature, K

di: inner tube diameter, m

T: combustion gas temperature, K

do: outer tube diameter, m

subscript o refers to the combustion gas side

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

$$hi(dp/k_f) = 2.58(Re)^{1/3}(Pr)^{1/3} + .094\ (Re)^{0.8}(Pr)^{0.4} \qquad (2\text{-}1\text{-}18)$$

where dp: equivalent particle diameter, m

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

Pr: Prandtl number

Re: partical Reynolds number

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

2.2 Modeling of Fuel Cell Stack Subsystem

In the fuel cell power section, air, in excess of the stoichiometric mixture, enters the cathode side of the cell, and effluents from the low temperature shift converter 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

$$H_2 + 1/2\ O_2 = H_2O \qquad (2\text{-}2\text{-}1)$$

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:

$$NX_{H2} = NI_{H2} - (\text{Imean } A)/(n\mathcal{F}) \qquad (2\text{-}2\text{-}2)$$

$$NX_{O2} = NI_{O2} - (\text{Imean } A)/(2n\mathcal{F}) \qquad (2\text{-}2\text{-}3)$$

$$NX_{H2O} = NI_{H2O} + (\text{Imean } A)/(n\mathcal{F}) \qquad (2\text{-}2\text{-}4)$$

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

Imean: mean current density, A/cm^2

A: effective area of cell plate, cm^2

n: number of Faraday equivalents transferred

$\mathcal{F}$: Faraday constant

The energy balance for the fuel cell is

$$-(Q+W_e) = \sum_{PF} n_j \left(\Delta h_f^\circ\right)_j - \sum_{rF} n_i \left(\Delta h_f^\circ\right)_i + \sum_{PF} n_j \int_{298}^{T_{fF}} (Cp)_j \, dT - \sum_{rF} n_i \int_{T_{iF}}^{298} (Cp)_i \, dT \quad (2\text{-}2\text{-}5)$$

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

$$Q = N_p \, Xn \, Yn \, Q_F \quad (2\text{-}2\text{-}6)$$

$$\text{and } Q_F = \left(\frac{\Delta Hr}{n\mathcal{F}} - V\right) I \quad (2\text{-}2\text{-}7)$$

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

Xn: width of cell plate, cm

Yn: length of cell plate, cm

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

ΔHr: heat of reaction, J/g-mole of H_2

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:

$$V = E - \eta \tag{2-2-8}$$

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

η: overpotential or polarization

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

$$E_o = E\ (T) + \frac{RT}{nF}\ \ln\ \frac{YH_2\sqrt{PtYO_2}}{YH_2O} \tag{2-2-9}$$

with Pt: total pressure, atm

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

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

YH_2: mean mole fraction of hydrogen at anode

YO_2: mean mole fraction of oxygen at cathode

YH_2O: mean mole fraction of water vapor at cathode

The polarization term η consists of four components,

$$\eta = \eta a + \eta r + \eta d + \eta co \tag{2-2-10}$$

where ηa: activation poparization at cathode, volts

ηr: resistance polarization, volts

ηd: diffusion polarization, volts

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

and

$$\eta a = \frac{RT}{\alpha oZF}\ \ln\ \frac{i}{(io)(SA)(CL)(CU)} \tag{2-2-11}$$

with αo: transfer coefficient

i: current density, mA/cm^2

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

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

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

CU: catalyst utilization factor

The exchange current is a function of the acid concentration, temperature, and partial pressure of the oxygen. The acid concentration is a function of the water vapor partial pressure which permits correlaion of io as a function of YO2, YH2O, and T. An empirical fit is

$$io = 232.7\ (PtYO2)^{0.8}\ \ (PtYH2O)^{0.4377}\ \exp\ (-6652/T) \qquad (2\text{-}2\text{-}12)$$

The resistance polarization is

$$\eta r = ir$$

where r: specific cell resistance, $ohm\text{-}cm^2$.

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

$$\eta co = 0.0782 PtYco \exp\left[9190\ \left(\frac{1}{T} - \frac{1}{450}\right)\right] \ln \frac{i}{CLa\ SA\ CU\ iao} \qquad (2\text{-}2\text{-}13)$$

where CLa: anode catalyst loading, mg

iao: anode exchange current, mA/cm^2

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

2.2.3 Stack Efficiency

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

$$\epsilon_{FC} = \epsilon_V \epsilon_I \epsilon_{TH} \epsilon_H, \ \cdots \qquad (2\text{-}2\text{-}14)$$

where the voltage efficiency ϵ_V, the current efficiency ϵ_I, the thermodynamic efficiency ϵ_{TH}, and the heating value efficiency ϵ_H, are defined as follows:

$$\epsilon_V = \frac{V}{E}, \ \cdots \qquad (2\text{-}2\text{-}15)$$

$$\epsilon_I = \frac{I}{I_F}, \ \cdots \qquad (2\text{-}2\text{-}16)$$

$$\epsilon_{TH} = \frac{\Delta G_r}{\Delta H_r}, \ \cdots \qquad (2\text{-}2\text{-}17)$$

$$\epsilon_H = \frac{\Delta H_r}{\Delta H_c}, \ \cdots \qquad (2\text{-}2\text{-}18)$$

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, ΔG_r is Gibb's free energy change, ΔH_C is lower heat of combustion of fuel cell feed, and Δh_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 itterative 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).

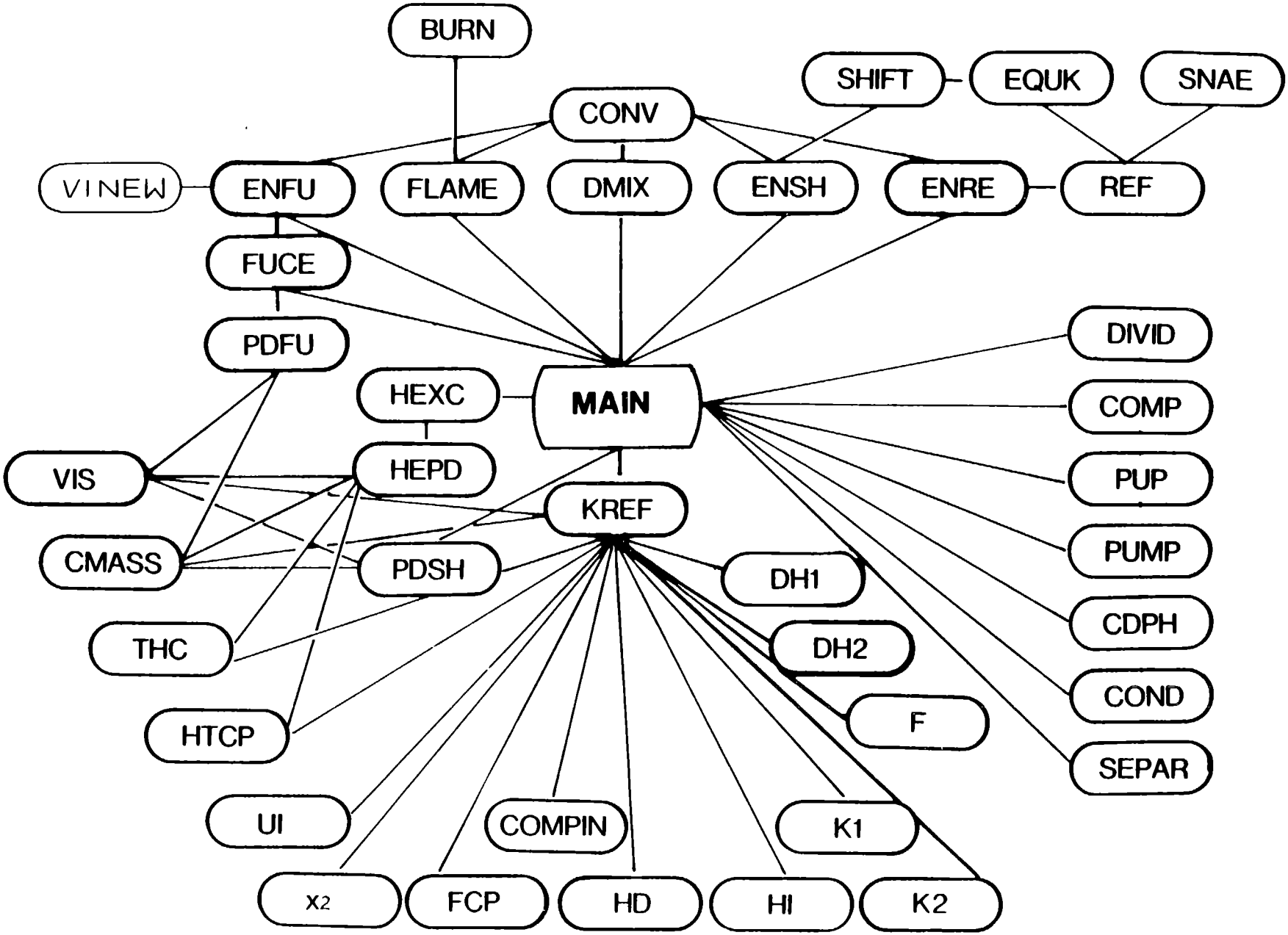


Figure 3. PERFORMANCE MODEL

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))  (3-1-1)
```

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

for methane, CK = 2

for methanol, CK = 1.5

for naphtha, CK = 15

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

```
T(22) = -B/(ALOG((DNSS(1,1)*SMRA-DNSS(21,6))/(DNSS(1,1)*SMRA-
        TKNSS(21))*POPS)-A)                                    (3-1-2)
```

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

A = 13.954316, atm

B = 5204.9597, atm-K

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

```
AC = (-1.0148+SQRT(1.0148*2-4*0.056/108*(0.0472*108-WK)))/2*0.0456/108) (3-1-3)
```

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

```
DNSS(36,6) = QQT(5)/1/18/(355-TAT)                             (3-1-4)
```

TABLE 1

MAIN PROGRAM NOMENCLATURE

A : Constant for calculating saturated condition of water, atm

AA1 : Thermal conductivity coeff. of gas I, Btu/hr-ft-R

AA2 : Viscosity coeff of gas I, lbm/ft-hr

AA3 : Specific heat capacity coeff. of gas I. Btu/R-lb-mole of the form:

$$AA3(1)+AA3(2)*T+AA3(3)*T^2+AA3(4)/T^2$$

AHLU : Mole fraction of available hydrogen

AHRN : Percent free gas space

AIRL : Length of air channel, ft

APPD : Total surface area of packing Acc. to the basis and oper. temp., ft^2

ATMP : Outlet temperature of gases, K

B : Constant for calculating saturated condition of water, atm-K

BPNA : Boiling point of naphtha, C

BSPAC : Baffle space, ft

CD : Current density, A/cm^2

CLENH : Length of tube in heat exchanger, ft

CLEPD : Length of shift converter (JK=1), reformer (JK-2 for methanol and naphtha), ft

CLH : Clearance in heat exchanger, ft

CN : U*A/CMIN in heat exchanger

DG : Standard free energy change, Cal/g-mole

DHIN : Enthalphy change due to temperature change of inlet fluid, Cal/g-mole

DHO : Integration constant to calculate H

DP : Catalyst pellet diameter, ft

TABLE 1

MAIN PROGRAM NOMENCLATURE
(cont'd)

DPD : Diameter of shift converter (JK=1), reformer (JK=2 for methanol and naphtha), ft

DSHO : Cathode inlet water of fuel cell, g-mole/hr

DSN : Cathode inlet nitrogen of fuel cell, g-mole/hr

DSO : Cathode inlet oxygen of fuel cell, g-mole/hr

DTH : Fraction of Delta T over inlet gas film in the heat exchanger

DX1 : Outside diameter of reformer center tube, ft

DX2 : Inside diameter of outside reformer tube, ft

DX3 : Outside diameter of outside reformer tube, ft

DZZ : Increment height of finite difference model in the reformer, ft

EA : Activation enegy for Arrhenius expression, Cal/g-mole CH4

EPS : Reactor void fraction

ERR : Convergence criteria

EXA : Fraction of extra air in fuel cell

EXT : Fraction of extra air in burner

FCO : Mole fraction of co contain

FLOAR : Flow area in heat exchanger, ft^2

FULE : Length of fuel channel, ft

HNA : Specific heat of naphtha, Btu/lbm-R

I : Gas number

I = 1 Fuel (methane, methanol, naphtha)
I = 2 Oxygen
I = 3 Carbon Monoxide
I = 4 Carbon Dioxide
I = 5 Hydrogen
I = 6 Water
I = 7 Nitrogen

TABLE 1

MAIN PROGRAM NOMENCLATURE
(cont'd)

ISSH : ID of shell in heat exchanger, ft

IDTH : ID of tube in heat exchanger, ft

IFUEL : Fuel Type

1 = Methane CH4
2 = Methanol CH3OH
3 = Naphtha C7H16

IDNO : Number of trial-and-error loops

IHUI : Stoichiometric number

IP : Index of operation condition in the reformer and shift converters

IP = 1 Adiabatic Operation
IP = 2 Isothermal Operation

KO : Frequency factor for Arrhenius expression, lb-mole CH_4/lb cata.-hr-atm

NN : Stream number of exit of shift converter

NOR : Scale factor in the model of reformer

NPFU : Number of cell plates in the fuel cell stacks

NPH : Number of tube passes

NRH : Number of rows for tubes

NTAA : Number of air flow channel in one cell plate

NTAF : Number of fuel flow channel in one cell plate

NTPD : Number of tubes in shift converter (JK=1), Reformer (JK=2 for methanol and naphtha)

ODTH : OD of tube, ft

OU : O2 utilization

PAT : Ambient pressure, atm

TABLE 1

MAIN PROGRAM NOMENCLATURE
(cont'd)

PIN : Inlet pressure, atm

PINFU : Inlet pressure of fuel cell stacks, atm

PITCH : Pitch of heat exchanger, ft

POP : Operation pressure, atm

POUT : Outlet pressure, atm

PL : Platinum catalyst loading, $mgPT/CM^2$

RHOB : Bulk density of cata., lbs/ft^3

S : Side length of an assumed square flow duct for combustion gas, ft

SITS2 : Ratio of total inside-tube cross-sectional area per pass to header cross-sectional area per pass

SK : Equilibrium constant

SKI : Equilibrium constant with pressure different from 1 atm

SMRA : Steam/fuel ratio

SURFC : Surface per line, ft

SV(1) : Specific volume of fuel 1, ft^3/lbm

SVW : Specific volume of water, ft^3/lbm

TACOA : Inlet air temperature of fuel cell stack, K

TACOF : Inlet fuel temperature of fuel cell stack, K

TAT : Ambient temperature, K

TC : Critical temperature, K

TCAS : Total heat capacity constant A

TCBS : Total heat capacity constant B

TCCS : Total heat capacity constant C

TABLE 1

MAIN PROGRAM NOMENCLATURE
(cont'd)

TDNS : total amount of material, g-mole

TIN : Inlet fluid temperature, K

TOP : Operation temperature, K

TOVO : Total volume of inlet flow, m^3

TOUT : Outlet temperature, K

VHNA : Vaporized heat of naphtha, Cal/g-mole

WAT : Relative humidity of air, g water/g air

WIDAA : Width of square air channel in the fuel cell stack, ft

WIDAF : Width of square fuel channel in the fuel cell stack, ft

X : Necessary amount of oxygen in cathode, g-mole/hr

ZH : Reformer length, ft

DINSC(I) : Inlet amount of gas I, g-mole

DNS(I) : Inlet (outlet) amount of gas I, g-mole

HA(J) : Surface area of heat exchanger J, m^2

HCAS(I),

HCBS(I),

HCCS(I) : Heat capacity const. of gas I, Cal/g-mole-K of the form:

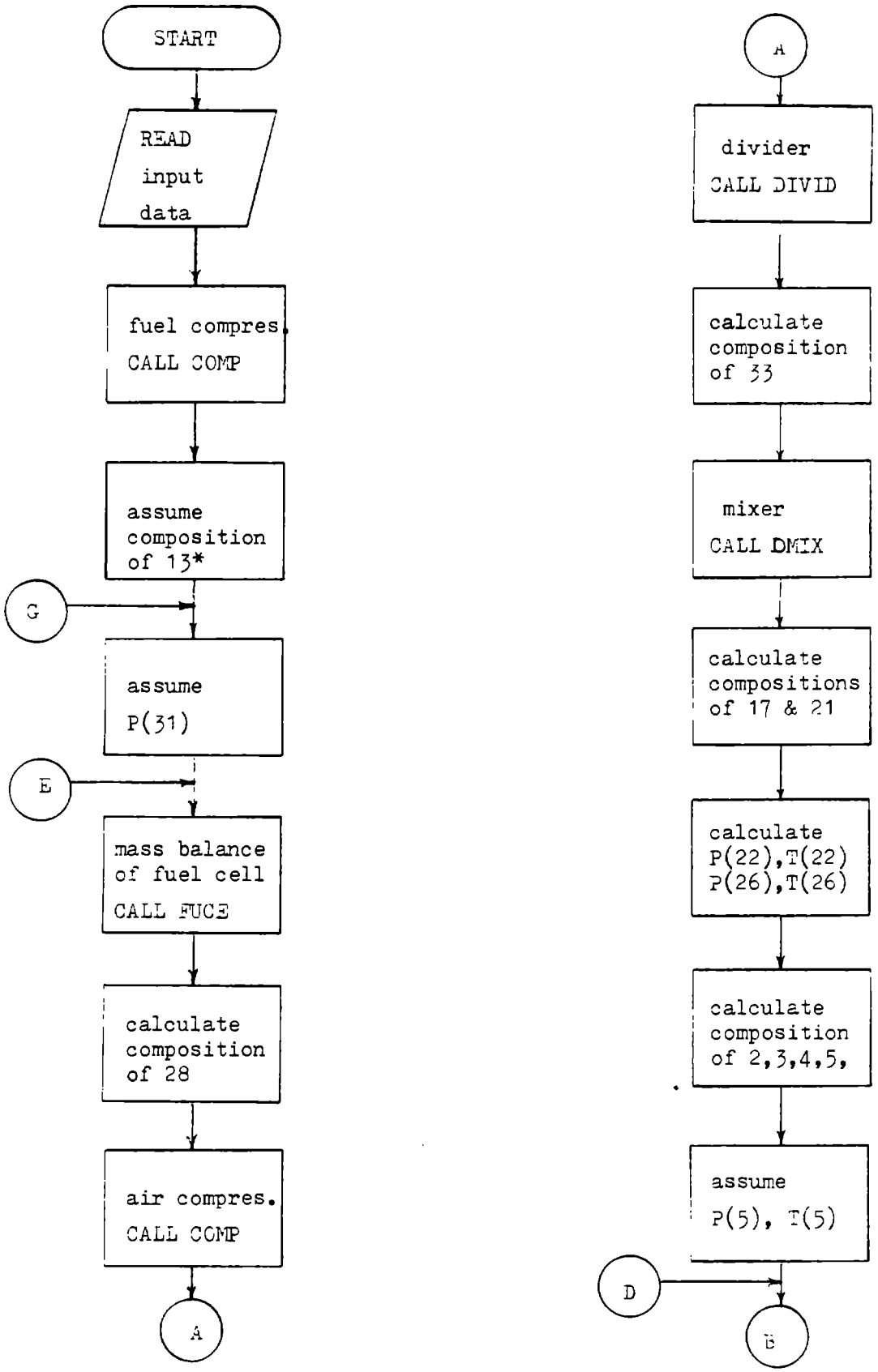
$$HCAS+HCBS*T+HCCS*T^2$$

HS(I) : Heat of formation of gas I at 298 K, 1 atm, Cal/g-mole

NNS(I) : Stoichiometric coefficient of gas I

WM(I) : Molecular weight of gas I, g/g-mole

DNSS(I,J): Flow rate of gas J in stream I, g-mole/hr



* stream number (refer to Figure 1)

Figure 4 Flow chart of executive program for simulating CSU's PAFC system steady state performance

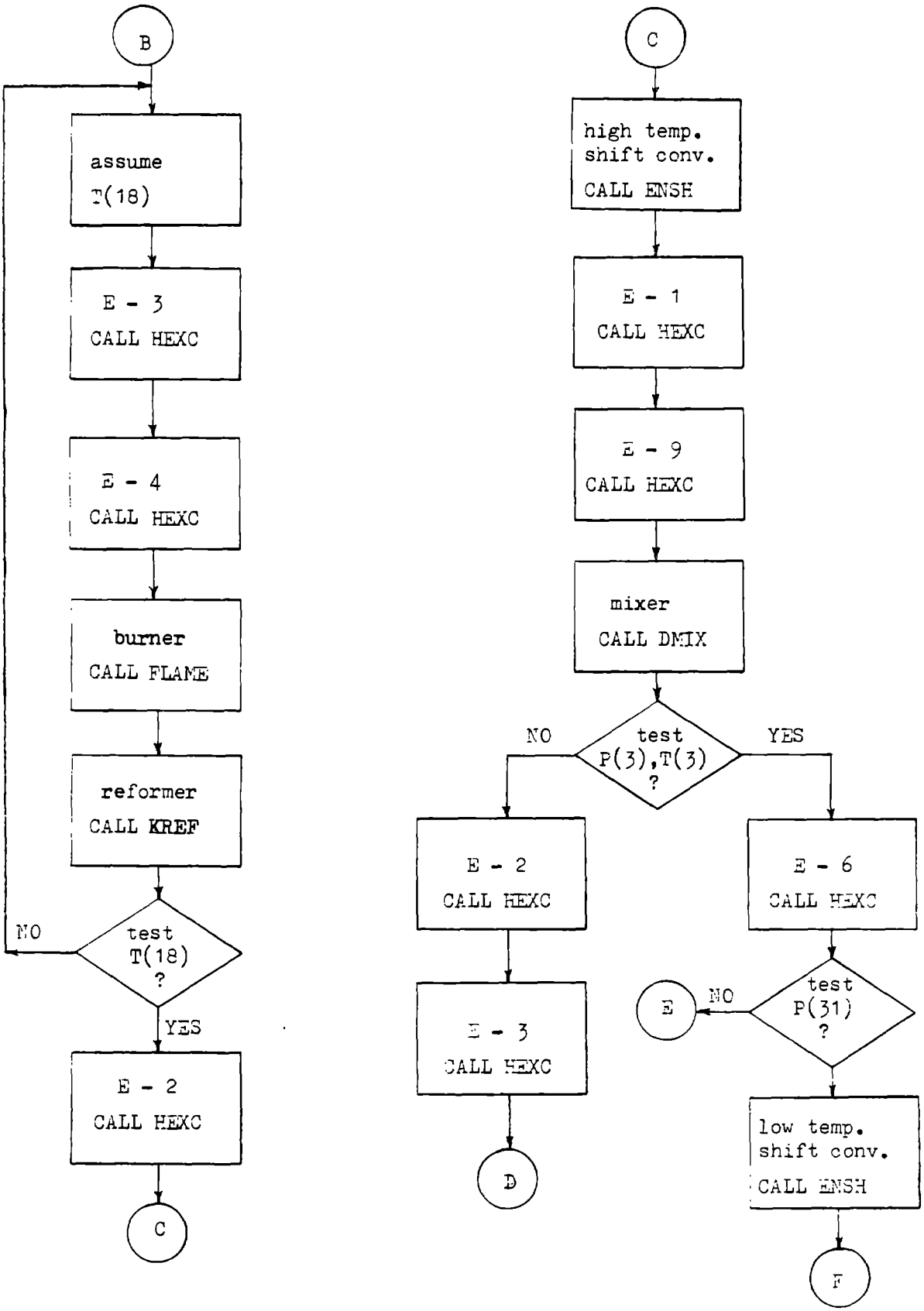


Figure 4 continued

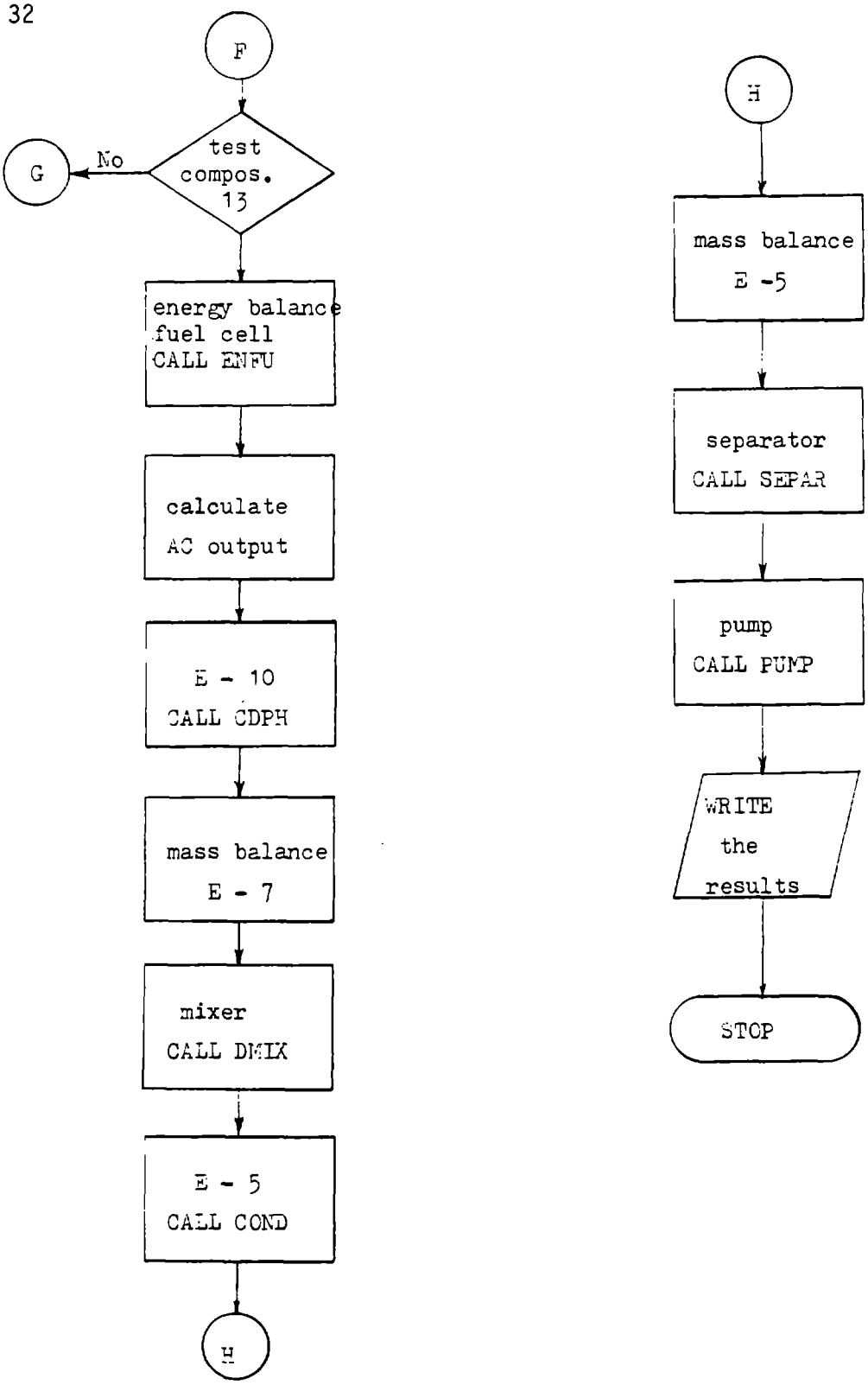


Figure 4 continued

3.2 Subroutines

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

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

1. Calculate the amount of oxygen reacted:

$$X = 0.5*DNS(3)+0.5*DNS(5)+2*DNS(1) \qquad (3\text{-}2\text{-}1)$$

2. Calculate the amount of carbon dioxide produced

$$XY = DNS(3)+DNS(1) \qquad (3\text{-}2\text{-}2)$$

3. Calculate the amount of water produced

$$Y + DNS(5)+2*DNS(1). \qquad (3\text{-}2\text{-}3)$$

4. Calculate the exit composition

$$DNS(1) = 0$$

$$DNS(3) = 0$$

$$DNS(5) = 0$$

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

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

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

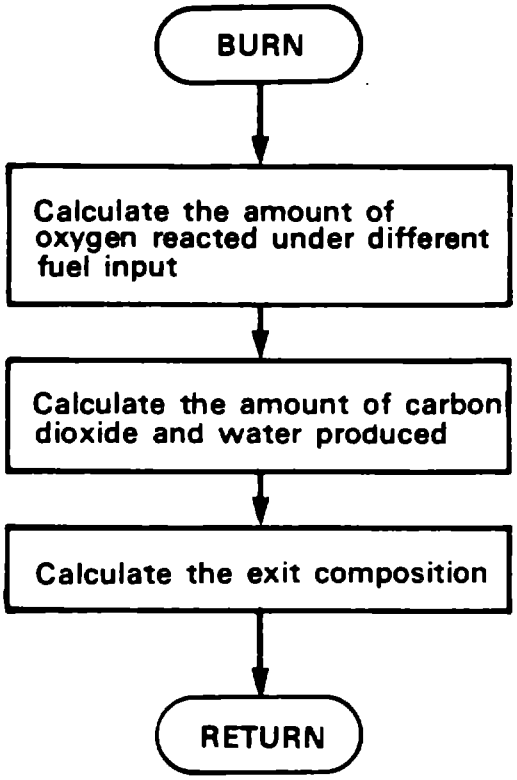


Figure 5 Flow Chart of BURN

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

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

