CELL AND STACK DESIGN ALTERNATIVES

FOURTH QUARTERLY REPORT

May 1, 1979 - July 29, 1979

Contract No. DE-AC03-78ET11300

D. Q. Hoover
Program Manager
August 1979

MASTER

Prepared for:

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TASK 1: STUDY OF SYSTEM DESIGN ALTERNATIVES

1.1 Electric Utility Load Sharing

For a preliminary evaluation of system operation, a model of the system was developed* using the power plant characteristics shown in NASA RFP No. 3-853309Q (dated Nov. 28, 1978) entitled "Study of Component Technologies for Fuel Cell On-Site, Integrated Energy Systems." The division of input energy is shown in Figure 1 as a function of percent electrical load on the power plant. This was transcribed to show the energy content in various streams (low temperature -165°F, high temperature 15-30 psig steam and unrecovered heat) as a function of electrical load. The resulting plot is shown in Figure 2.

The system to which this power plant was coupled consisted of three apartment buildings with the load profiles based upon an abbreviated 48 day year as described in the First Quarterly Report.

The principal purpose of the study was to evaluate hybrid operation with appreciable amounts of electrical energy being supplied by a connected utility. One goal was to reduce gas consumption of the OS/IES to a level comparable to that of a conventional system. Table I lists the major pertinent characteristics of the system.

The system was operated with a total of 10 different strategies with regard to load sharing with the electric utility. The first four studied were "uniform" strategies in which the fuel cell output was controlled to provide some fixed percentage of the electrical load over the entire year, except that the fuel cell was shut off if the electrical demand fell below 17.5%. Under maximum load conditions, it was limited to 110% of its rating. There were 7 other strategies employed in which the percent of the load generated locally was varied month by month. These seven strategies are listed in Table II.

*The development and operation of this code was accomplished using (W) funds. The results are, however, pertinent to this project.

Curve 715537-A

Fig. 1 — Fuel cell power plant patterned after figure B-1
RFP-3-853309Q

Fig. 2 — Fuel cell power plant patterned after figure B-1
RFP 3-853309Q

TABLE I

SIMPLIFIED SYSTEM STUDIED

- 1) Three Apartment Buildings
- 2) Abbreviated Load Profile (48 days)
- 3) Individual heat Pumps in each Apartment
(Rated at 18,000 Btu/hr)
- 4) Water Storage (25,000 gal) operable between 150°F and 200°F
- 5) Gas Cooking
- 6) Fuel Cell Plant Profile per NASA R.F.P.
- 7) 160°F available heat not stored
- 8) 15-30 psig Steam heat storable
- 9) If reject heat or storage cannot supply DHW, then DHW supplied
with I^2R
- 10) Priority for Building Thermal load Requirements:
Reject Heat, Storage, Heat Pump, (HP + I^2R .)
- 11) Fuel Cell capable of 10% overload and not operable below
17-18% rating
- 12) Fuel Cell System Auxiliaries take 7% of Fuel Cell output.

TABLE II
Non-Uniform Loading Strategies

FUEL CELL GENERATION PROFILES

Month	1	2	3	4	5	6	7
Jan	50%	70%	70%	100%	90%	90%	100%
Feb	50	70	70	100	90	90	70
Mar	50	70	70	100	90	90	50
Apr	50	70	70	75	70	60	40
May	50	70	70	45	55	40	30
June	30	0*	40	30	55	40	0*
July	30	0*	40	25	55	40	0*
Aug	30	0*	40	25	55	40	0*
Sept	30	0*	40	30	55	40	0*
Oct	50	70	70	60	70	60	30
Nov	50	70	70	90	90	90	70
Dec	50	70	70	100	90	90	100

*DHW Supplied with gas

The monthly gas and electrical consumption (from the utilities) was ratioed up to the actual days in each month from the abbreviated four day month and summed over the year. For each case the ratio of purchased energy with and without the OS/IES was computed and these ratios are plotted in Figure 3 for the "uniform" strategies. Also plotted on this figure are the annual savings in purchased energy based on 5¢/kWhr and \$3.00/MCF of gas. In addition the required size (or rating) of the fuel cell systems are plotted. From these curves one can deduce that for a "uniform" strategy which requires 46% of the system demand to be met by the fuel cell system, there would be no change (relative to a conventional system) in gas consumption and a reduction of 30% in consumption of electrical energy. The fuel cell size required for this strategy would be about 68 kW and the annual cost of purchased energy would be \$7800 less than for the conventional system. This would represent an annual energy savings of about \$115 per kW. As an upper limit, an apartment owner might be willing to capitalize this savings by a multiple of 10 to decide its value. It would require an installed cost below \$1150/kW to meet this criterion. The cost savings capitalized at both 10 and 6 times the annual energy savings for the "uniform" strategies are shown in Figure 4. It is believed that this range represents the range of practical interest to investors.

The "nonuniform" strategies tabulated in Table II were selected in an attempt to coincide with the monthly variations in thermal load. These are plotted as individual points on Figures 3 and 4 (keyed by number to Table II). No curves are drawn through these points since they do not represent variations (one to the others) that are amenable to functional representation. They are plotted so as to be directly comparable to the uniform strategies.

One conclusion of this preliminary study is that properly chosen strategies (for this type of HVAC system) offer advantages over "uniform" strategies. For example, strategy No. 6 for the same amount of purchased gas as the "uniform" strategy reduces bought electrical energy from about 48% of conventional to 40.5% of conventional.

Fig. 3 - Effect of generation profiles on operating results

Fig. 4 — Effect of generation profiles on capitalized cost savings

Utility Ownership Scenario

Using the data from strategy No. 7, an interesting analysis can be made based upon electric utility ownership of the OS/IES power plant. Table III shows certain significant results from strategy No. 7 (plotted in Figure 5) which was intended to result in no change in gas consumption. Also shown in Figure 6 (for this strategy) is a profile of both conventional demand and demand on the electric utility with the OS/IES power plant in place on the "worst" winter day of the study.

Also shown in Figure 6, for comparison, is a typical utility total demand curve for the peak load day in December (for a winter peaking utility). As can be seen, the peak load on the utility occurs in the 6-7 pm time period. It is this period of peak demand that defines their generation and transmission requirements, and the concomitant capital required to provide that capability. Thus with strategy No. 7, the 6-7 pm December peak kilowatt demand, with and without the OS/IES system is of importance with regard to how much load alleviation is available to the utility at the time of their peak demand. Table III shows, for this example, a 71.0 kW reduction in demand on the utility.

The ability of scheduling the OS/IES power plant in such a way as to provide peak-load reduction to the utility suggests that utility ownership of the OS/IES power plant could be of interest to electric utilities.

Figure 7 illustrates another benefit to the electric utility as a result of strategy No. 7. The maximum electrical energy purchased by the apartment complex occurs in July. Using this as 100%, the monthly purchased energies are plotted through the year. Also plotted for comparison is the monthly energy generated by a typical northeastern winter peaking utility. Although the match is not perfect across the year, it is clear that there is a strong tendency for the apartment complex purchased energy to fill in the "valley" of the utility system generated energy. Thus with significant penetration of OS/IES systems, the annual load factor of the utility would be improved.

