

TRANSIENT THERMODYNAMIC ANALYSIS
OF
A FUEL CELL SYSTEM

A Thesis
Presented to
the Faculty of the Department of Mechanical Engineering
University of Houston

In Partial Fulfillment
of the Requirements for the Degree of
Master of Science in Mechanical Engineering

by
William Emile Simon
August, 1966

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ABSTRACT

This presentation is concerned with the development of an analytical model capable of accurately predicting the transient temperature and voltage response characteristics of a fuel cell system. The Apollo fuel cell system was selected for analysis. For a given space mission, a complete time history of fuel cell temperature and voltage must be obtained before launch to determine (1) whether there are sufficient reactants aboard the spacecraft available for fuel cell consumption to complete the objectives of the mission—reactants consumed depend on the efficiency of the fuel cell, which is a function of operating temperature; (2) whether fuel cell voltage is always within its specification voltage band of 29 ± 2 volts.

In order to obtain the necessary relations for the variation of fuel cell temperature and voltage with time, a control volume was set up around the fuel cell stack, or heart of the system. Heat and mass balances were then used, time derivatives taken, and appropriate boundary and initial conditions applied. Due to the complexity of the system, it was necessary to introduce a set of simplifying assumptions in order to hold the number of varying parameters to a minimum. A certain amount of empirical (test) data was also needed.

After the transient equations were developed for all regions of normal operation, these relations were used to

formulate a computer program which accepts a given mission profile and calculates the temperature and voltage variations of the fuel cell with time.

From a comparison of analytical results with test data obtained on a qualified Apollo fuel cell powerplant in a thermal vacuum environment, it is concluded that the analysis presents an adequate mathematical model for predicting fuel cell performance, subject to the limitations imposed on the study.

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NOMENCLATURE

Subscripts

c/e	≡ Condenser Exit (Primary Side)
H ₂ cons	≡ Consumption Hydrogen
H ₂ O prod	≡ Water Produced
mix	≡ Mixture
O ₂ cons	≡ Consumption Oxygen
p/e	≡ Pump-Separator Exit (Primary Loop)
r	≡ Pressure Jacket Inlet
recir	≡ Recirculation Stream
recir in	≡ Recirculation stream entering stack
recir out	≡ Recirculation stream leaving stack
rin	≡ Reactant(s) in
s	≡ Stack Inlet
ss	≡ Steady State
w	≡ Water Vapor

Symbols

A	}	= A Collection of terms used in the analysis for simplification
a		
B		
b		
C_1		
c		
c_p		= Specific Heat at Constant Pressure (BTU/LBm-R)
E		= Module output voltage (volts)
E_a		= Actual electromotive force (volts)
E_c		= Cold-side effectiveness of primary regenerator
E_R		= Reversible electromotive force (volts)
G		= Free energy (Gibbs function) (BTU)
H		= Heat content (Enthalpy of Formation) (BTU)
HF		= Heat of Formation of Water ($\frac{\text{BTU}}{\text{LBm H}_2}$)
ΔHF_p		= Pressure Correction at Constant Temperature for Heat of Formation of Water (BTU/LBm H_2)
ΔHF_t		= Temperature Correction at Constant Pressure for Heat of Formation of Water (BTU/LBm H_2)
% H_2O		= Per cent water in electrolyte solution
h		= Specific enthalpy (BTU/LBmR)
I		= Module current (amp.)
K_1		= Electrochemical constant which in effect states Faraday's Law (amp-hr./LBm H_2 cons)
M		= Thermal Mass of the fuel cell stack (BTU/F DEG)
m		= Mass (LBm)
$\dot{m}$		= Mass flow rate (LBm/HR)

MW	=	Molecular Weight (LBm per pound mole)
P	=	Gross Electrical Power Output of the Fuel Cell Module (Watts)
p	=	Absolute Pressure (psia)
p_{H_2}	=	Partial Pressure of Hydrogen (psia)
p_w	=	Partial Pressure of Water Vapor (psia)
Q	=	Heat Generated Due to the Inefficiency of the Fuel Cell, Adjusted for the Difference in Temperature Between Incoming Reactants and Outgoing Products (BTU/HR)
q	=	Heat quantity (BTU); also in some parts of the analysis, a collection of terms used to form a discriminant
Q_A	=	Heat produced in an actual fuel cell (BTU)
Q_{gen}	=	Product of Hydrogen Consumption Flow Rate and Lower Heating Value (BTU/HR) at 77 F and 1 atmosphere.
Q_{htr}	=	In-line heater power (BTU/HR)
Q_L	=	Portion of waste heat generated in actual cell due to losses (BTU)
Q_{recir}	=	Heat removed by recirculating stream through stack (BTU/HR)
Q_s	=	Heat Stored in Stack (BTU/HR)
Q_{stack}	=	Stack Heat Loss (BTU/HR)
R	=	Gas Constant (FT-LB _f /LBm-R)
$\bar{R}$	=	Universal Gas Constant (FT-LB _f /pound mole - R)
S	=	Entropy (BTU/R)
s	=	Specific entropy (BTU/LBmR)
T	=	Fuel cell operating temperature (degrees F or degrees R)

T_{high}	$\equiv$	Upper limit of in-line (low-power) heater temperature deadband (F)
T_{low}	$\equiv$	Lower limit of in-line (low-power) heater temperature deadband (F)
t	$\equiv$	Time (hours)
T_o	$\equiv$	Reference temperature (deg. F or deg. R)
V	$\equiv$	Volume (FT^3); also in Chapter VII a dummy variable used in the solution of a differential equation
$\dot{V}$	$\equiv$	Volumetric flow rate (cfm)
v	$\equiv$	Specific Volume (FT^3/LBm)
W	$\equiv$	Work done by an actual cell (BTU or WATT-Hr.)

β_1
 β_2
 β_3
 β

} $\equiv$ Collection of terms used in the analysis for simplification

γ

$\equiv$ Specific Humidity ($\frac{\text{LBm WATER VAPOR}}{\text{LBm DRY HYDROGEN}}$)

δ_1
 δ_2
 δ_3
 δ_4

} $\equiv$ Collection of terms used in the analysis for simplification

η_{actual}

$\equiv$ Efficiency of an actual fuel cell

$\eta_{\Delta G}$

$\equiv$ Fuel cell efficiency based on free energy

$$\begin{aligned}
 \eta_{\Delta H} &\equiv \text{Fuel cell efficiency based on heat content} \\
 \eta_{\text{ideal}} &\equiv \text{Efficiency of an ideal fuel cell} \\
 \left. \begin{array}{l} \xi_1 \\ \xi_2 \\ \xi_3 \\ \xi_4 \end{array} \right\} &\equiv \text{Collection of terms used in the analysis} \\
 &\quad \text{for simplification} \\
 \phi &\equiv \text{Fraction of stack exhaust flow rate} \\
 &\quad \text{which bypasses the primary regenerator}
 \end{aligned}$$

CHAPTER I

INTRODUCTION

Analytic techniques directed to the prediction of system performance are important in the design of all systems. The prediction of the system's operating characteristics is based on the physical geometries of the system components and the behavior of working media. When various forms of energy are converted, non-isothermal systems may result. In this case the performance analysis may be significantly complicated because (1) the system performance is generally temperature dependent and (2) heat transfer mechanisms may be present. Generally, a thermal analysis extends beyond the system itself to include the influence of the surroundings. If the system is in thermodynamic equilibrium, it is classified as in the steady-state condition. If any of the system's variables are changing with time, it is in the transient state.

Accurate analysis of system performance is particularly critical for design considerations such as for the systems involved in space vehicles. This presentation is concerned with developing an analysis to describe the performance of a fuel cell system such as the one used in the Apollo spacecraft. The fuel cell system aboard the Apollo spacecraft accepts hydrogen and oxygen from a cryogenic storage and supply system and converts these reactants electrochemically

into waste heat, water and electrical energy. A thermal control system removes the waste heat for dissipation into space by spacecraft radiators.

The variables which govern the performance of a multi-component fuel cell system are numerous; analytical treatments rely to a certain extent on empirical (test) data and are limited by necessary simplifying assumptions. The most important single parameter governing the performance and life capability of this type of fuel cell is temperature. While performance increases with increasing temperature, fuel cell life is inversely proportional to temperature. The voltage output of the system is highly dependent on fuel cell temperature at any given load. Since the allowable range of voltage variation is very sensitive (only ± 2 volts about a nominal 29 volts), an accurate thermal analysis is most necessary in order to be able to predict the performance of a fuel cell system for a given space mission.

Thermodynamic analyses of fuel cell systems are largely limited to steady-state treatments and generally can be classified as "in-house" reports of the developers. A transient analysis must determine the proper relations for the variation of fuel cell temperature and voltage with time after a given step load change for all regions of operation. Inputs to an analysis of this type must include (1) load profiles (current as a function of time), (2) fuel cell coolant inlet-temperature profiles, (3) reactant inlet-temperature profiles,

and (4) variations in the environment temperature of the fuel cell system. The desired outputs of the analysis are the transient temperature and voltage response of the fuel cell in terms of such variables as electrolyte concentration.

This thesis presents a transient thermodynamic analysis of a fuel cell system exclusive of cryogenic supply system and external heat dissipation system. The results of simplified and more general analyses are compared, and the results of the more general analysis are compared with performance test data. The analysis is oriented toward a particular application, but the methods employed are sufficiently general to allow application of these concepts to most fluid-loop systems involving heat and mass transfer.

CHAPTER II

OPERATING PRINCIPLES AND CHARACTERISTICS
OF THE FUEL CELL

The conversion of chemical energy to electrical energy within the fuel cell is governed by Faraday's Law, which states^{1*} that during electrolysis, or while a voltaic cell is discharging, the passage of one faraday (96,500 coulombs) through the circuit is accompanied by the oxidation of one gram-equivalent weight of matter at one electrode and the reduction of one gram-equivalent weight at the other electrode.

The fuel cell converts chemical energy into electrical energy without an intermediate step of conversion into heat. In this way, the irreversibilities associated with the conversion of heat into electrical energy are eliminated. Thus the fuel cell has a higher ideal efficiency than the Carnot efficiency of the conventional heat engine.

From the second law of thermodynamics, the maximum useful work (change in "free energy") which can be obtained from a chemical reaction can be expressed mathematically as²

$$\Delta G = \Delta H - T\Delta S \quad (1)$$

where G = free energy (Gibbs function)
 H = heat content (Enthalpy of Formation)
 T = absolute temperature
 S = entropy

* Superscript numbers refer to references.

The change in the enthalpy of formation for the chemical process can be expressed from the heat and mass balance of Figure 1 as

$$\Delta H = \sum_i m_i h_i - \sum_j m_j h_j$$

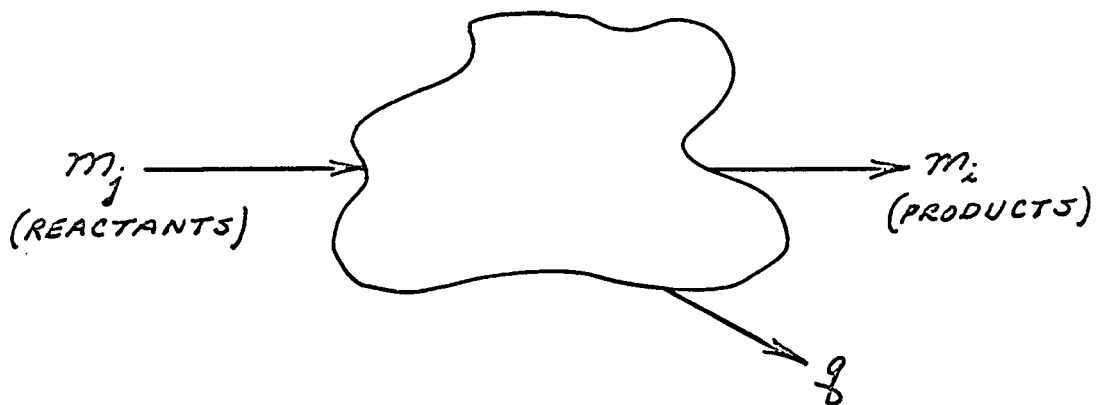


FIGURE 1. FUEL CELL HEAT AND MASS BALANCE

If all the chemical components are at a pressure of one atmosphere and a temperature of 77 F, then $\Delta H = q$ where q is the heat of combustion in the conventional combustion process. However, in the fuel cell arrangement, q is converted directly into electrical energy. The change in entropy of an isothermal chemical reaction is

$$\Delta S = \sum_i m_i s_i - \sum_j m_j s_j$$

The efficiency of a chemical process must be evaluated differently than for the conventional heat engine. Efficiency can be defined in two ways:

$$\eta_{\Delta G} \equiv \frac{\text{ACTUAL USEFUL WORK}}{\text{MAXIMUM USEFUL WORK}} = \frac{\text{POWER} \times \text{TIME}}{\Delta G}$$

$$\eta_{\Delta H} \equiv \frac{\text{ACTUAL USEFUL WORK}}{\text{CHANGE IN HEAT CONTENT}} = \frac{\text{POWER} \times \text{TIME}}{\Delta H}$$

Since $\Delta H = \Delta G + T\Delta S$, $\eta_{\Delta H} < \eta_{\Delta G}$ for the same power output.
This is shown in Figure 2.

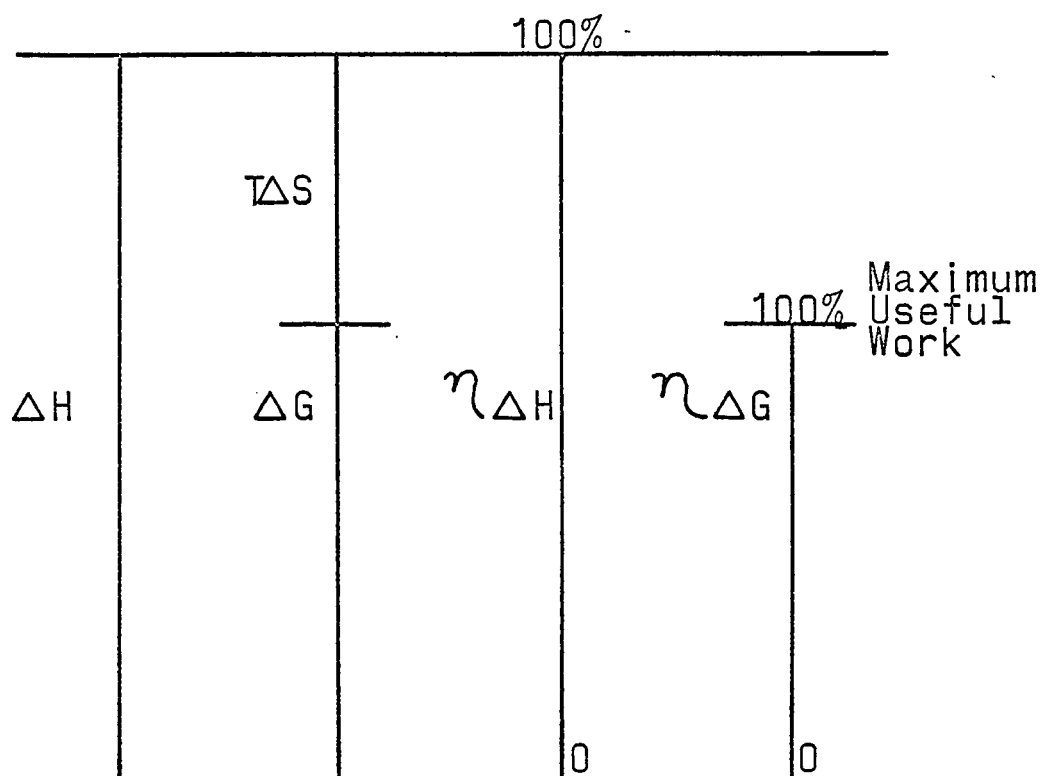
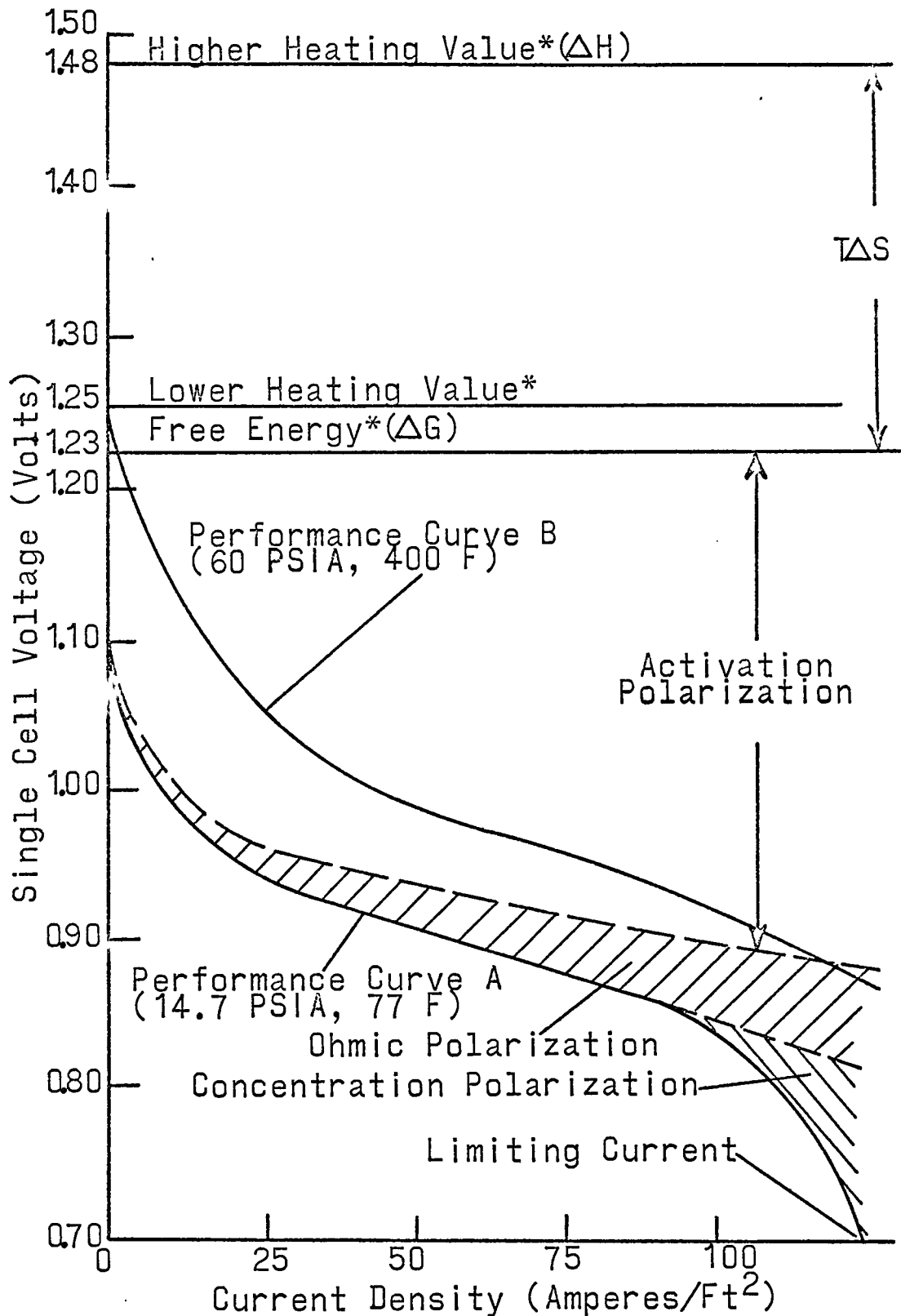


FIGURE 2
ENERGY DIAGRAM FOR THE FUEL CELL

If the total energy based on the higher heating value (reference 14.7 PSIA, 77 F) could be converted to electrical energy, then a theoretical potential of 1.48 volts/cell³ could be achieved, as shown in Figure 3. The theoretical potential based on the lower heating value for the same conditions is also shown for reference purposes. Because of the $T\Delta S$ limitation, the maximum theoretical potential of the cell at 14.7 PSIA and 77 F is 1.23 volts. This is the voltage which the cell would produce if the free energy could be entirely converted to electrical energy with no losses. The actual work in a real fuel cell is less than the maximum useful work because of other irreversible phenomena in the physical process. Three types of irreversibilities³ are encountered which are classified as (1) activation polarization, (2) ohmic polarization and (3) concentration polarization. Not much is known about activation polarization except that it is attributed to various irreversible effects and perhaps side reactions at the fuel cell electrodes. Ohmic polarization is due to the electrical resistance of the electrolyte to the flow of electrons. Concentration polarization is due to concentration gradients within the electrolyte (caused by an increased water production rate at the electrodes) and a possible density gradient effect within the reactant gas cavities (attributed to the



*Reference 14.7 PSIA, 77 F

FIGURE 3
HYDROGEN-OXYGEN FUEL CELL PERFORMANCE
BASED ON EQUILIBRIUM CONDITIONS

presence of impurities). Due to these losses, the performance curve of an actual fuel cell would be similar to performance curve A of Figure 3, for the reaction taking place at 14.7 PSIA and 77 F, with reactants and products entering and leaving under the same conditions. Performance in Figure 3 is expressed as voltage as a function of current density, where current density is defined as the current output of the cell per unit of active cell area. The actual output power of course would be

$$P = EI$$

At higher pressures and temperatures the maximum theoretical potential increases, due to increases in free energy at higher pressure and temperature. Since the Apollo fuel cell operates at a higher temperature and pressure than the standard conditions of performance curve A, its performance will be higher than that of performance curve A. Although it is a variable-temperature fuel cell, representative single cell performance is given by performance curve B for 60 PSIA and 400 F.

The efficiency of an ideal fuel cell based on heat content (ΔH) is given by²

$$\eta_{IDEAL} = \frac{\Delta G}{\Delta H}$$

or, using equation (1),

$$\eta_{IDEAL} = 1 - \frac{T\Delta S}{\Delta H} \quad (2)$$

Thus even an ideal fuel cell, operating reversibly and isothermally, will have an efficiency less than unity, with the heat quantity $T\Delta S$ being exchanged with the surroundings.

If all the free energy could be converted to electrical energy in the cell, then the maximum useful work is given by

$$\Delta G = E_r I t \quad (3)$$

where E_r is the reversible electromotive force of the cell, I is the current output and t is the time required to consume one mole of fuel. Ideal efficiency then becomes

$$\eta_{IDEAL} = \frac{E_r I t}{\Delta H} \quad (2-a)$$

Due to the losses described above, the waste heat produced in the actual cell (Q_A) is greater than the $T\Delta S$ heat of the ideal cell. This is expressed as

$$Q_A = T\Delta S + Q_L$$

where Q_L is that portion of the waste heat generated in

the actual cell due to losses. The work done by the actual cell is, then

$$W = E_a I t = \Delta H - Q_A \quad (4)$$

where E_a is actual cell voltage. From this the actual cell efficiency is

$$\eta_{\text{ACTUAL}} = \frac{E_a I t}{\Delta H} = 1 - \frac{Q_A}{\Delta H} \quad (5)$$

where $Q_A > T\Delta S$

The overall chemical reaction of the fuel cell is given by



Figure 4 illustrates the chemical balance within the cell which corresponds to this overall reaction. At the anode or hydrogen electrode, two hydrogen molecules are ionized to form four hydrogen ions and four electrons. The electrons travel through the external circuit and eventually reach the cathode or oxygen electrode, where they combine with one molecule of oxygen and two molecules of water taken from the electrolyte to form four hydroxyl ions. The four hydroxyl ions then combine with the four hydrogen ions from the anode

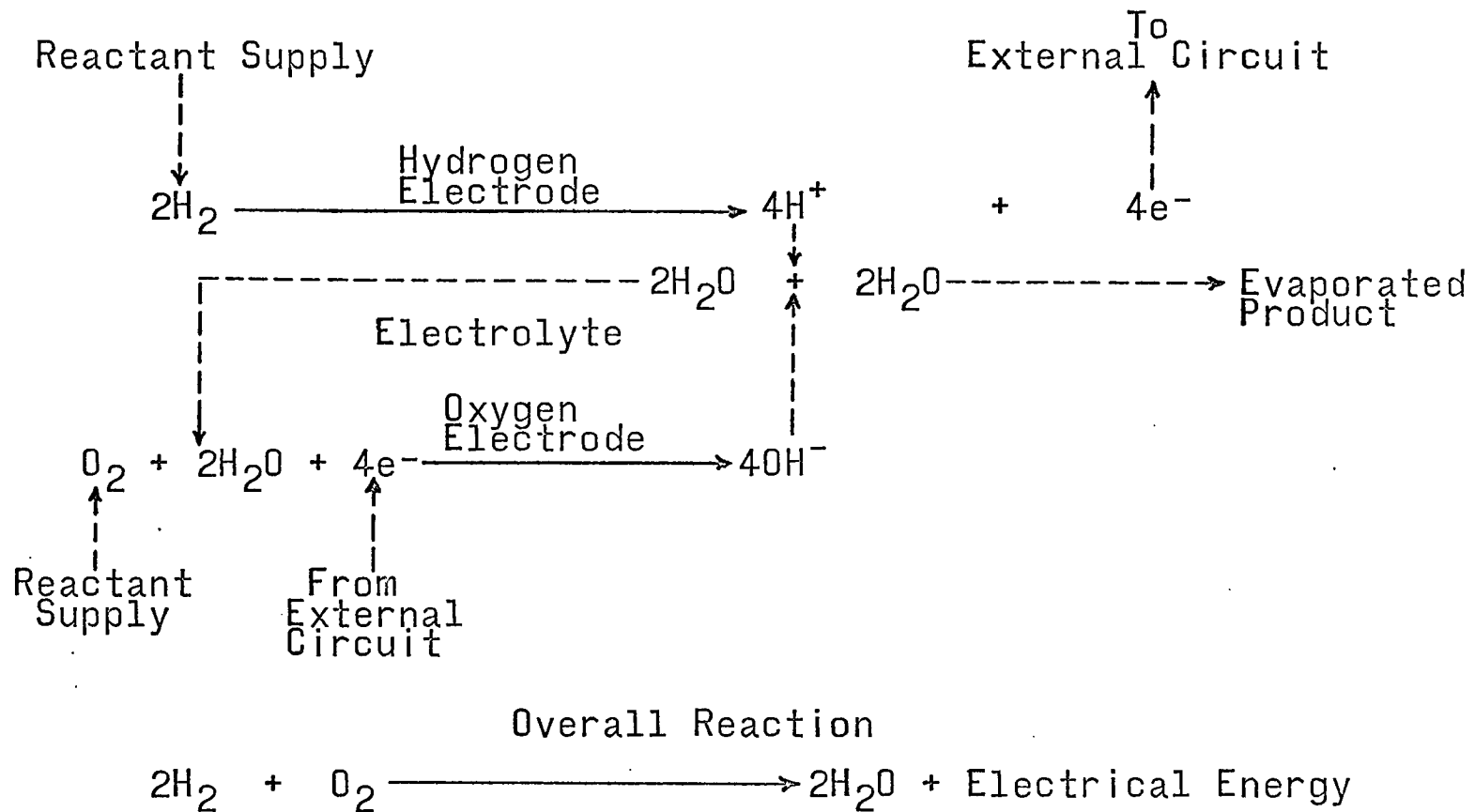


FIGURE 4
FUEL CELL CHEMICAL BALANCE

to form four molecules of water. The water is formed at the hydrogen electrode, from which two of the water molecules go to replenishing the potassium hydroxide-water electrolyte solution, while the other two molecules leave the cell as steam after having absorbed both sensible and latent heat.

Although the evaporated product water takes with it a considerable amount of heat on leaving the cell, the waste heat generated by the inefficiency of the reaction is greater than that removed by the water produced. The excess waste heat is removed by a recirculating hydrogen stream. The recirculating hydrogen also provides a mechanism for water removal.

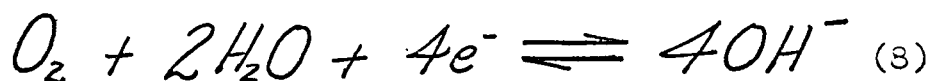
In order to better illustrate the reactions and their mechanisms within the fuel cell, the cell diagram of Figure 5 is presented.

Hydrogen enters the hydrogen gas cavity where it reacts at the hydrogen electrode according to the equation



The hydrogen electrode potential depends on hydrogen gas pressure and hydrogen ion concentration.