```
QT = ((I-TC1)/(1-0.577))**0.38*9700
     *DNSC(6)+(TCB-TC1)*1*18*DNSC(6).          (3-2-4)
```

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

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

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

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

1. Calculate the compressor shaft work assuming adiabatic conditions

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

2. Calculate the compressor shaft work assuming isothermal conditions

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

3. Calculate the compressor power requirements

```
POW = WS*TDNS/641400                           (3-2-7)
```

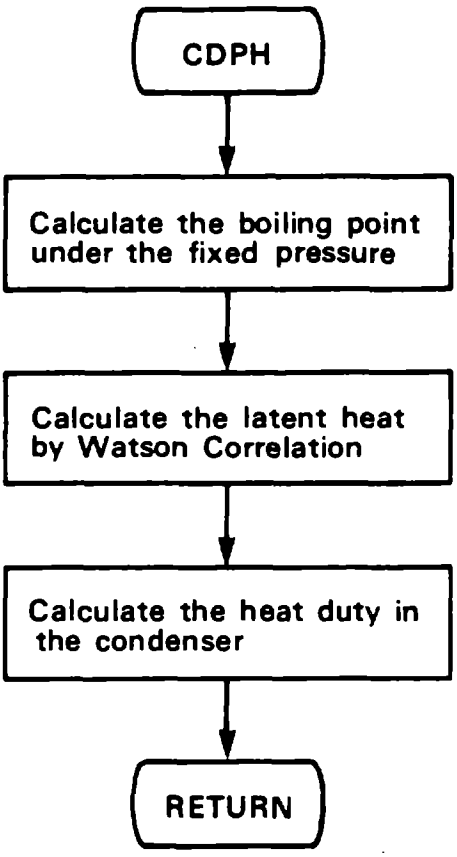


Figure 6 Flow Chart of CDPH

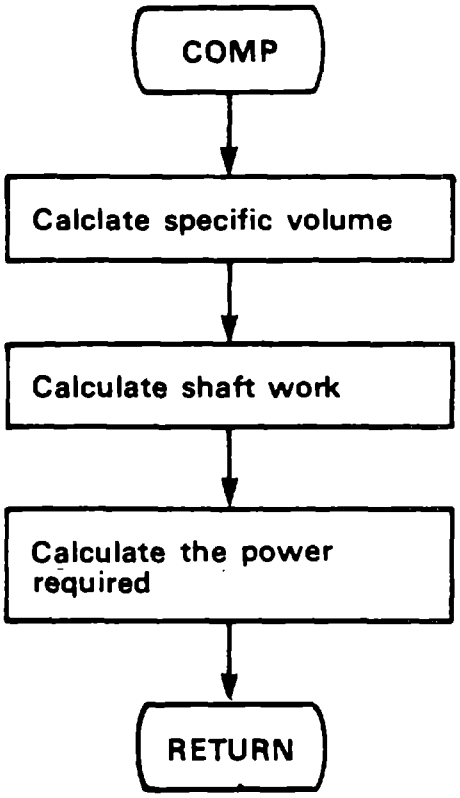


Figure 7 Flow Chart of COMP

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

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

```
QT = QT+DNSH(I)*(HCAS(I)*(THI-THO)+HCBS(I)*(THI**2-THO**2)
     +HCCS(I)*(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*9700*DNSH(6)             (3-2-9)
```

where Watson correction is given as,

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

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

T_{ri}: reduced temperature at condition i.

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

1. Calculate the roots of a given nonlinear function:

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

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

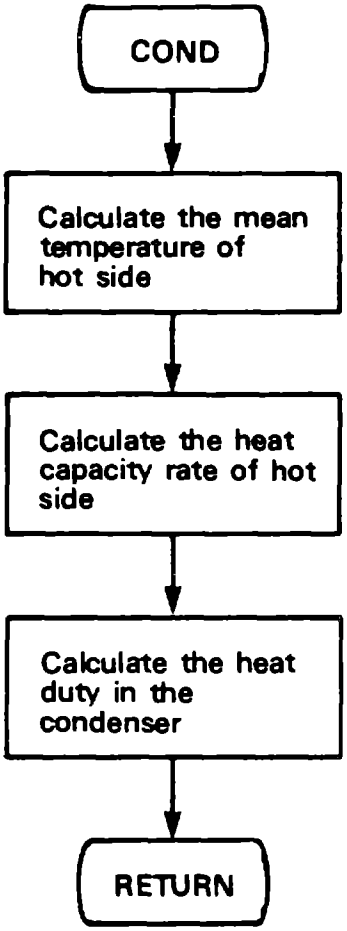


Figure 8 Flow Chart of COND

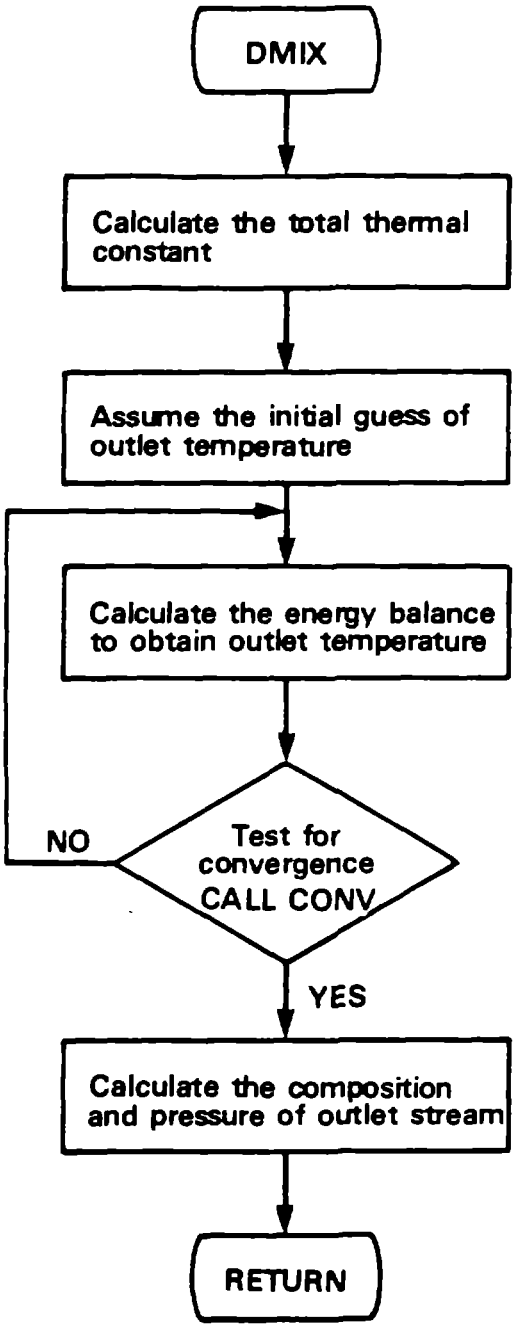


Figure 9 Flow Chart of DMIX

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

1. Calculate the outlet temperature

```
TOUTC = (TCAS1*TIN1+TCAS2*(TIN2-TOUT)+TCBS1/2.*
(TIN1**2-TOUT**2)+TCBS2/2.*(TIN2**2-TOUT**2)+TCCS1*
(TIN1**3-TOUT**3)/3.+TCCS2*(TIN2**3-TOUT**3)/3.)/TCAS1
```

(3-2-12)

2. Calculate the outlet pressure

```
POUT = (TDNS1+TDNS2)/(TDNS1*TINI/PINI+TDNS2*TIN2/PIN2)*TOUT
```

(3-2-13)

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

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

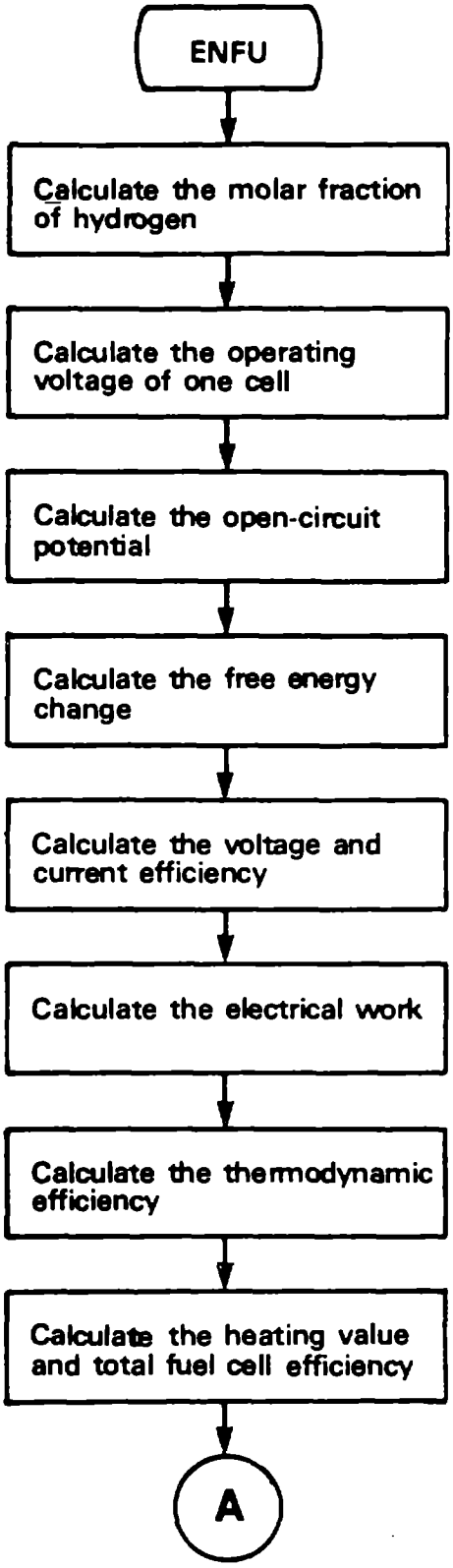


Figure 10 Flow Chart of ENFU

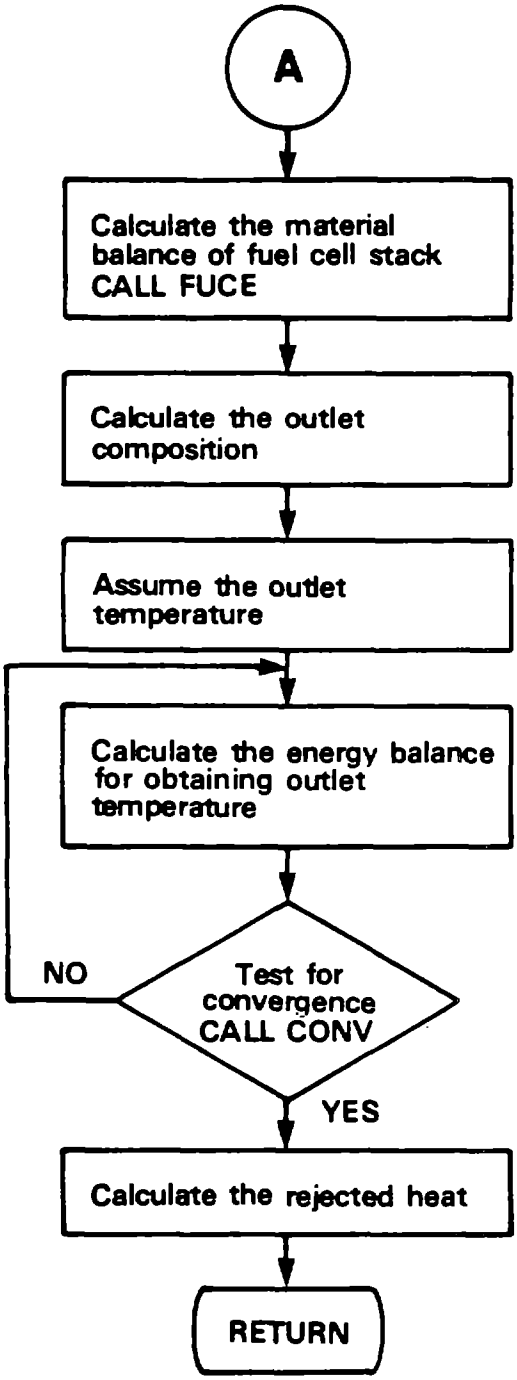


Figure 10 continued

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

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

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

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

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

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

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

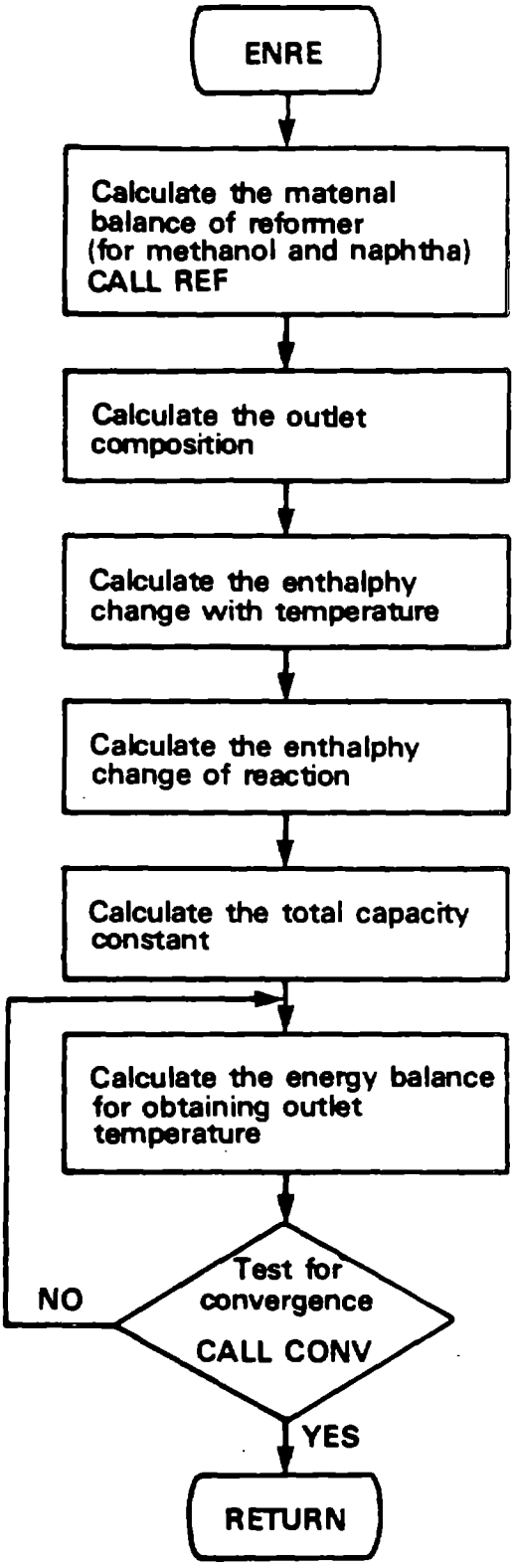


Figure 11 Flow Chart of ENRE

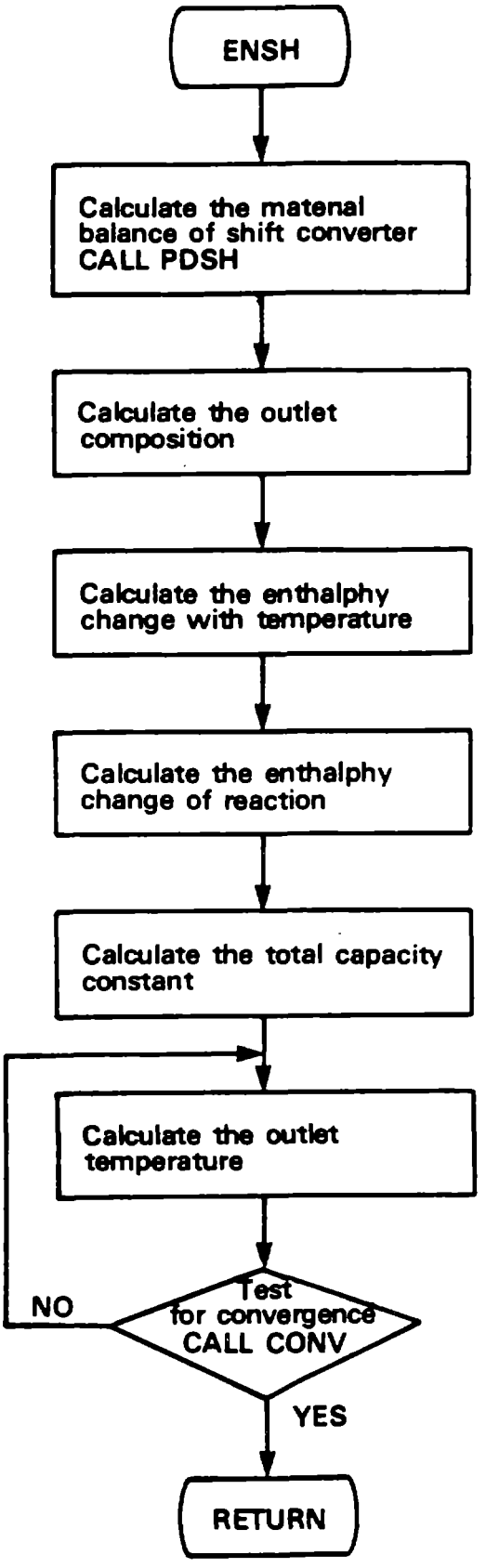


Figure 12 Flow Chart of ENSH

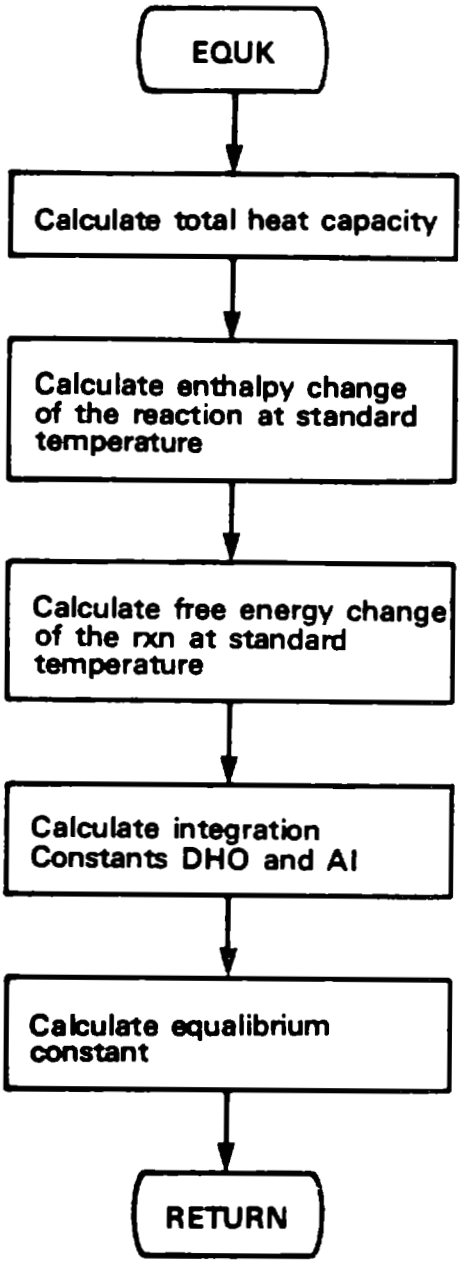


Figure 13 Flow Chart of EQUK

1. Calculate heat capacity constants

```
TCAS = TCAS+NNS(I)*HCAS(I)
TCBS = TCBS+NNS(I)*HCBS(I)                    (3-2-16)
TCCS = TCCS+NNS(I)*HCCS(I)
```

2. Calculate enthalpy of reaction change

```
DH = DH+NNS(I)*HS(I)                          (3-2-17)
```

3. Calculate free energy of reaction

```
DG = DG+NNS(I)*GS(I)                          (3-2-18)
```

4. Calculate constant DHO

```
DHO = DH-TCAS*TST-TCBS*TST**2/2-TCCS*TST*3/3  (3-2-19)
```

5. Calculate constant AI

```
AI = (DHO-DG-TCAS*TST*ALOG(TST)-TCBS/2*TST**2
     -TCCS/6*TST**3)/TST/R                    (3-2-20)
```

6. Calculate equilibrium constant

```
SK = EXP(-DHO/R/TOP+TCAS/R*ALOG(TOP)+TCBS/2*TOP/R
    +TCCS/6/R*TOP**2+AI)                      (3-2-21)
```

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

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

1. Calculate the enthalpy of reaction change at 298 K

```
DH = DH+DNS(I)*HS(I)-DINS(I)*HS(I)                    (3-2-22)
```

2. Calculate the sensible enthalpy change

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

3. Calculate total heat capacity constants