TABLE III – COMPARISON OF OS/IES WITH CONVENTIONAL SYSTEM

System	Annual Gas MCF	Annual kW hrs	6-7 PM December Peak kW
Conventional*	3552	513,275	77.3
Fuel Cell OS/IES	3550	359,050	6.3
Difference	—	154,225	71.0

• Gas Used For: Heating, DHW & Cooking
 Electricity Used For: Lights, Appliances and
 Air Conditioning

Curve 718079-A

Fig. 5— Load division profile - OS/IES vs. elec. utility

Curve 718080-A

Fig. 6 — Mid winter day of peak system load

Curve 718081-A

Fig. 7 — Monthly energy purchased from electric utility

Figure 8 shows a block diagram for the interfacing of a utility owned and operated OS/IES power plant with an apartment complex. The power plant would consist of the fuel conditioning equipment, the fuel cells, the power conditioning equipment and all piping, heat exchangers, auxiliaries, controls, etc., that are necessary to provide for efficient operation and interfacing of the power plant with the loads (electrical and thermal). This power plant would be owned and operated by the electric utility with a flat charge to the apartment owner to provide revenues sufficient to recover all charges required for capital and operation and maintenance. These charges should properly take into account reduction in charges elsewhere in the system by virtue of the alleviation of peak load. These would in effect be represented as a "credit" tied to the 71 kW reduction in peak load.

The apartment complex and OS/IES power plant would be connected to both a gas utility and the electric utility that owns the power plant through appropriate meters. The owner of the apartment complex would pay the appropriate utilities in accordance with the readings of both meters. Thus his total cost would be for the energy consumed (gas and electric) plus the "charge" for the OS/IES power plant.

For the example of strategy No. 7, the annual net energy cost savings to the apartment owner would be \$7720 based upon 5¢/kWhr and \$3.00/MCF. In order to test the validity or desirability of electric utility ownership of the power plant, the \$7720 must provide more than the Minimum Revenue Requirement (MRR) of the project as analyzed by the electric utility. Table IV expresses this MRR in terms of the Fixed

Table IV

Minimum Revenue Requirements

$$\begin{aligned} \text{MRR} &= [\text{Capital Cost of OS/IES}] \times [\overline{\text{FCR}} + \text{O.M.}]_1 \\ &\quad - [\text{Capital Cost of Credits}] \times [\overline{\text{FCR}} + \text{O.M.}]_2 \end{aligned}$$

Note: Subscript 1 Refers to $\overline{\text{FCR}} + \text{O.M.}$ of OS/IES
 Subscript 2 Refers to $\overline{\text{FCR}} + \text{O.M.}$ of Balance
 of Utility System

Operating Philosophy:

- Keep Reject Heat to Environment to Minimum
- Alleviate Utility Winter Peak Load to Greatest Extent Possible
- Make Total Gas Consumption from Gas Main Comparable to that for a Conventional System

Fig. 8 – System configuration

Charge Rate (FCR) and Operation and Maintenance costs (OM) as applied to the capital cost of the OS/IES power plant, less corresponding credits that result from the reduction in peak load.

These credits are real only for a system that is expanding, in that, penetration of OS/IES systems into the utility load will effect future generation, transmission and distribution needs. For a completely static utility (one that is exhibiting no growth), there would be no credits available because the existing equipment represents imbedded capital that cannot be realistically reduced. Assuming growth in load, the credits can be expressed in terms of the kilowatts necessary at the load point. Assuming that the credit of one kW of load is at the peak load condition for the utility, the installed generation required to supply this load would probably consist of combustion turbines. One kW at the load point would require 1.1 kW at the point of generation (allowing a 10% loss in transmission and distribution). In addition for each kW of required generation there should be 0.2 kW of reserve margin installed. Thus the total required generation to provide one kW at the point of load would be 1.32 kW. Using an average figure of \$250/kW for the installed cost of combustion turbines, this results in a credit of \$330/kW referred to a kW of load.

The credits for transmission can be highly variable depending upon the utility being impacted. An analysis was made for a typical north-eastern utility using historic data such as the ratio of kW miles of transmission added to the system per kW of added generation, the mix of various voltage classes of transmission added and the cost per kW mile of each voltage class. Using such data, an estimate of \$125/kW referred to the power demand at the point of load was arrived at. As pointed out, this credit would be extremely utility sensitivity. The electric utility industry has traditionally had relative capital expenditures as shown in Table V below:

Table V
Relative E.U. Expenditures*

Generation	62.5%
Transmission	11.3%
Distribution	21.4%
Miscellaneous	<u>4.8%</u>
TOTAL	100.0%

The \$125/kW for transmission credit as compared to \$330/kW for generation is not out of line with this table since the 62.5% of capital expenditures assigned to generation covers all forms of generation (nuclear, coal, oil, hydro, etc.) of which combustion turbines are the least expensive.

The credits for distribution savings are very elusive, requiring an in-depth study of a given locale and probably being most sensitive to penetration of the OS/IES system. An unpublished Westinghouse study on small distributed generation plants in an urban area indicated that (in 1979 dollars) there were potential credits of \$50 to \$55 per kW available in the subtransmission system (69 kV and below) which is considered part of distribution. Based on this value a total distribution credit of \$100/kW was selected for this analysis. This is conservative in the light of the data in Table V. The values of credits used in this analysis are shown in Table VI.

Table VI
Credits for Generation
Transmission & Distribution

Generation - \$330/kW (at Load Site)
Transmission - \$125/kW (at Load Site)
Distribution - \$100/kW (at Load Site)

*Twenty-Sixth Annual Electrical World Forecast (Sept. 15, 1975).

The Operation and Maintenance costs (O&M) can be expressed as a % of initial capital costs based upon experience with normal types of E.U. equipment. Over the broad spectrum of equipment (generation, transmission and distribution) an (O&M) factor of 1.5% of first cost is reasonable. However for the OS/IES power plant, major parts of the system contain catalysts which will not have a life of 30 years. For the purposes of this analysis, it will be assumed that those portions of the system that contain catalysts will have to be "changed-out" every five years. If we let γ equal an assumed annual inflation rate applied to the cost of the replacement modules and i equal the discount rate, the levelized cost of replacement in constant dollars would be,

$$C = ICC \left[\frac{(1+\gamma)^n \cdot 1}{(1+i)^n - 1} \right]$$

where ICC is initial capital cost; n is the number of years between replacements.

For n equal to 5 years, $\gamma = 0.07$ and $i = 0.11$, the ratio of C to ICC is 0.225. This means that the cost of replacing the module (assuming no salvage value) at the end of 5 years would be 22.5% of initial cost annually. If we assume a 10% salvage value, the levelized charge becomes 20% per year. Assuming 25% of the plant cost represents components or modules that must be changed-out every five years and the remaining 75% of the plant can be maintained at 1.5% of initial capital cost annually, the total annual maintenance cost would be 6.1% of initial capital cost. These O&M costs are summarized in Table VII. Later in this analysis, a sensitivity to the % of plant subject to a 5 year replacement schedule is discussed. This sensitivity can also be viewed as an O&M charge sensitivity.

Table VII
Operation & Maintenance Costs
 (% of Capital Costs)

OS/IES Power Plant*	6.1%/yr
Normal Utility System Equipment	1.5%/yr

*Assumes 25% of Capital Cost Items Replaced
 on 5 Year Schedule

In addition to the cost of operation and maintenance, the electric utility (EU) would expect to obtain revenues from the apartment owner to cover the costs associated with the EU ownership of the power plant. Figure 9 pictorially shows how the revenue streams from the apartment owner to the EU would be allocated. The first item would be the dividend or return to the stockholders at a "fair rate of return" on their equity as set by the Regulatory Commission. The second item of expected revenues would cover the cost of operation and maintenance (as discussed above). Since in this scenario, the apartment owner is paying for the metered gas and kilowatt hours, these do not appear in the EU operating costs. The next two items cover the cost of borrowed capital, namely the interest on the debt and the retirement of the debt. The next item is administrative expenses (including insurance). The next two items are state and local taxes and Federal income tax. Usually, in making an economic analysis, the taxes, administrative expenses, debt service (including debt retirement) and return on equity are lumped together in a Fixed Charge Rate (FCR) which represents the levelized value (over the project life) of all of these charges as a percent of the initial capital cost.