The oxygen electrode reaction is



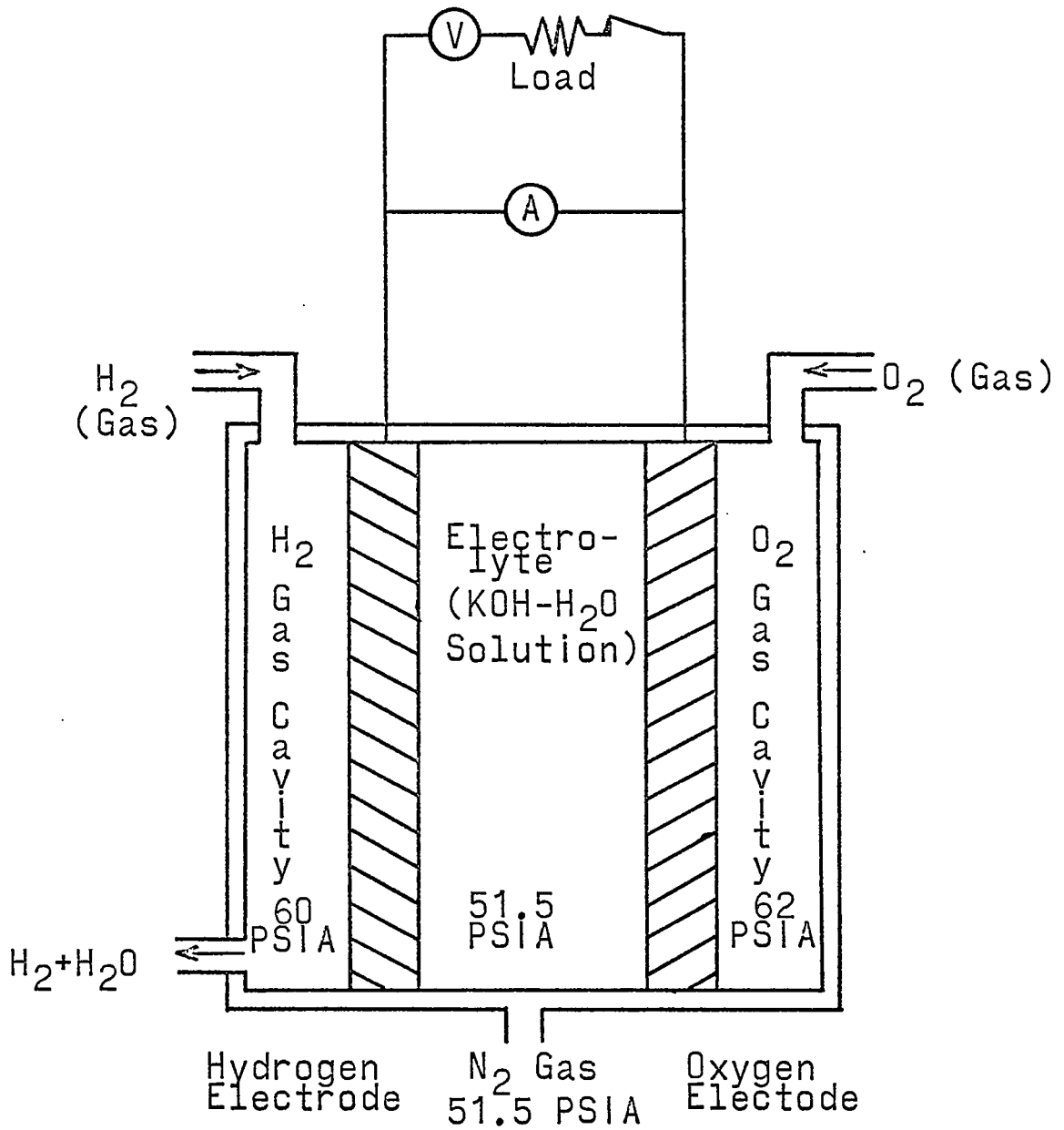


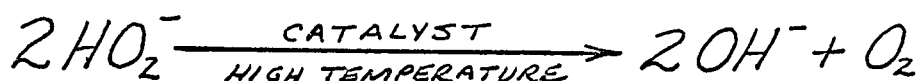
FIGURE 5
FUEL CELL ELECTROCHEMICAL FLOW SCHEMATIC

The oxygen electrode potential depends on oxygen gas pressure and hydroxyl ion concentration. The total cell voltage is the difference between the hydrogen and oxygen electrode potentials.

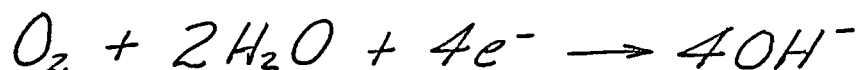
Two reaction mechanisms exist at the hydrogen electrode. In the first the hydrogen gas adsorbs on the dry nickel electrode surface. The adsorbed hydrogen migrates along the nickel surface until it is ionized, whereupon the hydrogen ions go into solution in the electrolyte. In the second mechanism the hydrogen gas dissolves in the electrolyte. The dissolved hydrogen diffuses to the nickel surface, where it is ionized; the hydrogen ions then go into solution in the electrolyte. It is thought that the second reaction mechanism dominates.

At the oxygen electrode the same two physical mechanisms occur as those described above, with the second mechanism again dominating. The chemical mechanism is controversial, however, and two theories are advanced. The first (the "four-electron reaction") is given by equation (8). This theory is favored for high-temperature ranges. The second theory (the "Berl mechanism") holds that hydrogen peroxide ions are produced at the oxygen electrode and subsequently decomposed at high temperatures. The chemical reactions corresponding to this theory are:





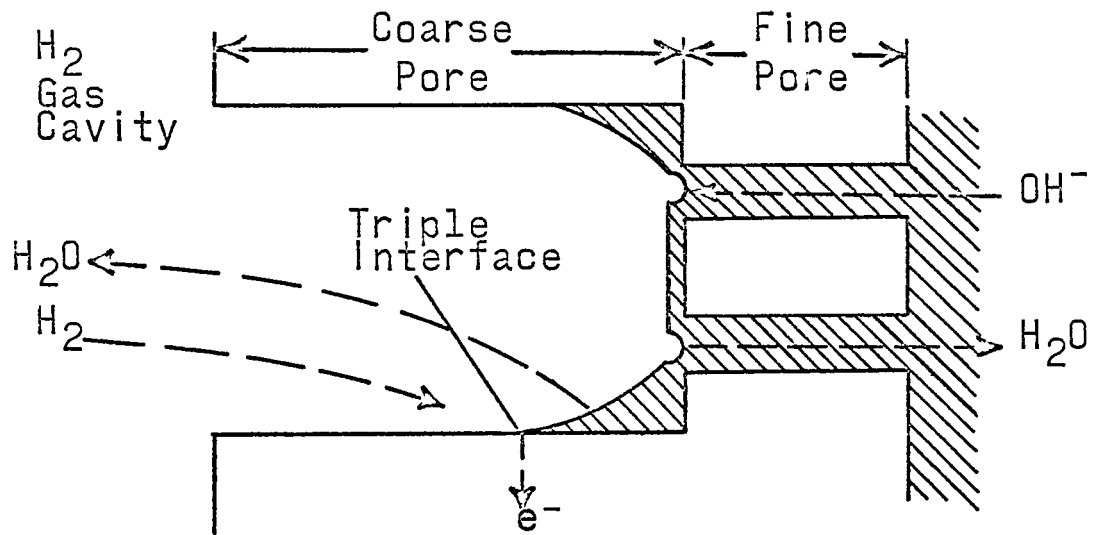
or expressed as an overall reaction



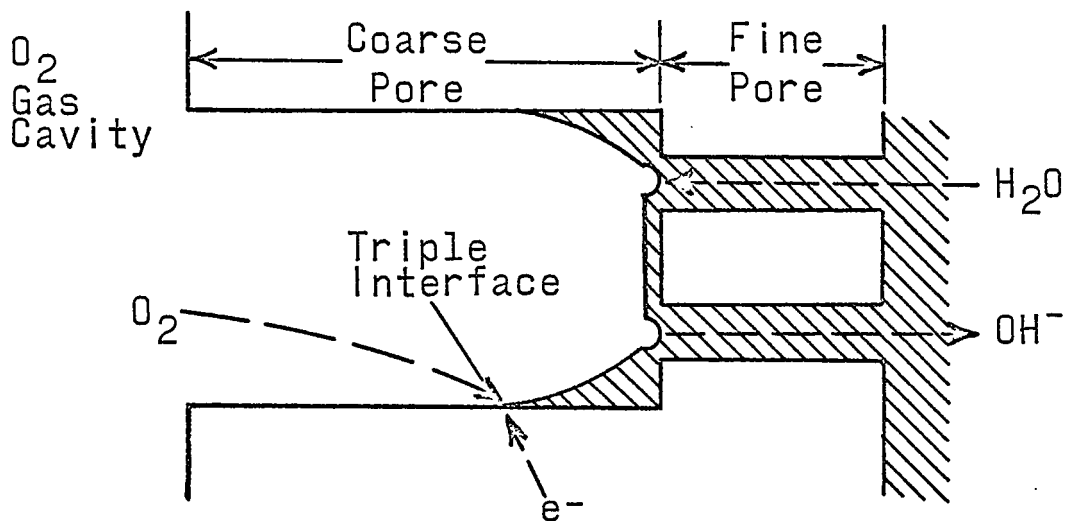
The overall reaction is the same as that of equation (8). The presence of hydrogen peroxide ions lowers electrode potential, thereby contributing to cell inefficiency. These ions are, however, decomposed more rapidly at higher temperatures.

Figure 6 shows schematically the reaction mechanisms occurring at the hydrogen and oxygen electrodes. The location where the electrode, electrolyte and reactant gas are all in contact is called the "triple interface point."

In Figure 6-a, the hydrogen gas flows down the coarse pore, where (by one or both of the two mechanisms discussed above) it is ionized at the triple interface. The hydrogen ions then go into solution in the electrolyte, where they react with the hydroxyl ions coming from the oxygen electrode to form water. One half of the water evaporates into the hydrogen gas, after which it diffuses out of the coarse pore and is carried away by the hydrogen recirculation stream. The remaining water diffuses through the fine pore and into the electrolyte. Hydroxyl ions diffuse from the electrolyte through the fine pore and to the reaction zone



(a) Hydrogen Electrode



(b) Oxygen Electrode

FIGURE 6
REACTION MECHANISMS AT HYDROGEN AND
OXYGEN ELECTRODES

to replace those used up in the reaction.

In Figure 6-b oxygen flows through the coarse pore to the triple interface, where it reacts with water from the electrolyte while removing electrons from the nickel to become hydroxyl ions. These hydroxyl ions diffuse through the fine pore and into the electrolyte to replace those used at the hydrogen electrode. Water from the electrolyte diffuses in through the fine pore to the reaction site.

The foregoing paragraphs summarize briefly the basic principles of operation and characteristics of the fuel cell.

CHAPTER III

DESCRIPTION OF FUEL CELL SYSTEM SELECTED FOR ANALYSIS

The Apollo fuel cell produces direct-current electrical power over a normal range of 563 watts to 1420 watts at a normal voltage range of 27 to 31 volts. The module is 44 inches high by 22.5 inches in diameter, and it weighs approximately 245 pounds. A photograph is shown in Figure 7. Three of these modules or powerplants, connected electrically in parallel, will be used in the Apollo spacecraft to provide electrical power and potable water. The module is composed of four distinct sections or systems: (1) an energy conversion section, (2) a reactant control system, (3) a thermal control and water removal system, and (4) necessary instrumentation. The last three are included in what is termed the accessory section.

The energy conversion section is shown in Figure 8. It consists mainly of a "stack" composed of thirty-one Bacon-type, series-connected cells with associated gas manifolds and connecting leads. The energy conversion section is housed in a pressurized jacket which rests in an insulated support assembly. The primary bypass valve shown in the figure will be discussed later.

The components forming the accessory section are mounted on a Y-frame which is shown in Figure 9. The three

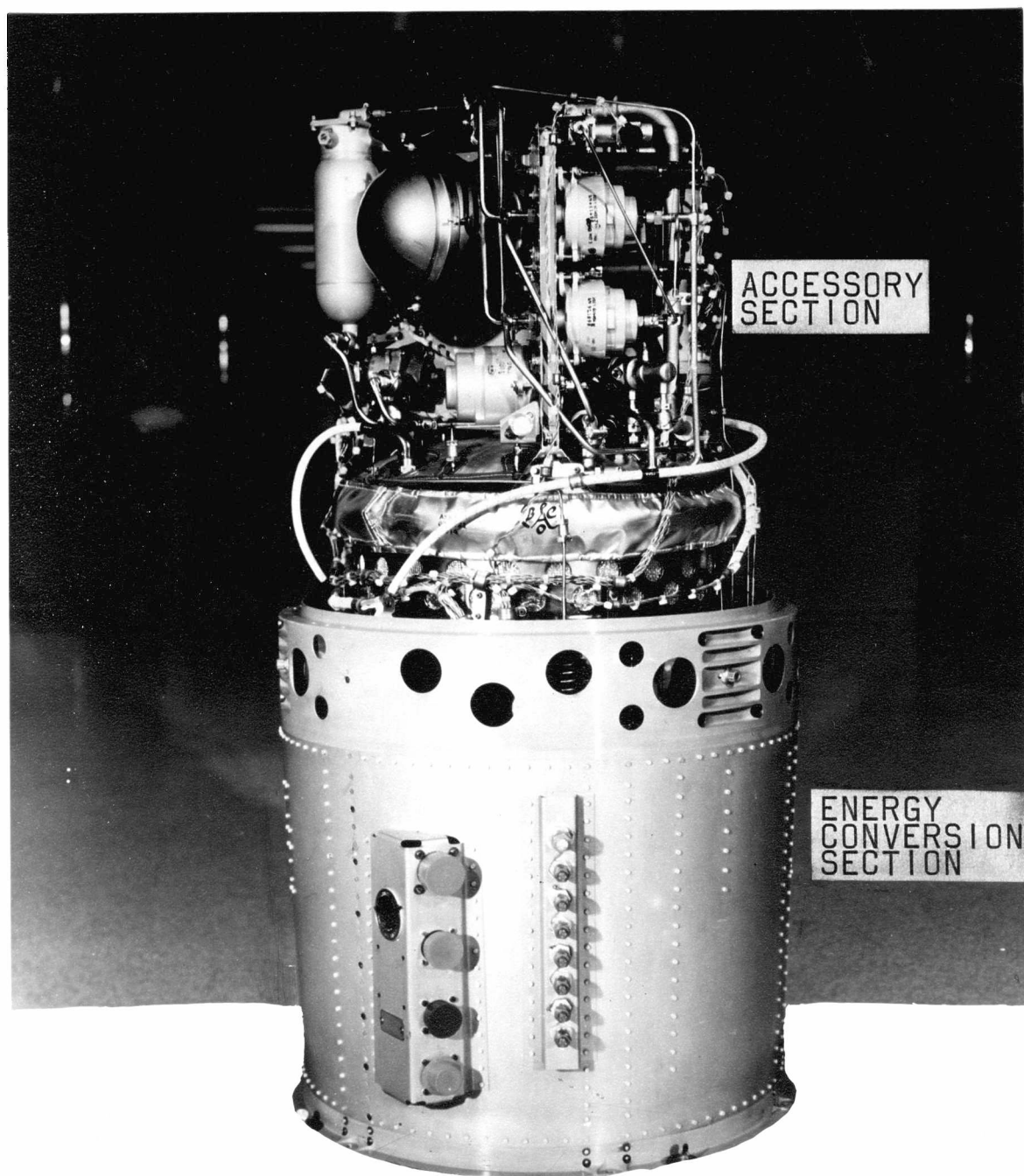


FIGURE 7
APOLLO FUEL CELL MODULE

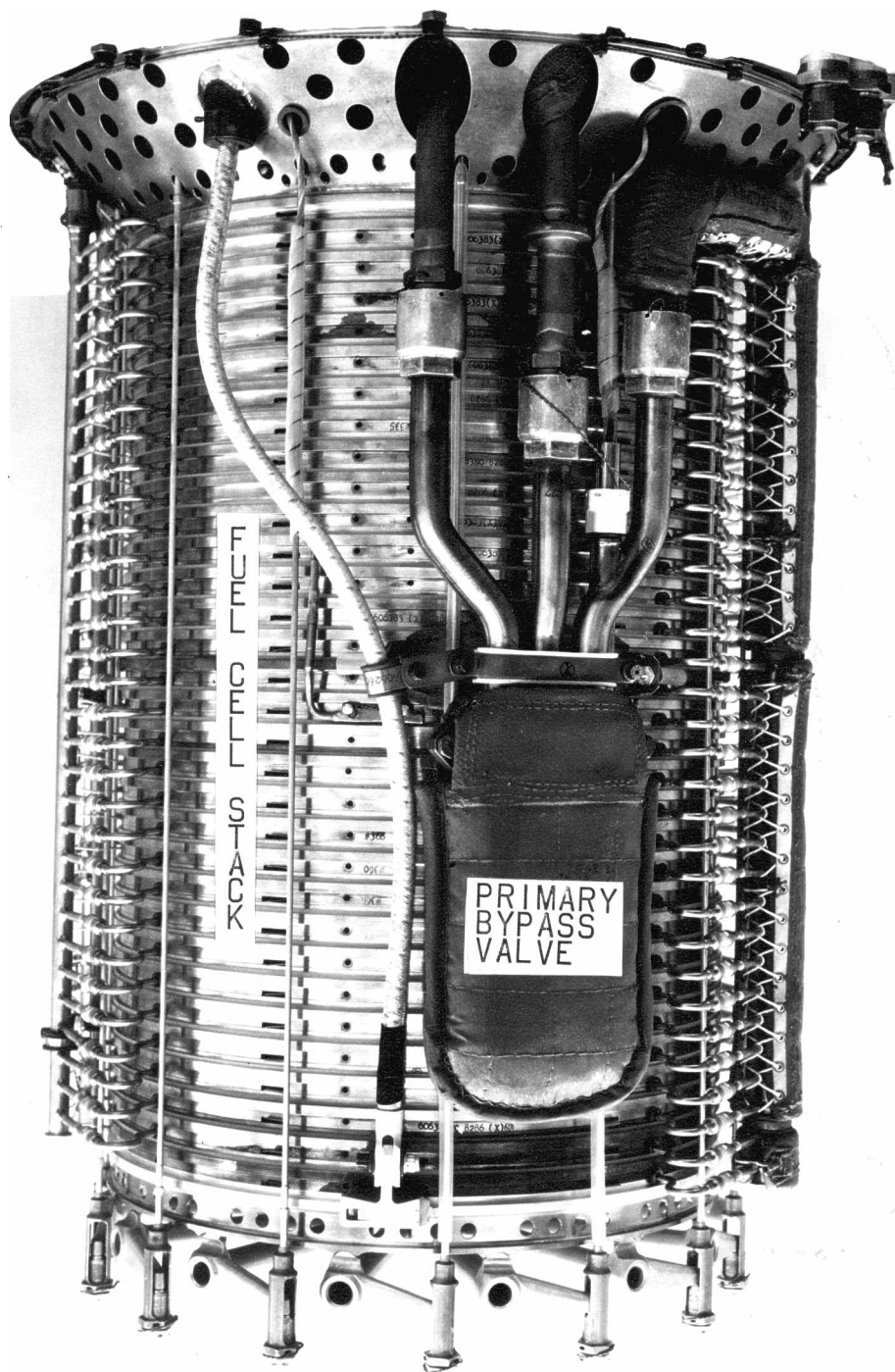


FIGURE 8
ENERGY CONVERSION SECTION

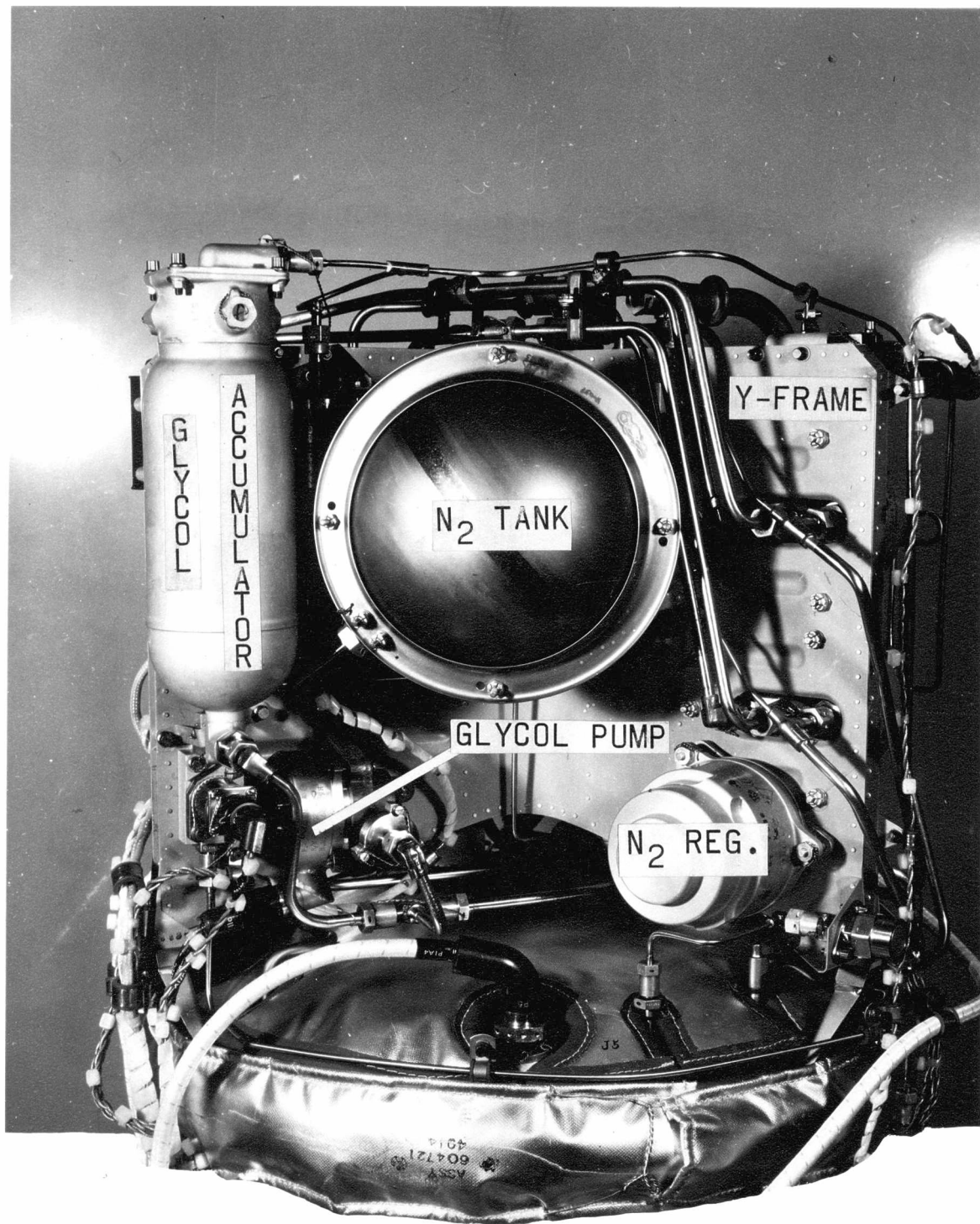


FIGURE 9
ACCESSORY SECTION--BAY 1

legs of the Y-frame are 120° apart. The accessory section consists of a nitrogen pressurization system, three regulators, a primary loop (hydrogen-water vapor) and a secondary loop (glycol-water), with heat exchangers, motor-driven pumps and plumbing. A condenser connects the two fluid loops. Figures 9, 10 and 11 show the various components of the accessory section mounted on the three legs of the Y-frame.

Before examining the system diagram, a discussion of single cell operation would be advantageous. In Figure 5 are shown the relative pressure differentials across the electrodes. The $\text{KOH} \cdot \text{H}_2\text{O}$ electrolyte solution is pressurized by a nitrogen blanket and regulated to 51.5 ± 0.5 psia. The reactant regulators, using the nitrogen pressure as a reference, maintain differential pressures of 8.5 ± 0.5 psi and 10.5 ± 0.5 psi for the hydrogen and oxygen, respectively above the nitrogen pressure. Two of the various parameters governing the performance of the fuel cell system are the operating pressure of the system and the relative pressure differentials across the electrodes. The pressure differential across an electrode determines the location of the triple interface discussed in Chapter II. Through extensive testing, the combination of pressure and pressure differentials shown in Figure 5 has been found to be optimum for this system from the combination standpoint of performance and operational feasibility.

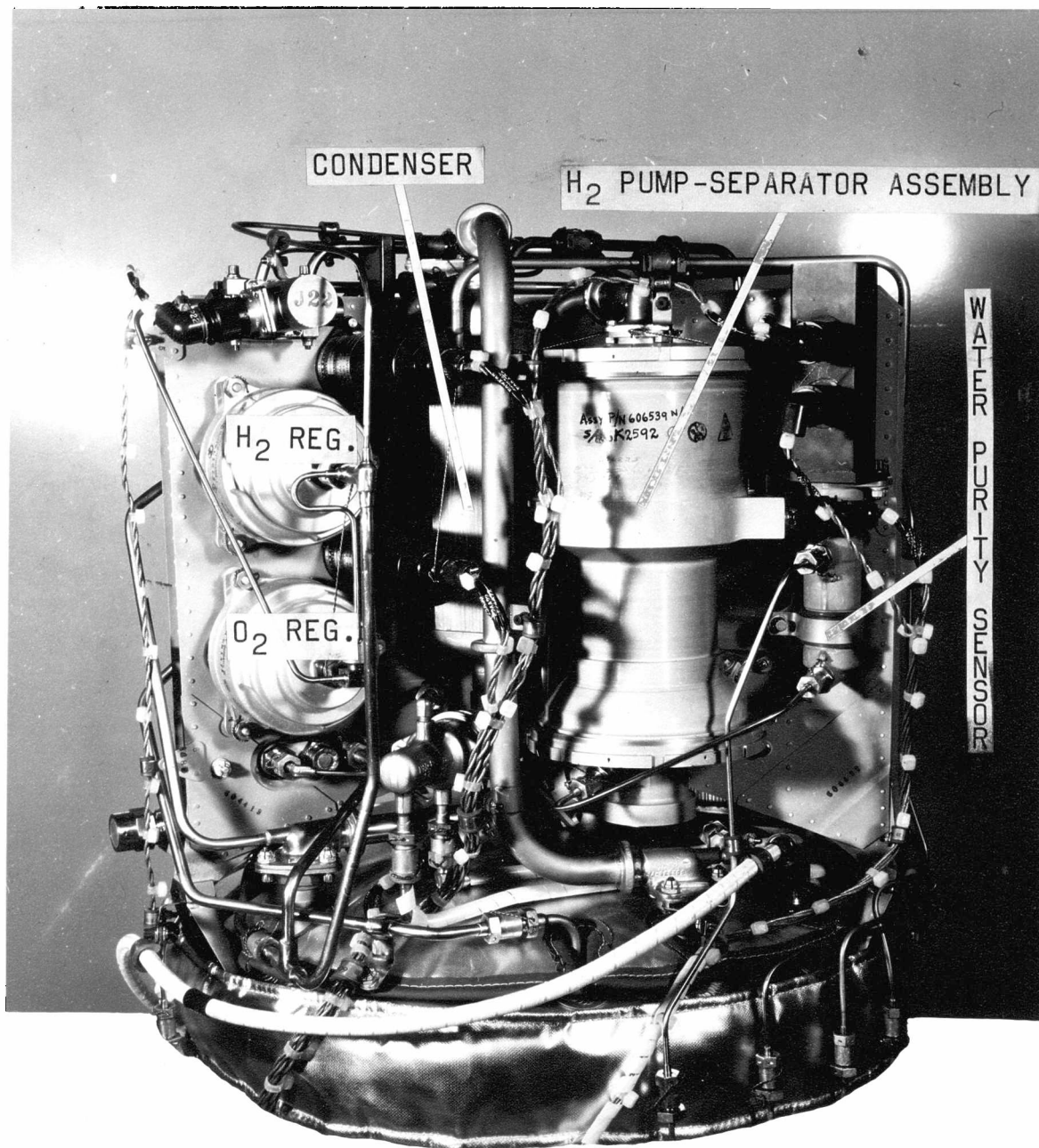


FIGURE 10

ACCESSORY SECTION--BAY II

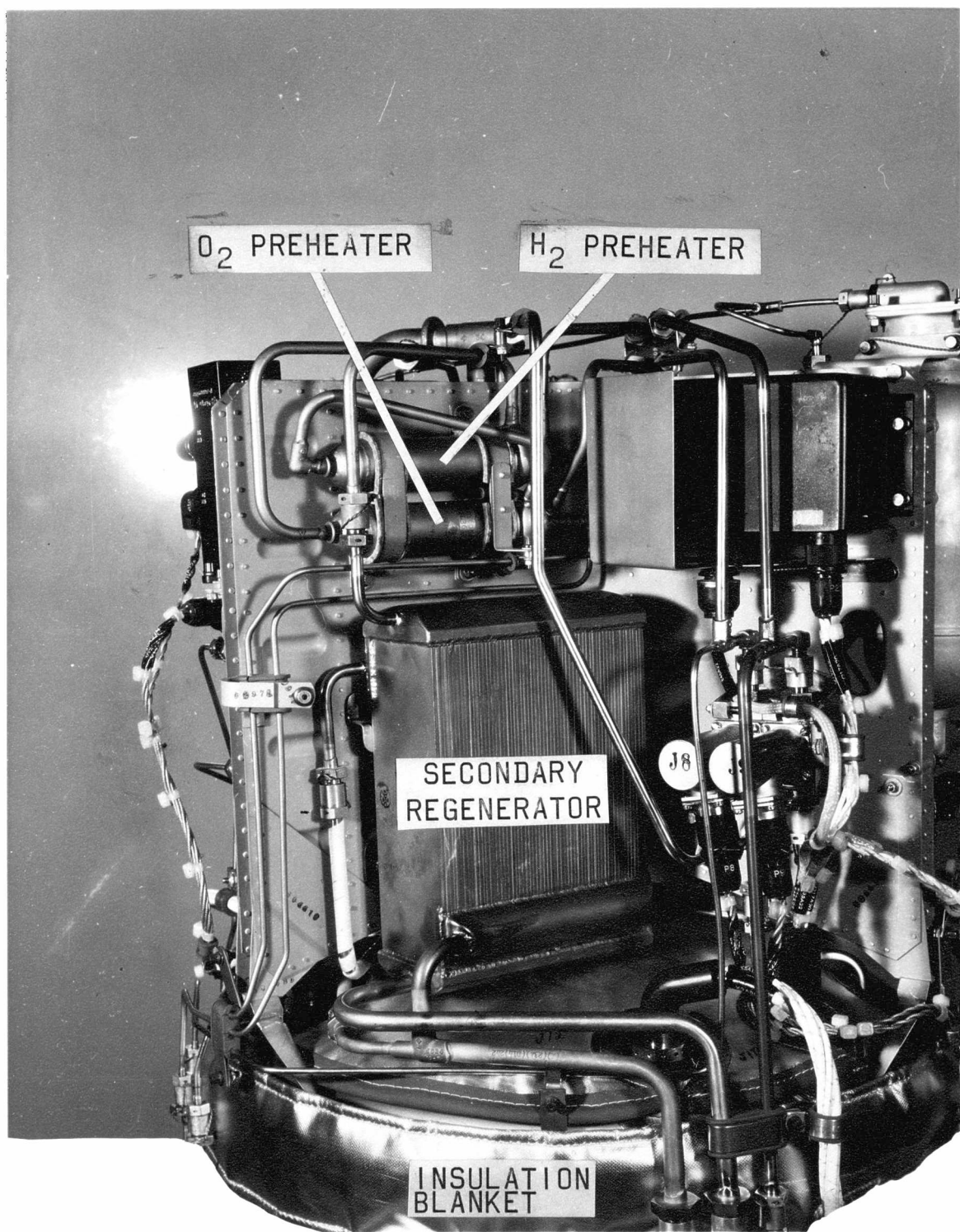


FIGURE 11
ACCESSORY SECTION--BAY III

Figure 12 illustrates the construction of an actual single cell. The two electrodes within each cell are made of dual porosity sintered nickel which is formed from nickel powder pressed into sheets. The coarse pores (approximately 40 microns) are on the gas side and the fine pores (approximately 10 microns) are on the electrolyte side. The two electrodes are similar in construction, but the oxygen electrode contains a coating of black lithium-impregnated nickel oxide on the electrolyte side to inhibit oxidation. The electrode materials serve as a catalyst in the electrochemical reaction and are resistant to corrosion by the electrolyte. A pure nickel back-up plate is used to support each electrode; it also acts as a gas housing. A teflon seal, which extends around the periphery of the cell, contains the electrolyte and acts as an electrical insulator. While the electrodes are only about $8\frac{1}{2}$ inches in diameter, the entire cell is approximately $11\frac{1}{4}$ inches in diameter. The diaphragm section (between the electrodes and the cell spacer) accommodates changes in electrolyte concentration as the flexible back-up plates expand and contract. The 31 cells are stacked in series and held together by torsion tie rods.

