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# SYSTEMS ANALYSIS OF ELECTRICITY PRODUCTION FROM COAL USING FUEL CELLS 



Final Report<br>Donald K. Fleming<br>November 1983

Prepared for

## CALIFORNIA INSTITUTE OF TECHNOLOGY JET PROPULSION LABORATORY 4800 Oak Grove Drive <br> Pasadena, CA 91103

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This work was performed for the Jet Propulsion Laboratory, California Institute of Technology, sponsored by the United States Department of Energy through an agreement with the National Aeronautics and Space Administration.

A program has been undertaken to evaluate alternative systems for the production of electricity from coal using coal gasification and power generation through molten carbonate fuel cells. The purpose of the work effort was to identify research and development effort that, if successful, could be cost-effective in reducing the overall cost of power from such systems.

The approach taken in the evaluation was the development of a versatile, computerized process simulator. The performance of individual subprocess elements was characterized mathematically; the subprocess elements were arranged in alternative configurations on the simulator to form a total process; and the relative performance of the systems was analyzed. For those systems showing efficiency promise, capital and operating costs for a 675 MW power plant were estimated using factored costing techniques. Finally, the 10-year levelized cost of power was obtained using standardized financial factors.

The above approach is cost-effective for the stated purpose of this program. However, it must be used with care and the results must be interpreted with mature engineering judgment for the following reasons:

1. By its nature, the overall system is quite sensitive to minor variations in inputted assumptions.
a. The systems analyst must use care to assure that only the desired variable has been altered in the analysis.
b. In a separate subtask, input assumptions were systematically varied for the same total base system. Process efficiencies varied from $46 \%$ to $57 \%$; yet all of the systems are operable.
c. Comparisons of systems analyzed by different investigators must be made with extreme care.
2. The cost of electricity developed by this approach is highly sensitive to capital-related chargea; with system efficiency having little impact. Yet, the factored-costing technique that was necessarily utilized cannot have great accuracy.
3. The financial assumptions used in developing the levelized cost of electricity also tend to emphasize capital costs, rather than system efficiency.
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A total of 66 cases were evaluated during the course of the study; several of these cases were iterated several times to assure greater comparability when the degree of sensitivity of the overall system became apparent.

Table ES-1 presents the nine systems that were analyzed economically; several other systems also incorporate features that warrant R\&D attention. The efficiency and cost data in Table ES-1 must be assessed while considering the caveats above. In particular, the degree of conservatism used in this analysis is somewhat greater than other efforts reported in the literature reported system efficiencies are considerably lower than estimated by other investigators.

The major conclusions drawn from this effort include

- Fluidized-bed gasification appears to be a viable alternative in this system if the relatively minor cost advantage can be realized. Although this approach has a total capital requirement that is only $2.5 \%$ 1ower than entrained flow gasification, this difference is apparently sufficient to counteract the three-percentage-point reduction in process efficiency.
- The development of steam reforming of methane, thermally and chemically integrated within the anode compartment of the fuel cell, offers significant efficiency and cost advantage when the system also includes a fluidized-bed gasifier. This advantage increases as the quantity of methane made in the gasifier is increased.
- High-temperature dust removal adds nearly two percentage points of process efficiency, without a capital cost penalty, by permitting process rearrangement. Additionally, this approach peimits incorporation of other advanced concepts.
- High-temperature desulfurization, when integrated with high-temperature dust removal, results in still higher efficiency and cost savings due to improved system simplicity.

Other R\&D effort was identified that may be cost-effective in reducing the cost of power or improving system simplicity:

- Improved definition of the carbon deposition phenomena, so that the quench system might be eliminated
- Development of countercurrent heat exchange for high-temperature, toxic, hazardous gases
- Development of a novel, single-stage, fluidized-bed gasifier that produces greater quantities of methane

Table ES-1. SUMMARY OF SYSTEMS ANALYZED

| System. No. | 1 | 2 | 3 | 4 | 5 |
| :---: | :---: | :---: | :---: | :---: | :---: |
| Gasifier Type Methane Make | $\begin{gathered} \text { Entrained } \\ \text { NL1 } \end{gathered}$ | $\begin{aligned} & \text { Entrained } \\ & \text { Nil } \end{aligned}$ | Fluldized Bed Minimal | Fluidize: Bed Minimal | Flusdized Bed Moderate |
| Heat Exchange Type | Countercurrent | Crobsflou | Croasflow | Crobsflow | Croseflou |
| Carbon Control | None | Quench | Quench | Quench | Quench |
| Dust Control | Water Wash | Water Wash | Water Wash | Water Wash | Water Wash |
| Sulfur Control | Selective AGR | Selective AGR | Selective AGR | Selective AGR | Selective AGR |
| $\mathrm{CO}_{2}$ Control | None | None | None | Hone | None |
| Fuel Cell | Conventional | Conventional | Conventional | Internal Reforming | Internal Reforming |
| System Efficiency, z | 42.1 | 41.6 | 38.4 | 44.9 | 45.8 |
| $\begin{aligned} & \text { Total Capital Requirement } \\ & \left(675 \mathrm{~mW}, \$ 10^{6}\right. \end{aligned}$ | 1024.1 | 1055.3 | 1029.1 | 981.6 | 970.4 |
| 10-Year Levelized Cost of Pover, \$/kWh |  |  |  |  |  |
| Capital Charge | 4.80 | 4.94 | 4.82 | 4.60 | 4.54 |
| Coal | 1.98 | 2.00 | 2.17 | 1.85 | 1.82 |
| Other Operating | 0.98 | 1.04 | 0.99 | 0.94 | 0.92 |
| Fuel Cell | 0.72 | 0.76 | 0.75 | 0.87 | 0.88 |
| Total | 8.5- | $8.7+$ | 8.7+ | $8.3-$ | 8.2- |
| System No. | 6 | + 7 |  | 8. | 9 |
| Gasifier Type Mechane Make | Fluidized Bed Moderate | Fluidi Mode | Bed | dized Bed derate | dized Bed derate |
| Heat Exchange Type | Crosaflow | Cros |  | ossflow | obsflow |
| Carbon Control | Quench | Que |  | Quench | uench |
| Dust Control | High-Temperature | High-Tem | rature | Her Wash Higi | empersture |
| Sulfur Control | Selective AGR |  |  | ctive AGR High | emperature |
| $\mathrm{CO}_{2}$ Control | None |  |  | Temperature | None |
| Fuel Cell | Internal Reforming | Sulfur Internal | erant Inte | 1 Reforming Inter | 1 Reforming |
| Syatem Efficiency, $z$ | 47.4 |  |  | 47.5 | 50.0 |
| Toral Capital Requirement $(675 \mathrm{~min}), \$ 10^{6}$ | 958.4 | 852 |  | 88.2 | 46.8 |
| 10-Year Levelized cost of Power, \&/kWh |  |  |  |  |  |
| Capltal Charge | 4.49 |  |  | 4.62 | 3.97 |
| Coal | 1.76 | 1. |  | 1.76 | 1.67 |
| other Operating | 0.91 |  |  | 0.94 | 0.80 |
| Fuel Cell | 0.86 | 0. |  | 0.86 | 0.81 |
| rotal | $8.0+$ |  |  | 8.2- | 7.2+ |

- Development of a dust-tolerant water-gas shift reactor, permitting the recovery of the exothermic heat of the shift reaction at elevated temperatures.

Additional R\&D effort that appears warranted, based upon engineering judgment, includes the following:

- Development of a sulfur-tolerant fuel cell
- Development of high-temperature carbon dioxide removal
- Continued systems analysis effort to assess additional novel systems that could not be evaluated within the constraints of this effort
- Improved catalytic combustion systems with lower light off temperatures and higher maximum temperature limits for reduced heat exchange and improved system simplification.

The above recommendations for identiffed R\&D effort are based upon an indepth analysis of the many ramifications of the overall system by mature chemical process and research engineers. The conclusions are based not only upon the calculated analysis, but also upon first-hand knowledge of the processes of coal gasification and fuel cell power generation.

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## OBJECTIVE

The purpose of the work effort described in this document is to evaluate, on a total systems basis, various means for integration of coal gasification with power gerieration (through molten carbonate fuel cells) with emphasis upon Identifying research and development effort that, if fruitful, could be costeffective in reducing the overall cost of power from such systems.

## INTRODUCTION

## Approach

The approach employed in evaluating the integration of coal gasification with high-temperature, molten carbonate fuel cells was the development of a versatile computer process simulator that can integrate the various subsystems and provide an analysis of the resulting overall system. Such an approach is useful because it permits the relatively quick comparison of alternative systems and, if used with care, provides a relative comparison of the benefits of process modifications.

Those process configurations that appeared to offer efficiency merit, based upon the process simulator, were then costed, using a factored-estimate approach, and the relative cost of power from each of the systems was projected. More accurate costing techniques could not be employed because the engineering basis underlying several of the novel processing systems was considered insufficient to warrant a more definative evaluation.

The approach has certain drawback. Unless excessively complex, the models for certain process elements (notably the gasifier, the acid-čas remoyat zystem, and the fuel cell) are simplified approximations of actual operation. Thus, unless engineering judgement is employed, it is possible that the approach may result in exercising the simulator, rather than actually comparing the anticipated performance of alternative systems.

With the overall system under sonsideration, extreme care is required to make each simulator test comparable to the others. Because many hundreds of millions of Btu's are being transferred or converted at each step of the process, and because the net power recovered from the system is the algebraic sum of large quantities of energy that are being produced and consumed, an apparently minor change in an assumption can readily cause a change of 25 to 50 million Btu's in recovered power - an apparently significant improvement. Thus, many of the systems discussed have been iterated several times to assure comparability.

As a corollary to the sensitivity discussed above, one must be extremely careful in comparing the evaluations of alternative investigators. The assumptions underlying the effort must be clearly defined and be precisely identical for comparlsons to be meaningful. Evaluations presented in this
effort consistently.show lower process efficiencies than others reported in the literature. In a separate subtask (Appendix Da), a systematic variation in the conservatism of the assumptions (underlying the same basic system) saused a change in apparent system efficiency from $45 \%$ to $57 \%$. When alternative systems are to be compared, they must be compared with precisely the same assumptions.

The approach is flawed by the high leverage of capital costa upon final cost of power; yet the factored estinating technique that must necessarily be employed cannot be highly accurate. Moreover, the financial factors employed in assessing the cost of power from capital and operating charges inherently tend to favor systems with reduced capital requirements.

In spite of the drawbacks cited above, the approach is quite valuable in providing a first-cut evaluation of alternative systems and is particularly valuable in projecting the anticipated benefits of R\&D on novel concepts. When used in conjunction with macure engineering judgement, it provides an excellent basis for assessing projected research effort.

Sonsistent with the limitations of the approach as set forth above, the following sections describe the procese simulator employed and define the assumptions used throughout the effort.

## Basic Process Element Simulators

Many of the elements of the process simulator were adapted from an earlier effort that evaluated alternative approaches for the production of substitute natursi gas from coal. 1 The elements were modified to include oxidizing speeies and additional process subsections were added for this effort.

Before discussing the individual elements in the overall system, the general process configuration will be outlined. Figure 1 presents the process configuration that wa. found to be preferred in many of the evaluations; improved systems were generally modifieations of this basic configuration. Appendix Cd presents the computerized process simulatior printout for the specific case presinted. Each page of the printout represents one step in the overall process; approximately 75 pages of printout are required to character-
ize a given configuration.* Figure 1 , the printout, and the disosssion below, when analyzed together, provide the necessary background for evaluating the process simulator employed.

In Figure 1, fuel gas is produced from coal, steam, and oxygen in the primary con\%\%ter. After preliminary dust removal, the gases are quenched for carbon stability and heat is recovered in a waste heat boiler (WHB). The gas is cooled in a train of crossflow heat exchangers and an air cooler, finally washing out the dust in a non-condensing venturi scrubber (operating at the temperature that is the dewpoint of the gas). The gas is then roheated in the above train, reacted for initial shift conversion, and expanded to fuel cell operating pressure at the maximum temperature of the departiculated gas. After additional heat recovery through a waste heat boiler, another stage of shift conversion is included; followed by a heat exchange train, with intermediate $C O S$ hydrolysis; final cooling for condensate removal; and selective acid/gas removal (AGR) for recovery of $\mathrm{H}_{2} \mathrm{~S}$ but only the cost-effective removal of carbon dioxide. The fuel gas is then reheated in the second heat exchange train, purified over zinc oxide, and steam is added for control of carbon stability in the feed to the fuel cell. Eighty-five percent of the moles of reductant $\left(\mathrm{H}_{2}+\mathrm{CO}+\mathrm{CH}_{4}\right)$ are electrochemically converted to power in the fuel cell; the rest are catalytically combusted. At the fuel cell station, recycle (with heat recovery) is employed for 1) temperature control of the fuel cell and 2) maintaining correct temperatures for the booster fans (on both the anode and cathode exhaust gases) as well as the catalytic combustor. In addition to power recovery in the fuel cell, a steam bottoming cycle and a cathode exhaust-gas expander also provide net power output from the system.

## Gasifiers

The entrained-flow gasifier model, used in the initial simulations, is a simplified transfer-function model employing the inputs and outputs provided by the prime contractor in the reference case for the system (Appendixes Aa and Ab ). The printout page includes gas quantities and compositions, oxygen demand, and outlet stream conditions. Also included is an empirical factor to allow for the power required for coal preparation and feeding of the unit. In

[^0]
an analysis of this operation by others, the subsystem was found to be optimistic. For example, $100 \%$ of the carbon in the coal is converted to gaseous species with an oxygen requirement of 0.84 lb of oxygen per lb of coal, while pumping a slurry with $70 \%$ fecd solids concentration.

Four different operating conditfons were considered for fluidized-bed gasifiers during this program. The gasifier models are based upon extrapolation of pilot plant performance to higher operating pressures, employing known effects of pressure upon gasification rates and the product gas spectrum. In each case, carbon conversion is $96.9 \%$, reflecting pilot plant data for the amount of carbon lost to dust and gasifier ash. Three of the gasifiers were specified with a steam/carbon ratio of $1: 1$ molar and an operating pressure of 500 psi. The fourth gasifier was operated with a steam/carbon ratio of $0.75: 1$ and a pressure of 600 psi - operating conditions that are less conservative considering the state of current technology. (This fourth gasifier was employed in the analysis of variations of initial assumptions, presented in Appendix Da.) The quantity of methane in the fluidized bed gasifier product varies, depending upon the mode of operation as predicted from pilot plant and theoretical evaluations. In one conceptual gasifier, higher methane yield was allotted to correspond with predictions for the novel gasification system. Heat and material printouts for the nonconfidential fluidized-bed gasifiers are presented in Appendix Ce.

The printout for the fluidized-bed gasification output includes gas composition and yuantity, off-gas temperature and pressure, steam demand (as inputed), oxygen requirements (as dictated by material and energy balance), and the quantity of recycle gas required to inject the coal into the gasifier. A power demand is indicated to account for coal preparation and gasifier requirements.

## Heat Transfer

Each side of a heat exchanger was calculated independently. In many cases, heat transfer was calculated from known inlet and assumed outlet temperatures, using the composition of the flowing gas and three-factor heat capacity correlations. In other cases, for example when heat is being transferred from one gas to another, the quantity of heat to be transferred is fixed and the outlet temperature of the exchanger is calculated.


When integrating the flow sheet, care was taken to avoid temperature crosses in most instances. In other words, because crossflow heat exchange is generally considered, the temperature to which the cool gas is heated may not be warmer than the temperature to which the hot gas is cooled. In most cases, a temperature of approach (approximately $50^{\circ} \mathrm{F}$ ) was imposed. In future work, it is suggested that, when using gas-to-gas heat exchange, the temperature of approach be the controlling design factor and the heat exchangers be designed as a unit. Such a modification would make test-to-test comparisons more valid. and minimize operator error in the analysis.

The typical heat exchanger printout page provides gas compositions and quantities, inlet and outlet temperatures, process gas sensible enthalpies, and heat exchanger duty.

## Gas Stability

The thermodynamic stability of the gas for carbon deposition is calculated from thermodynamic equilibria (based upon the carbon activities for both amorphous and graphitic carbon) ${ }^{2}$, using free energies based upon six-term* functions of temperature. The quantity of water required to inhibit the carbon deposition is calculated as a function of the assumed temperature, pressure, and initial gas composition.

Quench
The addition of water (as either liquid or steam) to the gas stream results in a temperature redistribution based upon heat capacity data and an empirical representation of water or steam enthalpies. The quantity of water used for this quench is determined from the preceeding step, as derived for inhibition to the limits described by the activity of either amorphous carbon (in the assumption sensitivity study - Appendix Da) or for most of the work effort, midway between amorphous and graphitic carbon, which includes a safety factor in the operation.

Water-Gas Shift Reaction
Steam, carbon monoxide, carbon dioxide, and hydrogen are equilibrated according to the water-gas shift reaction based upon the free energy

[^1]calculated at an assumed temperature by using standard free energy data and six-term thermodjnamic expressions. The heat of reaction is calculated and the exit gas temperature is determined assuming an adiabatic reactor.

In this step, the equilibrium temperature is assumed and the resulting calculated exit gas temperature is manually compared with the assumptions, to determine if the temperature of approach to equilibrium is satisfactory. The preferred future system would incorporate an inputted desired temperature of approach to equilibrium and iterate the process element to close the heat balance and degree of reaction.

When the water-gas shift reaction occurs within the fuei cell, the equilibrium temperature is assumed to be the "characteristic" temperature of the cell, as discussed later.

## Reforming-Methanation

The steam-reforming of methane, or the reverse reaction of methane formation from hydrogen and carbon monoxide, is calculated similarly to the watergas shift reaction. Although not used as an independent reactor step in this effort, the capability exists in the generalized computer simulator. It was used as a subroutine to modify fuel cell gas composition within the anode corpartment of the fuel cell in many of the cases studied.

## Other Catalytic Reactions

Most systems include a $\operatorname{COS}$ hydrolysis reactor in the heat exchange train as the gas is cooled. The reaction of COS with water to produce $\mathrm{H}_{2} \mathrm{~S}$ is favored at a lower temperature; therefore, the reactor is located at a point where the gas is slightly above its dewpoint. The reported thermodynamics of this reaction vary over a wide range, depending upon the data source. This effort has assumed equilibrium conversion of $\operatorname{COS}$ according to the recent UCI data ${ }^{3}$ (which are more conservative than JANAF or NASA tables).

After acid-gas removal, traces of $\mathrm{H}_{2} \mathrm{~S}$ and COS are removed by zinc oxide at about $750^{\circ} \mathrm{F}$. The consumption of zinc oxide is presented, based on the estimated sulfur leakage through the acid-gas removal system (as discussed below).

## Compressors and Expanders

Rotating power equipment is calculated at the inputted efficiency of enthalpy change into work based upon isentropic pressure differential. Process inefficiencies appear as heat in the outlet gas. A mechanical efficiency is also assumed in the conversion of shaft horsepower into work.

For multiple stage compression, interstage cooling to $90^{\circ} \mathrm{F}$ is assumed, and the cooling duty as well as the energy requirements per stage, are printed。

## Acid-Gas Removal

Process element algorithms are available for amine, hot potassium carbonate, and physical solvent systems for acid-gas removal (AGR). Although other acid-gas systems were checked during the course of the work to determine if advantages existed, the AGR system employed throughout this system was the "Selexol" acid-gas removal process.

The algorithm for this process is a transfer function that removes 1 ) $H_{2} S$ from the process gas, 2) $\mathrm{CO}_{2}$ in accordance with an assumed $\mathrm{H}_{2} \mathrm{~S}$ soncentration in the resultant acid-gas, 3) approximately $50 \%$ of the $\operatorname{COS}$, and 4) almost all of the water content of the feed gas (a small quantity of water is left in the gas to avoid computational problems in the downstream fuel cell). Steam and power demands are based on an extensive in-house data bank and are functions of the operating pressure, acid-gas partial pressures, and degree of concentration of the $\mathrm{H}_{2} \mathrm{~S}$ in the resulting acid-gas.

In this work, the Selexol acid-gas removal system was not specified for total carbonyl sulfide removal because this AGR process option requires extensive power demands for pumping and refrigeration. Rather, in most cases, a $C O S$ hydrolysis reactor was included upstream of the AGR and the estimated distribution of COS in the $\mathrm{H}_{2} \mathrm{~S}$-selective system was reported.

The simulator algorithm appears directionally correct. For example, it predicts increased steam usage with changes in the subsystem parameters that would increase the solvent flowrate in the AGR subsystem. Similarly, it predicts increased power demands for modifications that would increase the pumping required, the refrigeration load, or the flash gas recompression duty. However, the algorithm is based upon an empirical correlation of published results, rather than upon the basic principles of the AGR system. Therefore,
the algorithm cannot be extrapolated beyond the normal operating regime of such a system.

In addition to the selective AGR described above, the simulator also includes algorithms for bulk removal of acid-gas. Such a process unit was employed in a few tests of the overall system. In this case, the nitrogen required for stripping the solvent of $\mathrm{CO}_{2}$ is also included.

The Fuel Cell
The fuel cell simulator is also a simplified approximation of the complex operation of the subsystem. The simulator was derived from a Physical
Sciences, Inc. (PSI) package that employs a characteristic temperature input for calculations of free energy, open circuit voltage, and cell polarizations. The Nernst concentration polarizations are calculated at the characteristic temperature, using the $\log$ mean concentrations of the inlet and outlet gases at both the anode and the cathode. In its original form, the program also calculated electrode polarizations, using a wetted-pore model, and the same gas compositions. The total heat released in the system was calculated and both the anode and cathode exhaust gases leave at the same temperature for an adiabatic cell.

The initial PSI simulator was modified twice during the project. First, the features external to the fuel cell within the PSI-supplied tape were dropped and the fuel cell simulator was incorporated as a subroutine in the overall project computer package. Reforming and shift equilibria were drawn from the project subroutines rather than from the initial PSI package. The PSI simulator, in this form, still contained a relatively thick electrolyte and electrode polarizations that were based upon data published by IGT about seven years ago. Thus, the simulator is not representative of state-of-theart fuel cell electrodes, nor the new, thinner electrolyte systems being developed in several laboratories. However, at a 10-atmosphere operating pressure, the simulator projects about 925 mV , IR-free, when operated on simulated reformed methane (at $160 \mathrm{~mA} / \mathrm{cm}^{2}$ ). Extrapolated experimental data ${ }^{4}$ indicate a potential of 935 mV under these conditions. With allowances made for the differing fuel utilizations, the correspondence is within 5 mV . Thus, the simulator, after the initial modifications, gave reasonable results at high-pressure operation. However, at 1-atmosphere operating pressure, the simulator projected oniy 520 mV (IR-free), much less than the 852 mV
experimental output. Thus, the use of the simulator at pressures much different than 10 atmospheres (or at gas partial pressures that vary greatly from the experimental conditions) should be avoided.

Midway through the project, it was found that the fuel cell subroutine would not function in conjunction with internal reforming within the fuel cell when the gas contained moderate methane concentrations. The conversion technique employed in the simulator was too sensitive with the changing quantities of hydrogen produced by reforming. At this point in the project, the internal programing of the simulator was modified in three ways:

1. The fuel cell hydrogen conversion was changed to a stepwise approach, with methane reforming, in shift equilibrium, after each step.
2. The electrode polarizations were modified to simple, current-dependent: approximations with a factor that resulted in the same polarization that had been noted in the prior tests.
3. The expression for the free energy of the reaction was adjusted to be more consistent with the JANAF tables.

The elimination of che wetted-pore model, and the substitution of a simpler expression, further limits the applicability of the subsystem simulator to near the range in which it was utilized. Application of the model to a higher pressure fuel cell, as had been considered in this project, was therefore not attempted.

The modification of the expression for the free energy caused a 54 mV loss in cell potential. This voltage loss, in the systems considered, caused a 39 MW change in the power delivered by the fuel cell, or about a 25 MW change in total plant output, a variation of 1.6 percentage points in system efficiency.* Thus, the modified fuel cell simulator is somewhat more conservative than results shown by 1980 fuel cell data. It is significantly more conservative (approximately 2.5 percentage points in efficiency) than recent fuel cell data. ${ }^{5}$

The fuel cell simulator is simplified. For example, it does not differentiate the directions of gas flow with the cell. Considering the imperative requirements of 1 ) uniform gas flow across the face of a single cell and 2) precise gas distribution, cell-toncell, in a fuel cell stack, it is likely

As presented in Appendix Da.
that future systems will be cocurrent in operation. Several of the projected designs were double-checked against total Nernst polarization, assuming zero current flow at the common outlet of a cocurrent cell. These results did not give a voltage less than the average total cell polarization provided by the simulator and were, therefore, not controlling. However, as is shown later, the total-system performance is quite sensitive to the fuel ceil operating characteristics and its off-gas temperature. An integrated, differential simulator for a cocurrent cell, including temperature effects, would be highly desirable for an improved process simulator.

## Catalytic Combustor

The combustion of the anode exhaust into the cathode feed is assumed to take place catalytically. The subsystem simulator integrates the heat of reaction with the chemical changes taking place and calculates an off-gas temperature. Warnings appear if the mixed feed temperature is less than the light-off temperature for conventional catalysts, or if the adiabatic reaction temperature is sufficiently high to cause long-term çtalyst degradation.

## Major Assumptions - System Simulator

## System Pressure Drops

Pressure drops of 5 psi were assumed across packed bed reactors such as the water-gas shift reactor, carbonyl sulfide hydrolysis reactor, zinc oxide bed, and catalytic combustion. Similarly, 5 psi was taken across the acid-gas removal absorbers.