In Table VIII are listed the pertinent factors that go into the computation of the FCR. The factor T in the equation for FCR represents the component of the FCR that is allocated to Federal income tax. This component is strongly influenced by both investment tax credits and methods used for depreciation. The methods for computing T are discussed in the reference at the bottom of the table. The Internal

Fig. 9 - Allocations of revenue streams

TABLE VIII — BACK UP FOR FIXED CHARGE RATE (FCR)

Life	30 yrs
Annual "Other Taxes" - % Capital Cost	4.0%
Annual Ins & Adm Exp - % Capital Cost	0.45%
Statutory Income Tax Rate	48%
Ratio of Debt to Total Capitalization	40%
Annual Rate of Return (Debt, Stock)	10.6%
Cost of Capital	10.6%
Investment Tax Credit (Regular)	10%
Investment Tax Credit (Spec. Energy Prop)	10%

$$\overline{\text{FCR}} = [(k + d) + T + \beta_1 + \beta_2]^{**}$$

$(k + d) = \text{CRF} = 0.115$; CRF = Capital Recovery Factor

$\beta_1 = \text{"Other Taxes"} = 0.040$

$\beta_2 = \text{Ins \& Other Adm Exp} = 0.0045$

T = Federal Income Tax Component

$\overline{\text{FCR}} = 0.165$ (Regular ITC)

$\overline{\text{FCR}} = 0.146$ (Regular + Special ITC) *

* Special ITC for "Special Energy Property" Under Energy Act. of 1978

** "Profitability & Economic Choice", P. H. Jaynes,
Iowa State University Press, Ames, Iowa 1968

Revenue Service will allow, for new properties, accelerated depreciation such as sum-of-years-digits or double-declining-balance. Investment tax credits of 10% are now available for EU's. The Energy Act of 1978 presents the interesting possibility that OS/IES power plants might qualify for additional tax credits as either "specially defined energy properties" under the conservation sections or as cogeneration properties. As can be seen in Table VIII, using the factors listed, the FCR is either 16.5% or 14.6% depending upon whether the OS/IES power plant qualifies for an additional 10% tax credit.

EPRI in a guide published for the purposes of technical and financial assessment of advanced energy projects, recommends the use of a FCR of 18%. This FCR has been seized upon by many Federal agencies as being typical of the EU industry. However, upon careful reading of the assessment guide, the basis of their recommendations is that one should ignore all preference items such as accelerated depreciation and investment tax credits. In the example they give with and without preference items the FCR's so calculated were 14.63% and 17.87%, respectively.

In the subsequent analysis the two FCR's of Table VIII are used. In any utility specific analysis, the FCR's appropriate to their operation should be used.

As indicated from Table III, the annual savings in metered energy would be \$7720. One question of interest is "what is the break-even cost of an OS/IES power plant that corresponds to a savings of \$7720/year?" If we let C equal the break-even cost per kW of the plant then the total plant cost is 90 C since the plant was sized as a 90 kW plant.

Assuming that the plant does not qualify for special investment tax credit, the fixed charges and O&M charges are 16.5% and 6.1% respectively of the initial capital costs. Thus the fixed charges are 22.6% of 90 C or 20.34 C dollars per year. However this plant alleviates the peak load by 71 kW and the total credits of Table VI would be

\$555/kW times the 71 kW of capacity credit or \$39,405. At a FCR of 16.5% it represents an annual credit of \$6502. The O&M credit for the displaced capital equipment is 1.5% of the displaced capital cost or \$591/year, making for a total credit of \$7093. The break-even cost is obtained by the following equation:

$$20.34 C - 7093 = 7720$$

This is an application of the equation shown in Table IV in which MRR is equal to the savings (break-even). Solving for C yields, C equal to \$728/kW. Figure 10 shows this point plotted as a function of both the percent of OS/IES plant capital cost subject to a 5 year replacement and the equivalent O&M cost. Also plotted is the break-even power plant cost that would result if the plant qualified for extra tax credits under the Energy Act of 1978. The present target cost for such a power plant is \$500/kW which is well below the break-even curves.

This figure is illustrative of a particular case and is not necessarily definitive for all utilities. There are a great many variables that can effect the result in a particular EU scenario. Among these are:

- Climatology
- Load characteristics in the face of the climatology
- Siting in the system
- Operational mode (including feedback to the utility)
- Effectiveness of waste heat utilization
- Penetration
- Application credits

To carry the analysis one step further, Figure 11 is a bar chart showing the results of the previous calculation. For the conventional system the annual bill for gas and kWhrs to the apartment owner would be \$36,320. In the example studied the energy costs would be \$28,600, or 78% of the normal bill. In addition the net annual charge by the utility for the power plant (ownership and O&M) would be \$3055 resulting in a savings of \$4665/year to the customer.

Curve 718082-A

Fig. 10 – Break even capital costs of OS/IES power plant

Curve 718083-A

Fig. 11 – Customer benefits of utility owned OS/IES power plant

1.2 Thermal Storage/Terminal Unit Interface

As shown in Figure 12, the method of delivering heat to the building load will employ an "ambient temperature reset controller" to control the temperature delivered to the terminal units. The terminal units in general could be fan/coil units with two coils (a fairly common construction where the terminal unit must provide both heating and air conditioning service). In addition the terminal unit would have I²R capability to provide ultimate back-up. During the heating season, a central (reverse cycle) heat pump would also back up the reject heat obtainable from the OS/IES power plant. This heat pump, in the heating season, would use the same coil of the terminal unit as would be used in the cooling season for air conditioning. Exact details of the interface of the central heat pump through its own storage with the second coil of the terminal unit are not shown in Figure 12.

The functioning of the ambient temperature reset controller can be explained by referring to Figure 13. This figure shows building load (net heating load required from HVAC systems for all three buildings) as a function of ambient temperature. The points plotted are taken from the hour-by-hour load profile over the heating season. Not all possible points are plotted, attention being concentrated on two time periods of the day which should give the greatest "spread" in results. These are times early in the morning when temperatures tend to reach their daily low point and solar effects are not present and times in the mid-afternoon when temperatures tend to reach their daily highs and solar effects might be prominent. As can be seen, there is significant scatter caused by variations in solar effects, building dynamics, occupancy patterns, etc. The static load lines for the group of buildings are drawn through 70°F and 65°F for comparison with the actual building loads.

Fig. 12— Fuel cell/HVAC interface - heating season

Fig. 13 — Heating load vs. ambient temperature

As can be seen, the specific hourly loads all fall below the static load line drawn through 65°F. The terminal units can be so designed that they will deliver the required Btu's design ambient temperature as obtained from the line drawn through 65°F. In this instance, at -2°F, that would be 740,000 Btu/hr, or approximately 15,500 Btu/hr per apartment. In sizing the terminal unit, the water supply and return temperatures would have to be specified. For example, these might be 180°F and 100°F, respectively, requiring about 0.4 gpm flow through the terminal heat exchanger. The ambient temperature reset controller would then reduce the temperature of the water flowing to the heat exchanger as ambient temperature increased so as to give a capacity that would follow the dotted line of Figure 13. At actual hourly operating points as exemplified by the points on Figure 13, the unit fans would cycle on and off under the control of the apartment's thermostat. If the storage temperature on OS/IES power plant water temperature were not sufficient to give the required capacity, the heat pump followed by I²R would pick up the load.

