CELL AND STACK DESIGN ALTERNATIVES

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SECOND QUARTERLY REPORT

November 1, 1978 - January 31, 1979

Contract No. ET-78-C-03-2031

D. Q. Hoover
Program Manager

February 14, 1979

Prepared for:

Department of Energy
20 Massachusetts Avenue NW
Washington, DC 20545

MASTER

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NASA-Lewis Research Center
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TABLE OF CONTENTS

	<u>Page</u>
NOTICE	i
ABSTRACT	ii
TASK 1: STUDY OF SYSTEM DESIGN ALTERNATIVES	1
1.1 Application	1
1.1.1 Load Patterns	1
1.1.2 Utility Interface	6
1.2 Development of Subsystem Models	7
1.2.1 Power Plant Model	7
1.2.2 OS/IES Power Plant Design Point	11
1.2.3 Fuel Conditioner Operation	13
TASK 2: FUEL CELL DESIGN ALTERNATIVES	29
2.1 Fuel Cell Analysis	29
2.2 Cell and Stack Tests	31
TASK 3: METHANE CONDITIONER STUDY	
3.1 Technology Assessment	34
3.2 Mathematical Model	39
4. MANAGEMENT AND DOCUMENTATION	40
4.1 Supervision and Coordination	40
4.2 Documentation and Reporting	41
4.3 Planning	42
APPENDIX A	43
APPENDIX B	62
NOMENCLATURE	74
DISTRIBUTION LIST	78

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ABSTRACT

This report summarizes the second-quarter progress on the four tasks of the Cell and Stack Design Alternatives Contract.

A mass and energy balance was completed for one operating point of a selected power generation sub-system with a power output of 119 kW. Potentially, 87 percent of the LHV of the input fuel is available as bus bar electricity or useful heat.

A 2 kW stack of conventional design and a 0.5 kW DIGAS cooled stack have been constructed and are on test at ERC. Renovation of a space for the Westinghouse stack test facility is underway and procurement of equipment has been initiated. The coupled cell temperature — current density analysis has been modified to include the effects of turbulent coolant flow and extended to permit analysis of up to 10 process plates between cooling plates.

The REFORM computer program was verified by comparison with data received from the government project manager. A method for predicting carbon deposition was developed and compared with data from the literature.

A detailed plan for Phase II was developed. A meeting of the program Advisory Committee and three monthly review meetings were held.

Task 1: STUDY OF SYSTEM DESIGN ALTERNATIVES

1.1 Application

1.1.1 Load Patterns

In calculating the HVAC thermal loads, the apartment building selected for the study is divided into four zones so that the effects of exposure can be included in the solar component. At the request of the government project manager, the individual apartment loads were calculated for several times of interest.

Figure 1 shows the load pattern at 10 AM on a spring day when the net building load is very low (approximately 3650 Btu/hr-heating). This is an average of only 228 Btu/hr per apartment with individual apartments deviating from this value by as much as 2134 BTU/hr heating and 1793 BTU/hr cooling. The average apartment loads in the four zones are +338, +1453, -987 and +109* Btu/hr for the NE, NW, SE and SW zones, respectively. Since the apartment loads are very small during the spring (and fall) transitional seasons, it is anticipated that any attempt to individualize the apartment loads (as contrasted with staying with the zone loads) would not be worth the effort in an annual energy consumption evaluation.

Figure 2 shows the individual apartment loads on a fall transitional day. As in the case of the spring transitional period, the loads (while varying considerably from each other) are small when related to the loads that occur in summer and winter.

Figure 3 shows the individual apartment loads on the summer day which had the highest dry bulb outdoor temperature of the year. At this time, all of the apartments required air conditioning so that no opportunity for energy interchange (via the HVAC system) between apartments exists. At a time such as this, the calculated energy requirements will be the same if zone loads, entire building load or individual apartment loads are used.

Figure 4 shows the individual apartment loads for the winter

* + indicates heating, - indicates cooling

<u>+2362</u> 12	<u>+1223</u> 11	<u>+1223</u> 10	<u>+65</u> 9
<u>+1875</u> 16	<u>-1126</u> 15	<u>-1126</u> 14	<u>-382</u> 13

SECOND FLOOR

All Loads are Btu/hr

<u>+1682</u> 4	<u>+543</u> 3	<u>+543</u> 2	<u>-480</u> 1
<u>+1201</u> 8	<u>-1515</u> 7	<u>-1515</u> 6	<u>-925</u> 5

FIRST FLOOR

Month: April Day: 3 Time: 10:00 a.m.

Figure 1. Individual Apartment Loads — Spring

<u>+1959</u> 12	<u>+914</u> 11	<u>+914</u> 10	<u>-655</u> 9
<u>+1783</u> 16	<u>-1980</u> 15	<u>-1980</u> 14	<u>-1120</u> 13

SECOND FLOOR

All Loads are Btu/hr

<u>+1369</u> 4	<u>+324</u> 3	<u>+324</u> 2	<u>-1131</u> 1
<u>+1153</u> 8	<u>-2187</u> 7	<u>-2187</u> 6	<u>-1596</u> 5

FIRST FLOOR

Month: October Day: 3 Time: 9:00 a.m.

Figure 2. Individual Apartment Loads — Fall

<u>-14,521</u> 12	<u>-11,688</u> 11	<u>-11,688</u> 10	<u>-14,737</u> 9
<u>-16,740</u> 16	<u>-13,267</u> 15	<u>-13,267</u> 14	<u>-16,692</u> 13

SECOND FLOOR

All Loads are Btu/hr

<u>-13,639</u> 4	<u>-10,800</u> 3	<u>-10,800</u> 2	<u>-13,840</u> 1
<u>-15,748</u> 8	<u>-12,270</u> 7	<u>-12,270</u> 6	<u>-15,688</u> 5

FIRST FLOOR

Month: July Day: 2 Time: 12 (noon)

Figure 3. Individual Apartment Loads — Summer

<u>+17,384</u> 12	<u>+12,480</u> 11	<u>+12,480</u> 10	<u>+17,298</u> 9
<u>+17,338</u> 16	<u>+12,405</u> 15	<u>+12,405</u> 14	<u>+17,162</u> 13

SECOND FLOOR

All Loads are Btu/hr

<u>+14,687</u> 4	<u>+9785</u> 3	<u>+9785</u> 2	<u>+14,605</u> 1
<u>+14,644</u> 8	<u>+9715</u> 7	<u>+9715</u> 6	<u>+14,475</u> 5

FIRST FLOOR

Month: December Day: 4 Time: 8:00 a.m.

Figure 4. Individual Apartment Loads — Winter

day having the lowest outdoor dry bulb temperature of the year. As in the case of the summer day, all loads are of the same sign (heating in this case) and the entire building load could validly be used as a load on the OS/IES.

1.1.2 Utility Interface

A number of considerations indicate that an electrical utility intertie for the OS/IES would be desirable. As a prelude to considering the economic effects of such an interface, based upon no energy revenues to the utility, an inquiry was directed to Niagara Mohawk Power Corporation, the utility that services the Albany area. In answer to the inquiry, they indicated that their current filed tariff would allow Niagara Mohawk to provide standby service (with no anticipated energy revenues) in the Albany area with the following options:

Option 1 - Provide 110 kW as dedicated standby--Cost \$860 per month.

Option 2 - Provide 110 kW as standby (if available)--Cost \$110 per month.

Option 3 - Provide 30 kW as dedicated standby, 80 kW as standby (if available)--Cost \$250 per month.