A 3-psi drop was taken across particulate scrubbers. A 2-psi drop was taken across each shell of a heat exchanger train and the fuel cell itself. Splitting or merging streams were assumed to require l-psi drop.

The above pressure drops would appear quite optimistic compared with normal chemical engineering practice. Yet several system designs in the literature have shown much lower pressure drops than presented here. The impact of lower pressure drops is improved energy recovery in the overall system. A few cases were evaluated at lower pressure drops (in the analysis of sensitivity to assumptions presented in Appendix Da) to indicate the magnitude of this effect.

## Efficiency of Rotating Power Equipment

In most instances, turboexpanders were taken at $92 \%$ isentropic efficiency and large axial compressors were taken at $88 \%$ efficiency. A mechanical efficiency of $98 \%$ was also imposed. These values were taken from the base case provided at the beginning of the project. Although slightly optimistic relative to the anticipated performance of generally available machinery, the values were maintained throughout the project for consistency. One series of calculations was made to indicate the impact of driver efficiency upon the overall system.

The compression efficiency of the multiple-stage oxygen compressor, feeding the gasifier, was taken at $62 \%$, to reflect the higher power demand of these non-lubricated, slow-speed, reciprocating machines.

The maxinum compression ratio was varied as a function of the gas being corpressed. For air, this maximum was normally a ratio of 3.5. However, with final stages of air compression, specialized outboard designs were considered that would permit higher compressed air temperatures and compression ratios as high as 4.0. Note that the humid air to the system is assumed to contain 14.3-psi partial pressure dry air, at reasonable site elevations above sea level.

## Heat Exchangers

Generally, heat exchangers were assumed to be crossflow with an approach temperature differential of $50^{\circ} \mathrm{F}$ between the maximum temperature of the cooler gas and the minimum temperature of the warmer gas. The assumption of countercurrent heat exchanger and/or reduced temperature of approach will decrease the heat losses of the system and improve the overall system efficiency.

Although countercurrent heat exchangnis were not normally employed, if the heat exchange duty was large and multiple shells of heat exchange would normally be required, the shells were arranged in series to provide more efficient heat transfer. This approach improves the heat recovery within the system at the expense of greater system pressure drops; however, it does not approach the temperature recovery for countercurrent heat exchangers by perhaps $100^{\circ} \mathrm{F}$ temperature loss in each heat exchanger train.

## Chemical Reactions

The water-gas shift reactors were assumed to have a temperature of approach to equilibrium of approximately $50^{\circ} \mathrm{F}$ to simulate end-of-1ife for the catalyst. A reduced approach to equilibrium will improve the overall system efficiency by converting more of the water vapor present into hydrogen, reducing heat loss to condensation, and reducing downstream humidification requirements.

The water-gas shift and reforming operations were assumed to reach equilibrium when these reactions take place within the fuel cell where the gas flow is laminar. However, the equilibrium is based upon the "characteristic" temperature of the cell. Should the outlet gas temperature of the cell be used, slightly improved system performance would be expected.

Complete combustion was assumed in the catalytic reactors on the anode tail gas.

The carbonyl sulfide hydrolysis reactors were assumed to reach equilibrium, using the free energies of carbonyl sulfide reeently developed by United Catalysts, Inc.

Zinc oxide beds were assumed to operate at $750^{\circ} \mathrm{F}$ and provide complete removal of both hydrogen sulfide and carbonyl sulfide.

## Steam System

Because the total facility for conversion of coal to power has not been described, and certain steam sources and demands have not been quantified, the steam system was nut defined in detail. Additional energy demands or production thet might be expected of the total system include:-

1. Both high- and low-pressure steam generation in the sulfur plant
2. The steam and reductant demand in the sulfur plant tall gas treatment unit
3. The steam demand, both low and moderate pressure, for waste water stripping and ammonia recovery
4. The power demands for activated sludge treatment of water before recycle
5. Boiler feedwater and cooling water pumping (for precess units)
6. The power demands for waste solide handling
7. Miscellaneous power demands for facilities, instrument air, flare, and other systems that will be required in the overall facility.

The impact of these miscellaneous steam, power, and reductant demands, or sources, indicates that the total system cannot be quantified with the available information. Therefore, the steam system was not optimized.

In the project, the steam required for humidification of the anode fuel was assumed to be recovered as high-pressure, superheated steam, similar to the reference case supplied by the prime contractor. Likewise, that steam recovered into power was also assumed as high-pressure, superheated steam, with reheat. Other steam demands within the system were assumed to be recovered at the conditions for which they were required. For example, the gasifier steam requirement was assumed to be recovered at $600 \mathrm{psi}, 750^{\circ} \mathrm{F}$, and the AGR steam demands were assumed to be recovered at 50 psi.

In the appended discussion on variation of assumptions, the total heat recoverable to high-pressure steam was also assumed to be manageable for the production of high-pressure, superheated steam. Boiler feed water was preheated in an economizer and by contact with the cooling gas stream. Lower temperature heat was assumed to be available for vaporizing the water and higher temperature heat was available for providing superheat. The effort was not made to quantify the source of heat as a function of temperature; rather, it was assumed that the total heat discharged to the system could be recovered in this fashion. In that optimization study, significant power could be recovered by expanding the high-pressure steam to the duty required in the system.

The high-temperature, superheated steam was assumed to be recoverable to power at $35.28 \%$ efficiency. This efficiency includes allowances for boiler feedwater heating and pumping, as well as cooling tower duty and cooling water pumping. This efficiercy might be considered low by modern power plant standards (土f stack gas scrubbing is not required) and, in the assessment of the assumptions, an alternative efficiency of $40 \%$ was also assumed.

In future efforts, it is recommended that the energy sources and requirements outside the basic plant be identified and factored into the overall energy balance. Then, the steam system could be quantified to 1 /hentify heat sources by quality of heat and verify that sufficient heat is available at the necessary quality to provide the steam power at the design conditions.

## The Fuel Cell Subsystem

Appendix Cb presents a discussion of the voltage and power produced in the fuel cell. The determination of voltage losses in the cell, as projected by the modified PSI simulator, was presented earlier. In general, current density was taken at $150 \mathrm{~mA} / \mathrm{cm}^{2}$ and the conversion of total fuel gas species $\left(\mathrm{H}_{2}+\mathrm{CO}+\mathrm{CH}_{4}\right)$ was $85 \%$. Although short optimization tests indicate that these assumptions are not ideal, they were maintained for comparability to other work.

An effort was made to specify operating units around the fuel cell subsystem that would be operable. The fans, or low-compression-ratio boosters, that are used on both the anode arts cathode exhausts have been protected against excessive temperature by heat exchange. Additionally, feeds to the catalytic combustor were properly temperature-conditioned such that this unit should be in the proper operating temperature range. Additional heat exchange equipment was required for this design consideration.

In general, the temperature of the feed gases to the fuel cell were greater than $1000^{\circ} \mathrm{F}$ to avoid excessive polarizaticn at the gas inlet. These streams were temperature-conditioned with additional heat exchange equipment. In most instances, the outlet gas temperatures were about $1260^{\circ} \mathrm{F}$. By careful tuning of the simulator, through adjustment of the cathode gas recycle rate, the exit gas temperature could be increased to $1300^{\circ} \mathrm{F}$, with a resultant increase in overall system power output.

## Major Assumptions - System Costing

The prime contractor provided a base case reference design and economic analysis to estimate the investment, operating costs, and levelized power costs for a 675 MW fuel cell power plant using an entrained-flow coal gasification system. That complete report is included with this document as Appendix Aa. The costing assumptions employed herein, together with the financial factors, came from the base case economics (included as Appendix Ab) and were used directly in the economic assessment of the current effort when applicable.

The nine cases evaluated economically in this document often contain gasification and other processing steps that are different from the base case, iequiring additional costing information. The assumptions listed in Table 1
wer：added to those presented in the reference design to evaluate alternative processing schemes．

Table 1．SYSTEM COSTING ASSUMPTIONS

| Fuel Processing Unit | Cost Base | Scaling <br> Capacity Factor | Scaling <br> Exponent |
| :--- | :--- | :--- | :--- |
| Fluidized Bed Gasification <br> and Ash Handling | M．W．Kellogg report <br> on Westinghouse and <br> U－Gas Processes for | Tons／day coal | 0.6 |
| Coal to SNG |  |  |  |

## General

During this project, 66 cases were examined for the integration of coal gasification with molten carbonate fuel cells for power generation. Of these, 20 cases were analysed for the change in system efficiency by variation in process configuratioa. These initial cases were based upon a constant 4991 tons/day of candidate coal input (the quantity required for the production of 675 MW in the reference case in an early iteration) and the resulting power output was assessed. When the sensitivity of the overall system to input assumptions was realized, many of these cases were iterated several times for more accurate comparisons. The results of this analysis are presented in Appendix Ca.

As discussed elsewhere, the system is very sensitive to the engineering assumptions inputted by the systems analyst. A subprogram was undertaken to indicate the effect of various input assumptions; this assessment (21 cases) is presented in Appendix Da. Summary printouts for these cases are presented in Appendix Db.

Many of the systems analyzed are not specifically presented herein. In general, many of these cases represent minor variations in a specific analysis or involved optimization studies by varying a single process parameter. In these cases, the results are discussed but not specifically analyzed in depth.

Nine of the conceptual systems were reevaluated at a constant 675 MW power output to provide a constant basis for the economic analysis of the alternatives. When recalculated on the process simulator, the necessary flows at all stages of the system were evaluated to aid in the system costing. The reevaluation of these systems for the economic analysis was made after the sensitivity assessment and, consequently, an effort was made while reassessing these data to ensure comparability between the systems. Therefore, the system efficiencies vary slightly from the initial work presented in Appendix Ca.

The nine cases were selected for economic analysis based upon anticipated efficiency improvements, as derived from the earlier work, the systematic incorporation of system advances to be expected through R\&D, and the potential for success in the R\&D effort. Because the overall goal of the program was to identify cost-effective R\&D efforts as applied to this system, the major
thrust was for advanced concepts, rather than shorter-term, engineering solutions.

A number of concepts were identified that could not be costed within the constraints of the program. These concepts are discussed, directionally, based upon the analyses of similar efforts.

The nine cases evaluated in the economic analysis, and the rationale for their selection, were as follows:

1. The Base Case: This system includes an entrained-flow gasifier, thermodynamically unstable raw gas, no shift reactor, and countercurrent heat exchange. The case is included to provide a direct comparison to earlier work.
2. Modified Base Case: The base case was reengineered for operability, adding a quench for carbon stability, water-gas shift reaction for improved raw gas hydrogen content, and crossflow heat exchange for improved operability. Location of the turboexpander was moved for greater energy recovery. This case was included to indicate the cost impact of the desired modifications and becomes a new reference for the remainder of the systems that are designed to a similar degree of operability.
3. Fluidized-Bed Gasifier: This case is similar to the Case 2 above, with the substitution of a fluidized-bed gasifier, producing low methane offgas (substituted for the entrained-flow gasifier). Although this case showed lower efficiency that Case 2 above, it was included because it is a starting point for further improvements indicated below.
4. Internal Reforming Fuel Ce11: Internal reforming capability was added to the fuel cell of the system in Case 3 (using the fluidized-bed gasifler) to indicate the merit of this concept.
5. Modified Fluidized Bed Gasifier; to produce greater methane content: Case 4, above, was modified only by the mechanical configuration of the gasifier so that it would produce greater quantities of methane for greater efficiency both in the gasifier and in the internally reforming fuel cell.
6. High-Temperature Dust Removal: The addition of high-temperature dust removal, per se, adds little to the overall system. However, it permits system modifications. In this case, the turboexpander could be relocated to provide significant improvement in process efficiency, as well as a cost reduction by elimination of much heat exchange equipment. The hightemperature dust removal is also employed in other systems below.
7. Sulfur-Tolerant Fuel Cell: The combination of high-temperature dust removal with a conceptual sulfur-tolerant fuel cell represents an extremely simple system, with minimum equipment, of relatively high thermal efficiency.
8. High-Temperature $\mathrm{CO}_{2}$ Transfer: The concept of removal of carbon dioxide from the raw fuel gas and transferring it to the cathode is attractive because of the higher-purity fuel feeding the fuel cell and greater fuel cell output. The system in Case 5 was modified to include this effect; somewhat greater efficiency was achieved.
9. High-Temperature Sulfur Removal: The integration of high-temperature dust removal with high-temperature sulfur removal provides a system that is similar in efficiency and complexity to the sulfur-tolerant fuel cell (Case 7) discussed above.

Other cases considered, but not specifically analyzed for cost, include the following:
10. Incorporation of a Novel Fluidized-Bed Gasifier: A nove1, single-stage fluidized-bed gasifier has been conceived that promises still higher methane production. From the efficiency analyses, incorporation of this gasifier into the system with an internally reforming fuel cell promises improved system efficiency.
11. Integration of High-Temperature Sulfur Removal with a Sulfur-Tolerant Fuel Cell: The system including the sulfur-tolerant fuel cell does not remove sulfur dioxide from the final stack. High-temperature sulfur removal, to the degree required for environmentally satisfactory utilization of coal, has now been demonstrated on the laboratory and bench scale. Although laboratory results on high temperature sulfur remeval to the degree required for conventional fuel cells appear promising, this combination appears attractive as a backup position.
12. Dust-tolerant Shift Reactor: A system incorporating a dust-tolerant shift reactor indicated improved process efficiency and system simplicity. It was not separately costed because extrapolations from Case 6 above would be applicable.
13. Advanced Systems: Several systems were conceived during the course of the program that could not be evaluated, even on an efficiency basis, because of the constraints of time, budget, or fnapplicability of the fuel cell simulator. Such systems appear promising, based upon first principles, but were beyond the scope of this investigation.

Table 2 presents the efficiency comparisons for the nine cases outlined above, as developed from the computerized process simulator. The reader is specifically directed to Appendix Ca for the discussion of the individual cases and the factors that impact the efficiency. More detailed discussions of the effects that occur in the system are presented in Appendix Cb and Appendix B presents summary printouts of the computerized analysis for the nine cases outlined above. Each of the cases is described briefly later in this report section, after the economic analysis is discussed.

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|  | $0 \cdot 05$ | ¢ 49 | $\varepsilon 1$ | Sss | く | $19 \cdot 7$ |  | IIA | $\iota$ |
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|  | 3] | тәल | $\begin{gathered} \begin{array}{c} \text { aivo } \\ \text { wivas } \\ \text { jind } \end{array} \end{gathered}$ |  |  |  |  |  | วडए |

Table 2 illustrates one of the basic tenets of systems analyses - an optimized overall system is not necessarily made up of components operating at their optimal condition. For example, the fluidized-bed gasifier of Case 3 has a higher efficiency than the entrained-flow gasifier of Case 2, with both operating in the same system. However, the entrained-flow gasifier yielded a higher overall system efficiency. This efficiency was recovered, including the benefits of the improved gasifier, when internal reforming was added to the fuel cell, as in Case 4.

Systems 7 and 9, incorporating either high-temperature sulfur removal or the sulfur-tolerant fuel cell (both in conjunction with high-temperature dust removal) produce nearly the lowest fraction of the total power from the fuel cell itself. This is because the gas fed to the fuel cell has relatively high concentrations of carbon dioxide and water vapor, suppressing the fuel cell voltage. Nevertheless, on the total systems basis, they show the highest overall efficiency. Thus, compromises taken in the fuel cell operating conditions result in favored overall system performance. Conversely, System 8, with high-temperature carbon dioxide transfer, shows the highest voltage from the fuel cell; yet the overall system performance is not as high as in Systems 7 and 9. Note that System 8 did not include the high-temperature dust removal in conjunction with the high-temperature carbon dioxide transfer. Should this combination have been included, it is conceivable that the overall system efficiency would again be higher.

Table 2 also indicates that, in general, high-temperature purification systems showed efficiency advantages over their low-temperature counterparts. High-temperature dust removal, $\mathrm{CO}_{2}$ transfer, and sulfur removal are all preferred system options.

Of note in Table 2 is the relative power recovered in system elements. For example, Systems 5 and 6 provide very little power from the steam cycle; It may be reasonable in these cases to simplify the overall system by optimizing the conversion taken across the fuel cell and completely eliminating the steam cycle from the system.

Tables 3, 4, and 5 provide the economic analysis for the nine cases evaluated. The techniques of calculation follow the format suggested by the prime contractor and were derived EPRI costing bases. The assumptions used in arriving at the capital cost and operating expenses were presented earlier in
Case No.*
Component
Gasificatio

| Case No.* | 1 | 2 | 3 | 4 | 5 | 6. | 7 | 8 | 9 |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  |  |  |  | $\$ 100^{6}$ |  |  |  | - |
| Component |  |  |  |  |  |  |  |  |  |
| Gasification Section |  |  |  |  |  |  |  |  |  |
| Oxygen Plant | 87.2 | 88.2 | 77.3 | 68.6 | 63.8 | 62.4 | 59.8 | 62.1 | 59.8 |
| Coal Handling | 18.8 | 19.1 | 20.3 | 18.0 | 17.6 | 17.3 | 16.6 | 17.2 | 16.6 |
| Coai Feed, Gasification and Ash Handling | 23.5 | 23.6 | 15.5 | 14.1 | 13.9 | 13.6 | 13.2 | 13.6 | 13.2 |
| Gasifier Effluent Cooling, Quench and Dust Removal | 45.4 | 45.9 | 19.3 | 16.9 | 17.0 | 15.6 | 14.7 | 15.4 | 15.9 |
| High-Temperature $\mathrm{CO}_{2}$ temoval. | - | -- | -- | -- | -- | - | -- | 28.5 | $\cdots$ |
| High-Temperature Sulfur Removal | - | -- | -- | $\cdots$ | $\cdots$ | - | - | -- | 18.6 |
| C0-Shift and Heat Recovery | - | 31.6 | 26.0 | 23.6 | 22.6 | 22.2 | - | 24.0 | - |
| Acid-Gas Removal | 38.5 | 47.0 | 50.6 | 46.0 | 43.7 | 42.9 | -- | 38.4 | - |
| Zinc Oxide Treatment | 4.6 | 5.7 | 5.9 | 5.4 | 5.0 | 4.9 | -- | 4.4 | - |
| Sulfur Recovery | 12.1 | 12.6 | 13.4 | 12.2 | 12.0 | 11.8 | - | 11.6 | 1.0 |
| Fuel Prucessing Section Subtotal | 230.1 | 273.7 | 228.1 | 204.8 | 195.6 | 190.7 | 104.3 | 215.2 | 124.9 |
| Power Recovery Spection |  |  |  |  |  |  |  |  |  |
| Fuel Cells Including Piping, etc. | 145.2 | 147.1 | 146.8 | 169.9 | 172.1 | 166.7 | 176.1 | 166.1 | 158.0 |
| Gas-Turbine and Steam Cycle | 91.9 | 57.2 | 95.3 | 51.5 | 50.8 | 58.3 | 81.9 | 44.1 | 73.7 |
| Inverters | 47.3 | 50.6 | 46.1 | 55.4 | 55.6 | 53.8 | 46.7 | 57.2 | 49.0 |
| Other Electrical Equipment | 25.6 | 25.6 | 25.6 | 25.6 | 25.6 | 25.6 | 25.6 | 25.6 | 25.6 |
| Power Recovery Section Subtotal | 310.0 | 280.6 | 313.8 | 302.4 | 304.2 | 304.4 | 330.3 | 293.0 | 306.3 |
| Total Process On-Site | 540.1 | 554.3 | 541.9 | 507.2 | 499.8 | 495.1 | 434.6 | 508.2 | 431.2 |

* Description of cases presented in Table 2.
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| $\Rightarrow$ | 0 | 0 | $\square$ |
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| $\Rightarrow$ | 0 | 0 | $\infty$ |
|  |  | 0 |  |



| 0 | 0 | 0 | 0 |
| :--- | :--- | :--- | :--- |
|  | 0 | 0 | 0 |
| $\infty$ |  |  |  |

CELL OPERATION

$\sim |$| 0 | $\infty$ | 0 | 0 | 0 | 0 | 0 |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| $\cdots$ | 0 | $n$ | $i$ | 0 | 0 | $\infty$ |
| $\infty$ | $\infty$ | 0 | 0 |  |  |  |



Table 4. SUMMARY OF CAPITAL REQUIRED FOR 675 MW POWER PLANT USING
COMBINED COAL GASIFICATION/FUEL
3
 1
$m$
55.4

$\begin{array}{cc}0 & 0 \\ - & \infty \\ & 0\end{array}$
$\stackrel{\square}{0}$


| 0 | $\overrightarrow{0}$ | $\dot{0}$ | $?$ |
| :--- | :--- | :--- | :--- |
| $\cdots$ | $\infty$ | 0 | $\ddots$ |
|  |  | 0 |  |



Case No*
A. Process
B. General


D. Process Contingency $\quad$ - Composite by Process Unit and State of Art -

F . Total (TPC)
Allowance for Funds During Construction (AFDC)
$\begin{aligned}= & 0.5 \% \text { (TPC - General Facilities - Project } \\ & \text { Contingencies on General Facilities) }\end{aligned}$ Contingencies on General Facilities)
Preproduction or StartUp Costs
Days Itisentory of Fuel, Catalyst, and
rial Catalyst and Chemical Charge
Cost, 164 Acres at $\$ 5500 /$ Acre
Total Capital Required (TCR) 1 Month Fixed Operating Coo's
1 Month Variable Operating Costs
1 Month Capacity Fuel $\times 0.25$
$2 \%$ of TPC
ntory Capital
60 Days Inventory of Fuel, Cataly
Chemical? at Full Rate
Initial Catalyst and Chemical cha
Land Cost, 164 Acres at $\$ 5500 /$ Act
Description of cases given in Table 2.
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OF POOR QUALITY

the "Assumptions" section of this document and are illustrated in Appendix $A b$. These assumptions were employed directly to give a consistent comparison basis. It should be emphasized, however, that variations in the assumed financial factors strongly influence the cost of electricity; further, such assumptions can affect the relative ranking of the systems.

The relative cost-of-power derived in this analysis must be used with care. Significant effort was expended in evaluating a number of alternative concepts to identify systems with relatively high overall system thermal efficiency. Yet, this system efficiency is often overshadowed by the extremely high leverage effects of capital upon cost of power.

The financial factors employed in the analysis of the cost of electricity for the various systems also tend to emphasize capital-related areas, rather than more highly efficient systems:

- The contingency allowances range from $43 \%$ to $50 \%$ of the estimated base capital cost. This assumption increases the relative capital cost charges in the electricity, and diminishes the relative importance of the cost of fuel.
- The levelized cost of electricity is taken over the first 10 years of plant life. This assumption tends to deemphasize the cost of fuel, which would continue to escalate and show greater relative importance over a 25 - or 30 -year levelized cost of electricity.
- The $65 \%$ load factor also emphasizes capital-related charges, relative to a higher load factor that might be anticipated on a base-loaded facility.

In the systems considered, the capital-related charges (including the fixed operating costs that are largely capital-driven) are approximately $70 \%$ of the cost of electricity; the coal costs, reflecting the efficiency of the system selected, represent $20 \%$ to $25 \%$ of the cost of power. Thus, with the underlying financial assumptions employed, an appreciable change in system efficiency can be readily overpowered by a moderate variation in initial capital requirement estimates.

For example, System 3 operates with a fluidized-bed gasifier in place of the entrained-bed gasifier of System 2, with the rest of the system essentially identical. System 3 had an overall system thermal efficiency of about $38 \%$, compared with $41 \%$ for System 2. Yet, because of the somewhat simpler or smaller gasifier, oxygen plant, and raw gas quench, System 3 has a process equipment cost advantage of $\$ 12$ million out of approximately $\$ 550$ million
(about $2.2 \%$ ). Yet, this small change in capital cost is sufficient to overcome the efficiency advantage of System 2, and both systems result in approximately the same cost-of-power.

It is, therefore, emphasized that mature engineering judgement must be employed in evaluating the alternative cases for cost-effective research and development, rather than absolute reliance upon the numbers that have been generated.

## Discussion of Systems Analyzed

The drawings presenting simplified process flow diagrams for the nine cases are included at the end of this discussion; these drawings are repeated in Appendix Ca, where more complete discussions of the cases are presented, along with discussions of the efficiency impacts of the various alternatives.

Case 1 - The Reference Case
The reference system for integration of coal gasification with power generation through molten carbonate fuel cells was supplied to the program by the prime contractor. It employed an entrained-flow gasifier and a simplified process configuration (Figure 2). When analyzed on the process simulator, the system provided a process efficiency of $42.1 \%$ and, when costed, resulted in a cost of electricity of $8.5 \$ / \mathrm{kWh}$. This cost of electricity is similar to that provided by the prime contractor in his base case analysis; however, the details of the cost factors are much different: The current process simulator results in much higher power output from the fuel cell but less energy recovered from the bottoming cycles.

## Case 2 - Conservative Base Case

Case 2 (Figure 3) employs the entrained flow gasifier but incorporates additional features to improve the operational stability, safety, and design conservatism. A quench step has been added to eliminate thermodynamic potential for carbon deposition and the heat exchange has been converted from countercurrent to crossflow operation. A portion of the loss in efficiency was recovered by incorporation of a shift reactor and improving the location of the fuel gas turboexpander in the system. Overall process efficiency fell to $41.6 \%$ and the cost of electricity increased to $8.7 \$ / \mathrm{kWh}$. Note that the decrease in efficiency caused only a minor change in the levelized revenue requirements; the coal accounts for only $23 \%$ of the total cost of power. The
major factor in the cost change is a $3 \%$ increase in the total capital required for the facility.