1.3 Domestic Hot Water System

Figure 14 shows a domestic hot water (DHW) heating system which uses the sensible and latent heat from the spent fuel and process air condensers. An auxiliary gas heater is also provided. The coils in the condensers are in series, with the DHW flowing through the spent fuel condenser first. Two additional coils (located downstream of the DHW coils) are supplied with cooling tower water to cool the streams to the required temperature for water self-sufficiency. A bypass valve in the cooling tower water supply to the process air condenser controls the level in the condensate storage tank.

Figures 15 and 16 show that the seasonal extremes of water temperatures delivered by this system vary from 138°F to 203°F. These temperatures are tempered by passing through the storage tank and controlled to 145°F by mixing with unheated city water.

The DHW computer model calculates water outlet temperatures and spent fuel or process air outlet temperatures as a function of water inlet temperature and flow, and spent fuel or process air flow. The model will be extended to include the DHW storage tank and tempering valve effects.

A heat transfer phenomenon which limits the temperature variations occurs on the coils in both condensers, due to the large difference in heat transfer coefficients between the condensing and non-condensing regions. When the hot side flows are high and cold side flow is low, significantly more area in the heat exchangers is non-condensing. The non-condensing area heat transfer coefficient is much lower than the condensing area heat transfer coefficient, so even though the log mean temperature difference is fairly high, the amount of heat flow and resulting temperature rise in cold fluid is limited. A reverse buffering effect occurs for low hot side flow and high cold side flow. In this case, much of the heat exchange area is condensing. The high heat transfer coefficient improves heat flow, and increases the temperature rise in the cold fluid since a large amount of latent heat is available.

In the spent fuel condenser, condensation will occur on 40 - 75% of the heat exchange area depending on inlet temperatures and flows. In

Fig. 14 - System to recover process water using city water as coolant

Fig. 15 — Spent fuel condenser - seasonal extremes (worst hour)

Curve 718087-A

Fig. 16 — Process air condenser-DHW side
in series with spent fuel condenser-seasonal
extremes (worst hour)

the process air condenser, condensation occurs on 5-60% of the area depending on inlet conditions.

1.4 Fuel Conditioner Performance

Further efforts to make the fuel conditioner operate solely on spent fuel has indicated a significant sensitivity to fuel conditioner outlet composition. That is, a very efficient fuel conditioner, with an outlet composition near equilibrium values, would leave little unreformed CH_4 to be burned in the combustion chamber of the reformer. An approximate cut off point appears to be a fuel conditioner conversion rate in excess of 90%. In other words, if less than 0.1 moles of unreformed CH_4 per mole of CH_4 feed are left, and assuming a heat exchanger effectiveness of 0.8 and an H_2 utilization of 80% in the fuel cell, there will be insufficient energy available for self-sustaining reformer operation. Figure 17 shows the required effectiveness of the reformer as a heat exchanger as a function of ΔT approach to equilibrium of the reformer in order to have self-sustaining operations. This curve can be used as a design criterion for the reformer. Additional quantitative investigation will be conducted when the reformer kinetic model becomes available.

Fig. 17 — Required heat exchanger effectiveness for self-sustaining reformer operation using spent fuel

TASK 2: FUEL CELL DESIGN ALTERNATIVES

2.1 Fuel Cell Analysis

The lumped parameter fuel cell model was used to calculate the relationship between voltage and makeup air flow for process and DIGAS cooled stacks. With 2 stoichs of makeup and with 15 percent of the flow through process channels DIGAS cooling reduces output voltage by about 10 mV due to higher oxygen depletion than occurs in process cooled stacks for equal mean temperatures. The benefits of DIGAS cooling are lower pressure drop and higher mean cell temperatures for a given maximum temperature in the stack. It is estimated that the higher temperature available by DIGAS cooling will add about 20 mV thus giving an overall improvement in both pressure drop and voltage output.

Cooling channel designs were developed for the two 23 cell DIGAS cooled 30.5 x 43.2 cm stacks. Cooling plates have been successfully machined for the first design.

The voltage-current characteristics of stack 551 were analyzed to determine the performance parameters of the lumped model at the three oxygen concentrations tested at ERC. The values of r , cell resistance, and CU , catalyst utilization factor, derived from the data are given in Table IX. Values of CU are consistent with values from other 12.7 x 38.1 cm stack tests. However, the cell resistance has an unexpected variation with oxygen concentration. Previous values of cell resistance varied between .5 and .7 ohm-cm². The high value of .969 obtained for the 10 percent inlet oxygen concentration may be due to the low water vapor pressure under this test condition which would cause high acid concentration. In the recirculation mode considered for the OS/IES system, the oxygen concentration would be about 10 percent and the water vapor concentration would be over 20 percent. This is approximately equal to the mean water concentration in the 100 percent oxygen feed case. If the high resistance is due to low water vapor concentration it will not be a problem in OS/IES operation.

TABLE IX
RESISTANCE AND CATALYST UTILIZATION FOR STACK 551 AT 350°F

Oxygen Mole Fraction at Inlet	Specific Cell Resistance ohm-cm ²	Catalyst Utilization
0.10	.969	.123
0.20	.736	.095
1.00	.556	.084

In reducing the data, it became apparent that a better method was needed for estimating the mean water vapor concentration in the cell. The previous approach used the geometric mean of inlet and outlet concentrations. Appendix A presents a derivation of the mean concentrations in terms of the inlet concentrations and utilization factors for fuel and oxygen. A current density weighted average value was assumed to eliminate the need to specify current density in the analysis. Results show that the geometric means are reasonably close to the current density weighted mean values for all concentrations except water vapor. In the case of water vapor, the simple arithmetic average concentration agrees reasonably well with the current density weighted mean and will be used in further analysis.

TASK 2.2 CELL AND STACK TESTS

During this quarter, four 12.7 x 38.1 cm stacks were tested. The description and status of each stack is presented in Table X. The objectives and achievements of the stacks tested are summarized in the following stack discussion.

Stack No. 553

Testing of Stack No. 553 (80 - 12.7 x 38.1 cm cells with process air cooling formerly called Stack No. 1) was completed this period and the stack was removed from the test loop. During final tests two thermocouples indicated excess temperature and flow tests indicated that a

TABLE X

SUMMARY OF 12.7 cm x 38.1 cm STACK TESTING FOR THIS QUARTER

Stack Number	551	552	553	554
Stack Size	.05kW	0.5kW	2kW	0.5kW
No. Cells	2	20	80	20
Cooling Mode	Process	DIGAS	Process	DIGAS
Cooling Channel Direction and Configuration	-	12.7 cm straight through	-	38.1 cm straight through
Peak Cell Performance*, mV	610	600	580	580
Run Time, Hours	2602	1076	72	†
Time Avg. Cell Performance*, mV	586	570	565	560**
Test Location	ERC	ERC	ERC/W	ERC/W
Status	Terminated	Terminated	Terminated	In Operation

* Current density = 113 mA/cm².

** During pretesting period.

† Still on testing.

hydrogen crossover had developed. The stack was torn down for visual inspection but no evidence of local overheating or crossover was found.