These are rates which are predicated upon very limited applications for such service. That such a rate appears reasonable, consider that a utility agrees to provide such service to only one such customer on a dedicated basis. If we assume that the allocation of capital plant cost for generation, transmission and distribution is 40%, 20% and 40%, respectively, the total capital cost dedicated to provide this service would be 2.5 times the average systems cost of generation. At an average system generation cost of \$250/kW, and a fixed charge rate of 16%, the revenue required to support the dedicated capital would be \$100/kW ($= 2.5 \times \$250/\text{kW} \times 0.16$). For a dedicated service of 110 kW this would amount to \$11,000/year or \$917/month.

This is quite comparable to Niagara Mohawk's published rates.

Niagara Mohawk indicated that widespread application of OS/IES in their service area would necessitate a revision of the published rates. The following reasoning would apply:

If the power plant of the OS/IES has a reasonably high reliability or availability (say 98%), the cost of dedicated standby service would be drastically reduced as the inclusion of such systems on the utility systems increased. This would be so because the probability of simultaneous outages of two OS/IES would be 4×10^{-4} and of three would be 8×10^{-6} . Thus, to a first approximation, the dedicated capital costs in generation and transmission could be divided by the total number of such installations and the dedicated capital costs in distribution would be divided by the number of installations serviced by each distribution subsystem.

It should also be pointed out that the cost of \$110/month for a standby service (when available) would be a reasonably viable alternative to dedicated standby. If it is assumed that the outages of the OS/IES are independent of the utility load, the probability of the OS/IES outage occurring at a time when the utilities load is at or near its peak would be small. Furthermore, the utility's planning would typically provide for a capacity margin of about 20% over its anticipated peak.

1.2 Development of Subsystem Models

1.2.1 Power Plant Model

A complete OS/IES diagram is shown in Figure 5, with an emphasis (at the detailed level) on the fuel conditioning-fuel cell subsystem as a power plant capable of supplying building loads, both electrical and thermal.

The fuel conditioner consists of the reformer, shift converter, steam generator and appropriate heat exchangers and condensers necessary to provide fuel for the fuel cell. The fuel cell subsystem consists

Fig. 5 - OS/IES - power plant schematic

of the fuel cell proper, its associated power conditioner, the heat exchangers necessary to cool the fuel cell and the condenser necessary to remove water for the fuel conditioner water supply.

The reformer consists of a packed catalytic bed counter flow heat exchanger which is fed with a mixture of CH_4 and super heated steam which derives its heat from the reformer effluent via heat exchanger No. 5. The reformer effluent is further cooled in the steam generator (no. 6) which produces saturated steam to be fed into the super heater (mixed with the proper proportions of CH_4). The effluent from the steam generator leaves at a temperature somewhat below 400°F and enters the shift converter. The shift converter consists of several catalytic beds. Direct contact heat exchangers between the beds use finely atomized water to remove the heat released by the reactions in the catalytic beds. The effluent from the first section would be cooled to a temperature comparable to that at which it entered so that the temperature of the reactant entering the second section would be comparable to that entering the first. This process of alternate reactions and cooling would be repeated in subsequent sections. Three reaction sections are shown in the figure but the actual number of sections will be determined by a design trade-off study. In the mathematical model developed for the shift converter, isothermal operation was assumed.

The shift converter effluent enters the fuel cell containing H_2 , CO , CH_4 , CO_2 , and H_2O . Approximately 80% of the H_2 is consumed in the fuel cell, the H_2O being formed passing out of the fuel cell with the depleted cathode air. The spent fuel from the fuel cell anode, as a consequence of the depletion of hydrogen, has a high enough partial pressure of H_2O to make water recovery in the condenser (No. 7) reasonably practical. Approximately $2/3$ of the water will be recovered if the fuel stream is cooled 105°F . The spent fuel then goes to the combustion chamber (No. 4) of the reformer to be burned with whatever additional CH_4 is necessary to provide the thermal energy necessary for

the reformer reaction. To improve the overall system efficiency, the reformer CH_4 feed and the air for combustion are preheated in stack heat exchangers No. 3 and No. 4 respectively. To further improve system efficiency, both the combustion air and the fuel cell make-up air are preheated by passing them over the components of the power conditioning equipment. Since the power conditioning equipment requires forced cooling, this is an effective way to improve system efficiency.

The fuel cell coolant is cooled (in No. 8) to a temperature that will be set by the fuel cell requirements. That portion of the cathode effluent that is not recirculated will then have about 2/3 of its water vapor removed in condenser No. 9. As in the case of the spent fuel condenser, this requires that the stream be cooled to a temperature of about 105°F. The recovered water will be pumped to pressures appropriate for the steam generator and shift converter. Over the complete turn-down range of operation of the OS/IES, there will not be complete matching of fuel conditioner water requirements with the water available from the condensers (e.g., on hot days when the electrical load is high). Condensate storage will be considered as a means of adjusting the match.

Waste heat recovery for the building loads will be obtained from heat exchanger No. 1 in the reformer stack as well as from heat exchanger No. 8 and condensers No. 7 and No. 9. At times, some of the potentially recoverable thermal energy will not be usable or storable (if storage is full). In those cases the excess thermal energy will be "dumped" via an external cooling tower, shown connected into the building load and storage subsystem.

In the system program, provision for the recirculation of stack gas back to the combustion chamber has been made. Recirculation may be necessary to control NO_x emissions and can be used to improve operating efficiency.

1.2.2 OS/IES Power Plant Design Point

A tentative design-point calculation for the power plant of Figure 5 has been made based upon a selection of a design point current of 345 amperes per cell (equivalent to 276 amperes per square foot). The calculated power output at the dc bus is 119 kW. The power conditioner efficiency is 90% so that the power available at the ac bus is 107 kW of which 9.75 kW is assumed to be consumed by power plant auxiliaries and the remainder is available for the building loads and HVAC system. Of the 9.75 kW auxiliary power, a portion is recoverable as thermal energy in the power plant, but no allowance has been made for that in computing the numbers given in Table 1. This point was chosen for illustration purposes and corresponds to a high power density (low efficiency) fuel cell operating point. As a consequence, the H_2 requirements per kilowatt are greater than they would be for a lower current density. The proper balance between fuel cell size, fuel conditioner capacity and fuel consumption is dependent on their relative costs and the load profile of the application. When these costs have been firmed up, a sub-optimization will be made to finalize a design point.

The heat and mass balance for the system of Figure 5 is tabulated in Table 1. The total CH_4 feed to the system is 73.43 lb /hr of which 58.00 lb /hr is fed to the reformer and the remainder is added to the spent fuel to provide the heat required by the endothermic reforming reaction process. This represents a total energy input to the system of 1.580×10^6 Btu/hr based on the lower heating value of CH_4 . The recoverable energy is as follows:

Ht. Exch. No. 1	-	157,040 Btu/hr.
Ht. Exch. No. 8	-	665,710 Btu/hr.
Condenser No. 7	-	34,030 Btu/hr.
Condenser No. 9	-	190,400 Btu/hr.
Delivered Electrical Power	-	332,940 Btu/hr.
		<hr/>
TOTAL		- 1,380,120 Btu/hr.

Table 1

OS/IES POWER PLANT DATA TABLE

(2.8% Excess Air, 15% Recirculation, 345 Amps Per Cell, 756 Cells, 119 kW)

*	$T_{h_i}^{**}$ (°F)	T_{h_o} (°F)	$\dot{m}_h$ (Lb/Hr)	Q (Btu/)	T_{c_i} (°F)	T_{c_o} (°F)	$\dot{m}_c$	$\dot{m}$ (lb/hr) Condensate
(1)	1,005	250	832	157,040	175	195	7,852	
(2)	1,347	1,005	832	77,051	145	736	523	
(3)	1,620	1,347	832	59,912	70	1,330	58	
(4)	3,200	1,620	832	379,679	1,100	1,520	161	
(5)	1,520	1,285	161	29,330	820	1,100	161	
(6)	1,285	400	161	110,704	120	250	103	
(7)	345	100	185	34,026	80	153	466	18
(8)	331	237	25,704	665,712	175	195	33,285	
(9)	237	100	1,512	190,400	80	153	2,608	136

*Numbers in this column refer to components in Figure 5.