## Case 3-Fluidized-Bed Gasifier

The procese design employed for Case 2 was modified only by changing the gasifier to a fluidized-bed type; the remaining process elements were kept the same (Figure 4). Temperatures and flows varied because of the different characteristics of the gasifier. The gasifier selected was designed for minimal methane production at the 500 psi operating pressure. This methane is not reacted in the fuel cell but, rather, is only recovered as heat in the steam bottoming cycle. The overall process efficiency dropped to $38.4 \%$. However, the cost of powar remained the same at $8.7 \phi / \mathrm{kWh}$. The reduced efficiency was economically counterbalanced by only a $2.5 \%$ change in total capital requirement. This reduction in cost was due to simpler heat recovery from the offgases of the lower temperature gasifier and the reduced oxygen demand of the system.

Although the reduced cost of the system is probably directionally correct, the technique of factored estimates used in the costing procedure can not have great accuracy, Because of the high leverage of capital costs on the final price of electricity, the relatively high loss in system efficiency is not of great importance. Thus, the results of this study, particularly the comparison of Cases 2 and 3, must be used with care. Nevertheless, the use of a fluidized-bed gasifier in such a system, although apparently of lower efficiency, merits further evaluation.

Case 4 - Internal Reforming
Case 4 (Figure 5) employs the identical system used in Case 3, incorporating a low-methane, fluidized-bed gasifier, but adds the developmental concept of reforming the methane within the fuel cell with chemical and thermal integration to the fuel cell. The remainder of this system is nearly identical, except for the variations in output energy allocation. In spite of the capital-related developmental charge applied against the novel fuel cell concept, the total capital requirement dropped by over $4 \%$, the efficiency increased by 6.5 percentage points, and the overall cost of power dropped to $8.3 \phi / \mathrm{kWh}$. Apparently, the concept of internai reforming in the fuel cell is desirable, when integrated with the fluidized bed gasifier.

## Case 5-Higher Methane Production

By niodification of operating techniques, the fluidized-bed gasifier can produce higher quantities of methane (Figure 6 - a repeat of Figure 1). Such a configuration was employed in the system described above; the cost-of-power dropped to $8.2 \dot{f} / \mathrm{kWh}$.

One case not analyzed economically (Case IVa of Appenaix Ca), included a conceptual fluidized gasifier that would permit even greater methane production. Analysis of the directional trends of Cases 4 and 5 indicates that this gasifier warrants development.

## Case 6 - High-Temperature Dust Removal

The process of Case 5 was modified to include removal of dust at high temperature from the raw gasifier product (Figure 7). This appruach simplifies the system, eliminates much heat exchange and gas washing equipment, and enables the gas expansion turbine to operate at higher inlet temperatures. The overall process efficiency increased by 1.6 percentage points, the capital costs dropped slightly, and the cost-of-electricity decreased to $8.0 \phi / \mathrm{kWh}$. Therefore, it is concluded that current work on high-temperature dust removal should be accelerated.

An alternative system that was not evaluated economically employes a dust-tolerant water-gas shíft reactor (Case V of Appendix Ca). This option resulted in the same process simplicity as the high-temperature dust removal and had a similar process efficiency. The concept is relatively straightforward and only a minor portion of the capital in the plant would be impacted by developmental charges. It is, therefore, suggested that this concept also merits investigation.

Case 7 - Sulfur-Tolerant Fuel Cell
This analysis assumed that a fuel cell can be developed that will operate directly on the raw gas after departiculation and cooling (Figure 8). Catalysts for this duty have been preliminarily identified. The system is considerably simplified and overall process efficiency increased to $50.0 \%$. The cost-of-power decreased to $7.2 \phi / \mathrm{kWh}$.

It shoulid be noted, however, that the system described does not treat the sulfur in the woal. Some type of stack gas scrubber should be added to the
system. If that stack gas scrubbing costs $\$ 150 / \mathrm{kW}$, the apparent benefits of the sulfur-tolerant cell are negated.

Nevertheless, the system has merit. High-temperature sulfur removal systems (similar to those discussed later) have now been identified and tested (on a PDU scale) to provide sulfur removal in excess of EPA New Source Performance Standards for coal combustion, although not to the extreme purity required for fuel cell application. The integration of this subsystem with a sulfur-tolerant cell may have significant potential. The concept also has value as a backup position should the current high-temperature desulfurization work, directed at the extreme purities required for fuel cells, not be fruitful when scaled up.

Case 8-High-Tamperature $\mathrm{CO}_{2}$ Transfer
A concept has been identified that permits energy-efficient transfer of carbon dioxide from the hot, high-pressure fuel gas directly to the cathode inlet (Figure 9). This approach improves the purity of the gas feeding the fuel cell because the carbon dioxide concentration has been reduced and the concentration polarization within the fuel cell is minimized. By incorporation of this subsystem, the system efficiency is improved by nearly 2 percentage points. However, the capital cost of this option appears to be about $1.7 \%$ greater than without the option, negating the efficiency improvement and resulting in an identical cost of power of $8.2 \phi / \mathrm{kWh}$ (when referred to Case 5 as the starting point).

The integration of high-temperature $\mathrm{CO}_{2}$ transfer with high-temperature dust removal may be an attractive option (similar to integration of the sulfur-tolerant cell with high temperature dust removal). The improved process simplicity and efficiency of the two systems would appear to be synergistic; that is, the high-temperature dust removal improves the fuel processing section and the high-temperature $\mathrm{CO}_{2}$ removal improves the fuel cell section such that the combination should work better than either of the alternatives alone.

Case 9 - High-Temperature Sulfur Removal
Several systems for high-temperature sulfur removal are under development. The approach considered here is a spinel-based system, which regenerates directly to elemental sulfur, under development at IGT (Figure 10). It
should be noted ihat this case is not strictly comparable to the remainder of the examples - an overall process is considered that results in elemental sulfur production. Other systems have included only the efficiency of the basic system, without $t$ energy penalties associated with sulfur production and tail-gas treatment. Nevertheless, the system offers a process efficiency of $50.5 \%$ and an apparent cost of power of $7.2 \$ / \mathrm{kWh}$.

Summary
Nine systems for integration of coal gasification with molten carbonate fuel celis have been evaluated econcrically to assess potential for cost sffective research in this application. The analysis is constrained by the high leverage of capital cost upon the cost-of-electricity and the necessary inaccuracies in the factored-costing approach utilized. The financial factors assumed for the analysis also impact the relative ranking of aiternative systems. The data, however, when combined with mature engineering judgement, Indicate that a number of process subsystems appear to offer merit for future development:

- Internally reforming fuel cell, chemically and thermally integrated, to be incorporated with fluidized bed gasifiers
- High-temperature desulfurization
- High-temperature dust removal
- High methane content, single-stage fluidized-bed gasifier
- Dust-tolerant shift catalyst
- High-temperature $\mathrm{CO}_{2}$ transfer
- Sulfur-tolerant fuel cell.

Additionally, a number of minor process improvements have been identified that, although apparently desirable, have not teen specifically analyzed in the economic assessment.

- Improved data base on carbon deposition phenomena
- Countercurrent heat exchangers for hazardous, high-temperature gases
- Improved catalytic combustion
- Continued systems analysis.
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Figure 2. process flow diagram of base case
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Figure 10. PROCESS FLOW DIAGRAM INCORPORATING HIGH-TEMPERATURE SULFUR REMOVAL

## CONCLUSIONS

Based upon the conduct of the project and the results obtained, the following conclusions have been drawn:

- The technique of systems analysis is a cost-effective approach for comparing the efficiency of alternative systems for power production from coal using gasification and molten carbonate fuel cells.
- In this system, the results are extremely sensitive to the process assumptions
a. The systems analyst must use great care to assure that two systems are identical in all respects except for that quantity being varied.
b. Caution must be exercised in comparing work of different investigators because of the probable difference in initial assumptions.
- Overall system efficiencies, for approximately the same system, may vary from $46 \%$ to $57 \%$, depending upon the initial assumptions employed.
- The cost of power is highly leveraged by capital cost, minimizing the impact of system efficiency. Additionally, the choice of financial assumptions does not tend to favor systems of higher efficiency.
- A 3-percentage-point loss in efficiency, from $41 \%$ to $38 \%$, is counterbalanced by only a $2.5 \%$ change in capital cost.
- The factored costing techniques employed, although directionally correct, cannot have high accuracy.
- Knowledgable engineering judgment must be employed in the interpretation of the relative cost data.
- Several systems were found that indicate promise for additional research and development. Such recommendations are listed in the following section.
- The incorporation of a methane-producing fluidized-bed gasifier and an internalling reforming fuel cell shows a 4.2-percentage-point gain in efficiency and a $10 \%$ reduction in capital cost when comparea with a conservative analysis of the reference case.
- The incorporation of high-temperature dust removal adds nearly 2 percentage points of process efficiency, without a capital cost penalty, because of improved placement of the fuel gas turboexpander. Additionally, this concept permits incorporation of other advanced concepts, listed below.
- The incorporation of high-temperature sulfur removal, together with high temperature dust removal, improves the system efficiency by another 2.5 percentage points with a significant capital savings due to system simplicity, resulting in a preferred cost of power.
- A number of other subsystem elements were identified that either a) were not costed so relative value could not be determined or b) showed lesser efficiency and/or cost gains but, in total, might be significant.
- Improved definition of the carbon deposition phenomena so that the quench system might be eliminated
- Development of countercurrent heat exchange for high-temperature, toxic, hazardous materials
- Development of dust-tolerant water-gas shift reactors
- Development of a sulfur-tolerant fuel cell
- Development of high-temperature carbon dioxide removal
- Development of a novel, single-stage, fluidized-bed gasifier that produces greater quantities of methane.
- Optimization of a subsystem element does not necessarily result in a preferred overall system.
- Optimization of the fluidized bed gasifier to the limits of currently available designs, compared to the conservative designs specified, did not improve the overall system efficiency.
- Systems with highest overall efficiency had relatively poor fuel cell operating characteristics because of high back pressures of carbon dioxide and water vapor in the fuel.

Additional systems have been conceived that are directed at minimizing the primary areas of energy loss in the system. These systems could not be evaluated within the budget constraints of the progran.

## RECOMMENDATIONS

The recommendations presented below are based upon engineering assessment of the direct calculated results of the program and include factors for both efficiency and cost improvement of novel processing schemes in recommending where identified R\&D may be fruitful. Also, additional systems analysis work is suggested.

## Identified R\&D Effort

A number of mechanical and/or chemical processing suggestions appear to offer promise for improving the efficiency and, in some cases, the costeffectiveness of production of electricity from coal through molten carbonate fuel cells. The suggestions are briefly outlined below and discussed in detail within the report. The suggestions below are not prioritized.

Improved Defindtion of Carbon Deposition Phenomenon
The raw gas from the gasifier, and also the purified fuel cell feed gas, have been humidified to the extent required to render the gases thermodynamically stable and eliminate the potential for carbon deposition.

The data base underlying the carbon deposition phenomenon is relatively sparse and includes only methane cracking and the Boudouard reactions, not the combination of gases that will be experienced in such a system. Further, a potential may exist for the inhibition of carbon deposition in the presenco of sulfur compounds.

Although systems have been developed that nearly overcome the efficiency penalty inherent with quenching the raw gas, these systems are cumbersome and expensive.

## Cost-Effective, Countercurrent, High-Temperature Gas-Gas Heat Exchange

Although countercurrent heat exchange between combustion products and combustion air is often practiced in the power industry, it is rarely employed in chemical engineering service, particularly with hazardous, toxic, or flammable materials at elevated pressure, because of the extreme complexity, poor maintainability, and costs of available designs. The problem with such units is the thermal expansion of the shell and tube components and the available means to allow for differential expansion within the exchanger. Should such units be available for operation with toxic, explosive gases at elevated
pressure, the heat exchange within the system would be simplified, efficiency would be improved, and cost of service would be reduced.

## The Combination of Methane-Producing Gasifiers and Internally Reforming Fuel Cells

A fluidized-bed gasifier, compared with an entrained flow gasifier, has lower parasitic power demands and is more efficient in converting the coal to fuel gas species rather than heat. In a conventional MCFC cell, however, the methane produced in such a gasifier cannot be readily consumed electrochemically to power. Introduction of reforming capability within the anode compartment of the cell, thermally and chemically integrated with the fuel cell operation, perwits substantial improvement in overall system performance. Initial R\&D efforts at internally reforming fuel cells are promising. Efforts sholid be accelerated, because the improved cost-wf-electricity appears to be significant.

## High-Methāne-Content Gasifiers

Patent action has been initiated on conceptual, single-compartment, fluidized-bed gasifier that should produce higher methane content in the fuel gas through control of the mixing patterns within the single fluidized bed. The gasifier cost should be similar to a conventional, singleastage, fluidized bed gasifier. If developed, such a gasifier would permit improved efficiency and lower cost in the overall system, when integrated with an internaily reforming fuel cell.

## High-Temperature Departiculation

By removing particulates from the raw gas while it is hot, the turboexpander can be moved within the system to operate on a hotter gas and provide greater power recovery. Process efficiency can be improved with this development; cost-of-power is apparently reduced.

## Dust-Tolerant Water-Gas Shift Reactors

Dust-tolerant catalytic reactors have been conceptualized and appear to offer little cost penalty relative to conventional systems. If implemented in the overall system, the process efficiency will improve; moreover, the system complexity is significantly reduced and the development appears to be costeffective.

## High-Temperature Desulfurization

The concept of high-temperature desulfurization, when used in conjunction with high-temperature particulate removal, offers improved system efficiency relative to currently available, low-temperature sulfur removal processes. The improvement in efficiency, however, is not the major benefit. Rather, this approash eliminates most of the heat exchangers, pressure vessels, and contacting towers associated with gas cooling, thus providing a significant cost reduction in the selling price of the electrictity.

Sulfur-Tolerant Fuel Cell
If a sulfur-tolerant fuel cell could be developed and integrated with high-temperature departiculation described above, the overall system efficiency would be improved and the overall system significantly sfmplified. The cost of such a system is currently conjectural, but the benefits appear to warrant an effort in this direction.

## High-Temperature $\mathrm{CO}_{2}$ Transfer

A subsystem for transfer of carbon dioxide from the fuel gas to the cathode feed has been concelved and analyzed. The overall system efficiency improved by over 2 percentage points; however, with the high leverage of capital costs used in this analysis, the bencfit did not outweigh the cost. Nevertheless, the $\mathrm{CO}_{2}$-transfer system appears to offer merit (particulariy in advanced systems that are beyond the scope of this program) and should be further evaluated.

## Improved Catalytic Combustion

The operating temperature range of commercial catalysts in the combustion of the anode tail gas requires significant heat exchange equipment for temperature control. Non-noble catalysts with lower light-off temperature and higher maximum-temperature limits are required for system simplification and cost reduction.

Continued Systems Analysis
Several systems were identified, but could not be evaluated within the time and budget constraints of the program. Specific areas of evaluation include the following:

## Recycle Systems

- Effective $100 \%$ conversion, rather than $85 \%$ conversion
- Recover latent heat of water vapor
- Air Blown Systems
- Save cost of oxygen system
- Use fuel cell as heat pump
- Incorporation of membranes
- The total syetem - from coal in the ground to delivered electricity
- May be cost effective to manufacture methane in large, central, mine-month facilities, transport methane, and produce electricity in smaller substations
- Relative transportation costs of coal, electricity, and gas, favor gas
- Makes maximum use of economies of scale.

The suggested effort is discussed in greater detail balone

## Improved Fuel Cell Simulator

The calculated system efficiency if sensitive to the fuel cell performance; yet the fuel cell simulator is simplified and based on out-of-date data. Additionally, the overall system is quite sensitive to the cathode offgas temperature, but the current simviator does not separately calculate this parameter. Current, publishable fuel cell performance data should be acquired and incorporated into an improved simulator.

Identified Systems Analysis Effort

## A1r-B1own Systems

It was discovered during the program that the molten carbonate fuel cell is an excellent heat source for a heat engine. The theoretical Carnot effielency from a fuel cell exhaust temperature of $1300^{\circ} \mathrm{F}$ approaches $69 \%$ the maximum fuel cell efficiency, considering isentropic losses, is 79\%. Thus, the heat content of the exhaust gases, when recovered by a gas turbine and a steam bottoming cycle, can approach high theoretical efficiency. Note that transferring the heat to the exhaust gases is preferred to a cathode recycle that exhausts heat directly to a steam cycle.

The system considered is to feed the gasifier with af.r, rather than oxygen, and allow the gas to pass through the total cycle. The gasiffer off-gas would contain approximately $50 \%$ nitrogen, which would be a significant diluent and increase the size of much of the processing equipment. Additionally, it would increase the polarization of both the anode and the cathode of the fuel cell. However, significant thermal energy will be stored in this nitrogen at the fuel cell cathode exhaust, and this energy may be recovered effectively by the gas turbine bottoming cycle downstream of the fuel cell. The system appears to offer merit; however, the relative tradeoff of positive and negative features cannot be ascertained without a careful comparison on the overall process simulator.

An alternative system considers the use of an air-blown gasifier with semipermeable membrane separation of the fuel hydrogen from the remainder of the species in the gas. Conceptually, the system would consist of a gasifier, quench, heat recovery, dust-tolerant shift reaction, cooling, and sulfur removal. The high-pressure fuel gas can then be separated by a semipermeable membrane recovering a hydrogen-rich stream. The membrane would operate between the pressure of the sweetened gas and the fuel cell operating pressure for the permeated hydrogen. Depending upon the operating conditions selected for the membrane, either a moderate fraction of the hydrogen could be recovered at high purity, or a much higher fraction of the hydrogen could be recovered at lower purity. The primary impurity in the hydrogen would be carbon dioxide, which has a moderate transport rate through commercially available membrane materials. Both the permeate hydrogen and the non-permeated, low-Btu fuel gas would then be reheated through the heat exchanger train. The hydrogen would pass to the fuel coll after zinc oxide treatment; the low-Btu gas could be fired into a combined cycle system, using hot cathode off-gas as the oxidant. A significant increase in earegy recovery from the exhaust gas turbine would be expected because of its much higher inlet temperature.

Note that the above system has increased merit if high-temperature membranes (which are now being developed) were available. After high-temperature sulfur removal, the hydrogen could be recovered directly at elevated temperature and passed to the fuel ceil. Cell operating voltage wculd be higher than in the high-temperature sulfur removal case considered herein because of the cleaner fuel gas. The cost associated with the heating and cooling trains would be eliminated.

## Recycle Systems

Analysis of the energy balances of the various systems considered indicates that the major losses in the system are 1) the $15 \%$ of the fuel value that is combusted directly and 2) the latent heat of vaporization of water vapor that is discharged through the cathode to the stack. A number of systems can be envisioned that would employ recycle to enhance the water vapor balance.

On the total systems basis, the primary fuel is carbon, but the fuel cell only consumes hydrogen. The carbon values are converted into hydrogen reductant by reacting with water. Because these reactions take place at elevated temperature, the reactant water muse have been vaporized and the latent heat of that water vapor is lost as available energy to the system.

Carbon fuel is converted to hydrogen fuel by the steam-carbon reaction, in the gasifier, and by the water-gas shift reaction, either within an external shift reactor or within the fuel cell.* Also, additional water vapor was added to the fuel cell feed to avoid carbon deposition. All of the water added to the system - either for the chemical reactions or to maintain carbon stability in the off-gas mas been vaporized. That heat of vaporization is a heat debit to the system, either in raw gas cooling or in the latent heat present in the final stack from the system. That latent heat consumed feed energy that was not recoverable to product power.

By recycling the hot, wet, anode exhaust back upstream in the system, the energy penalty for water vaporization can be minimized. As discussed in Appendix $C b$, the theoretical system need not require water make-up or discharge; rather, it may be in water balance. By recycling the wet anode exhaust upstream, all of the hydrogen value required for the fuel cell operation can be maintained in the recycle loop, without adding heat to vaporize water. Additionally, all of the fuel value in the raw gas is eventually converted to eleciricity in the fuel cell, without burning the anode exhaust into the Carnot-limited steam cycle.

[^2]Case $X$ of Appendix Ca was an initial attempt at a recycle system. In this case, the fuel cell was fed with dry, nearly $\mathrm{CO}_{2}$-free gas by recycle of the spent anode tail gas back to the feed of the acid-gas removal system. The system permitted $100 \%$ recovery of the hydrogen value in the fuel within the fuel cell and eliminated the need to add steam to the fuel cell feed, thus minimizing some of the heat losses from the system. Although that system had high fuel cell voltage and power recovery, the approach was found not to be a preferred alternative.

Other points for reinjection of the spent anode exhaust would result in further minimization of the water demand. The gas could be fed directly into the raw off-gas of the gasifier, displacing the steam required for quenching. Alternatively, the spent anode off-gas could be fed directly into the gasifier itself, displacing all of the steam or water required for the gasifier or the quench system. The chemistry discussed in Appendix Cb illustrates that this approach is feasible; preliminary calculations indicate that it is almost possible, although a small bleed stream must be taken from the recirculating gas loop to eliminate nitrogen build-up from the system.

Either approach would require removal of carbon dioxide from the recirculating loop and, preferably, would require the operation of the fuel cell at the gasifier operating pressure. In order to maintain the water in the vapor phase in the recirculating loup, a high-temperature $\mathrm{CO}_{2}$ recovery system is required. The proper location for this recovery system is on the anode discharge, where the partial pressure of carbon dioxide would be the greatest (assuming that the gasifier and fuel cell operate at the same pressure). Sufficient carbon dioxide could be transferred from the recirculating anode loop to the cathode feed to close the carbon dioxide balance of the system.

Preferably, the fuel cell should operate at the pressure of the gasifier. The volume of tail gas from the anode is mach greater than the feed; therefore, expansion and recompression would be uneconomical. Conversely, the volume of the cathode exhaust would be similar to its feed, so the penalty of air compression should not be severe. One of the reasons that improved recycle systems were not considered in the current program was the nonapplicability of the current fuel cell simulator to high-pressure fuel cell operation. The simulator, although relatively accurate at 150 psi, showed significant errors at lower operating pressures. The extrapolation to higher
operating pressure would, therefore, be tenuous. Part of the required program would be the development and evaluation of a fuel cell similator that would operate well at elevated pressures.

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APPENDIX Aa. Reference Case

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# BASE CASE REFERENCE DESIGN 

IND ECONONIC ASSUMPTIONS
FOR A COAL-BASED
FUEL CELL POHER PLANT

## Jet Propulsion Laboratory 4800 Oak Grove Drive Pasadena, California 91109

1. Description of Base Case Design

The base case, as shown in Figure 1 is a relatively simple two pressure level configuration incorporating a Texaco gasifier and gas cleanup system operating at 600 psia and a fuel cell system operating at 100 psia. Data on the composition, pressure, and temperat:re of designated streams is given in Table 1. The salient feature of this system is the injection of low pressure steam into the anode fuel gas to create a carbon-free equilibrium composition prior to entry into the fuel cell.

The Texaco gasifier is an entrained bed gasifier fed with a coal/water slurry and oxygen producing a high temperature fuel gas. A performance summary of the Texaco gasifies is given in Table 2. Product gas at $2450^{\circ} \mathrm{F}$ leaves the gasifier and passes through the heat recovery steam generator. Downstream of the steam generator, the raw gas flow is divided into two streams, one passing through a steam generator heat exchanger and the other passing through a regenerative heat exchanger for reheating clean gas. These heat exchangers are followed by a wet particulate scrubber in which the gas enters at a temperature slightly above its dew point. Following the scrubber is a second parallel arrangement of steam generators and regenerative heat exchangers, followed by a gas cooler, knockout drum, and the acid gas removal subsystem.