A schematic diagram of the system is shown in Figure 13. Certain detailed components not essential to the objectives of this analysis are omitted. The diagram is coded to aid in distinguishing the different fluid paths.

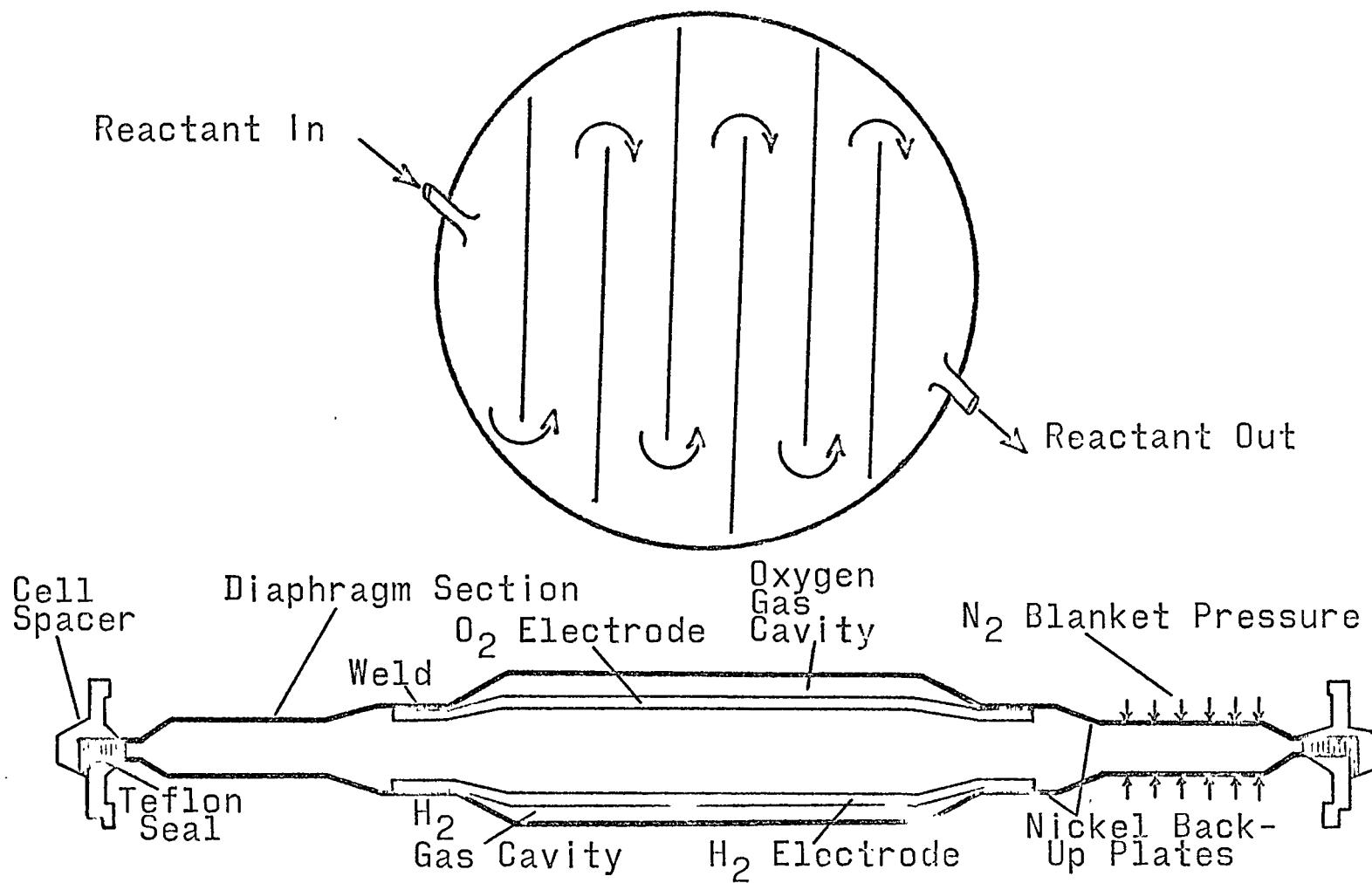


FIGURE 12
SINGLE CELL DIAGRAM ILLUSTRATING CELL CONSTRUCTION

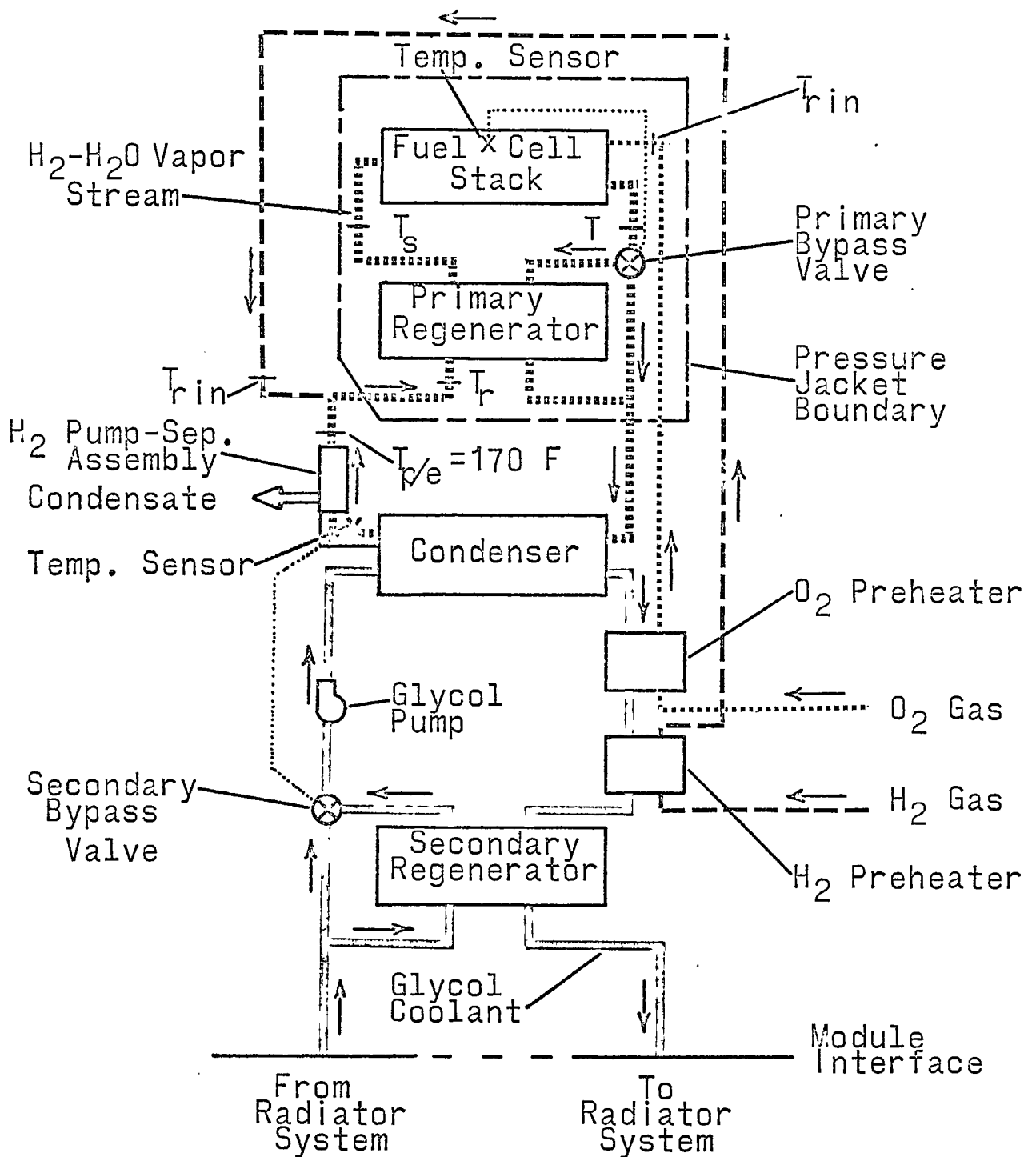


FIGURE 13
SCHEMATIC DIAGRAM OF FUEL CELL SYSTEM

The nitrogen subsystem (not shown in the diagram) is composed of a small nitrogen tank which holds approximately one half of a pound of nitrogen at 1500 psia, a nitrogen regulator, and connecting lines. The regulated nitrogen pressure (51.5 ± 0.5 psia) serves a three-fold purpose: (1) it is used as a reference pressure for the hydrogen and oxygen regulator; (2) it is used as a head pressure in the glycol accumulator; and (3) it pressurizes the jacket around the stack, thus pressurizing the electrolyte in each of the 31 single cells.

Hydrogen and oxygen are supplied to the module from a cryogenic storage system; the hydrogen is stored at a nominal 245 psia and the oxygen at a nominal 900 psia. The gases are warmed by flowing through the connecting lines between the cryogenic storage system and the fuel cell system; then they enter the reactant preheaters before being regulated to normal operating pressures. Both hydrogen and oxygen subsystems are equipped with purge valves which, when electrically energized, permit a continuous flow of additional reactant through the cells; the surplus is dumped overboard. The purging process is performed at regular intervals to remove impurities carried into the cells by the reactants.

The make-up (or consumption) hydrogen enters the primary loop at the pump-separator exit. Here it mixes with the recirculating hydrogen and water vapor and proceeds

into the pressure jacket, through the primary regenerator where the mixture is heated, and into the stack. The primary (or hydrogen) loop consists of the primary regenerator and bypass control, the hydrogen pump-separator-motor assembly, a condenser, and an in-line heater for temperature control at low-power conditions.

The primary bypass valve sensor detects stack exhaust temperature, which is essentially equal to stack temperature. The sensor is a bimetallic strip which also acts as a flow diverter. At high powers when a large amount of heat must be rejected, the stack temperature is high and the bypass valve is open (this is a proportional-control valve). At low powers when heat must be conserved, the bypass valve is closed, permitting maximum regeneration.

The pump-separator is a positive displacement (vane-type) unit. It circulates the hydrogen-water vapor mixture through the cells in order to remove waste heat and product water. Liquid water from the condenser is separated from the gas stream by centrifugal action. Input power to the motor (approximately 85 watts) is supplied by 3-phase, 400-cycle, 115-volt spacecraft inverters.

The condenser serves a two-fold purpose. First, it maintains the primary loop heat balance by rejecting waste heat to the glycol loop for transfer to the radiators. Secondly, it maintains the mass balance in the primary loop by condensing the product water vapor from the cells before

this liquid water is removed by the separator.

The secondary loop uses an ethylene glycol-water coolant mixture, and consists of a glycol pump, the condenser and preheaters discussed above, a coolant accumulator, and a secondary regenerator and bypass valve. The positive-displacement (vane-type) glycol pump circulates the coolant through the secondary loop components and the radiator system. Desired flow characteristics are obtained by using a bypass line with an internal orifice to decrease pump flow with increasing pressure differential across the pump. Power for the pump (approximately 25 watts) is provided by the same spacecraft inverters which supply the hydrogen pump.

The coolant accumulator maintains a constant pressure within the coolant system regardless of volumetric changes caused by coolant temperature variations.

The secondary regenerator controls the heat transferred from the module to the spacecraft heat rejection system in order to provide the condenser with a relatively constant coolant inlet temperature. The bypass valve, which is controlled by the condenser exit temperature on the primary side, modulates the glycol flow passing through the cold side of the secondary regenerator. If primary side condenser exit temperature becomes too high, more of the glycol flow is bypassed around the secondary regenerator. Less is bypassed as the temperature goes down.

CHAPTER IV

GENERAL ANALYTICAL APPROACH

The basic approach to an analysis of this type involves the formation of an analytical model for the fuel cell in a transient mode of operation, with the provision that as time approaches infinity, the model must represent the steady state operation of the fuel cell system. Another stipulation is that at some initial time t_0 , an initial fuel cell temperature T_1 is known. This initial temperature is an input to the system.

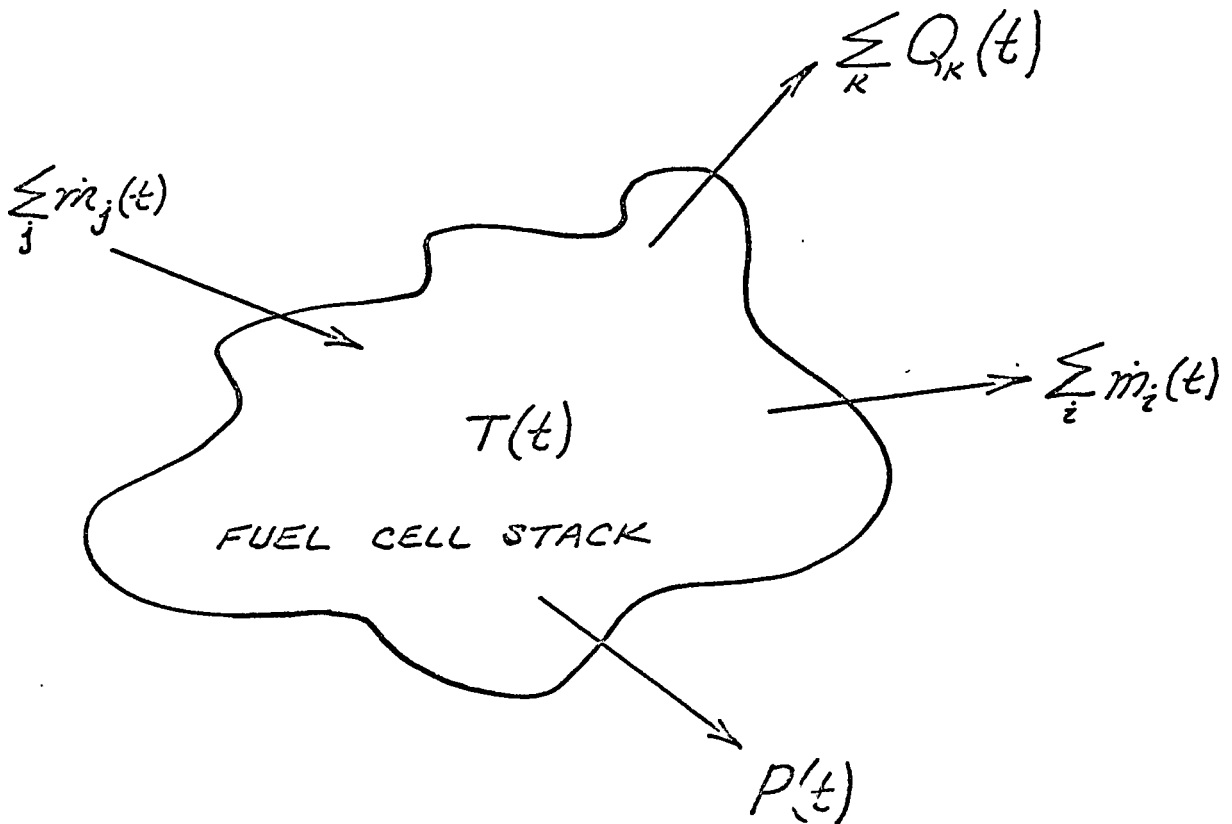


FIGURE 14. CONTROL VOLUME APPROACH TO THE ANALYSIS

As shown in Figure 14 above, a control volume is set up around the fuel cell stack, which is the heart of the system. By analyzing the incoming and outgoing fluid streams and the energy released within the system and transferred from it, a heat balance and a mass balance are obtained which form the basis of the analysis.

Because of the complexity of the system and the interactions of its many components, a completely theoretical approach to the transient problem would lead to a large and unwieldy set of simultaneous higher-order, non-linear partial differential equations. The numerical methods employed for the solution of such a set of equations would almost certainly be plagued with stability and convergence problems, which are beyond the scope of this presentation.

To circumvent these problems, an analytical approach is undertaken which utilizes powerplant and component performance data from various tests conducted throughout the development program. This semi-empirical approach, used in conjunction with a set of simplifying assumptions, helps in holding the number of varying parameters to a minimum. In this way the governing equation for the variation of fuel cell operating temperature with time will have an exact solution.

The necessary simplifying assumptions used in the analysis are discussed as follows:

- (1) TYPE OF TRANSIENT ANALYSIS. There are two

types of transients associated with the operation of this fuel cell system; namely, extremely short-term transients (on the order of milliseconds) and long-term transients (minutes or hours). The short-term electrical transients caused by the application of "pulse-loads," or "spikes," have come and gone before the fuel cell temperature has had time to change, and therefore do not contribute to transient thermal effects. The long-term transients, on the other hand, are associated with a change in stack temperature, and thus are the type with which this analysis will be concerned.

To illustrate the long-term thermal transient effect, consider first the operating characteristics of the power-plant on the polarization (voltage-current) curve of Figure 15. Suppose that the power-plant is initially at a steady state operating condition at temperature T_1 , current I_1 and voltage E_1 . At time t_0 a step load is applied, so that the current demand rises instantaneously from I_1 to I_2 . The voltage at this instant drops from E_1 to E_{2i} (subscript i is for initial) along the constant temperature line T_1 , neglecting the short-term electrical transient here. Now the stack is producing a higher current, hence I^2R losses are greater, and the stack temperature begins to rise at a constant current I_2 . If this current is maintained, both temperature and voltage will approach steady state values as time approaches infinity. As stack temperature rises,

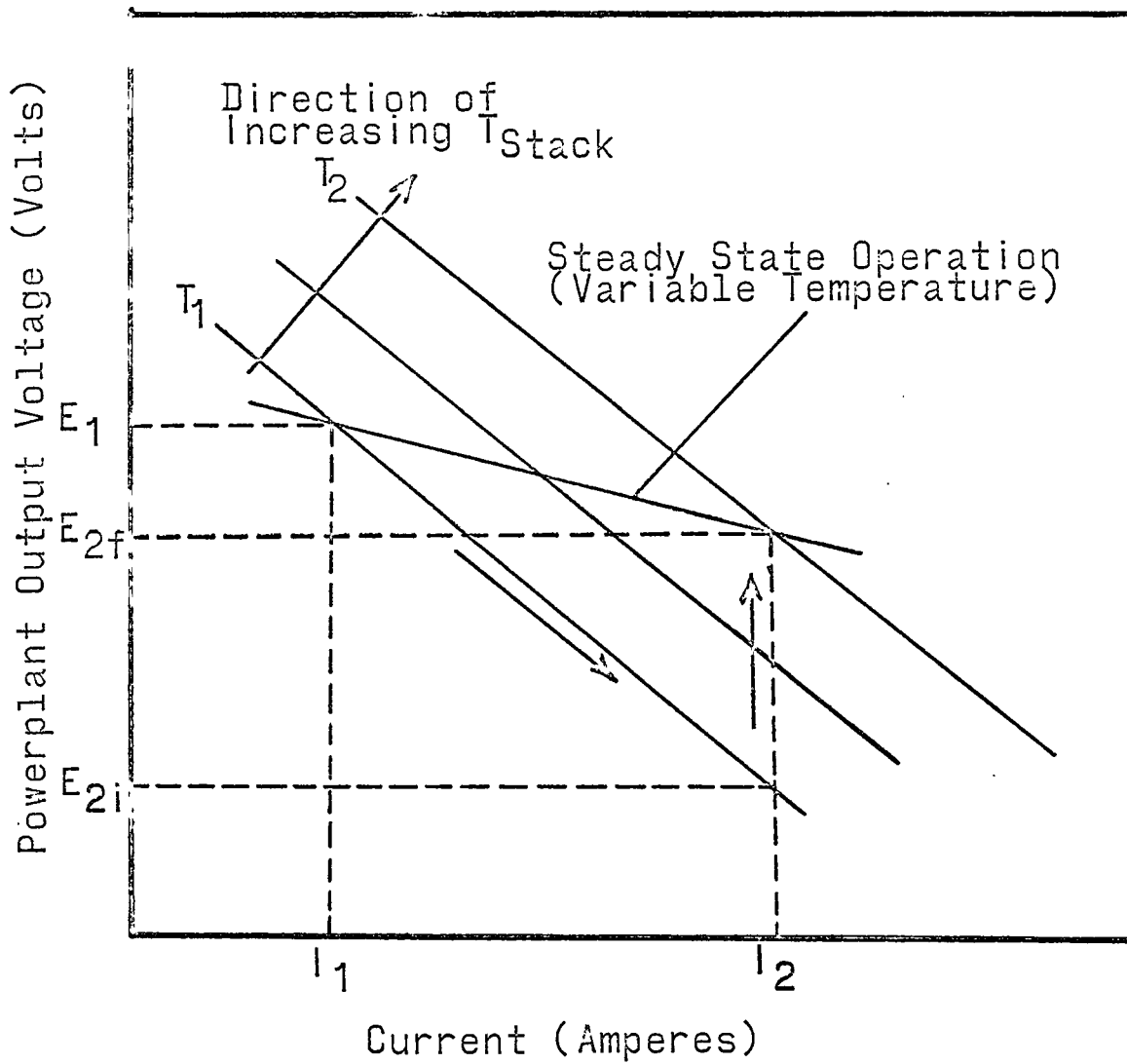


FIGURE 15
TRANSIENT FUEL CELL PERFORMANCE

so does performance (voltage). This performance increase with time is shown in Figure 16. Figure 17 shows the performance variation for a step load decrease in current.

(2) CURRENT VARIATIONS. Due to the nature of most spacecraft loads, only step current variations in load are considered, with the fuel cell output current to the spacecraft load being constant between each step load change. Actually, the current does change slightly due to fuel cell output voltage variations and the fact the voltage impressed upon a purely resistive load determines the current through it in accordance with Ohm's Law.

(3) FUEL CELL ENVIRONMENT TEMPERATURE. Variations in the environment temperature of the fuel cell module cause corresponding changes in the heat lost by the module to its surroundings. These changes in heat loss affect module temperature. This analysis is for a constant fuel cell environment temperature of 77 F.

(4) THERMAL MASS. Since the mass of each of the primary and secondary loop components is almost negligible compared to the mass of the stack, it will be assumed that the thermal masses of the components and connecting lines can be neglected. This is equivalent to stating that there is no thermal time lag associated with any components other than the stack.

(5) CHEMICAL EQUILIBRIUM. Chemical equilibrium is defined⁴ as that condition in a reversible reaction in

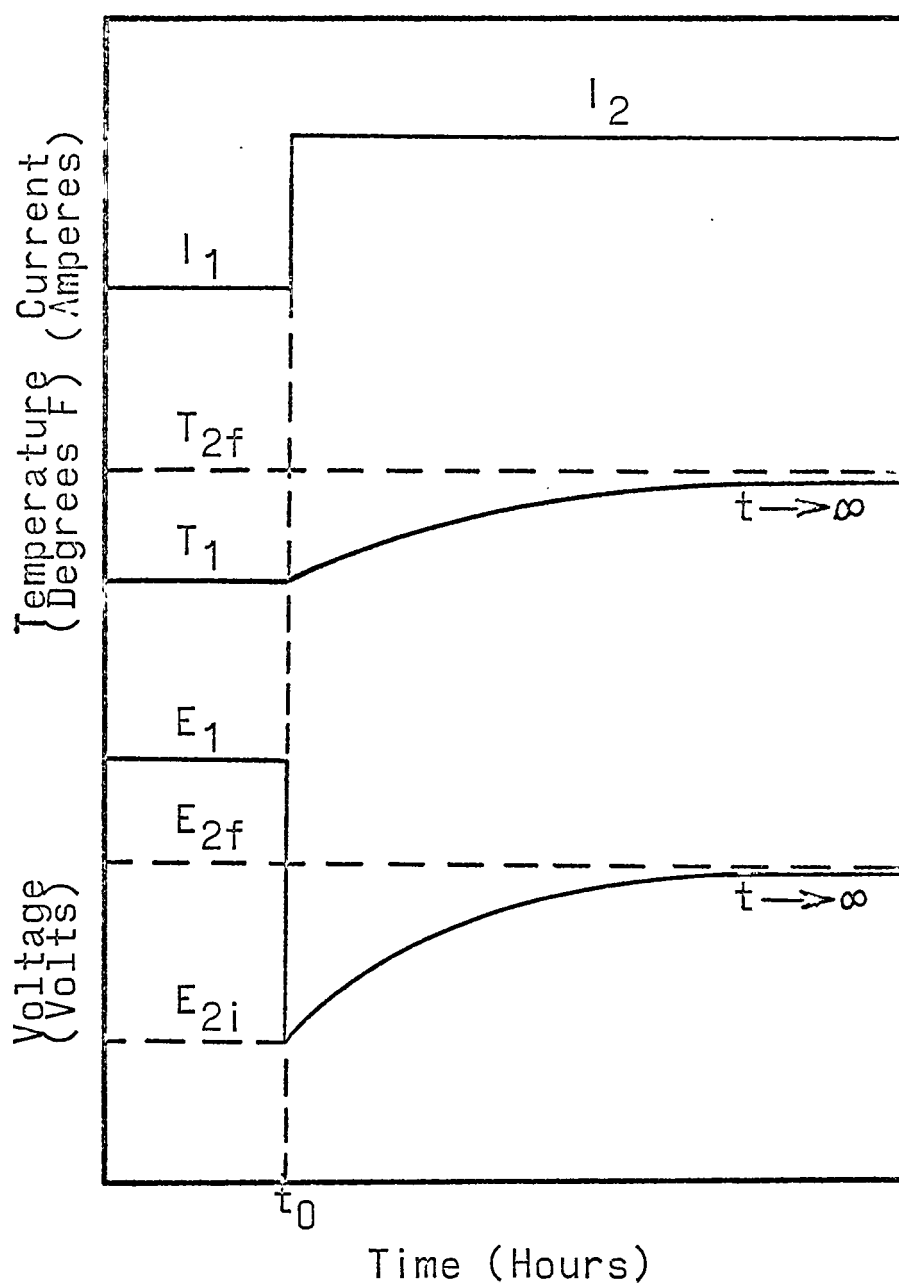


FIGURE 16
TRANSIENT FUEL CELL PERFORMANCE
(STEP CURRENT INCREASE)

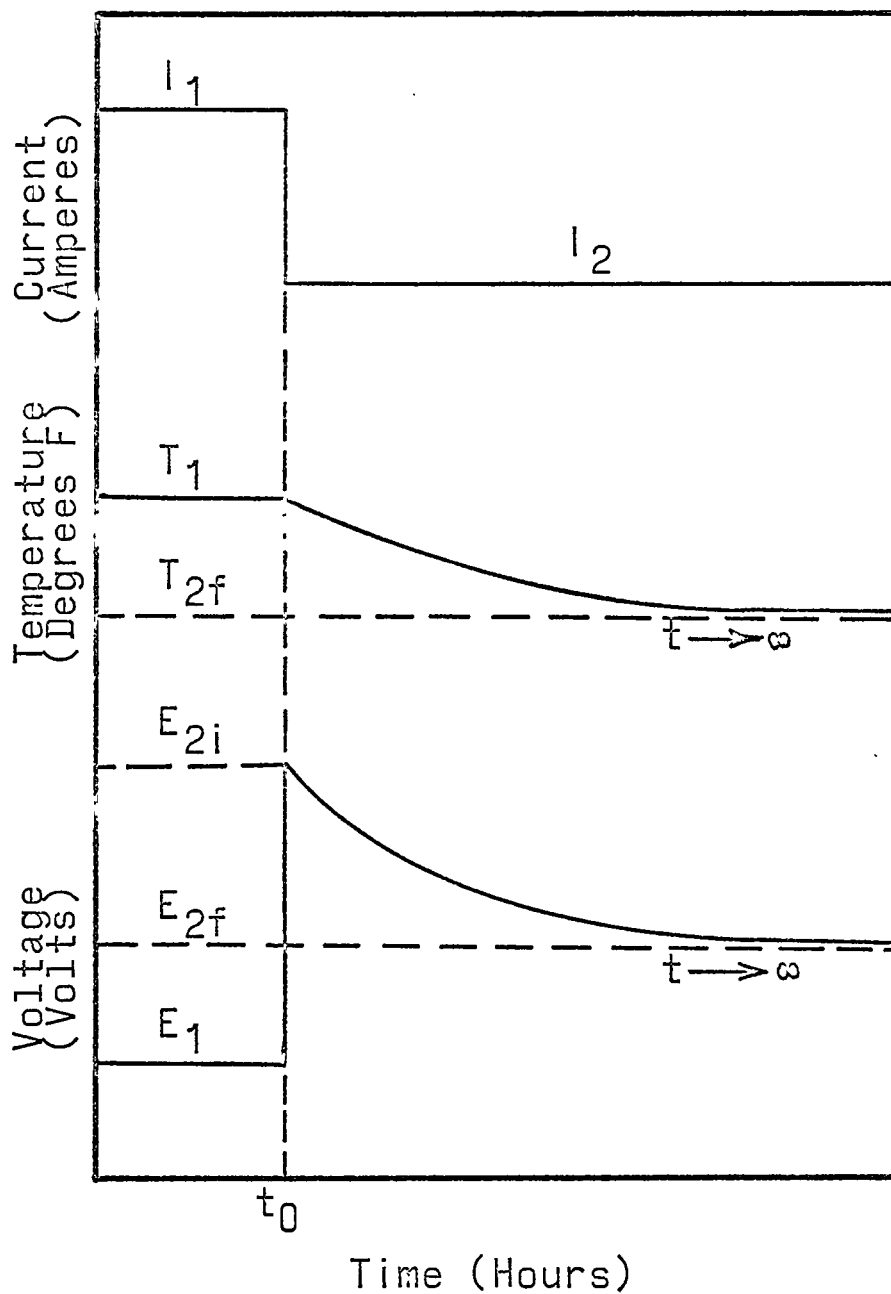


FIGURE 17
TRANSIENT FUEL CELL PERFORMANCE
(STEP CURRENT DECREASE)

which the speeds of the reactions in both directions are equal. The chemical equilibrium point within the cell depends on many things, one of which, for example, is the position of the triple interface at the electrodes. Three of the most important of these, however, are temperature, pressure and concentration. The analysis, of course, accounts for variations of temperature, concentration, and partial pressure of the water above the KOH in the hydrogen gas cavity. Since in a transient mode of operation the concentration of the electrolyte depends on partial pressure and temperature, which are always changing, the partial pressure of the water above the electrolyte can never really reach an equilibrium state. The condition of equilibrium is assumed, however, for purposes of calculating electrolyte concentration. Further, since the flow rates are small and the flow paths tortuous, it is assumed that the fluid stream leaving the stack is at the average temperature of the stack. It is also assumed that the partial pressure of the water vapor at the stack exit is equal to the average partial pressure of the water vapor in each cell. From this average stack temperature and partial pressure an average electrolyte concentration is calculated under the equilibrium assumption above. In other words, the concentration, temperature and pressure gradients across the 31-cell stack are neglected.