** h = hot stream
 c = cooler stream
 i = inlet
 o = outlet

This represents 87.35% of the lower heating value of the fuel. If half of the power consumed by power plant auxiliaries is recoverable, the factor would rise to 88.40%.

1.2.3 Fuel Conditioner Operation

Due to the limited residence times, the effluent gas composition from a chemical reactor generally differs from the equilibrium composition for the actual temperature and pressure. The use of "approach differential temperatures" (ADT) is one method of expressing this difference. In calculating the composition of the effluent gases, the equilibrium constant for each reaction is evaluated at a temperature determined by subtracting the ADT from the actual gas temperature. The appropriate value of the ADTs depend on reactor size relative to flow rate (space velocity) and rates of individual reactions under reactor conditions. Based on engineering judgement (i.e. shift conversion reaction is much faster than reforming) the following ADTs were used for the design point calculation discussed in Section 1.2.2:

Reforming Reaction	100°F
Shift Reaction in Reformer	25°F
Shift Reaction in Shift Converter	25°F

The fuel supplied to the fuel cell was constrained to have 1% CO on a wet basis. The reformer steam to methane ratio is selected to avoid carbon formation at the reactor temperature. The selection is based on available information on commercial reformer operation and is higher than the equilibrium values discussed in Section 3.1 of this report.

Figures 6, 7, 8, and 9 are operating maps for the above differential temperatures showing lines of constant % CO, mole fraction of unreacted CH_4 , moles of H_2O /mole of CH_4 feed required for the shift converter and moles of H_2 delivered per mole of CH_4 feed. On all figures, the reformer operating point of 1520°F and 1.57 $\text{H}_2\text{O}/\text{CH}_4$ corresponds to 1% CO and acceptable avoidance of carbon formations is shown.

Figures 10, 11, 12, and 13 are similar maps with the differential temperatures increased 50% and Figures 14, 15, 16, and 17 correspond to the differentials being doubled over the design-point values. The 1% CO operating point is shown on all maps consistent with avoidance of carbon formation.

Fig. 6 - Carbon Monoxide Map for 100°F Reforming Approach. Differential Temperature

Fig. 7 - Unreformed Methane Map for 100°F Reforming Approach Differential Temperature

Fig. 8 - Shift Converter Water Requirements Map for 100°F Reforming Approach Differential Temperature

Fig. 9 - Product Hydrogen Map for 100°F Reforming Approach Differential Temperature

Fig. 10 - Carbon Monoxide Map for 150°F Reforming Approach Differential Temperature

Fig. 11 - Unreformed Methane Map for 150°F Reforming Approach Differential Temperature

Fig. 12 - Shift Converter Water Requirements Map for 150°F Reforming Approach Differential Temperature

Fig. 13 - Product Hydrogen Map for 150°F Reforming Approach Differential Temperature

Fig. 14 - Carbon Monoxide Map for 200°F Reforming Approach Differential Temperature

Fig. 15 - Unreformed Methane Map for 200°F Reforming Approach Differential Temperature

Fig. 16 - Shift Converter Water Requirements Map for 200°F Reforming Approach Differential Temperature

Fig. 17 - Product Hydrogen Map for 200°F Reforming Approach Differential Temperature

Figure 18 shows the effect of the change in differential temperature on H_2O consumption of the reformer and shift converter. The H_2O requirements appear to be quite insensitive to differential temperature. However, the percent unreformed CH_4 and the moles of H_2 produced per mole of CH_4 feed are sensitive to the differential temperature as shown in Figure 19. Higher differential temperatures represent decreasing conversion effectiveness in the reformer and shift converter and would mean smaller equipment per mole of CH_4 feed.

Fig. 18 — Fuel conditioner water consumption as a function of approach to equilibrium temperature for 1% CO in shift converter output

Fig. 19 — Fuel conditioner performance as a function of approach to equilibrium temperature for 1% CO in shift converter output

Task 2: FUEL CELL DESIGN ALTERNATIVES

2.1 Fuel Cell Analysis

Current Density Distribution Computer Program

The current density distribution model discussed in the First Quarterly Report of this contract was modified to use average compositions of fuel and oxidant for each finite element of the cell. The results given in Figure 20 are based on the same conditions used for Figure 18 in the first quarterly. The major difference occurs near the inlet corner of the cell, where the compositions are changing most rapidly.

The iteration procedures and computer program used to calculate these current densities are described in Appendix B.

Analysis of Cell Temperature Distribution

The coupled heat transfer-current density model was modified to include turbulent friction factors and developing turbulent heat transfer coefficients in the cooling passages. A methodology that permits a group of N plates to be represented as a single layer with N times the thickness, heat generation, process channels, etc. was developed to permit analysis of a larger number of cells between cooling plates. Results for $N = 2$ were compared to results for $N = 1$ (old analysis) to verify the methodology. With 4 and 6 regular cells per cooling plate, the cell temperature uniformity agreed to within 1°C for the two methods. It is concluded that this approach is adequate for analyzing larger numbers of cells per cooling plate.

The new method (with $N = 2$) was then used to calculate the effect of larger numbers of cells on maximum to minimum temperature difference. The calculated values were 13.5 , 17.2 , 22.4 and 30.2°C for 4, 6, 8 and 10 cells per cooling plate respectively. In making this comparison, the cooling channels were designed to maintain 17 per cent of air flow through cathode channels in all cases with total air

Fig. 20—Distribution of current density (i) in 12" $\times$ 17" cell at 350°F

flow specified to give a 55°C air temperature rise. The analysis was based on the 12" x 17" cells with average current densities of 200 ASF. These cells will be operated at lower current densities for much of their life (part load) and the temperature uniformity will be better due to the reduced heat flows.

2.2 Cell and Stack Tests

Westinghouse Stack Test Facility

A laboratory space for testing the 2 to 10 kW fuel cells was selected and is being renovated. As indicated in Figure 21, the fuel cells will be located in walk-in canopy hoods (12 x 6 ft. floor area). The hoods in this space have an independent exhaust system. The room is presently supplied with H₂ and N₂ from the laboratory central system. Gas cylinders will be used to supply the CO and CO₂ for testing the 2 kW cells. Plans are underway to obtain a new hydrogen line for this laboratory from the central storage site so there will be no interference with other hydrogen users. As our needs increase for CO and CO₂, a new storage facility for these gases will be provided outside of the building.

Orders have been placed for the following long lead-time equipment:

- 1.) Model 209 Hagan Oxygen Monitor
- 2.) Georator model 30-002 frequency converter (500 VA output) 60-400 Hz.
- 3.) Two Rotron Propimax 3 Fans. (400 Hz, 21,900 rpm)
- 4.) 3 Brooks Hi-Accuracy Rotameters
- 5.) 3 Brooks ELF Gas Flow Controllers
- 6.) Chromalox process Air Heater with Electronic Proportional Power Controller

An air recirculation loop has been completely designed and shop drawings for fabricating the ductwork are being prepared. Additional quotes for the electronic three component gas blending system have been solicited and working meetings with potential suppliers have been scheduled.

Dwg. 7687A60

Fig. 21 — Westinghouse laboratory facility for testing of phosphoric acid fuel cells

Measurement of Local Current Densities

The fuel cell analysis indicates that even for isothermal cells, the current densities vary considerably over the cell area due to the change in reactant compositions as they proceed through the cell (Figure 20). Since the heat generation rate is nearly proportional to current density at a given point and the local cell life and performance are in turn dependent on the local temperature; the credibility of the current density calculation methodology is a critical component in the credibility of the fuel cell analysis and it should be experimentally verified. Due to the difficulty of directly measuring local current densities an indirect method based on the following discussion was developed.