Clean fuel gas leaving the acid gas removal subsystem is regeneratively reheated to a temperature of $750^{\circ} \mathrm{F}$ and passed through a ZnO polishing scrubber to remove any residual sulfur compounds. The gas is then admitted to an expander turbine in which pressure is reduced to the fuel cell pressure. Anode inlet gas is conditioned to carbon-free equilibrium composition by mixing it with steam extracted from the steam turbine and then it is heated by the anode outlet gas stream. The anode discharge stream is mixed
$\qquad$ IMTENTONALLK BL AMA


|  |  |  |  | BASE CA | CASE 'FLOM | Table 1 Stream gas | COMPO | SITIONS |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | 1 | 2 | $2^{\prime}$ | 3 | $3{ }^{1}$ | 4 | 5 | - 6 | 7 | 6 | 9 | $10$ |
| $\mathrm{H}_{2} \mathrm{MF}$ | 0.288 |  |  |  | $\longrightarrow$ | 0.361 |  | 0.360 | 0.034 |  |  | 유잉 |
| CO MF | 0.425 |  |  |  | $\longrightarrow$ | 0.532 |  | 0.116 | 0.017 |  |  | $\bigcirc$ |
| $\mathrm{CH}_{4} \mathrm{MF}$ | 0.001 |  |  |  | $\longrightarrow$ | 0.001 |  | 0.0005 | 0.0003 |  |  | 앙 |
| $\mathrm{C}_{2} \mathrm{H}_{4} \mathrm{MF}$ <br> $\mathrm{C}_{2} \mathrm{H}_{6} \mathrm{MF}$ |  |  |  |  |  |  |  |  | . |  |  |  |
| $\mathrm{CO}_{2} \mathrm{MF}$ | 0.087 |  |  |  | $\longrightarrow$ | 0.096 |  | 0.219 | 0.509 | 0.110 |  | 0.137 |
| $\mathrm{H}_{2} \mathrm{O} \mathrm{MF}$ | 0.179 |  |  |  | $\longrightarrow$ |  | 1.00 | 0.300 | 0.436 | 0.218 |  | 0.207 |
| $\mathrm{N}_{2} \mathrm{MF}$ | 0.008 |  |  |  | $\longrightarrow$ | 0.010 |  | 0.005 | 0.004 | 0.594 | 0.790 | 0.565 |
| $\mathrm{H}_{2} \mathrm{~S}$ MF | 0.010 |  |  |  | $\longrightarrow$ |  |  |  |  |  |  |  |
| COS MF | 0.001 |  |  |  | $\cdots$ |  |  |  |  |  |  |  |
| $\mathrm{O}_{2} \mathrm{MF}$ |  |  |  |  |  |  |  |  |  | 0.079 | 0.210 | 0.091 |
| $\mathrm{HH}_{3} \mathrm{MF}$ | 0.002 |  |  |  | $\rightarrow$ |  |  |  |  |  |  |  |
| Total Moles/ Mole Raw Gas | 1 | 0.79 | 0.21 | 0.73 | 0.27 | 0.80 | 0.70 | 1.50 | 2.10 | 4.55 | 3.41 | 19.12 |
| Pressure PSIA | 600 |  |  |  |  |  | 105 | 100 |  | 99 | 14.7 |  |
| Temp ( ${ }^{\circ} \mathrm{F}$ ) | 2450 | 800 | 800 | 330 | 330 | 75 | 600 | 1000 | 860 | 1300 | 60 | 1120 |

Table 2
TEXACO GASIFIER PERFORMANCE SUMMARY

| GASIFIER PRODUCT GAS COMPOSITION (Mole fraction) |  |  |
| :---: | :---: | :---: |
| $\mathrm{CH}_{4}$ | 0.0008 |  |
| $\mathrm{H}_{2}$ | 0.2884 |  |
| CO | 0.4245 |  |
| $\mathrm{CO}_{2}$ | 0.0871 |  |
| $\mathrm{H}_{2} \mathrm{~S}$ | 0.0101 |  |
| COS | . 0.0006 |  |
| $\mathrm{N}_{2}$ | 0.0078 |  |
| $\mathrm{H}_{2} \mathrm{O}$ | 0.1788 |  |
| $\mathrm{NH}_{3}$ | 0.0019 |  |
| FEEDS |  |  |
| $0_{2}: 0.84 \mathrm{Lb} / \mathrm{Lb}$ Coal |  |  |
| Water: $0.44 \mathrm{Lb} / \mathrm{Lb}$ Coal |  |  |
| Coal/Water Slurry Feed Temperature |  | $140^{\circ} \mathrm{F}$ |
| Oxygen Feed Temperature |  | $300{ }^{\circ} \mathrm{F}$ |
| Product Gas Temperature |  | $2450^{\circ} \mathrm{F}$ |
| Moles Product gas/Lb Coal |  | 0.10809 |
| $\mathrm{HHV}\left(\mathrm{CO}+\mathrm{H}_{2}+\mathrm{CH}_{4}\right)$ | HHV COA 1 | . 772 |

with air from the botzoming cycie gas turbine compressor and passed through a catalytic burner, to combust the remaining $\mathrm{H}_{2}, \mathrm{CO}$ and any $\mathrm{Cli}_{4}$. The burner discharge stream is mixed with additional air and cooled recycled cathode discharge gas before it is admitted to the cathode. The cathode discharge stream, after being partially recirculated thrsugh a steam generator heat exchanger for removal of fuel cell waste heat, is admitted to the bottoming cycle gas turBine. Downstream of this turbine is a compressor discharge preheater and an economizer heat exchanger for recovery of exhaust heat ahead of the stack. Steam generation for a $2400 \mathrm{psi} / 1000^{\circ} \mathrm{F} / 1000^{\circ} \mathrm{F}$ reheat steam bottoming cycle is accomplished in the economizer (feedwater heating), the gasifier heat recovery steam generator (final feedwater heating and evaporation) and in the bottoming cycle heat exchanger (superheat and reheat) which cools the fuel cell cathode recirculation stream.

The gasifier heat recovery steam generator heat exchanger, a standard feature of the Texaco gasification system is a combination radiant/convective unit with slag solidification and separation in the radiant portion and further gas cooling in the convective section. Tube metal temperatures are maintained below $800^{\circ} \mathrm{F}$ by restricting the heat exchanger auty to final feedwater heating and evaporation. Low pressure steam for stripping use in the acid gas removal process is generated in the secondary heat exchangers operating in parallel with the clean gas regenerative heat exchangers.

Air discharge flow from the gas turbine compressor is preheated dy heat exchange with the expansion turbine discharge in order to increase the amount of high level heat available to the steam cycle through the cathode recirculation loop heat exchanger.

The fuel cell anode operates at 0.85 utilization of the CO and $\mathrm{H}_{2}$ in the fuel gas. Unreacted CO and $\mathrm{H}_{2}$ in the anode exhaust, together with amall amount of methane generated in the gasifier which passes through the anode, are burned in the catalytic combustor. Most of the $\mathrm{CO}_{2}$ required by the cathode is generated by electrochemical conversion of the fuel in the anuie, however, small contributions are produced in the gasffier and in the catalytic combustor.

The gasifier pressure level of this system ( 600 psi) is that of an established Texaco design. It is also. a level which is suitable for relatively low cost heat exchangers in the heat recovery train, and for a Felatively $10 w$ cost physical absomption type of actd gas removal process. Power recovery in the fuel gas expander turbine, in which pressure is reduced to the level of the fuel cell, exceeds the power required by the intercooled oxygen eampressors in the oxidant supply to the gasifier.

The fuel cell perssure level ( 100 psi ) has been selectad at an approximately optimized value for suximpm power output from the bottoming cycle. Similarly, the overall excess afr ratio (100\%) hes been chosen to maximize the combined output of the gas and steam turbine generators.

Design requirements fif the acid gas removal process specify a reduction cf sulfur bearing gas species to a level less than 1 ppm ( 0.1 ppm), and that the loss of $\mathrm{CO}_{2}$ from the clean gas stream not exceed $12 \%$. It is also desirable that stripping steam requirements be low in order to minimize or avoid the need for turbine extraction steam to supplement that wich can be generated from the lower temperature level heat sources in the heat recovery
train. A single stage Selexol process appears to be capable of meeting these requirements for the conditions of this cycle. Some problem with $\operatorname{COS}$ removal may exist, but if necessary, final COS removal can be handed in the ZnO polishing units placed downstream of the clean gas regenerative heat exchangers.

An overall energy balance is given in Table 3. Altnough this system provides a modest fuel cell output ratio of 0.30 , it does achieve an excellent ratio of waste heat conversion in the gas and steam turbine bottoming cycle. Thus, very little low level heat is uselessly rejected in the cooling train. The net efficiency* of this system is 46.7\%, which is considered satisfactory for a near term plant and would probably be increased by advancements in molten carbonate fuel cell technology.

Compared to ofher aiternative cycles, this system configuration has an attractive simplicity. In addition, the gas composition at the fuel cell anode inlet is similar to that of fuel gases that have been used in laboratory testing of molten carbonate fuel ceils. Thus, uncertainties relative to carbon and methane formation and relative to the aceuracy of fuel cell voltage predictions are minimized.

The principal disadvantage of this system is the calculated fuel cell DC voltage of 0.69 volts (at the design current density of $160 \mathrm{~mA} / \mathrm{cm}^{2}$ ). Fuel cell voltage this low may result in electrochemical corrosion phenomena within the fuel cell stack, Although improvements in molten carbonate fuel cell

[^3]
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Table 3.
GAS STREAM ENERGY LWLANCE AND SYSTEM PERFORMANCE SUMMARY

| Energy Inputs | Energy Input | Energy Output |
| :---: | :---: | :---: |
| Coal HHV Input | 1.0 |  |
| Coal $/ \mathrm{H}_{2} \mathrm{O}$ Oxidant Sensible Energy | 0.008 |  |
| Injection Steam Energy | 0.144 |  |
| Plant Compressors | 0.02 |  |
| Total Energy Input to Gas Stream | 1.172 |  |
| Energy Outputs |  |  |
| Fuel Cell DC Output |  | 0.305 |
| Gas Tubine Shaft Output |  | 0.121 |
| Heat Delivered to Steam Turbine Cycle |  | 0.450 |
| Heat Available for Stripping Steam Generation |  | 0.011 |
| Stack Loss |  | 0.223 |
| Low Level Heat Rejection in Gas Heat Recovery Train | . | 0.016 |
| Residual Heat Loss |  | 0.046 |
| Total energy Output |  | 1.172 |


| Periormance Summary |  |
| :---: | :---: |
| ETectric Generation Outputs |  |
| Fuel Cell AC Output | 0.299 |
| Gas Turbine Generation Output | 0.119 |
| Steam Turbine Generation Output | 0.133 |
| Gross Electric Output | 0.551 |
| Auxiliary Power Requirements |  |
| Oxygen Plant | 0.034 |
| Oxygen Compressors | 0.015 |
| Plant Gas Compressors | 0.02 |
| Other Auxiliary Power | 0.015 |
| Total Auxiliary Power | 0.084 |

Plant Efficiency $=0.551-0.084=0.4 \epsilon$ Fuel Cell DC Voltage: 0.69
performance will probably ameliorate this concern in the future, the present uncertainty in predicting the voltage level at which this electrochemical corrosion will occur provides impetus for developing system configurations that result in higher fuel cell voltages than are currently predicted for this system configuration.
II. Technical Assumptions Used in Base Case Design For the Base Case the following assumptions apply:

## 1. Fuel Stack Performance

- Fuel Cell Temperatures

The anode inlet temperature is $1000^{\circ} \mathrm{F}$. Cathode outlet temperature is $1300^{\circ}$ f for this system and the cathode iniet temperature is selected to provide an anode outlet temperature under counterflow conditions of $1150^{\circ}$.

## - Carbon Formation Criterion

The anode inlet gas composition satisfies the criterion of freedom from carbon depositior. under the condition of complete C-H-O equilibrium.

- Methane Formation

It is assumed that the kinetics of the methanation and reforming reactions are sufficiently slow inside the anode stream of the fuel cell under load that methane can be treated as an inert species for purposes of determining gas composition variation through the cell anode.

- Fuel Cell Average Curient Denstty

The design value of the fuel cell stack average current density is $160 \mathrm{~mA} / \mathrm{cm}^{2}$.

- Calculation Procedure for Cell Terminal Voltage

Cell terminal voitage is calculated by use of the fuel cell nodal computer program deseribed in EPRI Report EM-1670. For
the Base Case, the fuel cell was represented by 10 segments. Nernst voltage is calculated for each node on the basis of average nodal anode and cathode gas concentration and the local temperature. Terminal voltage is determined by an iterative prosedure which establishes the current density distribution such that the difference between local Nernst voltage and the product of the polarization constant and local current density is equal for all segments. The program is capable of handing counterflow, cofiow or crossflow relationships between the anode and the cathode gas streams.

- Cell Polarization factor

The cell polarization constant for use in the calculation of cell voltage has been detemined from an empirical correlation of state-of-the-art MCFC test data.

0
Fuel Cell Stack Inverter
A D.C. to $A_{F} C$. power conversion efficiency of 0.98 is assumed.
2. PlantAuxiliary Power Requirements

Auxiliary power requirements are assumed to consist of the following:

- Oxygen Plant

Oxygen plant power is assumed to be 108\% of the power for
electrically driven high efficiency air separation process
compressors of 6.8 pressure ratio.

- Oxygen Compressors

Electrically driven high efficiency eompressors with three stages of intercooling are assumed.

- Plant Gas Recirculation Compressors

High efficiency electrically driven compressors are assumed.

- Additional auxiliary power for acid gas removal pumps and compressors, coal handling equipment, gasifier auxiliaries, etc., is assumed to equal 1.5 percent of the coal higher heating value (HHV) energy (approximately 3\% of the plant gross output).


## 3. Gas Turbomachinery Components

- Compressors

Efficiency is assumed to be 0.88 .

- Turbines
. Efficiency is assumed to be 0.92.

4. Electrical Machines

All motors and generators are assumed to have an efficiency of 0.98.
5. Acid Gas Removal Processes

- Gas Purification

Processes are assumed to remove all sulfur bearing species and
HCN to less than 1 ppm.

- Stripping Steam Requirements

A minimum requirement of 0.13 lbs of 50 psig saturated steam per pound of coal was assumed. This assumes the combined use of steam and $\mathrm{N}_{2}$ for stripping. This corresponds to an energy requirement of 0.012 of the coal HHV, and $80 \%$ of this energy must be available above a temperature level of approximately $330^{\circ} \mathrm{F}$. For systems similar to the Base Case, the 50 psia steam energy available may be lower than the stripping steam requirements. This would require the excess to be supplied by extraction from the steam turbine, at a cost per pound of coal of approximately 2 percentage points system perfomance loss per pound of steam required.

- $\mathrm{CO}_{2}$ Recovery

The Base Case employs a one stage acid gas removal process and $88 \% \mathrm{CO}_{2}$ recovery is assumed.
111. Economic Analysis Assumptions 8 Methods to be Used

1. Capital costs include the following basic components:

- TOTAL PLANT COST (TPC)
- Process (On-Site) Capital
- General Facilities (Off-Site) Capital
- Engineering and Hone Office Overhead Inciuding Fee
- Process Contingency
- Project Contingency
- TOTAL CAPITAL REQUIREMENT (TCR)
- Total Plant Investment
- Prepaid Royalties
- Preproduction (Start-up) Costs
- Inventory Capital
- Initial Chemical and Catalyst Charge
- Allowance for Funds Dur'ng Construction
- Land

Process capital is the total constructed cost of all on-site fuel processing and power generating units including all direct and indirect construction costs. Capftal costs for fuel processing items can be scaled from previous literature sources or in-house data, according to the following rule:

Cost Unit $A=\operatorname{Cost}$ Unit $B \times\left(\frac{\text { Size Unit } A}{\text { Size Unit } B}{ }^{C}\right.$

Scaling exponent $C$ and cost basis for several fuel processing units are given as follows:

| Fue] Processing Unit | Cost Base | Scaling Capacity Factor | Fraling Exionent $C$ |
| :---: | :---: | :---: | :---: |
| Oxygen Plant | AP-642* | Ton/Day $\mathrm{O}_{2}$ | 0.56 |
| Coal Storage \& Reclaiming/ Handling $\&$ Preparation | AP-1543* | Ton/Day Coal | 0.78 |
| Gasification \& Ash Handling | AP-1543* | Ton/Day Coal | 0.60 |
| Gasifier Gas Cooling |  | Gas Molar flow | 0.82 |
| Gas Cooling 8 Anmonia Scrubbing |  | Gas Molar flow | 0.67 |
| Acid Gas Removal | AP-1543* | Gas Molar flow | 0.60 |
| ZnO Unit |  | Gas Molar Flow | 0.65 |
| Sulfur Recovery | AP-1543* | Gas Molar flow | 0.60 |

The capital cost of the fuel cell should be estimated as if it were a "mature" technology; f.e., the cost would be that of the "nth" fuel cell unit and not the first, second, etc., unit ever to be built.

Seneral Facilities Capital includes roads, buildings, shops, laboratories, etc., and are generally in the range of $\mathbf{5 0 2 0 \%}$ of the Process Capital Cost. For this analysis, $10 \%$ should be used.

Engineering and Home Office Overhead Including Fees is generally about 10-15\% of the process capital. For this analysis, $10 \%$ should be used.

[^4]Process contingencies include costs added to Process Plant Investment for improved technology. Process Contisgencies for those units considered iaproved are as follows:
Gasification - conmercial units operated ..... 5\%

- 100-1000 TPD plant operated ..... 15\%
- 10-100 TPD pilot plant operated ..... 25\%
- concept with bench scale data ..... 50\%
- new concept with limited data ..... 60\%
Ash Handling ..... 5\%
High Temperature Gas Cooling ..... 15\%
High Temperature Sulfur Cleanup ..... 50\%
Tail Gas Treating ..... 5\%
Molten Carbonate Fuel Cell (Base Case) ..... 50\%
Molten Carbonate Internal Reforming Fuel Cell ..... $60 \%$
Other process contingencies san be cosed as follows:
State of Technology Devel opment
Percentage of Installed Section Cost
New concept with limited data ..... 60\%
Concept with bench-scale data available ..... 50\%
Small pilot plant data (e.g., 1 MW ) avallable ..... 25\%
A ful: size module has been operated (e.g., 10.100 MW ) ..... 25\%
Process used connerciei ivy with different feed or application ..... 5\%

Project Contingency includes costs added to the Total Plant Cost that would result from a more defintive design. A $30 \%$ Project Contingency cost should be used for this analysis.

Prepaid royalties include process royalty fees; a value of $0.5 \%$ of the Process Capital (exciuding contingencies) should be used for this anelysis.

Preproduction, or Start-up Costs, includes the following:
a) One month fixed operating costs (operating and maintenance labor, administrative and suppoft labor, and maintenance materials);
b) one month of variable costs (consumables) at full capacity exciuding fuel;
c) twenty-five percent of full capacity fuel cost for one month;
d) two percent of the TPC.

Inventory Capital includes the value of 60 days inventory of fuels, other consumables, and by-products at-full load (100\% capacity).

Initial Chemical and Catalyst Charge Costs include the initiai cost of the charge of catalysts or chemicals contained wititin the process equipment.

- Allowance for Funds During Construction is based on the annual interest: rate with annual end-of-year compounding and the following construction expenditure schedule:

| Year | Percent of Total <br> Plant Cost |
| :---: | :---: |
| 1 | $331 / 3$ |
| 2 | $331 / 3$ |
| 3 | $331 / 3$ |


| Year | Mid-1981 |
| :---: | :---: |
| Debt/Equity Ratio | 50/50 |
| Debt Cost | 8r/Yr. |
| Preferred Stock Ratio | 15\% |
| Preferred Stock Cost | 11\%/Yr. |
| Common Stock Ratio | 35\% |
| Common Stock Cost | 15.3\%/Vr. |
| Discount Rate | 12.5\%/Vr. |
| Federal and State Income Tax Rate | 50\% |
| Property Taxes and Insurance | 2\%/Yr. |
| Investment Tax Credit | 10\% |
| Book Life | $30 \mathrm{Yrs}$. |
| Tax Life | 15 Yrs. |
| Inflation Rate | 8.5\%/Yr. |
| Real Escalation Rate | 0\%/Yr. |
| Total Plant Capactty | 675 MH |

2. Operating costs are based on the following components:

0 FIXED

- Operating Labor
- Maintenance Costs
- Overhead Charges
- VARIABLE
- Consumables
- Fuel
- Water
- Ash Disposal

0 Catalysts and Chemicals

- Variable Maintenance Charges (if any)

0 FUEL CELL REPLACEMENT EXPENSE (40,000 HR LIFE)

An average labor rate(ALR) of $\$ 15,25 /$ person hour should be used. This ALR includes payroll burden.

Annual maintenance costs were estimated as a percentage of the instalied capital cost of each plant section. The percentage applied varies with the nature of the processing conditions and the type of design. The following percentages were used in this study as shown in Table 4.

The mafntenance costs can be broken down and expressed as maintenance labor and maintenance materials. A maintenance labor/materials ratio of $40 ; 50$ can be used for this breakdown.

## Table 4. MAINTENANCE COSTS

Percent/year. of Installed
Process Unft FunctionPlant Section Cost
Oxygen Production ..... 2.0
Coal Storage \& Preparation ..... 3.0
Gasification \& Ash Handling ..... 4.5
Gas Processing
A. Gas Cooling ..... 3.0
B. Gas Cooling \& Ammonia Serubbing ..... 3.0
C. Gas Reheat ..... 2.0
Acid Gas Removal
A. Selexol ..... 2.0
B. Trim Zno Unit ..... 0.5
Sulfur Recovery \& Tail Gas Treating ..... 2.0
Waste Water Treating ..... 3.0
Steam Generation ..... 1.5
Fuel Gas Expansion \& Air Compression ..... 3.0
Process Condensate Treating ..... 3.0
Steam, Condensate and BFW ..... 1.5
Support Facilities ..... 1.5
Fuel Cell Combined Cycles ..... 2.0
Fuel Cell Moctules ..... 0
Fuel Cell Inverters ..... 1.0

The Overhead Charges is for administrative and support labor; 30\% of the operating and maintenance labor should be used.

The variable operating costs are based on a 65\% yearly utilization of the total plant capacity suld are composed of the following chaiges:

- Fuel (Coal) Cost
- Raw Water
- Ash Disposal
o Catalysts and Chemicals

These ftems are discussed below.

The 1981. delivered coal cost is $\$ 1.65 / 10^{6}$ Btu (HHV) for an Illinois No. 6 coal with analyses as given in Table 5. Coal costs are expected to escalate in real year terms by $0.7 \% /$ year (apparent escalation of $9.3 \%$ including 8.5\% inflation).

The 1981 raw water acqifisition cost to be used is $50 \& / 1000$ gallons. Intake structures, treating costs and pumping costs are to be included in the process capital and operating and maintenance charges.

The catalyst, chemicols and other cisumable costs should be estimated from literature, in-house, or vendor sources.

The 1981 ash disposal charge to be used is $\$ 5 /$ ton.

Coal analysis is shown in Table 5 for an Illinois No. 6 coal.

Table 5
COAL ANALYSIS

| Type | Illinois No. 6 |
| :---: | :---: |
| PROXIMATE ANALYSIS (Wt \%) |  |
| Moisture | 4.2 |
| Ash | 9.6 |
| Fixed Carbon | 52.0 |
| Volatile Matter | 34.2 |
|  | 100.0 |
| ULTIMATE ANALYSIS - DAF COAL (WE \%). |  |
| Carban | 77.26 |
| Hydrogen | 5.92 |
| Oxygen | 11.14 |
| Nitrogen | 1.39 |
| Sulfur | 4.29 |
| Other | - |
|  | 100.00 |
| HEATING VALUE - AS RECEIVED |  |
| High Heating Value (HHV) (Btu/ib) Net Heating Value (LHV) (Btu/lb) | $\begin{aligned} & 12,235 \\ & 11,709 \end{aligned}$ |

3. Economic Analysis Method

The objective of the study is to identify RED activities that have the patential for making.significant improvements over the Base Case Reforence Design . Improvements should be quantified, for purposes of this study, as reductions in capital cost (\$/kW). reductions in operating costs (\$/year), and reductions in cost of electricity (COE; $\$ / k W h$ ). Capital and operating cost reductions should be calculated using the factors given above. COE reductions should the calculated using the revenue requirement method as explained in EPRI's 1982 Technical Assessment Guide (Report No. P-2410-SR). More specifically, the COE should be calculated using the lo-year, short-terti, levelized analyses.

Potential economic advantages of alternatives over the Base Case Reference Design should then be compared to estimated R\&D costs required to utilize the alternative in a coal based fuel cell plant.APPENDIX Ab. Economic Report for Reference Case
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# ECONOMICS FOR <br> base case reference design 

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The purpose of this report is to provide a standardized format for calculating the COSt of Electricity (COE). The report includes a Summary Section, which highlights the major capital and operating costs, plus Sections 1 through 5 which give further details on the calculation of capital costs, operating costs, and the COE calculation method. An Appendix section is included to give details of how units within the Reference Design were scaled and how the constructed costs were estimated.

Many of the economic assumptions were taken from EPRI's Technical Assessment Guide (TAG), Report No. P-2410-SR.

## SUMAARY

Calculation of the Cost of Electricity (COE) includes estimating the Total Capital Requirement, the Variable Operating Costs, the Fixed Operating Costs, and the Fuel Cell Replacement Expense.

The Total Capital Requirement can be broken into seven major elements as follows:

SMM

### 1.1 Total Plant Cost (TPC)

A. Process (On-Site) Costs
B. General Facilities Total Constructed Cost - 10\% of Process Capital 54.77
C. Engineering \& Home Office Overhead plus Fee - 10\% of Process Capital . 54.77
D. Process Contingency - composite by process unit and state of art 90.9
E. Project Contingency

- $30 \%$ of Total Plant Cost $-(A+B+C) \times 0.3$
F. Total 945.35
1.2 Allowance for Funds During Construction (AFDC)

| AFDC | $=$ TPC | $35.28, ~$ |
| ---: | :--- | ---: |
| (see TAG B-5-IV-1) | $=945.35(0.037 \overline{3})$ |  |

### 1.3 Prepaid Royalties

$=0.5 \%$ (TPC - Gen'1 Facilities - Project Cont. on Gen'l. Facilities) 4.37
$=0.005(945.35-54.77-0.3 \times 54.77)$
1.4 Preproduction or Start Up Costs
1 month fixed oper. costs 24.350 MM/yr-12 $=2.03 \mathrm{MM}$1 month variable oper. costs47.67 MM/yr - 0.65-12 $=6.1 \mathrm{MM}$1 month capacity fuel $\times 0.2546 .35 \mathrm{MM} / \mathrm{yr}-0.65-12 \times 0.25=1.5 \mathrm{MM}$$2 \%$ of TPCTotal$945.35 \times 0.02=18.9 \mathrm{MM}$28.53
1.5 Inventory Capital
60 days inventory of fuel, catalyst, and chemicals efull capacity
coal $=\frac{46.35}{0.65} \times \frac{60}{365}$ $=\$ 11.7 \mathrm{MM}$
Catalyst \& Chemicals $=\frac{0.31}{0.65} \times \frac{60}{365}=0.08 \mathrm{MM}$Total11.78
1.6 Initial Catalyst \& Chemical Charge
Basis: Prorate based on AP-1543
$\frac{\text { Initial Cat } \& \text { Chem }}{\text { Añual Cat \& Chem }}=\frac{2451}{455}=5.4$
$5.4 \times 0.31=1.7 \mathrm{MM}$ ..... 1.7
1.7 Land (est. 164 acres e 5500/acre) ..... 0.9
1.8 Total Capital Requirement (TCR)
TCR $=\sum 1.1$ thru 1.7 ..... 1027.91 MM

The Variable Operating Costs can be broken into 4 elements as follows:
2.0 Voriable Operating Costs
47.67

1981 MM \$/yr
2.1 Fuel
46.35
2.2 Water
2.3 Ash Disposal
0.46
2.4 Catalysts \& Chemicals
0.55
0.31
$-47.67$

The Fixed Operating Costs can be broken into 3 elements as follows:

### 3.0 Fixed Operating Costs

24.41

| 3.1 | Operating Labor | 3.74 |
| :--- | :--- | ---: |
| 3.2 | Maintenance Costs ( $60 \%$ Natis, $40 \%$ Labor) | 17.45 |
| 3.3 | Overheaó Cnarges ( $30 \%$ Oper + Maint. Labor | $\frac{3.22}{24.41}$ |

4.0 The fuel Cell Replacement Expense is treated as a yearly levelized sinking fund (for the first 10 years only). The cost is $\$ 25.66 \mathrm{MM} / \mathrm{yr}$.