(6) STOICHIOMETRY. For the chemical reaction .

which takes place within the cells, the condition of stoichiometry is assumed. Only two things would prevent stoichiometry, and these are (1) hydrogen diffusion through the electrolyte, and (2) hydrogen or oxygen leakage from the system. The former has been shown to be negligible by numerous experiments on single cells. Hydrogen leak detectors in the thermal vacuum chamber have failed to give evidence of hydrogen leakage on powerplants which have been properly connected to their reactant supply systems, and oxygen containment problems are even less severe than those of hydrogen.

(7) PERFECT GAS LAW. The conditions of pressure and temperature around the primary loop are approximately 60 psia total pressure, with the partial pressure of the water vapor never exceeding 10 psia, at temperatures between 150 F and 450 F. Under these conditions the perfect gas law is satisfactory,⁵ and hence is used throughout the analysis for the hydrogen-water vapor mixture.

(8) CONDENSER EXIT TEMPERATURE VARIATIONS. The variation of condenser exit temperature on the primary side is always less than ± 5 degrees from its nominal 160 F, except under adverse glycol coolant inlet temperature conditions. In order to account for these more extreme variations in primary side condenser exit temperature, a module glycol inlet temperature-time profile would be needed. Such a profile is not available at this time. For this reason,

and because the small variations in condenser exit temperature experienced during normal operation do little to change condenser performance and cause only a very small change in the latent heat (h_{fg}) of the water condensed, a constant 160 F will be used for primary side condenser exit temperature.

(9) PRESSURE CONDITIONS. Although certain very small pressure fluctuations will exist from time to time in the nitrogen blanket which pressurizes the electrolyte, causing corresponding fluctuations in pressure within the hydrogen and oxygen gas cavities, a constant nitrogen pressure of 52 psia is assumed for the analysis, with a constant 8.5 psid and 10.5 psid pressure differential for the hydrogen and oxygen, respectively, referenced to the nitrogen (see Figure 5). It is further assumed that the pressure drop in the components and connecting lines around the primary loop, the total of which is less than 1 psid, can be neglected. A constant total pressure of 60 psia is used for all locations in the primary loop.

(10) PRIMARY LOOP VOLUMETRIC FLOW RATE AND EFFICIENCY OF WATER SEPARATION. For primary loop calculations it is assumed that the volumetric flow rate of the hydrogen pump-separator assembly is constant at 3.5 cfm. Although changing condensate mass flow rates at the condenser exit due to changing water production rates and variations in condenser performance cause small fluctuations in torque at the motor shaft, bench tests have shown that the pump

volumetric flow rate is almost constant. These tests have also shown that the efficiency of separation of liquid water from the recirculating hydrogen-water vapor stream is very near 100%.

(11) PERFORMANCE DEGRADATION. Due to the build-up of impurities within the cells which are carried in by the reactant gases, the powerplant will experience a small degradation of voltage with time under given conditions of current and temperature. Over the operating lifetime for which the Apollo fuel cell is qualified (400 hours), this performance degradation is statistically less than 1%, and therefore will be neglected in the analysis.

(12) REACTANT INLET TEMPERATURE. A constant reactant inlet (hydrogen and oxygen) temperature of 77 F will be used for the purposes of this analysis, since no reactant temperature-time profiles are as yet available. It will be seen in the analysis that unless variations in reactant inlet temperature become very extreme, performance variations are almost undetectable.

(13) HOMOGENEITY OF HYDROGEN-WATER VAPOR MIXTURE. It will be assumed in the analysis that the recirculating hydrogen-water vapor mixture is homogeneous throughout. This is a realistic assumption, since although the flow rates are fairly low, the flow regime is always turbulent due to the many bends and turns in the primary loop and because of such components as heat exchangers, the in-line.

heater and the in-line condenser exit temperature sensor. At the condenser exit, where two-phase flow exists, the gas (mixture) stream and the condensate stream will be treated separately.

The foregoing analytical approach, combined with the above thirteen assumptions and the use of empirical data where necessary, will be used for the analysis.

CHAPTER V

DEVELOPMENT OF GOVERNING EQUATIONS

The analytical description of the physical behavior of fuel cell operation is based on the proper application of the principles of conservation of mass and energy. Since the processes within the fuel cell involve chemical and phase changes along with the flow of various fluids, the equations must be developed in such a way as to decrease the number of independent variables.

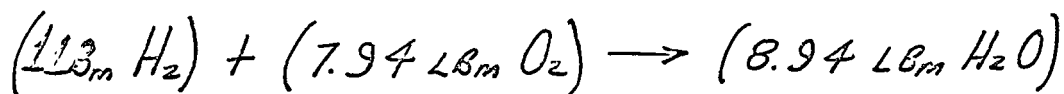
For purposes of developing the reactant consumption and water production equations, the overall chemical reaction for the formation of water can be written as



The mass balance is



or



Under the assumption of stoichiometry, the oxygen-consumption and water-production rates can be written in terms of the consumption rate of hydrogen as

$$\dot{m}_{O_2 \text{ CONS}} = 7.54 \dot{m}_{H_2 \text{ CONS}} \quad (1)$$

and

$$\dot{m}_{H_2O \text{ PROD}} = 8.94 \dot{m}_{H_2 \text{ CONS}} \quad (2)$$

The term reactant "consumption" is used to distinguish this quantity from total reactant usage, which is the sum of reactant consumption and purge (reactants which are vented to rid the cells of accumulated impurities).

On a time basis, Faraday's Law can be used to define the electrochemical constant K_1 as

$$\begin{aligned} K_1 &= \frac{50,500 \text{ AMP.}}{1.008 \text{ GM/SEC OF } H_2 \text{ CONSUMED}} \\ &= 95,730 \frac{\text{AMP.} - \text{SEC.}}{\text{GM. } H_2 \text{ CONSUMED}} \times \frac{453.6 \text{ GM.}}{\text{LB}_M} \bigg/ \frac{3600 \text{ SEC}}{\text{HR}} \\ &= 12,060 \text{ AMP-HR/LB}_M H_2 \text{ CONSUMED} \end{aligned}$$

Hence $\left(\frac{1}{K_1}\right) = 8.292 \times 10^{-5} \text{ LB}_M H_2 \text{ CONSUMED/AMP-HR.}$

Therefore, assuming stoichiometry the hydrogen consumption rate for each of the 31 cells is

$$\dot{m}_{H_2 \text{ CONS CELL}} = \left(\frac{1}{K_1}\right) \cdot I = 8.292 \times 10^{-5} I \quad (\text{per cell}).$$

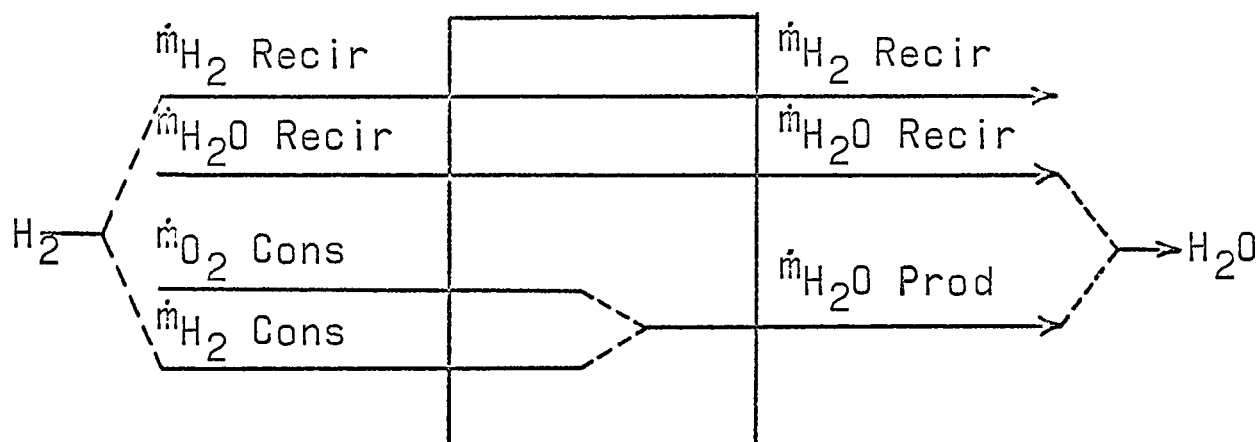
For a 31-cell module, the consumption rate is

$$\dot{m}_{H_2 \text{ CONS}} = 2.571 \times 10^{-3} I \quad (3)$$

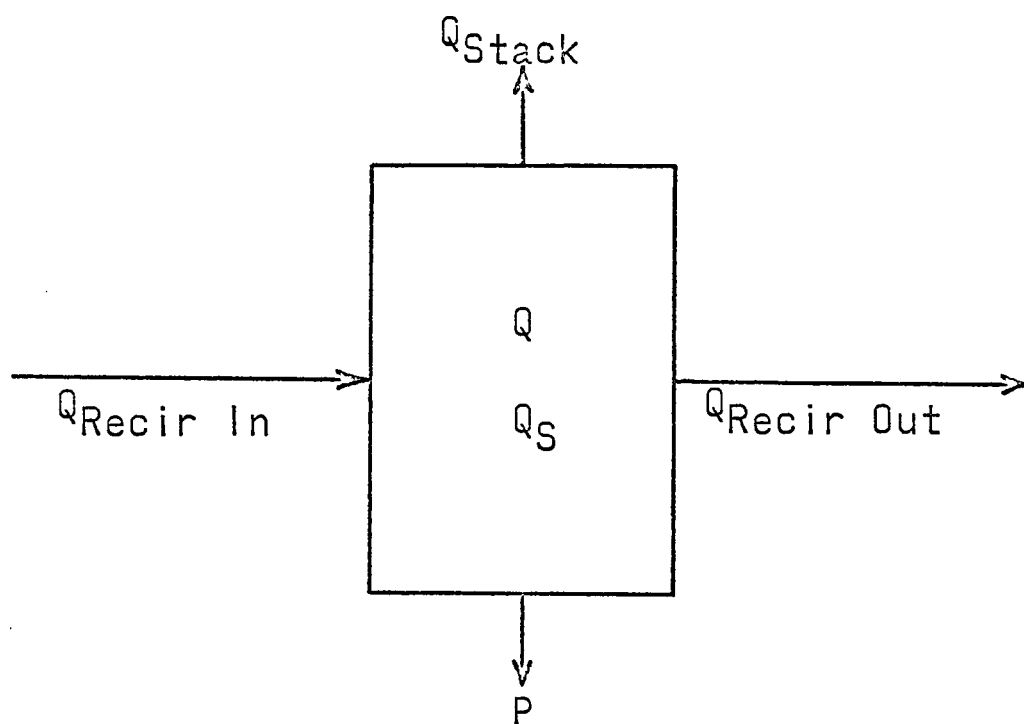
A flow diagram of the reactants, products and recirculating stream entering and leaving the fuel cell stack is shown in Figure 18-a. The fluids of the recirculating stream do not enter into the chemical reaction. The consumption hydrogen enters the stack with the recirculating stream; it joins outside the pressure jacket after passing through the hydrogen preheater. Consumption oxygen enters the stack after being conditioned in the oxygen preheater.

The stack heat loss (Q_{stack}), electrical power output (P), heat stored (Q_s) and waste heat generated (Q), as well as the heat entering and leaving the stack by means of the recirculating stream are shown in Figure 18-b. Now if the gases entering and leaving the stack are treated separately, then the First Law of Thermodynamics gives

$$\begin{aligned} & (\dot{m}h)_{H_2 \text{ CONS}_{IN}} + (\dot{m}h)_{O_2 \text{ CONS}_{IN}} + (\dot{m}h)_{H_2 \text{ RECIR}_{IN}} + \\ & (\dot{m}h)_{H_2 O \text{ RECIR}_{IN}} + (\dot{m}_{H_2 \text{ CONS}} \times HF) = (\dot{m}h)_{H_2 O \text{ PROD}_{OUT}} + \\ & (\dot{m}h)_{H_2 \text{ RECIR}_{OUT}} + (\dot{m}h)_{H_2 O \text{ RECIR}_{OUT}} + 3.413 P + Q_{\text{STACK}} \quad (4) \end{aligned}$$



(a) FLOW DIAGRAM



(b) HEAT BALANCE

FIGURE 18
FLUID FLOW DIAGRAM AND HEAT BALANCE
FOR FUEL CELL STACK

where for convenience all enthalpies are referenced to 77 F. Kinetic and potential energy changes across the stack are negligible. The heat of formation of water (HF) will be taken as the lower heating value of hydrogen (since superheated steam leaves the stack) and will also be referenced to 77 F. At one atmosphere and 77 F, $HF_{77} = 51,571 \text{ BTU/LB}_m \text{ H}_2$.⁵

Since the chemical reaction within the fuel cell occurs at temperatures near 400 F and at a pressure of approximately 4 atmospheres, pressure and temperature corrections should be investigated. The correction for pressure⁶ is

$$\Delta H_F_P = \int_{P_1}^{P_2} \left(\frac{\partial h}{\partial p} \right)_T dp \quad (5)$$

The correction for temperature⁷ can be written as

$$\Delta H_F_T = \int_{T_1}^{T_2} \Delta C_p dT \quad (6)$$

where for the reaction $\text{H}_2(\text{gas}) + \frac{1}{2} \text{O}_2(\text{gas}) \rightarrow \text{H}_2\text{O}(\text{gas})$,

$$\Delta C_p = \left\{ C_p(\text{H}_2\text{O VAPOR}) - \left[C_p(\text{H}_2 \text{gas}) + \frac{1}{2} C_p(\text{O}_2 \text{gas}) \right] \right\} \left(\frac{\text{BTU}}{\text{LB}_m - R} \right) \quad (6-a)$$

Since the reactants and products are treated as perfect gases, $\left(\frac{\partial h}{\partial p} \right)_T = 0$. Hence $\Delta H_F_P = 0$. The correction for temperature, ΔH_F_T , is included in the energy balance.

The sole purposes of the recirculating stream of water and hydrogen (Figure 13) are to remove heat and water. Hence the quantity Q_{recir} is defined as the heat removed by the recirculating stream and can be written as

$$Q_{\text{RECIR}} = \left[(\dot{m}h)_{\text{H}_2 \text{ RECIR OUT}} - (\dot{m}h)_{\text{H}_2 \text{ RECIR IN}} \right] + \left[(\dot{m}h)_{\text{H}_2\text{O RECIR OUT}} - (\dot{m}h)_{\text{H}_2\text{O RECIR IN}} \right] \quad (7)$$

Now the total energy available from the heat of formation of water is (before the temperature correction for HF)

$$Q_{\text{GEN}} = \dot{m}_{\text{H}_2 \text{ CONS}} \times HF_{77} \quad (8)$$

Substituting Equations (7) and (8) into Equation (4), the energy equation becomes

$$(\dot{m}h)_{\text{H}_2 \text{ CONS}} + (\dot{m}h)_{\text{O}_2 \text{ CONS}} + Q_{\text{GEN}} = (\dot{m}h)_{\text{H}_2\text{O PROD}} + Q_{\text{RECIR}} + 3.413 P + Q_{\text{STACK}} \quad (9)$$

Introducing the net heat produced in the stack (Q , BTU/HR) as a result of fuel cell inefficiency,

$$Q = Q_{GEN} + (\dot{m}h)_{H_2 \text{ CONS}} + (\dot{m}h)_{O_2 \text{ CONS}} - (\dot{m}h)_{H_2O \text{ PROD}} - 3.413 P \quad (10)$$

Substituting Equation (10) into Equation (9),

$$Q = Q_{STACK} + Q_{RECIR} \quad (11)$$

In other words, the net heat generated in the stack is the sum of the stack heat loss and the heat removed by the recirculating stream. Substituting Equations (1), (2), (3) and (8) into Equation (10),

$$Q = 2.57 \times 10^{-3} \frac{P}{E} \left\{ [C_p (T_{IN} - T_o)]_{H_2 \text{ CONS}} + 7.94 [C_p (T_{IN} - T_o)]_{O_2 \text{ CONS}} - 8.94 [C_p (T_{STACK} - T_o)]_{H_2O \text{ PROD}} + 51,571 \right\} - 3.413 P \quad (12)$$

where the reference temperature T_o is 77 F.

Now from Figure 19,⁸ the average C_p of hydrogen between 77 F and 450 F is 3.44 BTU/LB_m-R. For oxygen under these same conditions, $C_{p_{avg}} = 0.221$ BTU/LB_m-R; and similarly for water, $C_{p_{avg}} = 0.454$ BTU/LB_m-R. Hence Equation (12) can be written as

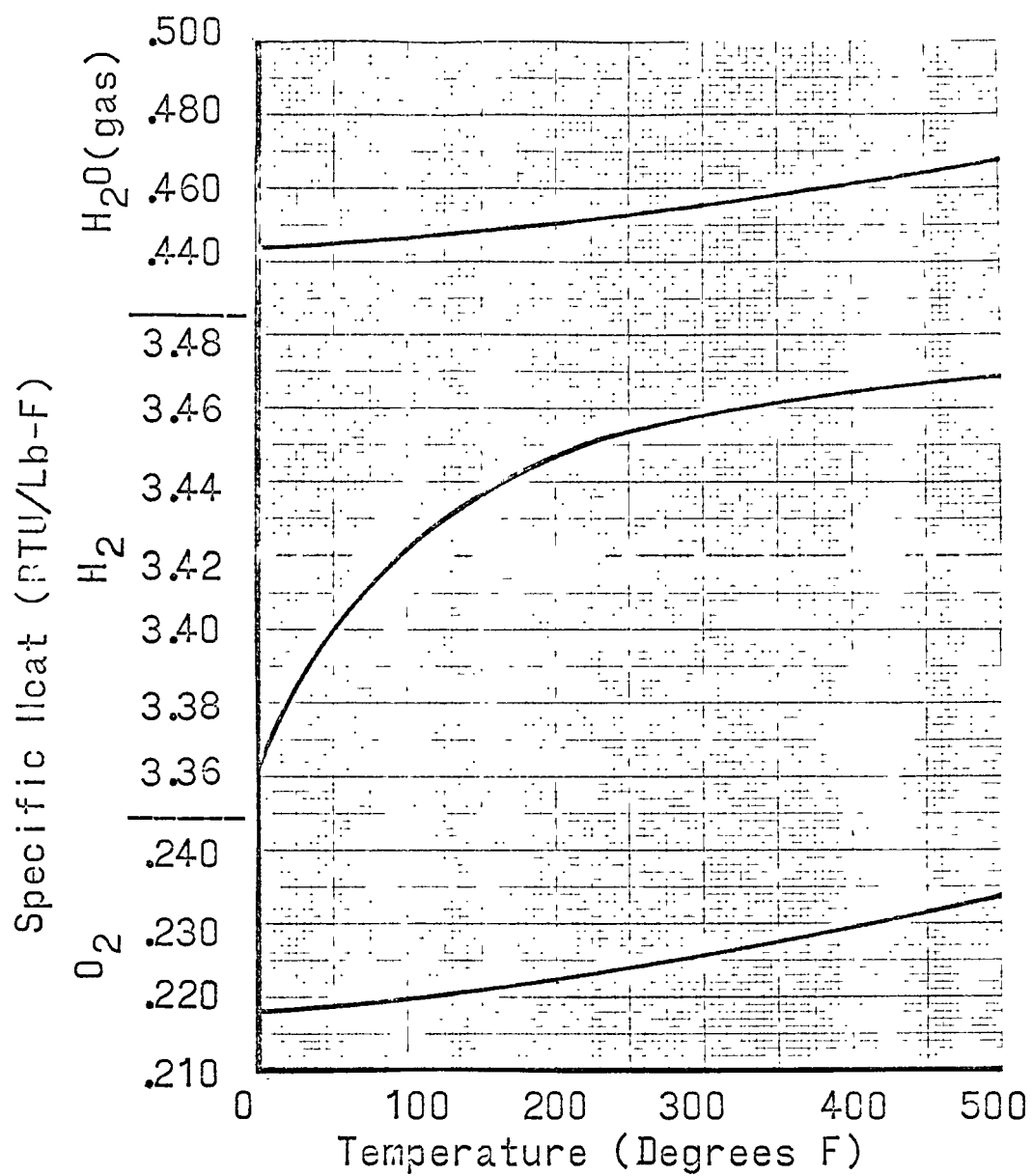


FIGURE 19
SPECIFIC HEATS AT CONSTANT PRESSURE
FOR OXYGEN, HYDROGEN, AND WATER VAPOR

$$Q = 2.57 \times 10^{-3} I \left\{ 3.44 (T_{IN} - 77)_{H_2 \text{ CONS}} + 7.94 (0.221) (T_{IN} - 77)_{O_2 \text{ CONS}} \right. \\ \left. - 8.94 (0.454) (T_{STACK} - 77)_{H_2O \text{ PROD}} + 51,571 \right\} \\ - 3.413 EI$$

Assuming $T_{H_2 \text{ in}} = T_{O_2 \text{ in}} = 77^\circ \text{ F}$ and denoting T_{stack} by T , this equation can be reduced to

$$Q = 133.3 I - 0.01043 IT - 3.413 EI \quad (13)$$

Now after a step load change, (Figure 16 or Figure 17) the fuel cell current will be constant at I_2 and (13) can be rewritten as

$$Q = 133.3 I_2 - 0.01043 I_2 T - 3.413 EI_2 \quad (13-a)$$

In order to be able to solve the differential equation readily, an ordinary differential equation is desired. Therefore the temperature and concentration gradients across the stack are neglected as a first approximation, and the only independent variable is time. Then, remembering that I is constant after a given step load change, the derivative of (13) becomes

$$\frac{dQ}{dt} = -0.01043 I \frac{dT}{dt} - 3.413 I \frac{dE}{dt} \quad (14).$$

This equation will be used subsequently in the analysis to obtain a relation for stack temperature as a function of time by expressing Q and E as functions of temperature and other variables.

Now from Figure 18, for a transient thermal condition in the stack

$$Q_{RECIR\ IN} + Q = Q_S + Q_{RECIR\ OUT} + Q_{STACK} \quad (15)$$

where the fuel cell power output P is included in the expression for Q in Equation (12).

It is assumed from calculations based on test data that the heat loss from the stack is constant, i.e.,

$$Q_{STACK} = 165 \text{ BTU/HR} \quad (16)$$

Now

$$[Q_{RECIR\ OUT} - Q_{RECIR\ IN}] = \left(\dot{m} C_p \Delta T \right)_{H_2 RECIR} + \left(\dot{m} C_p \Delta T \right)_{H_2 O RECIR} \quad (17)$$

where

$$\begin{aligned} \Delta T &= T_{STACK\ OUT} - T_{STACK\ IN} \\ &= T_{STACK} - T_{STACK\ IN} \\ &= T - T_{STACK\ IN} \end{aligned}$$

Assuming a constant condenser exit temperature of 160 F and a constant total pressure of 60 psia as well as a constant volumetric flow rate of 3.5 cfm for the positive displacement vane pump at the condenser exit, the perfect gas law may be applied to the fluid stream as follows:⁹

$$p\dot{V} = \dot{m}RT \quad (\text{for the mixture})$$

$$\therefore (\dot{m}R)_{\text{MIX}} = \frac{(60 \times 144) \times (3.5 \times 60)}{620}$$

$$= 2925 \left(\frac{\text{BTU}}{\text{HR} \cdot \text{DEG}} \right)$$

But $(\dot{m}R)_{\text{MIX}} = (\dot{m}R)_{\text{H}_2} + (\dot{m}R)_{\text{H}_2\text{O}}$

$$\therefore \frac{2925}{\dot{m}_{\text{H}_2 \text{ RECIR}}} = \left(\frac{\dot{m}_{\text{H}_2 \text{ RECIR}} \times 767}{\dot{m}_{\text{H}_2 \text{ RECIR}}} \right) + \left(\frac{\dot{m}_{\text{H}_2\text{O RECIR}} \times 85.3}{\dot{m}_{\text{H}_2 \text{ RECIR}}} \right)$$

or $\frac{2925}{\dot{m}_{\text{H}_2 \text{ RECIR}}} = 767 + 85.3 \gamma_{\text{C/E}} \quad (18)$

where $\gamma_{\text{C/E}} = \text{Specific Humidity at Condenser Exit} \left(\frac{\text{Lbm H}_2\text{O}}{\text{Lbm DRY H}_2} \right)$
 Using the perfect gas equation of state for each constituent of the mixture, and using Dalton's Law of Partial Pressures,

$$m_w = \frac{p_w V}{R_w T} \quad \text{and} \quad m_{\text{H}_2} = \frac{p_{\text{H}_2} V}{R_{\text{H}_2} T} \quad (19)$$

where the subscript W refers to the water vapor and the subscript H₂ refers to the dry hydrogen.

Now

$$\begin{aligned}
 Y &= \frac{m_w}{m_{H_2}} = \frac{P_w}{P_{H_2}} \times \frac{R_{H_2}}{R_w} \\
 &= \frac{P_w}{P_{H_2}} \times \frac{\bar{R}/MW_{H_2}}{\bar{R}/MW_w} \quad (\text{where } MW \equiv \text{Molecule Wt.}) \\
 &= \frac{P_w \times MW_w}{P_{H_2} \times MW_{H_2}} = \frac{P_w}{P_{H_2}} \times \frac{18.016}{2.016} \\
 &= 8.94 \frac{P_w}{P_{H_2}}
 \end{aligned}$$

But

$$\text{Total Pressure} = p = P_{H_2} + P_w$$

$$\therefore P_{H_2} = p - P_w = 60 - P_w$$

or

$$Y = 8.94 \frac{P_w}{(60 - P_w)} \quad (20)$$

or, for later use, Equation (20) can be written as

$$P_w = \frac{60}{\left(1 + \frac{8.94}{Y}\right)} \quad (21)$$

For a condenser exit temperature of 160 F, the partial pressure of the saturated water vapor is 4.741 psia.