Stack 553 was tested at approximately 25 steady state operating points with a total operating time of about 40 hours. Nine thermocouples were installed in the hydrogen channels to permit an accurate measure of average cell temperature and of temperature distribution in the air flow direction. Table XI presents typical cooling data for 4 tests at currents between 20 and 80 amperes. The total temperature difference across the plates was found to be approximately equal to the measured air rise across the stack as predicted by the detailed analytical model for process cooled stacks. The average gradient over the active area was 81 percent of the measured air rise. Comparison of calculated and measured air rises indicated a stack heat loss of about 300 W which is consistent with the calculated loss based on stack surface area and insulation thickness.

Voltage-current characteristics for makeup air flows of 2.5 and 5.0 stoichs are shown in Figure 18. Stack voltages for these conditions were lower than the values obtained during pretest by 1.5 to 2 volts (.019 to .025 V/cell). The difference is believed to be due to higher operating temperature and higher makeup air flow rate used in the pretests.

TABLE XI
COOLING DATA FOR STACK 553

I Current, Amps	Mean ΔT Over Active Area, °C	Mean ΔT of Plate in Cooling Direction, °C	Calculated Air Rise °C	Measured Air Rise °C
20	16.0	18.8	30.2	18.9
44	46.5	54.6	69.5	63.8
60	53.0	62.3	69.0	66.5
80	63.0	74.0	73.1	74.2

Fig.18 - Performance of 80 cell state-of-the-art stack

Additional work on the test loop included calibration of orifices and flowmeters using high accuracy wet test meters and installation of an O_2 gauge to monitor oxygen concentration in the test loop. Stack 554 was installed in the test loop for testing in August.

Stack No. 551 (Current Density Study)

Stack No. 551, a 2-cell stack with modified endplate heaters, was terminated this quarter after over 2600 hours of operation. The primary objective of these tests, as discussed in the Second Quarterly Report, was to verify the theoretical model of current density distribution under isothermal conditions. Figure 19 illustrates the performance history of this stack, including the open circuit voltage and on-load performance at 113 mA/cm^2 . During this period, peak performance was 610 mV and a time-averaged performance was 586 mV at 40A (113 mA/cm^2). The following results were obtained during the operating life of Stack No. 551:

- The distribution of current density under isothermal conditions was experimentally determined to corroborate the theoretical prediction shown in the Second Quarterly Report. The experimental results verified the theoretical model.
- The voltage-current response* was determined as a function of oxidant (air) utilization at a constant H_2 utilization ($\sim 80\%$). It was experimentally determined that cell performance was sensitive to air flow rates between 1 and 2 stoich due to severe oxygen depletion but was relatively insensitive to air flow above 2 stoich.
- The capability to operate at 2 stoich air flow without significant performance loss for an extended period was demonstrated. This ability is necessary in the DIGAS cooling concept, for which the design objective is 2 to 3 stoich air to the cells.

* Presented in the Third Quarterly Report.

FIGURE - 19
PERFORMANCE HISTORY of 2-CELL STACK, (STACK 55I)

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- Polarization data at different reactant concentrations was collected to verify the analytical model. The data, including cell temperature profiles, was taken at three anode and three cathode gas compositions** for 50% oxidant and 75% fuel utilization.

Figure 20 shows the effect of cathode gas composition at 2 stoich on iR-free performance. As illustrated, there was a 30 mV drop going from 20% O₂ (~ air) to 10% O₂, and a 70 mV gain going from 20% to 100% O₂ at 113 mA/cm² and 177°C. These results are within 5% of theoretical results predicted by the analytical model. The variation in anode gas composition (for fresh air as cathode gas) showed a 12 mV drop from 100% H₂ (dry basis) to 75% H₂/25% CO₂ and an additional ~ 15 mV drop with 1% CO present in the inlet feed. Slightly larger losses were observed when oxygen concentration in the inlet cathode gas was 10%.

Upon disassembly of Stack No. 551, the current collectors were found intact and the plates were in good condition. However some gas channels were blocked by electrolyte droplets.

Stack No. 552 (0.5 kW -12.7 x 38.1 cm DIGAS Stack)

Stack No. 552 a 20-cell DIGAS stack with cooling in the 12.7 cm direction was also terminated for post-test analysis of cell components and to free the test stand for the next DIGAS stack (No. 554). Test objectives of Stack No. 552 were to; 1) develop assembly procedures for DIGAS stacks, 2) verify design calculations dealing with air channel geometry and flow split between process and cooling channels, 3) determine temperature distribution in the stacking direction.

Figure 21 shows the performance history of this stack, including the open circuit voltage and performance at 40A (113 mA/cm²) for over 1000 hours of operation. The data was taken at 70 to 85% H₂ utilization and a

** Cathode gas compositions: 100% O₂, 20% O₂/80% N₂,
10% O₂/90% N₂.

Anode gas compositions: 100% H₂, 75% H₂/25% CO₂,
75% H₂/24% CO₂/1% CO.

FIGURE 20
EFFECT OF CATHODE GAS COMPOSITION AT 2 STOICH
ON IR-FREE PERFORMANCE (STACK 55I)

FIGURE 21
PERFORMANCE HISTORY OF 0.5kW DIGAS STACK (STACK 552)

total air flow of 15 to 20 stoich to the stack. This is equivalent to 2 to 3 stoich air into each cell since approximately 15% of total air flows through the cells.

A fairly steady performance of ~ 570 mV/cell at 113 mA/cm^2 (after the initial breaking-in period) indicates that DIGAS cooling is working well and that a DIGAS stack is capable of operating at 2 to 3 stoich air through cells continuously. This capability may be more difficult to achieve than operating a process air-cooled stack (such as Stack No. 551) at the same low (2 to 3 stoich) flow rate. In a process cooled stack, any blockage in some channels causes flow increase to other channels. This additional flow then produces a significant increase in pressure drop in the small process channels, discouraging maldistribution to some extent. However in a DIGAS cooled stack, the portion of rerouted flow passes through large, open cooling channels rather than small process gas channels, thus adding insignificant pressure drop. The flow through DIGAS cooling channels is several times that through process channels. Therefore channel blockage in a DIGAS stack could cause more severe maldistribution leading to high performance losses due to severe oxygen depletion and/or starvation at some local areas.

The following was observed during ~ 1000 hours of DIGAS stack operation:

- The observed split in flow between the cooling plates and cells was in good agreement with the intended design.
- DIGAS stacks are capable of operating well at high reactant utilization. An average cell performance was 590 mV at 40A (113 mA/cm^2), with 2 stoich air to cells and 85% H_2 utilization.
- DIGAS stacks are capable of operating continuously with 2 to 3 stoich air to cells for over 1000 hours without significant performance loss (less than 20 mV from time-averaged performance).
- The temperature gradient in the stacking direction was measured as $1.7^\circ\text{C}/\text{cell}$ on the average. This corresponds

to $\sim 40^{\circ}\text{C}$ rise from the cell adjacent to cooling plates to the center cell in a five cell group between the two cooling plates. This gradient is reasonable for a DIGAS stack.

Stack No. 554

Stack No. 554, a 20-cell (12.7 x 38.1 cm) DIGAS stack with cooling in the 38 cm direction, (Figure 22) was pretested at ERC before delivery to Westinghouse for additional testing. The main objectives of this stack are:

1. To generate thermal data similar to that which will be observed in a 30.5 x 43.2 cm DIGAS stack employing the same cooling channel configuration, i.e. straight-through cooling channels.
2. To measure IR drop in the cooling plates made with new fabrication methods and techniques.