The Total Annual Operating Costs equals the sum of $2.0,3.0$, and 4.0 , or $\$ 97.74$ MM/ yr in $1981 \$$.

The COE based on the levelized annual revenue requirement for the first 10 years is made up of the following charges:

Levelize凶
Revenūe Requirement
MN S/YR
185.0 - Capital Related Charges
36.3 - Fixed Operating Costs
73.5 - Variable Operating Costs
25.7 - Fuel Cell Replacement Expense
$\$ 320.5=$ Total Annual Revenue Requirement

COE $=\$ 0.0834$ per $\mathrm{kW}-\mathrm{hr}$ for 675 MW plant at $65 \%$ operating factor

### 1.0 TOTAL CAPITAL REQUIREMENT (TCR)

### 1.1 Total Plant Cost (See Appendix A for Unit Costing Bases):

$=\$ 945.35 \mathrm{MM}$

### 1.2 Allowance For Funds During Construction:

$$
\begin{aligned}
& \text { Basis: } 3 \text { yr Construction Period; } i=\text { discount rate }=.125 ; e_{i}= \\
& \text { inflation rate }=0.085
\end{aligned}
$$

$$
\text { mid'78 mid'79 mid' } 80 \text { mid' } 81
$$

$$
=T P C \frac{1}{3}(1+1.0751+1.0369)
$$

$$
=1.0373 \times T P C
$$

$$
\begin{aligned}
\text { AFDC } & =.0373 \times \text { TPC } \\
& =.0373 \times 945.35 \\
& =\$ 35.28 \mathrm{MM}
\end{aligned}
$$

(See also EPRI Tff P-2410 SR p. B-46)

## 1.? Prepaid Royalties:

$=(0.005) \times(T . P . C .-G e n ' l$ Facilities - Project Cont. on Gen'l Facilities)
$=(.005) \times(945.35-54.77-0.3 \times 54.77)$
$=\$ 4.37 \mathrm{MM}$
1.4 Preproduction Or Start-up Costs:
a) 1 Month Fixed Oper. Costs
$=1 / 12 \times \$ 24.35 \mathrm{MM} / \mathrm{Yr}$
$=\$ 2.03 \mathrm{MM}$
b) 1 month of variable operating costs at full capacity

$$
=\frac{\$ 47.67}{.65} \times \frac{1}{12}=\$ 6.1 \mathrm{MM}
$$

c) $25 \%$ of fuil capacity fuel cost for 1 , mionth:

$$
=\frac{\$ 46.35}{.65} \times \frac{1}{12} \times .25
$$

$=\$ 1.5 \mathrm{MM}$
d) $2 \%$ of the Total Plant Cost

$$
\begin{aligned}
& =.02 \times \$ 945.35 \\
& =\$ 18.9 \mathrm{MM}
\end{aligned}
$$

Total Pre-Production or Start-Up Costs

$$
\begin{aligned}
& =a \$ 2.03 \\
& \text { b } 6.1 \\
& \text { c } \quad 1.5 \\
& \text { d } 18.9 \\
& \$ 28.53 \text { MM (1981 \$) }
\end{aligned}
$$

1.5 Inventory Capital:

$$
\begin{aligned}
& =60 \text { days inventory of fuel + catalysts + chemicals } \\
& \text { o full capacity }
\end{aligned}
$$

Coal:

$$
\begin{array}{ll}
\frac{\$ 46.35}{.65} \times \frac{60}{365}= & \$ 11.7 \\
\text { Cat. \& Chemicals: } & \frac{0.31}{.65} \times \frac{60}{365}=\$ 0.08
\end{array}
$$

$\$ 11.78$ MM (1981 \$)

### 1.6 Initial Chemical \& Catalyst Charge:

Basis: Prorate based on AP-1543
Initial Chem. + catalyst Charge $=2,451=5.4$
Annual Cat. \& Chem. charge

$$
\text { Initial Charge }=5.4 \times \$ 0.31 \mathrm{MM} / \mathrm{Yr}
$$

$=\$ 1.7 \mathrm{MM} / \mathrm{Yr}$ (1981)
1.7 Land Cost (scaled from AP-1543)

AP-1543: $1200 \mathrm{MW}(10,000 \mathrm{TPD}$ Coal) requires 210 acres

- Coal Storage Area $=105$ acres
- Process Area $=105$ acres

Assume for 675 MW plant that proress area is the same while the coal strorage area is proportional to power output.

Area $=105+675 / 1200 \times 105=164$ acres
Cost e $\$ 5500$ /acre $=\$ 902,000$
1.8 Total Capital Requirement
$=\sum 1.1$ thru 1.8
$=\$ 1027.91$ MM

### 2.0 VARIABLE OPERATING COSTS

Fuel 46.35
Water
0.46

Ash Disposal
0.55

Catalysts \& Chemicals
0.31
\$47.67 MM @ 65\% capacity (1981 \$)

### 2.1 Fuel:

Yearly Coal Costs 065 operating factor:

$$
\text { 403, } \begin{aligned}
& \frac{1991 \text { bs }}{\mathrm{hr}} \times \frac{12,235}{10} \text { Btu } \times 365 \times 24 \times .65 \times \frac{\$ 1.65}{10^{6} 8 t u \cdot \mathrm{~s}} \\
& =\$ 46.35 \mathrm{MM}(1981 \$)
\end{aligned}
$$

### 2.2 Water:

assume the following

1. $90 \%$ of water use is from cooling tower
2. $90 \%$ of cooling tower use is for steam cycle condenser
3. Steam Cycle efficiency $=38 \%$

$$
\frac{\text { Ratio of Condenser Duty }}{\text { Steam turoine power }}=\frac{1-.38}{.38}
$$

Steam turbine input $=192 \mathrm{MW}$ $=655.3 \mathrm{MM} \mathrm{Btu} / \mathrm{hr}$

Condenser cooling $=\quad 655,3 \times 1-, 38$


Total cooling Twr duty $=\frac{1,069}{.9}$ MY Btu/hr
$=1,188 \mathrm{MM} \mathrm{BEu} / \mathrm{hr}$
CTW make-up $=1,188 \times 10^{6} \frac{\mathrm{Btu}}{\mathrm{hr}} \times \frac{\frac{1 \mathrm{~b}}{\mathrm{H}} \mathrm{H} \mathrm{O} \text { M.U.U }}{1000 \mathrm{BLU} \mathrm{S}}$
$=1,188 \times 10^{3} \mathrm{jbs} \mathrm{H}_{2} \mathrm{O} / \mathrm{hr}$
$=142,600 \mathrm{gal} / \mathrm{hr}$
Total Water use $/ \mathrm{hr}=\frac{142,600}{.9}=158,440 \mathrm{gal} / \mathrm{hr}$

Variable Operating Costs (Contd)
Costs per year @ 65\% capacity
$\Gamma$

$$
\begin{aligned}
& 158,440 \frac{\mathrm{gal}}{\mathrm{hr}} \times 365 \times 24 \times .65 \frac{\$ .50}{1000} \mathrm{gal} \\
& =\quad \$ 0.46 \mathrm{MM} / \mathrm{Yr} \quad(1981 \$)
\end{aligned}
$$

Note: Total Water Use $=\frac{3,900 \mathrm{gpm}}{1000 \mathrm{MW}}$
2.3 Ash Disposal Costs:

Assume Costs $=\$ 5 /$ ton

$$
\begin{aligned}
& \text { Costs @ 65\% Cap. }
\end{aligned}=-1 \begin{aligned}
& 4838 \frac{\text { CPD }}{\text { dat }} \times .096 \times 365 \times .65 \times \$ 5 \\
&=\$ 0.55 \mathrm{mM} / \mathrm{Yr} \quad(1981 \$)
\end{aligned}
$$

2.4 Catalysts + Chemicals:
prorate from AP-1543
1976 costs $=\$ .455 \mathrm{MM} / \mathrm{Yr} 1976$
for 10,000 TPD coal
1981 costs for $65 \%$ per. factor:

$$
\begin{aligned}
& =\$ .455 \times 10^{6} \times \frac{4838}{10,000} \times 1.54 \times \frac{.65}{.7} \\
& =\$ 0.31 \mathrm{MM} / \mathrm{Yr} 1981 \$
\end{aligned}
$$

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### 3.0 FIXED OPERATING COSTS

| Operating Labor | $=$ | 3.7 |
| :--- | :--- | :---: |
| Maintenance costs | $=$ | 17.45 |
| Overhead Charges | $=$ | -3.2 |
|  |  |  |
|  |  | $\$ 24.35$ |

3.1 Operating Labor:

$$
1981 \text { ALK }=\$ 15.25 / \text { person-hour }
$$

- using AP-1543 as basis:

Total Plant operating labor $=28$ people per shift

$$
\begin{aligned}
& =245,280 \mathrm{man}-\mathrm{hrs} / \text { year } \\
& =\$ 3.74 \mathrm{MM} / \mathrm{Yr} \text { for } 1981 \$
\end{aligned}
$$

3.2 Maintenance Costs: Malierials (60\%) + Labor (40\%)

|  | \% of <br> Capital <br> Cost | Unit <br> Maintenance <br> Cost <br> MMS | Unit <br> Capital <br> Cost <br> MMS |
| :--- | :--- | :--- | :--- |
| O2 |  |  |  |

3.3 Overhead Charges: ( $30 \%$ of Oper. + Main. Labor)

$$
\begin{aligned}
& =0.3(3.74+7)(3.2 \mathrm{mM} / y \mathrm{~F} \\
& =0 .
\end{aligned}
$$

### 4.0 FUEL CELL REPLACEMENT COST (as Operating Expense)

### 4.1 1981 Fuel Cell Stock Cost Caluculation

4.1.1 Ref. EPRI EM-1670:

$$
\begin{array}{ll} 
& \$ 97.63 / \mathrm{kW} \\
= & 1978 \text { costs } \\
- & \$ 133 / \mathrm{kw} \\
\text { for } 675 \mathrm{MW} \text { plant, } 442 \mathrm{MW} \text { is MCFC } \\
\text { Cost }=\$ 58.8 \mathrm{MM} & 1981
\end{array}
$$

4.1.2 Assume

$$
\begin{aligned}
& \text { - } \frac{\$ 13.60}{2} \text { ( } 1981 \text { Costs w/out contingencies) } \\
& \text { ft. } 2 \text { active area } \\
& 0160 \frac{\mathrm{milliamps}}{\mathrm{~cm}^{2}} \times \frac{\mathrm{amps}}{1000 \mathrm{milliamps}} \times \frac{929 \mathrm{~cm}^{2}}{\mathrm{ft}^{2}}=149 \frac{\mathrm{Amps}}{\mathrm{ft} .{ }^{2}} \\
& 0.69 \text { volts } \times 149 \frac{\mathrm{amps}}{\mathrm{ft} .2}=\frac{103 \text { watts }}{\mathrm{ft} .2} \\
& 0 \text { Total ft. } 2=442 \times 10^{6} \text { watts } \times \frac{\mathrm{ft.} .2}{103 \text { watts }} \\
& =4.29 \times 10^{6} \mathrm{ft} .{ }^{2} \\
& \begin{aligned}
\text { Cost } & =4.29 \times 10^{6} \times \$ 13.60 \\
& =\$ 58 \mathrm{MM} \text { in } 1981 \$
\end{aligned}
\end{aligned}
$$

4.2 FUEL CELL REPLACEMENT COST

Use Level Annual Payment $=\mathbf{x}$
Use Ten Year Period
Replacement @ 5 yrs \& © 10 Yrs
Base Cost @ $\mathrm{Yr}=0 ;=\$ 58 \mathrm{MM}$
Apparent Escalation $\quad=8.5 \% / Y r=e_{a} \quad e_{a}=\left(1+e_{r}\right) /\left(1+e_{i}\right)$
Real Escalation $\quad=0.0 / \mathrm{Yr}=e_{r}$
Inflation Rate $=8.5 \% / \mathrm{Yr}=\mathrm{e}_{\mathbf{i}}$
Discount Rate $=12.5 \% / \mathrm{Yr}=\mathrm{i}$
Cost to replace e end of $5 \mathrm{yrs}=\$ 58(1.085)^{5}$
$=\$ 87.21 \mathrm{MM}$

Cost to replace end of $10 \mathrm{yrs}=58(1.085)^{10}$

$$
=\$ 13 i .14
$$

$x\left[1+i j^{5}+(1+i)^{4}+(1+i)^{3}+(1+i)^{2}+(1+i)\right]=7.21829 x$ $=5 \mathrm{yr}$. Sinking Fund

Anount remaining after lst replacement: -
$7.21829 \times-87.21$
Amount end of $10 \mathrm{yr}=\$ 131.14 \mathrm{~mm}=$
ARtount Remaining after lst Payment + Accumulated 5 yr. Sinking Fund
$=(7.21829 x-87.21)(1.125)^{5}+7.21829 x=131.14$
$\begin{aligned} 20.23 X-157.16 & =131.14 \\ X & =\$ 14.25 \mathrm{~mm} / \mathrm{yr}\end{aligned}$

+ Process Cont. @ $50 \%=7.13 \mathrm{~mm} / \mathrm{yr}$
+ Project Cont. $30 \%=\frac{-4.28}{-\underline{~} \mathrm{~mm} / \mathrm{yr}}$
$\frac{25.66 \times 10^{6}}{442.000}=\$ 0.01068 / \mathrm{KW}-\mathrm{hr}$ $442,000 \mathrm{KW} \times 0.65 \times 365 \times 24$ of F.C. power


### 5.0 COST OF ELECTRICITY (COE) CALCULATION

### 5.1 Calculate short-term 10 yr , levelized COE:

$1 s t 10$ Years Levelized Revenue Requirement
$=(T C R) P_{f}+$ (Expenses) $\times L F_{f} \quad-\quad$ Notes (1) \& (2)
$=1027.91 \times .180+$ (Expenses) $\times L F_{f}$
Expenses $=$ Fixed + Coal + Other Variable + Fuel Cell Replacement

|  |  | $\begin{aligned} & \frac{1981}{\text { Exps }} \end{aligned}$ | Int. Rate | Real Escal. | Inflat. Rate | Apparent Esc. | Level Factor | $\frac{\text { Level }}{\text { Exps }}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  |  | (i) | ( $\mathrm{er}_{\mathrm{r}}$ ) | $\left(e_{j}\right)$ | $\left(e_{a}\right)$ | ( $L_{10}$ ) |  |
| 0 | Fixed | 24.41 | . 125 | 0 | . 085 | . 085 | 1.4878 | 36.32 |
| 0 | Var.-Coal | 46.4 | " | 0.007 | " | . 0926 | 1.5434 | 71.6 |
|  | -Others | 1.3 | " | 0 | " | . 085 | 1.4878 | 1.9 |
| 0 | Fuel Cell | 25.66 | " | " | " | " | - | 25.66 |
|  |  |  |  |  |  |  |  | 135.48 |

Levelized Revenue Requirement for first 10 years $=$

| (mm \$/yr) | (\%) |  |
| :---: | :---: | :---: |
| 185.0 | 57.8 | Capital Related Charges |
| 36.3 | 11.3 | Fixed Operating Costs |
|  |  | Variable Operating Costs |
| 71.6 | 22.3 | - Coal |
| 1.9 | 0.6 | - Others |
| 25.7 | 8.0 | Fuel Cell Replacement Expense |
| \$320.5 | 100.0 |  |
| C.O.E. $=$ | $\begin{aligned} & 20.5 \mathrm{x} \\ & .0834 \mathrm{p} \end{aligned}$ | $\div\left(675 \times 10^{3} \times .65 \times 24 \times 365\right)$ |

## Notes:

(1) $P_{f}=$ factor for cumulative present value of carrying charges for the first f years of project
(2) $L F_{f}=$ levelizing factor for $f$ years
(3) Factors found in EPRI TAG p. A-3 and A-5

## APPENDIX A

## Total Plant Cost Via Unit Costing For Base Case Reference Design



| Anode <br> Out | Cathode <br> Out | Cuthede <br> Recycle |
| :---: | :---: | :---: |
|  |  |  |
| 3,214 | - | - |
| 1,560 | - | - |
| 35 | - | - |
| 46,584 | 87,568 | 65,585 |
| 39,862 | 172,655 | 129,509 |
| 340 | 471,179 | 353,433 |
| - | - | - |
| - | - | - |
| - | 62,442 | 46,838 |
| - | - | - |
| 91,419 | 793,844 | 595,465 |

Molar Flow, mph
Notes: Molar flows are approximate and used for cost scalling purposes only.


E



#### Abstract

APPENDIX B. Summary Printouts of Cases for Economic Analysis


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## Case 1

The Base Case at 675 MW Output
GASIFICATION AUS ELECTOJCY:YICAL TUEL SFLLS, ALCNS WITM COHVENTIOYAL POWEP GENEQATION MACHIVERY.





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COAL CONSUMDTION IS 4?3. THJUSANDS DOUNDS PER HDUD, OP AROUT 5471. MILLIONS ETU. PRJCESS STEAM CONSUYOTICN IS JO1. THOUSANDS DOUNDS PER HOUR.

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297050 . \text { KILOWATTS } \\
113978 . \text { KILCWATTS } \\
553352 . \text { KILCWATTS } \\
675000 . \text { KILOWATTS }
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CASE 2
Add Quench, Shift, Crossflow Heat Exchange
GASIFITATION AND ELETTROCHEMICAL FUEL CELLS. ALONG WITY CONVENTIONAL POWER GENERATION MACHINERY.


















THIS IS THE FINAL SYNOPSIS OF THE ENERGY QUDGET OF AN ENTEGPATED POWE
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THE AREA OF THE FUEL CELL IS
OVERALL PLANT EEFICIENCY, COAL PILE TO BUSGAR, IS 4.5.5 PEREENT.

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CASE 3
Change to Fluidized-Bed Gasifier, Producing Low Methane




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-346231. KILOWATTS
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-48638.1 \text { KILOWATTS } \\
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-2486.6 \text { KILONATTS }
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COAL CONSUMPTION IS 4823. TONS PER DAY.

## NET DELIVERED POWER IS 675. MEGAWATTS.

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COAL CONSUMPTION IS LOZ. THOUSANDS POUNDS PER HOUR, OR ABOUT SIS?. MILLIONS BTU.
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PROCESS STEAM CONSUMPTION IS $7 S$. THOUSANDS POUNDS PER HOUR.
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$\begin{array}{rr}0.8411 & \text { VOL.TS. } \\ 5374565 . & 50 . F T .\end{array}$
-264590. KiLOWATTS
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OVERALL PLANT EFFPCIENCY, COAL PILE TO BUSBAR, IS 44.9 PEREENT.


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## CASE 5

Change Gasifier to High Methane Production

CASE LAAIR.4E
SUMMARY FES BJ $95: 35: 37$
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CQYOGENIC OXYGEN COMPRESSOQ FOR SUPPLY TO COAL GASIFIER

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& \text { G EXPAN STACK GAS THROUGH TURGNE TO RECOVER POWER. } \\
& 70 \text { COPRESS RECYCLE GAS TO SHJECT FEEED COAL TO SASIFIER. }
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CASE 6
Employ High-Temperature Dust Removal



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CASE 7
Emp1oy Sulfur-Tolerant Fuel Cell


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GASIFICATION AMD ELECTRDCHEMICAL FUEL CELLS, ALOHS HITH CONVENTIONAL POWER GENERATION MACHINEPY.

> NET DELIVERED POWER IS 6?5. MEGAUATTS.
> *********

*     *         *             *                 *                     *                         *                             * 

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## CASE 8

## Employ High -Temperature $\mathrm{CO}_{2}$ Transfer

THIS IS THE FINAL SYNOPSIS OF THE PNERGY QUDGET OF AN INTEGQATED PAUER PLANT USING COAL
GASIFICATION AND ELEGTOOCHEMICAL FUEL GELLS, ALOVG WITH CONVENTIDNAL POWER GENERATION MACHINERY.

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4584. TONS PER DAY.
NET DELIVERED POWER IS 675. MEGAWATTS.

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## ORIGINAL EFFICIENCY COMPARISON

During the course of the program, 66 separate cases were examined for the integration of coal gasification for molten carbonate fuel cells for power generation. of these, 20 cases were analyzed for variations in system efficiency by modification of process configurations. These cases were undertaken early in the program, on the basis of a constant coal feedstock to the system with varying power production, and are discussed in this appendix of the report. Additionally, nine of these 20 cases were revised to a constant power output basis, with slight modifications in system parameters to make them more truly comparable, and analyzed on an economic basis in the main body of this report. Twenty additional cases were evaluated to indicate the effects of primary assumptions upon the total system efficiency; these cases are presented in Appendix Da. The remaining cases are not specifically presented. Many of these represent minor variations in a specific analysis or involved short optimization studies by varying a single process parameter. In these cases, the results are discussed below but not specifically analyzed in depth.

Many of the cases were reanalyzed periodically during the program. As the output from later systems was assessed, it became apparent that the overall system was extremely sensitive to minor variations in specific inputs. Therefore, earlier cases were reassessed, with particular attention paid to these inputs, so that the results would be more comparable. An example of the complete printout. for a single case is included as Appendix cd In this document, to illustrate the types of calculations that were made to integrate the entire system. Complete printouts of the major systems analyzed were placed on file with the prime contractor; however, only summary sheets are included (Appendixes $C c, D b$, and $B$ ) with this document because of the bulk that would result.

## Efficiency Comparison of Alternative Systems

The primary charge of the project was to evaluate alternative systems that might be conceived for integration of coal gasification with power generation by molten earbonate fuel cells. Emphasis was to be placed on identifying development effort that may be cost-effective in reducing the overall cost of future power generation. Twenty systems, incorporating various features of this integration, are summarized in Table Ca-l.


Additional systems were also analyzed, but are not presented in depth, either because they showed little potential or were primarily optimization studies on the systems included.

This appendix presents the results of the initial analysis (after several iterations for comparability) of the twenty systems. The cases all present the power output obtained from a constant 4991 tons/day of coal - the amount required for 675 MW of power from an early iteration of the base case. The analysis reflects the learning experience that was encountered as the project progressed. The cases are closely comparable, based upon knowledge gained on the system sensitivity. However, the final iteration, presented in the body of the report, shows slight discrepancies from the analysis below.

## Case I T The Base Case

The prime contractor prepared a reference design, derived from evaluations by others, as a starting point for this systems analysis effort. That contractor's report, together with its economic analysis, is included as Appendixes $A a$ and $A b$. The discussion of the system in that document is detailed; only the major features of the system are described below, together with deviations and evaluations used in the current analysis.

The basic configuration of the base case is presented in Figure Ca-1. In that base case, an entrained-bed gasifier produces a high-temperature raw gas. The gas is cooled by waste heat recovery to high-pressure steam. The gas is further cooled by "regenerative" heat recovery (to the purified gas). After scrubbing for dust removal and condensation, the gas is treated for selective $\mathrm{H}_{2} \mathrm{~S}$ removal at ambient or reduced temperature. The sweetened gas is reheated by the raw gas in the heat exchange described above. Because not all of the heat available in the raw gas is required for reheat to the purified gas, additional high-pressure steam is recovered by parallel cooling of the raw gas. The hot, purified gas is tuboexpanded to the fuel cell operating pressure, humidified for carbon control, and fed to the fuel cell. After 85\% conversion of the hydrogen and carbon monoxide within the fuel cell, the spent anode exhaust is catalytically combusted with hot, compressed air and fed to the fuel cell cathode. An additional cathode feed is a recirculating stream derived from the cathode exhaust and cooled (to high-pressure, superheated steam production) for fuel cell temperature control. The remainder of the spent cathode gas is exhausted through a turboexpander and heat recovery to

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Figure Ca-1. PROCESS flow diagram of base case
the incoming air. Isentropic compressor efficiencies are $88 \%$ and expander efficiencies are $92 \%$. Other assumptions used in the analysis were -

1. The fuel cell operating pressure was taken as 150 psia so that the output from the process simulator would closely approximate fuel cell data. (See "Assumptions" section of main text).
2. The spent cathode exhaust was discharged from the stock at approximately $500^{\circ} \mathrm{F}$ to avoid potential plume formation.
3. The gas purification by a selective Selexol system was specified for $19 \%$ $\mathrm{H}_{2} \mathrm{~S}$ in the acid-gas, a value that has been found to be a satisfactory feed for split-flow Claus sulfur plants. No effort was made to recover $\operatorname{COS}$ in the acid-gas removal system, because of the high steam and power demands of the Seloxol system when applied for this duty
4. Steam addition for carbon control, feeding the fuel cell, was selected as midway tetween the theoretical requirements for inhibition of graphite and amorphous carbon deposition.
5. The power production from the high-pressure steam system, with reheat, was taken as $35.28 \%$ efficiency to include factors for boller feedwater pumping and the cooling water system.
6. The precise estimation of temperature levels available for high-pressure steam production and reheat was not attempted because of the additional energy production and demands within the overall system (sulfur plant, tailgas system, water stripping, ammonia recovery, and water treatment system) have not been quantified.