Hence

$$Y_{c/E} = 8.94 \times \frac{4.741}{(60 - 4.741)}$$

or
$$\gamma_{C/E} = 0.767 \quad (22)$$

Now substituting Equation (22) into Equation (18),

$$\frac{2925}{\dot{m}_{H_2O RECIR}} = 767 + 85.3 \times 0.767 = 832.5$$

or
$$\dot{m}_{H_2O RECIR} = 3.51 \text{ LBM/HR} \quad (23)$$

$$\begin{aligned} \% \dot{m}_{H_2O RECIR} &= \gamma_{C/E} \times \dot{m}_{H_2 RECIR} \\ &= 0.767 \times 3.51 \end{aligned}$$

or
$$\dot{m}_{H_2O RECIR} = 2.70 \text{ LBM/HR} \quad (24)$$

Now substituting Equations (23) and (24) into Equation (17), for the average values of specific heat stated before, denoting stack inlet temperature by T_s ,

$$\begin{aligned} [Q_{RECIR OUT} - Q_{RECIR IN}] &= (\dot{m} C_p \Delta T)_{H_2 RECIR} + (\dot{m} C_p \Delta T)_{H_2O RECIR} \\ &= (3.51)(3.44)(T - T_s) + (2.70)(0.454)(T - T_s) \end{aligned}$$

or
$$[Q_{RECIR OUT} - Q_{RECIR IN}] = 13.3 (T - T_s) \quad (25)$$

Now the thermal mass of the stack, $M \left(\frac{BTU}{F DEG} \right)$, is known from test data:

$$M = 32 \text{ BTU/F DEG} \quad (26)$$

Hence, the heat quantity stored in the stack by raising it from temperature T_1 to temperature T is

$$\begin{aligned} q_s (\text{BTU}) &= \int_{T_1}^T M dT = M \int_{T_1}^T dT \\ &= M(T - T_1) \end{aligned}$$

or
$$\frac{dq_s}{dt} = Q_s \left(\frac{\text{BTU}}{\text{hr}} \right) = M \frac{dT}{dt} \quad (27)$$

Finally, substituting Equations (16), (25), (26) and (27) into Equation (15), we get

$$\begin{aligned} Q &= 32 \frac{dT}{dt} + 13.3(T - T_s) + 165 \\ \text{or } Q &= 32 \frac{dT}{dt} + 13.3T - 13.3T_s + 165 \end{aligned} \quad (28)$$

Hence
$$\frac{dQ}{dt} = 32 \frac{d^2T}{dt^2} + 13.3 \frac{dT}{dt} - 13.3 \frac{dT_s}{dt} \quad (29)$$

Substituting Equation (29) into Equation (14),

$$32 \frac{d^2T}{dt^2} + (13.3 + 0.01043I) \frac{dT}{dt} - 13.3 \frac{dT_s}{dt} + 3.413I \frac{dE}{dt} = 0 \quad (30)$$

Now from Appendix A, neglecting the time degradation of performance due to the build-up of impurities, the variation of moduel output voltage with temperature, current and

electrolyte concentration is

$$E = (7.96 \times 10^{-4} T - 0.481) I + (0.026 T + 23.0) - 0.2473 (\% H_2O - 27.0) \quad (31)$$

where:

$$360F \leq T \leq 480F$$

$$5 \text{ AMP.} \leq I \leq 55 \text{ AMP.}$$

$$22 \leq \% H_2O \leq 32$$

For the current region from open circuit to 5 amp., the equation corresponding to (31) is

$$E = (2.775 \times 10^{-3} T - 1.903) I + (0.0157 T + 30.24) - 0.2473 (\% H_2O - 27.0) \quad (32)$$

$$360F \leq T \leq 440F$$

$$0 \leq I \leq 5 \text{ AMP.}$$

$$22 \leq \% H_2O \leq 32$$

Equations (30), (31) and (32) are the principal governing equations describing the transient behavior of the fuel cell system. Other expressions will be introduced as needed in solving these three equations for appropriate boundary and initial conditions.

CHAPTER VI

SIMPLIFIED TRANSIENT ANALYSIS

By a simplified transient analysis is meant an analysis of the fuel cell stack only, neglecting the various heat exchangers and other parts of the system. Such an analysis is developed as a first step toward mathematical formulation of the transient fuel cell problem prior to incorporating the auxiliary components into the analysis.

Although the results of the simplified analysis are not in good agreement with test data (especially at higher temperatures), they do provide satisfactory results within limitations.

The governing energy equation for the system is Equation (30). For the simplified analysis, however, the temperature T_s at which the hydrogen-water vapor stream enters the stack (see Figure 13) is assumed a constant 350 F; hence, $\left(\frac{dT_s}{dt}\right) = 0$ in Equation (30). This is equivalent to assuming a heat exchanger between the condenser exit and the stack inlet which will always raise the temperature of the stream flowing through it to 350 F, regardless of any other changing conditions. With this assumption, the governing equation becomes

$$32 \frac{d^2T}{dt^2} + (13.3 + 0.01243I) \frac{dT}{dt} + 3.413I \frac{dE}{dt} = 0 \quad (33)$$

From Equation (31), neglecting variations of electrolyte concentration with time and assuming a constant 27% water by weight for the electrolyte solution, the variation of voltage with current and temperature is

$$E = (7.96 \times 10^{-4} T - 0.481) I + (0.026 T + 23.0) \quad (34)$$

$$360 F \leq T \leq 480 F$$

$$5 \text{ amp.} \leq I \leq 55 \text{ amp.}$$

$$\% H_2O = 27.0$$

It should be noted that the low-current region from open circuit to 5 amp. is excluded in the simplified analysis.

Now
$$\frac{dE}{dt} = (7.96 \times 10^{-4} I + 0.026) \frac{dT}{dt} \quad (35)$$

Substituting (35) into (33) and rearranging,

$$32 \frac{d^2 T}{dt^2} + (2.717 \times 10^{-3} I^2 + 9.913 \times 10^{-2} I + 13.3) \frac{dT}{dt} = 0$$

or
$$A \frac{d^2 T}{dt^2} + B \frac{dT}{dt} = 0 \quad (36)$$

where: $A = 32$

$$B = 2.717 \times 10^{-3} I^2 + 9.913 \times 10^{-2} I + 13.3$$

The solution to Equation (36) is

$$T = a + b e^{-\lambda t} \quad (37)$$

where: $\lambda = \frac{B}{A}$ and a, b are constants of integration
 The value of λ is always positive since $5 \text{ amp.} \leq I \leq 55 \text{ amp.}$ Evaluation of a can be accomplished by using the boundary condition that as time becomes infinite, the fuel cell stack temperature (T) will approach its steady state temperature (Tss); i.e.,

$$\text{As } t \rightarrow \infty, \quad T \rightarrow T_{ss}$$

Substituting this condition into Equation (37) it is seen that $a = T_{ss}$. Evaluation of b uses the initial condition that at time t_0 (i.e., when the fuel cell current changes instantaneously from I_1 to I_2), the stack is at an initial temperature T_1 , where T_1 is not necessarily a steady state temperature.

Hence

$$b = (T_1 - T_{ss}) \cdot e^{\lambda t_0}$$

Substituting the values of a and b into Equation (37), the equation for the change in stack temperature with

time becomes

$$T = T_{ss} + (T_i - T_{ss}) \cdot e^{\lambda t_0} \cdot e^{-\lambda t}$$

or

$$T = T_{ss} - (T_{ss} - T_i) \cdot e^{-\lambda(t-t_0)} \quad (38)$$

The change in voltage with time can be computed by substituting Equation (38) into Equation (34).

The steady state stack temperature (T_{ss}) is found by rewriting Equation (15),

$$Q = Q_s + Q_{RECIR} + Q_{STACK}$$

where $Q_{RECIR} = Q_{RECIR\ OUT} - Q_{RECIR\ IN}$

But in a steady state condition, the heat stored (Q_s) is zero. Hence

$$Q = Q_{RECIR} + Q_{STACK} \quad (39)$$

Now $Q = I(133.3 - 0.01043T - 3.413E)$ from (13-a)

and $Q_{RECIR} = 13.3(T - T_s)$ from (25)

$$= 13.3(T - 350)$$

Using the assumption
of a constant stack
inlet temperature

$$= 13.3T - 4655$$

And $Q_{STACK} = 165 \text{ BTU/hr}$ from (16)

Substituting the relations for Q , Q_{recir} and Q_{stack} into Equation (39) and using Equation (34) for the variation of voltage with temperature and current, the steady state temperature of the fuel cell stack is a function of current only and can be expressed as

$$T_{ss} = \frac{(1.642I^2 + 5.18I + 1490)}{(2.717 \times 10^{-3}I^2 + 9.91 \times 10^{-2}I + 13.3)} \quad (40)$$

And the steady state voltage is computed as

$$E_{ss} = (7.96 \times 10^{-4}T_{ss} - 0.481)I + (0.026T_{ss} + 23.0) \quad (41)$$

The steady state power level of the fuel cell is, then

$$P_{ss} = E_{ss} \times I_z \quad (42)$$

In Chapter VIII the results of this simplified analysis are compared to those of the more general transient analysis.

CHAPTER VII

GENERAL TRANSIENT ANALYSIS

The analysis is now extended to the more general situation with the incorporation of the primary bypass control and primary regenerator characteristics into the system. Although this analysis will be termed a "general" transient analysis, it is only general in comparison with the simplified analysis, and is still subject to the simplifying assumptions of Chapter IV. As shown later by comparing the results of the simplified analysis to those of this more general analysis, the incorporation of the bypass control and regenerator produces a feedback effect in the temperature region where regeneration occurs. This feedback effect quickens the thermal response of the system considerably in this region, as well as narrows the operating temperature range of the system.

In this analysis the following assumptions previously used in the simplified analysis will be eliminated:

- (a) The temperature at which the hydrogen-water vapor mixture enters the stack (T_s), earlier assumed constant, will now be allowed to vary in accordance with the response of the primary bypass valve and primary regenerator.
- (b) The previous assumption of constant electrolyte concentration will no longer be used. The concen-

tration of the KOH electrolyte solution will be allowed to change according to variations in electrolyte (stack) temperature and partial pressure of the water vapor above the KOH at the gas-electrode-electrolyte interface. The assumption of pressure and temperature equilibrium at the gas-liquid interface will be retained for purposes of calculating electrolyte concentration. It will further be assumed, as with stack temperature, that the partial pressure of the water vapor at the stack exit is equal to the average partial pressure of the water above the KOH within the stack.

In addition, the analysis will include the following considerations:

- (a) The effects of the heat input to the mixture stream at the hydrogen pump due to the inefficiency of the pump are considered.
- (b) Thermal effects due to the cycling of the in-line heater at low power levels are included.
- (c) The low-current region (0 to 5 amp.) is included in the analysis in order to provide the capability of analyzing the hot standby or no-load condition.

All previous assumptions, such as a constant condenser exit temperature of 160 F and a constant fuel cell system environment temperature of 77 F, will be retained.

In the schematic diagram of Figure 13, the heat input to the system at the hydrogen pump is calculated as follows. The pump-separator motor is a three-phase, Y-connected motor drawing approximately a 0.76-amp. line current, which is equivalent to 0.76 amp. per phase. The spacecraft inverter supplies the motor with 115 volts per phase. Hence the motor is supplied with 87.3 volt-amp. per phase, or 262 volt-amp. total for the three phases. At a nominal power factor of 0.32, the power input to the motor is approximately 84 watts.

Some of this power input is dissipated in the motor due to losses, the remainder being shaft output power. This can be expressed as

$$P_{H_2 \text{ PUMP IN}} (\text{WATTS}) = P_L + P_S$$

where: P_L = Power dissipated in motor due
to losses (watts)

P_S = Shaft output power of motor (watts)
= Shaft HPx746

The power losses can be divided into three general categories:

$$P_L = P_{F\&W} + P_{H\&E} + P_{ELEC}$$

where: $P_{F\&W}$ = (Combined) Friction and
Windage Losses (watts)

$P_{H\&E}$ = (Combined) Hysteresis and
Eddy Current Losses (watts)

$$P_{ELEC} = I^2 R \text{ loss in motor}$$

Since the motor torque is 32.5 oz-in at 2125 rpm,

$$\begin{aligned} \text{SHAFT HP} &= Tn / 63,060 \\ \text{WHERE: } T &= \text{TORQUE (LB}_f\text{-IN)} \\ n &= \text{RPM} \\ \text{SHAFT HP} &= \frac{(\frac{32.5}{16}) \times 2125}{63,060} \\ &= 0.0684 \end{aligned}$$

so that $P_S = 51$ watts. This means that $P_L = 33$ watts, or that the motor efficiency, defined as the ratio of shaft output power to total input power times 100, is approximately 61%. The 51 watt-equivalent of shaft horsepower operates the pump and the water separator.

The losses associated with the pump and the water separator can also be calculated. The input power to the motor can then be expressed as the sum of all these losses plus the flow work required to pump the mixture stream around the primary loop, plus the work required to impart a sufficient amount of kinetic energy to the liquid water to remove it from the system by means of centrifugal force.

Regardless of the amount of the total input power converted either directly or indirectly to heat within the pump-separator assembly via losses, the remainder will also eventually appear in the system as heat (although not.

entirely in the pump-separator assembly) due to friction. This heat due to friction, which is dissipated in other parts of the system, is only a very small part of the overall power input; it will be assumed that the total input power to the pump-separator assembly is dissipated as heat in that same assembly. Not all of this heat enters the recirculating stream, however. The fraction which is absorbed by the stream will now be calculated. From Figure 13, the temperature of the mixture stream at the pump exit is found from the thermal vacuum test data¹⁰ to be approximately 170 F when the fuel cell system is in a nominal 77 F environment. Neglecting the small preheating effect, the reactant or make-up hydrogen enters the primary loop at the mixing tee at 77 F.

Using the specific heat values and flow rates of the hydrogen and water vapor from Chapter V, that temperature to which the stream would rise if the total power input were absorbed by the stream is calculated from the following energy balance:

$$\begin{aligned}
 Q_{\substack{\text{PUMP-SEP.} \\ \text{ASS'Y. INPUT}}} &= \sum (\dot{m} C_p) (T_{P/E} - 160) \\
 &= (\dot{m}_{H_2 \text{ RECIR}} \times C_{p_{H_2}} + \dot{m}_{H_2O \text{ RECIR}} \times C_{p_{H_2O}}) (T_{P/E} - 160)
 \end{aligned}$$

But $Q_{\text{PUMP-SEP ASS'Y. INPUT}} = 84 \text{ WATTS} \times 3.413 = 287 \text{ BTU/HR}$

$$\therefore T_{P/E \text{ THEOR}} = \frac{287}{(3.51 \times 3.44) + (2.70 \times 0.454)} + 160$$

$$= 181.6 \text{ F}$$

Since from test data the actual temperature to which the recirculating stream rises as it flows through the pump-separator assembly is only 170 F, the heat lost at the pump due to radiation and conduction is

$$Q_L = \sum (\dot{m} C_p) \cdot (181.6 - 170.0)$$

$$= 13.296 \times 11.6$$

$$= 154.1 \text{ BTU/HR}$$

Hence the actual heat input to the recirculating stream at the pump is 132.9 BTU/HR, or only about 46.3% of the total input power.

Using the notation of Figure 13, the mixing equation for the hydrogen make-up tee is

$$\dot{m}_{H_2 \text{ CONS}} \times C_{p_{H_2}} (T_{RIN} - T_0) + \dot{m}_{H_2 \text{ RECIR}} \times C_{p_{H_2}} (T_{P/E} - T_0) +$$

$$\dot{m}_{H_2 O \text{ RECIR}} \times C_{p_{H_2 O}} (T_{P/E} - T_0) = \dot{m}_{H_2 \text{ RECIR}} \times C_{p_{H_2}} (T_R - T_0) +$$

$$\dot{m}_{H_2 O \text{ RECIR}} \times C_{p_{H_2 O}} (T_R - T_0) + \dot{m}_{H_2 \text{ CONS}} \times C_{p_{H_2}} (T_R - T_0)$$

where: T_0 is a reference temperature

T_R is the temperature of the mixture entering the primary regenerator, assuming no heat loss in line connecting the mixing tee and the regenerator.

$T_{P/E}$ is the actual pump exit temperature (170 F)

All terms containing the reference temperature T_0 subtract out. Rearranging the above equation, and substituting the known temperatures, flow rates and specific heats into the equation as well as Equation (3), the expression for T_R becomes

$$T_R = \left(\frac{0.681 I + 2261}{8.841 \times 10^{-3} I + 13.3} \right) \quad (43)$$

where I is fuel cell current in amperes and T_R is in degrees F. It is assumed that this temperature changes instantaneously with a step current change although there is some small time lag associated with the mixing tee.

In order to calculate T_s , the mixture temperature at the cold side exit of the primary regenerator, the cold side effectiveness of the regenerator must be considered. The effectiveness of a counter-flow heat exchanger such as

this one is defined as¹¹

$$E_c \equiv \frac{\sum (\dot{m} C_p)_c (T_s - T_r)}{X (T - T_r)} \quad (44)$$

$$\begin{aligned} \text{where: } \sum (\dot{m} C_p)_c &= \left[(\dot{m} C_p)_{H_2 \text{ REGR}} + (\dot{m} C_p)_{H_2 \text{ CONS}} + (\dot{m} C_p)_{H_2 O \text{ REGR}} \right] \\ &\equiv \text{THERMAL CAPACITY RATE OF} \\ &\quad \text{COLD SIDE STREAM (BTU/HR-DEG)} \end{aligned}$$

$$\begin{aligned} X &\equiv \text{SMALLER OF } \sum (\dot{m} C_p)_c \text{ AND } \sum (\dot{m} C_p)_H \\ \text{WHERE } \sum (\dot{m} C_p)_H &\equiv \text{THERMAL CAPACITY RATE OF HOT SIDE STREAM (BTU/HR-DEG)} \end{aligned}$$

In order to determine X, the characteristic of the primary bypass control must be introduced. A plot of per cent bypass-versus-temperature is shown in Figure 20 for the bypass valve, which is biased to stack temperature (T) by means of a bimetallic strip within the valve which is placed in the stack exhaust stream. The two solid curves in the figure show the effects of hysteresis inherent in the valve. For example, if the stack temperature is at 430 F and rising, then the valve is following curve A. If, however, after reaching 444 F, the stack temperature starts decreasing, the valve will continue to bypass 50% of the total flow around the regenerator until the stack temperature reaches 441 F, at which time the per cent bypass will start to decrease along curve B.

Since the temperature deadband of the valve due to hysteresis is relatively small, it is neglected in this analysis. Also, since the normal operating temperature

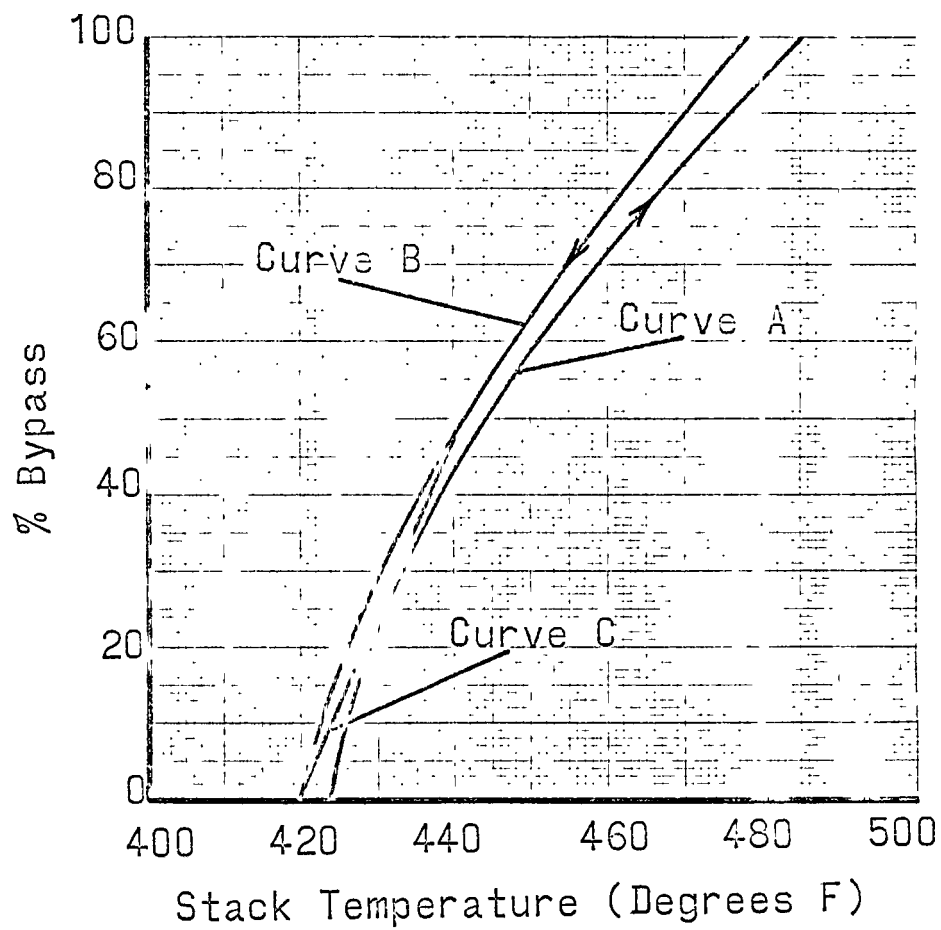


FIGURE 20
PRIMARY BYPASS VALVE CHARACTERISTIC

range of the powerplant is 380 F to 440 F from minimum to maximum power, the linear bypass-valve characteristic of curve C is used.

$$\begin{aligned} \text{Now } \sum (\dot{m} C_p)_C &= (\dot{m}_{H_2 RECIR} + \dot{m}_{H_2 CONS}) C_{p_{H_2}} + (\dot{m}_{H_2 O RECIR} \times C_{p_{H_2 O}}) \\ &= (3.51 + 2.57 \times 10^{-3} I) \times 3.44 + (2.70)(0.454) \end{aligned}$$

$$\text{or } \sum (\dot{m} C_p)_C = 8.841 \times 10^{-3} I + 13.3 \quad (45)$$

Letting the bypass fraction be denoted by ϕ ,

$$\text{i.e., } \phi = \% \text{ BYPASS} \times 10^{-2} \quad (46)$$

$$\begin{aligned} \sum (\dot{m} C_p)_H &= (1 - \phi) \left\{ (\dot{m}_{H_2 RECIR} \times C_{p_{H_2}}) \right. \\ &\quad \left. + (\dot{m}_{H_2 O RECIR} + \dot{m}_{H_2 O}) \cdot C_{p_{H_2 O}} \right\} \end{aligned}$$

where $\dot{m}_{H_2 O}$ is that portion of the water produced which exits from the stack. This term can be expressed as

$$\dot{m}_{H_2 O} = \dot{m}_{H_2 O PROD} + \left(\frac{d\dot{m}_{H_2 O}}{dt} \right) dt$$

where $\left(\frac{d\dot{m}_{H_2 O}}{dt} \right) \leq 0$

In a steady state condition all the water produced leaves the stack and $\left(\frac{d\dot{m}_{H_2 O}}{dt} \right) = 0$. Hence, for steady state operation

$$\dot{m}_{H_2O} = \dot{m}_{H_2O PROD}$$

For the transient condition $\left(\frac{d\dot{m}_{H_2O}}{dt}\right) < 0$.

The portion of the water produced which leaves the stack changes as electrolyte concentration ($\%H_2O$) changes, and therefore

$$\left(\frac{d\dot{m}_{H_2O}}{dt}\right) = \left(\frac{d(\%H_2O)}{dt}\right)\left(\frac{d\dot{m}_{H_2O}}{d(\%H_2O)}\right)$$

However, since changes in electrolyte concentration are very small, this term can be neglected with only a very small error. Hence

$$\dot{m}_{H_2O} \approx \dot{m}_{H_2O PROD}$$

Then the expression for the hot side thermal capacity rate is

$$\begin{aligned} \Sigma(\dot{m}C_p)_H &= (1-\phi) \left[(\dot{m}_{H_2O RECIR} \times C_{p_{H_2}}) \right. \\ &\quad \left. + (\dot{m}_{H_2O RECIR} + \dot{m}_{H_2O PROD}) \times C_{p_{H_2O}} \right] \\ &= (1-\phi) \left[(3.51 \times 3.44) + (2.70 + \right. \\ &\quad \left. 8.94 \times 2.57 \times 10^{-3} I)(0.454) \right] \\ &= (1-\phi) (10.431 \times 10^{-3} I + 13.3) \quad (47) \end{aligned}$$

or $\Sigma (\dot{m} C_p)_H = (1-\phi) \cdot \mathcal{L}$

where $\mathcal{L} = \mathcal{L}(I) = (10.431 \times 10^{-3} I + 13.3)$

From Figure 20 it is seen that there are two distinct stack temperature regions to be considered, namely the region of variable regeneration from 420 F to 440 F (440 F is used as an upper limit since this temperature roughly corresponds to the temperature of the stack at its rated maximum continuous output power, 1420 watts). Also, from Appendix A, there are two current regions. The various regions of current and temperature result in five cases to be considered. These cases are listed in Table 1 below.

CASE No.	CURRENT REGION		TEMPERATURE REGION			IN-LINE HEATER	
	(I)		REGENERATION		TEMP. RANGE (T)	ON	OFF
	0-5 amp.	5-55 amp.	FULL ($\phi=0$)	PARTIAL ($\phi \neq 0$)			
1		✓	✓		$360F \leq T \leq 420F$		✓
2		✓		✓	$420F \leq T \leq 440F$		✓
3		✓	✓		$360F \leq T \leq 420F$	✓	
4	✓		✓		$T_{HIGH} \leq T \leq 420F$		✓
5	✓			✓	$420F \leq T \leq 440F$		✓

TABLE 1. CASES CONSIDERED IN THE DEVELOPMENT OF THE TRANSIENT EQUATIONS FOR DIFFERENT CURRENT AND TEMPERATURE REGIONS OF OPERATION

The transient equations for the variation of stack temperature with time after a given step load change will now be derived for all cases.

Case I

$$5 \text{ amp.} \leq I \leq 55 \text{ amp.}$$

$$360F \leq T \leq 420F$$

Full Regeneration ($\phi=0$)

In-line Heater Off

To determine X for use in Equation (44), the values of $\sum (\dot{m} C_p)_c$ and $\sum (\dot{m} C_p)_H$ can be compared from Equations (45) and (47), where in Equation (47) $\phi=0$.

$$\text{At } I = 5 \text{ amp., } \sum (\dot{m} C_p)_c = 13.344 \left(\frac{\text{BTU/H}^2}{F \text{ DEG}} \right)$$

$$\text{and } \sum (\dot{m} C_p)_H = 13.352 \left(\frac{\text{BTU/H}^2}{F \text{ DEG}} \right)$$

$$\text{At } I = 55 \text{ amp., } \sum (\dot{m} C_p)_c = 13.786 \left(\frac{\text{BTU/H}^2}{F \text{ DEG}} \right)$$

$$\sum (\dot{m} C_p)_H = 13.874 \left(\frac{\text{BTU/H}^2}{F \text{ DEG}} \right)$$

$$\text{Hence } 0.008 \leq [(\dot{m} C_p)_H - (\dot{m} C_p)_c] \leq 0.088$$

It is seen from these calculations that the difference in hot side and cold side thermal capacity rates is always less

than $0.1 \left(\frac{370/3.2}{F_{DES}} \right)$ in the region of full regeneration, with $\sum (\dot{m} C_p)_H$ only very slightly greater than $\sum (\dot{m} C_p)_C$. Hence it will be assumed that $\sum (\dot{m} C_p)_H = \sum (\dot{m} C_p)_C$ and therefore X is chosen as $\sum (\dot{m} C_p)_C$. The equation for cold side regenerator effectiveness is then simplified considerably to

$$E = \frac{(T_3 - T_R)}{(T - T_R)} \quad (48)$$

Using a constant cold side effectiveness of 0.84, the inlet temperature to the stack is found from Equation (48) to be

$$T_3 = 0.84 T + 0.16 T_R \quad (49)$$

Substituting Equation (49) into Equation (25) and denoting $[Q_{RECIR OUT} - Q_{RECIR IN}]$ by Q_{RECIR} , the heat removed from the stack by the recirculation stream is

$$Q_{RECIR} = 2.128 (T - T_R) \quad (50)$$

To calculate the steady state temperature of the fuel cell as a function of current, the steady state heat balance is

$$Q = Q_{RECIR} + Q_{STACK} \quad (51)$$

where Q is given by Equation (28) with $\left(\frac{dT}{dT}\right)=0$ and Q_{stack} is assumed constant at 165 BTU/HR.