```
TCAS = TCAS+DNS(I)*HCAS(I)
TCBS = TCBS+DNS(I)*HCBS(I)                            (3-2-24)
TCCS = TCCS+DNS(I)*HCCS(I)
```

4. Calculate the adiabatic FLAME temperature

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

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

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

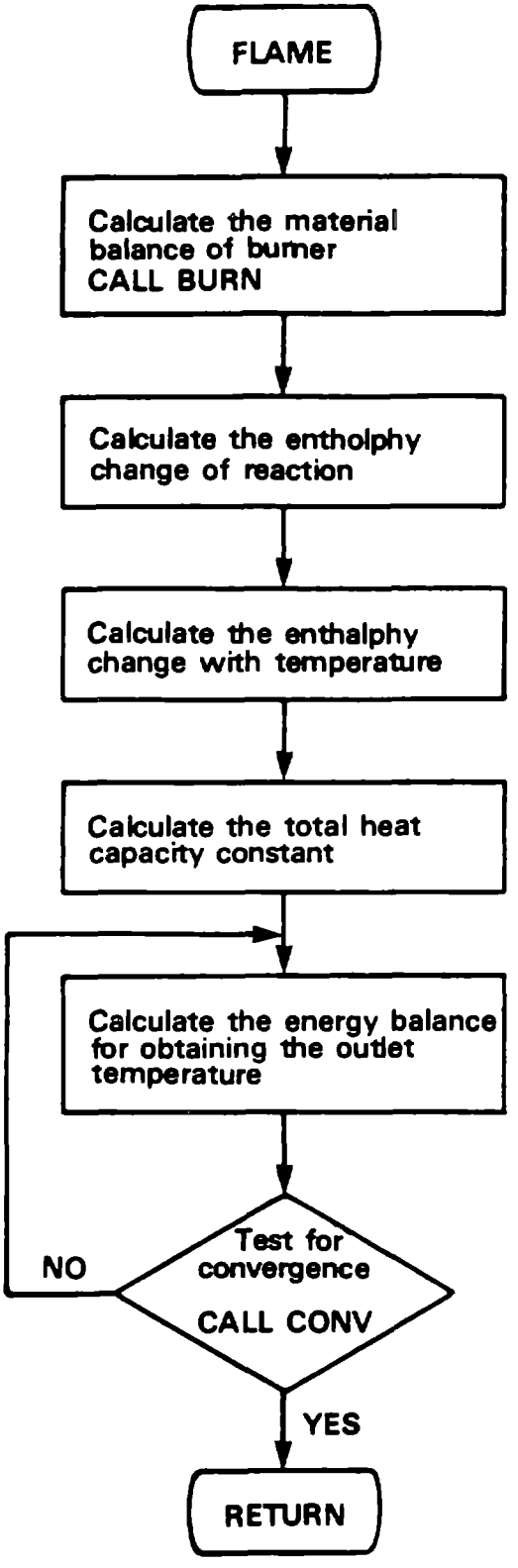


Figure 14 Flow Chart of FLAME

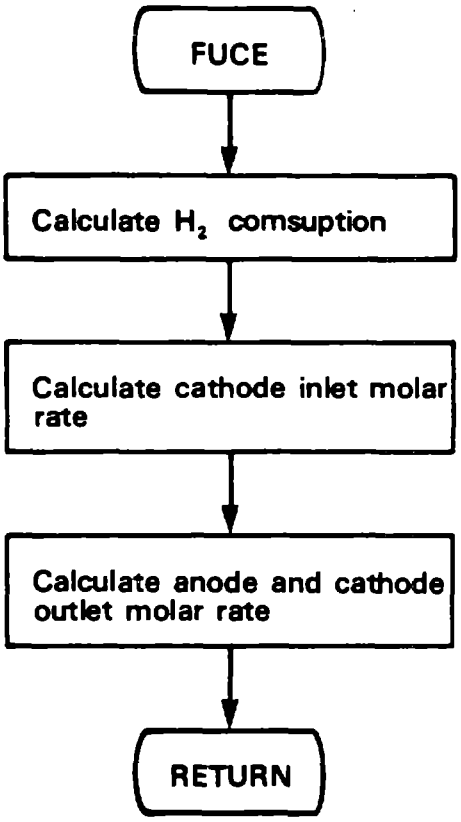


Figure 15 Flow Chart of FUCE

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

1. Calculate the number of tubes

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

2. Calculate number of baffles

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

3. Calculate free area between baffles

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

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

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

5. Calculate friction factor

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

6. Calculate pressure drop

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

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

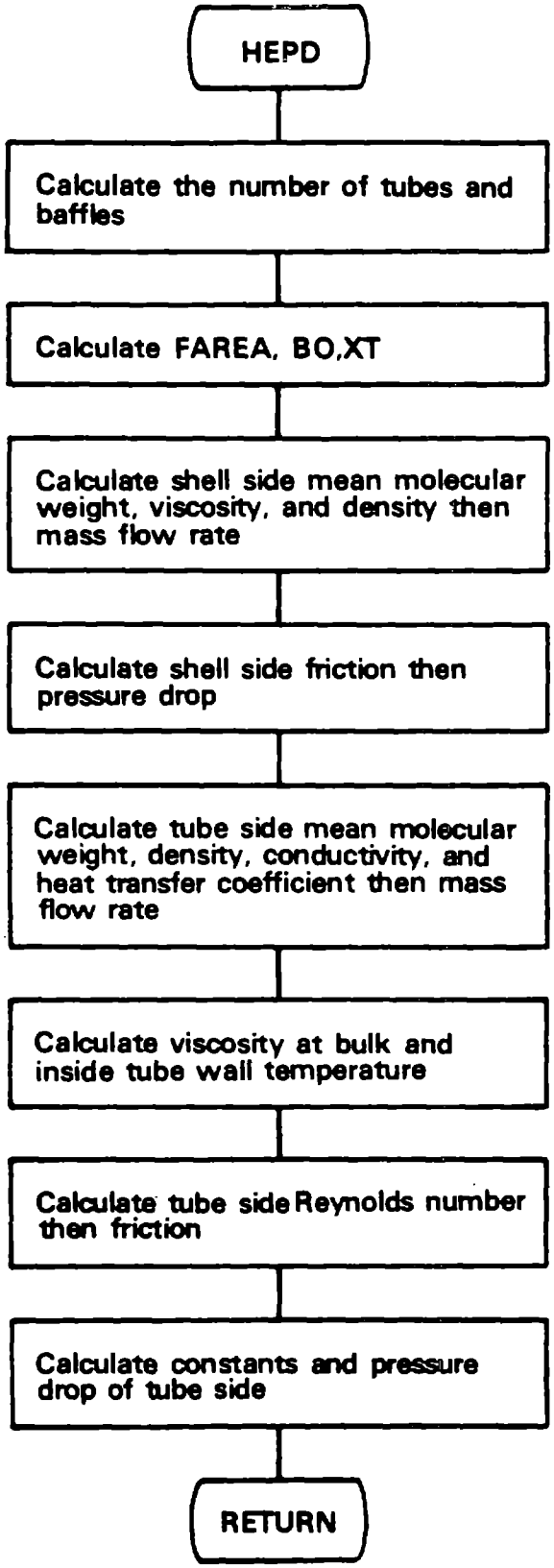


Figure 16 Flow Chart of HEPD

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

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

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

1. Calculate the power required to pump water

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

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 $f2\ (X_1, X_2) = 0$:

$$X_1 \text{ NEW} = X_1 \text{ old} + \Delta X_1$$
$$X_2 \text{ NEW} = X_2 \text{ old} + \Delta X_2 \qquad (3\text{-}2\text{-}33)$$

where

$$\Delta X_1 = \frac{f_2 \frac{\partial f_1}{\partial x_2} - f_1 \frac{\partial f_2}{\partial x_2}}{D}$$
$$\Delta X_2 = \frac{f_1 \frac{\partial f_2}{\partial x_1} - f_2 \frac{\partial f_1}{\partial x_1}}{D} \qquad (3\text{-}2\text{-}34)$$

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

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

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

$$XW = (TDNS-DNS(6)/(DK-1) \qquad (3\text{-}2\text{-}35)$$

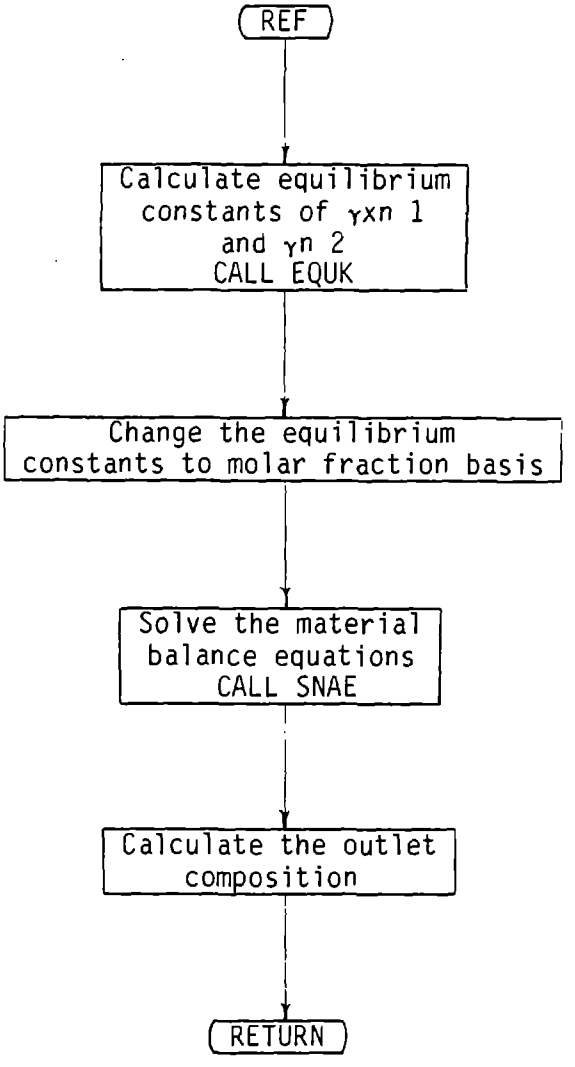


Figure 17: Flow Chart of Subroutine REF

where XW: amount of water in liquid phase

DK: equilibrium constant of liquid-vapor system, which equals to (PSAT/POP)

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

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

3.3 Subroutine KREF

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

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

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

TABLE 2

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

1. Demethanation Reaction Kinetic Mass Balance

$$X1(i+1) = X1(i) = \frac{\epsilon_B \; P \; \Delta Z}{U_o \; C_o} \; Ko^{\,-EA/R[TA(i+1)+460]} \; XMCOMP(i,1)$$

2. Water Gas Shift Equilibrium

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

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

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

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

3. Reforming Gas Energy Balance

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

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

4. Combustion Gas Energy Balance

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

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

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

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

5. Pressure Drop of Reforming Gas

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

where ΔP can be calculated from Ergun equation (Equation (2-1-7)).

TABLE 3

NOMENCLATURE OF VARIABLES AND FUNCTIONS IN SUBROUTINE KREF

Component	Compound
1	CH_4
2	CO
3	CO_2
4	H_2O
5	H_2
6	N_2
7	O_2

Variable	Definition
FL for J = 0 to 7	Total reformer gas feed flow rate and component feed flow rates for components 1 thorugh 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
KO	Frequency factor for Arrhenius expression $k + k_0 \exp(-Eact/RT)$
WM	Molecular weight
EA	Activation energy for demethanation reaction
RHOB	Catalyst bulk density
EPS	Reactor void volume
D1	Reformer center tube outside diameter
D2	Reformer outer tube inside diameter
D3	Reformer outer tube outside diameter
S	Characteristic dimension of the combustion gas flow duct (geometry is square)
DP	Catalyst particle diameter
P	Pressure

TABLE 3

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

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

TABLE 3

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

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

TABLE 3

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

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

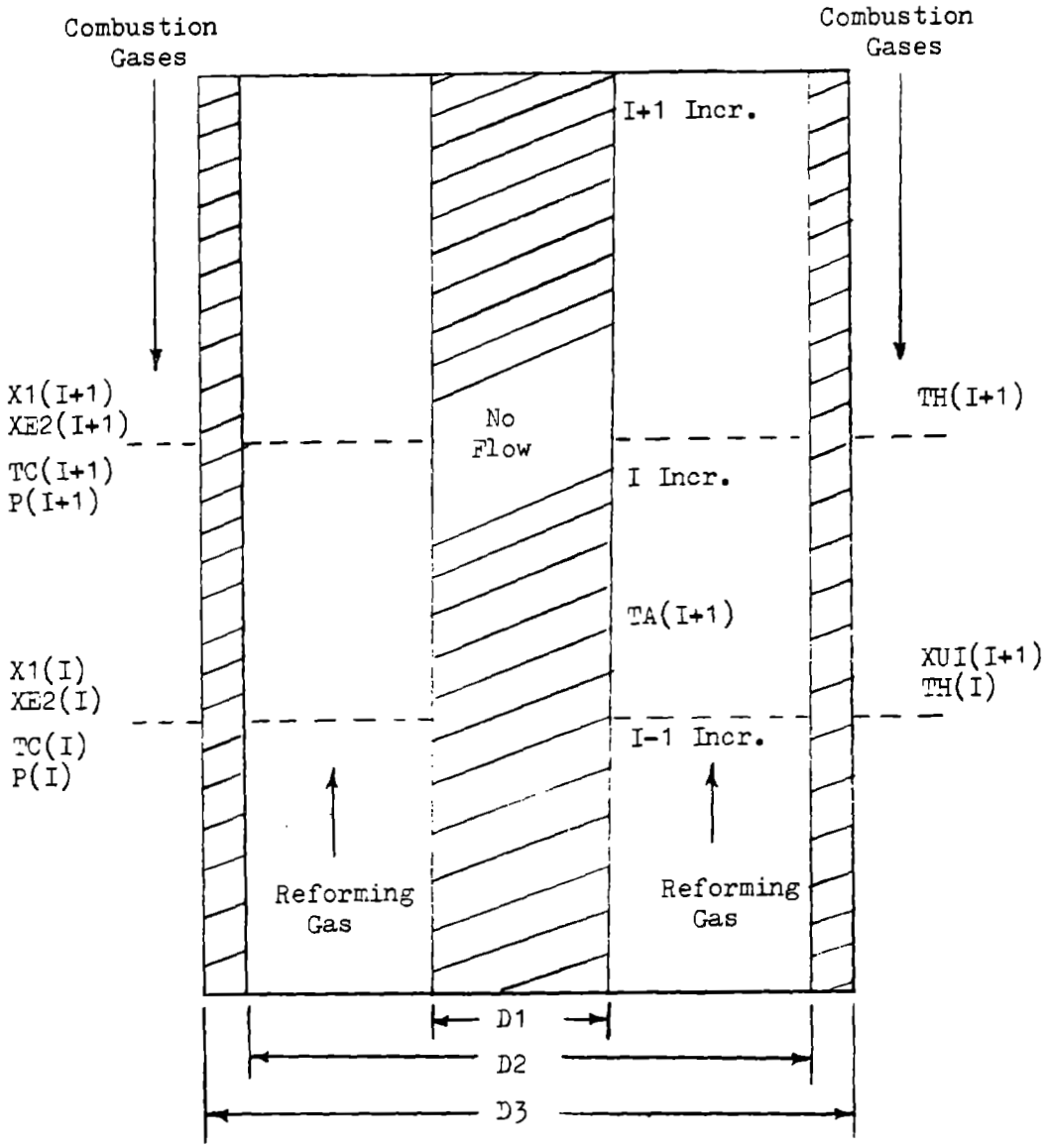


Figure 18 Single Tube Kinetic Reformer Model

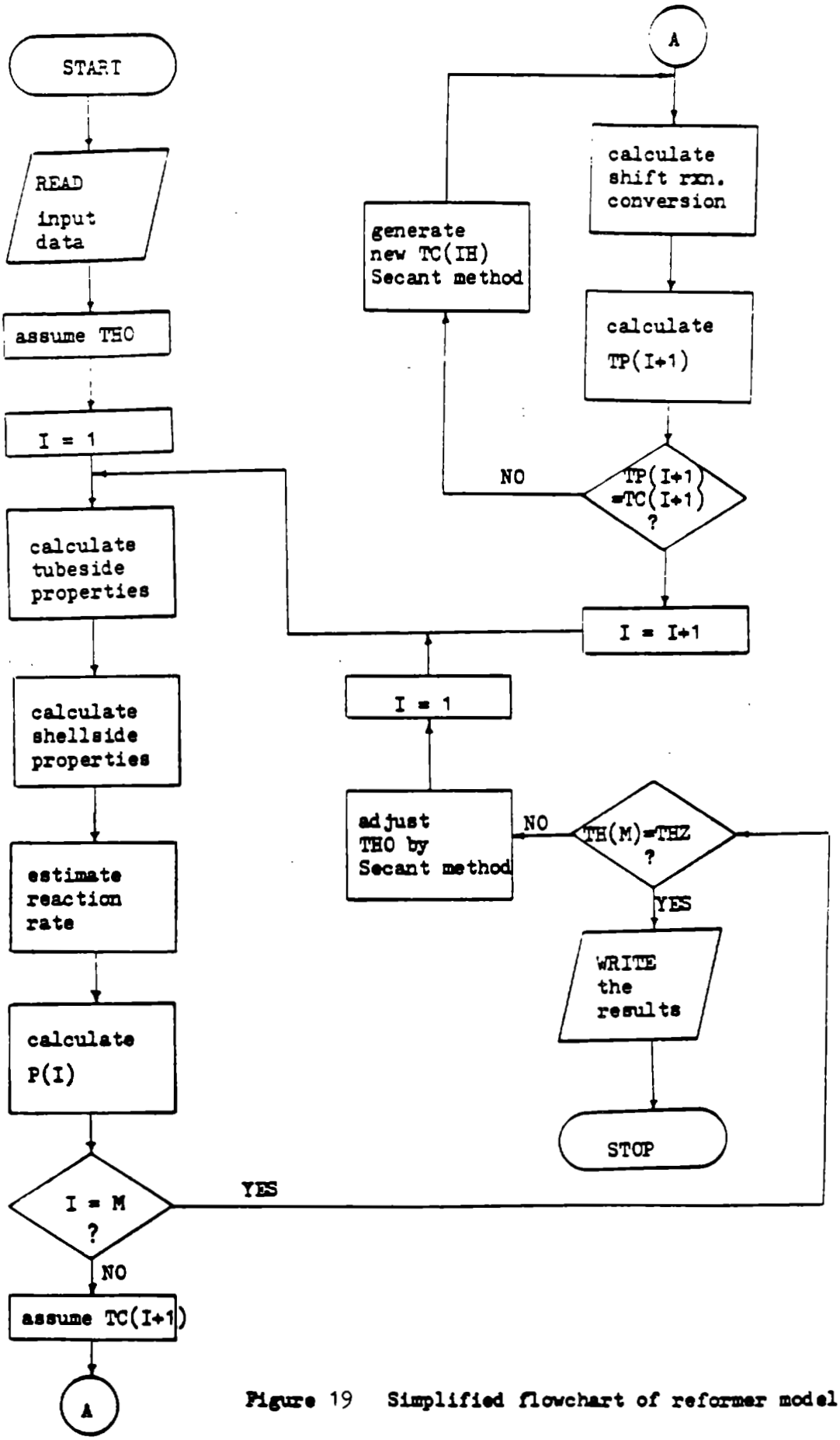


Figure 19 Simplified flowchart of reformer model

3.4 Program Operation

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

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

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

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

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

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

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

TABLE 4

INPUT DATA FOR SIMULATION OF CSU PAFC SYSTEM STEADY STATE PERFORMANCE

(SAMPLE RUN)

NAMELIST LIST	VARIABLE NAME	DIMENSION	SAMPLE VALUE	UNIT	DEFINITION
OPFC	TOPFC		443	K	Operating temperature in fuel cell stack
OPFC	UT		0.8		Utilization of H2 in stack
OPFC	CD		325	mA/cm^2	Designed current density
INIT	DNSM	1	1216.	g-mole/hr	Input mole flow rate of CH_4
		2	0	g-mole/hr	Input mole flow rate of O_2
		3	1.36	g-mole/hr	Input mole flow rate of CO
		4	21.8	g-mole/hr	Input mole flow rate of CO_2
		5	166.	g-mole/hr	Input mole flow rate of H_2
		6	0	g-mole/hr	Input mole flow rate of H_2O
		7	0	g-mole/hr	Input mole flow rat of N_2
INIT	TAT		298	K	Ambient temperture
INIT	PAT		1	atm	Ambient temperature
INIT	SMRA		3.0		Steam to carbon ratio
INIT	POPR		5.0	atm	Operating pressure of reformer
CONDT	IFUEL		1		= 1 Input fuel is methane
					= 2 Input fuel is methanol
					= 3 Input fuel is naphtha
CONDT	ERR		0.01		Criterion of convergence in system trial and error procedure

TABLE 4 (cont'd)

INPUT DATA FOR SIMULATION OF CSU PAFC SYSTEM STEADY STATE PERFORMANCE

(SAMPLE RUN)

NAMELIST LIST	VARIABLE NAME	DIMENSION	SAMPLE VALUE	UNIT	DEFINITION
CONDT	IP		2		= 1 adiabatic operation in shift converters = 2 isothermal operation in shift converters
CONDT	I		7		Number of components in whole system
CONDT	EXT		100		Extra percentage of needed air in burner
CONDT	WAT		0.015	g water/g air	Relative humidity of air
CONDT	EXA		100		Extra percentage of air in fuel cell stack
REPEN	ZH		6	ft	Height of reformer
REPEN	DX1		0	ft	Outside diameter of regenerative tube
REPEN	DX2		0.15	ft	Inside diameter of reforming tube
REPEN	DX3		0.1667	ft	Outside diameter of reforming tube
REPEN	KO		10400	lb-moleCH_4/ lb cata-hr-atm	Rate constant of demethanation reaction
REPEN	EA		20000	Cal/g-mole CH_4	Activity energy of demethanation reaction
REPEN	RHOB		80	lb/ft^3	Density of packing in refomer
REPEN	EPS		0.487		Void fraction in reformer
REPEN	S		0.25	ft	Width of combustion gas square duct
REPEN	DP		0.00328	ft	Diameter of catalyst in reformer
REPEN	DZZ		0.25	ft	Height of finite-difference section
HEATX	CN		1.3	m^2-K	QxA/C min in heat exchanger

TABLE 4 (cont'd)

INPUT DATA FOR SIMULATION OF CSU PAFC SYSTEM STEADY STATE PERFORMANCE

(SAMPLE RUN)

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

TABLE 4 (cont'd)

INPUT DATA FOR SIMULATION OF CSU PAFC SYSTEM STEADY STATE PERFORMANCE

(SAMPLE RUN)

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

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

3.5 Sample Problem

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

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

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

```
&OPFC TOPFC=443.,UT=0.8,CD=325.,
&END
&INIT DNSM=1216.,0.,1.360,21.8,166.,0.,0.,TAT=298.,PAT=1.,SMRA=3.,POPR=5.0
&END
&CONDT IFUEL=1,ERR=0.01,IP=2,I=7,EXT=100.,WAT=0.015,EXA=100.,
&END
&REPEN ZH=6.,DX1=0.,DX2=0.15,DX3=0.1667,K0=1.040E+04,EA=20000.,RHOB=80.
 ,EPS=0.487,S=0.25,DP=0.00328,DZZ=0.25,
&END
&HEATX CN=1.3,U=48825.1,HA(7)=0.2,HA(10)=0.2,
&END
&HEPDC NPH=2,NRH=5,BSPAC=1.,ODTH=.0625,PITCH=.0833,CLH=.0208,IDSH=.833,
IDTH=.04667,FLOAR=.001716,SURFC=.1466,CLENH=2.,S1TS2=0.5,DTH=0.7,
&END
&PDSHH DPD=1.18,0.,AHRN=0.66,.0,APPD=69.,0.,CLEPD=5.91,0.,
NTPD=1,0,
&END
&PDFUH NTAF=140,FULE=1.42,WIDAF=.009744,NPFU=3365,
NTAA=40,AIRL=1.,WIDAA=.00515
&END
&CATAI SRO=.44,SA=400.,CU=.15,CL=.75,ALFA=.5,SN=2.,FCONST=96500.,
DKC=2.4E5,
&END
```

Figure 20 Sample Input Data

```
&OPFC
TOPFC= 443.0
UT= 0.80
CD= 325.0
&END
&INIT
DNSM= 1216.0, 0.0, 1.360, 21.79999, 166.0, 2*0.0
TAT= 298.0
PAT= 1.0
SMRA= 3.0
POPR= 5.0
&END
&CONDT
IFUEL= 1
ERR= 0.9999998E-02
IP= 2
I= 7
EXT= 100.0
WAT= 0.150E-01
EXA= 100.0
&END
&REPEN
ZH= 6.0
DX1= 0.0
DX2= 0.150
DX3= 0.1666999
KO= 10400.0
EA= 20000.0
RHOB= 80.0
EPS= 0.4870
S= 0.250
DP= 0.3280E-02
DZZ= 0.250
&END
&HEATX
CN= 1.299999
U= 48825.10
HA= 6*0.0, 0.20, 2*0.0, 0.20
&END
&HEPDC
NPH= 2
NRH= 5
BSPAC= 1.0
ODTH= 0.6250E-01
PITCH= 0.8329999E-01
CLH= 0.2080E-01
IDSH= 0.8329999
IDTH= 0.46670E-01
FLOAR= 0.17160E-02
SURFC= 0.1465999
CLENH= 2.0
S1TS2= 0.50
DTH= 0.70
&END
&PDSHH
DPD= 1.179999, 0.0
AHRN= 0.660, 0.0
APPD= 69.0, 0.0
CLEPD= 5.910, 0.0
```

Figure 21 Sample Computer Run

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

Figure 21 continued

```
 THE STEAM/METHANE RATIO IN THE REFORMER IS   3.00

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

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

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

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

THE FRACTION OF CO IN THE FEED IS 0.00029

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



THE AC OUTPUT IS  113.77KW
```

Figure 21 continued

STREAM	METHANE	OXYGEN	CAR. MONOXIDE	CAR. DIOXIDE	HYDROGEN	WATER	NITROGEN	FLOW RATE	TEMP.(K)	PRE.(ATM)
1	1216.00	0.00	1.36	21.80	166.00	0.00	0.00	1405.16	298.00	5.1000
2	1216.00	0.00	1.36	21.80	166.00	0.00	0.00	1405.16	612.96	5.0996
3	1216.00	0.00	1.36	21.80	166.00	3648.00	0.00	5053.16	588.38	4.8983
4	1216.00	0.00	1.36	21.80	166.00	3648.00	0.00	5053.16	784.59	4.8975
5	1216.00	0.00	1.36	21.80	166.00	3648.00	0.00	5053.16	1035.87	4.8965
7	141.97	0.00	531.09	566.10	3932.37	2029.68	0.00	7201.20	920.63	4.7243
8	141.97	0.00	531.09	566.10	3932.37	2029.68	0.00	7201.20	755.26	4.7242
9	141.97	0.00	312.87	784.31	4150.58	1811.46	0.00	7201.20	755.26	4.7242
10	141.97	0.00	312.87	784.31	4150.58	1811.46	0.00	7201.20	678.77	4.7241
11	141.97	0.00	312.87	784.31	4150.58	1811.46	0.00	7201.20	591.03	4.7240
12	141.97	0.00	312.87	784.31	4150.58	1811.46	0.00	7201.20	399.68	4.7239
13	141.97	0.00	2.09	1095.10	4461.37	1500.68	0.00	7201.20	399.68	4.7245
14	141.97	0.00	2.11	1095.06	892.25	1500.74	0.00	3632.13	443.00	4.7245
15	141.97	1462.25	2.11	1095.06	892.25	1667.78	5498.04	10759.47	353.52	4.7195
16	141.97	1462.25	2.11	1095.06	892.25	1667.78	5498.04	10759.47	744.09	4.7181
17	0.00	731.12	0.00	1239.15	0.00	2843.97	5498.04	10312.29	1575.99	4.4192
18	0.00	731.12	0.00	1239.15	0.00	2843.97	5498.04	10312.28	1182.31	4.1983
19	0.00	731.12	0.00	1239.15	0.00	2843.97	5498.04	10312.29	1033.81	4.1975
20	0.00	731.12	0.00	1239.15	0.00	2843.97	5498.04	10312.29	664.94	4.1970
21	0.00	2515.63	0.00	1239.15	0.00	6820.70	18917.51	29492.99	525.95	4.4154
22	0.00	2515.63	0.00	1239.15	0.00	6820.70	18917.51	29492.99	357.34	4.4198
23	0.00	2515.63	0.00	1239.15	0.00	3172.68	18917.51	25844.97	357.34	4.4198
24	0.00	0.00	0.00	0.00	0.00	3648.02	0.00	3648.02	357.34	4.4198
25	0.00	0.00	0.00	0.00	0.00	3648.00	0.00	3648.00	357.34	5.0025
26	0.00	0.00	0.00	0.00	0.00	3648.00	0.00	3648.00	421.65	5.0025
27	0.00	0.00	0.00	0.00	0.00	3648.00	0.00	3648.00	586.60	5.0018
28	0.00	5031.25	0.00	0.00	0.00	574.77	18917.50	24523.52	298.00	1.0000
29	0.00	5031.25	0.00	0.00	0.00	574.77	18917.50	24523.52	298.00	4.8139
30	0.00	3569.01	0.00	0.00	0.00	407.72	13419.46	17396.19	298.00	4.8139
31	0.00	3569.01	0.00	0.00	0.00	407.72	13419.46	17396.19	386.41	4.7900
32	0.00	1784.50	0.00	0.00	0.00	3976.73	13419.47	19180.70	443.00	4.7899
33	0.00	1462.25	0.00	0.00	0.00	167.05	5498.04	7127.34	298.00	4.8139
34	0.00	0.00	0.00	0.00	0.00	134510.94	0.00	134510.94	333.00	1.0000
35	0.00	0.00	0.00	0.00	0.00	134510.94	0.00	134510.94	355.00	1.0000
36	0.00	0.00	0.00	0.00	0.00	106332.44	0.00	106332.44	298.00	1.0000
37	0.00	0.00	0.00	0.00	0.00	106332.44	0.00	106332.44	355.00	1.0000

Figure 21 continued

```
THE DUTY OF HEAT EXCHANGER (CAL.) (0 MEANS NO THIS NO. HEAT EXCHANGER)
     E-1          E-2          E-3          E-4          E-5          E-6          E-7          E-8          E-9          E-10
 0.45316E 07  0.99787E 07  0.14123E 08  0.33156E 08  0.10910E 09  0.10777E 08  0.53266E 08      0.00000  0.51060E 07  0.37070E 08

THE SURFACE AREA OF HEAT EXCHANGER (M**2) (0 MEANS NO  THIS NO. HEAT EXCHANGER)
     E-1          E-2          E-3          E-4          E-5          E-6          E-7          E-8          E-9          E-10
 0.38308E 00  0.13541E 01  0.14964E 01  0.22603E 01  0.21182E 02  0.14996E 01  0.20000E 00      0.00000  0.82420E 00  0.20000E 00

THE EFFICIENCY OF HEAT EXCHANGER (0 MEANS NO THIS NO.  HEAT EXCHANGER OR IS CONDENSER)
     E-1          E-2          E-3          E-4          E-5          E-6          E-7          E-8          E-9          E-10
 0.68881E 00  0.59056E 00  0.63181E 00  0.57412E 00    0.00000  0.65302E 00    0.00000      0.00000  0.64153E 00    0.00000

THE POWER OF AIR COMPRESSOR:      64.04HP
THE POWER OF METHANE COMPRESSOR:       3.80HP
THE POWER OF PUMP :    0.00146HP
```

Figure 21 continued

3.6 Discussion

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

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

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

3.7 Further Developments

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

Further developments have been completed, which include 3-D temperature and current density distributions (distributed model) of fuel cel 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).

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Listing of the Steady State Performance Lumped Model