During the first quarter of this program it was postulated that if a current collector in contact with a stack of cells be cut into two or more pieces (insulated from each other) and these pieces be held at the same potential; the current associated with each piece will be that generated by that portion of the cell directly beneath it. This follows directly from Ohm's law - no current will flow between conductors at the same potential. Separation of the current collector into a large number of discrete sections will permit localized characterizations as well as validation of the computer model. The initial step in this work has been carried on under subcontract with ERC and is reported in Appendix A. In this work, the current collectors of a 3 cell stack were cut into two separate insulated sections. Each section was brought to the same voltage by inserting suitable resistances in each circuit and the current measured using appropriate ammeters. Using a combination of experimental and calculated values, the same theoretical voltage was calculated for each half of the cell (See Appendix A). The preliminary tests agree qualitatively with the calculated results (Figure 20) but the test results were confounded by cell temperature variations due to heat losses and to poor distribution of air flow to the cell. A 2 cell stack with a split guard heater and improved air flow manifold is being constructed and will be tested soon. Fabrication of the first 2kW stack has been completed and it is currently being tested. A 20 cell DIGAS cooled stack is also on test.

TASK 3: METHANE CONDITIONER STUDY

3.1 Technology Assessment

Fuel Processor Capital Costs

Capital cost information for nine methane reformer systems was plotted to obtain an indication of the costs of fuel processor sub-systems for the PAFC On-Site Integrated Energy System. Included were data from six commercial plants, reported in Hydrocarbon Processing Magazine,⁽¹⁾ quotations from the files of project personnel, and information presented in an A. D. Little study⁽²⁾ for naphtha reforming. The quotations from Girdler and DeMarkus and the 6 plants reported in Hydrocarbon Processing included methane reforming, carbon monoxide shift conversion and removal of carbon dioxide. The plant in the A. D. Little study was based on naphtha, did not consider carbon dioxide removal, and was thermally integrated into an overall fuel cell system. Figure 22 indicates that the cost of a thermally integrated naphtha fuel processor without CO₂ removal is very nearly the same as that for a non-integrated methane fuel processor with CO₂ removal.

The A. D. Little study included an estimate of the cost of the 100th fuel processing subsystem in addition to the prototype unit and this point is included in Figure 22. Learning curves are commonly used in estimating the cost of volume production of identical items. The slope of the learning curve (s) is defined as the ratio of the cost of the 2N unit to the cost of the N unit. For an arbitrary ratio of production (K/N) then the ratio of the cost of the K unit to that of the N unit is:

$$C_K = C_N S^{\frac{\log K/N}{\log 2}}$$

for the first and the hundredth units of the A. D. Little Study, the costs were $\$1.8 \times 10^6$ and $\$0.9 \times 10^6$ respectively. Solving for S gives:

$$S = \left(\frac{.9}{1.8}\right)^{\frac{\log 2}{\log 100}} \\ = .9$$

(1) Hydrocarbon Processing, September 1967 and December 1967.

(2) EPRI EM-695, "Assessment of Fuels for Power Generation by Electric Utility Fuel Cells," Prepared by Arthur D. Little, Inc., March 1978.

Fig. 22 — Capital costs of fuel processors for H_2 via reforming

Assuming that the same learning slope applies to the PAFC for the OS/IES and that the economy of scale indicated in Figure 22 applies to mass-produced fuel processor subsystems, the cost for the 10,000 and 100,000 fuel processor subsystems for a 120 kW fuel cell would be 295 and 207 dollars per kW respectively.

Review of Engelhard Methane Reforming Data

A comparison has been made of methane reforming data developed by Engelhard Minerals and Chemicals Corporation with that calculated by the Westinghouse REFORM computer program. A graph, labeled Figure 2 — Methane Reforming, was provided by the government project manager as part of a larger package. These data were apparently calculated from equilibrium considerations of the following equations:

Data were compared at 1200, 1400 and 1600°F. Results are as follows:

<u>Temp-°F</u>	<u>H₂O/C</u>	<u>Mole Percent H₂ (Water Free)</u>	
		<u>Westinghouse</u>	<u>Engelhard</u>
1200	2	73.1	73.1
1400		76.0	76.0
1600		76.0	76.1
1200	3	76.0	75.9
1400		77.0	77.0
1600		76.7	76.8
1200	4	77.3	77.3
1400		77.6	77.5
1600		77.2	77.3
1200	5	78.0	78.0
1400		78.0	77.9
1600		77.6	77.6

The greatest variation between the two sets of data is ± 0.1 percent H₂ (water free). Such a variation is well within the accuracy of the thermodynamic data from which the compositions are derived.

Carbon Formation During Reforming

A possibility exists that during reforming elemental carbon may form and deposit on the catalyst bed. Primary control is by proper selection of a suitable steam/methane ratio. Several analytical methods were used to establish the minimum steam/methane ratios required at various temperatures and pressures, in order to avoid potential carbon formation.

The reference method used to establish minimum steam/methane ratios was that outlined by Hougen and Watson⁽³⁾. This method assumes that equilibrium is attained and that the steam/methane ratio is sufficiently high that carbon is not present at equilibrium.

Equilibrium compositions for a number of steam/methane ratios were calculated, using the REFORM computer program. The resultant compositions served to establish the required activity ratios for the following reactions,

These activity ratios are $(A_{\text{H}_2})^2/(A_{\text{CH}_4})$ and $(A_{\text{CO}})(A_{\text{H}_2})/(A_{\text{H}_2\text{O}})$, respectively. The minimum steam /methane ratio to prevent carbon formation occurs where the activity ratio is equal to the respective equilibrium constant, as follows:

$$(A_{\text{H}_2})^2/(A_{\text{CH}_4}) = K_1$$

$$(A_{\text{CO}})(A_{\text{H}_2})/(A_{\text{H}_2\text{O}}) = K_2$$

The calculated minimum steam/methane ratios are summarized in Table 3.1. Results were found to be consistent for the two carbon formation reactions and there appears to be little or no effect of pressure, up to 2 atmospheres.

(3) Hougen, O.A. and K. Watson, Chemical Process Principles Part Two- Thermodynamics, John Wiley & Sons, Inc., New York, 1947, pp. 731-732

Table 3.1

MINIMUM STEAM-METHANE RATIO FOR ABSENCE OF CARBON

Temp, °F	Pressure, Atm	Minimum Steam-Methane Ratio		Avg Minimum Steam-Methane Ratio
		$K_1 = \frac{A_{H_2}^2}{A_{CH_4}}$	$K_2 = \frac{A_{CO}A_{H_2}}{A_{H_2O}}$	
1200	1	1.30	1.30	1.30
1400	1	1.07	1.05	1.06
1600	1	0.95	0.98	0.96
1800	1	0.93	0.95	0.94
1200	2	1.30	1.28	1.29
1400	2	1.07	1.07	1.07

A second method was used for comparison with the method outlined by Hougan and Watson. This method utilizes data obtained by General Electric.⁽⁴⁾⁽⁵⁾ The General Electric information presents equilibrium data for the CHO system, using triangular coordinate graphs. Curves are plotted at constant temperature, with each graph at a fixed pressure. Various ratios of steam/methane are located on the line connecting CH_4 and H_2O . The point where this line crosses a particular constant temperature curve defines the equilibrium points and the minimum steam/methane ratio at that temperature. Ratios above the equilibrium curve indicate carbon formation. The General Electric data indicate minimum steam/methane ratios that are essentially the same as developed by using the Hougen and Watson method.