Substituting Equations (28) and (41) into Equation (51),

$$I(133.3 - 0.01043T - 3.413E) = 2.128(T - T_R) + 165 \quad (52)$$

where E is given by Equation (31), repeated here for convenience

$$E = (7.96 \times 10^{-4}T - 0.431)I + (0.026T + 23.0) - 0.2473(\%H_2O - 27.0) \quad (31)$$

From Appendix A, % H_2O is given by

$$\%H_2O = 61.78 - 0.0997T + P_w \quad (53)$$

where P_w is the partial pressure of the water above the KOH, assumed here as the equilibrium pressure, in psia, and calculated at the stack exit. T is in $^{\circ}F$. From Equation (21),

$$P_w = \frac{60}{1 + \frac{8.94}{Y}}$$

where Y is the specific humidity $\left(\frac{\text{Lbm WATER VAPOR}}{\text{Lbm DRY HYDROGEN}}\right)$ of the mixture stream at the stack exit. By definition,

$$\gamma = \frac{\dot{m}_{H_2O \text{ RECIR}} + \dot{m}_{H_2O \text{ PROD}}}{\dot{m}_{H_2 \text{ RECIR}}}$$

or

$$\gamma = \frac{2.70 + 22.98 \times 10^{-3} I}{3.51} \quad (54)$$

Substituting Equation (21) into Equation (53), then substituting Equation (53) into Equation (31), the voltage relation of Equation (31) becomes

$$E = (7.96 \times 10^{-4} T - 0.481) I + 0.05066 T + \Gamma' \quad (31-a)$$

where γ is given by Equation (33) and

$$\Gamma' = \Gamma(I) = 14.399 - \left(\frac{14.838}{1 + \frac{8.94}{\gamma}} \right) \quad (55)$$

Substituting Equation (31-a) into Equation (52), simplifying, and rearranging, the steady state stack temperature, denoted by T_{ss} , becomes:

$$T_{ss} = \left\{ \frac{1.642 I^2 + [133.3 - 3.413 \Gamma'] I + (2.128 T_R - 165)}{27.17 \times 10^{-4} I^2 + 0.1833 I + 2.128} \right\} \quad (56)$$

This steady state temperature will later be used as a boundary condition. The steady state voltage for this case is given by Equation (31), with $T = T_{ss}$.

For the transient condition, substituting Equations (31-a) and (49) into the governing differential equation (30), the

following linear second-order equation is obtained:

$$32 \frac{d^2 T}{dt^2} + (27.17 \times 10^{-4} I^2 + 0.1333 I + 2.128) \frac{dT}{dt} = 0 \quad (57)$$

Letting $A = 32$

$$B = 27.17 \times 10^{-4} I^2 + 0.1333 I + 2.128$$

and $\lambda = B/A$

the solution to Equation (55) is

$$T = a + b e^{-\lambda t} \quad (58)$$

where a and b are constants of integration.

Using the same boundary and initial conditions of the simplified analysis, i.e.,

$$\begin{aligned} \text{At } t = t_0, \quad T &= T_i \\ \text{As } t \rightarrow \infty, \quad T &\rightarrow T_{ss} \end{aligned}$$

it is found that

$$\begin{aligned} a &= T_{ss} \\ b &= (T_i - T_{ss}) \cdot e^{\lambda t_0} \end{aligned}$$

Substituting the value of these constants into Equation (58) and rearranging, the solution is

$$T = T_{ss} - (T_{ss} - T_i) \cdot e^{-\lambda(t-t_0)} \quad (59)$$

Case II

$$5amp \leq I \leq 55amp.$$

$$420F \leq T \leq 440F$$

Partial Regeneration

In-line Heater Off

Since with full regeneration $\sum (\dot{m} C_p)_c$ and $\sum (\dot{m} C_p)_H$ are approximately equal, it is evident that with any amount of regeneration $\sum (\dot{m} C_p)_H$ will always be less than $\sum (\dot{m} C_p)_c$.

Hence $X = \sum (\dot{m} C_p)_H$ and Equation (44) becomes

$$E_c = 0.84 = \frac{\sum (\dot{m} C_p)_c \cdot (T_s - T_R)}{\sum (\dot{m} C_p)_H \cdot (T - T)} \quad (60)$$

Now the linear primary bypass valve characteristic of Figure 20 can be expressed mathematically as

$$\% \text{ BYPASS} = 2.167 T - 910.4 \quad (61)$$

Substituting Equations (45), (47) and (61) into Equation (60), simplifying, and solving for T_s , it is seen that

$$T_s = T_R + \left[\frac{1}{\sum (\dot{m} C_p)_c} \right] \left[(0.0182 \alpha) T^2 + (8.845 \alpha + 0.0182 \alpha T_R) T - (8.485 \alpha T_R) \right]$$

or $T_s = T_R + \beta_1 T^2 + \beta_2 T + \beta_3 \quad (62)$

where: $\beta_1 = \left[\frac{1}{\Sigma(\dot{m}c_p)_c} \right] \cdot (-0.0182 \Delta C)$

$$\beta_2 = \left[\frac{1}{\Sigma(\dot{m}c_p)_c} \right] \cdot (8.485 \Delta C + 0.0182 \Delta T_R)$$

$$\beta_3 = \left[\frac{1}{\Sigma(\dot{m}c_p)_{\text{COLD}}} \right] \cdot (-8.485 \Delta T_R)$$

Substituting Equation (26) into Equation (25),

$$Q_{\text{RECIR}} = (-13.3\beta_1)T^2 + 13.3(1-\beta_2)T - 13.3(T_R + \beta_3)$$

or $Q_{\text{RECIR}} = \mathcal{J}_1 T^2 + \mathcal{J}_2 T + \mathcal{J}_3$ (63)

where $\mathcal{J}_1 = -13.3\beta_1$

$$\mathcal{J}_2 = 13.3(1-\beta_2)$$

$$\mathcal{J}_3 = -13.3(T_R + \beta_3)$$

Again the steady state heat balance as given by Equation (51) is

$$Q = Q_{\text{RECIR}} + Q_{\text{STACK}}$$

Substituting Equation (28) with $\frac{dT}{dt} = 0$ and Equation (63) into Equation (51), still using $Q_{\text{stack}} = 165 \text{ BTU/HR}$, and solving for the steady state fuel cell temperature T_{ss} , it is found that

$$T_{ss} = \frac{-\xi_2 \pm \sqrt{\xi_2^2 - 4\xi_1\xi_3}}{2\xi_1}$$

where: $\xi_1 = \delta_1$

$$\xi_2 = (\delta_2 + 27.17 \times 10^{-4} I^2 + 9.917 \times 10^{-2} I)$$

$$\xi_3 = (\delta_3 - 1.642 I^2 - 54.8 I + 165)$$

An order-of-magnitude analysis for the current region under consideration reveals that the positive root must be chosen in the above expression for T_{ss} in order to make the mathematical model compatible with the actual fuel cell.

Hence

$$T_{ss} = \frac{-\xi_2 + \sqrt{\xi_2^2 - 4\xi_1\xi_3}}{2\xi_1} \quad (64)$$

The order-of-magnitude analysis also ensures that for the current region considered, the discriminant $(\xi_2^2 - 4\xi_1\xi_3)$ is always greater than zero, avoiding the possibility of imaginary roots.

By using Equation (31) in conjunction with Equation (64), the steady state voltage for this case can be obtained.

The differential equation for the transient condition is derived by substituting Equations (31-a) and (62) for E and T_s , respectively, into Equation (30). This yields

$$32 \frac{d^2 T}{dt^2} + (2\mathcal{J}_1 T + \mathcal{J}_2 - \mathcal{J}_4) \frac{dT}{dt} = 0 \quad (65)$$

$$\text{where } \mathcal{J}_4 = \mathcal{J}_4(I) = -(27.17 \times 10^{-4} I^2 + 0.1026 I)$$

Equation (65) is non-linear, but easily solved by making the substitution

$$\text{Then } V = \frac{dT}{dt} \\ \frac{d^2 T}{dt^2} = \frac{dV}{dt} = \frac{dT}{dt} \frac{dV}{dT} = V \frac{dV}{dT}$$

Substituting these relations for $\frac{dT}{dt}$ and $\frac{d^2 T}{dt^2}$ into Equation (65), the equation is reduced to a linear equation in V:

$$32 \frac{dV}{dT} + (2\mathcal{J}_1 T + \mathcal{J}_2 - \mathcal{J}_4) = 0$$

Since the $\mathcal{J}_i$ are functions of current only, this equation is easily integrated to give

$$32 \frac{dT}{dt} = -\mathcal{J}_1 T^2 + (\mathcal{J}_4 - \mathcal{J}_2) T + C_1 \quad (66)$$

where the constant of integration C_1 is evaluated by using the fact that as $t \rightarrow \infty$, $T \rightarrow T_{ss}$ and $\frac{dT}{dt} \rightarrow 0$. This results in

$$C_1 = \mathcal{J}_1 T_{ss}^2 + (\mathcal{J}_2 - \mathcal{J}_4) T_{ss} \quad (67)$$

Equation (66) can be rearranged and integrated as follows:

$$\int_{T_1}^T \frac{32 dT}{(a+bT+cT^2)} = \int_{t_0}^t dt \quad (68)$$

where: $a = C_1$
 $b = (\mathcal{L}_4 - \mathcal{L}_2)$
 $c = -\mathcal{L}_1$

Now, defining q as $4ac-b^2$, the value of the stack temperature at any time after a step load change from I_1 to I_2 , where the stack temperature was T_1 at time t_0 when the load changed instantaneously, is

$$T = -\frac{b}{2c} + \left(\frac{\sqrt{q}}{2c}\right) \cdot \tan \left\{ \tan^{-1} \left(\frac{2cT_1+b}{\sqrt{q}} \right) + \frac{\sqrt{q}}{64} (t-t_0) \right\} \quad (69)$$

for $q > 0$

and

$$T = -\frac{b}{2c} + \left(\frac{\sqrt{-q}}{2c}\right) \cdot \tanh \left\{ \tanh^{-1} \left(\frac{2cT_1+b}{\sqrt{-q}} \right) - \frac{\sqrt{-q}}{64} (t-t_0) \right\} \quad (70)$$

for $q < 0$

where the positive root is always used for $\sqrt{q}$ and $\sqrt{-q}$.

The voltage at any temperature T is given by Equation (31).

Case III

$$5 \text{ amp.} \leq I \leq 55 \text{ amp.}$$

$$360 F \leq T \leq 420 F$$

Full Regeneration ($\phi = 0$)

In-line Heater On

Although the equations for this case are good for $360 F \leq T \leq 420 F$, the in-line heater is designed to sense stack temperature such that if the stack temperature is falling, the heater is activated when the temperature reaches some temperature T_{low} , which is in the range of $380 F \pm 5 \text{ degrees F}$. The heater then stays on until the stack temperature has risen to some temperature T_{high} , which is in the range of $390 F \pm 5 \text{ degrees F}$. The actual values of T_{low} and T_{high} vary from powerplant to powerplant. The in-line heater dumps heat into the powerplant for low-power operation according to the equation

$$Q_{\text{HTR}} = \frac{3.413 E^2}{R_{\text{HTR}}} \quad (71)$$

Since the voltage varies only slightly within the relatively narrow temperature deadband (only 3 or 4 degrees on most powerplants) in which the heater is on, a constant heater power based on 31 volts will be used in the analysis. Heater resistance is 6.02 ohms. Substituting these values into Equation (71), the heater power is found to be 159.6 watts, or 544.8 BTU/HR. It is assumed that all of this heat goes to raising the temperature of the powerplant.

For purposes of calculating a steady state temperature with the heater on, Equation (11) becomes

$$Q + Q_{HTR} = Q_{STACK} + Q_{RECIR} \quad (72)$$

Using the voltage equation (31) in conjunction with Equation (28) with $\left(\frac{dT}{dt}\right) = 0$ for Q , Equation (50) for Q_{recir} , $Q_{stack} = 165$ BTU/HR and $Q_{htr} = 544.8$ BTU/HR, the steady state stack temperature with the heater on is

$$T_{ss} = \left\{ \frac{1.642 I_{TOT}^2 + (133.3 - 3.413 \Gamma) I_{TOT} + (2.128 T_R + 379.8)}{27.17 \times 10^{-4} I_{TOT}^2 + 0.1833 I_{TOT} + 2.128} \right\} \quad (73)$$

where: Γ is calculated on the basis of total current (I_{TOT}) and

$$\begin{aligned} I_{TOT} &= I + I_{HTR} \\ &= I + 31/6.02 \end{aligned}$$

$$\text{or} \quad I_{TOT} = I + 5.15 \quad (74)$$

The transient equation for this case is the same as that of Equation (59) for Case I, except that the steady state temperature (T_{ss}) is that of Equation (73).

Case IV

$$0 \leq I \leq 5 \text{ amp.}$$

$$T_{HIGH} \leq T \leq 420F$$

Full Regeneration ($\phi = 0$)

In-line Heater Off

In order to calculate T_{ss} for this case, Equation (32) is modified by substituting Equation (21) into Equation (53), then substituting Equation (53) into Equation (32) to obtain

$$E = (2.775 \times 10^{-3} T - 0.481) I + 0.0404 T + \Gamma \quad (32-a)$$

$$\text{where: } \Gamma = 14.962 + \frac{14.838}{1 + \frac{8.94}{\gamma}}$$

For this case the steady state temperature, obtained by substituting Equation (32-a) into Equation (52), is

$$T_{ss} = \left\{ \frac{6.495 I^2 + (133.3 - 3.413 \Gamma) I + (2.128 T_R - 165)}{9.471 \times 10^{-3} I^2 + 0.1483 I + 2.128} \right\} \quad (75)$$

For the transient condition, substituting Equations (32-a) and (49) into Equation (30), the governing equation becomes

$$32 \frac{d^2 T}{dt^2} + (9.471 \times 10^{-3} I^2 + 0.1483 I + 2.128) \frac{dT}{dt} = 0$$

for which the solution is given by Equation (58) with the exception that

$$B = 9.471 \times 10^{-3} I^2 + 0.1483 I + 2.128$$

Case V

$$0 \leq I \leq 5 \text{ amp.}$$

$$420F \leq T \leq 440F$$

Partial Regeneration ($\phi \neq 0$)

In-line Heater Off

For this case the only two parameters which are different from Case II are ξ_2 , ξ_3 and δ_4 . These are derived using the same techniques as were used in Case II, except that Equation (32-a) is used instead of Equation (31-a) for the voltage. The relations for ξ_2 , ξ_3 and δ_4 are

$$\xi_2 = 9.471 \times 10^{-3} I^2 + 0.1383 I + \delta_2 \quad (76)$$

$$\xi_3 = -6.495 I^2 - (133.3 - 3.413 \Gamma') I + (165 + \delta_3) \quad (77)$$

$$\delta_4 = -(9.471 \times 10^{-3} I^2 + 0.1483 I) \quad (78)$$

where Γ' is that of Equation (32-a)

The steady state and transient temperature equations are the same as for Case II, with the exception that the new values of ξ_2 , ξ_3 and Γ' are used for this case.

The foregoing equations were used to formulate a computer program which accepts a given current profile and predicts the thermal response of the fuel cell to the demand load imposed upon it. The computer program is described in Appendix B. A computer program was also written for the simplified analysis presented in Chapter VI.

CHAPTER VIII

COMPARISON OF ANALYTICAL RESULTS

Before comparing the results of the general analysis to test data obtained in the thermal vacuum chamber, the results of the simplified and general analyses will be compared. Figure 21 shows this comparison for a sample current profile. From the figure it is seen that the incorporation of the primary regenerator and bypass valve into the analysis, which is the major difference between the simplified and general analyses, has two main effects: (1) the thermal response time of the fuel cell using the equations of the general analysis is much smaller than the response time obtained from the simplified analysis; (2) the operating temperature range of the fuel cell is narrowed considerably, particularly at high-power loads, using the equations of the general analysis.

The steady state voltage-current characteristic of the fuel cell module obtained by using the equations of the general analysis is compared to the thermal vacuum characteristics of various qualified Apollo fuel cell modules¹⁰ in Figure 22. The steady state voltage-current characteristic obtained with the simplified analysis is also included for comparison. In this figure the large error incurred by use of the simplified analysis is shown clearly. As seen from the figure the general analysis

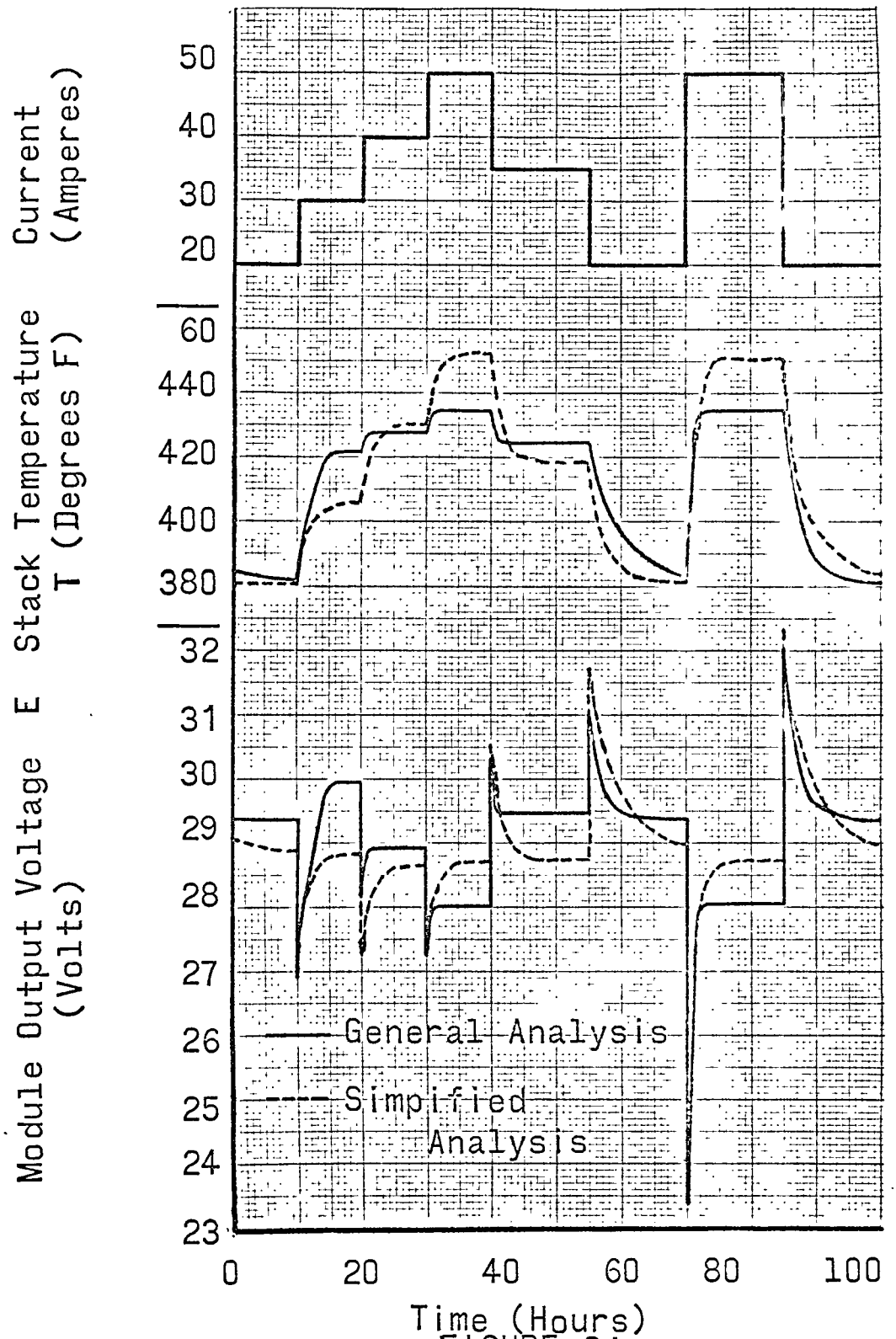


FIGURE 21
COMPARISON OF RESULTS OF SIMPLIFIED
AND GENERAL ANALYSES

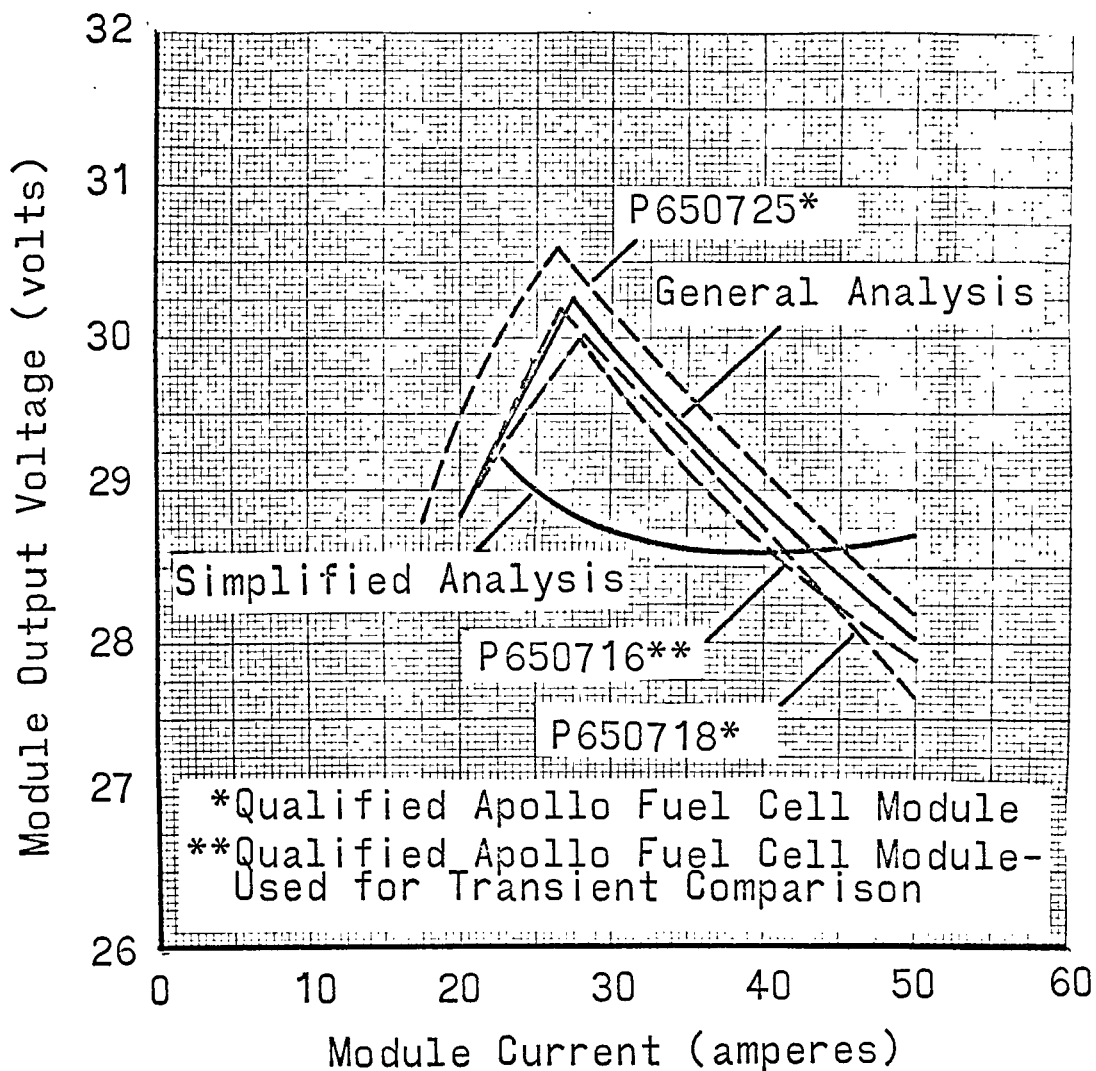


FIGURE 22

COMPARISON OF STEADY STATE
VOLTAGE-CURRENT CHARACTERISTICS

gives a more realistic approximation to actual fuel cell performance.

It must be emphasized that the empirical data used in the equations is a statistical average of data obtained from many actual powerplants and components, and that each powerplant is a separate entity in itself, although all are made to the same specifications, and as such the performance of each will be slightly different. These differences are due to slight variations in manufacturing tolerances from powerplant to powerplant, which result in differences in physical geometry, and ultimately in performance differences. As such, it should not be expected that the results of the general analysis will compare exactly with the test data. These differences in performance between actual powerplants are illustrated in Figure 22 by variations in the steady state voltage-current characteristic between various qualified powerplants.

The discontinuity in the characteristic curves of the general analysis and the qualified powerplants shown in Figure 22 is that point at which the primary bypass valve is fully closed, and the powerplant is in a condition of full regeneration. If the current is further decreased from this point, no more regeneration is obtained, and the stack temperature settles to a lower steady state value, thereby lowering the steady state voltage.

The constant temperature lines shown in the voltage-

current plot of Appendix A for a constant electrolyte (H_2O) concentration of 27% are not included in Figure 22, because at each different point on the steady state characteristic, the electrolyte concentration has a different value. If both lines of constant temperature and constant concentration were shown, a three-dimensional plot would be needed.

The transient performance results of the general analysis are compared to actual test data¹⁰ obtained on a qualified Apollo fuel cell module for various step load changes in Figures 23 through 27. It should be kept in mind in making the comparison that the steady state voltage values of the general analysis will always be higher than those of the qualified powerplant to which they are compared by the values shown in Figure 22, except for very low currents, where the two steady state lines approach each other. In the figures, the glycol coolant inlet temperature to the module, as well as the glycol flow rate through the condenser, are given for the test module. These two quantities determine the primary side condenser exit temperature ($T_{c/e}$) for any given fuel cell load. The maximum and minimum values of $T_{c/e}$ observed during the various test sequences are also shown on the figures for comparison with the constant 160 F condenser exit temperature assumed in the general analysis. The variations in condenser exit temperature are due to the fact that as fuel cell load increases, more water is produced, causing an increase in partial pressure of the water vapor