```
0000020C      BLOCK DATA
0000040CC
0000060 C******BLOCK DATA FOR CSU PROGM FUEL CELL POWER PLANT PERFORMANCE
0000100C      DIMENSION GS(7),HS(7),HCAS(7),HCBS(7),HCCS(7),WM(7),SV(3),
0000120C     1HLHV(7),A1(2,7),A2(2,7),A3(4,7)
0000140C      COMMON /ETHDA/ GS,HS,HCAS,HCBS,HCCS
0000160C      COMMON /TC/ TC/CONS/ A,B
0000180C      COMMON /GAG/ GAGM,GAGA
0000200C      COMMON /NAPH/HNA,BPNA,WMNA,VHNA
0000220C      COMMON /WM/ WM
0000240C      COMMON/SV/ SV,SVW
0000260C      COMMON/HLHV1/ HLHV
0000280C      COMMON/THCC/A1/VIPC/A2/HTCPC/A3
0000300CC
0000320CC STANDARD VALUE OF FREE ENERGY, ENTHALPHY AND HEAT CAPACITY CONSTANT
0000340C      DATA GS/-12140.,0.,-32781.,-94258.,0.,-54635.,0./
0000360C      DATA HS/-17889.,0.,-26416.,-94051.,0.,-57798.,0./
0000380C      DATA HCAS/3.381,6.148,6.42,6.214,6.947,7.256,6.524/
0000400       DATA HCBS/.018044,.003102,.001665,.010396,-.0002,.002298,.00125/
0000420       DATA HCCS/-4.3E-06,-9.23E-07,-1.96E-07,-3.545E-06,4.81E-07,2.83E-07,1.E-09/
0000440CC THE MOL. WEIGHT OF GASES
0000460C      DATA WM/16.,32.,28.,40.,2.,18.,28./
0000480CC THE THERMAL DATA OF NAPHTHA
0000500CC     DATA HNA/0.58/,BPNA/103.4/,VHNA/7680./
0000520CC THE CONST. FOR CAL. SATURATED PRESSURE (EXP(A-B/T))
0000540C      DATA A,B/13.954316,5204.9597/
0000560CC CRITICAL TEMPERATURE OF WATER
0000580C      DATA TC/646.447/
0000600CC INSERT RATIO OF HEAT CAPASITY
0000620C      DATA GAGM/1.3/,GAGA/1.4/
0000640CC INSERT THE SPECIFIC VOLUME OF FUEL AND WATER
0000660       DATA SV/0.,.02034,.021/,SVW/.0162/
0000680CC INSERT THE HEATING VALUE
0000700C      DATA HLHV/-191762.,0.,-67636.,0.,-57798.,0.,0./
0000720CC INSERT THE SPECIFIC HEAT CAPACITIES, BTU/R-LB-MOLE
0000740C      DATA A3/5.34,6.39E-03,0.,0.,6.60,6.67E-04,0.,0.,10.34,1.52E-03,0.,
0000760C     1-6.33420E+05,8.22, 8.3E-05,4.136E-07,0.,6.62,4.5E-04,0.,0.,6.5,
0000780C     25.56E-04,0.,0.,6.732,8.36E-03,5.53E-09,0./
0000800CC INSERT VISCOSITY, LBM/FT-HR
0000820C      DATA A2/3.4373E-05,2.5861E-02,3.8185E-05,4.8688E-02,5.0368E-05,
0000840C     13.3634E-02,5.221E-05,1.7532E-02,1.8789E-05,2.312E-02,4.2318E-05,
0000860C     24.6721E-02,2.4580E-05,5.5613E-02/
0000880CC INSERT THERMAL CONDUCTIVITY, BTU/HR-FT-F
0000900C      DATA A1/6.6539E-05,7.4614E-03,1.5349E-05,1.6581E-02,2.0451E-05,
0000920C     11.1726E-02,4.046E-05,1.8765E-03,1.1899E-04,1.0126E-01,1.6774E-05,
0000940C     21.5182E-02,1.792E-05,1.67E-02/
0000960C      END
0000980 C
0001000 C     ***************************************************************
0001020 C     THIS PROGRAM IS USING FORTRAN TO SIMULATE THE PHOSPHORIC ACID FUEL
0001040 C     CELL SYSTEM
0001060 C     ***************************************************************
0001080 C
0001100 C     DEFINITION:
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0001120 C     A  : CONSTANT FOR CAL. SATURATED CONDITION OF WATER
0001140 C     AA1: THERMAL CONDUCTIVITY COEFF. OF GAS I, BTU/HR-FT-F
0001160 C     AA2: VISCOSITY COEFF. OF GAS I, LBM/FT-HR
0001180 C     AA3: SPECIFIC HEAT CAPACITY COEFF. OF GAS I, BTU/R-LB-MOLE
0001200 C       OF THE FORM:AA3(1)+AA3(2)*T+AA3(3)*T**2+AA3(4)/T**2
0001220 C     AHLU: MOLE FRACTION OF AVAILABLE HYDROGEN
0001240 C     AHEN: PERCENT FREE-GAS SPACE
0001260 C     AIRL: LENGTH OF AIR CHANNEL, FT
0001280 C     ALFA: TRANSFER COEFF.
0001300 C     APFD: TOTAL SURFACE AREA OF PACKING ACC. TO THE BASIS AND OPER.
0001320 C     TEMPERATURE, FT**2
0001340 C     ATMP: OUTLET TEMP. OF GASES, K
0001360 C     B  : CONSTANT FOR CAL. SATURATED CONDITION OF WATER
0001380 C     BPNA: BOILING POINT OF NAPHTHA, C
0001400 C     BSPAC: BAFFLE SPACE, FT
0001420 C     CD: CURRENT DENSITY,MAMP/CM**2
0001440 C     CL: CATALYST LOADING,MG/CM**2
0001460 C     CLENH: LENGTH OF TUBE IN HEAT EXCHANGER, FT
0001480 C     CLEFD: LENGTH OF SHIFT CONVERTER(JK=1),REFORMER(JK=2 FOR METHANOL
0001500 C        NAPHTHA), FT
0001520 C     CLH: CLEARANCE IN HEAT EXCHANGER, FT
0001540 C     CN: Q*A/CMIN IN HEAT EXCHANGER
0001560 C     CU: CATALYST UTILIZATION
0001580 C     DG: STANDARD FREE ENERGY CHANGE,CAL/G-MOLE
0001600 C     DH: STANDARD ENTHALPHY CHANGE AT REACTION,CAL/G-MOLE
0001620 C     DHIN: ENTHALPHY CHANGE DUE TO TEMPERATURE CHANGE OF INLET FLUID
0001640 C     CAL./G-MOLE
0001660 C     DKC: CONST. TO CALC. LIMITING CURRENT DENSITY
0001680 C     DHO: INTEGRATION CONSTANT IN CALCULATE H
0001700 C     DP: CATALYST PELLET DIAMETER, FT
0001720 C     DPD: DIA. OF SHIFT CONVERTER(JK=1),REFORMER(JK=2 FOR METHANOL AND
0001740 C       NAPHTHA), FT
0001760 C     DSHO: CATHODE INLET WATER OF FUEL CELL, G-MOLE/HR.
0001780 C     DSN: CATHODE INLET NITROGEN OF FUEL CELL, G-MOLE/HR.
0001800 C     DSO: CATHODE INLET OXYGEN OF FUEL CELL, G-MOLE/HR.
0001820 C     DTH: FRACTION OF DELTA T OVER INLET GAS FILM IN THE HEAT EXCHANGER
0001840 C     DX1: OUTSIDE DIAMETER OF REFORMER CENTER TUBE, FT
0001860 C     DX2: INSIDE DIAMETER OF OUTSIDE REFORMER TUBE, FT
0001880 C     DX3: OUTSIDE DIAMETER OF OUTSIDE REFORMER TUBE, FT
0001900 C     DZZ: INCREMENT HEIGHT OF FINITE DIFFERENCE MODEL IN THE REFORMER,
0001920 C     EA: ACTIVATION ENERGY FOR ARRHENIUS EXPRESSION, CAL/GMOLE CH4
0001940 C     EPS: REACTOR VOID FRACTION
0001960 C     ERR: CONVERGE CRITERIA
0001980 C     EXA: FRACTION OF EXTRA AIR IN FUEL CELL
0002000 C     EXT: FRACTION OF EXTRA AIR IN BURNER
0002020 C     FCO: MOLE FRACTION OF CO CONTAIN
0002040 C     FCONST: FARADAY CONSTANT,23061 CAL/VOLT-GM EQUIV.
0002060 C     FLOAR:FLOW AREA IN HEAT EXCHANGER, FT**2
0002080 C     FULE: LENGTH OF FUEL CHANNEL, FT
0002100 C     HNA: SPECIFIC HEAT OF NAPHTHA, BTU/LBM-R
0002120 C     I  : GAS NUMBER
0002140 C      I=1 FUEL(METHANE,METHANOL,NAPHTHA)
0002160 C      I=2 OXYGEN            OR CARBON MONOXIDE(IN SUB. KREF AND
0002180 C                            RELATED SUBROUTINES)
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0002200 C      I=3 CARBON MONOXIDE   OR CARBON DIOXIDE(   "    )
0002220 C      I=4 CARBON DIOXIDE    OR WATER(    "    )
0002240 C      I=5 HYDROGEN
0002260 C      I=6 WATER             OR NITROGEN(    "    )
0002280 C      I=7 NITROGEN          OR OXYGEN(    "    )
0002300 C     IDSH: ID OF SHELL IN HEAT EXCHANGER, FT
0002320 C     IDTH: ID OF TUBE IN HEAT EXCHANGER, FT
0002340 C     IFUEL: FUEL TYPE
0002360 C       1: METHANE CH4
0002380 C       2: METHANOL CH3OH
0002400 C       3: NAPHTHA  C7H16
0002420 C     IDNO: NO. OF REDO
0002440 C     IHUI: STOICHIOMETRIC NUMBER
0002460 C     IP: INDEX OF OPERATION CONDITION IN THE REFORMER(NOT FOR METHANE)
0002480 C       SHIFT CONVERTOR
0002500 C      IP=1 ADIABATIC OPERATION
0002520 C      IP=2 ISOTHERMAL OPERATION
0002540 C     K0: FREQUENCY FACTOR FOR ARRHENIUS EXPRESSION, LB MOLE CH4/LB
0002560 C     CATA.-HR-ATM
0002580 C     NN: STREAM NU-BER OF EXIT OF SHIFT CONVERTER
0002600 C     NCR: SCALE UP FACTOR IN THE MODEL OF REFORMER
0002620 C     NPFU: NO. OF CELL PLATE IN THE FUEL CELL STACK
0002640 C     NPH: NO. OF TUBE PASSES
0002660 C     NRH: NO. OF ROWS FOR TUBES
0002680 C     NTAA: NO. OF AIR FLOW CHANNEL IN ONE CELL PLATE
0002700 C     NTAF: NO. OF FUEL FLOW CHANNEL IN ONE CELL PLATE
0002720 C     NTPD: NO. OF TUBES IN SHIFT CONVERTER(JK=1),REFORMER(JK=2 FOR
0002740 C     METHANOL AND NAPHTHA)
0002760 C     ODTH: OD OF TUBE, FT
0002780 C     OU: O2 UTILIZATION
0002800 C     PAT: AMBIENT PRESSURE, 1ATM
0002820 C     PIN: INLET PRESSURE, ATM
0002840 C     PINFU: INLET PRESSURE OF FUEL CELL STACK, ATM
0002860 C     PITCH: PITCH OF HEAT EXCHANGER, FT
0002880 C     POP: OPERATION PRESSURE, ATM
0002900 C     POUT: OUTLET PRESSURE, ATM
0002920 C     RHOB: BULK DENSITY OF CATA., LBS/FT**3
0002940 C     S: SIDE LENGTH OF AN ASSUMED SQUARE FLOW DUCT FOR COMBUSTION GAS,
0002960 C     SITS2: RATIO OF TOTAL INSIDE-TUBE CROSS-SECTIONAL AREA PER PASS TO
0002980 C        HEADER CROSS-SECTIONAL AREA PER PASS
0003000 C     SA: CATALYST SURFACE,CM**2/MG
0003020 C     SK: EQUALIBRIUM CONSTANT
0003040 C     SK1: EQUALIBRIUM CONSTANT WITH PRESSURE DIFFERENT FROM 1 ATM
0003060 C     SMRA: STEAM/FUEL
0003080 C     SN: NUMBER OF FARADAY EQUIVALENTS TRANSFERED
0003100 C     SRO: CELL RESISTANCE AT 480 K,OHM-CM**2
0003120 C     SURFC: SURFACE PER LINE, FT
0003140 C     SV(I): SPECIFIC VOLUME OF FUEL I, FT**3/LBM
0003160 C     SVW: SPECIFIC VOLUME OF WATER, FT**3/LBM
0003180 C     TACOA: INLET AIR TEMP. OF FUEL CELL STACK, K
0003200 C     TACOF: INLET FUEL TEMP. OF FUEL CELL STACK, K
0003220 C     TAT: AMBIENT TEMPERATURE, 298 K
0003240 C     TC: CRITICAL TEMPERATURE, K
0003260 C     TCAS: TOTAL HEAT CAPACITY CONSTANT A
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0003280 C     TCBS: TOTAL HEAT CAPACITY CONSTANT B
0003300 C     TCCS: TOTAL HEAT CAPACITY CONSTANT C
0003320 C     TDNS: TOTAL AMOUNT OF MATERIAL, G-MOLE
0003340 C     TIN: INLET FLUID TEMPERATURE, K
0003360 C     TOP: OPERATION TEMPERATURE, K
0003380 C     TOVO: TOTAL VOLUME OF INLET FLOW, M**3
0003400 C     TOUT: OUTLET TEMPERATURE, K
0003420 C     VHNA: VAPORIZED HEAT OF NAPHTHA, CAL/G-MOLE
0003440 C     WAT: RELATIVE HUMIDITY OF AIR, G WATER/G AIR
0003460 C     WIDAA: WIDTH OF SQUARE AIR CHANNEL IN THE FUEL CELL STACK, FT
0003480 C     WIDAF: WIDTH OF SQUARE FUEL CHANNEL IN THE FUEL CELL STACK, FT
0003500 C     X   : THE NECESSARY AMOUNT OF OXYGEN IN CATHODE, G-MOLE/HR.
0003520 C     ZH: REFORMER LENGTH, FT
0003540 C     DINS(I): INLET AMOUNT OF GAS I, G-MOLE
0003560 C     DNS(I): INLET (OUTLET) AMOUNT OF GAS I, G-MOLE
0003580 C     HA(J): SURFACE AREA OF HEAT EXCHANGER J
0003600 C     HCAS(I),HCBS(I),HCCS(I): HEAT CAPACITY CONST. OF GAS I, CAL/G-MOLE
0003620 C                              OF THE FORM:HCAS+HCBS*T+HCCS*T**2
0003640 C     HS(I): HEAT OF FORMATION OF GAS I AT 298 K, 1ATM
0003660 C     NNS(I): STOICHIOMETRIC COEFFICIENT OF GAS I
0003680 C     WM(I): MOLECULAR WEIGHT OF GAS I, G/G-MOLE
0003700 C     DNSS(I,J): FLOW RATE OF GASJ IN STREAM I, G-MOLES/HR
0003720 C
0003740       REAL K0,IDSH,IDTH
0003760       DIMENSION GS(7), HS(7), HCAS(7), HCBS(7), HCCS(7), WM(7)
0003780       DIMENSION DNSL(7), DNSV(7), HLHV(7)
0003800       DIMENSION DNSS(39,7), T(39), P(39), TDNSS(39)
0003820       DIMENSION DNS1(7), DNS2(7), DNS(7), DNSM(7), DNSAN(7), DNSCA(7), D-
0003840      1NSAI(7), DNSC(7), DNSH(7)
0003860       DIMENSION QQT(10), HA(10), EFF(10), NT(10)
0003880       DIMENSION DNSR(7), DNSF(7)
0003900       DIMENSION DPD(2), AHRN(2), APPD(2), CLEPD(2), NTPD(2), SV(3)
0003920       DIMENSION AA1(2,7), AA2(2,7), AA3(4,7)
0003940       NAMELIST /REPEN/ ZH,DX1,DX2,DX3,K0,EA,RHOB,EPS,S,DP,DZZ
0003960       NAMELIST /HEATX/ CN,U,HA
0003980       NAMELIST /OPFC/ TOPFC,UT,CD
0004000       NAMELIST /INIT/ DNSM,TAT,PAT,SMRA,POPR
0004020       NAMELIST /CONDT/ IFUEL,ERR,IP,I,EXT,WAT,EXA
0004040       NAMELIST /HEPDC/ NPH,NRH,BSPAC,ODTH,PITCH,CLH,IDSH,IDTH,FLOAR,SURF-
0004060      1C,CLENH,S1TS2,DTH
0004080       NAMELIST /PDSHH/ DPD,AHRN,APPD,CLEPD,NTPD
0004100       NAMELIST /PDFUH/ NTAF,FULE,WIDAF,NPFU,NTAA,AIRL,WIDAA
0004120       NAMELIST /TR/ TOPR
0004140       NAMELIST /CATAI/ SRO,SA,CU,CL,ALFA,SN,FCONST,DKC
0004160 C
0004180       COMMON /TC/ TC/CONS/A,B/GAG/GAGM,GAGA
0004200       COMMON /CONST/ I
0004220       COMMON /EXA/ EXA
0004240       COMMON /ETHDA/ GS,HS,HCAS,HCBS,HCCS
0004260       COMMON /HUMI/ WAT
0004280       COMMON /EXT/ EXT
0004300       COMMON /U1/ U
0004320       COMMON /CONFC/ E,ETH,EI,EV,EC,EFC
0004340       COMMON /HE/ HE
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0004360       COMMON /CN1/ CN
0004380       COMMON /NAPH/ HNA,BPNA,WMNA,VHNA
0004400       COMMON /WM/ WM
0004420       COMMON /HEPDT/ NPH,NRH,BSPAC,ODTH,PITCH,CLH,IDSH,IDTH,FLOAR,SURFC,-
0004440      1CLENH,SITS2,DTH
0004460       COMMON /PDSHT/ DPD,AHRN,APPD,CLEPD,NTPD
0004480       COMMON /PDFUT/ NTAF,NTAA,FULE,AIRL,WIDAF,WIDAA,NPFU
0004500       COMMON /REP/ KO,EA,RHOB,EPS,DZZ
0004520       COMMON /SV/ SV,SVW
0004540       COMMON /HLHV1/ HLHV
0004560       COMMON /THCC/ AA1/VIPC/AA2/HTCPC/AA3
0004580       COMMON /CATAL/ SRO,SA,CU,CL,ALFA,SN,FCONST,AREAF,DKC
0004600 C
0004620       DATA DNSS/273*0./
0004640 C     READ   THE OPERATION CONDITION OF FUEL CELL
0004660       READ (5,OPFC)
0004680       WRITE (6,OPFC)
0004700 C     READ   THE INLET AMOUNT AND CONDITION
0004720       READ (5,INIT)
0004740       WRITE (6,INIT)
0004760 C     READ OPERATION CONDITION
0004780       READ (5,CONDT)
0004800       WRITE (6,CONDT)
0004820 C     READ OPERATING COEFFICIENT IN THE REFORMER(METHANE FUEL ONLY)
0004840       IF (IFUEL.EQ.1) READ (5,REPEN)
0004860       IF (IFUEL.EQ.1) WRITE (6,REPEN)
0004880 C     READ CONDITION OF HEAT EXCHANGER
0004900       READ (5,HEATX)
0004920       WRITE (6,HEATX)
0004940 C     READ THE CONSTRUCTION OF HEAT EXCHANGER FOR CAL. PRESSURE DROP
0004960       READ (5,HEPDC)
0004980       WRITE (6,HEPDC)
0005000 C     READ CONFIGURATION COEFF. OF SHIFT CONVERTER FOR CAL. PRESSURE DRO
0005020       READ (5,PDSHH)
0005040       WRITE (6,PDSHH)
0005060 C     READ CONFIGURATION COEFF. OF FUEL CELL FOR CAL. PRESSURE DROP
0005080       READ (5,PDFUH)
0005100       WRITE (6,PDFUH)
0005120 C     READ THE OPERATING TEMP. OF REFORMER FOR FUEL NAPHTHA AND METHANOL
0005140       IF (IFUEL.NE.1) READ (5,TR)
0005160       IF (IFUEL.NE.1) WRITE (6,TR)
0005180 C     READ CATALYST CONSTANTS
0005200       READ (5,CATAI)
0005220       WRITE(6,CATAI)
0005240 C
0005260 C
0005280 C     CHANGE THE THERMAL DATA FOR DIFFERENT FUEL INPUT
0005300       IF (IFUEL.EQ.2) GO TO 1
0005320       IF (IFUEL.EQ.3) GO TO 2
0005340       GO TO 3
0005360     1 GS(1)=-38810.
0005380       HS(1)=-48050.
0005400       HCAS(1)=4.394
0005420       HCBS(1)=0.024274
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0005440       HCCS(1)=-0.0000069
0005460       WM(1)=32.
0005480       HLHV(1)=-159258.
0005500       AA3(1,1)=4.394
0005520       AA3(2,1)=0.013486
0005540       AA3(3,1)=-2.1157E-06
0005560       AA3(4,1)=0.
0005580       AA1(1,1)=3.E-05
0005600       AA1(2,1)=1.5E-02
0005620       AA2(1,1)=1.8E-05
0005640       AA2(2,1)=0.0092
0005660       GO TO 3
0005680     2 GS(1)=6520.
0005700       HS(1)=-42275.
0005720       HCAS(1)=7.094
0005740       HCBS(1)=0.123447
0005760       HCCS(1)=-0.0000387
0005780       WM(1)=100.
0005800       HLHV(1)=-1099580.
0005820       AA3(1,1)=7.488
0005840       AA3(2,1)=0.062467
0005860       AA3(3,1)=-1.0945E-05
0005880       AA3(4,1)=0.
0005900       AA2(1,1)=2.66E-05
0005920       AA2(2,1)=0.0157
0005940       AA1(1,1)=2.5E-05
0005960       AA1(2,1)=0.7E-02
0005980     3 CONTINUE
0006000       IDNO=1
0006020 C     FUEL INPUT COMPRESSOR(PUMP)***
0006040       P(1)=POPR*1.02
0006060       IF (IFUEL.EQ.1) CALL COMP (DNSM,TAT,TOUT,PAT,P(1),POWM,GAGM,I,IP)
0006080       IF (IFUEL.NE.1) CALL PUP (DNSM,TAT,TOUT,PAT,P(1),POWN,I,IFUEL)
0006100       DO 301 IA=1,I
0006120 301           DNSS(1,IA)=DNSM(IA)
0006140       T(1)=TOUT
0006160 C     ASSUME THE COMP. OF 13TH FLOW
0006180       DNSS(13,2)=0.
0006200       DNSS(13,7)=0.
0006220       IF (IFUEL.EQ.2) GO TO 4
0006240       IF (IFUEL.EQ.3) GO TO 5
0006260       DNSS(13,1)=0.147*DNSS(1,1)
0006280       DNSS(13,3)=0.0018*DNSS(1,1)+DNSS(1,3)
0006300       DNSS(13,4)=0.85*DNSS(1,1)+DNSS(1,4)
0006320       DNSS(13,5)=3.4*DNSS(1,1)+DNSS(1,5)
0006340       DNSS(13,6)=SMRA*DNSS(1,1)-1.7*DNSS(1,1)
0006360       GO TO 6
0006380     4 DNSS(13,1)=0.000863487*DNSS(1,1)
0006400       DNSS(13,3)=0.01
0006420       DNSS(13,4)=0.999128*DNSS(1,1)
0006440       DNSS(13,5)=2.9974*DNSS(1,1)
0006460       DNSS(13,6)=0.60087*DNSS(1,1)
0006480       GO TO 6
0006500     5 DNSS(13,1)=0.
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0006520        DNSS(13,3)=0.0221*DNSS(1,1)
0006540        DNSS(13,4)=6.971*DNSS(1,1)
0006560        DNSS(13,5)=21.956*DNSS(1,1)
0006580        DNSS(13,6)=SMRA*DNSS(1,1)-13.9645*DNSS(1,1)
0006600 C      ASSUME THE PRESSURE OF 13TH FLOW
0006620      6 P(13)=POPR*0.958
0006640 C      ASSUME THE PRESSURE OF 31ST FLOW
0006660      7 IF (IDNO.GT.1) GO TO 8
0006680        P(31)=P(13)
0006700        T(31)=TAT
0006720      8 PINF=P(13)
0006740        PINA=P(31)
0006760        POPFC=P(31)
0006780        DO 9 IB=1,I
0006800      9 DNS(IB)=DNSS(13,IB)
0006820 C       FUEL CELL MASS BALANCE***
0006840        CALL FUCE(DNS,TOPFC,POPFC,DNSAN,DNSCA,DSO,DSN,DSHO,UT,I,PINF,PINA -
0006860       1,IFUEL)
0006880        P(14)=PINF
0006900        P(32)=PINA
0006920        DO 10 IC=1,I
0006940        DNSS(32,IC)=DNSCA(IC)
0006960     10 DNSS(14,IC)=DNSAN(IC)
0006980        T(32)=TOPFC
0007000        T(14)=TOPFC
0007020        IF (IFUEL.EQ.2) CK=1.5
0007040        IF (IFUEL.EQ.1) CK=2.
0007060        IF (IFUEL.EQ.3) CK=15.
0007080 C      CAL. THE DIVIDER FACTOR FOR THE ASSUMPTION OF DEFINED EXTRA AIR IN
0007100 C      NER
0007120        GARM=1./(((1.+EXT*0.01)*((DNSS(14,3)+DNSS(14,5))/2.+CK*DNSS(14,1))-
0007140       1)/DSO+1.)
0007160        DO 11 ID=1,I
0007180     11 DNSS(28,ID)=0.
0007200        DNSS(28,2)=DSO/GARM
0007220        DNSS(28,6)=DSHO/GARM
0007240        DNSS(28,7)=DSN/GARM
0007260        P(28)=PAT
0007280        DO 12 IE=1,I
0007300     12 DNSAI(IE)=DNSS(28,IE)
0007320 C      AIR COMPRESSOR***
0007340        T(28)=TAT
0007360        POUT=POPFC*1.005
0007380        CALL COMP (DNSAI,T(28),TOUT,P(28),POUT,POWA,GAGA,I,IP)
0007400        P(29)=POUT
0007420        DO 13 I8=1,I
0007440     13 DNSS(29,I8)=DNSAI(I8)
0007460        DO 14 IG=1,I
0007480     14 DNS(IG)=DNSS(29,IG)
0007500        T(29)=TOUT
0007520 C      DIVIDER***
0007540        CALL DIVID (T(29),T(30),T(33),DNS,DNS1,DNS2,GARM,I)
0007560        DO 15 IH=1,I
0007580        DNSS(33,IH)=DNS2(IH)
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0007600        DNSS(30,IH)=DNS1(IH)
0007620     15 DNSS(31,IH)=DNSS(30,IH)
0007640        P(30)=P(29)
0007660        P(33)=P(29)
0007680 C      CAL. THE 33RD FLOW COMP. UNDER THESE ASSUMPTION:
0007700 C      (1). COMPLETE COMBUSTION
0007720        DNSS(33,2)=(1.+EXT*0.01)*((DNSS(14,3)+DNSS(14,5))/2.+CK*DNSS(14,1)-
0007740       1)
0007760        DNSS(33,7)=DNSS(33,2)*3.76
0007780        DNSS(33,6)=((DNSS(33,2)+DNSS(33,7))*28.8)*WAT/18.
0007800        T(33)=TAT
0007820        DO 16 II=1,I
0007840        DNS1(II)=DNSS(14,II)
0007860     16 DNS2(II)=DNSS(33,II)
0007880 C      MIXER***
0007900        CALL DMIX (DNS1,DNS2,DNS,T(14),T(33),T(15),I,P(14),P(33),POUT)
0007920        P(15)=POUT
0007940        DO 17 IJ=1,I
0007960        DNSS(15,IJ)=DNS(IJ)
0007980     17 DNSS(16,IJ)=DNSS(15,IJ)
0008000 C      CAL. THE COMP. OF 17TH FLOW UNDER THE SAME ASSUMPTION AS BEFORE
0008020        IF (IFUEL.NE.3) DNSS(17,4)=DNSS(15,3)+DNSS(15,4)+DNSS(15,1)
0008040        IF (IFUEL.EQ.3) DNSS(17,4)=DNSS(15,3)+DNSS(15,4)+7.*DNSS(15,1)
0008060        IF (IFUEL.NE.3) DNSS(17,6)=DNSS(15,5)+DNSS(15,6)+2.*DNSS(15,1)
0008080        IF (IFUEL.EQ.3) DNSS(17,6)=DNSS(15,5)+DNSS(15,6)+8.*DNSS(15,1)
0008100        DNSS(17,2)=DNSS(15,2)-0.5*(DNSS(15,3)+DNSS(15,5))-CK*(DNSS(15,1))
0008120        DNSS(17,7)=DNSS(15,7)
0008140        DO 18 IK=1,I
0008160        DNSS(18,IK)=DNSS(17,IK)
0008180        DNSS(19,IK)=DNSS(18,IK)
0008200        DNSS(20,IK)=DNSS(19,IK)
0008220     18 CONTINUE
0008240 C      CAL. THE COMP. OF 21ST FLOW
0008260        DO 19 IL=1,I
0008280     19 DNSS(21,IL)=DNSS(20,IL)+DNSS(32,IL)
0008300        TDNSS(21)=0.
0008320        DO 20 IM=1,I
0008340     20 TDNSS(21)=TDNSS(21)+DNSS(21,IM)
0008360 C      CAL. TEMP. OF 26TH FLOW
0008380 C      ASSUMPTION:
0008400 C      (1). SATURATED PRESSURE IS ESTIMATED BY (EXP(A-B/T))
0008420 C      (2). UNDER SATURATED CONDITION
0008440 C ASSUME THE PRESSURE OF 26TH FLOW IS IDENTICAL TO 25TH FLOW (THE PRESS.
0008460 C DROP IS SMALL)
0008480        P(25)=POPR*1.0005
0008500        P(26)=P(25)
0008520        T(26)=B/(A-ALOG(P(26)))
0008540        DNSS(26,6)=DNSS(1,1)*SMRA
0008560        DO 21 IN=1,I
0008580     21 DNSS(25,IN)=DNSS(26,IN)
0008600        DO 22 IO=1,I
0008620        IF (IFUEL.NE.2) DNSS(27,IO)=DNSS(26,IO)
0008640     22 DNSS(2,IO)=DNSS(1,IO)
0008660        DO 23 I9=1,I
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0008680       IF (IFUEL.NE.2) DNSS(3,I9)=DNSS(2,I9)+DNSS(27,I9)
0008700       IF (IFUEL.EQ.2) DNSS(3,I9)=DNSS(2,I9)+DNSS(26,I9)
0008720       IF (IFUEL.NE.2) DNSS(4,I9)=DNSS(3,I9)
0008740       IF (IFUEL.EQ.2) DNSS(5,I9)=DNSS(3,I9)
0008760       IF (IFUEL.NE.2) DNSS(5,I9)=DNSS(4,I9)
0008780    23 CONTINUE
0008800 C     ASSUME THE TEMP. AND PRESSURE OF 5TH FLOW
0008820       IF (IDNO.GT.1) GO TO 24
0008840       IF (IFUEL.EQ.1) T(5)=1110.88
0008860       IF (IFUEL.EQ.2) T(5)=661.59
0008880       IF (IFUEL.EQ.3) T(5)=1052.
0008900       P(5)=POPR
0008920    24 CONTINUE
0008940       IF (IDNO.GT.1) GO TO 25
0008960 C     ASSUME THE TEMP. OF 18TH FLOW
0008980       IF (IFUEL.EQ.1) T(18)=1222.
0009000       IF (IFUEL.EQ.2) T(18)=863.88
0009020       IF (IFUEL.EQ.3) T(18)=1398.94
0009040 C ASSUME P(16)
0009060       P(16)=P(15)*0.99
0009080 C DESIGN THE TUBE TO LET PRESSURE DROP THROUGH BURNER BE 6%
0009100  604  P(17)=P(16)*(1.-0.06)
0009120 C ASSUME PRESSURE DROP OF COMBUSTIAN GAS THROGH REFORMER TO BE 5%
0009140       P(18)=P(17)*0.95
0009160    25 CONTINUE
0009180 C     E-3***
0009200       DO 26 IQ=1,I
0009220       DNSH(IQ)=DNSS(17,IQ)
0009240    26 DNSC(IQ)=DNSS(5,IQ)
0009260       PT=P(5)
0009280       PS=P(18)
0009300       IF (IFUEL.NE.2) CALL HEXC (T(18),DNSH,DNSC,T(4),T(19),T(5),QT,1,HA-
0009320      1(3),3,2,I,PT,PS,NT(3),IFUEL)
0009340       IF (IFUEL.EQ.2) CALL HEXC (T(18),DNSH,DNSC,T(3),T(19),T(5),QT,1,HA-
0009360      1(3),3,2,I,PT,PS,NT(3),IFUEL)
0009380       IF (IFUEL.NE.2) P(4)=PT
0009400       IF (IFUEL.EQ.2) P(3)=PT
0009420       P(19)=PS
0009440       EFF(3)=HE
0009460       QQT(3)=QT
0009480 C     E-4***
0009500       DO 27 IR=1,I
0009520       DNSH(IR)=DNSS(19,IR)
0009540       DNSC(IR)=DNSS(15,IR)
0009560    27 CONTINUE
0009580       PT=P(15)
0009600       PS=P(19)
0009620       CALL HEXC (T(19),DNSH,DNSC,T(15),T(20),T(16),QT,1,HA(4),4,1,I,PT,P-
0009640      1S,NT(4),IFUEL)
0009660       IF(ABS((PT-P(16))/(PT+P(16))).LT.ERR) GO TO 605
0009680       P(16)=(PT+P(16))/2.
0009700       GO TO 604
0009720  605  P(16)=PT
0009740       P(20)=PS
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0009760       EFF(4)=HE
0009780       QQT(4)=QT
0009800 C     BURNER ENERGY BALANCE***
0009820       DO 28 IS=1,I
0009840    28 DNS(IS)=DNSS(16,IS)
0009860       CALL FLAME (DNS,T(16),T(17),I,IFUEL)
0009880       DO 29 IT=1,I
0009900    29 DNSS(17,IT)=DNS(IT)
0009920       IF (IFUEL.NE.1) GO TO 33
0009940 C     REFORMER(METHANE)***
0009960       NOR=DNSS(1,1)/60.
0009980       DO 30 IU=1,I
0010000       DNSR(IU)=DNSS(5,IU)/453.6/NOR
0010020    30 DNSF(IU)=DNSS(17,IU)/453.6/NOR
0010040       CALL KREF(DNSR,DNSF,DX1,DX2,DX3,P(5),T(5),T(17),ZH,P(7),T(7)      -
0010060      1,TTEST,S,DP,1)
0010080 C     TEST THE ASSUMPTION OF 18TH FLOW
0010100       IF (ABS((TTEST-T(18))/(TTEST+T(18))).LT.ERR) GO TO 31
0010120       T(18)=TTEST
0010140       GO TO 25
0010160    31 DO 32 IV=1,I
0010180       DNSS(7,IV)=DNSR(IV)*453.6*NOR
0010200    32 DNSS(18,IV)=DNSF(IV)*453.6*NOR
0010220       T(18)=TTEST
0010240       GO TO 39
0010260 C     E-8(METHANOL AND NAPHTHA)***
0010280    33 DO 34 IW=1,I
0010300       DNSH(IW)=DNSS(17,IW)
0010320    34 DNSC(IW)=DNSS(5,IW)
0010340       PTEST=P(17)
0010360       PS=P(5)
0010380       CALL HEXC (T(17),DNSH,DNSC,T(5),TTEST,T(6),QT,2,HA(8),8,1,I,PTEST,-
0010400      1PS,NT(8),IFUEL)
0010420 C     TEST THE ASSUMPTION OF 18TH FLOW
0010440       IF ((ABS((TTEST-T(18))/(TTEST+T(18))).LT.ERR).AND.(ABS((PTEST-P(18-
0010460      1))/(PTEST+P(18))).LT.ERR)) GO TO 35
0010480       T(18)=(TTEST+T(18))/2.
0010500       P(18)=(P(18)+PTEST)/2.
0010520       GO TO 25
0010540    35 QQT(8)=QT
0010560       T(18)=TTEST
0010580       P(18)=PTEST
0010600       P(6)=PS
0010620       EFF(8)=HE
0010640       DO 36 IX=1,I
0010660       DNSS(6,IX)=DNSC(IX)
0010680    36 DNSS(18,IX)=DNSH(IX)
0010700 C     REFORMER(METHANOL AND NAPHTHA)***
0010720       DO 37 IY=1,I
0010740    37 DNS(IY)=DNSS(6,IY)
0010760       CALL ENRE (DNS,TOPR,POPR,T(6),T(7),I,IP,IFUEL)
0010780       DO 38 IZ=1,I
0010800    38 DNSS(7,IZ)=DNS(IZ)
0010820 C     CAL. PRESSURE DROP
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0010840       CALL PDSH (DNS,P(6),P(7),TOPR,2,IFUEL)
0010860       IF (IFUEL.EQ.2) GO TO 56
0010880    39 DO 40 IAA=1,I
0010900       DNSH(IAA)=DNSS(7,IAA)
0010920    40 DNSC(IAA)=DNSS(3,IAA)
0010940 C     E-2***
0010960       PT=P(4)
0010980       PS=P(7)
0011000       IF(IFUEL.EQ.1) CALL HEXC(T(7),DNSH,DNSC,T(3),T(8),T(4),QT,1,HA(2),-
0011020      12,2,I,PT,PS,NT(2),IFUEL)
0011040       IF(IFUEL.EQ.3) CALL HEXC(T(7),DNSH,DNSC,T(3),T(9),T(4),QT,1,HA(2),-
0011060      12,2,I,PT,PS,NT(2),IFUEL)
0011080       P(3)=PT
0011100       IF (IFUEL.EQ.1) P(8)=PS
0011120       IF (IFUEL.EQ.3) P(9)=PS
0011140       EFF(2)=HE
0011160       QQT(2)=QT
0011180       DO 41 IBB=1,I
0011200       IF (IFUEL.EQ.1) DNSS(8,IBB)=DNSH(IBB)
0011220       IF (IFUEL.EQ.3) DNSS(9,IBB)=DNSH(IBB)
0011240    41 DNSS(4,IBB)=DNSC(IBB)
0011260       IF (IFUEL.EQ.3) GO TO 46
0011280 C     HIGH TEMP. SHIFT CONVERTER***
0011300       TOPHS=T(8)
0011320    42 CONTINUE
0011340       POPHS=P(8)
0011360       DO 43 ICC=1,I
0011380    43 DNS(ICC)=DNSS(8,ICC)
0011400       CALL ENSH (DNS,T(8),T(9),TOPHS,POPHS,I,IP,IFUEL)
0011420       P(9)=POPHS
0011440       TM=(T(9)+T(8))/2.
0011460       IF ((IP.EQ.2).OR.(ABS((TM-TOPHS)/(TM+TOPHS)).LT.ERR)) GO TO 44
0011480       TOPHS=TM
0011500       GO TO 42
0011520    44 CONTINUE
0011540       DO 45 IDD=1,I
0011560    45 DNSS(9,IDD)=DNS(IDD)
0011580    46 CONTINUE
0011600       DO 47 IEE=1,I
0011620       DNSH(IEE)=DNSS(9,IEE)
0011640    47 DNSC(IEE)=DNSS(1,IEE)
0011660       IF (IFUEL.EQ.3) GO TO 48
0011680 C     E-1(METHANE AND NAPHTHA)***
0011700       PT=P(1)
0011720       PS=P(9)
0011740       CALL HEXC (T(9),DNSH,DNSC,T(1),THO,TCO,QT,1,HA(1),1,1,I,PT,PS,NT(1-
0011760      1),IFUEL)
0011780       P(10)=PS
0011800       P(2)=PT
0011820       EFF(1)=HE
0011840       QQT(1)=QT
0011860       T(2)=TCO
0011880       T(10)=THO
0011900       GO TO 52
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0011920    48 CONTINUE
0011940 C     DESIGN THE HEAT EXCHANGER 1 TO VAPORIZE NAPHTHA AND RISE THE TEMP.
0011960 C     TO 400
0011980 C     K FOR NAPHTHA FUEL
0012000       T(2)=400.
0012020       QQT(1)=HNA*252./453.6*100.*1.8*DNSS(1,1)*(BPNA+273.-T(1))+DNSS(1,1-
0012040      1)*VHNA+HCAS(1)*(T(2)-T(1))+HCBS(1)*(T(2)**2-T(1)**2)/2.+HCCS(1)*(T-
0012060      2(2)**3-T(1)**3)/3.
0012080 C     ASSUME EFFICIENCY OF H-E 1 IS 0.7
0012100       EFF(1)=0.7
0012120       HA(1)=CN*QQT(1)/EFF(1)/(T(9)-T(1))/U
0012140 C     ASSUME AVERAGE TEMP. OF HOT SIDE
0012160       TAVG=T(9)-50.
0012180    49 CHH=0.
0012200       DO 50 IB=1,I
0012220    50 CHH=CHH+DNSS(9,IB)*(HCAS(IB)+HCBS(IB)*TAVG+HCCS(IB)*TAVG**2)
0012240       T(10)=T(9)-QQT(1)/CHH
0012260 C     TEST THE ASSUMPTION OF AVERAGE TEMP.
0012280       IF (ABS((T(10)+T(9))/2.-TAVG).LT.ABS((T(10)+T(9))/2.+TAVG)*0.001) -
0012300      1GO TO 51
0012320       TAVG=(T(9)+T(10))/2.
0012340       GO TO 49
0012360    51 CONTINUE
0012380 C     ASSUME PRESSURE DROP IS NEGLECTABLE
0012400       P(2)=P(1)
0012420       P(10)=P(9)
0012440    52 DO 53 IFF=1,I
0012460       IF (IFUEL.EQ.3) DNSS(10,IFF)=DNSS(9,IFF)
0012480    53 IF (IFUEL.EQ.1) DNSS(10,IFF)=DNSH(IFF)
0012500       DO 54 IGG=1,I
0012520       DNSH(IGG)=DNSS(10,IGG)
0012540    54 DNSC(IGG)=DNSS(26,IGG)
0012560 C     E-9***
0012580       PT=P(26)
0012600       PS=P(10)
0012620       CALL HEXC (T(10),DNSH,DNSC,T(26),T(11),T(27),QT,1,HA(9),9,1,I,PT,P-
0012640      1S,NT(9),IFUEL)
0012660       P(11)=PS
0012680       P(27)=PT
0012700       EFF(9)=HE
0012720       QQT(9)=QT
0012740       DO 55 IHH=1,I
0012760       DNSS(11,IHH)=DNSH(IHH)
0012780       DNSS(27,IHH)=DNSC(IHH)
0012800       DNS1(IHH)=DNSS(2,IHH)
0012820       DNS2(IHH)=DNSS(27,IHH)
0012840    55 CONTINUE
0012860       GO TO 60
0012880 C     E-1(METHANOL)***
0012900    56 DO 57 III=1,I
0012920       DNSH(III)=DNSS(7,III)
0012940    57 DNSC(III)=DNSS(1,III)
0012960       PT=P(1)
0012980       PS=P(7)
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0013000       CALL HEXC (T(7),DNSH,DNSC,T(1),THO,TCO,QT,1,HA(1),1,1,I,PT,PS,NT(1-
0013020      1),IFUEL)
0013040       PTE=PS
0013060       P(2)=PT
0013080       EFF(1)=HE
0013100       QQT(1)=QT
0013120       DO 58 IJJ=1,I
0013140    58 DNSS(2,IJJ)=DNSC(IJJ)
0013160       T(2)=TCO
0013180       T(13)=THO
0013200       DO 59 IJJ=1,I
0013220       DNS1(IJJ)=DNSS(2,IJJ)
0013240       DNS2(IJJ)=DNSS(26,IJJ)
0013260    59 CONTINUE
0013280 C     MIXER***
0013300       CALL DMIX (DNS1,DNS2,DNS,T(2),T(26),TESTT,I,P(2),P(26),PTEST)
0013320       GO TO 61
0013340    60 CALL DMIX (DNS1,DNS2,DNS,T(2),T(27),TESTT,I,P(2),P(27),PTEST)
0013360 C     TEST TEMP. OF 3RD FLOW
0013380    61 IF ((ABS((TESTT-T(3))/(TESTT+T(3))).LT.ERR).AND.(ABS((PTEST-P(3))/-
0013400      1(PTEST+P(3))).LT.ERR)) GO TO 70
0013420       IF (IFUEL.EQ.2) GO TO 66
0013440 C     E-2***
0013460       DO 62 IKK=1,I
0013480       DNSS(3,IKK)=DNS(IKK)
0013500       DNSH(IKK)=DNSS(7,IKK)
0013520    62 DNSC(IKK)=DNSS(3,IKK)
0013540       P(3)=(P(3)+PTEST)/2.
0013560       T(3)=(TESTT+T(3))/2.
0013580       PT=P(3)
0013600       PS=P(7)
0013620       IF (IFUEL.EQ.3) GO TO 63
0013640       CALL HEXC (T(7),DNSH,DNSC,T(3),T(8),T(4),QT,1,HA(2),2,1,I,PT,PS,NT-
0013660      1(2),IFUEL)
0013680       P(4)=PT
0013700       P(8)=PS
0013720       GO TO 64
0013740    63 CALL HEXC (T(7),DNSH,DNSC,T(3),T(9),T(4),QT,1,HA(2),2,1,I,PT,PS,NT-
0013760      1(2),IFUEL)
0013780       P(4)=PT
0013800       P(9)=PS
0013820 C     E-3***
0013840    64 DO 65 ILL=1,I
0013860       DNSS(4,ILL)=DNSC(ILL)
0013880       DNSH(ILL)=DNSS(18,ILL)
0013900    65 DNSC(ILL)=DNSS(4,ILL)
0013920       PT=P(4)
0013940       PS=P(18)
0013960       CALL HEXC (T(18),DNSH,DNSC,T(4),T(19),T(5),QT,1,HA(3),3,1,I,PT,PS,-
0013980      1NT(3),IFUEL)
0014000       P(5)=PT
0014020       P(19)=PS
0014040       GO TO 68
0014060    66 DO 67 IMM=1,I
```

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0014080       DNSS(3,IMM)=DNS(IMM)
0014100       DNSH(IMM)=DNSS(18,IMM)
0014120    67 DNSC(IMM)=DNSS(3,IMM)
0014140       T(3)=(T(3)+TESTT)/2.
0014160       PT=P(18)
0014180       PS=(P(3)+PTEST)/2.
0014200       CALL HEXC (T(18),DNSH,DNSC,T(3),T(19),T(5),QT,1,HA(3),3,1,I,PT,PS,-
0014220      1NT(3),IFUEL)
0014240       P(19)=PT
0014260       P(5)=PS
0014280       EFF(3)=HE
0014300       QQT(3)=QT
0014320    68 DO 69 INN=1,I
0014340    69 DNSS(5,INN)=DNSC(INN)
0014360       IDNO=IDNO+1
0014380       GO TO 24
0014400    70 CONTINUE
0014420       IF (IFUEL.EQ.2) GO TO 77
0014440       DO 71 IPP=1,I
0014460       DNSH(IPP)=DNSS(11,IPP)
0014480    71 DNSC(IPP)=DNSS(30,IPP)
0014500 C     E-6***
0014520       PT=P(30)
0014540       PS=P(11)
0014560       CALL HEXC (T(11),DNSH,DNSC,T(30),T(12),T(31),QT,1,HA(6),6,1,I,PT,P-
0014580      1S,NT(6),IFUEL)
0014600       P(12)=PS
0014620       PTEST=PT
0014640 C     TEST THE PRESSURE OF 31ST FLOW
0014660       IF (ABS((PTEST-P(31))/(PTEST+P(31))).LT.ERR) GO TO 72
0014680       P(31)=(PTEST+P(31))/2.
0014700       GO TO 8
0014720    72 EFF(6)=HE
0014740       QQT(6)=QT
0014760       DO 73 IQQ=1,I
0014780       DNSS(12,IQQ)=DNSH(IQQ)
0014800    73 DNSS(31,IQQ)=DNSC(IQQ)
0014820 C     LOW TEMP. SHIFT CONVERTER***
0014840       TOPLS=T(12)
0014860       POPLS=P(12)
0014880    74 CONTINUE
0014900       DO 75 IRR=1,I
0014920    75 DNS(IRR)=DNSS(12,IRR)
0014940       CALL ENSH (DNS,T(12),T(13),TOPLS,POPLS,I,IP,IFUEL)
0014960       TM=(T(12)+T(13))/2.
0014980       IF ((IP.EQ.2).OR.(ABS((TM-TOPLS)/(TM+TOPLS)).LT.ERR)) GO TO 76
0015000       TOPLS=TM
0015020       GO TO 74
0015040    76 CONTINUE
0015060 C     TEST THE ASSUMPTION OF 13TH FLOW
0015080    77 DO 78 ISS=1,I
0015100       IF ((IFUEL.NE.2).AND.(DNS(ISS).LT.0.50).AND.(DNSS(13,ISS).LT.0.50)-
0015120      1) GO TO 78