3.2 Mathematical Model

Work was completed on the development of a preliminary mathematical model which describes the functional performance of the fuel processor and the basic equations were reported in the last quarterly report.⁽⁶⁾

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- (4) Cairns, E.J. and A.D. Tevebaugh, "CHO Gas Phase Compositions in Equilibrium with Carbon and Carbon Deposition," J. Chem. and Eng. Data, 9, No. 3, pp.453-462, July 1964.
 - (5) Tevebaugh, A.D. and E.J. Cairns, "Carbon Deposition Boundaries in the CHO System at Several Pressures", J. Chem. and Eng. Data, 10, No. 4, pp.359-362, Oct. 1965.
 - (6) "Cell and Stack Design Alternatives, First Quarterly Report," August 1, 1978-October 31, 1978, January 1979.

4. MANAGEMENT AND DOCUMENTATION

4.1 Supervision and Coordination

The first meeting of the program Advisory Committee was held at the Westinghouse R&D Center on December 5. All members of the committee, named in the proposal, were present. Prepared discussions were presented by the task leaders and these were all followed by interactive discussions with the committee members. Several recommendations made by the Advisory Committee members have been implemented.

Approval of the ERC subcontract was received from DOE and the subcontract was executed on December 6.

A more suitable location for the Westinghouse fuel cell test laboratory was identified during this quarter. The facilities modifications are underway and are being coordinated by Mr. Pollack. Mr. Makiel has defined the needed instrumentation and initiated procurement.

Mr. S. Abens was appointed as the ERC project manager replacing Dr. H. C. Maru.

At the request of Mr. King, the detailed planning and scheduling of the Phase I fuel cell tests was started in January by Dr. Köthmann and Mr. Abens. The plans and schedule should be complete by February 19.

As a result of a suggestion by Mr. King, a purchase order was placed with Burt Hill Kosar Rittleman Associates for four days of consulting time (\$1,000). This is a firm of architects which has previously worked with Westinghouse and is very actively involved in R&D and application of energy conservation techniques. They will review our system study, particularly the building design, to assure that it is realistic in terms of the anticipated time frame.

Dr. Kirschbaum calculated the heating and cooling loads for individual apartments to answer a questions about the effects of slab and roof losses raised by Mr. Simons of NASA.

Information on the future price and availability of natural gas and electricity has been collected from various sources for use in the system study.

4.2 Documentation and Reporting

Monthly review meetings were held on November 15, December 14 and January 17 at the Westinghouse R&D Center. Mssrs. King, Pickrell and Simons of NASA were present at all meetings as were the Westinghouse and ERC task leaders for Phase I tasks. The meetings provide a valuable forum for exchange of information and discussion among the participants.

At the December meeting, Mr. Putkovich of the Power Electronics Laboratory discussed some of the projects that his group had successfully completed. The discussion was followed by a tour of the laboratories to view on-going projects. At the January meeting, the group inspected the space selected for the fuel cell test facility.

Six patent disclosures were included with and discussed in the pre-patent clearance copies of the first quarterly report according to the agreed upon procedure for advising the government project manager of patent disclosures resulting from contract work. The modifications required for patent clearance of the first quarterly report were received early in January. The document was modified and copies of the report were sent to those people on the list provided by DOE.

Mr. King has supplied the information on procedures for requesting waivers of the government's patent rights. This was an action item resulting from the January review meeting.

The monthly Milestone Plan and Management Reports, Contract Management Summary Reports and Cost Management Reports were prepared and delivered as required by the contract. The Technical Status Reports were submitted for patent clearance following the procedure developed in the first quarter. Patent clearance for the November

report has been received and it will be mailed to the people on the distribution list provided by DOE.

4.3 Planning

A detailed plan for Phase II was submitted to the government project manager early in November. The plan was discussed during the November meeting and several points clarified. Mr. Pickrell pointed out that our Aerospace Electrical Division has worked on power conditioning equipment for solar and fuel cell applications and suggested that we make use of their expertise. As a result, Don Shireman of AED attended the December monthly meeting and AED has agreed to participate in the Phase II power conditioning task.

APPENDIX A

ENERGY RESEARCH CORPORATION

PROGRAM TO DEVELOP AND TEST FUEL CELL
DRIVEN TOTAL ENERGY SYSTEMS

Subcontract 34-JP-76802-A
(DOE Contract No. ET-78-C-03-2031)

TECHNICAL PROGRESS REPORT NO. 6

Second Quarterly Report for
November, 1978 to January, 1979

SUMMARY

During the second quarter of the project, work was in progress at ERC on Task 2.2, Design of Corroborating Experiments and Task 2.3, Fuel Cell Design and Fabrication. Distribution of current in a subscale stack was determined at various air flow rates to verify results predicted by the analytical model. A 0.5 kW stack was constructed and tested to study plate manufacturing and stack assembly methods for DIGAS cooling. A 2 kW stack utilizing 5 x 15 in. cell components was constructed and is currently undergoing initial performance testing.

TASK 2.2 CORROBORATING EXPERIMENTS

The primary objectives of this task are:

- to verify and compare the results predicted by the analytical model with the experimental results obtained from an operating stack.
- to generate additional information needed in the design of phosphoric acid fuel cell stack for OS/IES.

2.2.1 Current Density Distribution

In support of the Westinghouse effort in the analytical cell model development, ERC has fabricated 2 short stacks

(5 in. x 15 in. cells) with divided current collectors. This arrangement allows independent measurement of current across the leading and trailing halves of the cell in the air flow direction.

Optimum cell performance can be expected to occur under operating conditions leading to relatively uniform current distribution across the cell. The major factors affecting current density at any location in the cell are reactant gas concentration and temperature profiles across the cell. The effect of these variables has been studied analytically⁽¹⁾, and the present effort was designed as a corroborative experiment for support of the modeling effort. Study of the density distribution in an operating cell will also provide useful information for the design of DIGAS cooling systems, including design of the cooling plate itself, manifolding, and possibly cell channels.

2.2.1.A 3-Cell Stack for Current Density Study

As described in the First Quarterly Report, ERC fabricated a 3-cell stack for preliminary study of current density distribution in an operating stack. In this stack, the flow of current was divided into two equal zones with respect to the active area of the cells, i.e., upper and lower zones⁽²⁾, which is adequate to determine the effect of oxygen depletion expected in a DIGAS-cooled stack (at ~ 2 stoichiometric air/oxygen flow rate). Theory⁽³⁾ (based on electrochemical reactions) predicts that there is a significant variation in current density due to reactant depletion in a cell. This was

(1) First Quarterly Report, Figure 18, p. 52.

(2) A schematic of one side of the stack is shown in Figure 2 in the ERC section of the First Quarterly Report. Fresh air enters the upper zone, and the partially reacted air leaving the upper zone enters the lower zone.

(3) A theoretical example of current density distribution under an isothermal condition was presented in Figure 18 in the First Quarterly Report. Also refer to the Appendix for a theoretical explanation.

experimentally verified for 2.2 times stoichiometric air flow rate (see Table 1).

TABLE 1

CURRENT DENSITY DATA (Run #1)

	<u>Upper Zone</u>	<u>Lower Zone</u>
Exp. Voltage, mV/cell	520	516
Exp. Current, Amp.	18.3	13.7
Avg. Temp., °F	337	330
Calculated Voltage ⁽⁴⁾ , mV/cell	694	694

As shown above, the upper zone generated significantly higher current (18.3 A) than the lower zone (13.7 A) as expected. This result can be attributed to reactant depletion in a cell. Detailed discussion of the theoretical calculations is presented in the Appendix.

Figures 1 and 2 describe a general trend of experimental data showing the effect of air flow rate on current density generation in the two separate zones (Run #2).

As shown, as the air flow rate decreases below 2 stoichs, the effect of oxygen concentration becomes pronounced. As a result, the upper zone where fresh air is supplied produces a much higher current than the lower zone where current generation becomes limited by reactant supply. The data on this uneven current generation is plotted in Figure 2, and the stack volts at these points in Figure 3. The sharp change in slope (Figure 1) shows a transition point where the performance of the bottom zone becomes very sensitive to the oxygen concentration/supply rate.