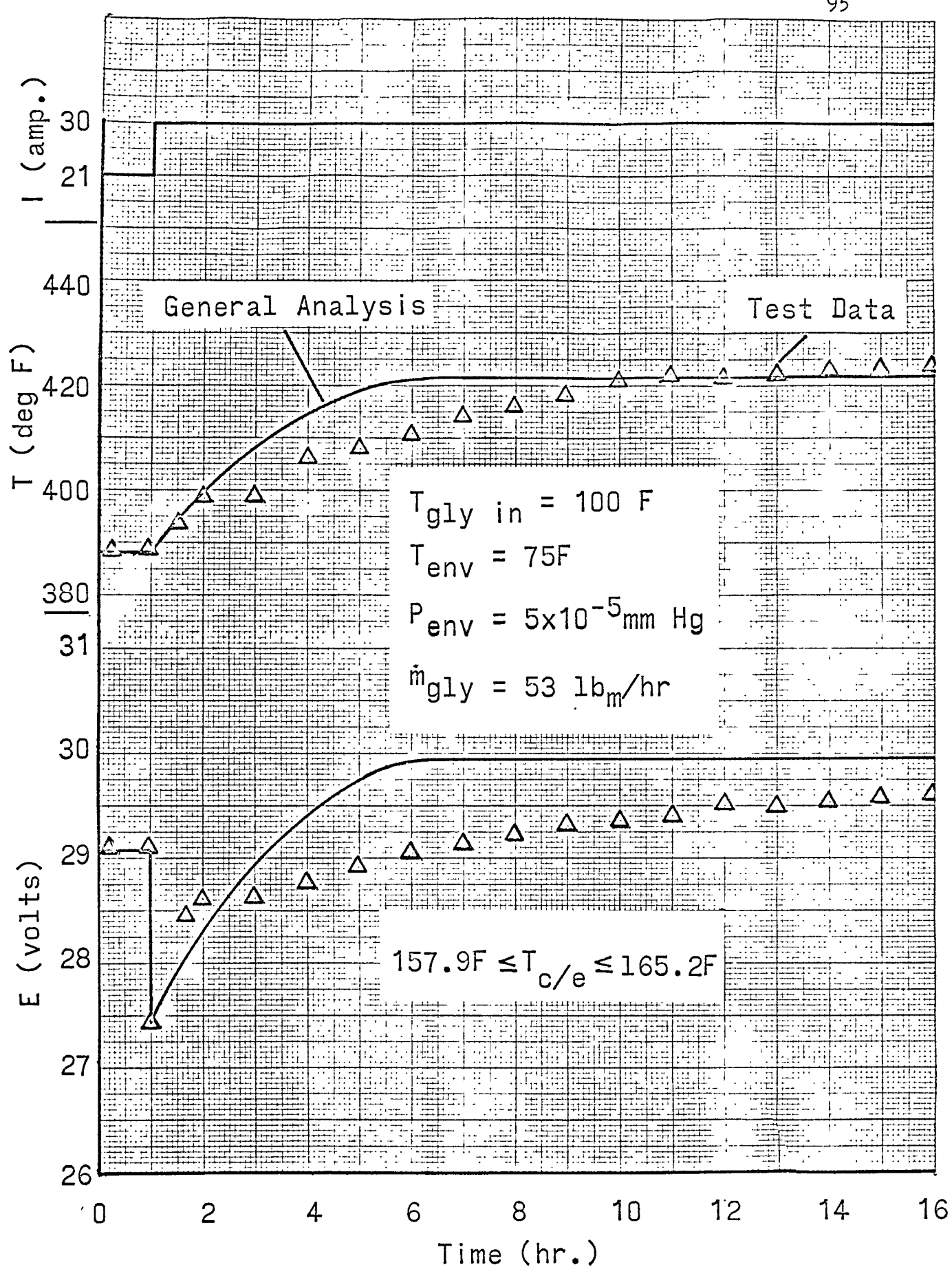


FIGURE 23. COMPARISON OF RESULTS OF GENERAL ANALYSIS WITH VACUUM CHAMBER TEST DATA

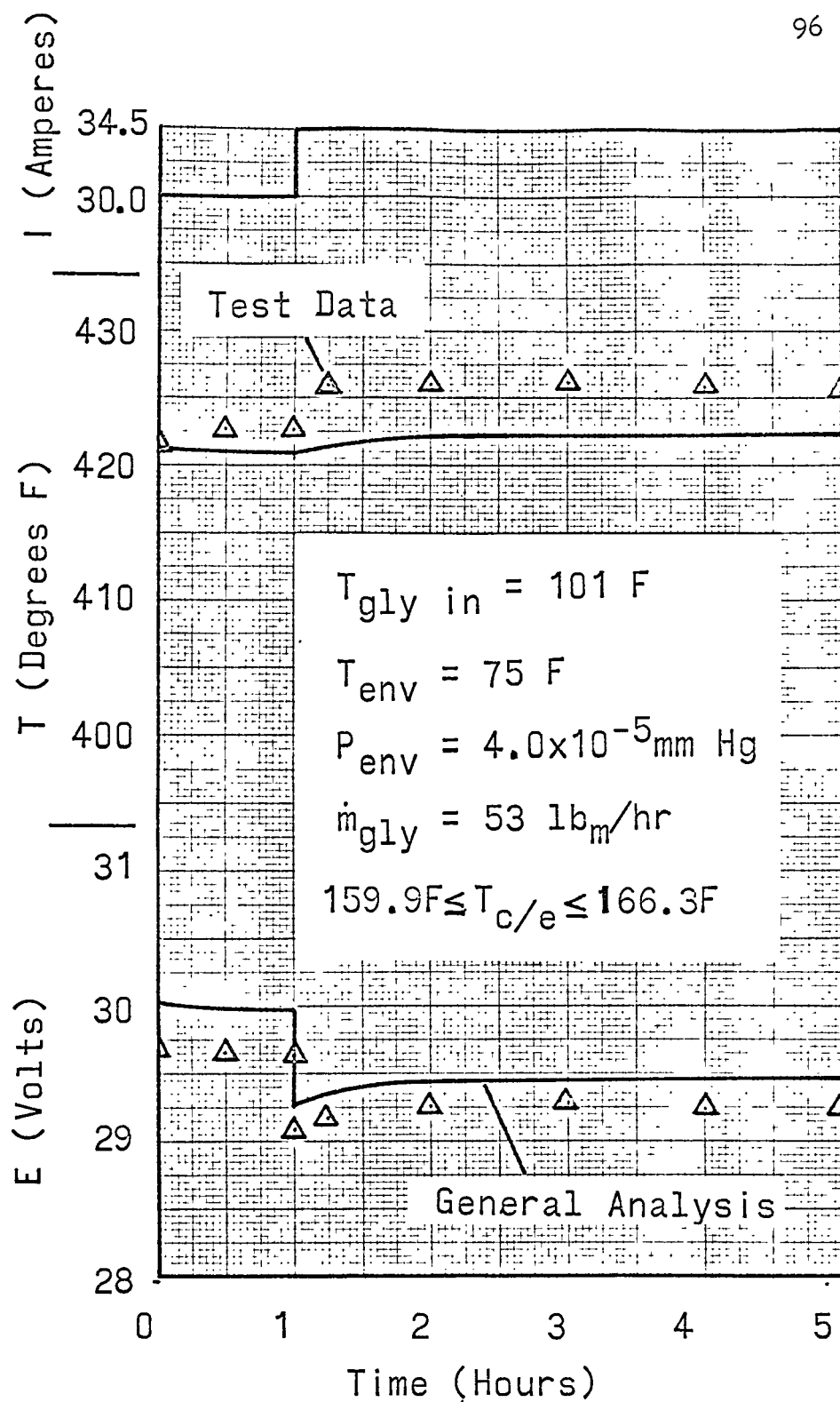


FIGURE 24
 COMPARISON OF RESULTS OF GENERAL ANALYSIS
 WITH VACUUM CHAMBER TEST DATA

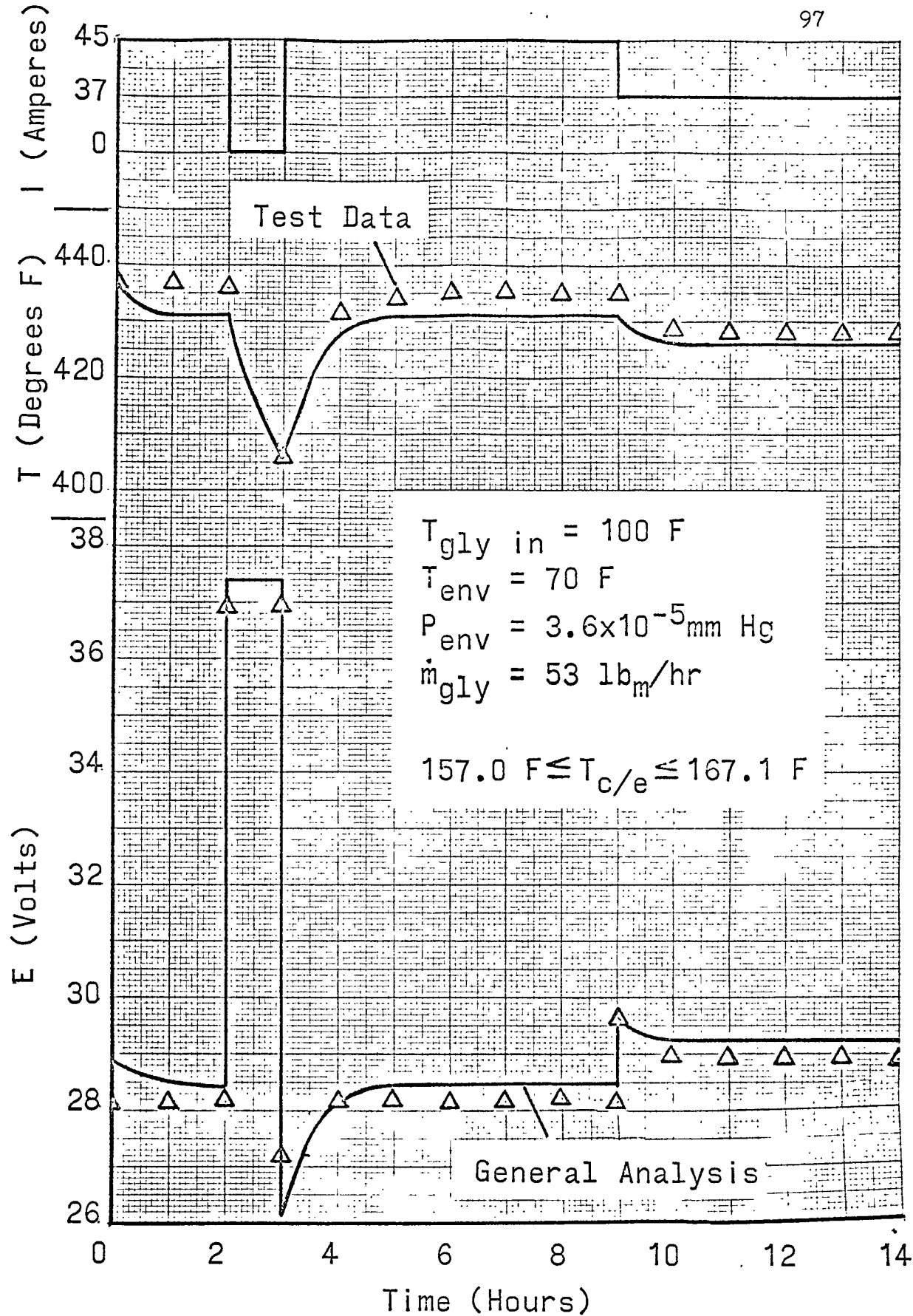


FIGURE 25
COMPARISON OF RESULTS OF GENERAL ANALYSIS
WITH VACUUM CHAMBER TEST DATA

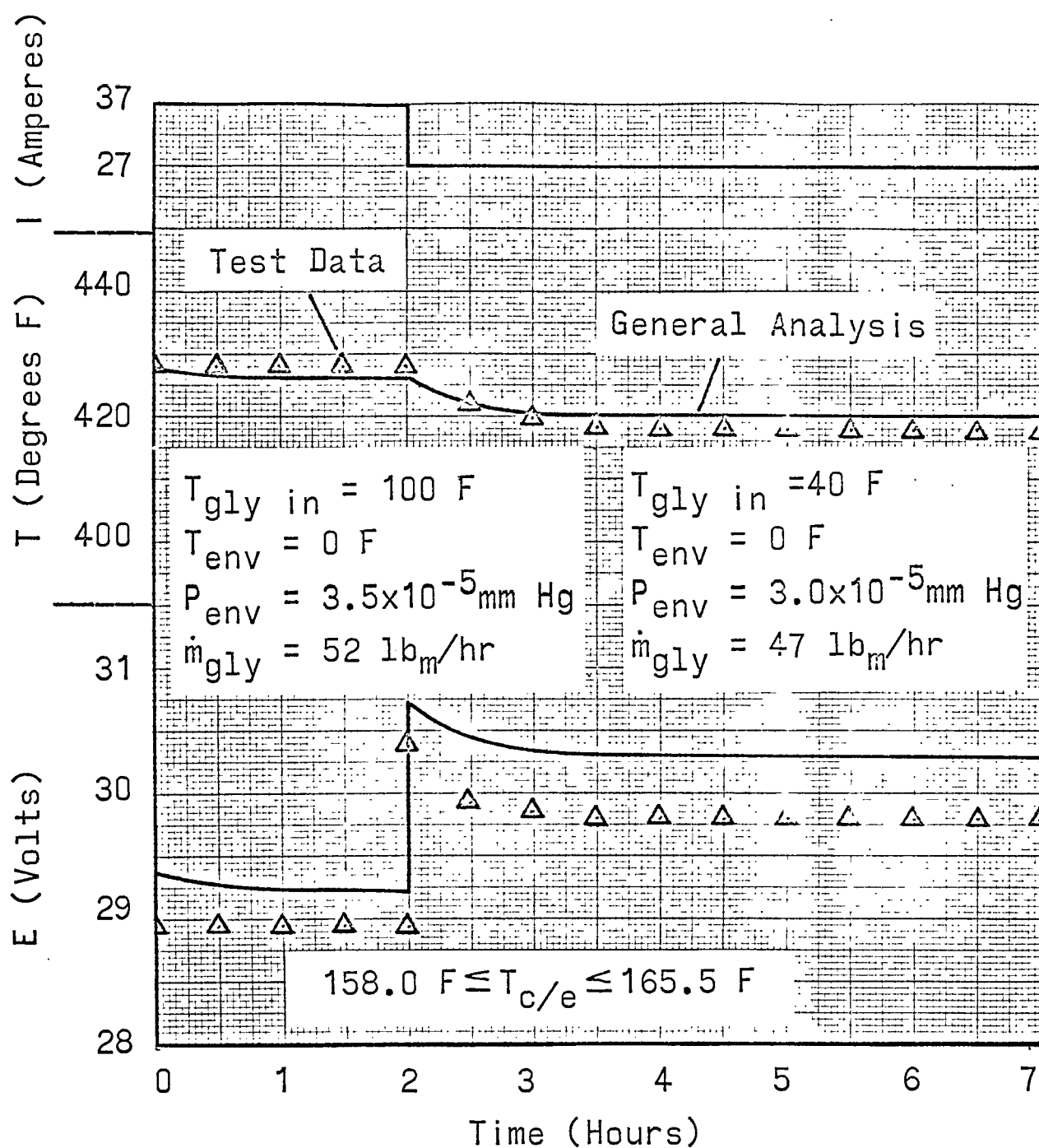


FIGURE 26
COMPARISON OF RESULTS OF GENERAL ANALYSIS
WITH VACUUM CHAMBER TEST DATA

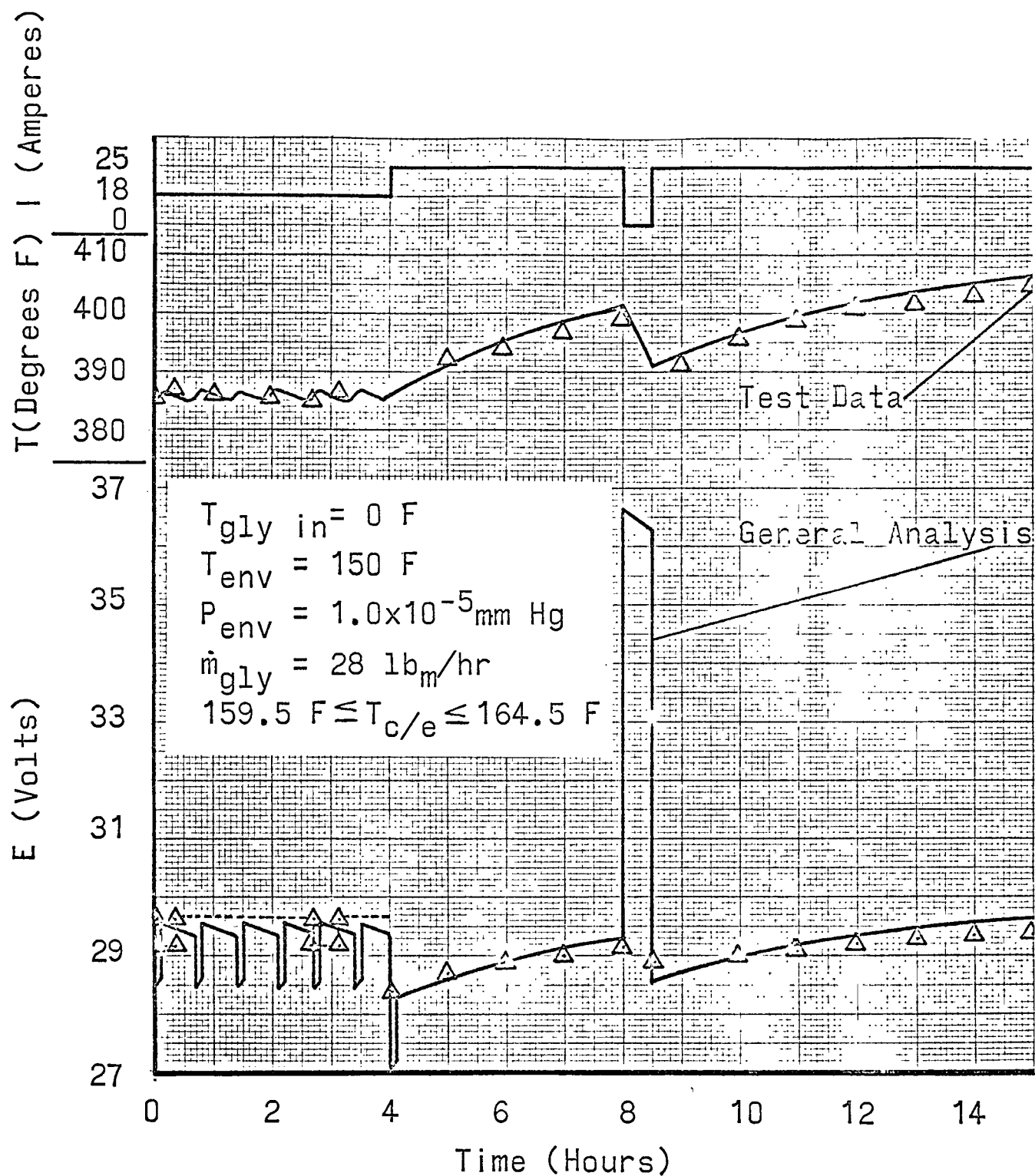


FIGURE 27
COMPARISON OF RESULTS OF GENERAL ANALYSIS
WITH VACUUM CHAMBER TEST DATA

in the primary loop and a consequent increase in condenser exit temperature.

Figure 23 shows the comparison for a step load change from steady state conditions at 21 amp. to 30 amp. Condenser exit temperature varies from 157.9 F to 165.2 F for this case. From this figure it is noted that when the stack temperature reaches 420 F for the analytical model, the bypass valve begins to open, and the temperature of the stack is then quickly regulated by the valve. It is difficult to tell where the bypass valve begins to open on the test module, because of the scatter in the data.

Figure 24 shows a step from 30.0 to 34.5 amp., with condenser exit temperature varying between 159.9 F and 166.3 F on the test module. As in Figure 23, the steady state voltage of the test module is lower than that of the analytical model, while the steady state temperature of the test module is higher than that of the analytical model. Thus it is evident that the loss of the test module is somewhat greater than that of the analytical model, resulting in a lower efficiency, or voltage, for the test module.

In Figure 25, the stack temperature is allowed to settle for two hours at 45 amp., then the powerplant is put on open circuit. Since data for the test module was recorded only every hour in the test report from which the data was taken, the exact shape of the curve for the temperature decrease of the test module is not known, but the

analytical model and the test module compared favorably in temperature just before the load was increased once more to 45 amp. Six hours later, the load was decreased to 37 amp., for which a comparison is shown. Figure 26 also illustrated the temperature and voltage response comparison for a step load decrease in current.

The first part of Figure 27 illustrates the operation of the low-power in-line heater. The temperature deadband of the analytical model was set at between 385 F and 387 F, and thus compares favorably with the test module. It is not known at this time, however, why the output voltage of the test module drops only a half volt while that of the analytical model drops a whole volt when the heaters are energized. One possible explanation is that the resistance of the in-line heater on the test module is slightly less than that of the analytical model. It should also be noted that the in-line heater of the analytical model was energized more frequently than that of the test module. This is because the fuel cell environment temperature of the test module was 150 F, whereas a 77 F environment temperature was used in the general analysis. This increased environment temperature of the test module caused a lower stack heat loss than that used in the general analysis. A very interesting feature of Figure 27 is the fact that at $t = 4$ hrs., when the load is increased from 18 amp. to 25 amp., the stack temperature for the analytical model

has just dropped to 385 F, causing the heaters to be energized simultaneously with application of the step load. This results in a total instantaneous current demand of 12.15 amp., since for the analytical model the heater current is assumed constant at 5.15 amp.; thus the voltage drops to 27.1 volts. In the test module the in-line heater was still on, however, when the step load was applied, and hence the voltage only dropped to 28.6 volts. Several minutes after $t = 4$ hr., the stack temperature of the analytical model reached 387 F causing the heater to be de-energized, and the voltage rose instantaneously to 28.55 volts, from which point the normal transient voltage build-up continued. At $t = 8$ hr., the powerplant was put on open circuit for 31 minutes. The 25-amp. load was then resumed. No open circuit data was recorded here for the test module, but the open circuit voltage would be similar to that of Figure 25.

CHAPTER IX

DISCUSSION AND CONCLUSIONS

From the steady state voltage-current characteristic comparison of Figure 22, it is seen that the general analysis yields a characteristic curve which can be considered to be statistically representative of the performance of a qualified Apollo fuel cell module. It should be emphasized, however, that the fuel cell performance characteristics which were used as a basis for formulating the mathematical model are statistical characteristics which represent the average performance obtained from many powerplant and component performance tests.

From the transient response comparison of the general analysis to the response of the qualified fuel cell module in Figures 23 through 27, it is concluded that the equations derived in the general analysis, as well as the representative performance characteristics which served as inputs to the analysis, are adequate to describe the performance of an actual fuel cell system throughout its normal operating range, for both the steady state and transient modes of operation.

The principal limitations of the analysis are summarized as follows: (1) the predicted values of the analysis are only valid for a fuel cell powerplant operating in a vacuum environment. (2) The analysis is restricted to a

normal range of glycol coolant-inlet temperatures such that the condenser exit temperature on the primary side remains within approximately ± 10 degrees from 160 F; (3) the environment temperature of the fuel cell is restricted to temperatures in the region of 77 F. It is felt that a ± 20 F variation from 77 F would be tolerable; (4) the stack heat loss is assumed constant at 165 BTU/HR. Actually, little is known about the stack loss, since the stack and primary regenerator are both inside the pressure vessel where it is very difficult to place instrumentation. It is known, however, that since the two modes of heat transfer from the stack are radiation and conduction, the stack heat loss will be a function of stack temperature. As was seen in Chapter VIII the results achieved using the constant stack heat loss assumption are in fairly good agreement with the test data. (5) The cold-side effectiveness of the primary regenerator was assumed to be constant at 84%. It is known that cold-side effectiveness is a function of temperature, per cent bypass and specific humidity. This assumption, as well as assumption (4), does not appear to cause serious errors in the computations, however. (6) In the actual spacecraft, assuming a purely resistive load, Ohm's law dictates that the current through this load is a function of the voltage impressed upon it, which is fuel cell output voltage. This voltage, however, changes with fuel cell temperature and concentration, as well as other variables, as was seen in

the analysis, causing fluctuations in fuel cell output current. Although these fluctuations are usually small, this effect should be taken into account.

In conclusion, it is felt that this analysis presents an adequate mathematical model for predicting fuel cell performance, subject to the limitations imposed upon the study.

Areas of further study are as follows, in order of priority: (1) considering the effects of variable current. This would mean an iterative-type solution in which at any given time, a fuel cell output voltage is assumed for a given resistance input and from this a current is calculated. Using this current as an input to the general analysis, fuel cell temperature and voltage are calculated for this time. The calculated voltage is then compared to the assumed voltage, and if the two are not equal, some new voltage is assumed and the process repeated until the calculated and assumed voltages are within a reasonable tolerance. The computation then proceeds to the next time step and the whole iteration process is repeated. (2) accounting for variations of fuel cell performance with environmental temperature changes; this would include trying to more accurately define the stack heat loss, as it is a function of environment temperature as well as stack temperature; (3) taking into consideration the effects of voltage degradation with time due to the build-up of impurities within

the cells. (4) accounting for variations in fuel cell performance due to changes in condenser exit temperature on the primary side; this would entail an analysis of condenser and secondary loop performance.

The analytical techniques needed to formulate a mathematical model for a complex system such as the fuel cell system may appear at first to be unique and lacking in general applicability; however, there is a common body of knowledge in modeling and simulation which is broadly applicable and of great help to the systems engineer. This thesis is only one application of these general techniques, but the approach taken and the methods used are sufficiently general to allow application to other types of systems.

APPENDIX A

DEVELOPMENT OF EMPIRICAL RELATION FOR FUEL CELL
POWERPLANT OUTPUT VOLTAGE AS A FUNCTION OF CURRENT,
TEMPERATURE AND ELECTROLYTE CONCENTRATION

In order to obtain the necessary relation for the module output voltage, a statistical compilation of test data taken from many powerplants is plotted as shown by the triangular points of Figure A-1. Test data is not readily available for the open circuit condition at temperatures above 440 F or for the current region between open circuit and approximately 15 amp. Hence values in this region can only be estimated. Figure A-1 is for a constant electrolyte concentration of 27 per cent water by weight.

Since the fuel cell normally operates at temperatures between 380 and 440 F and currents between 20 and 55 amp. at voltages between 27 and 31 volts, the data points in the shaded area only were considered for the 5 amp. to 55 amp. current region. From these points it is seen that at any specified temperature, the module output voltage is essentially a linear function of current. The voltage equation would then have the form

$$E = m_1 I + b_1 \quad (A-1)$$

where m_1 is the slope and b_1 the y-intercept

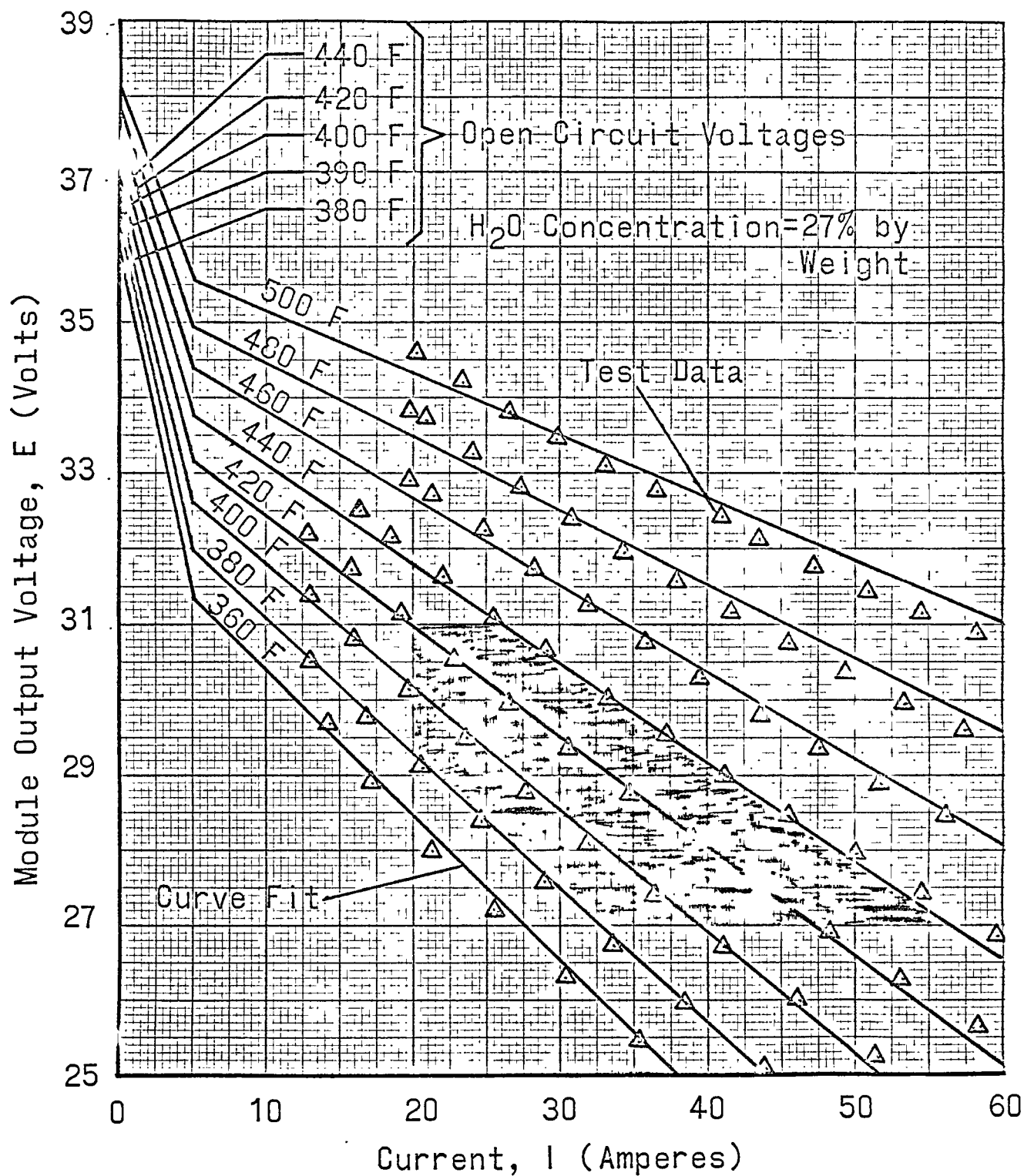


FIGURE A-1
COMPARISON OF POLARIZATION CURVES OF ANALYTICAL
MODEL WITH THOSE OF STATISTICAL TEST DATA

Assuming linearity, the slope and y-intercept are calculated for each constant-temperature line between 380 F and 440 F. A plot of m_1 -versus- T and b_1 -versus- T is shown in Figure A-2. Calculations show that the use of a first-order approximation in the most-frequented operating temperature range (400-440 F) produces only a very small error in the voltage calculation for the region between 380 F and 400 F. This approximation yields relations for the slope and y-intercept as a function of temperature as follows:

$$m_1 = 7.96 \times 10^{-4} T - 0.481 \quad (\text{A-2})$$

$$b_1 = 0.026 T + 23.0 \quad (\text{A-3})$$

Substituting Equations (A-2) and (A-3) into Equation (A-1), the voltage variation with current and temperature at a constant electrolyte concentration of 27 per cent water is

$$E_{27\%, \text{H}_2\text{O}} = (7.96 \times 10^{-4} T - 0.481) I + (0.026 T + 23.0) \quad (\text{A-4})$$

where: $5 \text{ amp.} \leq I \leq 55 \text{ amp.}$

$$380 \text{ F} \leq T \leq 440 \text{ F}$$

From Figure A-1 it is seen that agreement between the test data and Equation (A-4) is quite good within the region considered, and even well outside this region.