This DIGAS stack (described in the Third Quarterly Report) exhibited marked improvements in the DIGAS cooling plate IR drop over the previous DIGAS Stack No. 552 (with cooling air in the 5-inch direction).

During the break-in period (in which the stack accumulated 93 hours of operation), the average cell performance was 565 mV at 40A (113 mA/cm²) and the open circuit voltage was 895 mV which is ~ 50 mV lower than typically obtained with 12.7 x 38.1 cm stacks. This can be attributed to the large temperature gradient in the stack ($\sim 39^{\circ}\text{C}$) which is a result of the cooling channel configuration used. As the DIGAS cooling channel pattern is refined and optimized, it is expected to attain a more uniform temperature gradient ($\sim 19^{\circ}\text{C}$) and higher performance.

Test Stand Design and Construction

Air Recirculating System

Ductwork and manifolding have been designed and fabricated. Figure 23 is a photograph of the air recirculating system. Figure 24 is a schematic of this system. Figure 25 shows the automatic damper assembly which controls the amount of air recirculated to the stack on the basis of ("outlet air") temperature. The details of the damper, bimetallic coil and linkage appear in Figure 30. The ratio of recycled air to fresh air

FIGURE 22 STACK NO. 554, 20-CELL DIGAS STACK

FIGURE 23 STACK 555 AND RECIRCULATING AIR DUCT

FIGURE 24 SCHEMATIC OF RECIRCULATING AIR SYSTEM

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FIGURE 25 DAMPER ASSEMBLY AND AIR EXHAUST DUCT

FIGURE 26 DAMPER ASSEMBLY

is regulated automatically by the damper in the air exhaust duct. The damper blade is controlled by a temperature sensitive bimetallic coil located in the air exhaust stream. Teflon bearings and a linkage with stainless steel shafts minimize friction in the damper movement to maximize temperature sensitivity. Outside adjustment of the tension in the bimetallic spring and a window installed in the duct at the location of the damper (which allows visual inspection of the position of the damper blade) enable calibration of the damper during stack operation by using a velometer.

Test Panel

The test panel to pretest Stack 555 has been completed (Figure 27). The instrumentation (flow meters, electrical instruments, etc.) has been calibrated and the auxiliary components such as load banks, thermocouples, variacs, etc. are now ready for operation.

TASK 2.3 STACK MANUFACTURING

DIGAS Stack Construction

Cell and cooling plate assembly procedures for DIGAS stacks were developed as well as other aspects of stack design and construction, including manifold and seal designs and a means for electrolyte introduction.

The only previous experience in DIGAS stack construction was with an intermediate size (27.9 x 35.6 cm) 10-cell stack built for the DOE technology program in 1978 that had only one cooling plate between the 5th and 6th cells. In this stack, acid was introduced from each side of the stack but not through the cooling plate. In Stack 552, acid was successfully wicked in the cells with acid-fill channels that ran through the four cooling plates. The experience and knowledge gained with this stack were a valuable basis for a DIGAS stack fabrication procedure. The cooling plates in Stack 552 consisted of two molded half-plates which had process gas channels on one side and were flat on the other. The cooling air channels were then machined into the flat side of each plate and the two halves were cemented together. These cooling plates produced much higher IR drop than expected, ~ 190 mV per cooler at 113 mA/cm^2 . Therefore, in the following stack fabrication, additional emphasis was placed on improving cooling plate fabrication to reduce resistive losses.

FIGURE 27 TEST PANEL FOR 12 in. x 17 in. STACKS

It was thought that the method of curing the graphite cement and uneven compression when joining the two halves contributed significantly to the high resistance of the coolers of Stack No. 552. In Stack No. 554, this was improved by a longer curing time at a lower temperature. The slower, lower temperature cure allowed better, more uniform escape of the solvent from the cement and less formation of gaps and air bubbles in the joint. Two of the DIGAS plates in Stack No. 554 were also shimmed with graphite paper and thin metallic sheets to improve contact and to compensate for steps in the plates (where the electrodes are recessed). All plates were compressed between two flat aluminum plates during the cure of the cement. The four coolers in Stack No. 554 exhibited an IR drop of ~ 10 mV per ohm on average (at 113 mA/cm^2), confirming the improvements made in assembly procedures.

For Stack No. 554, thick cathode half plates (~ 0.210 in.) were successfully molded which made it possible to machine cooling grooves only on one half-plate*. This was cemented to a thin, flat half-plate. (Two machined grooved half-plates were used in Stack 552.) This reduced labor costs (for machining and assembly) and material costs.

Stack No. 555 (the first 2 kW, 30.5×43.2 cm stack) has been assembled with four cooling plates with straight-through cooling channels (Figure 28). Each cooler consists of a thick (~ 0.53 cm) molded cathode half-plate and a thin (~ 0.25 cm) molded anode half-plate and was assembled similarly** to that in Stack 554. This stack is now ready for electrolyte introduction. A wicking assembly has been specially designed to introduce electrolyte into the stack. Phosphoric acid will be introduced through the bottom three hydrogen channels on the anode side of each plate since the present 30.5×43.2 cm bipolar plates do not have other provisions for acid introduction. Thus the anodes have been trimmed back from the bottom

* Details of the cooling plates used in Stack 554 were presented in the Third Quarterly Report.

** Straight-through cooling channels (~ 0.25 cm deep $\times$ 0.48 cm wide $\times$ 30 cm long) were machined into the flat side of a cathode half-plate only.

FIGURE 28 30.5 x 43.2 cm 2 kW DIGAS Stack No. 555

edge of the plate to accommodate the electrolyte in these three channels. Also provisions were incorporated in the design of the wicking assembly to prevent the acid from contacting or seeping into the glued joint in the DIGAS plates. After electrolyte introduction, the stack will be pretested at ERC before delivery to Westinghouse for further testing. The target date for shipment of Stack No. 555 to Westinghouse is ~ August 31.

The cooling half-plates for the second 30.5 x 43.2 cm 2 kW stack (No. 556) were sent to the vendor on July 20 for machining an innovative cooling channel design. It is expected that this configuration will result in a significant reduction in the temperature gradient observed experimentally in Stack 554 (~39°C) which employed straight-through cooling channels in the 38.1 cm direction. A more uniform temperature profile will result in a corresponding increase in stack performance.

Currently the cell subassemblies and auxiliary stack components are being manufactured for Stack 556.

Cooling Plate Manufacture

Expertise in molding thick 30.5 x 43.2 cm (DIGAS) cooling half-plates with process channels on one side and cooling channels on the other is being developed at ERC's own initiative and expense. Thus far, 0.53 cm thick cooling-half plates have been molded successfully. A set of the molded cooling plates is shown in Figure 29. The platten was machined to mold 44 straight cooling channels 0.25 cm deep x 0.64 cm wide in the 30 cm direction. The ability to mold deep cooling grooves is an important step toward molding the cooling channel configurations for the innovative design to be tested later.

Metallic Cooling Plates

Under our current concept, the DIGAS cooling plates in the fuel cell modules are made of the same graphite-phenolic composite as the bipolar plates. The use of metallic plates appears to have several advantages;

1. Simpler, less expensive and faster fabrication -
could be stamped

FIGURE 29 MOLDED COOLING PLATE ASSEMBLY

2. Higher electrical and thermal conductance
3. More intricate flow passages might be possible
4. Higher strength and ductility

The suggestion that 316 SS be used for the plates was made in one of our review meetings and the discussion centered on its corrosion resistances under stack operating conditions. The results of a brief survey of the literature indicated corrosion rates approaching 2.5 cm per year (cpy) for 316 SS under operating conditions similar to those in the stack. However, the corrosion rate for this Hastelloy B under the same conditions was less than .13 cpy. While this is probably unsatisfactory, it does suggest that further study of this concept may be justified.