(4) For 100% catalyst utilization.

Run #2

Temperature: 350°F

Fuel: H₂, 1.3 x stoichiometric

FIGURE 1 EFFECT OF AIR FLOW RATE ON CURRENT GENERATION
IN TWO ZONES - UPPER AND LOWER

FIGURE 2 EFFECT OF AIR FLOW RATE ON CURRENT GENERATION

FIGURE 3 STACK POTENTIAL VS. AIR FLOW RATE
(FOR FIGURES 1 AND 2)

2.2.1.B 2-Cell Stack for Current Density Study

Since the rate of heat generation is a function of current density, temperature variations were encountered in the 3-cell stack. In order to minimize these variations, a 2-cell stack with modified endplate heaters has been fabricated (Figure 4).

This stack is similar to the first stack but improvements have been made so that the temperatures of the upper zone and lower zone of the stack can be controlled independently, employing separate heater blankets. As can be seen in Figure 5, Teflon has been incorporated into the aluminum side plates of the stack to provide thermal insulation between the heater blankets and the metallic plates. In addition, a modified manifold design was used to insure more uniform air flow distribution to the cells as well as a more uniform air inlet temperature.

The 2-cell stack is currently being filled with electrolyte. The stack will be operated first with the air flow introduced as in the previous manner (shown in Figure 6) to establish a base-line performance for comparison. Then the effect of the new manifold orientation on current density and the stack temperature profile will be studied. The test stand for this 2-cell stack is shown in Figure 7. The test panel of the 3-cell stack was modified to accommodate the separate temperature control on the upper and lower zones.

2.2.2 20-Cell DIGAS Stack

A DIGAS-cooled, 5 inch x 15 inch, 20-cell stack (Figure 8) has been fabricated for the following important objectives:

- ③ To verify design calculations (channel geometries, flow distribution, temperature distribution, etc.)
- ③ To check manifold and seal designs
- ③ To develop assembly procedures for DIGAS-cooled stacks

FIGURE 4 2-CELL (5 in. x 15 in.) STACK WITH SPLIT CURRENT COLLECTORS

P0057

FIGURE 5 SCHEMATIC OF STACK FOR CURRENT DENSITY STUDY

FIGURE 6 SCHEMATIC OF NEW MANIFOLD DESIGN

FIGURE 7 2-CELL TEST STAND

FIGURE 8 20-CELL (5 in. x 15 in.) DIGAS STACK

(cell and cooling plate assembly, electrolyte introduction, stack construction, etc.)

The information and experience gained with this stack will be applied to the design of future DIGAS-cooled stacks.

Design of the 20-cell stack, including four DIGAS cooling plates and the assembly of the stack with standard cell components, has been completed. The cooling plates consist of two molded half-plates cemented together as shown in Figure 9. To minimize labor and material costs, each half of the cooling plate has been designed to serve a dual purpose. One face of each half was molded to provide the reactant flow area for an adjacent cell. On the other face, grooves for the cooling plate channels are machined.

A test stand and manifolding for this stack have also been designed for operation on compressed air. The necessary instruments and flowmeters have been received, calibrated, and installed and construction of the test stand has been completed.

Special manifolds for the stack have been designed and fitted to the stack. Both the air and fuel manifolds have been designed to insure an even flow distribution of reactants to all cells and, correspondingly, a more uniform reactant inlet temperature.

TASK 2.3 FUEL CELL DESIGN AND FABRICATION

The first 80-cell (5 in. x 15 in.) 2 kW stack (Figure 10) has been assembled with strain gauges installed on the tie rods and is being filled with electrolyte. The stack will be pretested before delivery to Westinghouse.

FIGURE 9
DIGAS COOLING PLATES

in inches

FIGURE 10 30-CELL (5 in. x 15 in.) 2kW STACK

P0061

NOMENCLATURE

- α = transfer coefficient, assumed to be 0.5
- CL = catalyst loading
- CU = catalyst utilization, fraction
- E = Nernst potential (reversible open circuit E.M.F.)
- E° = standard E.M.F. of the cell, volts
- F = Faradays Constant, 96500 coulombs/mole - equivalent
- i = current density, A/cm²
- i_o = exchange current density, A/cm²
- K = (SA) (CL) (CU)
- n = number of electrons transferred per mole of hydrogen,
n = 2
- r = cell resistance, ohm-cm²
- R = gas constant, 8.314 joules/(mole - °K)
- SA = catalyst surface area
- T = temperature, °K
- V = cell voltage, volts
- Y_{H_2} = mole fraction of hydrogen at anode
- Y_{H_2O} = mole fraction of water vapor at cathode
- Y_{O_2} = mole fraction of oxygen at cathode

APPENDIX

Since the two (upper and lower) zones of the 3-cell stack were operated at the same potential (to provide equipotential⁽⁵⁾ surfaces), theoretical voltage calculations were made as a simple means to check the experimental results. Verification of the equipotential condition (with the observed experimental values) rather than calculating the current densities, was preferred in consideration of the fact that the cell voltage V can be expressed as an explicit function of reactants, product, and current density, while the calculation of the current density involves a trial and error procedure. An expression for the cell voltage V can be obtained from

$$V = E^{\circ}(T) + \frac{RT}{nF} \ln \frac{Y_{H_2} Y_{O_2}^{1/2}}{Y_{H_2O}} - \frac{RT}{\alpha nF} \ln \frac{i}{Ki_o} - ri \quad (1)$$

for negligible diffusion polarization and atmospheric operation. Equation 1 then provides two equations, i.e., one for the upper and one for the lower zone, which were evaluated with the following expressions⁽⁶⁾:

$$E^{\circ}(T) = 1.2605 - 0.00025T \quad (2)$$

$$r = r_o \exp. \left[3650 \left(\frac{1}{T} - \frac{1}{450} \right) \right] \quad (3)$$

Y_{H_2} , Y_{O_2} , Y_{H_2O} , are geometric averages in each zone.

$$i_o = 0.2327 Y_{O_2} Y_{H_2O}^{0.4377} \exp. (-6652/T) \quad (4)$$

$$K = (SA) (CL) (CU)$$

$$SA = 500 \text{ cm}^2/\text{mg}$$

$$CL = 0.6 \text{ mg}/\text{cm}^2$$

$$CU = 1.00 \text{ (i.e., 100\% catalyst utilization)}$$

$$r_o = 0.44 \text{ ohm-cm}^2$$

(5) This was checked with a high accuracy digital voltmeter. The difference in the two zones was less than 1% (upper 520 mV/cell; lower 516 mV/cell).

(6) Presented in the First Quarterly Report.

ENERGY RESEARCH CORPORATION

For example, the experimental data and data calculated from experimental conditions for the upper zone for the 2.2 stoich air flow rate can be substituted into Equations 1, 2, 3, and 4.

The results were as follows:

	<u>Upper Zone</u>	<u>Lower Zone</u>
T	442 °K (337°F)	438 °K (330°F)
E°, V	1.150	1.151
Y _{H₂}	0.943	0.956
Y _{O₂}	0.173	0.121
Y _{H₂O}	0.0393	0.1475
i, A/cm ²	0.107	0.0737
i _o , A/cm ²	2.89 (10 ⁻⁹)	3.10 (10 ⁻⁹)
r, Ω-cm ²	0.506	0.546
Eqn. 1	<u>0.694 V</u>	<u>0.694 V</u>

The same potential, i.e., equipotential conditions in the two zones, is found.