0015140       IF ((IFUEL.EQ.2).AND.(DNSH(ISS).LT.0.50).AND.(DNSS(13,ISS).LT.0.50-
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0015160      1)) GO TO 78
0015180       IF ((IFUEL.NE.2).AND.(ABS((DNS(ISS)-DNSS(13,ISS))/(DNS(ISS)+DNSS(1-
0015200      13,ISS))).LT.ERR)) GO TO 78
0015220       IF ((IFUEL.EQ.2).AND.(ABS((DNSH(ISS)-DNSS(13,ISS))/(DNSH(ISS)+DNSS-
0015240      1(13,ISS))).LT.ERR)) GO TO 78
0015260       GO TO 79
0015280    78 CONTINUE
0015300       IF (IFUEL.EQ.2) POPLS=PTE
0015320       IF (ABS((POPLS-P(13))/(POPLS+P(13))).LT.ERR) GO TO 81
0015340    79 DO 80 ITT=1,I
0015360       IF (IFUEL.EQ.2) DNSS(13,ITT)=(DNSS(13,ITT)+DNSH(ITT))/2.
0015380    80 IF (IFUEL.NE.2) DNSS(13,ITT)=(DNSS(13,ITT)+DNS(ITT))/2.
0015400       P(13)=(POPLS+P(13))/2.
0015420       GO TO 7
0015440    81 CONTINUE
0015460       DO 82 IUU=1,I
0015480       IF (IFUEL.EQ.2) DNSS(13,IUU)=DNSH(IUU)
0015500    82 IF (IFUEL.NE.2) DNSS(13,IUU)=DNS(IUU)
0015520       TDN13=0.
0015540       DO 83 IVV=1,I
0015560    83 TDN13=TDN13+DNSS(13,IVV)
0015580       FCO=DNSS(13,3)/TDN13
0015600       DO 84 IWW=1,I
0015620       DNSAN(IWW)=DNSS(13,IWW)
0015640    84 DNSCA(IWW)=DNSS(31,IWW)
0015660 C    FUEL CELL ENERGY BALANCE***
0015680       AREAF=FULE*AIRL*30.48**2
0015700       CD=CD/1000.
0015720       OU=1./(EXA*0.01+1.)
0015740       CALL ENFU(DNSAN,DNSCA,T(31),T(13),TOUT,TOPFC,POPFC,VOP,UT,1,I,QY, -
0015760      1WK,OU,CD,CL,IFUEL)
0015780       QRT=QY
0015800 C CALCULATE THE OUTPUT OF AC POWER
0015820       AC=(   -1.0148+SQRT(1.0148**2-4.*0.0456/108.*(0.0472*108.-WK)))   -
0015840      1/(2.*0.0456/108.)
0015860       DO 86 IYY=1,I
0015880    86 DNSC(IYY)=DNSS(25,IYY)
0015900       DO 87 IZZ=1,I
0015920       DNS1(IZZ)=DNSS(20,IZZ)
0015940    87 DNS2(IZZ)=DNSS(32,IZZ)
0015960 C     MIXER***
0015980       CALL DMIX (DNS1,DNS2,DNS,T(20),T(32),TOUT,I,P(20),P(32),POUT)
0016000       P(21)=POUT
0016020       DO 88 I1=1,I
0016040       DNSS(21,I1)=DNS(I1)
0016060    88 DNSH(I1)=DNSS(21,I1)
0016080       T(21)=TOUT
0016100 C ASSUME P(22)
0016120       P(22)=P(21)*1.001
0016140   602 T(22)=-B/(ALOG((DNSS(1,1)*SMRA-DNSS(21,6))/(DNSS(1,1)*SMRA-       -
0016160      1TDNSS(21))*P(22))-A)
0016180 C     E-10***
0016200       T(25)=T(22)
0016220       CALL CDPH (QRT,T(25),T(26),DNSC,P(25),I,QQT(10))
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0016240       QQT(7)=QRT
0016260 C     ASSUME HOT WATER IS FEEDING IN AT 333OK AND FEEDING OUT AT 355 K
0016280       DNSS(34,6)=QQT(7)/(355.-333.)/1./18.
0016300       DNSS(35,6)=DNSS(34,6)
0016320       T(34)=333.
0016340       T(35)=355.
0016360       P(34)=PAT
0016380       P(35)=PAT
0016400 C     E-5***
0016420       CALL COND (T(21),T(22),DNSH,QT,HCH,I)
0016440       QQT(5)=QT
0016460 C     ASSUME HOT WATER IS FEEDING IN AT TAT   AND FEEDING OUT AT 355OK
0016480       DTL=((T(21)-355.)-(T(22)-TAT))/ALOG((T(21)-355.)/(T(22)-TAT))
0016500       T(36)=TAT
0016520       T(37)=355.
0016540       P(36)=PAT
0016560       P(37)=PAT
0016580       DNSS(36,6)=QQT(5)/1./18./(355.-TAT)
0016600       DNSS(37,6)=DNSS(36,6)
0016620 C     ASSUME E-5 IS THE TYPE OF COUNTERFLOW
0016640       HA(5)=QQT(5)/U/1./DTL
0016660       THM=(T(36)+T(37))/2.
0016680       TCM=(T(22)+T(21))/2.
0016700       CALL HEPD(DNS,DNSH,THM,TCM,HA(5),P(21),P(36),5,DPJ,DP,NT,T(22),   -
0016720      1T(21),4)
0016740       P22TE=P(21)-DPJ
0016760       IF(ABS((P22TE-P(22))/(P22TE+P(22))).LT.ERR) GO TO 603
0016780       P(22)=(P(22)+P22TE)/2.
0016800       GO TO 602
0016820   603 DO 89 I2=1,I
0016840       DNSS(22,I2)=DNSH(I2)
0016860    89 DNS(I2)=DNSS(22,I2)
0016880 C     SEPARATER***
0016900       POPS=P(22)
0016920       CALL SEPAR (T(22),POPS,T(23),T(24),DNS,DNSL,DNSV,I)
0016940       DO 90 I3=1,I
0016960       DNSS(24,I3)=DNSL(I3)
0016980    90 DNSS(23,I3)=DNSV(I3)
0017000       P(24)=POPS
0017020       P(23)=POPS
0017040 C     PUMP***
0017060       DO 901 I4=1,I
0017080   901 DNS(I4)=DNSS(24,I4)
0017100       CALL PUMP (DNS,T(24),T(25),P(24),P(25),POWS,I)
0017120       DO 92 IB=1,39
0017140       TDNSS(IB)=0.
0017160       DO 91 IA=1,I
0017180       TDNSS(IB)=TDNSS(IB)+DNSS(IB,IA)
0017200    91 CONTINUE
0017220    92 CONTINUE
0017240 C     WRITE THE RESULT
0017260       IF (IFUEL.EQ.1) WRITE (6,108) SMRA
0017280       IF (IFUEL.EQ.2) WRITE (6,109) SMRA
0017300       IF (IFUEL.EQ.3) WRITE (6,110) SMRA
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0017320       WRITE (6,103) P(5),P(7),T(5),T(7)
0017340       IF (IFUEL.EQ.1) WRITE (6,104) TOPHS,P(8),T(8),T(9)
0017360       IF (IFUEL.NE.2) WRITE (6,105) TOPLS,P(13),T(12),T(13)
0017380       WRITE (6,106) T(22),POPS
0017400       WRITE (6,99) FCO
0017420       WRITE (6,118) TOPFC,POPFC,E,VOP,CD,CL,UT,OU
0017440       WRITE (6,102) T(13),T(31)
0017460       WRITE (6,100) ETH,EI,EV,EC
0017480       WRITE (6,107) EFC
0017500       WRITE (6,101) WK,QRT
0017520       WRITE (6,117) AC
0017540 C     WRITE THE MATERIAL IN JTH FLOW
0017560 18280 WRITE(6,119)
0017580       IF (IFUEL.EQ.1) WRITE (6,94)
0017600       IF (IFUEL.EQ.2) WRITE (6,95)
0017620       IF (IFUEL.EQ.3) WRITE (6,96)
0017640       IF (IFUEL.EQ.1) WRITE (6,93) (((J,(DNSS(J,IA),IA=1,I),TDNSS(J),T(J-
0017660      1),P(J)),J=1,5),((II,(DNSS(II,IA),IA=1,I),TDNSS(II),T(II),P(II)),II-
0017680      2=7,37))
0017700       IF (IFUEL.EQ.2) WRITE (6,93) (((J,(DNSS(J,IA),IA=1,I),TDNSS(J),T(J-
0017720      1),P(J)),J=1,3),((II,(DNSS(II,IA),IA=1,I),TDNSS(II),T(II),P(II)),II-
0017740      2=5,7))
0017760       IF (IFUEL.EQ.3) WRITE (6,93) (((J,(DNSS(J,IA),IA=1,I),TDNSS(J),T(J-
0017780      1),P(J)),J=1,7),((II,(DNSS(II,IA),IA=1,I),TDNSS(II),T(II),P(II)),II-
0017800      2=9,37))
0017820 C     WRITE DUTY OF HEAT EXCHANGER OR CONDENSER
0017840       WRITE(6,119)
0017860       WRITE (6,111)
0017880       WRITE (6,97)
0017900       WRITE (6,98) (QQT(IA),IA=1,10)
0017920 C     WRITE SURFACE AREA OF HEAT EXCHANGER
0017940       WRITE (6,112)
0017960       WRITE (6,97)
0017980       WRITE (6,98) (HA(IA),IA=1,10)
0018000 C     WRITE THE EFFICIENCY OF HEAT EXCHANGER
0018020       WRITE (6,113)
0018040       WRITE (6,97)
0018060       WRITE (6,98) (EFF(IA),IA=1,10)
0018080       IF (IFUEL.EQ.1) WRITE (6,114) POWA,POWM,POWS
0018100       IF (IFUEL.EQ.2) WRITE (6,115) POWA,POWN,POWS
0018120       IF (IFUEL.EQ.3) WRITE (6,116) POWA,POWN,POWS
0018140       STOP
0018160 C
0018180    93 FORMAT (1X,2X,I2,2X,F8.2,1X,F8.2,1X,3X,F8.2,6X,F8.2,5X,F8.2,F10.2,-
0018200      11X,F8.2,3X,F10.2,4X,F7.2,2X,F6.4)
0018220    94 FORMAT (1X,'STREAM  METHANE  OXYGEN  CAR. MONOXIDE  CAR. DIOXIDE  -
0018240      1HYDROGEN  WATER  NITROGEN    FLOW RATE   TEMP.(K)   PRE.(ATM)')
0018260    95 FORMAT (1X,'STREAM  METHANOL OXYGEN  CAR. MONOXIDE  CAR. DIOXIDE  -
0018280      1HYDROGEN  WATER  NITROGEN    FLOW RATE   TEMP.(K)   PRE.(ATM)')
0018300    96 FORMAT (1X,'STREAM  NAPHTHA  OXYGEN  CAR. MONOXIDE  CAR. DIOXIDE  -
0018320      1HYDROGEN  WATER  NITROGEN    FLOW RATE   TEMP.(K)   PRE.(ATM)')
0018340    97 FORMAT (1X,'     E-     1     E-2          E-3          E-4       -
0018360      1 E-5          E-6          E-7         E-8          E-9           -
0018380      2 E-10')
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0018400    98 FORMAT (1X,10(E12.5,1X)/)
0018420    99 FORMAT (1X,'THE FRACTION OF CO IN THE FEED IS',F8.5/)
0018440   100 FORMAT (1X,'THE THERMODYNAMIC EFFICIENCY OF FUEL CELL IS',E13.5,'T-
0018460      1HE CURRENT EFFICIENCY IS',E13.5/' THE VOLTAGE EFFICIENCY IS',E13.5-
0018480      2,'THE HEATING VALUE EFFICIENCY IS',E13.5)
0018500   101 FORMAT (1X,'THE ELECTRICAL WORK IS',E13.5,'KW '/' THE TOTAL HEAT R-
0018520      1ELEASE IS',E13.5,'CAL'//)
0018540   102 FORMAT (1X,'THE ANODE SIDE INLET TEMP. IS',F7.2,' K'/' THE CATHODE-
0018560      1 SIDE INLET TEMP. IS',F7.2,' K')
0018580   103 FORMAT (' THE REFORMER IS OPERATING UNDER THESE CONDITIONS ',6X,/'-
0018600      1 INLET PRESSURE',F7.2,'ATM',' OUTLET PRESSURE',F7.2,'ATM'/      ' -
0018620      2 INLET TEMP. :',F7.2,' K',' OUTLET TEMP. :',F7.2,' K'/)
0018640   104 FORMAT (' THE HIGH TEMP. SHIFT CONVERTER IS OPERATING UNDER THESE -
0018660      1CONDITIONS ',6X,/                                                -
0018680      2    ' OPERATING TEMP.:',F7.2,' K'/' OPERATING PRESSURE:',F7.2,'ATM-
0018700      3'/' INLET TEMP.:',F7.2,' K'/' OUTLET TEMP.:',F7.2,' K'/)
0018720   105 FORMAT (1X,'THE LOW TEMP. SHIFT CONVERTER IS OPERATING UNDER THESE-
0018740      1 CONDITIONS  ',6X,/                                              -
0018760      2    ' OPERATING TEMP.:',F7.2,' K'/' OPERATING PRESSURE:',F7.2,'ATM-
0018780      3'/' INLET TEMP.:',F7.2,' K'/' OUTLET TEMP.:',F7.2,' K'/)
0018800   106 FORMAT (' THE LIQUID SEPERATER IS OPERATING UNDER THESE CONDITIONS-
0018820      1 ',6X,/' OPERATING TEMP.:',F7.2,' K'/' OPERATING PRESSURE:',F7.2,'-
0018840      2ATM'/)
0018860   107 FORMAT (1X,'THE FUEL CELL EFFICIENCY IS',F6.4)
0018880   108 FORMAT ('1',1X,'THE STEAM/METHANE RATIO IN THE REFORMER IS',F7.2/)
0018900   109 FORMAT ('1',' THE STEAM/METHANOL RATIO IN THE REFORMER IS',F7.2/)
0018920   110 FORMAT ('1',' THE STEAM/NAPHTHA RATIO IN THE REFORMER IS',F7.2/)
0018940   111 FORMAT (1X,'THE DUTY OF HEAT EXCHANGER (CAL.) (0 MEANS NO THIS NO.-
0018960      1 HEAT EXCHANGER)')
0018980   112 FORMAT (1X,'THE SURFACE AREA OF HEAT EXCHANGER (M**2) (0 MEANS NO -
0019000      1 THIS NO. HEAT EXCHANGER)')
0019020   113 FORMAT (1X,'THE EFFICIENCY OF HEAT EXCHANGER (0 MEANS NO THIS NO. -
0019040      1 HEAT EXCHANGER OR IS CONDENSER)')
0019060   114 FORMAT (1X,'THE POWER OF AIR COMPRESSOR:',F10.2,'HP'/1X,'THE POWER-
0019080      1 OF METHANE COMPRESSOR:',F10.2,'HP'/1X,'THE POWER OF PUMP :',F10.5-
0019100      2,'HP')
0019120   115 FORMAT (1X,'THE POWER OF AIR COMPRESSOR:',F10.2,'HP'/1X,'THE POWER-
0019140      1 OF METHANOL COMPRESSOR:',F10.5,'HP'/1X,'THE POWER OF PUMP :',F10.-
0019160      25,'HP')
0019180   116 FORMAT (1X,'THE POWER OF AIR COMPRESSOR:',F10.2,'HP'/1X,'THE POWER-
0019200      1 OF NAPHTHA PUMP:',F10.5,'HP'/1X,'THE POWER OF PUMP :',F10.5,'HP')
0019220   117 FORMAT (//1X,'THE AC OUTPUT IS ',F7.2,'KW'//)
0019240   118 FORMAT(' THE FUEL CELL IS OPERATING UNDER THESE CONDITIONS ',6X,/'-
0019260      1 THE OPERATING TEMPERATURE :',F7.2,'K'/' THE OPERATING PRESSURE:',-
0019280      2F5.2,'ATM'/' THE OPEN CIRCUIT POTENTIAL:',F8.3,' V'/             -
0019300      3' THE OPERATING POTENTIAL:',F8.3,' V'/' THE CURRENT DENSITY:',F8.3-
0019320      4,'A/CM**2'/' THE CATALYST LOADING:',F8.3,'PT/CM**2'/             -
0019340      5 ' THE FUEL UTILIZATION:',F5.3/                                  -
0019360      6' THE OXYGEN UTILIZATION:',F5.3)
0019380   119 FORMAT('1')
0019400       END
0019800       SUBROUTINE BURN(DNS,I,IJ)
0019900 C*************************************************************************
0020000 C THIS SUBROUTINE IS TO CALCULATE THE MASS BALANCE OF BURNER
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0020100 C*************************************************************************
0020200 C ASSUMPTION:
0020300 C           (1) THE COMBUSTION IS COMPLETE
0020400 C  X  : THE AMOUNT OF O2 REACTED
0020500 C XY  : THE AMOUNT OF CO2 PRODUCED
0020600 C  Y  : THE AMOUNT OF H2O PRODUCED
0020700 C   IJ: 1 =MATHANE AS INPUT GAS
0020800 C       2 =METHANOL AS INPUT GAS
0020900 C       3 =NAPHTHA AS INPUT GAS
0021000       DIMENSION DNS(I)
0021100 C CALCULATE THE NECESSARY AMOUNT OF O2
0021200       IF(IJ.EQ.3) GO TO 4
0021300       IF(IJ.EQ.2) GO TO 2
0021400       X=1./2.*DNS(3)+1./2.*DNS(5)+2.*DNS(1)
0021500       GO TO 3
0021600     2 X=.5*DNS(3)+.5*DNS(5)+1.5*DNS(1)
0021700       GO TO 3
0021800     4 X=0.5*DNS(3)+0.5*DNS(5)+15.*DNS(1)
0021900       XY=DNS(3)+7.*DNS(1)
0022000       Y=DNS(5)+8.*DNS(1)
0022100       GO TO 5
0022200     3 CONTINUE
0022300       XY=DNS(3)+DNS(1)
0022400       Y=DNS(5)+2.*DNS(1)
0022500 C CALCULATE THE EXIT COMPOSITION
0022600     5 DNS(1)=0.
0022700       DNS(3)=0.
0022800       DNS(5)=0.
0022900       DNS(2)=DNS(2)-X
0023000       DNS(4)=DNS(4)+XY
0023100       DNS(6)=DNS(6)+Y
0023200       RETURN
0023300       END
0023400       SUBROUTINE CDPH(QTI,TCI,TCO,DNSC,P,I,QTS)
0023500 C*************************************************************************
0023600 C THIS SUBROUTINE IS TO CAL. THE ENERGY ANALYSIS FOR E-7 AND E-10
0023700 C*************************************************************************
0023900 C DEFINITION:
0024000 C  QTI: TOTAL HEAT TRANSFER FROM FUEL CELL
0024100 C  TCB: BOILING POINT OF FIXED PRESSURE
0024200       DIMENSION GS(7),HS(7),HCAS(7),HCBS(7),HCCS(7)
0024300       DIMENSION DNSC(I)
0024400       COMMON /ETHDA/ GS,HS,HCAS,HCBS,HCCS
0024500       COMMON/TC/TC/CONS/A,B
0024600       COMMON/U1/ U
0024700 C ASSUME THE SATURATED PRESSURE IS EXP(A-B/T)
0024800       TCB=B/(A-ALOG(P))
0024900 C ASSUME THE SATURATED STEAM OUTPUT
0025000       TCO=TCB
0025100 C ASSUME THE LATENT HEAT CAL. BY WATSON CORRELATION
0025200       TC1=TCB/TC
0025300 C ASSUME THE AVERAGE HEAT CAPACITY OF WATER IS 1 CAL/G-K
0025400       QT=((1.-TC1)/(1.-0.577))**0.38*9700.0*DNSC(6)+(TCB-TCI)*1.*18.    -
0025500      1*DNSC(6)
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```
0025600       IF(QT.GE.QTI) GO TO 1
0025700       QTI=QTI-QT
0025800       QTS=QT
0025900       GO TO 2
0026000     1 TCO=TCB
0026100     2 CONTINUE
0026200       RETURN
0026300       END
0026302       SUBROUTINE COMP(DNS,TIN,TOUT,PIN,POUT,POW,GAG,I,IP)
0026304 C*****************************************************************
0026306 C THIS SUBROUTINE CALCULATES THE BALANCE OF COMPRESSOR
0026308 C*****************************************************************
0026310 C ASSUMPTION:
0026312 C           (1). IDEAL GAS BEHAVIOR
0026314 C  GAG: RATIO OF HEAT CAPACITY
0026316 C   WS: SHIFT WORK
0026318 C  POW: POWER REQUIRED; HP
0026320 C   VO: SPECIFIC VOLUME OF GAS AT APPLIED CONDITION; M**3/G-MOLE
0026322       DIMENSION DNS(I)
0026324       TDNS=0.
0026326       DO 1 IA=1,I
0026328       IF(DNS(IA).EQ.0.) GO TO 1
0026330       TDNS=TDNS+DNS(IA)
0026332     1 CONTINUE
0026334       IF(IP.EQ.2) GO TO 2
0026336       TOUT=TIN*(POUT/PIN)**((GAG-1.)/GAG)
0026338       WS=GAG*1.987*TIN*1.8*((POUT/PIN)**((GAG-1.)/GAG)-1.)/(GAG-1.)
0026340       POW=WS*TDNS/641400.
0026342       RETURN
0026344     2 TOUT=TIN
0026346       WS=1.987*TIN*1.8*ALOG( POUT/PIN)
0026348       POW=WS*TDNS/641400.
0026350       RETURN
0026352       END
0026400       SUBROUTINE COND(THI,THO,DNSH,QT,CH,I)
0026500 C*****************************************************************
0026520 C THIS SUBROUTINE ESTIMATES THE HEAT DUTY IN THE CONDENSER
0026700 C*****************************************************************
0026800 C DEFINITION IS THE SAME AS HEXC
0026900       DIMENSION GS(7),HS(7),HCAS(7),HCBS(7),HCCS(7)
0027000       DIMENSION DNSH(I)
0027100       COMMON /ETHDA/ GS,HS,HCAS,HCBS,HCCS
0027120       COMMON/TC/TC
0027200 C CAL. THE MEAN TEMP. OF HOT SIDE
0027300       THM=(THI+THO)/2.
0027400 C CAL. THE CAPACITY RATE OF FLUID OF HOT SIDE
0027500       CH=0.
0027600       DO 1 IA=1,I
0027700       IF(DNSH(IA).EQ.0.) GO TO 1
0027800       CH=CH+DNSH(IA)*(HCAS(IA)+HCBS(IA)*THM+HCCS(IA)*THM**2)
0027900     1 CONTINUE
0028000       QT=0.
0028100       DO 2 IA=1,I
0028200       QT=QT+DNSH(IA)*(HCAS(IA)*(THI-THO)+HCBS(IA)*(THI*THI-THO*THO)
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0028300      1+HCCS(IA)*(THI**3-THO**3))
0028400     2 CONTINUE
0028420       QTL=((1.-(THO/TC))/(1.-0.577))**0.38*9700.*DNSH(6)
0028440       QT=QT+QTL
0028500       RETURN
0028600       END
0028700       SUBROUTINE CONV(XV,YV,NR,NC)
0028800 C*****************************************************************
0028820 C THIS SUBROUTINE USES WEGSTEIN METHOD FOR ALGEBRAIC CONVERGENCE
0029100 C*****************************************************************
0029200 C DEFINITION:
0029300 C   XV: TRIAL VALUE
0029400 C   YV: CALCULATED VALUE
0029500 C   NC: CONVERSE INDEX
0029600 C       NC=1 CONVERGE
0029700 C       NC=2 NONCONVERGE
0029800       DIMENSION XA(2),YA(2)
0029900       IF(ABS((XV-YV)/(XV+YV)).LT.0.001) GO TO 2
0030000       IF(NC.LE.1) GO TO 1
0030100       XT=(XA(NR)*YV-YA(NR)*XV)/(XA(NR)-XV+YV-YA(NR))
0030200       XA(NR)=XV
0030300       YA(NR)=YV
0030400       XV=XT
0030500       RETURN
0030600     1 XA(NR)=XV
0030700       YA(NR)=YV
0030800       XV=YV
0030900       NC=2
0031000       RETURN
0031100     2 XV=YV
0031200       NC=1
0031300       RETURN
0031400       END
0031500       SUBROUTINE DIVID(TIN,TOUT1,TOUT2,DNS,DNS1,DNS2,GARM,I)
0031600 C*****************************************************************
0031700 C THIS SUBROUTINE CALCULATES THE BALANCE AROUND THE DIVIDER
0031800 C*****************************************************************
0031900 C GARM: DIVIDER FACTOR OF STREAM 32
0032000       DIMENSION DNS(I),DNS1(I),DNS2(I)
0032100 C CAL. THE OUTLET CONDITION
0032200       DO 1 IA=1,I
0032300       DNS1(IA)=GARM*DNS(IA)
0032400     1 CONTINUE
0032500       DO 2 IA=1,I
0032600       DNS2(IA)=(1.-GARM)*DNS(IA)
0032700     2 CONTINUE
0032800       TOUT1=TIN
0032900       TOUT2=TIN
0033000       RETURN
0033100       END
0033200       SUBROUTINE DMIX(DNS1,DNS2,DNS,TIN1,TIN2,TOUT,I,PIN1,PIN2,POUT)
0033300 C*****************************************************************
0033400 C THIS SUBROUTINE CALCULATES THE BALANCE AROUND THE MIXER
0033500 C*****************************************************************
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0033600       DIMENSION GS(7),HS(7),HCAS(7),HCBS(7),HCCS(7)
0033700       DIMENSION DNS1(I),DNS2(I),DNS(I)
0033800       COMMON /ETHDA/ GS,HS,HCAS,HCBS,HCCS
0033900 C CAL. THE TOTAL THERMAL CONST.
0034000       TCAS1=0.
0034100       TCBS1=0.
0034200       TCCS1=0.
0034300       TCAS2=0.
0034400       TCBS2=0.
0034500       TCCS2=0.
0034600       DO 1 IA=1,I
0034700       TCAS1=TCAS1+DNS1(IA)*HCAS(IA)
0034800       TCAS2=TCAS2+DNS2(IA)*HCAS(IA)
0034900       TCBS1=TCBS1+DNS1(IA)*HCBS(IA)
0035000       TCBS2=TCBS2+DNS2(IA)*HCBS(IA)
0035100       TCCS1=TCCS1+DNS1(IA)*HCCS(IA)
0035200       TCCS2=TCCS2+DNS2(IA)*HCCS(IA)
0035300     1 CONTINUE
0035400 C ASSUME THE INITIAL VALUE
0035500       TOUT=(TIN1+TIN2)/2.
0035600 C CAL. THE ENERGY BALANCE
0035700     2 TOUTC=(TCAS1*TIN1+TCAS2*(TIN2-TOUT)+TCBS1/2.*(TIN1**2-TOUT**2)    -
0035800      1+TCBS2/2.*(TIN2**2-TOUT**2)+TCCS1*(TIN1**3-TOUT**3)/3.+TCCS2      -
0035900      2*(TIN2**3-TOUT**3)/3.)/TCAS1
0036000       CALL CONV(TOUT,TOUTC,1,NC)
0036100       GO TO (3,2),NC
0036200 C CAL. AND WRITE THE OUTLET COMPOSITION
0036300     3 DO 4 IA=1,I
0036400       DNS(IA)=DNS1(IA)+DNS2(IA)
0036500     4 CONTINUE
0036600       TDNS1=0.
0036700       TDNS2=0.
0036800       DO 5 IA=1,7
0036900       TDNS1=TDNS1+DNS1(IA)
0037000       TDNS2=TDNS2+DNS2(IA)
0037100     5 CONTINUE
0037200 C ASSUME PRESSURE DROP TO BE 3% AT MIXER
0037300       POUT=(TDNS1+TDNS2)/(TDNS1*TIN1/PIN1+TDNS2*TIN2/PIN2)*TOUT*0.97
0037400       RETURN
0037500       END
0037600       SUBROUTINE ENFU(DNSA,DNSC,TINC,TINA,TOUT,TOP,POP,VOP,UT,M,I,QT,WE,-
0037700      1OU,CD,PT,IJ)
0037800 C*************************************************************************
0037900 C THIS SUBROUTINE IS TO CAL. ENERGY BALANCE OF FUEL CELL
0038000 C*************************************************************************
0038100 C DEFINITION:
0038200 C  DGR: FREE ENERGY CHANGE AT FUEL CELL CONDITION
0038300 C    E: FUEL CELL EQU. POTENTIAL
0038400 C   EC: HEATING VALUE EFFICIENCY
0038500 C  EFC: FUEL CELL EFFICIENCY
0038600 C   EI: CURRENT EFFICIENCY
0038700 C   EO: FUEL CELL STANDARD EQU. POTENTIAL
0038800 C   EV: VOLTAGE EFFICIENCY
0038900 C FCH4: FRACTION OF METHANE
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0039000 C   FME: FRACTION OF METHANOL
0039100 C FNAP: FRACTION OF NAPHTHA
0039200 C    M: INDEX OF OUTLET CONDITION
0039300 C       M=1 OUTLET TEMP. IS FIXED TO TOPFC
0039400 C       M=2 OUTLET TEMP. IS NOT FIXED
0039500 C  PCO: MOL. FRACTION OF CO
0039600 C    Q: TOTAL HEAT RELEASE PER HR.
0039700 C  SIS: INTEGRATION CONST. IN CALCULATING S
0039800 C TAUHO: MOL. FRACTION OF AVAILABLE H2O
0039900 C   UT: FUEL UTILIZATION
0040000 C  VOP: ACTUAL FUEL CELL POTENTIAL
0040100 C   WE: ELECTRICAL WORK
0040200 C HLHV(I):LOWER HEATING VALUE OF GAS I
0040300       DIMENSION GS(7),HS(7),HCAS(7),HCBS(7),HCCS(7)
0040400       DIMENSION HLHV(7),DNSA(7),DNSC(7),DNS(7),DNSCI(7),DNSAO(7),       -
0040500      1DNSAI(7)
0040600       COMMON /ETHDA/ GS,HS,HCAS,HCBS,HCCS
0040700       COMMON/CONFC/ E,ETH,EI,EV,EC,EFC
0040900       COMMON/HLHV1/ HLHV
0041000 C CAL. THE MOL. FRACTION OF AVAILABLE HYDROGEN
0041100       TDNS=0.
0041200       TDNSC=0.
0041300       DO 1 IA=1,I
0041400       IF(DNSA(IA).EQ.0.) GO TO 1
0041500       TDNS=TDNS+DNSA(IA)
0041600       IF(DNSC(IA).EQ.0.) GO TO 1
0041700       TDNSC=TDNSC+DNSC(IA)
0041800     1 CONTINUE
0041900       IF(IJ.EQ.1) FCH4=DNSA(1)/TDNS
0042000       IF(IJ.EQ.2) FME=DNSA(1)/TDNS
0042100       IF(IJ.EQ.3) FNAP=DNSA(1)/TDNS
0042200       AHLU=DNSA(5)/TDNS
0042300       TAUHO=DNSA(6)/TDNS
0042400       PCO=DNSA(3)/TDNS
0042500       PPH2=SQRT(DNSA(5)/TDNS*DNSA(5)*(1-UT)/(TDNS-DNSA(5)*UT))
0042600       PPCO=SQRT(DNSA(3)/TDNS*DNSA(3)/(TDNS-DNSA(5)*UT))
0042700       PPO2=SQRT(DNSC(2)/TDNSC*DNSC(2)*(1-OU)/(TDNSC+DNSC(2)*OU))
0042800       PPH2O=SQRT(DNSC(6)/TDNSC*DNSC(6)/(TDNSC+DNSC(2)*OU))
0042900       CALL VINEW(1,VOP,CD,TOP,POP,PPH2,PPO2,PPH2O,PPCO,                 -
0043000      1X0)
0043100 C CAL.THE OPEN-CIRCUIT POTENTIAL
0043200       DHCAS=HCAS(6)-1./2.*HCAS(2)-HCAS(5)
0043300       DHCBS=HCBS(6)-1./2.*HCBS(2)-HCBS(5)
0043400       DHCCS=HCCS(6)-1./2.*HCCS(2)-HCCS(5)
0043500       DHO=HS(6)-1./2.*HS(2)-HS(5)-DHCAS*298.-1./2.*DHCBS*298.**2-1./3.* -
0043600      1DHCCS*298.**3
0043700       SIS=DHO/298.+DHCAS-(GS(6)-1./2.*GS(2)-GS(5))/298.-DHCAS*ALOG(298.)-
0043800      1-DHCBS*298./2.-DHCCS*298.**2/6.
0043900       DG=DHO+(DHCAS-SIS)*TOP-DHCAS*ALOG(TOP)*TOP-DHCBS/2.*TOP**2        -
0044000      1-DHCCS/6.*TOP**3
0044100       IF(TOP.EQ.463.) DG=-52798.
0044200       EO=-DG/2./23060.
0044300       E=EO+1.987*TOP/2./23060.*ALOG(AHLU*0.21**0.5/TAUHO*POP**0.5)
0044400 C CAL. FREE ENERGY CHANGE AT FUEL CELL CONDITION
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0044500       DGR=-2.*23060.*E*AHLU*TDNS
0044600 C CAL. THE EFFICIENCY
0044700       EV=VOP/E
0044800       EI=UT
0044900 C CAL. THE ELECTRICAL WORK
0045000       WE=-EV*EI*DGR
0045100 C CAL. THE THERMODYNAMIC EFFICIENCY
0045200       DH=(-57798.+DHCAS*(TOP-298.)+DHCBS/2.*(TOP**2-298.**2)+DHCCS*     -
0045300      1(TOP**3-298.**3)/3.)*AHLU
0045400       IF(TOP.EQ.463) DH=-58186.*AHLU
0045500       ETH=DGR/DH/TDNS
0045600       IF (IJ.EQ.1)                                                      -
0045700      1DHC=FCH4*(HLHV(1)+(HCAS(4)+2.*HCAS(6)-HCAS(1)-2.*HCAS(2))         -
0045800      1*(TOP-298.)+(HCBS(4)+2.*HCBS(6)-HCBS(1)-2.*HCBS(2))/2.           -
0045900      2*(TOP**2-298.**2)+(HCCS(4)+2.*HCCS(6)-HCCS(1)-2.*HCCS(2))/3.     -
0046000      3*(TOP**3-298.**3))
0046100       IF (IJ.EQ.2)                                                      -
0046200      1DHC=FME*(HLHV(1)+(HCAS(4)+2.*HCAS(6)-HCAS(1)-1.5*HCAS(2))        -
0046300      1*(TOP-298.)+(HCBS(4)+2.*HCBS(6)-HCBS(1)-1.5*HCBS(2))/2.          -
0046400      2*(TOP**2-298.**2)+(HCCS(4)+2.*HCCS(6)-HCCS(1)-1.5*HCCS(2))/3.    -
0046500      3*(TOP**3-298.**3))
0046600       IF (IJ.EQ.3)                                                      -
0046700      1DHC=FNAP*(HLHV(1)+(7.*HCAS(4)+8.*HCAS(6)-HCAS(1)-15.*HCAS(2))    -
0046800      2*(TOP-298.)                                                      -
0046900      1+(8.*HCBS(6)+7.*HCBS(4)-HCBS(1)-15.*HCBS(2))* (TOP**2-298.**2)/2. -
0047000      3+(8.*HCCS(6)+7.*HCCS(4)-HCCS(1)-15.*HCCS(2))/3.                  -
0047100      3*(TOP**3-298.**3))
0047200       DHC=DHC+FCO*(HLHV(3)+(HCAS(4)-HCAS(3)-0.5*HCAS(2))                -
0047300      4*(TOP-298.)+(HCBS(4)-HCBS(3)-1./2.*HCBS(2))/2.                   -
0047400      5*(TOP**2-298.**2)+(HCCS(4)-HCCS(3)-1./2.*HCCS(2))/3.*(TOP**3-298. -
0047500      6**3))+AHLU*(HLHV(5)+(HCAS(6)-HCAS(5)-1./2.*HCAS(2))*(TOP-298.)    -
0047600      7+(HCBS(6)-HCBS(5)-1./2.*HCBS(2))/2.*(TOP**2-298.**2)+(HCCS(6)     -
0047700      8-HCCS(5)-1./2.*HCCS(2))/3.*(TOP**3-298.**3))
0047800       EC=DH/DHC
0047900       EFC=ETH*EV*EI*EC
0048000       DO 2 IA=1,I
0048100       DNSCI(IA)=DNSC(IA)
0048200     2 DNSAI(IA)=DNSA(IA)
0048300       CALL FUCE(DNSAI,TOP,POP,DNSA,DNSC,DSO,DSN,DSHO,UT,I,PINF,PINA,IJ)
0048400       DHIN=0.
0048500       DO 3 IA=1,I
0048600       DHIN=DHIN+DNSAI(IA)*(HCAS(IA)*(298.-TINA)+HCBS(IA)/2.*(298.**2    -
0048700      1-TINA**2)+HCCS(IA)/3.*(298.**3-TINA**3))+DNSCI(IA)*(HCAS(IA)*     -
0048800      2(298.-TINC)+HCBS(IA)/2.*(298.**2-TINC**2)+HCCS(IA)/3.*            -
0048900      3(298.**3-TINC**3))
0049000     3 CONTINUE
0049100       DH=-57973.*(DNSAI(5)-DNSA(5))
0049200 C CAL. THE OUTLET COMPOSITION
0049300       DO 4 IA=1,I
0049400     4 DNS(IA)=DNSA(IA)+DNSC(IA)
0049500       TCAS=0.
0049600       TCBS=0.
0049700       TCCS=0.
0049800       DO 5 IA=1,I
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0049900       TCAS=TCAS+DNS(IA)*HCAS(IA)
0050000       TCBS=TCBS+DNS(IA)*HCBS(IA)
0050100       TCCS=TCCS+DNS(IA)*HCCS(IA)
0050200     5 CONTINUE
0050300       TOUT=TOP
0050400       IF(M.EQ.1) GO TO 7
0050500 C CAL. THE OUTLET TEMP.
0050600     6 TOUTC=(-DHIN-DH-WE  -TCBS/2.*((TOUT)**2-(298.)**2)-TCCS/3.       -
0050700      1*((TOUT)**3-(298.)**3))/TCAS+298.
0050800       CALL CONV(TOUT,TOUTC,1,NC)
0050900       GO TO (8,6),NC
0051000 C CAL. THE TOTAL HEAT REJECTED PER HR.
0051100     7 QT=-DHIN-DH-WE  -TCAS*(TOUT-298.)-TCBS/2.*(TOUT**2-298.**2)       -
0051200      1-TCCS/3.*(TOUT**3-298.**3)
0051300     8 CONTINUE
0051400 C 1 KWHR=860076CAL
0051500       WE=WE/860076.
0051600       RETURN
0051700       END
0051800       SUBROUTINE ENRE(DNS,TOP,POP,TIN,TOUT,I,IP,IJ)
0051900 C*****************************************************************
0052000 C THIS SUBROUTINE CALCULATES THE ENERGY BALANCE OF REFORMER
0052100 C*****************************************************************
0052200       DIMENSION GS(7),HS(7),HCAS(7),HCBS(7),HCCS(7)
0052300       DIMENSION DNS(7),DINS(7),X(2)
0052400       COMMON/ETHDA/ GS,HS,HCAS,HCBS,HCCS
0052500 C STORE THE INLET COMPOSITION
0052600       DO 1 IA=1,I
0052700       DINS(IA)=DNS(IA)
0052800     1 CONTINUE
0052900 C CALCULATE THE OUTLET COMP.
0053000       CALL REF(DNS,TOP,POP,X,I,IJ)
0053100       IF(IP.EQ.1) GO TO 2
0053200       TOUT=TIN
0053300       GO TO 6
0053400     2 CONTINUE
0053500 C CALCULATE THE ENTHALPY CHANGE WITH TEMP. OF INLET GAS
0053600       DHIN=0.
0053700       DO 3 IA=1,I
0053800       IF(DINS(IA).EQ.0.) GO TO 3
0053900       DHIN=DHIN+DINS(IA)*(HCAS(IA)*(298.-TIN)+HCBS(IA)/2.*((298.)**2    -
0054000      1-TIN**2)+HCCS(IA)/3.*((298.)**3-(TIN)**3))
0054100     3 CONTINUE
0054200 C CALCULATE THE ENTHALPY CHANGE OF REACTION
0054300       IF (IJ.EQ.1)                                                     -
0054400      1DH1=(HS(3)+3.*HS(5)-HS(1)-HS(6))*X(1)
0054500       IF (IJ.EQ.2)                                                     -
0054600      1DH1=(HS(4)+3.*HS(5)-HS(1)-HS(6))*X(1)
0054700       IF (IJ.EQ.3)                                                     -
0054800      1DH1=(7.*HS(3)+15.*HS(5)-HS(1)- 7.*HS(6))*X(1)
0054900       IF(IJ.EQ.2)                                                      -
0055000      1DH2=(HS(3)+2.*HS(5)-HS(1))*X(2)
0055100       IF ((IJ.EQ.1).OR.(IJ.EQ.3))                                      -
0055200      1DH2=(HS(4)+HS(5)-HS(3)-HS(6))*X(2)
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0055300       DH=DH1+DH2
0055400 C CALCULATE THE TOTAL HEAT CAP. CONSTANT OF OUTLET GAS
0055500       TCAS=0.
0055600       TCBS=0.
0055700       TCCS=0.
0055800       DO 4 IA=1,I
0055900       IF(DNS(IA).EQ.0.) GO TO 4
0056000       TCAS=TCAS+DNS(IA)*HCAS(IA)
0056100       TCBS=TCBS+DNS(IA)*HCBS(IA)
0056200       TCCS=TCCS+DNS(IA)*HCCS(IA)
0056300     4 CONTINUE
0056400 C CALCULATE THE MAX. TEMP. OF OUTLET GAS
0056500       TOUT=TOP-500.
0056600     5 TOUTC=(-DH-DHIN-TCBS/2.*((TOUT)**2-(298.)**2)-TCCS/3.*((TOUT)**3  -
0056700      1-(298.)**3))/TCAS+298.
0056800       CALL CONV(TOUT,TOUTC,1,NC)
0056900       GO TO (6,5),NC
0057000     6 CONTINUE
0057100       RETURN
0057200       END
0057300       SUBROUTINE ENSH(DNS,TIN,TOUT,TOP,PIN,I,IP,IJ)
0057400 C*********************************************************************
0057500 C THIS SUBROUTINE CALCULATES THE ENERGY BALANCE OF SHIFT CONVERTER
0057600 C*********************************************************************
0057700       DIMENSION GS(7),HS(7),HCAS(7),HCBS(7),HCCS(7)
0057800       DIMENSION DNS(7),DINS(7)
0057900       COMMON/ETHDA/ GS,HS,HCAS,HCBS,HCCS
0058000 C STORE THE INITIAL COMPOSITION
0058100       DO 1 IA=1,I
0058200     1 DINS(IA)=DNS(IA)
0058300       CALL PDSH(DINS,PIN,POUT,TOP,1,IJ)
0058400       POP=(PIN+POUT)/2.
0058500 C CALCULATE THE OUTLET COMPOSITION
0058600       CALL SHIFT(DNS,TOP,POP,X,I)
0058700       IF(IP.EQ.1) GO TO 2
0058800       TOUT=TIN
0058900       GO TO 6
0059000     2 CONTINUE
0059100 C CALCULATE THE ENTHALPY CHANGE WITH TEMP. OF INLET GAS
0059200       DHIN=0.
0059300       DO 3 IA=1,I
0059400       IF(DNS(IA).EQ.0.) GO TO 3
0059500       DHIN=DHIN+DINS(IA)*(HCAS(IA)*(298.-TIN)+HCBS(IA)/2.*((298.)**2-   -
0059600      1(TIN)**2)+HCCS(IA)/3.*((298.)**3-(TIN)**3))
0059700     3 CONTINUE
0059800 C CALCULATE THE ENTHALPY CHANGE OF REACTION
0059900       DH=(HS(4)+HS(5)-HS(3)-HS(6))*X
0060000       TCAS=0.
0060100       TCBS=0.
0060200       TCCS=0.
0060300       DO 4 IA=1,I
0060400       IF(DNS(IA).EQ.0.) GO TO 4
0060500       TCAS=TCAS+DNS(IA)*HCAS(IA)
0060600       TCBS=TCBS+DNS(IA)*HCBS(IA)
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0060700       TCCS=TCCS+DNS(IA)*HCCS(IA)
0060800     4 CONTINUE
0060900 C CALCULATE THE MAX. TEMPERATURE OF OUTLET GAS
0061000       TOUT=TOP+10.
0061100     5 TOUTC=(-DH-DHIN-TCBS/2.*((TOUT)**2-(298.)**2)-TCCS/3.*((TOUT)**3  -
0061200      1-(298.)**3))/TCAS+298.
0061300       CALL CONV(TOUT,TOUTC,1,NC)
0061400       GO TO (6,5),NC
0061500     6 CONTINUE
0061600       RETURN
0061700       END
0061800       SUBROUTINE EQUK(NNS,TOP,SK,I)
0061900 C*************************************************************************
0062000 C THIS SUBROUTINE CALCULATES THE EQUALIBRIUM CONSTANT
0062100 C*************************************************************************
0062200 C    R: GAS CONSTANT;G-CAL/G-MOLE-K
0062300 C  TST: STANDARD TEMPERATURE; K
0062400 C
0062500       DIMENSION GS(7),HS(7),HCAS(7),HCBS(7),HCCS(7)
0062600       DIMENSION NNS(I)
0062700       COMMON /ETHDA/ GS,HS,HCAS,HCBS,HCCS
0062800       DATA R/1.987/
0062900       DATA TST/298./
0063000 C CAL. THE TOTAL HEAT CAPACITY CONSTANT
0063100       TCAS=0.
0063200       TCBS=0.
0063300       TCCS=0.
0063400       DO 1 IA=1,I
0063500       IF(NNS(IA).EQ.0) GO TO 1
0063600       TCAS=TCAS+NNS(IA)*HCAS(IA)
0063700       TCBS=TCBS+NNS(IA)*HCBS(IA)
0063800       TCCS=TCCS+NNS(IA)*HCCS(IA)
0063900     1 CONTINUE
0064000 C CAL. HEAT CHANGE OF REACTION
0064100       DH=0.
0064200       DO 2 IA=1,I
0064300       IF(NNS(IA).EQ.0) GO TO 2
0064400       DH=DH+NNS(IA)*HS(IA)
0064500     2 CONTINUE
0064600 C CAL. FREE ENERGY OF REACTION
0064700       DG=0.
0064800       DO 3 IA=1,I
0064900       IF(NNS(IA).EQ.0) GO TO 3
0065000       DG=DG+NNS(IA)*GS(IA)
0065100     3 CONTINUE
0065200 C CAL. HEAT CONST.
0065300       DHO=DH-TCAS*TST-TCBS*TST**2/2.-TCCS*TST**3/3.
0065400 C CAL. CONST. AI
0065500       AI=(DHO-DG-TCAS*TST*ALOG(TST)-TCBS/2.*TST**2-TCCS/6.*TST**3)/TST/R
0065600 C CAL. EQU. CONST.
0065700       SK=EXP(-DHO/R/TOP+TCAS/R*ALOG(TOP)+TCBS/2.*TOP/R+TCCS/6./R*TOP**2 -
0065300      1+AI)
0065900       RETURN
0066000       END
```