Future Work Plan

- The immediate goal is to pretest Stack No. 555 (first 2 kW 30.5 x 43.2 cm DIGAS stack) and to deliver it to Westinghouse by the end of August.
- Fabrication of cell subcomponents (electrodes, matrices, bipolar plates, etc.) and auxiliary stack components (tie bars, end plates, etc.) will continue
- Delivery of the machined cooling half-plates is expected to be ~ October 4. If they arrive as scheduled the stack assembly is expected to take place on ~November 1. The target date for shipment of Stack No. 556 will then be November 20.

TASK 3: METHANE CONDITIONER STUDY

3.1 Mathematical Model

Work continued during this quarter to expand the equilibrium reformer model into a sizing and performance reformer model. The expanded model includes equations representing the chemical kinetics and equilibrium of the reforming reaction, the heat transfer from the combustion products to the reforming stream and the material and energy balances of the combustion and reforming streams. Various physical properties have been correlated in equation form for convenient use in the model.

A computer program, developed to numerically solve the various equations used in the model, has been debugged and is now operable. The program will be used to estimate the reformer size required for the design conditions and to calculate its performance under off-design operation. Calculated output values include equilibrium constants, heat transfer coefficients, mole fractions, mass fractions and the molar flow rates anywhere in the reactor, as well as the reaction conversions and temperatures.

The reforming equations, the finite element equations developed to model the reformer, a glossary of terms, and the algorithm being programmed to solve them are described in the following paragraphs.

The reforming reactions are;

The rate of conversion of methane by Equation (1) in an element of reformer height (dz) is;

$$\frac{dX_1}{dz} = \frac{e_B p k_o e^{-E/RT_c}}{u_o c_o} \left[\frac{F_1(1-X_1)}{F+2X_1F_1} - \frac{F_1(1-X_E)}{F+2X_EF_1} \right] \quad (3)$$

Equation (2) is assumed to be at equilibrium.

The equilibrium constants for Equations (1) and (2) in terms of the computer model variables are respectively;

$$[K_1(T_c)] = \frac{[F3+XEF1+X2(F3+XEF1)][F5+4XEF1+X2(F3+XEF1)]^4 p^2}{F1(1-XE)[F4-2XEF1-X2(F3+XEF1)]^2 [F+2XEF1]^2} \quad (4)$$

$$[K_2(T_c)] = \frac{[F3+XEF1+X2(F3+XEF1)][F5+4XEF1+X2(F3+XEF1)]}{[F2-X2(F3+XEF1)][F4-2XEF1-X2(F3+XEF1)]} \quad (5)$$

The reforming stream and combustion products stream energy equations are respectively;

$$F1 C_{pA} dT_c = U_1 (T_H - T_c)_{avg} \pi D_2 dz + F1(-\Delta H_{R1})dX1 + (F3+X1F1)(-\Delta H_{R2})dX2 \quad (6)$$

$$M_H C_H dT_H = U_1 (T_H - T_c)_{avg} \pi D_2 dz \quad (7)$$

For each incremental height of reformer these equations 3 through 7 are solved iteratively by the computer to determine the exit conditions for the specified inlet conditions.

The overall iterative algorithm for the reformer model is;

- (a) assume the exit combustion gas temperature, $(T_H)_o$
- (b) choose an element height, dz
- (c) calculate all outputs from the element given the inputs
- (d) repeat the calculations sequentially for all elements in the reformer bed using the outputs of the previous element as inputs
- (e) recalculate the combustion gas exit temperature and iterate if required.
- (f) check the element size by recalculating the values using a smaller element, and compare the exit values for the two sizes. Iterate as required.
- (g) write the values when these conditions are met.

This solution algorithm has been rigorously defined using the equations involved.

Glossary of terms for the equations

X1	is the fractional conversion of methane (as a function of position in the reformer)
X2	is the fractional conversion of carbon monoxide (as a function of position in the reformer)
e_B	is the catalyst density in the reformer, lb/ft ³ of bed
p	is the total pressure, atm
$k_o e^{-E/RT_c}$	is the rate constant, lb mols/(hr · lb catalyst · atm CH ₄)
T _c	is the reformer gas temperature, °R
z	is the height in the catalyst bed in the direction of flow, ft
u _o	is the initial linear velocity in the reformer, ft/hr
c _o	is the initial methane concentration, lb mol/ft ³
F	is the total moles of feed
F1(1-X1)	are the number of moles of methane present at any location
F+2X1F1	are the total number of moles
XE	is the equilibrium fractional conversion of methane (as a function of position in the reformer)
F1(1-Xe), F+2XE F1	are the equivalent molar quantities at equilibrium
[K ₁ (T _c)]	is the equilibrium constant for reaction (1)
[K ₂ (T _c)]	is the equilibrium constant for reaction (2)
[F3+XE F1+X2(F3+XE F1)]	are the moles of carbon dioxide present
[F5+4XE F1+X2(F3+XE F1)]	are the moles of hydrogen present
[F4-2XE F1-X2(F3+XE F1)]	are the moles of water present
[F2-X2(F3+XE F1)]	are the moles of carbon monoxide present
F1	is the initial number of moles of methane present
C _{pA}	is the heat capacity of the reformer feed per mole of entering methane, BTU/lb mol CH ₄ , °R
E	is the activation energy, Btu/lb mol
R	is the gas constant, Btu/(lb mol · °R)

- U_I is the overall heat transfer coefficient based upon the internal surface area, BTU/hr ft² °R
 T_H is the combustion gas temperature, °R
 D_2 is the internal tube diameter, ft
 ΔH_{R1} is the heat of reaction (1), BTU/lb mol CH₄
 ΔH_{R2} is the heat of reaction (2), BTU/lb mol CO₂
 $(F_3 + X_1 F_1)$ is the total number of moles of carbon dioxide before reaction (2) proceeds
 M_H is the combustion gas flow rate, lb/hr or lb mol/hr
 C_H is the combustion gas heat capacity, BTU/lb °R or BTU/lb mol °R
 $(T_H)_O$ is the assumed combustion gas outlet temperature, °R
 $(T_H)_Z$ is the calculated combustion gas inlet temperature for the corresponding $(T_H)_O$, °R
 $(T_H)_Z^k$ is the actual combustion gas inlet temperature, °R
 τ is the residence time of the reactants in the catalyst bed, sec.

The computer program described above has been successfully operated to converge on both $(T_H)_O$, combustion gas outlet temperature, and Δz , incremental bed height. In order to minimize iterations in achieving convergence, a secant correction method was adopted to correct the assumed $(T_H)_O$ after each iteration step, as demonstrated by Figure 1. For a given reformer gas inlet temperature, $(T_C)_O$, and combustion gas outlet temperature, $(T_H)_O$, the material and energy balances for the reformer determine what the combustion gas inlet temperature, $(T_H)_Z$, should be to obtain the combustion gas outlet temperature, $(T_H)_O$. These balances then determine $(T_H)_Z$ as a function of $(T_H)_O$ for a fixed reactant inlet gas temperature, $(T_C)_O$. Figure 30 shows this function in a modified form, where it is subtracted from the actual combustion gas inlet temperature $[(T_H)_Z^k]$ to yield an error function defined as follows:

$$E \equiv (T_H)_Z^k - (T_H)_Z$$

Curve 718089-A

Fig. 30 - Secant correction method

At $E \equiv 0$, $(T_H)_z = (T_H)_z^k$, and convergence is achieved. The secant method takes two functional pairs of temperatures such as $[(T_H)_o, (T_H)_z]_1$ and $[(T_H)_o, (T_H)_z]_2$ and draws a secant to the curve to predict the next guess $[(T_H)_o, (T_H)_z]_3$. It proceeds in this manner until convergence is achieved.