Evaluations of the system include -

1. The overall system, with the conservative approach indicated above, calculates as $42.1 \%$ efficient, compared with $46.7 \%$ calculated by others for this system. Power generated in the fuel cell stack in the current design is much greater, proportionally, than that shown by others; the recovery of waste heat is reduced because of the more conservative design employed.
2. The entrained-bed-gasifier design appears optimistic. The design assumes the capability to pump slurry at $70 \%$ feed solids concentration, and the oxygen demand is relatively low, particularly for the $100 \%$ carbon utilization claimed.
3. The raw gas leaving the gasifier is thermodynamically unstable for carbon deposition when cooled to the temperatures of waste heat recovery.
4. The temperature profile of the "regenerative" heat exchange system indicates a degree of countercurrency not often encountered in chemical engineering practice, particularly when operating with hazardous, toxic gases at elevated temperature and pressure.
5. The heat balance indicates major energy losses to latent and sensible heat of the system exhaust, to steam cycle losses, and to fuel cell air compression.
6. The gasification efficiency of the coal in the entrained-bed gasifier is relatively low. Although $100 \%$ conversion of the carbon is assumed, the heating value of the gas is only $77.2 \%$ of the coal fed to the system.

## Base Case Re-engineering

A number of cases were considered to ensure system operability for the base case. In particular, carbon stability of the raw gas was examined, the countercurrent heat exchange was converted to a safer operation, and the efficiency of rotating equipment was reviewed. Additionally, subsystems were added or moved within the process to achleve greater recovery of energy.

The first evaluation was the relative efficiency of the compressors and expanders within the system. The base case was reevaluated at three levels of assumed compressor and expander efficiency. It was found that an assumed 5 percentage point reduction in the efficiency of rotating equipment caused a decrease of 1.5 percentage points in the system efficiency. This efficiency loss was approximately constant for all efficiencies greater than $75 \%$. The primary reason for the loss was the compressor. In multistage compressors, interstage cooling is used to condition the gas to an acceptable temperature prior to each stage of operation. With lower efficiencies of compression, more of the energy supplied as work of compression is removed as waste heat in the interstage coolers. With expanders, on the other hand, efficiency loss is not as critical. Energy that is not recovered to the shaft still exists as thermal energy in the expanded gas, to be recovered downstream in the steam cycle.

After consultation with experts in the field, it was determined that efficiencies approaching those assumed in the base case design would be achieved in the field, although guarantees offered by equipment vendors may be about 5 percentage points lower. Therefore, it was decided to employ the efficiencies of the base case for rotating turbo equipment throughout the remainder of the program.

Case Id evaluates more conventional heat exchange equipment, as applied to the base case design.

The reference design employs the use of highly efficient, apparently countercurrent, "regenerative" heat exchange. In the chemical process industries, regenerative heat exchange is defined as the alternating heating and cooling of inert solids. For example, refractory checkerwork may be heated by contact with a hot gas. After an interval of time, the hot gas is valved off, cold gas is valved in, and the heat stored within the checkerwork is transferred to the colder gas. Conventional nomenclature defines energy recovery by heat transfer through metal walls as "recuperative."

In the chemical process industries, conventional heat exchange is not countercurrent, but rather crossflow. The cost of double-pipe heat exchangers, required to approach countercurrency, is excessive, primarily because of the mechanical problems that arise from the thermal stresses encountered. The differential expansion of the shell and tubes must be considered and usually packing glands are employed. Such a design would be questionable with toxic, flammable, hazardous, high-pressure, high-temperature gases.

In crossflow heat exchange, normal engineering practice is to assign a temperature differential between the temperature to which the hot gas is cooled and the temperature to which the cold gas is heated. Thus, in the general case, crossflow heat exchange cannot approach the efficiency of the countercurrent heat exchange.

An exception for improved temperature recovery is the use of several crossflow heat exchangers is series. If the quantity of heat being transferred is large, and the surface area required for the heat exchangers is therefore also large, a number of heat exchangers (or shells) may be required. Rather than arrange these shells in parallel, a series configuration can tend to approach countercurrency in the heat exchange.

In the current system, because the quantities of heat being transferred are quite large, the series heat exchange approach is reasonable. Engineering judgment was used to assign a practical number of shells at each point in the heating and cooling of the fuel gas stream, and the system was evaluated with specific heat exchangers identified.

This approach necossitated an energy loss in the system, relative to the countercurrent exchangers; approximately $100^{\circ} \mathrm{F}$ of energy will be lost from the
gas stream to air cooling and/or cooling water for each heat exchanger train included. The overall system efficiency drops by approximately 0.3 percentage points when this type of heat exchange is included.

Case Ie was developed to evaluate the performance penalties encountered if conservative engineering were employed in the design to counteract potential carbon deposition from the gasifier raw gas.

Raw gas from the entrained-bed gasifier has significant thermodynamic potential to deposit carbon. When analyzed on the triangular $\mathrm{C}-\mathrm{H}-0$ diagram, the raw gas composition contains relatively more carbon atoms that can theoretically exist in a thermodynamically stable gas. (See Appendix Cb for further discussion.) Although mechanisms may exist to inhibit carbon deposition in such a system, current prudent engineering practice would dictate that the gas should be treated to be stable with respect to carbon deposition before it is cooled to the temperature where this effect would be expected.

For this case, sufficient water was added to the raw gas to yield an overall gas composition that would be thermodynamically stable. The water was added as liquid. The quantity of water added to the quench was somewhat greater than actually required to control carbon deposition. The theoretical quantity of water was determined and a short optimization study was performed to find the preferred quantity of water for the most efficient overall system.

Rather than lose the hydrogen content of the water that was added for quenching the raw gas, this case also included a water-gas shift reactor on the raw gas to convert much of the water to hydrogen before condensation. For this effort, two stages of water-gas shift reaction were employed for a reasonable degree of water conversion.

The net effect of these counter-acting system changes was a decrease in the overall system efficiency by 2 percentage pcints, to $39.8 \%$. The addition of the quench water removes heat from the high-temperature gas - heat that was recovered to the steam system in the base case. For this case, much of that heat was not recoverable to power. The use of the shift reactor, however, converts a portion of the water to hydrogen for eventual consumption In the fuel cell and reduces the quantity of steam that must be added just prior to feeding the fuel cell. As discussed in Appendix $C b$, the addition of
steam at that point is a second-order effect, but higher hydrogen content to the fuel cell is a preferred option.

Case If was developed to indicate the impact of a preferred location for the turboexpander employed on the raw gas. In the initial base case design, the expansion turbine was located on the purified gas. With the inclusion of the shift reactor, as in Case $I e$, the temperature of the gas leaving the first shift reactor is much greater than the gas temperature feeding the turboexpander. Additionally, this gas contains water vapor and carbon dioxide, at temperature and pressure, that are unavailable to the turboexpander in Case Ie. Consequently, Case If was designed to evaluate the system with the turboexpander moved to the discharge of the first shift reactor. Figure Ca-2 illustrates the configuration of the system.

With the improved temperature and gas quantity for the fuel gas expansion turbine, the system efficiency increased to $40.9 \%$, approximately 1.2 percentage points lower than the original base case design. However, this case contains several system modifications for improved process operability, safety, and system control. Consequently, the use of raw gas quench, watergas shift reaction, and improved location of the expansion turbine were used in further systems for analysis.

Case II - Fluidized-Bed Operation
Case II was developed to evaluate the performance of a fluidized-bed gasifier within the system, rather than the entrained-bed gasifier used above. The overall processing scheme for the fluidized-bed gasifier is presented in Figure Ca-3; the scheme is essentially identical to that used in Case If, with the substitution of the fluidized-bed gasifier for the entrained-bed system.

The entrained-bed gasifier requires relatively high oxygen demands because of the high temperature of the product gas. Therefore, on the overall systems basis, more of the carbon in the coal is converted to carbon dioxide, rather than fuel gas species. The single-stage fluidized-bed gasifier should provide operating advantages because it requires less oxygen for operation. A fluidized-bed gasifier was specified to operate with relatively conservative design conditions. The operating pressure of the gasifier was selected as 500 psi to give a margin of safety relative to current limits of lockhopper


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technology. Coal injection gas requirements were identified, as well as dust losses and carbon content in the ash, to assure a realistic design.

The chemistry for a single-stage coal gasifier, operating at $1875^{\circ} \mathrm{F}$ at 500 psi , indicates that approximately $8.3 \%$ of the carbon fed to the gasifier will be present in the off-gas as methane, if the gasifier is designed to minimize methane procisction. This methane content translates to $3.7 \%$ of the raw gasifier effluent. The summary printout of the gasifier design is included in Appendix Ce.

The gasifier, as expected, was somewhat more efficient than the entrained-bed gasifier. The steam/carbon ratio in the gasifier was assumed at 1.0 molar and the oxygen required, for the system to be in mass and energy balance, was 0.35 moles/mole of carbon in the coal. Approximately $3.1 \%$ of the carbon in coal was lost to the dust and ash losses; the higher heating value of the product gas is $82.4 \%$ of the heating value of the coal.

The downstream processing was similar to Case If and optimization studies showed that the preferred amount of water quenching of the raw gas, on a total system basis, should be minimized. For the conservative design, the quantity of water added at that point was taken to be midway between the water demand * for carbon control to graphitic carbon thermodynamic equilibrium and amorphous carbon equilibrium.

Case II was over 3 percentage points lower in system efficiency, compared with Case If, which employed the same system components but with the entrained-bed gasifier. The fuel cell power production was considerably lower, because the methane fuel content of the gas was not available as power from the fuel cell, but rather was burned to the steam cycle. Even the steam cycle power output was not considerably higher than Case If, because of the steam demands of the fluidized-bed gasifier.

Alternative gasifier configurations have been developed that minimize the steam demand for fluidizing the gasifier. For example, some systems have employed recycle of product gas as a primary fluidization medium with only minimal steam addition for reaction control. however, in other systems analysis efforts, the gas composition in these configurations is much more unstable with respect to carbon deposition; therefore, with the greater energy penalty for additional quench, the overall system is not more efficient.

In the economic analysis work that followed, and is reported in the body of the text, the Case II system offers promise. Although the system with the fluidized-bed gasifier shows much lower efficiency than the entrained gasifier, enoint capital savings was realized that the two systems are essentially identical in the cost of electricity. Therefore, the use of fluidized-bed gasifiers in conjunction with molten carbonate fuel cell power production appears to warrant further investigation.

## Case III - Internally Reforming Fuel Cell

Case III was developed to evaluate the concept of a fuel cell that incorporates internal reforming of the methane to hydrogen and carbon monoxide, with thermal and chemical integration of the reforming with the fuel cell unit. Although the concept of an internally reforming fuel cell is relatively old, attention has again been focused on the operation of fuel cells that incorporate this feature. Active catalysts have been identified and evaluation is under way at several fuel cell laboratories.

The chemistry of the overall system is discussed in detail in Appendix Cb. That chemistry is summarized briefly below.

The steam-methane reforming reaction is the chemical recombination of methane and water vapor to produce carbon monoxide and hydrogen. Thermodynamically, high conversions are favored at the fuel cell operating temperature and pressure. When incorporated within the anode compartment of the fuel cell, the reforming reaction utilizes water vapor that is generated within the fuel cell, thus decreasing the back-pressure of water vapor in the Nernst concentration polarization effect. Additionally, the quantity of hydrogen in the cell is increased, further improving the polarization. The steam-methane reforming reaction is endothermic - 1000 Btu of methane heating value is converted to approximately 1300 Btu heating value in the product gases, requiring an input to the reaction of approximately 300 Btu. The excess heat released in the fuel cell can be used to drive this reaction, rather than be discharged to a steam cycle. On a total systems basis, the reduced heat load in the gasifier (with decreased carbon and oxygen consumption) results from the production of methane in the gasifier, but this methate can be converted to hydrogen fuel within the fuel cell, using excess heat from that cell.

As illustyated in Figure $\mathrm{Ca}-4$, the configuration of Case III is essentially identical to Case II, with the incorporation of the reforming reaction within the fuel cell.

Thermal and chemical integration of methane reforming, within the anode cavity of the fuel cell, produces exceptional advantages when combined with a methane producing gasifier. Case III exhibited a full 7 percentage points greater efficiency than Case II, with most of the advantage occuring in the fuel cell output. The most inefficfent form of power generation - the steam cycle - was reduced to a low level. It is concluded that the concept of an internally reforming, molten carbonate fuel cell, deserves increased attention.

Case IV - Operation of the Gasifier With Higher Methane Production
Case III, above, indicated high promise for a fluidized-bed gasifier integrated with an internally reforming molten earbonate fuel cell. The乡asifier operating characteristics had been specified for relatively low methane production. By proper mechanical construction of the gasifier, the methane production can be increased. Such a gasifier is more efficient, has lower oxygen demand, and higher product gas heating value.

Sase IV was developed to determine if the higher methane content from the product in the roduct gas would be desirable in the overall system. New gasifier material and energy talances (Appendix Ce) were developed for the candidate coal and the gasifier design that would convert $13.5 \%$ of the carbon in the coal to methane ( $6.1 \%$ methane in the product gas). This gasifier design was similar to that used by M. W. Kellogg in its evaluation of fluidized-bed gasifiers for SNG production. ${ }^{6}$ For the current case, conservatism in design was maintained: the steam requirements of the gasifier were maintained constant at 1 mole of steam/mole of carbon fed to the gasifier. Oxygen requirements of the gasifier decreased to 0.31 mole/mole of carbon, as required by the gasifier heat balance. Carbon lost to dust and ash was maintained at $3.1 \%$ of the feed and the heating value of the resulting product gas was $82.7 \%$ of that in the coal.

At this time, it is of value to review the gasifier operating parameters for those systems which were used in this study. Although two other gasifiers are used in later analyses, they are efther conceptual or showed no real

operating advantage. Therefore, the three gasifiers discussed at this point are sumamrized below in Table Ca -2.

The fluidized-bed gasiffers have lower oxygen demand and convert a greater fraction of the coal heating value into $t^{2}$. oroduct gas that may be employed in the fuel cell. When one considers the ey rall chemistry of the system (Appendix Cb ), the carbon in the coal is converted to hydrogen for consumption in the fuel cell through either the water-gas shift or the internal reforming reactions. The equivalent hydrogen produced per unit of coal is considerably higher for the fluidized-bed gasifiers and the gasiffer producing increased methane appears to be preferred from this analysis. From the triangular $\mathrm{C}-\mathrm{H}-0$ diagram of Appendix Cb , one notes that the fluidized-bed gasifier requires much less water addition for stabilizing carbon deposition; the gasifier with the increased methane production requires greater water addition than the low-methane fluidized-bed gasifier. This effect will counterbalance part of the advantage of the increased methane production.

The overall system considered for the analysis is identical to Cases If, II, and III, but incorporating the improved gasifier with the internally reforming fuel cell; it is illustrated in Figure $\mathrm{Ca}-5$.

The increased methane content of the gasifier, combined with the decreased oxygen requirement, increased the overall system efficiency by about 0.7 percentage points. Thus, this system is apparently preferred, but not with the degree of improvement anticipated.

## System Modifications

Several cases were evaluated to optimize the system of Case IV and to indicate the impact of operating variables. In an unreported analysis, the current density of the fuel cell was varied over a narrow range and the overall impact upon system efficiency was found to be minor. From this effort, a fuel cell current density of $150 \mathrm{~mA} / \mathrm{cm}^{2}$ was used in the remainder of the work.

In another optimization study, the air flow rate to the cathode was varied and found to be an important variable upon the system output. From this effort, the air flow to the enthode was set at $160 \%$ of stoichiometric requirements.

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Table Ca-2. GASIFIER SUMMARIES

Entrained Bed

Fluidized Bed Low Methane High Methane

Product Gas

Temperature, ${ }^{\circ} \mathrm{F} \quad 2450$
Pressure, psia 600
Composition, mol \%

| $\mathrm{H}_{2}$ | 29.4 | 29.3 | 25.8 |
| :--- | ---: | ---: | ---: |
| $\mathrm{CH}_{4}$ | 0.1 | 3.7 | 6.1 |
| CO | 43.3 | 24.9 | 24.8 |
| $\mathrm{CO}_{2}$ | 8.9 | 14.3 | 15.1 |
| $\mathrm{H}_{2} \mathrm{O}$ | 18.3 | 27.8 | 28.2 |

HHV/HHV Coal
0.772
0.47
0.776

Equivalent $\mathrm{H}_{2}{ }^{*} \mathrm{HHV} / \mathrm{HHV}$ Coal
0.824
0.827
$\mathrm{O}_{2}$ Demand, mols/mol C
0.35
0.31
0.868
0.895

* Equivalent $\mathrm{H}_{2}=\left(\mathrm{HHV} \mathrm{H}_{2}\right)\left(\mathrm{H}_{2}+\mathrm{CO}+4 \mathrm{CH}_{4}\right) / \mathrm{HHV} \mathrm{Coal}$.


Case IVa was developed to evaluate the impact of a conceptual gasifier that is anticipated to produce greater methane contents than systems currently under development. IGT has initiated patent action on a modified gasifier configuration that, through control of operating conditions within the single fluidized bed, is anticipated to enhance methane production within the gasifier. The operating conditions have been identified and the methane content of the product gas has been estimated. Gasifier heat material balances were developed for the candidate coal and the gasifier was integrated into the system to indicate the impact. With the exception of the modified gasifier, the system was identical to that of Case IV, as illustrated in Figure Ca-5. The use of the conceputal gasifier improved the system performance by 2.5 percentage points, significantly higher than the earlier cases. Because the gasifier is conceptual, however, the system was not employed in later design evaluations.

Cases IV $b_{2} c$, and $d$ were developed to illustrate the impact of relative fuel conversion, taken within the fuel cell, upon the overall system efficiency. Apparently the system is not optimized at the $85 \%$ conversion that had been employed as a basis for this study - even greater efficiency can be achieved at $90 \%$ conversion efficiency across the fuel cell. Careful study of this case, however, indicates that the effect might be a result of the mathematical fuel cell simulator employed in the analysis, and these effects might not necessarily occur in practice. Therefore, the value of $85 \%$ fuel gas conversion efficiency (hydrogen, carbon monoxide, and methane) was maintained constant for the work in this effort. Also, this conversion efficiency was maintained to improve comparability to other analyses.

Case IVe is essentially identical to Case IV, but includes the results of several small optimization studies. It includes the preferred air flow to the cathode, as discussed above. It also incorporates a two-stage compressor on the cathode aif supply. At an overall air compression ratio of 10 , conventional practice would suggest that a three-stage compressor be utilized. However, by technology transfer from other compressor applications, it is known that outboard bearings and labyrinth seals may be used to permit higher gas discharge temperatures. With this modification, a two-stage compressor could be employed. This option permits increased heat recovery from the compression energy into the cathode air, permitting a slightly increased system efficiency of 0.4 percentage points.

Cases IVf and g, taken together with Case IV, indicate the impact of the amount of quench water used in the system. Case IV is based upon a conservative utilization of quench water, IVf employs minimum theoretical amount of quench water, and $\operatorname{IVg}$ assumes that quenching will not be required, perhaps because of the inhibition of carbon deposition by the presence of other species in the raw fuel gas. Note that if the quench operation could be completely eliminated, the process efficiency improves by 1.4 percentage points. Therefore, an in-depth evaluation of the carbon deposition phenomena, and the possible inhibition of carbon deposition, should be undertaken.

## Case V -- Dust-Tolerant Water-Gas Shift Reaction

Case $V$ was developed to indicate the potential for process improvement if the water-gas shift reaction could be operated on a dusty gas, rather than one that had been previously washed for dust removal. Five systems were evaluated incorporating a dust-tolerant shift reactor; the system presented as Case $V$ in 'Table Ca-1 is the preferred variation. Catalyst configurations for such an operation have been identified and the penalty for inclusion of such a system is a moderate decrease in the space velocity required to achieve a specified degree of reaction.

Because this process modification was not selected for system costing and economic analysis, a separate drawing has not been prepared to illustrate the system. The system may be described as follows:

The raw gas from a fluidized-bed gasifier (taken from Case IV) is quenched for carbon stability and heat is recovered through a waste heat boiler to the required inlet temperature for the water-gas shift reaction. Although the gas has undergone primary solids removal through the cyclone associated with the gasifier, it still contains a dust loading that would have been washed out in prior systems. For this case, however, the dusty gas is fed directly to the water-gas shift reaction system. The shifted gas is cooled through a heat exchanger train; scrubbed for dust, ammonia, and excess water removal, and selectively desulfurized in an acid gas removal system. The purified gas is reheated in the heat exchanger train, expanded to fuel cell operating pressure, and humidified for carbon control before feeding the internally-reforming fuel cell. This system permits elimination of one gas washing train prior to the shift reactor, resulting in an energy saving equivalent to a $100^{\circ} \mathrm{F}$ temperature rise in the gas. The turbine operates on
the desulfurized gas; therefore, the mass of water vapor and $\mathrm{CO}_{2}$ present in the inlet to the gas turbine has been reduced. However, the heat of the shift reaction is still available to the turbine through the recuperative heat exchange train.

The overall efficiency of the modified system is $47.5 \%, 1.7$ to 2.1 percentage points greater than systems without the dust-tolerant water-gas shift reactor. The overall system is somewhat simpler than Case IV because of the elimination of one heat exchange train. Therefore, it is suggested that the concept of the dust-tolerant shift reactor should be investigated more thoroughly.

This system was not selected for economic analysis for the main body of the report. Similar system simplification and efficiency were determined for Case VI (below) and the economic evaluation of Case VI should be indicative of the economic advantages of the dust-tolerant shift reaction system.

Case VI - High-Temperature Dust Removal
Case VI was developed to indicate the potential for high-temperature dust removal in the coal gasification/fuel cell power generation system. Several techniques for high-temperature dust removal are being developed in various laboratories; the techniques are primarily being developed because of the need for this subsystem with pressurized fluidized-bed combustors when integrated with combined cycle power generation. The results of this analysis indicate that high-temperature dust removal is also applicable in the integration of coal gasification with molten carbonate fuel cell power generation.

Figure Ca-6 indicates that the high temperature dust removal subsystem considerably simplifies the overall process. Three cases were examined employing high-temperature dust removal; the preferred embodiment is shown in Eigure $\mathrm{Ca}=6$. In this system, the raw off-gas from the fluidized-bed gasifier (producing the moderate methane content of Case IV) is treated for high temperature dust removal, immediately after the cyclones that return most of the gasifier dust for regasification. The gas is then expanded. At this point, the gas temperature is high and the temperature drop across the turbine is not so great that carbon deposition is to be expected. Because of the higher temperature, the power recovered from this turbine is greater than in earlier systems. The gas then passes through quench, heat recovery, cooling,

and acid-gas removal before reheating through the single heat exchanger train. The fuel cell incorporates the internal reforming concept.

Note that the turbine could also be employed after the initial quench. In this case, the mass of gas that is passing through the turbine is increased, but the inlet temperature is reduced. After analyais, the placement of the turbine before quench appears to be a preferred embodiment of the system.

The overall efficiency of this system calculates at $47.3 \%$, neariy identical to the dust-tolerant shift catalysis considered in Case V. On the overall systems basis, the concepts of high-temperature dust removal and dusttolerant shift reaction appear to be complementary - either system offers approximately the same value with approximately the same degree of system complexity. Both systems should be developed because each becomes a backup system for the other, improving the probability of success in the overall research effort.

## Case VII - Sulfur-Tolerant Fuel Cell

The overall system for integration of coal gasification with molten carbonate fuel cell power generation would have the maximum simplicity if the fuel cell could be modified to operate directly on the fuel gas after quenching and cooling to the fuel cell operating temperature, without sulfur treatment. Conceptually, this problem appears solvable - sulfur-tolerant electrodes for this duty have been preliminarily identified and the electrolyte composition issue appears capable of resolution, based upon thermodynamic considerations.

The overall system (Figure Ca-7), employing a sulfur-tolerant fuel cell stack, is quite simple - minimal heat exchange, no water-gas shift reactor, and no condensation of water from the gas. The fluidized-bed gasifier with the moderate methane make is employed, as is high-temperature dust removal and the internal-reforming capability within the fuel ce11. The relatively high concentrations of carbon dioxide and water vapor in the fuel cell feed tend to suppress the fuel cell voltage and hence its power output. However, the overall system shows an excellent overall efficiency (49.3\%), about 3.5 to 4 percentage points better than the systems with low-temperature sulfur removal.
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One note of caution should be considered in the energy analysis of this system: The debits and credits for $\mathrm{SO}_{2}$ removal from the final stack were not considered (similar to the assumptions in the other cases that a final sulfur recovery from the acid-gas was not considered). Such stack desulfurization processes are relatively energy-intensive and may modify the relative ranking of this concept when analyzed in depth.

Final stack gas desulfurization, however, might not be required. Case IX (below) presents an analysis of a system that includes high-temperature desulfurization to the level required for current fuel cells. Such desulfurization capability has now been proved at only the laboratory scale. However, high-temperature desulfurization that is sufficient for environmental considerations has now been tested on larger equipment. Should that process be incorporated with a sulfur-tolerant fuel cell, the economic and system advantages would still be impressive. Therefore, it is recommended that efforts to develop sulfur-tolerant fuel cells should be undertaken.