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0066100       SUBROUTINE FLAME(DNS,TIN,TF,I,IJ)
0066200 C*************************************************************************
0066300 C THIS SUBROUTINE CALCULATES THE MAX. ADIABATIC FLAME TEMPERATURE
0066400 C FOR 200% THEORETICAL AIR
0066500 C*************************************************************************
0066600 C ASSUMPTION:
0066700 C           (1). THE COMBUSTION PROCESS GOES TO COMPLETION
0066800 C           (2). HEAT LOSSES ARE NEGLIGIBLE
0066900 C           (3). NEGLIGIBLE DISSOCIATION OF THE PRODUCTS OF COMBUSTION
0067000 C           (4). PRESSURE IS LOW AROUND 1ATM
0067100 C  TF: MAX. TEMPERATURE OF ADIABATIC FLAME
0067200       DIMENSION GS(7),HS(7),HCAS(7),HCBS(7),HCCS(7)
0067300       DIMENSION DNS(7),DINS(7)
0067400       COMMON/ETHDA/ GS,HS,HCAS,HCBS,HCCS
0067500       COMMON /EXT/EXT
0067600 C STORE THE INLET FLUID
0067700       DO 1 IA=1,I
0067800       DINS(IA)=DNS(IA)
0067900     1 CONTINUE
0068000 C CALCULATE THE EXIT FLUID
0068100       CALL BURN(DNS,I,IJ)
0068200 C CALCULATE THE HEAT CHANGE OF REACTION AT 298 K
0068300       DH=0.
0068400       DO 2 IA=1,I
0068500       IF(DNS(IA).EQ.0.) GO TO 2
0068600       DH=DH+DNS(IA)*HS(IA)
0068700     2 CONTINUE
0068800       DO 3 IA=1,I
0068900       IF(DINS(IA).EQ.0.) GO TO 3
0069000       DH=DH-DINS(IA)*HS(IA)
0069100     3 CONTINUE
0069200 C CALCULATE THE ENTHALPY WITH TEMP. CHANGE
0069300       DO 4 IA=1,I
0069400       IF(DINS(IA).EQ.0.) GO TO 4
0069500       DH=DH+DINS(IA)*(HCAS(IA)*(298.-TIN)+HCBS(IA)/2.*((298.)**2-TIN**2)-
0069600      1+HCCS(IA)/3.*((298.)**3-TIN**3))
0069700     4 CONTINUE
0069800 C CALCULATE THE TOTAL HEAT CAPACITY CONSTANT
0069900       TCAS=0.
0070000       TCBS=0.
0070100       TCCS=0.
0070200       DO 5 IA=1,I
0070300       IF(DNS(IA).EQ.0.) GO TO 5
0070400       TCAS=TCAS+DNS(IA)*HCAS(IA)
0070500       TCBS=TCBS+DNS(IA)*HCBS(IA)
0070600       TCCS=TCCS+DNS(IA)*HCCS(IA)
0070700     5 CONTINUE
0070800 C CALCULATE THE MAX. TEMPERATURE
0070900       TF=TIN+500.
0071000     6 TFC=(-DH-TCBS/2.*((TF)**2-(298.)**2)-TCCS/3.*((TF)**3-(298.)**3)) -
0071100      1/TCAS+298.
0071200       CALL CONV(TF,TFC,1,NC)
0071300       GO TO (7,6),NC
0071400     7 CONTINUE
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```
0071500       RETURN
0071600       END
0071700       SUBROUTINE FUCE(DNS,TOP,POP,DNSA,DNSC,DSO,DSN,DSHO,UT,I,PINF,PINA,-
0071800      1IJ)
0071900 C*****************************************************************
0072000 C THIS SUBROUTINE CALCULATES THE MASS BALANCE OF FUEL CELL
0072100 C*****************************************************************
0072200 C  X  : CONSUMPTION OF H2 IN THE FUEL CELL UNDER UT UTILIZATION
0072300       DIMENSION GS(7),HS(7),HCAS(7),HCBS(7),HCCS(7)
0072400       DIMENSION DNS(7),DNSA(7),DNSC(7),NNS(7)
0072500       COMMON /EXA/ EXA
0072600       COMMON /HUMI/ WAT
0072700       X=UT*DNS(5)
0072800 C CAL. AND WRITE THE INLET COMPOSITION OF AIR
0072900     1 DSO=(1.+EXA/100.)*(1./2.*X-DNS(2))
0073000       DSN=DSO*3.76
0073100       DSHO=((DSO+DSN)*28.8)*WAT/18.
0073200 C CAL. AND WRITE THE OUTLET COMPOSITION
0073300       DO 2 IA=1,I
0073400       DNSA(IA)=DNS(IA)
0073500     2 CONTINUE
0073600       DNSA(5)=DNS(5)-X
0073700       DO 3 IA=1,I
0073800       DNSC(IA)=0.
0073900     3 CONTINUE
0074000       DNSC(2)=EXA/100.*(1./2.*X-DNS(2))
0074100       DNSC(6)=DSHO+X
0074200       DNSC(7)=DSN
0074300       CALL PDFU(DNSA,DNSC,DNS,DSO,DSN,DSHO,POP,TOP,PINF,PINA,IJ)
0074400       RETURN
0074500       END
0074600       SUBROUTINE HEPD(DNSA,DNSC,THM,TCM,HA,PINT,PINS,N,DPJ,DP,NT,TCO,TCI-
0074700      1,IJ)
0074710 C*****************************************************************
0074740 C THIS SUBROUTINE CALCULATES PRESSURE DROP IN THE HEAT EXCHANGER
0074760 C*****************************************************************
0074765 C DP : PRESSURE DROP ON THE SHELL SIDE
0074770 C DPJ : PRESSURE DROP ON THE TUBE SIDE
0074775 C REJ : REYNOLDS NUMBER OF TUBE SIDE
0074780 C GS : SHELL SIDE MASS VELOCITY
0074785 C FPRI : FRICTION FACTOR
0074800       REAL IDT,IDS,DNSA(7),DNSC(7)
0074900       DIMENSION FLI(7),C(7),CM(7),WM(7),FLJ(7),CMJ(7),CJ(7)
0075000       COMMON /WM/ WM
0075100       COMMON /HEPDT/ NP,NR,BSPAC,ODT,PITCH,CL,IDS,IDT,FLOAR,SURFC      -
0075200      1,CLEN,SITS2,DTH
0075300 C*****************************************************************
0075400 C  HEAT EXCHANGER BASIS: 3/4 IN TUBE OD AND BWG 14
0075500 C*****************************************************************
0075600 C CALCULATE NO. OF TUBES
0075700       NT=  HA    /0.3048**2/NP/CLEN/SURFC
0075800 C CAL. NO. OF BAFFLES
0075900       NB=CLEN/BSPAC
0076000 C CAL. FREE AREA BETWEEN BAFFLES
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0076100       FAREA=IDS/(ODT+CL)*CL*BSPAC
0076200 C CAL. CORRECTION FACTOR
0076300       BO=NB+1.
0076400 C CAL. RATIO OF PITCH TRANSVERSE TO FLOW TO TUBE DIA.
0076500       XT=PITCH/ODT
0076600       IF (IJ.GT.3) GO TO 2
0076700 C INSERT FLOW RATE OF EACH GAS
0076800 C SHELLSIDE CALCULATIONS
0076900       FLI(1)=DNSA(1)/453.6
0077000       FLI(2)=DNSA(3)/453.6
0077100       FLI(3)=DNSA(4)/453.6
0077200       FLI(4)=DNSA(6)/453.6
0077300       FLI(5)=DNSA(5)/453.6
0077400       FLI(6)=DNSA(7)/453.6
0077500       FLI(7)=DNSA(2)/453.6
0077600       FI=FLI(1)+FLI(2)+FLI(3)+FLI(4)+FLI(5)+FLI(6)+FLI(7)
0077700       DO 1 I=1,7
0077800       CM(I)=FLI(I)/FI
0077900     1 CONTINUE
0078000       AMW=CM(1)*WM(1)+CM(2)*WM(3)+CM(3)*WM(4)+CM(4)*WM(6)+CM(5)*WM(5)   -
0078100      1+CM(6)*WM(7)+CM(7)*WM(2)
0078200       TF=(THM   -273.16)*1.8+32.
0078300       CALL CMASS(C,FLI,FI)
0078400       AMUI=VIS(C,TF,IJ)
0078500       RHO=(AMW*PINS)/(0.7302*(TF+460.))
0078600 C CAL. SHELL SIDE MASS VELOCITY ACROSS TUBES
0078700       GS=FI*AMW/FAREA
0078800 C CAL. CONST. SBO (FOR STAGGERED TUBES)
0078900       SBO=0.23+0.11/(XT-1.)**1.08
0079000 C CAL. FRICTION FACTOR
0079100       FPRI=SBO*(ODT*GS/AMUI)**(-0.15)
0079200 C CAL. PRESSURE DROP OF SHELL SIDE FLOW
0079300       DP= BO*2.*FPRI*NR*GS**2/32.174/3600.**2/RHO/2116.2
0079400     2 CONTINUE
0079500 C TUBESIDE CALCULATIONS
0079600       FLJ(1)=DNSC(1)/453.6
0079700       FLJ(2)=DNSC(3)/453.6
0079800       FLJ(3)=DNSC(4)/453.6
0079900       FLJ(4)=DNSC(6)/453.6
0080000       FLJ(5)=DNSC(5)/453.6
0080100       FLJ(6)=DNSC(7)/453.6
0080200       FLJ(7)=DNSC(2)/453.6
0080300       FJ=FLJ(1)+FLJ(2)+FLJ(3)+FLJ(4)+FLJ(5)+FLJ(6)+FLJ(7)
0080400       DO 3 JJ=1,7
0080500       CMJ(JJ)=FLJ(JJ)/FJ
0080600     3 CONTINUE
0080700       AMM=CMJ(1)*WM(1)+CMJ(2)*WM(3)+CMJ(3)*WM(4)+CMJ(4)*WM(6)           -
0080800      1+CMJ(5)*WM(5)+CMJ(6)*WM(7)+CMJ(7)*WM(2)
0080900       DT=DTH*(THM-TCM)
0081000       TW=DT+TCM
0081100       TWF=(TW-273.16)*1.8+32.
0081200       TCF=(TCM-273.16)*1.8+32.
0081300       CALL CMASS(CJ,FLJ,FJ)
0081400       AMUJ=VIS(CJ,TCF,IJ)
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0081500       AMUW=VIS(CJ,TWF,IJ)
0081600       IF((AMUJ.LE.0.).OR.(AMUW.LE.0.)) GO TO 10
0081700       TKC=THC(CJ,TCF,IJ)
0081800       CP=HTCP(CJ ,TCF,IJ)
0081900       AROH=(AWM*PINT)/(0.7302*(TCF+460.))
0082000       GJ=FJ*AWM /FLOAR/NT
0082100       REJ=GJ*IDT/AMUJ
0082200       IF(REJ.LE.2100.)GO TO 4
0082300       SF=0.046/REJ**0.2
0082400       GO TO 5
0082500     4 SF=16./REJ
0082600     5 CONTINUE
0082700       IF(S1TS2.GT.0.715) GO TO 6
0082800       CKC=0.4*(1.25-S2TS1)
0082900       GO TO 7
0083000     6 CKC=0.75*(1.-S2TS1)
0083100     7 CONTINUE
0083200       CK1=(1.-S2TS1)**2+CKC+0.5*(NP-1.)/NP
0083300       IF(REJ.GT.2100.) GO TO 8
0083400       PHI=1.1*(AMUJ/AMUW)**0.25
0083500       BI=1.+CK1*IDT*PHI/4./SF/CLEN
0083600       GO TO 9
0083700     8 PHI=1.02*(AMUJ/AMUW)**0.14
0083800       BI=1.+0.51*CK1*NP*(TW -TCM)*(AMUJ/AMUW)**0.28/(TCO-TCI)          -
0083900      1/(CP*AMUJ/TKC/AWM )**0.6667
0084000 C CAL. TUBESIDE DP
0084100     9 DPJ= BI*2.*SF*GJ**2*CLEN*NP/32.17/3600.**2/AROH/IDT/PHI/2116.2
0084200       GO TO 12
0084300    10 DPJ=0.
0084400       WRITE(6,11)
0084500    11  FORMAT('THE TRYING TEMP. IS BELOW THE LIMIT OF CAL. VISCOSITY')
0084600    12  CONTINUE
0084700       RETURN
0084800       END
0084900       SUBROUTINE HEXC(THI,DNSH,DNSC,TCI,THO,TCO,QT,MOD,HA,N,M,I,PT,PS,NT-
0085000      1,IJ)
0085100 C*************************************************************************
0085200 C THIS SUBROUTINE IS TO CAL. THE ENERGY ANALYSIS FOR HAET EXCHANGER
0085300 C*************************************************************************
0085400 C   CC: CAPACITY RATE OF FLUID ON COLD SIDE ,DNSC*CPC
0085500 C   CH: CAPACITY RATE OF FLUID ON HOT SIDE, DNSH*CPH
0085600 C CMAX: MAX. CAPACITY RATE
0085700 C CMIN: MIN. CAPACITY RATE
0085800 C  CPC: SPECIFIC HEAT OF COLD SIDE FLUID
0085900 C  CPH: SPECIFIC HEAT OF HOT SIDE FLUID
0086000 C   HE: HEAT EXCHANGER EFFECTIVENESS
0086100 C   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  THO: HOT SIDE OUTLET TEMPERATURE
0086700 C   UA: OVERALL HEAT TRANSFER COEFFICIENT OF EXCHANGER
0086800 C  MOD: TYPE OF HEAT EXCHANGER
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0086900 C       MOD=1 COUNTERFLOW
0087000 C       MOD=2 CROSS FLOW
0087100 C       MOD=3 CONDENSER
0087200 C   THM: MEAN TEMP. OF HOT SIDE
0087300 C   TCM: MEAN TEMP. OF COLD SIDE
0087400 C     N: THE NUMBER OF HEAT EXCHANGER
0087500 C     M: THE INDEX OF INITIAL CONDITION
0087600 C       M=1 TEMP. OF BOTH SIDES ARE KNOWN
0087700 C       M=2 TEMP. OF HOT SIDE INLET AND COLD SIDE OUTLET ARE KNOWN
0087800        DIMENSION GS(7),HS(7),HCAS(7),HCBS(7),HCCS(7)
0087900        DIMENSION DNSH(7),DNSC(7)
0088000        COMMON /ETHDA/ GS,HS,HCAS,HCBS,HCCS
0088100        COMMON/U1/ U
0088200        COMMON/CN1/ CN
0088300        COMMON/HE/ HE
0088400 C ASSUME THE MEAN TEMP. AT COLD AND HOT SIDE
0088500        IF(M.EQ.2) GO TO 1
0088600        THM=(THI+10.+TCI)/2.
0088700        TCM=(THI-10.+TCI)/2.
0088800        GO TO 2
0088900      1 THM=(THI+TCO-50.)/2.
0089000        TCM=(TCO*2.-200.)/2.
0089100 C CAL. CC AND CH
0089200      2 CC=0.
0089300        CH=0.
0089400        DO 4 IA=1,I
0089500        IF(DNSC(IA).EQ.0.) GO TO 3
0089600        CC=CC+DNSC(IA)*(HCAS(IA)+HCBS(IA)*TCM+HCCS(IA)*TCM**2)
0089700      3 IF(DNSH(IA).EQ.0.) GO TO 4
0089800        CH=CH+DNSH(IA)*(HCAS(IA)+HCBS(IA)*THM+HCCS(IA)*THM**2)
0089900      4 CONTINUE
0090000 C CHOOSE THE CMAX. ,CMIN.
0090100        IF(CC.GT.CH) GO TO 5
0090200        CMAX=CH
0090300        CMIN=CC
0090400        GO TO 6
0090500      5 CMAX=CC
0090600        CMIN=CH
0090700      6 CONTINUE
0090800        HA=CN*CMIN/U
0090900        UA=HA*U
0091000 C CAL. THE HEAT EXCHANGER EFFECTIVENESS
0091100        IF(MOD.GE.2) GO TO 8
0091200        IF((CMIN/CMAX).GT.0.01) GO TO 7
0091300        HE=1.-EXP(-UA/CMIN)
0091400        GO TO 12
0091500      7 HE=(1.-EXP((-UA/CMIN)*(1.-CMIN/CMAX)))/(1.-(CMIN/CMAX)*EXP((-UA    -
0091600       1/CMIN)*(1.-CMIN/CMAX)))
0091700        GO TO 12
0091800      8 IF(MOD.GT.2) GO TO 11
0091900        IF(ABS(CMIN/CMAX-1.).GE.0.01) GO TO 9
0092000        HE=(UA/CMIN)/(UA/CMIN+1.)
0092100        GO TO 12
0092200      9 IF((CMIN/CMAX).GT.0.01) GO TO 10
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0092300       HE=1.-EXP(-UA/CMIN)
0092400       GO TO 12
0092500    10 IF(CMAX.EQ.CH) HE=1.-EXP((-CMAX/CMIN)*(1.-EXP(-UA/CMAX)))
0092600       IF(CMIN.EQ.CH) HE=(CMAX/CMIN)*(1.-EXP((-CMIN/CMAX)*(1.-EXP(-UA/   -
0092700      1CMIN))))
0092800       GO TO 12
0092900    11 HE=1.-EXP(-UA/CMIN)
0093000 C CAL. THE OUTLET CONDITION AND TOTAL HEAT TRANSFER RATE
0093100    12 IF(M.EQ.2) GO TO 13
0093200       THO=THI-HE*(CMIN/CH)*(THI-TCI)
0093300       TCO=HE*(CMIN/CC)*(THI-TCI)+TCI
0093400       QT=HE*CMIN*(THI-TCI)
0093500       GO TO 14
0093600    13 TCI=(HE*(CMIN/CC)*THI-TCO)/(HE*(CMIN/CC)-1.)
0093700       THO=THI-HE*(CMIN/CH)*(THI-TCI)
0093800       QT=HE*CMIN*(THI-TCI)
0093900    14 IF((ABS((THO+THI)/2.-THM).LT.(ABS((THO+THI)/2.+THM)*0.005)        -
0094000      1).AND.(ABS((TCO+TCI)/2.-TCM).LT.(ABS((TCO+TCI)/2.+TCM)*0.005)))   -
0094100      2 GO TO 15
0094200       THM=(THO+THI)/2.
0094300       TCM=(TCI+TCO)/2.
0094400       GO TO 2
0094500   15  THM=(THO+THI)/2.
0094600       TCM=(TCO+TCI)/2.
0094700       CALL HEPD(DNSH,DNSC,THM,TCM,HA,PT,PS,N,DPJ,DP,NT,TCO,TCI,IJ)
0094800       IF(M.EQ.2) GO TO  16
0094900       PT=PT-DPJ
0095000       PS=PS-DP
0095100       GO TO 17
0095200   16  PT=PT+DPJ
0095300       PS=PS-DP
0095400    17 CONTINUE
0095500       RETURN
0095600       END
0095700       SUBROUTINE PDFU(DNSA,DNSC,DNS,DSO,DSN,DSHO,POP,ATMP,PINF,PINA,IJ)
0095710 C*************************************************************************
0095720 C THIS SUBROUTINE CALCULATES PRESSURE DROP IN THE FUEL CELL STACK
0095730 C*************************************************************************
0095800       REAL L(2),DP(4)
0095900       DIMENSION FLI(7),C(7),CM(7),WM(7),DNSA(7),DNSC(7),DNS(7),DNSI(7)
0096000       DIMENSION NTA(2),     WIDA(2),D(2)
0096100       COMMON/PDFUT/ NTA,L,WIDA,NP
0096200       COMMON /WM/ WM
0096300 C*************************************************************************
0096400 C  BASIS: NO. 522 STACK
0096500 C*************************************************************************
0096600       IT=1
0096700       DO 1 IA=1,7
0096800     1 DNSI(IA)=0.
0096900       DNSI(4)=DSHO
0097000       DNSI(6)=DSN
0097100       DNSI(7)=DSO
0097200 C CAL. THE PRESSURE DROP OF FUEL SIDE
0097300       JJ=1
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0097400       D(1)=WIDA(1)
0097500       FLI(1)=DNS(1)/453.6
0097600       FLI(2)=DNS(3)/453.6
0097700       FLI(3)=DNS(4) /453.6
0097800       FLI(4)=DNS(6) /453.6
0097900       FLI(5)=DNS(5) /453.6
0098000       FLI(6)=DNS(7)/453.6
0098100       FLI(7)=DNS(2)/453.6
0098200       GO TO 3
0098300     2 FLI(1)=DNSA(1)/453.6
0098400       FLI(2)=DNSA(3)/453.6
0098500       FLI(3)=DNSA(4)/453.6
0098600       FLI(4)=DNSA(6)/453.6
0098700       FLI(5)=DNSA(5)/453.6
0098800       FLI(6)=DNSA(7)/453.6
0098900       FLI(7)=DNSA(2)/453.6
0099000     3 CONTINUE
0099100       TK=ATMP
0099200       FI=FLI(1)+FLI(2)+FLI(3)+FLI(4)+FLI(5)+FLI(6)+FLI(7)
0099300       DO 4 I=1,7
0099400       CM(I)=FLI(I)/FI
0099500     4 CONTINUE
0099600       AMW=CM(1)*WM(1)+CM(2)*WM(3)+CM(3)*WM(4)+CM(4)*WM(6)+CM(5)*WM(5)    -
0099700      1+CM(6)*WM(7)+CM(7)*WM(2)
0099800       G=FI*AMW/WIDA(IT)**2/NP/NTA(IT)
0099900       TF=(TK-273.16)*1.8+32.
0100000       CALL CMASS(C,FLI,FI)
0100100       AMUI=VIS(C,TF,IJ)
0100200       RHO=(AMW*POP)/(0.7302*(TF+460.))
0100300       RE=D(IT)*G/AMUI
0100400       CONS=57.2
0100500       FRIC=CONS/RE
0100600       DP(JJ)=RHO*(G/RHO)**2/2.*(0.5+1.+0.6+FRIC*L(IT)/D(IT))/2116.2      -
0100700      1/3600.**2/32.174
0100800       JJ=JJ+1
0100900       IF(JJ.EQ.2) GO TO 2
0101000       IF(JJ.EQ.3) GO TO 5
0101100       IF(JJ.EQ.4) GO TO 6
0101200       IF(JJ.EQ.5) GO TO 8
0101300 C CAL. THE PRESSURE DROP OF AIR SIDE
0101400 C INSERT THE FLOW RATE OF EACH GAS
0101500     5 FLI(1)=DNSC(1)/453.6
0101600       FLI(2)=DNSC(3)/453.6
0101700       FLI(3)=DNSC(4)/453.6
0101800       FLI(4)=DNSC(6)/453.6
0101900       FLI(5)=DNSC(5)/453.6
0102000       FLI(6)=DNSC(7)/453.6
0102100       FLI(7)=DNSC(2)/453.6
0102200       IT=IT+1
0102300       D(2)=WIDA(2)
0102400       GO TO 3
0102500     6 DO 7 IA=1,7
0102600     7 FLI(IA)=DNSI(IA)/453.6
0102700       GO TO 3
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0102800     8 CONTINUE
0102900       PINF=PINF-(DP(1)+DP(2))/2.
0103000       PINA=PINA-(DP(3)+DP(4))/2.
0103100       RETURN
0103200       END
0103300       SUBROUTINE PDSH(DNS,PIN,POUT,TK,JK,IJ)
0103400 C*********************************************************************
0103500 C THIS SUBROUTINE CALCULATES PRESSURE DROP IN THE SHIFT CONVERTER
0103600 C*********************************************************************
0103700       DIMENSION D(2),AHRN(2),AP(2),CLEN(2),NT(2)
0103800       DIMENSION FLI(7),C(7),CM(7),WM(7),DNS(7)
0103900       COMMON/PDSHT/ D,AHRN,AP,CLEN,NT
0104000       COMMON /WM/ WM
0104100 C JK=1 SHIFT CONVERTER
0104200 C JK=2 REFORMER FOR METHANOL AND NAPHTHA FUEL
0104300       TF=(TK-273.16)*1.8+32.
0104400       DP=6.*(1.-AHRN(JK))/AP(JK)
0104500       FLI(1)=DNS(1)/453.6/NT(JK)
0104600       FLI(2)=DNS(3)/453.6/NT(JK)
0104700       FLI(3)=DNS(4)/453.6/NT(JK)
0104800       FLI(4)=DNS(6)/453.6/NT(JK)
0104900       FLI(5)=DNS(5)/453.6/NT(JK)
0105000       FLI(6)=DNS(7)/453.6/NT(JK)
0105100       FLI(7)=DNS(2)/453.6/NT(JK)
0105200       FI=FLI(1)+FLI(2)+FLI(3)+FLI(4)+FLI(5)+FLI(6)+FLI(7)
0105300       DO 1 I=1,7
0105400       CM(I)=FLI(I)/FI
0105500     1 CONTINUE
0105600       AMW=CM(1)*WM(1)+CM(2)*WM(3)+CM(3)*WM(4)+CM(4)*WM(6)+CM(5)*WM(5)    -
0105700      1+CM(6)*WM(7)+CM(7)*WM(2)
0105800       G=FI*AMW*4./(3.14159*D(JK)**2)
0105900       CALL CMASS(C,FLI,FI)
0106000       AMUI=VIS(C,TF,IJ)
0106100       RHO=(AMW*PIN)/(0.7302*(TF+460.))
0106200       DELP=CLEN(JK)*(1.-AHRN(JK))/AHRN(JK)**3*G**2/DP/4.18E+08          -
0106300      1/RHO*(150.*(1.-AHRN(JK))*AMUI/DP/G+1.75)/2116.2
0106400       POUT=PIN-DELP
0106500       RETURN
0106600       END
0106700       SUBROUTINE PUMP(DNS,TIN,TOUT,PIN,POUT,POW,I)
0106800 C*********************************************************************
0106900 C THIS SUBROUTINE IS TO CAL. THE BALANCE OF PUMP FOR WATER
0107000 C*********************************************************************
0107100 C ASSUMPTION AND DEFINITION IS THE SAME AS COMPR
0107200       DIMENSION DNS(7)
0107300       DIMENSION SV(3),WM(7)
0107400       COMMON/WM/ WM
0107500       COMMON/SV/ SV,SVW
0107600       TOUT=TIN
0107700 C CAL. THE WORK
0107800 C ASSUME AVERAGE SPECIFIC VOLUME OF WATER IS 0.0162 FT**3/LBM
0107900       POW=SVW*144.*5.05051*0.0000001*WM(6)*14.7*(POUT-PIN)*DNS(6)       -
0108000      1/453.6
0108100       RETURN
```

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

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

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

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

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

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0120560   92  XY(1)=X
0120580       XY(2)=Y
0120600       RETURN
0120620       END
0120640       SUBROUTINE VINEW (M,V,Z,TK,POP,PPH2,PPO2,PPH2O,PPCO,X0)
0120660       COMMON/CATAL/SRO,SA,CU,CL,ALFA,SN,FCONST,AREAF,DKC
0120680 1     R=8.314
0120700       ERR=0.005
0120720       CLA=CL
0120740       EZ=1.261-.00025*TK
0120760       SR=SRO*EXP(3650.*(1./TK-1./450.))
0120780       SIO=.2327*(PPO2*POP)**.8*(PPH2O*POP)**.4377*EXP(-6652./TK)
0120800       C=SIO*SA*CU*CL
0120820       EX=11.85*.0066*PPCO*POP*EXP(9190.*(1./TK-1./450.))
0120840       A=ALOG(PPH2/PPH2O*(PPO2*POP)**0.5)
0120860       C1=CLA*SA*CU*.000053
0120880       D=R*TK/SN/FCONST
0120900       B=EZ+D*A
0120920       DA=D/ALFA
0120940       CDL=DKC/AREAF*(PPO2*POP)
0120960       IF (M.EQ.2) GO TO 2
0120980       V=B-DA*ALOG(Z/C)-Z*SR-EX*ALOG(Z/C1)-D*ALOG(CDL/(CDL-Z))
0121000       GO TO 6
0121020 2     Z=X0
0121040 3     CONTINUE
0121060       DO 5 I=1,50
0121080       FZ=Z*SR+DA*ALOG(Z/C)+V-B+EX*ALOG(Z/C1)+D*ALOG(CDL/(CDL-Z))
0121100       DFZ=SR+DA/Z+EX/Z+D/(CDL-Z)
0121120       DZ=FZ/DFZ
0121140       Z=Z-DZ
0121160 4     IF (Z.LE.0.) GO TO 7
0121180       IF (ABS(DZ).LT.ERR) GO TO 6
0121200 5     CONTINUE
0121220 7     Z=X0
0121240       DO 8 I=1,50
0121260       GFZ=(DA*ALOG(Z/C)+V-B+EX*ALOG(Z/C1)+D*ALOG(CDL/(CDL-Z)))/(-SR)
0121280       GZ=Z
0121300       Z=GFZ
0121320       IF (Z.LE.0.) GO TO 19
0121340       IF (ABS((GZ-Z)/(Z+GZ)).LT.ERR) GO TO 6
0121360 8     CONTINUE
0121380       WRITE(6,201)
0121400   201 FORMAT(1X,'CURRENT DENSITY LOOPING')
0121420       GO TO 6
0121440 19    ERR=ERR+0.001
0121460       GO TO 2
0121480    6  CONTINUE
0121500       RETURN
0121520       END
0121540       SUBROUTINE KREF(DNSR,DNSF,DX,DY,DQ,PX,TCO,THZ,Z,POUT,TCOUT
0121560      1,THOUT,S1,DP1,IFUEL)
0121580       REAL K0,MH,K1,K2
0121600       COMMON F0,F1,F2,F3,F4,F5,F6,MH,CG1,CG2,CG3,CG4,CG5,CG6
0121620       COMMON/REP/ K0,EA,RHOB,EPS,DZZ
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0121640       COMMON/ADDRE/ D1,D2,D3,S,DP,P
0121660       COMMON /WM/ WM
0121680       COMMON /FCG/ F7,CG7
0121700       DIMENSION X1( 50),TAX2( 50),XE2( 50),TC( 50),                  -
0121720      1TH( 50),XE( 50),TA(50),TAK1( 50),TAK2( 50),                    -
0121740      2XF( 50),XCOMP( 50,7),XMCOMP( 50,7),XC( 50,7),                  -
0121760      3XU1( 50),TP( 50),FL(7),C(7),WM(7),COM(7),CGCOMP(7),TCGC(7)
0121780       DIMENSION REN( 50)
0121800       DIMENSION P( 50)
0121820       DIMENSION DNSR(7),DNSF(7)
0121840       DATA ERROR/0.01/
0121860       DATA XCOMP/ 350*0./
0121880       IDEBUG=0
0121900       D1=DX
0121920       D2=DY
0121940       D3=DQ
0121960       DP=DP1
0121980       S=S1
0122000       P(1)=PX
0122020       F1=DNSR(1)
0122040       F2=DNSR(3)
0122060       F3=DNSR(4)
0122080       F4=DNSR(6)
0122100       F5=DNSR(5)
0122120       F6=DNSR(7)
0122140       F7=DNSR(2)
0122160       F0=F1+F2+F3+F4+F5+F6+F7
0122180       CG1=DNSF(1)
0122200       CG2=DNSF(3)
0122220       CG3=DNSF(4)
0122240       CG4=DNSF(6)
0122260       CG5=DNSF(5)
0122280       CG6=DNSF(7)
0122300       CG7=DNSF(2)
0122320       WM=CG1+CG2+CG3+CG4+CG5+CG6+CG7
0122340       X1(1)=0.
0122360       XE2(1)=0.
0122380       TCO=(TCO-273.16)*9./5.+32.
0122400       THZ=(THZ-273.16)*9./5.+32.
0122420       KING=0
0122440       C0=(F1*(1.-X1(1))*P(1))/(.7302*(F0+2.*X1(1)*F1)*(TCO+460.))
0122460       U0=(4.*.7302*(F0+2.*X1(1)*F1)*(TCO+460.))/(3.1415927*P(1)       -
0122480      1*(D2**2-D1**2)*EPS)
0122500 C FIRST ASSUMPTION -- THO
0122520       X=.9
0122540       AX=Z*RHOB*K0*P(1)*F1*(2.*F0+X*(2.*F1-F0))/(2.*F0*(F0+2.*X*F1)*   -
0122560      1U0*C0)
0122580       T=-.9045*EA/ALOG(X/AX)-460.
0122600       TK2=K2(T)
0122620       TX2=X2(X,TK2)
0122640       TDH1=-DH1(T)
0122660       TDH2=-DH2(T)
0122680       AY=F1*TDH1*X+(F3+X*F1)*TDH2*TX2
0122700       FL(1)=F1*(1.-X)
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0122720       FL(2)=F2-TX2*(F3+X*F1)
0122740       FL(3)=F3+X*F1+TX2*(F3+X *F1)
0122760       FL(4)=F4-2.*X*F1-TX2*(F3+X *F1)
0122780       FL(5)=F5+4.*X*F1+TX2*(F3+X *F1)
0122800       FL(6)=F6
0122820       FL(7)=F7
0122840       TF=F(X)
0122860       CALL CMASS(C,FL,TF)
0122880       TVIS=VIS(C,T,IFUEL)
0122900       TTHC=THC(C,T,IFUEL)
0122920       THI=HI(TVIS,TTHC)
0122940       CGCOMP(1)=CG1
0122960       CGCOMP(2)=CG2
0122980       CGCOMP(3)=CG3
0123000       CGCOMP(4)=CG4
0123020       CGCOMP(5)=CG5
0123040       CGCOMP(6)=CG6
0123060       CGCOMP(7)=CG7
0123080       CALL CMASS(TCGC,CGCOMP,MH)
0123100       CGVIS=VIS(TCGC,THZ,IFUEL)
0123120       CGTHC=THC(TCGC,THZ,IFUEL)
0123140       CGHTCP=HTCP(TCGC,THZ)
0123160       THO=HO(CGVIS,CGTHC,CGHTCP,Z,THZ,RE)
0123180       TUI=UI(THI,THO,T)
0123200       AZ=3.1415927*TUI*Z*D2/2.
0123220       CALL COMPIN(COM,X1(1),XE2(1))
0123240       TFCP=FCP(T,COM)
0123260       AW=(MH*CGHTCP*TFCP)/AZ+MH*CGHTCP-TFCP
0123280       THO=(AW*THZ+2.*TFCP*TCO+AY)/(AW+2.*TFCP)
0123300       IF(THO.LT.TCO) THO=TCO+250.
0123320       IDEA=1
0123340       IHOPE=1
0123360    75 I=1
0123380       TAK1(1)=0.
0123400       TAK2(1)=0.
0123420       XU1(1)=0.
0123440       TA(1)=TCO
0123460       TAX2(1)=0.
0123480       XF(1)=F0+2.*F1*X1(1)
0123500       DO 80 J=1,7
0123520       XCOMP(1,J)=COM(J)
0123540       XMCOMP(1,J)=XCOMP(1,J)/XF(1)
0123560    80 CONTINUE
0123580       WMM1=0.
0123600       DO 81 J=1,7
0123620       WMM1=WMM1+(XCOMP(1,J)*WM(J))/XF(1)
0123640    81 CONTINUE
0123660       DO 82 J=1,7
0123680       XC(1,J)=(XCOMP(1,J)*WM(J))/(XF(1)*WMM1)
0123700    82 CONTINUE
0123720       TC(1)=TCO
0123740       TH(1)=THO
0123760 C SECOND ASSUMPTION --TC(I+1)
0123780    72 TC(I+1)=TC(I)
```

```
0123800    70 TA(I+1)=(TC(I)+TC(I+1))/2.
0123820       TAK1(I+1)=K1(TA(I+1))
0123840       TAK2(I+1)=K2(TA(I+1))
0123860       B1=DZZ*RHOB*K0*P(I)/(U0*C0)
0123880       B2=EXP(-.9045*EA/(TA(I+1)+460.))
0123900       X1(I+1)=X1(I)+B1*B2*XMCOMP(I,1)
0123920       XE2(I+1)=X2(X1(I+1),TAK2(I+1))
0123940       XDH1=-DH1(TA(I+1))
0123960       XDH2=-DH2(TA(I+1))
0123980       AL1=F1*XDH1*(X1(I+1)-X1(I))
0124000       AL2=(F3+X1(I+1)*F1)*XDH2*(XE2(I+1)-XE2(I))
0124020       AL=AL1+AL2
0124040       FL(1)=F1*(1.-X1(I+1))
0124060       FL(2)=F2-XE2(I+1)*(F3+X1(I+1)*F1)
0124080       FL(3)=F3+X1(I+1)*F1+XE2(I+1)*(F3+X1(I+1)*F1)
0124100       FL(4)=F4-2.*X1(I+1)*F1-XE2(I+1)*(F3+X1(I+1)*F1)
0124120       FL(5)=F5+4.*X1(I+1)*F1+XE2(I+1)*(F3+X1(I+1)*F1)
0124140       FL(6)=F6
0124160       FL(7)=F7
0124180       XF(I+1)=F(X1(I+1))
0124200       CALL CMASS(C,FL,XF(I+1))
0124220       DO 10 J=1,7
0124240       XCOMP(I+1,J)=FL(J)
0124260       XMCOMP(I+1,J)=XCOMP(I+1,J)/XF(I+1)
0124280       XC(I+1,J)=C(J)
0124300    10 CONTINUE
0124320       XVIS=VIS(C,TA(I+1),IFUEL)
0124340       XTHC=THC(C,TA(I+1),IFUEL)
0124360       V=WM(1)*F1+WM(3)*F2+WM(4)*F3+WM(6)*F4+WM(5)*F5+WM(7)*F6+WM(2)*F7
0124380       GMV=(V*4.)/(3.1415927*(D2**2-D1**2))
0124400       AMW=V/F0
0124420       RHO=(AMW*P(I))/(0.7302*(T+460.))
0124440       DELP=(1.-EPS)/EPS**3*GMV**2/DP/4.18E+08/RHO*(150.*(1.-EPS)*XVIS/DP-
0124460      1/GMV+1.75)*DZZ/2116.8
0124480       P(I+1)=P(I)-DELP
0124500       XHI=HI(XVIS,XTHC)
0124520       XCGVIS=VIS(TCGC,TH(I),IFUEL)
0124540       XCGTHC=THC(TCGC,TH(I),IFUEL)
0124560       XGHTCP=HTCP(TCGC,TH(I))
0124580       XHO=HO(XCGVIS,XCGTHC,XGHTCP,Z,TH(I),RE)
0124600       REN(I+1)=RE
0124620       XU1(I+1)=UI(XHI,XHO,TA(I+1))
0124640       AM=(3.1415927*XU1(I+1)*DZZ*D2)/2.
0124660       XFCP=FCP(TA(I),FL)
0124680       AN=(MH*XGHTCP*XFCP)/AM-XFCP+MH*XGHTCP
0124700       TH(I+1)=TH(I)*(AN+2.*XFCP)/AN-2.*XFCP*TC(I)/AN-AL/AN
0124720       TP(I+1)=TH(I+1)*(AM-MH*XGHTCP)/AM+TH(I)*(AM+MH*XGHTCP)/AM-TC(I)
0124740 C TEST SECOND ASSUMPTION
0124760       EE=ABS((TP(I+1)-TC(I+1))/TC(I+1))
0124780       IF(IDEBUG.NE.0)
0124800      1WRITE(6,2020) TP(I+1),TC(I+1),EE
0124820  2020 FORMAT('OTP=',1PE15.7,5X,'TC=',E15.7,5X,'EE=',E15.7)
0124840       IF(EE.LE.ERROR ) GO TO 71
0124860       IF(KING.LE.15) TC(I+1)=(TC(I+1)+TP(I+1))/2.
```