Figure 31 shows a typical problem. Table XII summarizes the results from the sample problem, obtained by using the secant correction method. The system, a ten foot reformer tube, converged at 80 increments (not shown). A low conversion ($\sim 35\%$) was obtained due to a short residence time (high space velocity = 1200 hr^{-1}).

Further work is planned, using the computer program, to investigate various cases of interest.

$$F = 12 \text{ lb. Moles/Hr.}$$

$$P = 1.5 \text{ ATM}$$

$$(T_C)_0 = 1290^\circ\text{F}$$

$$U_0 = 1.2027 \times 10^5 \text{ ft/hr}$$

$$\tau = 0.3 \text{ Sec.}$$

Fig. 31 — Typical sample problem

TABLE XII
SAMPLE CASE SUMMARY

Number of Increments	Iter. No.	(T_{H_o}) [Combustion Gas Outlet Temp. (°F)]	(T_{H_z}) [Combustion Gas Inlet Temp. (°F)]	(T_{c_z}) [Reformer Gas Outlet Temp. (°F)]
10	1	1476*	2343	1553
	2	2332**	5308	2800
	3	1724	3302	1882
	4	1693	3186	1843
	5	1696	3200	1847
20	1	1696*	3186	1850
	2	1713**	3246	1872
	3	1701	3200	1856
40	1	1701*	3192	1856
	2	1709**	3222	1867
	3	1703	3200	1860

Notes: (T_{H_o}) = Iteration Variable

(T_{c_o}) = 1290°F for all runs

* = Initial Assumption

** = Corrected Initial Assumption

TASK 4: MANAGEMENT AND DOCUMENTATION

The Third Quarterly Report and the May report were prepared, DOE patent approval was received and they, plus the March report, were distributed in accordance with the distribution lists provided by the government technical manager. The June report was submitted for patent approval.

A program review meeting was held at the Westinghouse R&D Center on May 31. Plans for a program review meeting on August 3 were made.

A proposal for Phase II was submitted to NASA. After discussions between ERC and Westinghouse and the government technical management team and Westinghouse a revised plan for Phase II was submitted to NASA-LERC. Several tasks were deleted to bring the level of effort into line with the available funds. Since the deleted tasks were not on the critical path for the overall program, no negative effects will occur if these tasks can be started during the second year of Phase II via modification of the base contract or under a separate contract.

The fuel cell fabrication and test schedule was revised as required by delays in receiving equipment from suppliers. Arrangements were made to expedite machining of components by using Westinghouse qualified suppliers.

A paper describing some of the results of the ongoing effort was delivered at the National Fuel Cell Seminar. During the seminar, informal discussions on plans and project coordination were held among the team members and the government technical manager and important information on other ongoing work was obtained.

A meeting on fuel processing was held at Westinghouse R&D. The discussions focused on developing relationships with catalyst suppliers to utilize their expertise to the extent possible.

Work on drafting a subcontract for the ERC Phase II work was started. If government approval can be obtained prior to contract award, the Phase II work will be expedited.

APPENDIX A MEAN MOLE FRACTIONS FOR CALCULATING FUEL CELL VOLTAGE

For the lumped parameter fuel cell model, fuel and oxidant streams are specified in terms of inlet composition and utilization factors. Calculation of cell voltage requires a mean concentration for each reacting component. The Nernst and cathode polarization terms involve $\ln Y$ terms which are to be "averaged" over the cell to obtain an "average" cell voltage. It is assumed that a current density weighted average provides a reasonable mean value. The crossflow configuration causes variation in current density between and along reactant channels in both directions. Consider a reactant channel which has mean current density equal to the average current density. Then, since depletion of a reacting component is proportional to current density, the fraction (Z) used between 0 and X of the amount used between 0 and L is

$$Z = \frac{1}{i_a L} \int_0^x i \, dx \quad (1)$$

where

- i_a = average current density
- i = current density at x
- L = length of the flow channel

If Y_m is the mean value of Y such that $\ln Y_m$ equals the current density weighted average value of $\ln Y$ over the flow path, then

$$\ln Y_m = \frac{\int_0^L (\ln Y) i \, dx}{\int_0^L i \, dx} = \int_0^1 (\ln Y) \, dz \quad (2)$$

which applies for O_2 , H_2O and H_2 mole fractions.

Air Side of Fuel Cell

Assume that S moles of O_2 enter a given flow path and that one mole is utilized. Then the moles of O_2 at x are $S-Z$. The total moles of flow entering the flow path are S/a where a is the mole fraction of O_2 at inlet. The total moles at x is $Z + S/a$ since Z moles of O_2 have been used and $2z$ moles of H_2O are produced. Thus the mole fractions of O_2 and H_2O at x are

$$Y_{O_2} = \frac{S - Z}{S/a + Z} \quad (3)$$

$$Y_{H_2O} = \frac{Sb/a + 2Z}{S/a + Z} \quad (4)$$

where

b = mole fraction of H_2O at inlet

Performing the integration indicated by Equation (2) gives

$$Y_{O_2m} = a \left(\frac{S}{S-1} \right)^{S-1} \left(\frac{S}{S+a} \right)^{\frac{a+S}{a}} \quad (5)$$

$$Y_{H_2Om} = \left(b + \frac{2a}{S} \right) \left(\frac{S}{S+a} \right)^{\frac{S+a}{a}} \left(1 + \frac{2a}{bS} \right)^{\frac{bS}{2a}}$$

Note that the oxygen utilization factor is defined by $\eta_{O_2} = 1/S$.

Fuel Side of Fuel Cell

For a fuel utilization factor of η , there are $1/\eta$ moles of H_2 at inlet for each mole consumed and $1/C\eta$ total moles at inlet where

C = inlet mole fraction of H_2

At x there are $1/\eta - Z$ moles of H_2 and $1/C\eta - Z$ total moles. Thus the mole fraction of H_2 at x is

$$Y_{H_2} = \frac{1 - \eta Z}{\frac{1}{C} - \eta Z} \quad (7)$$

and the mole fraction of CO at x is

$$Y_{CO} = \frac{d}{1 - C\eta Z} \quad (8)$$

where

d = mole fraction of CO at inlet.

Upon integration of Equation (2) one obtains

$$Y_{H_{2m}} = C (1 - C\eta)^{\frac{1}{C\eta} - 1} (1 - \eta)^{1 - \frac{1}{\eta}}$$

The effect of CO on voltage is assumed to be directly proportional to the mole fraction of CO. Thus the mean mole fraction of CO is defined by

$$Y_{CO_m} = \int_0^1 Y_{CO} dz$$

which gives

$$Y_{CO_m} = - \frac{d}{C\eta} \ln (1 - C\eta)$$

Under conditions of recirculation cooling of fuel cells, the geometric mean concentrations are within 5 percent of the mean concentrations. However, for once through air flow, the geometric mean concentration of water vapor is low by more than 20 percent. It is found that the simple arithmetic average water vapor concentration is within 10 percent of the mean under all conditions and thus should be used as an alternative to the more complicated expression derived here.

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