## Case VIII - High-Temperature Carbon Dioxide Transfer

A system has been conceived for pressure swing absorption of carbon dioxide from high-temperature, high-pressure gases. The sorbent would be regenerated by contacting with the compressed cathode air (which has a low concentration of carbon dioxide prior to being merged with other streams). Sorbents have been identified for this duty and the energy debits and credits for the sorption and regeneration phenomena have been calculated. The sorption of carbon dioxide takes place as shorin in Figure Ca-8, following the water-gas shift reactor, where the partial pressure of carbon dioxide is the highest. Approximately $50 \%$ to $60 \%$ of the carbon dioxide is removed from this gas stream. The sorbent is regenerated by the cathode air; significant heat exchange is required to heat this air and provide a thermal balance for the system. Purge steam is passed through the sorbent bed on both sides of the sorption and regeneration cycles to avoid mixing of oxidizing and reducing species.

This approach permits transfer of sufficient carbon dioxide from the hot fuel gas such that humidification of the feed to the fuel cell is not required. Thus, the gas feeding the fuel cell has higher purity and the cell exhibits excellent voltage. Similarily, the carbon dioxide is transferred directly to the cathode where it is required for the chemical reactions.

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The system with $\mathrm{CO}_{2}$ transfer is compared to Case IVe, which also uses a fluidized-bed gasifier of moderate mothane production and the internallyreforming fuel cell. The impact of transferring the carbon dioxide is about 2.5 percentage points gain in system efficiency. As noted in the economics discussion in the body of the report, however, this efficiency gain approximately offsets the increased capital requirement for the processing subsystem. Nevertheless, it is believed that the concept merits additional study; the approach offers significant advantages in certain recycle systems that culul not be evaluated within the constraints of the present program. Case IX - Hich-Temperature Desulfurization

Several concepts are under development at laboratories throughout the country for removal of sulfur from raw fuel gases at elevated temperature. The concept considered here is the mixed metal oxide system being deteloped at the Institute of Gas Technology. This system has particular attraction because the sorbent, when regenerated, produces elemental sulfur directly, rather than a dilute gas containing $\mathrm{SO}_{2}$ that must then be concentrated and reduced. Three cases were considered in the evaluation of this process, varying the technique employed for regeneration of the sorbent and recovery of the sulfur values in the gas. In the system as shown in Figure Ca-9, the raw gas first passed through high-temperature dust removal, quench; and waste heat recovery to the operating temperature of the sorbent. The sorbent is anticipated to purify the gas to the degree required for the molten carbonate fuel cell. If the gas is not purified to this degree, however, sulfur guards are under development that will operate at elevated temperature. Nevertheless, the gas was then cooled through turbo expansion and a recuperative heat exchanger train to $750^{\circ} \mathrm{F}$ before zinc oxide treatment. After reheating, the gas passed to the internally reforming fuel cell to consume the fuel values that were produced in the methane-producing fluidized-bed gasifier.

As mentioned above, three systems were considered for regeneration of the loaded sorbent. The systems were engineered sufficiently so feel confident of the operability, and energy balances were developed. The system solected for Table Ca-l produced elemental sulfur directly with essentially no tail gas strean. Note, therefore, that this system is not strictly comparable to the earlier systems - the energy balance has included all the systems necessary for sulfur removal. recovery, and environmental control, in contrast to the other systems analyzed.


Although the gas feeding the fuel cell has ligh concentration of water vapor and $\mathrm{CO}_{2}$, the overall system efficiency is high - about $50 \%$. In the economic analysis of the body of the report, thils system shows a preferred cost-of-electricity and the concept appears to warrant additional research effort.

Case X - Anode Tail Gas Recycle
Early in the program, it was recognized that $15 \%$ of the fuel values in the raw gas were being exhausted to the steam cycle because the fuel cell could not be driven to $100 \%$ conversion of the fuel. A system was conceived for recycling the spent anode exhaust back through the condensation and acid gas removal systems, permitting recovery of this fuel to the fuel cell. In this case, the acid-gas removal was total - carbon dioxide was removed from the gas as well as hydrogen sulfide. The carbon dioxide was removed selectively and recompressed into the cathode to supply the necessary fuel cell reactants. In this manner, the feed to the fuel cell could be dry and nearly $\mathrm{CO}_{2}$-free, thus providing the maximum voltage from the fuel cell. Also, all of the hydrogen value in the fuel is recovered electrochemically in the fuei cell, except for a small purge stream taken to eliminate nitrogen from the recirculating gas 1000 . This purge stream was burned into the cathode exhaust to provide the maximum temperature for the expansion turbine.

Significant effort was expended in trying to develop an operable system on the simulator. The primary problem was the excellent performance of the fuel cell - insufficient heat was discharged from the fuel cell at bigh temperatures to bootstrap the system to the fuel cell operating temperature. Thus, extreme heat exchange was incornorated into the system to provide proper energy management. Nevertheless, this system showed relatively poor efficiency and was not included in the economic analysis. No illustration of this system is provided; because the system could not be improved sufficiently to merit economic analysis, an illustration was not developed. The overall concept of recycle systems, however, deserves additional attention. Several other recycle systems have been conceived that may offer greater merit than the one attempted here.

## APPENDIX Cb.

Discussion of System Elements and Interrelated Effects

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## DISCUSSION OF SYSTEM ELEMENTS AND INTERRELATED EFFECTS

General

The work effort described in this document is an evaluation of alternative means for production of electricity from coal using molten carbonate fuel cells.

The overall system involves 1) gasification of the coal, 2) purification of the fuel gas produced, 3) fuel cell conversion of the fuel gas to electricity, and 4) various bottoming cycles to recover heat from the system and convert that heat to power. Discussion of the major system elements are presented below.

The approach used in this program is systems analysis. In this approach, the operation of each element of the process is described mathematically and the subprocess units are integrated by machine computation to define the operating performance of the total system. With this approach, the individual subelements are not optimized; rather, their operating regimes are varied so that the overall system performs in a preferred mode.

This approach is contrasted to that which has been historically followed. For example, a gasifier manufacturer might define his preferred operating mode and the fuel cell developer might specify his preferred feed; however, the required interfacing might be so complex that the overall system is less desirable than alternatives. In the preferred case, compromises might be taken in the gasifier and/or fuel cell operating condifions to minimize the complications of interfacing.

As is shown in Appendix Da, the system is extremely sensitive to assumed changes in operating variables. Basically, because large quantities of energy are being exchanged, transferred, or transformed in the various steps within the overall system, slight changes in the efficiency of any subsystem can severely impact the overall output efficiency that, marginally, becomes the difference between two large numbers.

Therefore, to better understand the overall system and its interrelated effects, one must not only comprehend the first principles involved in each process elemerit, but second=order effects are also important.

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A fuel cell is a device that electrochemically converts the free energy of a chemical oxidation-reduction reaction directly into electricity. As such, it is similar to an electrical storage battery, except that reactants are continuously supplied to the fuel cell and the reaction products are removed from the system.

Because electricity is thermodynamically equivalent to work, the fuel cell effectively produces work directly from the chenical process, without the temperature limitations of a Carnot cycle.

The free energy of formation of water vapor in a fuel cell is about $79 \%$ of the enthalpy of formation. Therefore, an ideal fuel cell can generate 79 kWh of power from $341,300 \mathrm{Btu}$ of hydrogen fuel. An ideal heat engine operating between $1200^{\circ}$ and $95^{\circ} \mathrm{F}$ can only generate 69 kWh from the same amount of fuel. Further, real heat engines are considerally less efficient than their conceptually ideal models. Real heat engines, with all their associated parasitic auxiliaries, typically yield a net power output of $35 \%$ to $40 \%$ of fuel input.

The fuel cell operates by physically separating the two halves of a chemical redox reaction, forcing the necessary electron transfer to take an external path and do useful work. The two locations for the half-reactions are electrically interconnected by some interiticiate of the chemical reaction, usually an ion in an electrolyte, thus closing the elecrical circuit.

The general chemical reaction employed in nost fuel cells is the reaction of hydrogen with oxygen to make water. In the simplest fuel cell, called the low temperature, acid fuel cell, molecular hydrogen reacts at the anode to produce hydrogen ions and electrons. At the cathode, the hydrogen ions react with oxygen to make water, removing electrons from the external circuit:

$$
\begin{equation*}
\frac{\mathrm{H}_{2}+2 \mathrm{H}^{+}+2 \mathrm{e}}{2 \mathrm{H}^{+}+1 / 2 \mathrm{O}_{2}+2 \mathrm{e}+\mathrm{H}_{2} \mathrm{O}} \mathrm{H}_{2}+1 / 2 \mathrm{O}_{2} \rightarrow \mathrm{H}_{2} \mathrm{O} \tag{Anode}
\end{equation*}
$$

The two electrodes are separated by an acidic medium containing $\mathrm{H}^{+}$ions and the nesessary electron transfer takes an external path between the electrodes.

```
*) 1
```

The free energy of this reaction is approximately $-55 \mathrm{kcal} / \mathrm{g}-\mathrm{mole}$ (to produce water vapor), resulting in a theoretical open circuit voltage of $1.185 \mathrm{~V} / \mathrm{ce} 11$ when conversion factors are included.

At higher temperatures (about $1200^{\circ}$ to $1300^{\circ} \mathrm{F}$ ) molten carbonate ion is the electrolytic transfer medium:

$$
\begin{equation*}
\frac{\mathrm{H}_{2}+\mathrm{CO}_{3}-\mathrm{H}_{2} \mathrm{O}+\mathrm{CO}_{2}+2 \mathrm{e}}{1 / 2 \mathrm{O}_{2}+\mathrm{CO}_{2}+2 \mathrm{e}+\mathrm{CO}_{3}-} \tag{Anode}
\end{equation*}
$$

(Cathode)
(Overall)
At elevated temperature, the free energy of the reaction is reduced to about $47.3 \mathrm{kcal} / \mathrm{g}$-mole or 1.027 V theoretical open circuit voltage. Note that carbon dioxide must be transferred between the electrodes in order to maintain the system. This is the fuel cell reaction that is the primary subject of the current project.

The molten carbonate cell, as mentioned above, requires the recycle of carbon dioxide around the system. Heat management at elevated temperatures is more complex (and is the primary subject of this document); yet, waste heat from the system may be recovered to valuable use.

The fuel cell converts, at most, the free energy of the chemical reaction合 alectricity. The total enthalpy change of the hydrogen-oxygen reaction in the molten carbonate cell is $59.12 \mathrm{kcal} / \mathrm{g}$-mole. If the fuel cell could sperate without losses, about $79 \%$ of the heat of reaction could be withdrawn as electricity (equivalent to the free energy of the reaction of 47.3 kcal / $g-m o l e)$. The remainder of the fuel heating value is released as heat. Note that any cell losses, as reflected by a decrease in cell voltage, also result in additional heat production.

The theoretical open circuit voltage of the molten carbonate fuel cell $1.027 \mathrm{~V} / \mathrm{cell}$ at $1200^{\circ} \mathrm{F}$ - is based upon free energy calculations and assumes that all reactants and products of the reaction occur at one atmosphere partial pressure. In real cells, however, these gases are usually present at different concentrations (or pressures) and this concentration changes as the gas is consumed (or produced) In the cell. In the anode compartment, the proper partial pressure ratio factor to be used is $\left(\mathrm{H}_{2}\right) /\left(\mathrm{H}_{2} 0\right) \cdot\left(\mathrm{CO}_{2}\right)$. A change in this ratio by a factor of 10 causes a change in the Nernst (or
concentration) potential of 91.5 mV at $1200^{\circ} \mathrm{F}$. At the cathode, where no reaction products are formed, the partial pressure factor is $\left(\mathrm{CO}_{2}\right)\left(\mathrm{O}_{2}\right)^{0.5}$. In both cases, reducing the factor causes a reduction in cell voltage and an increase in the heat release.

In the fuel cell simulator used in this project, the log mean average concentrations (i.e., the log mean average of the concentration at the inlet and at the outlet of the gas compartment) are used for calculating the concentration polarization effects within the cell. This is a reasonable approximation to the losses, depending upon the direction of gas flow within the system. Concentration effects at the cathode were generally minimal in this program; the reduced concertration of reacting species was counterbalanced by the 10 atmosphere cell operating pressure. At the anode, however, the Nernst polarizations were typically 70 to 75 mV at the $85 \%$ fuel utilization.

Other losses exist within the fuel cell. Notable among these are the socalled electrode polarizations and internal resistance of the cell. The internal resistance of the cell is the resistivity to current flow through the cell and the migration of the electrolyte ions. The total losses here are proportional to cell current. The primary aspect of cell construction that affects the resistivity is the thickness of the electrolyte used within the cell. With the avaliable fuel cell model, the internal resistance of the cell caused a voltage loss of about 49 mV at $160 \mathrm{~mA} / \mathrm{cm}^{2}$.

The electrode polarizations are a combination of factors. The true site for the electrochemical reaction is projected to be the area of those electrolyte pores that ace wall-wetted (but not filled) with electrolyte. The reactant gases must dissolve into the electrolyte (perhaps as governed by Henry's law) and diffuse to the electrode surface for reaction, with counterdiffusion and volatilization of reaction products. These effects are controlled by the partial pressures of the gases within the electrode pore and the current density of the cell. Some investigators claim very low power losses for this effect; the fuel cell simulator used in this project reported losses that were comparable in magnitude to the anode gas polarization.

In the project effort, the fuel cell was simulated at: a power density of about 150 to $160 \mathrm{~mA} / \mathrm{cm}^{2}$ and $85 \%$ fuel ucilization, factors that had been previously selected as preferred from earlier investigations. Optimization
studies in this effort did not always agree with these previous studies; however, these parameters were held constant for comparability. The operating pressure of 10 atm was selected because of the reasonable agreement of the model to experimental data at that pressure.

The overall fuel cell potential, as estimated by the fuel cell simulator, varied from 954 mV for a fuel feed gas with $10 w \mathrm{CO}_{2}$ and water concentrations to 815 mV for a system with relatively high contents of these species.

Currently, sulfir species are poisonous to molten carbonate fuel cells. When sulfur is present in the fuel gas, the nickel electrode material is deactivated, apparently by the formation of nickel sulfide. If sulfur is present in the anode gas, not only is the anode polarized but, because the anode exhaust gas is recycled after combustion into the cathode chamber, the cathode is also polarized. Additionally, sulfate ions form in the electrolyte, further degrading the overall cell performance. One of the major functions of the overall work effort is to find acceptable means for removal of sulfur from coal gas with minimum performance penalties.

For the total system, the maximum energy of the original fuel should be recovered in the fuel cell, because of its relatively higher efficiency, compared to the recovery of waste heat through Carnot-limited bottoming cycles. Directionally, certain effects should be expected in the fuel cell, based upon the fuel cell performance characteristics discussed above:

1. Higher-pressure operation is slightly preferred.
2. The fuel should be relatively dry and $\mathrm{CO}_{2}$-fiee.
3. The presence of $C 0$ in the fuel gas has a mixed effect because it impacts (through the water-gas shift reaction discussed later) the relative quantities of the terms in both the numerator and the denominator of the Nernst effect ratio. Generally, it was found that lower C0 concentrations are preferred.
4. If internal reforming of the methane present in the fuel can be accomplished, the Nernst effect is doubly adjusted to higher voltage.

The above effects are based upon operation of the fuel cell alone. When the fuel cell is integrated into the total system, counterbalancing effects may occur and the optimal operation of the fuel cell may not result in an optimal overall system.

## The Coal Gasifier

The overall system of conversion of coal to electricity, using molten carbonate fuel cells, requires a coal gasifier to convert the natural reductant - coal - into the species that is normally corsumed by the fuel cell - hydrogen. As will be shown later, this function should be expanded to include the production of $\underline{a l l}$ gaseous species that may be readily converted into hydrogen for use in the fuel cell.

The primary chemical reaction in a coal gasifier is the steam-carbon reaction:

$$
\mathrm{C}+\mathrm{H}_{2} \mathrm{O} \rightarrow \mathrm{H}_{2}+\mathrm{CO}
$$

The above reaction is highly endothermic and occurs, at reasonable rates, at temperatures greater than about $1700^{\circ} \mathrm{F}$. In most gasifier configurations, the endothermic heat of the reaction is supplied by burning a portion of the feed coal with air or oxygen:

$$
\mathrm{C}+\mathrm{O}_{2}+\mathrm{CO}_{2}
$$

The combination of the two primary reactions in the gasifier - the steam-carbon reaction and the carbon combustion reaction - yields an off-gas that contains primarily hydrogen, carbon monoxide, carbon dioxide, and water vapor. The water vapor is present because an excess of steam was used to drive the gasification reaction towards completion. The exact composition of the gas will be a function of the relative quantities of steam and coal that were used and the amount of oxygen required to sustain the reaction. Similarily, the proportions of the relative constituents will be governed by the chemical thermodynamics of the system at the operating temperature and pressure.

Based on heat balance, if carbon were the only constituent gasified, approximately $23 \%$ of the feed must be consumed with oxygen to supply the endothermic heat of the remaining $77 \%$ of the carbon that reacts with steam to form hydrogen and carbon monoxide. This carbon consumed by combustion is not a heat loss from the syster but, rather, supplies the additional heat that is available in the fuel gases as heat of combustion.

Most gasifiers require more oxygen than the theoretical minimum oxygen/carbon molar ratio of 0.23 required to support the steam-carbon
reaction. The increased oxygen is required to raise the temperature of the gasifier system to the level required for satisfactory kinetics. The additional combustion of carbon results in sensible heat in the off-gases; heat that can only be recovered to Carnot-limiting thermal cycles, rather than as fuel hydrogen for the fuel cell.

The entrained-flow gasifier of this study employs an oxygen/carbon molar ratio of about 0.47 at the operating temperature of $2450^{\circ} \mathrm{F}$. Thus, only slightly more than half of the feed carbon reports to the product gas as hydrogen and carbon monoxide. The fluidized-bed gasifier, operating at $1875^{\circ} \mathrm{F}$, requires an oxygen/carbon molar ratio of about 0.35 , converting much more of the coal into fuel gas species.

An alternative chemical reaction, termed hydrogasification, may also take place in the gasifier. In this reaction, carbon reacts directly with hydrogen to form methane.

$$
\mathrm{C}+2 \mathrm{H}_{2} \rightarrow \mathrm{CH}_{4}
$$

This reaction is exothermic. If it is promoted in the gasifier, it can help supply the heat for the steam-carbon reaction and displace part of the need for the carbon combustion reaction. In one conceptual gasifier evaluated in this study, the hydrogasification reaction is enhanced and the oxygen demand is markediy reduced, resulting in more efficient conversion of the feed coal into fuel gas species.

In the conventional molten carbonate fuel cell system, the methane produced by the hydrogasification reaction is not an acceptable fuel. Rather, the heating value of this material is only recovered to a thermal cycle. However, as discussed in detail later, the fuel cell may be integrated with steum-reforming of the methane to permit its utilization in the fuel cell for a more efficient overall system.

Gasifiers that promote the hydrogasification reaction are inherently more efficient because of reduced oxygen consumption (and burning of feed carbon to $\mathrm{CO}_{2}$ ). Developmental gasifiers such as HYGAS ${ }^{(2)}$, Exxon Catalytic, and Hydrane require little or no oxygen for supplemental heat, because of the vexy high methane production. Although conceptually advantageous in this system, these gasifiers were not assessed in the program because they generally add system complexity which, with the high leverage of plant capital on cost-of $\rightarrow$ electricity, would probably not be cost-effective at the plant scale used.

Note that it is possible to write the chemical reaction between carbon and oxygen to produce carbon monoxide rather than carbon dioxide. With this approach, all of the carbon value in the coal appears as fuel gas species. However, as will be shown later, any such gas produced is thermodynamically unstable at lower temperatures, tending to deposit carbon from the gas according to the Boudouard reaction:

$$
2 \mathrm{CO} \rightarrow \mathrm{C}+\mathrm{CO}_{2}
$$

This effect will be discussed in more detail in the next subsection. Other Chemical Reactions

## Carbon Deposition

Gas compositions that may be thermodynamically stable at elevated temperatures may, upon cooling, become unstable and have high potential for carbon deposition. The two primary reactions that are responsible for carbon deposition from the coal-gas compositions considered are -

$$
\begin{array}{r}
2 \mathrm{CO} \rightarrow \mathrm{C}+\mathrm{CO}_{2} \\
\mathrm{H}_{2}+\mathrm{CO} \rightarrow \mathrm{C}+\mathrm{H}_{2} \mathrm{O}
\end{array}
$$

Note that both of these reactions are the reverse of gasification reactions and are interconnected by the water/gas shift reaction (discussed later).

The thermodynamics of the above chemical reactions have been evaluated; the stability of the gas mixtire is a strong function of temperature, preser, e , and the allotropic form of the carbon that is deposited. Figure $\mathrm{Cb}-$ 1 is a representation of the carbon stability limits on the triangular $\mathrm{C}-\mathrm{H}-0$ diagram for the deposition of amorphous carbon at $1200^{\circ} \mathrm{F}$ at the operating pressures encountered in this program. The raw off-gas compositions from typical gasifiers encountered in this program are indicated, illustrating instability of these gases at the operating conditions specified. In general, the maximum instability will occur at a temperature of abou: $1050^{\circ}$ to $1200^{\circ} \mathrm{F}$, depending upon the precise gas composition. The carbon deposition reaction is catalyzed, particularly by nickel (as found in stainless sceel or fuel cell electrodes), and is also self-catalytic: Once carbon has been formed from an unstable gas mixture, the remaining unstable carbon falls out quickly.

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Figure $\mathrm{Cb}-1$. THERMODYNAMIC STABILITY OF FUEL GAS MIXTURES

The usual technique to avoid carbon deposition is to add sufficient water vapor to the gas so that the second of the carbon deposition reactions above is driven to the left. Similarly, the first of the reactions does not occur beacause of the interdependence of the water-gas shift reaction in converting carbun monoxide to hydrogen. Figure $\mathrm{Cb}-2$ illustrates the effect of steam addition on carbon deposition and further illustrates the impact of temperature on carbon deposition.

Most of the systems encountered in the current study include a water quench to add water vapor to the unstable gas and avoid the thermodynamic potential for carbon fallout. The water may have been added directly after the gasifier so that the gas, when cooled, would remain stable. Similarly, steam is added to the intermediate gas (which has been dehydrated in the course of sweetening) to avoid carbon deposifion within the fuel cell.

When water is added to the hot gas after the gasifier, the system efficiency is impaired because, somewhers in the system, heat is adred to liquid water to convert it to steam and the latent heat of vaporization is los:. Also, the steam absorbs some of the heat of the gasifier exhaust and part of this sensible heat is lost to cooling water.

When steam is added to the fuel cell feed, a similar effect takes place - the latent heat of vaporization is lost from the system, as is a portion of the sensible heat of the water vapor. Additionally, the water vapor present in the fuel cell feed depresses the hydrogen concentration in the feed and causes a Nernst concentration polarization.

Note, however, these effects are minimal if significant excess heat must be removed from the system as steam power. As discussed later in "turbine operations," the heat converted to steam power still loses the latent heat of vaporization of the steam. The expansion of the water vapor (in the fuel gas) through the various gas turbines in the system approximates the performance of the steam turbine, although it does not exhaust the heat at as low a temperature as the steam turbine. Generally, water vapor added to the fuel gas is a second-order effect for efficiency loss, when compared to a steam turbine, unless that water is condensed from the system under pressure and except for Nernst effects within the fuel cell.

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Figure $\mathrm{Cb}-2$. EFFECT of WATER ADDITION ON STABILITY of a fuel gas mixture

## Water-Gas Shift Reaction

Most of the carbon monoxide produced by the gasifies is eventually converted to hydrogen for utilization within the fuel cell by the water-gas shift reaction:

$$
\mathrm{CO}+\mathrm{H}_{2} \mathrm{O} \rightarrow \mathrm{H}_{2}+\mathrm{CO}_{2}
$$

This reaction is mildly exothermic. It may take place within the fuel cell, where the carbon monoxide is reacted with water vapor present in the feed or generated by the fuel cell reaction. If it takes place within the fuel cell, it alters both the numerator and the denominator of the concentration polarization equation. Generally, carbon monoxide is not preferred in the fuel cell feed because it dilutes the hydrogen.

If the water-gas shift reaction is included in the system prior to the fuel cell, a separate catalytic reactor is employed. To use available sulfurtolerant water-gas shift catalysts, the gas must be heated to a light-off temperature of approximately $550^{\circ}$ to $600^{\circ} \mathrm{F}$. The heat of the reaction is recovered at approximately $600^{\circ}$ to $800^{\circ} \mathrm{F}$, if a separate reactor is employed, compared with the $1250^{\circ}$ to $1300^{\circ} \mathrm{F}$ if the reaction takes place within the fuel cell. If a separate water-gas shift reaction step is included in the overall. system, the water added for quenching the raw gas is partially converted to hydrogen, minimizing the effects of heat loss in the initial quench. The additional hydrogen in the sweetened gas improves the fuel cell voltage and reduces the need for steam in the fuel cell feed (as discussed above, a second-order effect). However, the higher hydrogen content of the feed gas changes the relative quantities of water vapor and carbon dioxide in the fuel cell exhaust and, hence, the final stack in the system. Thus, higher hydrogen content to the cell increases the quantity of latent heat that is lost to the stack. Overall, several counterbalancing effects occur and the impact of an external water-gas shift reactor is not obvious. In general, the results of the project indicate that the inclusion of the water-gas shift reactor improves the overall system performance, if the quench water is condensed in the systein.