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0124880       TC2=TC(I+1)
0124900       EETC2=TH(I+1)*(AM-MH*XGHTCP)/AM+TH(I)*(AM+MH*XGHTCP)/AM-  -
0124920      1TC(I)-TC2
0124940       IF(KING.LE.15) GO TO 97
0124960       IF(EETC1.NE.EETC2) TC3=TC2-(EETC2/(EETC2-EETC1))*(TC2-TC1)
0124980       IF(EETC1.EQ.EETC2) TC3=(TC2+TP(I+1))/2
0125000       TC(I+1)=TC3
0125020    97 KING=KING+1
0125040       TC1=TC2
0125060       EETC1=EETC2
0125080       IF(KING.GE.40) GO TO 959
0125100       GO TO 70
0125120    71 CONTINUE
0125140       TC(I+1)=TP(I+1)
0125160       AA=I
0125180       AAA=AA*DZZ
0125200       IF(AAA.GE.Z) GO TO 73
0125220       I=I+1
0125240       KING=0
0125260       GO TO 72
0125280    73 N=I+1
0125300 C TEST FIRST ASSUMPTION
0125320       AB=ABS((TH(I+1)-THZ)/THZ)
0125340       IF(AB.LE.0.001) GO TO 74
0125360       THO2=THO
0125380       THZ2=TH(N)
0125400       IF(IDEA.LT.2) THO3=THO+THZ-THZ2
0125420       IF(IDEA.EQ.2) THO3=(THO1-THO2)/(THZ1-THZ2)*(THZ-THZ2)+THO2
0125440       IDEA=2
0125460       THZ1=TH(N)
0125480       THO1=THO
0125500       THO=THO3
0125520       IF(THO.LT.TCO) IHOPE=IHOPE+1
0125540       IF(THO.LT.TCO) THO=TCO+50.
0125560       IF(IHOPE.EQ.5) GO TO 975
0125580       GO TO 75
0125600    74 CONTINUE
0125620       IF(K.EQ.1) L=N
0125640       GO TO 954
0125660   975 CONTINUE
0125680       WRITE(6,976) THO
0125700   976 FORMAT(1H1,'***INSUFFICIENT COMB. GAS HEAT CAPACITY'/          -
0125720      1'0THO=',F17.3,'THIS IS LESS THAN TCO'/'0RAISE THZ AND/OR COMB.  -
0125740      2GAS FLOW RATES')
0125760       GO TO 954
0125780   959 WRITE(6,958) KING,I
0125800   958 FORMAT(1H1,'LOOPING ON TC FOR ',I4,'ITERATIONS IN INCRM',I4)
0125820   954 CONTINUE
0125840       TCO=(TCO-32.)*5./9.+273.16
0125860       THZ=(THZ-32.)*5./9.+273.16
0125880       POUT=P(N)
0125900       TCOUT=(TC(N)-32.)*5./9.+273.16
0125920       THOUT=(TH(1)-32.)*5./9.+273.16
0125940       DNSR(1)=XCOMP(N,1)
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0125960       DNSR(3)=XCOMP(N,2)
0125980       DNSR(4)=XCOMP(N,3)
0126000       DNSR(5)=XCOMP(N,5)
0126020       DNSR(6)=XCOMP(N,4)
0126040       DNSR(7)=XCOMP(N,6)
0126060       RETURN
0126080       END
0163100       SUBROUTINE CMASS(C,FL,F)
0163200       DIMENSION C(7),WM(7),FL(7)
0163300       COMMON /WM/ WM
0163400       WMM=(FL(1)*WM(1)+FL(2)*WM(3)+FL(3)*WM(4)+WM(6)*FL(4)+FL(5)*WM(5)+ -
0163500      1FL(6)*WM(7)+FL(7)*WM(2))/F
0163600       C(1)=FL(1)*WM(1)/(F*WMM)
0163700       C(2)=FL(2)*WM(3)/(F*WMM)
0163800       C(3)=FL(3)*WM(4)/(F*WMM)
0163900       C(4)=FL(4)*WM(6)/(F*WMM)
0164000       C(5)=FL(5)*WM(5)/(F*WMM)
0164100       C(6)=FL(6)*WM(7)/(F*WMM)
0164200       C(7)=FL(7)*WM(2)/(F*WMM)
0164300       RETURN
0164400       END
0164500       SUBROUTINE COMPIN(COM,X1,X2)
0164600       REAL MH
0164700       COMMON F0,F1,F2,F3,F4,F5,F6,MH,CG1,CG2,CG3,CG4,CG5,CG6
0164800       COMMON/ADDRE/ D1,D2,D3,S,DP,P
0164900       COMMON /FCG/F7,CG7
0165000       DIMENSION COM(7)
0165100       DO 8 J=1,7
0165200       IF(J.EQ.1) COM(J)=F1*(1.-X1)
0165300       IF(J.EQ.2) COM(J)=F2-X2*(F3+X1*F1)
0165400       IF(J.EQ.3) COM(J)=F3+X1*F1+X2*(F3+X1*F1)
0165500       IF(J.EQ.4) COM(J)=F4-2.*X1*F1-X2*(F3+X1*F1)
0165600       IF(J.EQ.5) COM(J)=F5+4.*X1*F1+X2*(F3+X1*F1)
0165700       IF(J.EQ.6) COM(J)=F6
0165800       IF(J.EQ.7) COM(J)=F7
0165900     8 CONTINUE
0166000       RETURN
0166100       END
0166200       FUNCTION DH1(T)
0166300       DH1=-2.7285E-03*(T**2)+12.698*T+7.002E+04
0166400       RETURN
0166500       END
0166600       FUNCTION DH2(T)
0166700       DH2=2.3280*T-18111.4
0166800       RETURN
0166900       END
0167000       FUNCTION F(X1)
0167100       REAL MH
0167200       COMMON F0,F1,F2,F3,F4,F5,F6,MH,CG1,CG2,CG3,CG4,CG5,CG6
0167300       COMMON/ADDRE/ D1,D2,D3,S,DP,P
0167400       COMMON /FCG/F7,CG7
0167500       F=F0+2.*X1*F1
0167600       RETURN
0167700       END
```