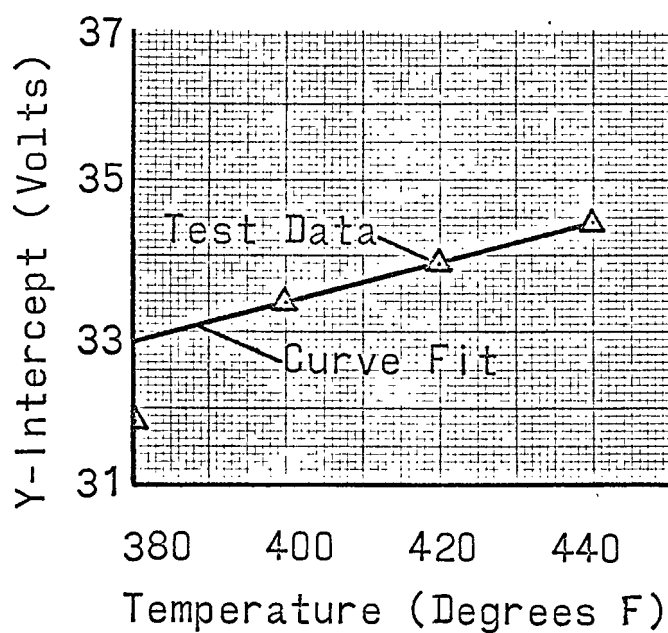
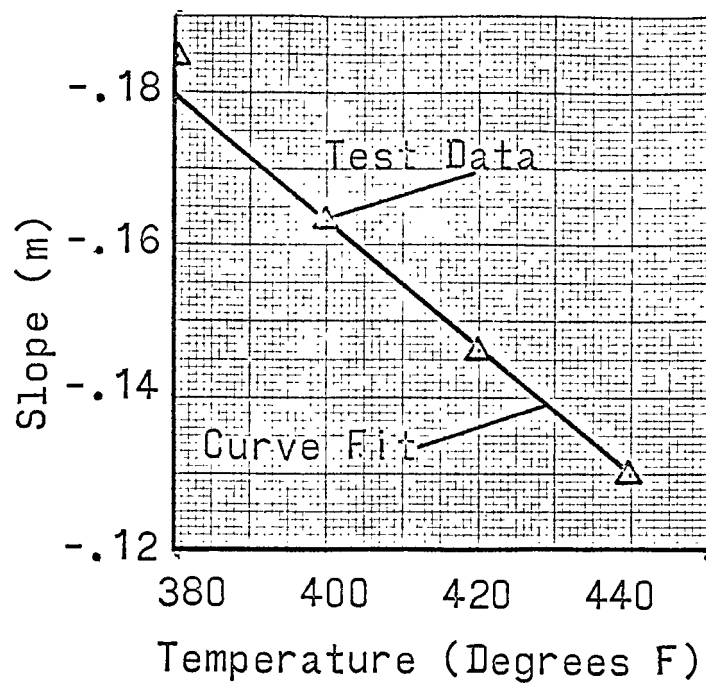


FIGURE A-2
VARIATION OF SLOPE AND Y-INTERCEPT OF CONSTANT-
TEMPERATURE VOLTAGE LINES WITH TEMPERATURE

To account for changes in electrolyte concentration, a correction factor K_c is introduced, where the units of K_c are volts per % change in electrolyte water concentration from the 27% baseline. Then the general voltage equation can be written as

$$E = E_{27\%H_2O} + K_c (\%H_2O - 27.0)$$

Extensive tests conducted on single cells, six-cell stacks and complete modules have shown that K_c is essentially constant over the normal operating electrolyte concentration range of the fuel cell, which is less than $\pm 2\%$ H_2O about the nominal 27% H_2O . The value of K_c from these tests is

$$K_c = -0.2473 \text{ volt}/\Delta\%H_2O \text{ ABOVE } 27\%$$

The general equation for the variation of module output voltage with current, temperature and electrolyte concentration is, then

$$E = (7.96 \times 10^{-4} T - 0.481) I + (0.026 T + 23.0) - 0.2473 (\%H_2O - 27.0) \quad (A-5)$$

$$5 \text{ amp.} \leq I \leq 55 \text{ amp.}$$

$$380 F \leq T \leq 440 F$$

$$22 \leq \%H_2O \leq 32$$

From Equation (A-5) it is seen that an increase in fuel cell operating (stack) temperature will raise the voltage output of the module correspondingly. For the temperature range considered, the term $(7.96 \times 10^{-4}T - 0.481)$ is always negative, and as such a current increase causes a decrease in module output voltage.

The quantity $\%H_2O$ is calculated using the assumption of equilibrium for the partial pressure of the water vapor above the KOH within the stack. Under this assumption, electrolyte concentration is a function of (1) the partial pressure of the water above the KOH and (2) temperature. A plot of a statistical average taken from actual laboratory data for $\%KOH$ as a function of these two variables is shown by the triangles in Figure (A-3). For a nominal 160 F fuel cell condenser exit temperature on the primary side, the partial pressure of the water above the KOH will always be between 4.6 and 7.0 psia. A first-order approximation is again used here, biased to the most-frequented region, and plots of the variations of slope and y-intercept are shown in Figure A-4. Using a straight-line fit for the y-intercept of Figure A-4 and noting that the slope is approximately constant at -1.0 per cent change in KOH per unit change in partial pressure, the relation for electrolyte concentration as a function of partial pressure and temperature is

$$\%KOH = 0.0997T + 38.22 - P_w$$

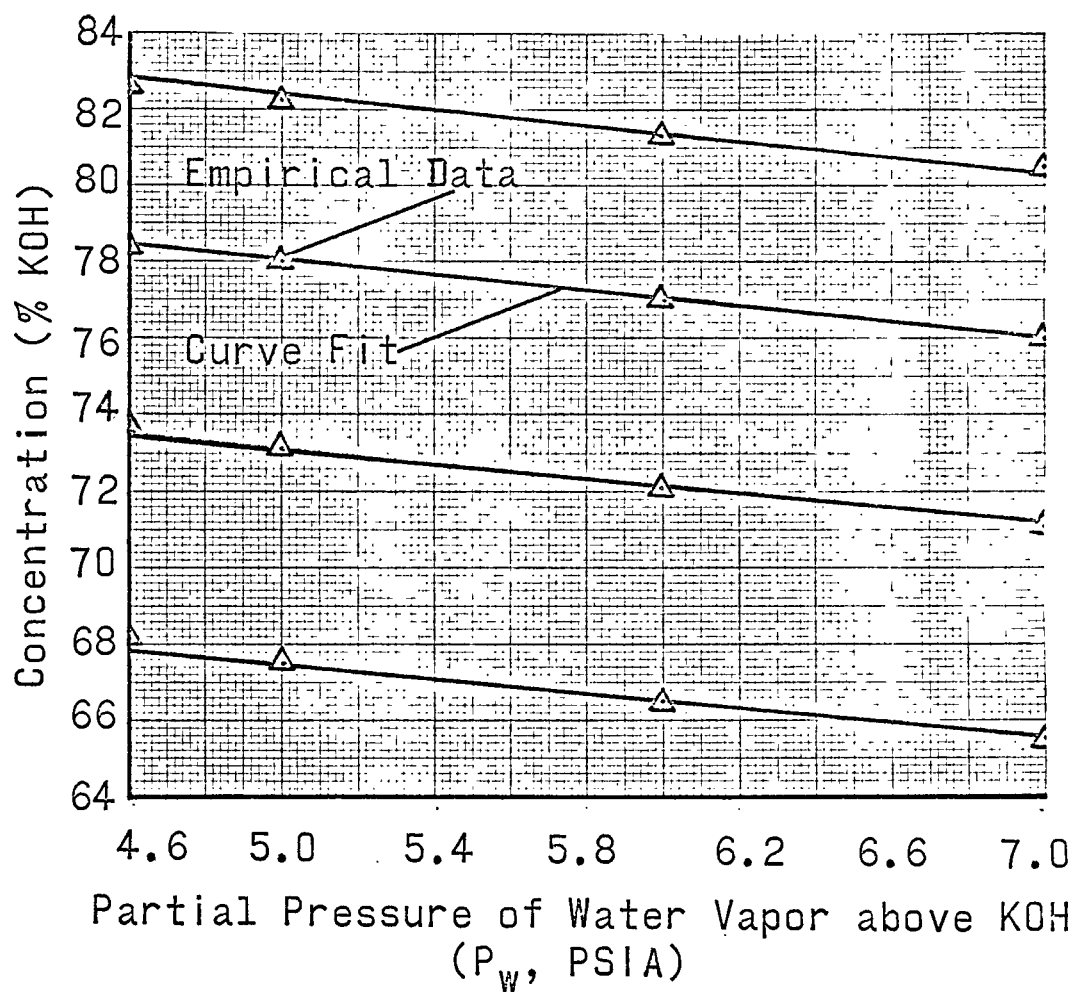


FIGURE A-3
VARIATION OF ELECTROLYTE CONCENTRATION WITH
TEMPERATURE AND PARTIAL PRESSURE

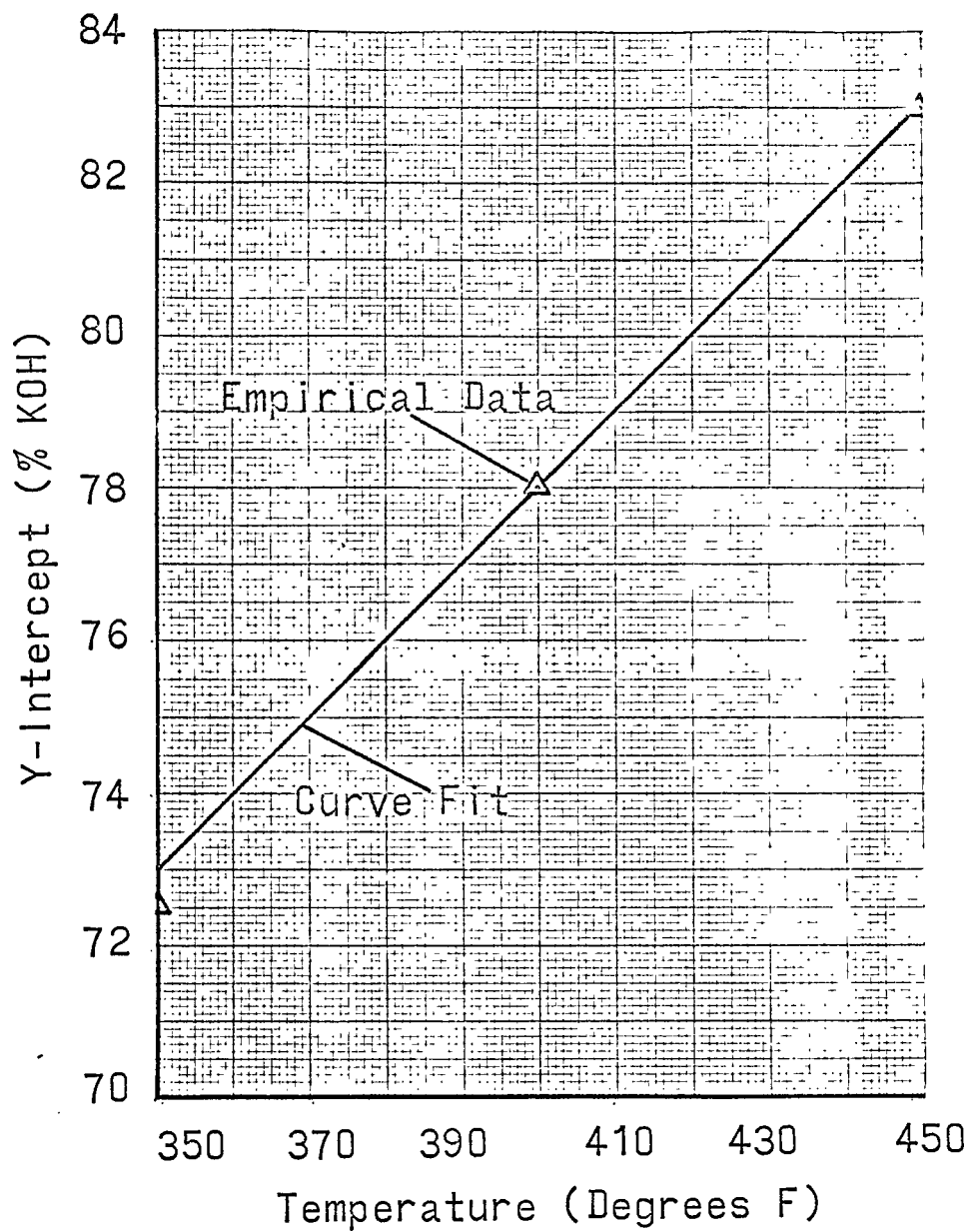


FIGURE A-4
VARIATION OF Y-INTERCEPT OF CONSTANT-
TEMPERATURE CONCENTRATION LINES WITH
TEMPERATURE

from which

$$\% H_2O = 61.78 - 0.0997T + P_w \quad (A-6)$$

$$350F \leq T \leq 500F$$

$$4.6 \text{ psia} \leq P_w \leq 7.0 \text{ psia}$$

Equation (A-6) is used in conjunction with Equation (A-5) in the analysis.

Since very little data could be obtained for this analysis between open circuit and 20 amp., the linear fit of Equation (A-4) is used down to 5 amp. Then, using test data values for open circuit voltage, the same procedure used in the derivation of Equation (A-4) is used for the low-current region (0 to 5 amp.), the result being

$$E = (2.775 \times 10^{-3}T - 1.903) I + (0.0157T + 30.24) - 0.2473(\%H_2O - 27.0) \quad (A-7)$$

where the same correction factor used before for concentration changes is applied. The quantity $\%H_2O$ is calculated from Equation (A-6), the limits of which are sufficient to include operation down to open-circuit conditions. A plot of Equation (A-7) is shown for various temperatures in

Figure (A-1) by the solid lines.

In summary, Equations (A-5) and (A-7) represent the empirical relations used in the analysis for the high-current (5 to 55 amp.) and low-current (0 to 5 amp.) regions, respectively. These two equations should be used with Equation (A-6) for %H₂O. P_w is calculated from Equation (21) of Chapter V.

APPENDIX B

COMPUTER PROGRAM

A digital computer program was written for the simplified analysis of Chapter VI and later expanded for the general analysis presented in Chapter VII. The program for the general analysis is presented in this appendix, along with a list of programming symbols and definitions.

The digital program accepts a current-time profile and for this profile predicts the transient temperature and voltage response of the fuel cell module. The five current/temperature regions of operation for which transient equations were developed in Chapter VII are included in the program.

```

;SEQUENCE,024500
;JOB,3103,WES,10
;EQUIP,5=60
;EQUIP,6=61
;FTN,L,X,*
  PROGRAM MAIN
  REAL I1,I2,IHTR,I,LAMBDA
  THON=385.0
  THOF=387.0
  WRITE(6,1)
  1 FORMAT(55H1TRANSIENT THERMODYNAMIC ANALYSIS OF A FUEL CELL SYSTEM/
  17H SIMON //)
  70 READ(5,9) DT
  READ(5,9) TSTART
  9 FORMAT(F10.0)
  TIME1=0.0
  T1=TSTART
  T=T1
  5 READ(5,10) TIME2,I2
  10 FORMAT(2F10.0)
  IF(TIME2)2000,70,80
  80 WRITE(6,999)
  T0=TIME1
  RT=T0
  2 IF(T.LT.350.) GO TO 24
  TR=(0.681*I2+2261.)/(8.641E-03*I2+13.3)
  GAMA=(2.70+22.976E-03*I2)/3.51
  PW=60.0/(1.0+8.94/GAMA)
  AGAMA=14.399-14.838/(1.0+8.94/GAMA)
  IF(T.LE.420.) GO TO 3
  IHTR=0.0
  17 IF(T.GT.450.) GO TO 4
  COLD=8.841E-03*I2+13.3
  Z=10.431E-03*I2+13.3
  Y1=(-0.0182*Z)/COLD
  Y2=(8.485*Z/COLD)+(0.0182*Z*TR/COLD)
  Y3=(-8.485*Z*TR)/COLD
  Z1=-13.3*Y1
  Z2=13.3*(1.0-Y2)
  Z3=-13.3*(TR+Y3)
  W1=Z1
  IF(I2.LT.5.0) GO TO 34
  W2=Z2+0.18333*I2+27.167E-04*I2**2
  W3=-1.642*I2**2-(133.3-3.413*AGAMA)*I2+165.0+Z3
  28 DISCRM=W2**2-4.0*W1*W3
  IF(DISCRM.LT.0.0) GO TO 20
  TSS=(-W2+SQRT(DISCRM))/(2.0*W1)
  PCH20=61.78-0.0997*TSS+PW
  ESS=(7.96E-04*TSS-0.481)*I2+(0.026*TSS+23.00)-0.2473*(PCH20-27.0)
  IF(I2.GE.5.0) GO TO 35
  Z4=-0.1483*I2-9.471E-03*I2**2
  GO TO 29
  35 Z4=-0.1833*I2-27.17E-04*I2**2
  29 C1=Z1*TSS**2+(Z2-Z4)*TSS
  A=C1

```

B=Z4-Z2

119

C=-Z1

Q=4.0*A*C-B**2

IF(Q)6,7,8

6 G=SQRT(-Q)

X1=(2.0*C*T1+B)/G

14 X2=-TANH((G*(RT-T0))/64.0)

T=-B/(2.0*C)+(G/(2.0*C))*((X1+X2)/(1.0+X1*X2))

PCH20=61.78-0.0997*T+PW

E=(7.96E-04*T-0.481)*I2+(0.026*T+23.00)-0.2473*(PCH20-27.0)

11 IF(T.GT.450.)GO TO 4

IF(T.LE.420.)GO TO 12

BP=2.167*T-910.14

WRITE(6,1000)RT,I2,E,T,BP,PCH20

IF(RT.GE.TIME2)GO TO 60

RT=RT+DT

GO TO 14

34 W2=9.471E-03*I2**2+0.1383*I2+Z2

W3=-6.495*I2**2-(133.3-3.413*AGAMA)*I2+(165.0+Z3)

GO TO 28

4 WRITE(6,2001)

2001 FORMAT(///15X28H STACK TEMP. EXCEEDS 450 F)

GO TO 2000

12 IF(Q.GT.0.) GO TO 13

RT=RT-DT

S=RT

DT1=DT/10.0

RT1=RT+DT1

21 X2=-TANH((G*(RT1-T0))/64.0)

T=-B/(2.0*C)+(G/(2.0*C))*((X1+X2)/(1.0+X1*X2))

RT=RT1

IF(T.GT.419.999) GO TO 22

RT=RT-DT1

DT1=DT1/10.0

RT1=RT+DT1

GO TO 21

22 IF(T.LT.420.001) GO TO 15

RT1=RT1+DT1

GO TO 21

15 PCH20=61.78-0.0997*T+PW

E=(7.96E-04*T-.481)*I2+(0.026*T+23.00)-0.2473*(PCH20-27.0)

T1=T

BP=0.0

WRITE(6,1000)RT1,I2,E,T,BP,PCH20

IF(RT1.GE.TIME2) GO TO 60

RT=S+DT

T1=420.0

T0=RT1

GO TO 3

3 IF(T.LE.THON)GO TO 16

IHTR=0.0

IF(I2.GE.5.0) GO TO 25

TR=(0.681*I2+2261.)/(8.841E-03*I2+13.3)

GAMA=(2.70+22.976E-03*I2)/3.51

PW=60./(1.+8.94/GAMA)

AGAMA=14.962-14.838/(1.+8.94/GAMA)

```

TSS=(6.495*I2**2+(133.3*I2-3.413*AGAMA)*I2+(2.128*TR-165.0))/(9.47
11E-03*I2**2+0.1483*I2+2.128)
PCH20=61.78-0.0997*TSS+PW
ESS=(2.775E-03*TSS-1.903)*I2+(0.0157*TSS+30.24)-0.2473*(PCH20-27.)
A=32.0
B=9.471E-03*I2**2+0.1483*I2+2.128
LAMBDA=B/A
27 T=TSS-(TSS-T1)*EXP(-LAMBDA*(RT-T0))
PCH20=61.78-0.0997*T+PW
E=(2.775E-03*T-1.903)*I2+(0.0157*T+30.24)-0.2473*(PCH20-27.0)
BP=0.0
IF(T.GT.420.) GO TO 32
IF(T.LE.THON) GO TO 33
IF(T.LT.350.) GO TO 24
WRITE(6,1000)RT,I2,E,T,BP,PCH20,IHTR
IF(RT.GE.TIME2) GO TO 60
RT=RT+DT
GO TO 27
25 TR=(0.681*I2+2261.)/(8.841E-03*I2+13.3)
GAMA=(2.70+22.976E-03*I2)/3.51
PW=60.0/(1.0+8.94/GAMA)
AGAMA=14.399-14.838/(1.0+8.94/GAMA)
TSS=(1.642*I2**2+(133.3-3.413*AGAMA)*I2+(2.128*TR-165.))/( 27.17E-
104*I2**2+0.1833*I2+2.128)
PCH20=61.78-0.0997*TSS+PW
ESS=(7.96E-04*TSS-.481)*I2+(0.026*TSS+23.00)-0.2473*(PCH20-27.0)
A=32.0
B=27.17E-04*I2**2+0.1833*I2+2.128
LAMBDA=B/A
18 T=TSS-(TSS-T1)*EXP(-LAMBDA*(RT-T0))
PCH20=61.78-0.0997*T+PW
E=(7.96E-04*T-0.481)*I2+(0.026*T+23.00)-0.2473*(PCH20-27.0)
BP=0.0
IF(T.GT.420.) GO TO 37
IF(T.LE.THON) GO TO 36
WRITE(6,1000)RT,I2,E,T,BP,PCH20,IHTR
IF(RT.GE.TIME2) GO TO 60
RT=RT+DT
GO TO 18
37 TB=420.0
GO TO 19
36 TB=THON
GO TO 19
33 TIME=T0-(1./LAMBDA)*ALOG((TSS-THON)/(TSS-T1))
T=THON
PCH20=61.78-0.0997*T+PW
E=(2.775E-03*T-1.903)*I2+(0.0157*T+30.24)-0.2473*(PCH20-27.0)
BP=0.0
WRITE(6,1000)TIME,I2,E,T,BP,PCH20,IHTR
T1=T
T0=TIME
HTIME=TIME
GO TO 26
32 TIME=T0-(1./LAMBDA)*ALOG((TSS-420.)/(TSS-T1))
T=420.0
PCH20=61.78-0.0997*T+PW

```

```

E=(2.775E-03*T-1.903)*I2+(0.0157*T+30.24)-0.2473*(PCH20-27.0)
BP=0.0
WRITE(6,1000)TIME,I2,E,T,BP,PCH20,IHTR
T1=T
T0=TIME
IF(TIME.GE.TIME2) GO TO 60
GO TO 17
16 IHTR=5.15
I=I2+5.15
TR=(0.681*I+2261.)/(8.841E-03*I+13.3)
GAMA=(2.70+22.976E-03*I)/3.51
PW=60./(1.+8.94/GAMA)
AGAMA=14.399-14.838/(1.+8.94/GAMA)
TSS=(1.642*I**2+(133.3-3.413*AGAMA)*I+(2.128*TR+379.8))/(27.17E-04
1*I**2+0.18333*I+2.128)
PCH20=61.78-0.0997*TSS+PW
ESS=(7.96E-04*TSS-0.481)*I+(0.026*TSS+23.0)-0.2473*(PCH20-27.0)
A=32.0
B=27.17E-04*I**2+0.1833*I+2.128
LAMBDA=B/A
DELHT=RT-TIME
23 T=TSS-(TSS-T1)*EXP(-LAMBDA*(RT-T0))
PCH20=61.78-0.0997*T+PW
E=(7.96E-04*T-0.481)*I+(0.026*T+23.0)-0.2473*(PCH20-27.0)
BP=0.0
IF(T.GT.THOF) GO TO 30
IF(T.LT.350.0) GO TO 24
WRITE(6,1000)RT,I2,E,T,BP,PCH20,IHTR
IF(RT.GE.TIME2) GO TO 31
RT=RT+DT
DELHT=DELHT+DT
GO TO 23
31 WRITE(6,1004) DELHT
GO TO 60
30 TIME=T0-(1.0/LAMBDA)*ALOG((TSS-THOF)/(TSS-T1))
DELHT=DELHT-(RT-TIME)
T=THOF
PCH20=61.78-0.0997*T+PW
E=(7.96E-04*T-0.481)*I+(0.026*T+23.0)-0.2473*(PCH20-27.0)
BP=0.0
WRITE(6,1000)TIME,I2,E,T,BP,PCH20,IHTR
WRITE(6,1004) DELHT
T0=TIME
26 T1=T
IF(TIME.GE.TIME2) GO TO 60
GO TO 3
19 TIME=T0-(1./LAMBDA)*ALOG((TSS-TB)/(TSS-T1))
T=TB
PCH20=61.78-0.0997*T+PW
E=(7.96E-04*T-0.481)*I2+(0.026*T+23.00)-0.2473*(PCH20-27.0)
BP=0.0
WRITE(6,1000)TIME,I2,E,T,BP,PCH20
T1=T
T0=TIME
IF(TIME.GE.TIME2) GO TO 60
IF(T.LE.400.) GO TO 16

```

```

GO TO 17
20 WRITE(6,2003)
2003 FORMAT(///15X31H DISCRIMINANT IS LESS THAN ZERO)
GO TO 2000
7 WRITE(6,2004)
2004 FORMAT(///15X25H DISCRIMINANT EQUALS ZERO)
GO TO 2000
13 X3=ATAN(((2.0*C*420.0)+B)/G)
X4=ATAN(((2.0*C*T1)+B)/G)
TIME=T0+(64.0/G)*(X3-X4)
T=420.0
RT1=TIME
GO TO 15
8 THETA1=ATAN((2.0*C*T1+B)/SQRT(Q))
THETA2=(SQRT(Q)*(RT-T0))/64.0
THETA=THETA1+THETA2
TAN=SIN(THETA)/COS(THETA)
T=(-B)/(2.0*C)+(SQRT(Q)/(2.0*C))*TAN
PCH20=61.78-0.0997*T+PW
E=(7.96E-04*T-0.481)*I2+(0.026*T+23.00)-0.2473*(PCH20-27.0)
G=SQRT(Q)
GO TO 11
24 WRITE(6,2005)
2005 FORMAT(///15X27H STACK TEMP. IS BELOW 350 F)
GO TO 2000
60 PSS=ESS*I2
TIME1=TIME2
I1=I2
T1=T
WRITE(6,1001)TSS
WRITE(6,1002)ESS
WRITE(6,1003)PSS
GO TO 5
999 FORMAT(7X4HTIME7X1HI11X1HE11X1HT8X2HBP5X4HCONC5X4HIHTR/7X3HHRS7X4H
1AMP57X5HVOLTS7X4HDEGF6X5HPRCNT2X7HPRCTH203X4HAMPS)
5000 FORMAT(//4F15.7)
1000 FORMAT(F12.4,2F11.4,F12.4,F8.2,F9.2,F8.2)
1001 FORMAT(//14X20H TEMP STEADY STATE = F13.8)
1002 FORMAT(14X24H VOLTAGE STEADY STATE = F13.8)
1003 FORMAT(14X22H POWER STEADY STATE = F13.8////////)
1004 FORMAT(//14X10HHTR ON FORF9.4,4H HRS)
3000 FORMAT(14F8.3)
2000 CONTINUE
END

```

SCOPE

```

;LOAD
;RUN,10,10000
.1
388.0
1.0      21.
16.0     30.
0.0      0.0
.1
422.7
1.0      30.
5.0      34.5

```

List of Symbols

A	A collection of terms used in the equations for simplification
AGAMA	A collection of terms used in the equation for simplification. AGAMA is a function of GAMA, and is denoted by $\sqrt{\prime}$ in the analysis
B	A collection of terms used in the equations for simplification
BP	Per cent bypass around primary regenerator
C	A collection of terms used in the equations for simplification
Cl	A collection of terms used in the equations for simplification
COLD	$\sum(\dot{m}C_p)$ for H_2 and H_2O vapor at side inlet to primary regenerator (BTU/DEG F)
DELHT	Length of time the in-line heater stays on (hr.)
DISCRM	Discriminant of the polynomial in W_1, W_2, W_3
DT	Time increment for transient temperature and voltage calculations (hr.)
DT1	Dummy variable (time increment) used in calculating the time at which the bypass valve closes (hr.)
E	Module voltage (volts)
ESS	Steady state module voltage (volts)
G	Dummy variable, equal to $\sqrt{q}$ or $\sqrt{-q}$, depending on whether q is positive or negative
GAMA	Specific humidity of hydrogen-water vapor mixture at stack outlet (LB_m water vapor per LB_m dry hydrogen)
HTIME	Time index used to calculate the length of time the in-line heater stays on (hr.)
I	Total fuel cell current (amp.) after a given step load change ($I=I_{\text{step}}+I_{\text{HTR}}$)
I1	Current before step load change (amp.)

I2	Current after step load change (amp.)
IHTR	Current drawn by in-line (low-power) heater (amp.)
LAMBDA	Time ₁ constant for fuel cell transient response (hr. ⁻¹)
PCH2O	%H ₂ O in electrolyte solution
PSS	Steady state power level (watts)
PW	Partial pressure of water vapor at stack outlet (psia)
Q	Negative discriminant of polynomial in A,B,C
RT	Variable time (hr.), used to calculate the transient temperature and voltage values between TIME1 AND TIME2 (hr.)
RT1	Dummy variable (time) used in calculating the time at which the bypass valve closes (hr.)
S	Time index used in calculating the time at which the primary bypass valve closes (hr.)
T	Fuel cell (stack) temperature at any time (F)
T1	Initial fuel cell temperature at each step load change (F)
TAN	A collection of terms used in the equations for simplification
TB	Dummy variable (temperature)
THETA	A collection of terms used in the equations for simplification
THETA1	
THETA2	
THOF	Temperature at which the in-line heater is de-energized (F)
THON	Temperature at which the in-line heater is energized (F)
TIME	Dummy variable used in calculating the time at which the primary bypass valve opens (hr.)

TIME1	Dummy variable used to initialize time at each step load change (hr.)
TIME2	Time at which the load changes from I2 (or I, if in-line heater is on) to some new value of current (hr.). The fuel cell current has the value I2 from TIME1 to TIME2
TO	Initial time of current I2 (or I, if in-line heater is on), in hr.; TO=TIME1
TR	Temperature of hydrogen-water vapor mixture at cold side inlet of primary regenerator (F)
TSS	Steady state fuel cell (stack) temperature (F)
TSTART	Initial temperature of fuel cell stack at time t=0 (F)
W1	A collection of terms used in the equations for simplification; denoted by ϵ_1 , ϵ_2 and ϵ_3 in the analysis
W2	
W3	
X1	A collection of terms used in the equations for simplification
X2	
X3	
X4	
Y1	A collection of terms used in the equations for simplification; denoted by β_1 , β_2 and β_3 in the analysis
Y2	
Y3	
Z	A collection of terms used in the equations for simplification; denoted by α in the analysis
Z1	A collection of terms used in the equations for simplification; denoted by δ_1 , δ_2 , δ_3 and δ_4 in the analysis
Z2	
Z3	
Z4	

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