APPENDIX B

Current Density Distribution Calculation Procedures

A finite element method for calculating the current density distribution in a cell of a DIGAS stack has been developed. The procedure divides a large fuel cell into elements that are small enough that variations in fuel and oxidant compositions and temperature are negligible. The following is a description of the methods used in calculating the boundary conditions for each element and iterating until a solution is found that satisfies the input specifications (e.g. average current density, fuel utilization, reactant flow rates). The nomenclature used in the program is defined in a table at the end of this appendix and a flow chart of the program is given in the three parts of Figure B1.

Inlet Flow Specifications

The input variables of the subroutine FLOW (X, LAMDA, V1, DTKFLO and W) are specified in the input of the main program. As shown in the flow chart, this subroutine calculates S and the mole fractions Y2O2 and Y2H2O using the relationships derived in Reference 1 for a DIGAS stack. From the definition of S, the oxygen utilization ETAO2 is equal to the reciprocal of S. These and the total current for the plate are sufficient to determine the total flow rate and component flow rates for the oxidant.

The total current IAMPS is determined from the current density, IDNSO, and the dimensions for the active plate area, XLENTN and YLENTN, which are input variables. The product of IDNSO, XLENTN and YLENTN in appropriate units yields the current IAMPS in amperes.

The total oxidant flow rate and component oxidant flow rates are determined with Z=2 from the following equations:

1) First Quarterly Report of this Contract, January 1979

Fig. B1 - Flow chart of the calculation procedure (part 1)

Fig. B1—Flow chart of the calculation procedure (part 2)

Subroutines:

Flow (X, LAMDA, V1, DTKFLO, W,
F, S, Y2O2, Y2H2O)

MOLFRA (I, J, N1UH2', N1UCO2,
N1UH2O, N1UCO, N2UO2,
N2UH2O, N2UN2, YHY,
YOX, YWA, YCO1)

VI* (MVB or MID, VGUESS, IDNSO,
TKAVG, SRO, SA, CU, CL, CLA,
YBH2, YBO2, YBH2O, YBCO,
DVCO, D)

* MVB = 1 Yields Voltage

* MID = 2 Yields Current Density

Fig. B1—Flowchart of the calculation procedure (part 3)

$$N2O2 = IAMPS / (2 * Z * FCONST * ETAO2) \quad (1)$$

$$Y2N2 = 1 - Y2O2 - Y2H2O \quad (2)$$

$$N2TOT = N2O2 / Y2O2 \quad (3)$$

$$N2N2 = N2TOT * Y2N2 \quad (4)$$

$$N2H2O = N2TOT * Y2H2O \quad (5)$$

Other variables which are specified in the input of the program are Y1CO2, Y1H2O and Y1CO which represent the mole fractions of carbon monoxide, water and carbon monoxide, respectively, in the inlet fuel. The final variable which is specified in the input of the program is the hydrogen utilization, ETAH2.

With the total current IAMPS, there is sufficient information available to determine the total flow rate and component flow rates for the fuel. These rates are determined with $Z = 2$ from the following equations:

$$N1H2 = IAMPS / (Z * FCONST * ETAH2) \quad (6)$$

$$N1TOT = N1H2 / Y1H2 \quad (7)$$

$$N1CO2 = N1TOT * Y1CO2 \quad (8)$$

$$N1H2O = N1TOT * Y1H2O \quad (9)$$

$$N1CO = N1TOT * Y1CO \quad (10)$$

Finite Element Definition

The total cell current may be attributed to a plate with a flow of fuel on one side and a flow of oxidant on the other. These flows may be oriented with respect to a coordinate system fixed in the plate as depicted in Figure B2. A total flow rate of fuel N1TOT may be considered to flow across the top surface of the plate, originating along edge 1 and representing flow in grooves perpendicular to edge 1. Similarly, a total flow rate of oxidant N2TOT may be considered to flow across the bottom surface of the plate, originating along edge 2 and representing flow in grooves perpendicular to edge 1. The fuel is considered to flow in the X-direction and the oxidant is considered to flow in the Y-direction. The integers NX and NY are used to specify

Fig. B2 —Coordinates for bipolar plate current distribution study

the number of elements used for the X and Y lengths of the cell respectively. The lengths of the X- and Y-divisions are designated DELX and DELY, respectively. A block is identified by a set of indices (I,J). Since the area of a single block is equal to $\Delta X \cdot \Delta Y$, the active area of the cell is equal to $\Delta X \cdot \Delta Y \cdot N_X \cdot N_Y$.

The flow entering a particular block along one of its edges is considered as a unit of the total flow entering a row of blocks along a common line (i.e. the sum of the unit flows $N1UTOT(1,1)$, $N1UTOT(1,2)$, ... $N1UTOT(1,N_Y)$ equals the total flow, $N1TOT$, and the sum of the unit flows $N2UTOT(1,1)$, $N2UTOT(2,1)$, ... $N2UTOT(N_X,1)$ equals the total flow $N2TOT$). Figure B3 depicts the unit flows for various representative blocks along edges 1 and 2 of the plate and also a generalization of the inlet flows to a block referred to as Block (I,J). The latter shows that any block with indexes I,J will have the inlet flows $N1UTOT(I,J)$ and $N2UTOT(I,J)$.

Any unit flow may also be expressed as the sum of its component flows as illustrated in Figure B4 for Block (I,J). The unit flow $N1UTOT(I,J)$ is composed of $N1UH2(I,J)$, $N1UCO2(I,J)$, $N1UH2O(I,J)$, and $N1UCO(I,J)$. The unit flow $N2UTOT(I,J)$ is composed of $N2UO2(I,J)$, $N2UH2O(I,J)$, and $N2UN2(I,J)$. The figure also illustrates the total and component exit unit flows for Block (I,J).

For each element the average of the inlet and exit mole fractions are employed in the Nernst equation when the subroutine VI is called. It should be clear from the use of the various suffixes in the previous paragraph what component mole fraction is represented when a particular suffix is appended to a letter Y to form a Y-symbol relating to Block (I,J). The symbol (I,J) is applicable whether or not it is visibly present.

Boundary Conditions

The inlet flows must be specified for any block that lies along a leading edge of the plate (i.e., along edge 1 or 2). These flows are found by apportioning the flow $N1H2$, $N1CO2$, $N1H2O$ and $N1CO$ to the

Fig.B3 --Total inlet flow rates for various blocks of plate

* Total Inlet Flow Rate for Next Block

Fig. B4 -- Total and component flow rates for Block(I, J) (General case)

blocks along edge 1 and by apportioning the flows N_{2O2} , N_{2N2} and N_{2H2O} to the blocks along edge 2. The block inlet component flows along edge 1 are then found to be $N_{1UH2}(1,J)$, $N_{1UCO2}(1,J)$, $N_{1UH2O}(1,J)$ and $N_{1UCO}(1,J)$ for all J from $J = 1$ to NY . Also, the block inlet component flows along edge 2 are then found to be $N_{2UO2}(I,1)$, $N_{2UH2O}(I,1)$ and $N_{2UN2}(I,1)$ for all I from $I = 1$ to NX . Collectively, all the inlet unit flows represent initial conditions for a mathematical marching problem on a two-dimensional field with Block (I,J) as the general field element.

The program has been provided with a means of introducing to the inlet flows a variation with position along a leading edge. This was accomplished by assigning apportioning multipliers to the inlet unit component flows $N_{1UH2}(1,J)$, ... $N_{1UCO}(1,J)$ and $N_{2UO2}(I,1)$, ... $N_{2UN2}(I,1)$. These multipliers are designated $FRN1(J)$ and $FRN2(I)$, along edge 1 and 2 respectively.

Description of Method

The overall method for determining the distribution of current density over the plate is to specify first a desired average current density $\bar{i}$ for the whole plate and to determine then the corresponding voltage V for the plate. This voltage will be determined such that it produces unique local current densities over the plate whose average value approximates $\bar{i}$ within a specified tolerance. The method is tractable if the inlet flows and the cell temperature distribution are specified and a starting value of V is selected.