```
0167800       FUNCTION FCP(T,COM)
0167900       DIMENSION COM(7),A(4,7)
0168000       DATA A/5.34,6.39E-03,0.,0.,6.60,6.67E-04,0.,0.,10.34,1.52E-03,0., -
0168100      1-6.33420E+05,8.22, 8.3E-05,4.136E-07,0.,6.62,4.5E-04,0.,0.,6.5,   -
0168200      25.56E-04,0.,0.,6.732,8.36E-03,5.53E-09,0.0/
0168300       TP=T+460.
0168400       FCP=0.
0168500       DO 9 I=1,7
0168600       FCP=FCP+COM(I)*(A(1,I)+A(2,I)*TP+A(3,I)*TP**2+A(4,I)/(TP**2))
0168700     9 CONTINUE
0168800       RETURN
0168900       END
0169000       FUNCTION HI(VIS,THC)
0169100       REAL MH
0169200       DIMENSION WM(7)
0169300       COMMON F0,F1,F2,F3,F4,F5,F6,MH,CG1,CG2,CG3,CG4,CG5,CG6
0169400       COMMON/ADDRE/ D1,D2,D3,S,DP,P
0169500       COMMON/WM/ WM
0169600       COMMON /FCG/F7,CG7
0169700       HI=0.
0169800       V=(WM(1)*F1+WM(3)*F2+WM(4)*F3+WM(6)*F4+WM(5)*F5+WM(7)*F6          -
0169900      1+WM(2)*F7)
0170000       GMV=(V*4.)/(3.1415927*(D2**2.-D1**2.))
0170100       HID=(.813*(GMV*DP/VIS)**.9)*EXP(-6.*DP/(D2-D1))
0170200       HI=(HID*THC)/(D2-D1)
0170300       RETURN
0170400       END
0170500       FUNCTION HO(VIS,THC,HTCP,Z,T,RE)
0170600       REAL MH
0170700       DIMENSION WM(7)
0170800       COMMON F0,F1,F2,F3,F4,F5,F6,MH,CG1,CG2,CG3,CG4,CG5,CG6
0170900       COMMON/ADDRE/ D1,D2,D3,S,DP,P
0171000       COMMON /FCG/F7,CG7
0171100       COMMON/WM/ WM
0171200       AMW=(CG1*WM(1)+CG2*WM(3)+CG3*WM(4)+CG4*WM(6)+CG5*WM(5)+CG6*WM(7)  -
0171300      1+CG7*WM(2))/MH
0171400       HO=0.
0171500       G=MH/(S**2-(3.1415927*D3**2)/4.)
0171600       DE=4.*(S**2-3.1415927*D3**2./4.)/(3.1415927*D3+4.*S)
0171700       RE=(DE*G*AMW)/VIS
0171800       PR=(HTCP*VIS)/(THC*AMW)
0171900       RHO=(AMW*P)/(0.7302*(T+460.))
0172000       GR=(Z**3)*(RHO**2)*4.18E08*100./(VIS**2)
0172100       IF(RE.GE.10000.) GO TO 300
0172200       IF(RE.LE.2100.) GO TO 200
0172300 C          2100<RE<10000
0172400       HO21=(1.*THC/DE)*(2100.**.45)*SQRT(PR)*(DE/Z)**.4*(S/D3)**.8       -
0172500      1*GR**.05
0172600       HO10=(.02*THC/DE)*(10000.**.8)*(PR**.333)*(S/D3)**.53
0172700       SLOPE=(HO10-HO21)/(10000.-2100.)
0172800       HO=HO21+SLOPE*(RE-2100.)
0172900       RETURN
0173000 C          RE<=2100
0173100   200 HO=(1.02*THC/DE)*(RE**.45)*SQRT(PR)*(DE/Z)**.4*(S/D3)**.8          -
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0173200      1*GR**.05
0173300       RETURN
0173400 C          RE>=10000
0173500   300 HO=(.02*THC/DE)*(RE**.8)*(PR**.333)*(S/D3)**.53
0173600       RETURN
0173700       END
0173720C      FUNCTION HTCP(CM,T)
0173740C      DIMENSION CM(7),C(7),A(4,7),WM(7)
0173760C      DATA A/5.34,6.39E-03,0.,0.,6.60,6.67E-04,0.,0.,10.34,1.52E-03,0.,
0173780C     1-6.3342E+05,8.22, 8.3E-05,4.136E-07,0.,6.62,4.5E-04,0.,0.,6.5,
0173800C     25.56E-04,0.,0.,6.732,8.36E-03,5.53E-09,0./
0173820C      DATA WM/16.,28.,44.,18.,2.,28.,32./
0173840       TC=CM(1)/WM(1)+CM(2)/WM(2)+CM(3)/WM(3)+CM(4)/WM(4)+CM(5)/WM(5)     -
0173860      1+CM(6)/WM(6)+CM(7)/WM(7)
0173880       C(1)=CM(1)/WM(1)/TC
0173900       C(2)=CM(2)/WM(2)/TC
0173920       C(3)=CM(3)/WM(3)/TC
0173940       C(4)=CM(4)/WM(4)/TC
0173960       C(5)=CM(5)/WM(5)/TC
0173980       C(6)=CM(6)/WM(6)/TC
0174000       C(7)=CM(7)/WM(7)/TC
0174020C      TP=T+460.
0174040C      HTCP=0.
0174060C      DO 1 I=1,7
0174080C    1 HTCP=HTCP+C(I)*(A(1,I)+A(2,I)*TP+A(3,I)*TP**2+A(4,I)/TP**2)
0174100C      RETURN
0174120C      END
0175400       REAL FUNCTION K1(T)
0175500       TP=T+460.
0175600       B=-8.7153E+08/(TP**3)+5.2409E+06/(TP**2.)-4.6299E+04/TP+27.849
0175700       K1=EXP(B)
0175800       RETURN
0175900       END
0176000       REAL FUNCTION K2(T)
0176100       TP=T+460.
0176200       B=-9.0283E+08/(TP**3)+3.5603E+06/(TP**2)+4.3662E+03/TP-3.0526
0176300       K2=EXP(B)
0176400       RETURN
0176500       END
0176600       FUNCTION THC(C,T,IJ)
0176700       DIMENSION C(7),A(2,7)
0176800       COMMON/THCC/ A
0176900       THC=0.
0177000       DO 5 I=1,7
0177100       THC=THC+C(I)*(A(1,I)*T+A(2,I))
0177200     5 CONTINUE
0177300       RETURN
0177400       END
0177500       FUNCTION UI(HI,HO,T)
0177600       REAL MH
0177700       COMMON/ADDRE/ D1,D2,D3,S,DP,P
0177800       COMMON /FCG/F7,CG7
0177900       DLM=(D3-D2)/ALOG(D3/D2)
0178000       R=0.005
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0178100       THMET=4.659E-03*T+6.248
0178200       UI=1./(1./HI+D2/(D3*HO)+((D3-D2)*D2)/(THMET*DLM)+R)
0178300       RETURN
0178400       END
0178500       FUNCTION VIS(C,T,IJ)
0178600       DIMENSION A(2,7),C(7)
0178700       COMMON/VIPC/ A
0178800       VIS=0.
0178900     5 DO 4 I=1,7
0179000       VIS=VIS+C(I)*(A(1,I)*T+A(2,I))
0179100     4 CONTINUE
0179200       RETURN
0179300       END
0179400       FUNCTION X2(X,K2)
0179500       REAL MH
0179600       REAL K2
0179700       COMMON F0,F1,F2,F3,F4,F5,F6,MH,CG1,CG2,CG3,CG4,CG5,CG6
0179800       COMMON/ADDRE/ D1,D2,D3,S,DP,P
0179900       COMMON /FCG/F7,CG7
0180000       A=(K2-1.)*(F3+X*F1)**2
0180100       B=(F3+X*F1)*(2.*X*F1*K2-K2*F2-K2*F4-5.*X*F1-F3-F5)
0180200       C=K2*F2*F4-2.*F1*F2*K2*X-(F3+X*F1)*(F5+4.*F1*X)
0180300       X2=(-B-SQRT(B**2-4.*A*C))/(2.*A)
0180400       IF(X2.LT.-1..OR.X2.GT.0.) X2=(-B+SQRT(B**2-4.*A*C))/(2.*A)
0180500       RETURN
0180600       END
0180700  &OPFC TOPFC=443.,UT=0.8,CD=325.,
0180800  &END
0180900  &INIT DNSM=1216.,0.,1.360,21.8,166.,0.,0.,TAT=298.,PAT=1.,SMRA=3.,POPR=5.0
0181000  &END
0181100  &CONDT IFUEL=1,ERR=0.01,IP=2,I=7,EXT=100.,WAT=0.015,EXA=100.,
0181200  &END
0181300  &REFEN ZH=6.,DX1=0.,DX2=0.15,DX3=0.1667,K0=1.040E+04,EA=20000.,RHOB=80.
0181400   ,EPS=0.487,S=0.25,DP=0.00328,DZZ=0.25,
0181500  &END
0181600  &HEATX CN=1.3,U=48825.1,HA(7)=0.2,HA(10)=0.2,
0181700  &END
0181800  &HEPDC NPH=2,NRH=5,BSPAC=1.,ODTH=.0625,PITCH=.0833,CLH=.0208,IDSH=.833,
0181900  IDTH=.04667,FLOAR=.001716,SURFC=.1466,CLENH=2.,SITS2=0.5,DTH=0.7,
0182000  &END
0182100  &PDSHH DPD=1.18,0.,AHRN=0.66,.0,APPD=69.,0.,CLEPD=5.91,0.,
0182200  NTPD=1,0,
0182300  &END
0182400  &PDFUH NTAF=140,FULE=1.42,WIDAF=.009744,NPFU=3365,
0182500  NTAA=40,AIRL=1.,WIDAA=.00515
0182600  &END
0182700  &CATAI SRO=.44,SA=400.,CU=.15,CL=.75,ALFA=.5,SN=2.,FCONST=96500.,
0182800  DKC=2.4E5,
0182900  &END
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16. Abstract

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

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