The local or block current density is determined first for Block $(1,1)$, then for Block $(1,2)$ until Block $(1,NY)$. Thereafter, it is determined first for Block $(2,1)$, and so on, until Block (NX, NY) .

A brief description of the calculations of local current density will now be presented, with Block $(1,1)$ used as an example. Since the inlet flows are known from specifications, the inlet mole fractions $Y_{1H2}(1,1)$, $Y_{1CO}(1,1)$, $Y_{2O2}(1,1)$ and $Y_{2H2O}(1,1)$ may be determined. The molar conversion equations derived from Faraday's law are

now used to determine the exit flows of those components that are electrochemically affected. For an initial guess of current density ($IDFRST = \bar{i}$) the exit flow of hydrogen from Block (1,1) is

$$N1XH2(1,1) = N1UH2(1,1) - (IDFRST * DELX * DELY) / (2.0 * FCONST) \quad (11)$$

which in turn yields by definition

$$N1UH2(2,1) = N1XH2(1,1) \quad (11a)$$

The exit flow of oxygen from Block (1,1) is similarly

$$N2XO2(1,1) = N2UO2(1,1) - (IDFRST * DELX * DELY) / (4.0 * FCONST) \quad (12)$$

which in turn yields by definition

$$N2UO2(1,2) = N2XO2(1,1) \quad (12a)$$

and the exit flow of water from Block (1,1) in the oxidant stream is

$$N2XH2O(1,1) = N2UH2O(1,1) + (IDFRST * DELX * DELY) / (2.0 * FCONST) \quad (13)$$

which in turn yields by definition

$$N2UH2O(1,2) = N2XH2O(1,1) \quad (13a)$$

The flows that are not affected by the electrochemical process do not change across the block and the following relations exit:

$$N1UCO2(2,1) = N1UCO2(1,1) \quad (14)$$

$$N1UH2O(2,1) = N1UH2O(1,1) \quad (15)$$

$$N1UCO(2,1) = N1UCO(1,1) \quad (16)$$

$$N2UN2(1,2) = N2UN2(1,1) \quad (17)$$

All inlet components are now available for the two adjacent blocks (i.e., Block (1,2) and Block (2,1)) based on the initial value of current density and the march could continue. However, more accurate values are determined iteratively from upgraded values of the current density for the block using the subroutine VI. The mole fractions at the exit sides of Block (1,1) are determined from the exit flows and the average mole fractions for the block are calculated.

Using this average composition, subroutine VI calculates a current density which is compared with the previous value. If agreement is not obtained within a specified tolerance, the exit flows for Block (1,1) are recalculated and the procedure is repeated until agreement between these successively calculated current densities is obtained. The procedure for other blocks will be the same as for Block (1,1).

All the various steps discussed in the above presentation of the analysis were used to create the computer program. These steps are summarized together with other unstated but obvious steps in the flow chart of the computer program presented in Figure B1. The loop MZ should be particularly noted because it represents the calculation of the average current density for all blocks.

Results

A distribution of current density over a bipolar plate whose active dimensions are 12 inch x 17 inch and whose temperature is 350°F has been determined from the computer program. This distribution is presented in Figure 2.1 of this report as a field plot of lines of constant current density. The compositions of the fuel and oxidant streams, the fuel and oxidant utilization, and the cell resistance are shown in the figure. The specified average current density for the plate is 0.150 A/cm^2 and the resulting cell voltage is 0.533 volt. It will be noted that the current density is a maximum in the corner of the plate common to the two inlet streams and a minimum in the opposite corner. The variation of current density over the plate can be seen to be substantial for typical operating values.

NOMENCLATURE

<u>Universal Symbol</u>	<u>Computer Symbol</u>	<u>Definition of Symbol</u>
	ALFA1(J)	Arbitrary number assigned to Block (1,J) such that $ALFA1(J) / \sum_{J=1, NY} ALFA1(J) = FRN1(J)$
	CU*	Catalyst utilization
	CL*	Catalyst loading (gm/cm ²)
	CLA*	Anode catalyst loading (gm/cm ²)
	D*	Exponent for partial pressure of oxygen in expression for exchange current IO*
ΔX	DELX	Length of X-division (inch)
ΔY	DELY	Length of Y-division (inch)
	DTKFLO [†]	Mixed mean temperature rise (°K)
	DVCO*	Cell voltage drop for 1 percent carbon monoxide and 0.8 hydrogen utilization (ETAH2 = 0.8)
η_H	ETAH2	Hydrogen utilization
η_O	ETAO2	Oxygen utilization
	F	Ratio of recirculation flow to exhaust flow
$\mathcal{F}$	FCNST	Faraday constant (96,520 coulomb per gram mole equivalent)

	FRNI(J)	Fraction of NITOT entering leading edge 1 of plate at inlet side of Block (1,J)
ΔH		Enthalpy change for chemical reaction. $2H_2 + O_2 \rightarrow 2H_2O$, at 450°K (watt-sec/gm mole)
	IATPS	Total current of cell (A)
$\bar{i}$	IDNSO	Specified average current density of plate (A/cm^2)
	IDNSAV	Average current density of plate (A/cm^2)
i	IDNS(I,J)	Current density of Block (I,J) (A/cm^2)
	IDFRST	Current density of Block (I,J) in single block iteration loop NZ (A/cm^2)
	IDLAST	Update of IDFRST in single block iteration loop NZ (A/cm^2)
λ	LAMDA [†]	Fraction of combined makeup flow and recirculation flow entering process channels
	LZ	Number of iterations required to achieve an initial voltage estimate compatible with inlet conditions for convergence defined by tolerance TOLLZ
	MZ	Number of iterations relative to all blocks of plate needed to achieve convergence of IDNSAV vs. IDNSO defined by tolerance TOLMZ
	NZ	Number of iterations relative to one block needed to achieve convergence of IDFRST vs. IDLAST defined by tolerance TOLNZ.
	NX	Number of X-divisions of plate
	NY	Number of Y-divisions of plate

	Flow rate (mole/sec)
NITOT	Total fuel flow at leading edge 1 of plate (mole/sec)
N2TOT	Total oxidant flow at leading edge 2 of plate (mole/sec)
N1H2	Hydrogen portion of flow N1TOT (mole/sec)
N2O2	Oxygen portion of flow N2TOT (mole/sec)
N1UH2(I,J)	Hydrogen portion of flow N1H2 crossing DELY at inlet side of Block (I,J) (mole/sec)
N1XH2(I,J)	Hydrogen portion of flow N1H2 crossing DELY at exit side of Block (I,J) (mole/sec)
S ⁺	Ratio of moles of oxygen entering process channels to moles of oxygen consumed (S=1/ETA02)
SA*	Catalyst surface area (cm ² /gm)
r	SRO* Cell resistance at 450°K (ohm-cm ²)
TK	Cell temperature (°K)
V	Voltage drop per plate (volt)
V1	Initial guess for V
VGUESS	Variable used for updating V
W ⁺	Ratio of moles of water per mole of dry air in makeup flow
X ⁺	Ratio of moles of oxygen in makeup flow to moles of oxygen consumed
XLENTH	Active length of plate in fuel flow direction (inch)
YLENTH	Active length of plate in oxidant flow direction (inch)
Y	Mole fraction
Y1H2	Mole fraction of hydrogen in inlet fuel flow

Y2O2	Mole fraction of oxygen in inlet process flow
Y2H2O	Mole fraction of water in inlet process flow
YH2(I,J)	Mole fraction of hydrogen at inlet side of Block (I,J)
YXH2(I,J)	Mole fraction of hydrogen at exit side of Block (I,J)
Z	Number of Faraday equivalents transferred

* Used in subroutine VI

† Used in subroutine FLOW

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