Carbonyl Sulfide Hydrolysis
The conversion of carbonyl sulfide to hydrogen sulfide by reaction with water vapor does not have a direct effect upon the overall system efficiency.

However, the relative quantity of carbonyl sulfide in the raw gas has an importani bearing upon the performance of the acid-gas removal system and the quantity of zinc oxide that is required for final gas purification. This reaction system was therefore included in most systems to enhance the practicality of the simulation and reduce the power and steam demands of the acid-gas removal process.

## Methane-Steam Reforming

Methane reacts with steam endothermically over nickel catalysis to produce hydrogen and carbon monoxide:

$$
\mathrm{CH}_{4}+\mathrm{H}_{2} \mathrm{O} \rightarrow 3 \mathrm{H}_{2}+\mathrm{CO}
$$

Significarit neat is absorbed when this reaction occurs. At lower pressures, such as found in these system, the thermodynamics favor methane decomposition at temperatures greater than about $1200^{\circ} \mathrm{F}$.

Thermodynamically, the steam-reforming reaction is ideally suited to be chemically and thermally integrated within anode compartment of the fuel cell. The fuel cell anode reaction produces the steam required to drive the reaction, and the cell provides the heat necessary to sustain the reaction. Several laboratories have been evaluating this integration: Catalysts to be incorporated within the anode chamber have been identified and tested. The overall system appears technically feasible at any condition where the fuel cell operating voltage is less than approximately 1.0 V , thus providing sufficient heat (total $\Delta \mathrm{H}$ ) to sustain the reaction. Consequently, in this effort, the reforming reaction was generally incorporated, chemically and thermally, within the anode compartment of the fuel cell.

Several other techniques are available for incorporation of the steamreforming reaction within the system. The waste heat in the anode exhaust can be used to reform that exhaust, down to an equilibrium temperature level. Also, the reforming reaction can be incorporated thermally (but not chemically) within the stack, using non-active sections of the stack. These approaches were not employed in the current study because of the high promise of the integrated intenally reforming system.

The total chemistry of the overall system can be summarized according to the reactions that occur. If the steam-carbon reaction is the only gasification mechanism, as encountered in entrained-flow gasifiers:

$$
\begin{aligned}
\mathrm{C}+\mathrm{H}_{2} \mathrm{O} & \rightarrow \mathrm{CO}+\mathrm{H}_{2} \\
\mathrm{CO}+\mathrm{H}_{2} \mathrm{O} & \rightarrow \mathrm{H}_{2}+\mathrm{CO}_{2} \\
2 \mathrm{H}_{2}+2 \mathrm{CO}_{3}^{--} & \rightarrow 2 \mathrm{H}_{2} \mathrm{O}+2 \mathrm{CO}_{2}+4 \mathrm{e} \\
\mathrm{O}_{2}+2 \mathrm{CO}_{2}+4 \mathrm{e} & +2 \mathrm{CO}_{3}^{--} \\
\mathrm{C}+\mathrm{O}_{2} & \rightarrow \mathrm{CO}_{2}
\end{aligned}
$$

(gasification)
(water-gas shift)
(anode)
(cathode)
(overall)
The everall reaction is the oxidation of carbon with oxygen to produce $\mathrm{CO}_{2} \cdot$ Intermediates include hydrogen, which is the material oxidized in the fuel cell. At perfect utilization, all the carbon monoxide is reacted by the water-gas shift reaction. Carbon dioxide must be recycled from the anode to the cathode and carbonate ion is an additional intermediate. Note that exactly as much water is produced in the system as is required for the chemical reaction. Note, however, that in the real systems considered, steam is raised and water vapor is discharged to the stack (including significant heat of vaporization). The techniques conceived for recycle of this vapor within the system could not be included within the constraints of the program.

If the hydrogasification reaction can be promoted within the gasifier, the reaction sequence changes to the following:

$$
\begin{aligned}
\mathrm{C}+2 \mathrm{H}_{2} & \rightarrow \mathrm{CH}_{4} \\
\mathrm{CH}_{4}+\mathrm{H}_{2} \mathrm{O} & \rightarrow 3 \mathrm{H}_{2}+\mathrm{CO} \\
\mathrm{CO}+\mathrm{H}_{2} \mathrm{O} & +\mathrm{CO}_{2}+\mathrm{H}_{2} \\
2 \mathrm{H}_{2}+2 \mathrm{CO}_{3}^{--} & \rightarrow 2 \mathrm{H}_{2} \mathrm{O}+2 \mathrm{CO}_{2}+4 \mathrm{e} \\
\mathrm{O}_{2}+2 \mathrm{CO}_{2}+4 \mathrm{e} & +2 \mathrm{CO}_{3}- \\
\mathrm{C}+\mathrm{O}_{2} & +\mathrm{CO}_{2}
\end{aligned}
$$

(hydrogasfication)
(steam-methane reforming)
(water-gas shift)
(anode)
(cathode)
(overall)
In this system, the sum of the first two reactions equals the first reaction of the previous set. However, the heat demand of the second reaction is supplied by the fuel cell, rather than by burning oxygen within the gasifier.

The individual species of $\mathrm{H}_{2} \mathrm{O}$ and $\mathrm{H}_{2}$ must either be recycled within the system or else the species must be provided externally. For example, the $H_{2}$ of the first reaction could be supplied by the first reaction of the earlier set of equations presented, if both reactions occur simultaneously.

Power Recovery Turbines
Although, on first examination, gas turbires appear to provide a means for recovery of pressure values of a gas into energy, they actually can be considered to operate on temperature. The value of the pressure is merely to define the temperature difference that can be recovered i:ito power across the turbine.

In general, the highest temperature feed to the turbine will result in the highest total power output because of the Carnot laws of heat engines. The steam turbine is generally limited to approximately $1000^{\circ} \mathrm{F}$ temperature on the input because of materials problems. However, the gas turbine concurrently operates at much higher temperatures. The combination of the gas turbine and the steam turbine - known as a combined cycle - is capable of much higher efficiency than the steam turbine alone because the heat discharged from the gas turbine can be recovered into steam and hence into the relatively low-temperature exhaust that corresponds to 2 to 4 inches of mercury absolute pressure in the condenser.

Consequently, on the overall system, it is preferred to operate the gas turbine at the maximum inlet temperature possible. The outlet temperature w11l be determined by the pressure ratio and the efficiency of the turbine. Note that the enthalpy difference extracted from the gas is directly translated into power, with only a small depreciation for mechanical efficiency, because the turbine inefficiency appears as heat in the outlet gas. Most of the heat in the outlet gas, eventually, is recovered into a steam cycle.

The steam cycle is depreciated in efficiency by the latent heat of vaporization of the water that must be converted into steam in the system. This inefficiency will exist, whether the steam cycle is used directiy or the steam is injected into the process gas for eventual recovery in the system.

Consider the case of the steam that is injected into the sweeten- gas, upstream of the fuel ce11. Under the assumptions of the system, this steam is
raised at relatively high pressure and $1000^{\circ} \mathrm{F}$. This steam is expanded across a power recovery turbine and injected into the gas stream to finhibit carbon deposition. In passing through the fuel cell, the mass of the steam is heated to fuel cell operating temperature and, eventuaily, exhausts with the pressurized cathede outlet gas. At this point, the mass of the water vapor is further expanded to atmospheric pressure, recovering power from part of the heat in the gas. Finally, the cathode gas, containing water vapor, is cooled through heat exchange and perhaps economizers before exhausting to the atmosphere. The final outlet temperature of the gas is $250^{\circ}$ to $500^{\circ} \mathrm{F}$, depending upon whether economizers are used or not. Relative to the same mass of steam passing through the standard steam cycle, the heat content of the anode gas injection steam has been recovered into power, or to reheat more water, to nearly the degree that would have been realized had the steam operated in a steam turbine alone. Thus, the injection of steam into the anode gas does not cause a direct loss of the power equivalent of that steam; rather, only a fraction of that power is lost because of the higher exhaust gas temperature. In order words, the effect of injecting steam into the anode feed gas is a second-order effect on efficiency as it impacts the overall system.

## Summary

In general, one can often evaluate the impacts of a change in the gasifier/fuel cell system on first principles. For example, the use of a methane-producing gasifier, in conjunction with an internally reforming fuel cell, is a relatively straightforward applicaition of first principles. The gasifier operates more efficiently, converting a greater fraction of the feed carbon into fuel gas species and consumes less parasitic power for the oxygen plant. The fuci cell converts its waste heat into reforming methane and maintains a higher concentration of hydrogen within the cell. Less heat is withdrawn from the fuel cell to the steam cycle; rather, that heat is used more effectively by producing hydrogen from methane.

In other systems, second-order effects occur and the solution is not so straightforward. For example, the incorporation of a separate, external shift reactor has several positive and negative effects. The summation of these impacts becomes minor in importance in affecting power outputs. Directionally, a separate water-gas shift reactor is a preferred alternative,
particularly if prudent design is followed, the raw gasifier off-gas is quenched for carbon control, and that quench water is condensed from the system.

Of particular interest was one case evaluated with a less conservative gasifier design. Less steam was fed to the gasifier and the overall gasifier performance was significantly improved. However, the altered gas composition required more severe quenching and the overall system did not benefit. In order words, optimization of the gasifier operating conditions did not optimize the overall system. Similarly, cases that gave extreme purification of the fuel cell feed, at a very high fuel cell voltage output, required sufficient parasitic power demand that the overall system did not benefit.

In the more detailed discussions of the individual systems presented in the body of the document and in Appendixes Ca and Da , the relative importance of each element in the system becomes more apparent.

# APPENDIX Cc. Summary Printouts for Cases 

 in Appendix Ca
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## CASE I

The Base Case

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## CASE Ie

## Carbon Control and Shift


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## Fluidized-Bed Gasifier

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## CASE III

Internally Reforming fuel Cell


## CASE IV

High-Methane Gasifier
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4 JAN 63 14:35:14
CASt JHI UG:4


-




## CASES IVb, $c$, and d

Vary Fuel Cell Conversion
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## METHーRIEN UOGAS HITM ANODE METNANE REFORMING $13.5 X C T O C$



| THE VOLTAGE OF THE FUEL CELL IS |
| :--- |
| THE AREA OF THE FUEL CELL IS |
| OVERALL PLANT EFEICIENCY, COAL PILE TO BUSBARE IS GI AB REREENIE |

OVERALL PLANT EFFICIENCY, COAL PILE TO OUSBAR IS GI BB PEREENT.

-u-upu-u
B-
CONVBO FLUZD BEDO REFORM, 85X CONV QUENGH, PREOSHIFT, COSX, $13.5 X$ CHK RAW


1



# 1 



## TABULATION OF SHAFT ENERGY AVAILABLE OR NEEOED:

AIR COMPRESSOR FOR SUPPLY TO CRYOGENIC OXYGEN PLANT
2 EXPIND SMIFS (ES EXIT GAS FHROUGN POUER RECOVERY TURESNE
29 REMOVE SULFLR RROM RAY GAS EY SELEXOL SYSTEE.
द2 ADD STEAM VIA TURSINE; PREVENT CARBON DROP IN FUEL CELL.
51 THE FUEL CELL, NAXIMUUA CONVERSTON, REREAM WITHIN ANODE.
57 ANJDE EXIT GAS BOOSTER FAN: TO EEED CATALYTIC BURMER.

| 64. EXPAND STACK GAS THROGG TURGINE TO RECOVER POUER. |
| :--- |
| 70 COMPRESS RECYCLE GAS TO INSECT FEED COAL TO GASIFIER. |


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$\sigma$
$\square$

## i

B
D


4

## CASE IV e

## Optimized Fluidized-Bed System

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gasif ication anu flectruchemical fuel cellis. al ong with cunvenitional power generation machinery.





电事"





 *

LIONS ETU.
-268075. KILOWATTS
$327910 . ~ K I L O W A T T S$
$1290 . ~ K I L O W A T T S$
$651336 . ~ R I L O W A T T S ~$
$712461 . ~ K I L O W A T T S$280
$\qquad$

## CASE IVf

Minimum Humidification


 24 JAN B3_14:43100



$\operatorname{Lin} 1$ itat
CASE OKF.4
STEAM LISI-
$\mathbf{1 2 ~ J A N ~} 83$ 15:18:23

500.0 PSIA 24072. MOLS STEAM 2 U-GAS GASIFIER NORMAL OPERATION. STAEAM AZ 2 NET MAKE. 5698. MOLS STEAM- 42 ADD STEAM VIA TUREINE: PREVENT GARBON DROP IN FUEL CELL.
ـ
$\qquad$
Dust-Tolerant Shift Reactor
THIS IS THE FINAL SYNUPSIS OF THE ENERGGY BUDGEI OF AN INTEGRATED PUWER PLANT USING COAL
GASIFICATION ANU ELECTROCHEMICAL FUEL CELLS ALONG WITH CUNVENTIONAL POWER GF:NFHATION MACHINERY.



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$$
\begin{aligned}
& \text { MO No日env } \\
& \text { S } 70 \times 773 \mathrm{c}
\end{aligned}
$$

TtN: FUEL
CELL.



[^7]PRECEDING PAGE BLANK NOT FILMED;

PROEESS STEAM CJNSUMOTION IS 7כ2. THOUSANDS POUHDS PED HOUR.
-2603:4. KILCWATTS

735908. KILOWATTS

DPDCZSS MACHINEDY (CONODESSODS AND MAJOR PUMPS) NEED
DROCESS GAS TURJO-EXDANDEOS G CLOSELY-ASSOCIATED STEAM TUDGINES GIVE SラAIT (1V,Nza

THE NET POWER DELIVERED TO GUSEAE IS
THE VOLTAGE OF THE FUEL CELL IS
THE AREA OF THE FUEL CELE IS
5744277. 52.FT.

OVEZALL PLANT EFFICIENTY, EOAL PILE TO GU'G•R, IS 47.3 DERCENT.

TABULATIO
NEEDED:

$$
\cdots \mathrm{N}
$$

$$
\begin{aligned}
& \text { n } \quad 315 \\
& 48 \equiv 15 \\
& n . j 15
\end{aligned}
$$

$$
\begin{aligned}
& 15 \\
& 15
\end{aligned}
$$

$$
\begin{array}{r}
553.2 \text { PSIA } \\
63.0 \text { SSIA } \\
1509.0 \text { PSIA }
\end{array}
$$

$$
\begin{array}{lll}
24072 . & 731 \\
14007 & 30 \\
7094 . & 80
\end{array}
$$

$$
\begin{aligned}
& 324 \\
& =945 \\
& =045
\end{aligned}
$$

$$
\begin{aligned}
& \text { U-GAS GASIFIEL NORMAL OPERATIOV. STREAY \#2 = NET MAKE. } \\
& \text { GEMOVE SULFUD FROM RAH GAS GY SELEXOL SYSTEM. }
\end{aligned}
$$

ADD STEAM VIA TUREINE: PREVENT CAREON ORDP IN FUEL CELL.

$$
\cdots
$$

## 1

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## CASE VII

## Sulfur-Tolerant Fuel Cell


24072. VIJLS STEAM 2 U-GAS GASIFIER NORMAL OPERATION. STREAM UZ = NET MAKE.



CASE VIII
High-Temperature $\mathrm{CO}_{2}$ Transfer

## ORIGINAL PAGE IS OF POOR QUALITY


17 FEE 33 7:19:13

COAL CONSUMDFION IS 496. THDUSANDS DOUNDS PER MOUR, OR AGOUT 5314. MILLIONS BTU.
PROCESS STEAM: CONSUMOTION IS 7L\&. THOUSANDS POUNOS PER HOUR
-264691. KILOWATTS
632848. KILOWATTS
750301. KILCWATTS
$\qquad$


TAZULATION OF SHAFT ENEDGY AVAILAMLE GO NEEDED.


L. U-FAS 5ASIFIER NDGMAL ODEAATIOH. STPEAM H2 ENET MAKE. ELEXDL SYSTEM.
CAPZON DRON IN FUEL GELL Cap30 DRO NJAJya
Ae $5 \forall 9$
$H \perp \forall 2 N I$ V Iáa an
 47 senove sulfur
$\qquad$

$\qquad$ 5:7. 4
-3:
$\qquad$
 553.0
1202.0
1202.0
65.0
1500.0
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Nongor317

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## CASE 1X

High-Temperature Sulfur Removal
$A M$
$A M$
$A M$

$$
\begin{array}{rl}
\text { TAEULATION OF STEAM NEEOED IN PROCSSS. } \\
2 & 550.0 \\
14 & 1200.0 . P S I A
\end{array} \quad 24072 . \text { MOLS }
$$

RUN.C 3 28 FEG 83 T4:11:14


$$
15 \text { DECLAIM ZN SPINEL (OXIOES GY OXYGEN: MAKE SULFUR. }
$$

$$
\begin{aligned}
& \text { 24072. MOLS STEAM } 2 \text { U-GAS GASIFIEP NORMAL OPERATION STREAM WZ E NET MAKE. } \\
& 192 \text {. MOLS STEAM } 14 \text { ADSORG HZS OHTO ZINC SPINEL: A NEW IGT DEVELOPMENT. }
\end{aligned}
$$

$$
\cdot
$$



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CASE X
Anode Exhaust Recycle






#### Abstract

I

APPENDIX Cd. Complete System Computer Printout for Case 5 (Similar to Case Ca-lVe, Da-C)





********
********




## KiLo

THE VOLTAGE OF THE FUEL CELL IS $\quad$ O.8303 VOLTS.
IHE AREA UF THE FUEL CELL IS
OVEKALL PLANT EFFICIENCY, COAL PILL 10 UUS日AR, 1545.8 PERCENT.

> TAGULATIUN OF SHAFI ENERGY AVAILAGLE OK NEEDED.


| $\begin{aligned} & \text { CASE AMALI } \\ & 14 \text { JNEAM } 83 \text { ISt } \end{aligned}$ |
| :---: |
|  |  |
|  |  |



2A CUOL 10 AMBIEIN：UROP CONUENSATE：UUMP HEAT TO AIH \＆$C W$ ． 29 REMUVE SULFUR FROM RAW GAS HY SELEXOL SYSTEM．
 54 CUOL ANOUE EXII GAS IN WHB－RAISE STEAM． $\stackrel{n}{0}$ bj Cathuue hecylle gas cinculation fan．

$$
\vdots+
$$

$$
7
$$

SS-*BSI

$$
\dot{N}_{\underset{\sim}{n}}^{\stackrel{n}{n}} \stackrel{0}{n}
$$

$$
\begin{aligned}
& 150 . \\
& 150 .
\end{aligned}
$$ 36 COMPRESS CUMGUSTION AIR TO FUEL CELL PRESSURE．

46 H46F62－WAKM COMBUSTIUN AIR FROM CATHOUE RECYCLE M62．
45 H45F65－WAKM COMBUSTION AIR FRON STACK GAS 465. 47 R47F6l－WAhm COMBUSTIUN AIR FROM CATHODE RECYCLE M6I． 48 MERGE FRESH AIR W47 WITH FECYCLED CATHODE EXIT GAS 463. 49 BURN ANUDE EXHAUST GAS W57 WITH DILUTED AIR \＃48． 50 JOIN THE IWU FUEL CELL FEEOS，ANODE \＃42，CATHODE 49. 5I TME FULL CELL，MAXIMUM CONVERSION，REFORM WITHIN ANODE． SEPAHATE ANUUE EXIT GAS．WS2．FROM CATHODE EXIT GAS．W53．

$$
55 \text { R36F5S COUL ANUDE EXİT GAS TO WARM ANOUE FEED GAS \#36. }
$$

$$
56 \text { This Sitep oeleieo. }
$$ 56 ThIS STEP OELEIED．

57 andode exit gis houstrir fan，to feev catalytic burner． 0.396 SPLIT CATHUDE EXIT．COOLED RECYCLE（M58），STACK EXIT（W59）． 60 cUol cathuut recycle gas in whb－railse steam． 61 K47F6I COUL CATIHODE RECYCLE TO WARM COMBUSTION AIR \＃47． 62 H46F62 COOL CAIHOUE RECYCLE TO WARM CUMSUSTION AIK M46．
$150 .{ }^{3}$
15 m
 in 162． $\stackrel{0}{0}$烒 © $\stackrel{\infty}{5}$ 4.4 $152 .{ }^{2}$ $145 .{ }^{3}$ 143.1 14．1．
我我我我我我 54， 5304 142． .2 T

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$$
\begin{array}{lll}
\text { CASt. } & \text { AIR4.150 } \\
\text { STEF } & 97 & 9 \\
14 & \text { JAN } 83 & 9121114
\end{array}
$$

$$
\begin{aligned}
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\end{aligned}
$$


THIS STEP DESCHIBES A PRUCESS GAS CUMPRESSUR OF 2 STAGES.
COMPONENT STREAM NUMGEK 97
$\begin{array}{lrr}\mathrm{CUZ} & 0.0 & 0.0 \\ \mathrm{HCO} & 1185.1 & 2.5\end{array}$
$0 \mathrm{OC} \quad 977 \mathrm{B.O} \quad 20.4$

> AIR COMPRESSOR $\mathfrak{f}$ UK SUPPLY TO CKYUGENIC OXYGEN PLAN
> - *********************
A1R4. 160


$\begin{array}{lr}\text { CuZ } & 0.0 \\ \text { H2O } & 0.00 \\ \text { N2 } & 34.04 \\ 0< & 7813.8\end{array}$
$\begin{array}{cc} & \text { STREAM NUMBER } 99 \\ \text { CUMPONENT } \\ \text { NOLS } & \%\end{array}$

## TOTAL



recyele gas fo inject coal fetu. stream "3 = Total exit gas.

$\square$
a aous stream 2671 to hhuuvce stream 3


 | 0 |
| :--- |
| 0 |
| 8 |



$$
\begin{array}{ll}
\text { CASE } & \text { AIR4.160 } \\
\text { STEN } & 4 \\
14 \text { JAN } 63 & 9121114
\end{array}
$$


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\% WVIHIS NOHS NOILISNHWOS SVS
CAREUN STAHILITY REIPOHTEU AS STHEAM
TEMPERATURE: 1200. 0 DEGREES F
PRESSURE: 490.0 PSIA GRAPHITE AMORPHOUS GAS Stream GAS STREAM AT 1000.0 DEGHEES F AND 490.0 PSLA GAS NEEUS 4399.06 MOLS WATER. 0.1677 EAMORPHOUS CAREOA LIMIT AT 900.0 DEGRELS F AND 490.0 PSIA GAS NEEDS 3001.31 MOLS WATER. O.IBOI I AMORPNOUS CARUUN LIMIT.

$$
\begin{aligned}
& \text { IFIS IS A TEST WHEIHER THE GAS IS SIAHLE WITH RESPECT TO CARBON DEPOSITION. }
\end{aligned}
$$

G QUENCH TU STAHILIzE GAS \& HREVENT CARHUN DEPOSITIUN.
THIS STEH IS AN AUGARATIC GUEACH OF HUT GAS WITH lIQUID water to avold carbun deposition.

THIS STEH IS AN AUGARATIC QUENCH OF MUT GAS WITH LIQUID WATER $\begin{array}{cc}\text { FEED STRLAM } \\ \text { MULS } & 3 \\ 15503.4 & 27.6 \\ 3513.2 & 6.3 \\ 12314.5 & 21.9 \\ 9197.6 & 16.4 \\ 14906.7 & 26.5 \\ 200.5 & 0.4 \\ 0.0 & 0.0 \\ 477.9 & 0.4 \\ 74.4 & 0.1 \\ 13.7 & 0.0 \\ 56208.0 & 100.0 \\ 1875.0 & \\ 500.0 & \text { PSIA } \\ & \\ 4622.7 \text { MULS }\end{array}$



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$\begin{array}{ll}\text { EXITE } & 640.0 \text { DEGREES FAHRENHEIT. } \\ \text { EXITE } & 279.63 \text { MILLIONS ETU. }\end{array}$
THE UUTY UF THIS PHOCESS COOLEH IS: -31.77 MILLIONS GTU PER HOUR.

 71312:6 EA NVF ot - \#**

THE DUTY UF THIS PKOCESS COOLEH IS! -31.42 MILLIONS BIU PER HOUR.
11 R11T17 COOL NAM GASI WARM CLEAN GAS M17.

|  | COMPONENT | STREAM NUM MOLS | $\text { BER } \frac{1}{9}$ |  |
| :---: | :---: | :---: | :---: | :---: |
|  | H2 | 15505.4 | 25.5 |  |
|  | Ch4 | 3513.2 | 5.8 |  |
|  | CU | 12314.5 | 20.3 |  |
|  | Cuz | 9197.6 | 15.1 |  |
|  | HCO | 19529.4 | 32.1 |  |
|  | NC | 200.5 | 0.3 |  |
|  | C2H6 | 0.0 | 0.0 |  |
|  | HCS | 477.9 | 0.8 |  |
|  | NH 3 | 74.4 | 0.1 |  |
|  | cus | 13.7 | 0.0 |  |
|  | tolal | 60830.6 | 100.0 |  |
| PROCESS GAS | TSMPEAATURE, | FEED: | 640.0 | EXITE |
| PRUCESS GAS | ENTHALPY, | FeED $=$ | 279.63 | EXITE |



16 R1ZT16 WARM SHIFT FEEU GAS FHUM RAW GAS WIZ.

 EXIT: 226.日S MILLIONS BTU.

ORIGINAL PAGE :
IH RIOTIA mAPM SHIJF FEEU UAS FRGM RAH GAS MLO.
THIS STEP RECURERATES HEAT AEAINST SIEF M 10
THE ENTHALPY THANSFERREU IS: 34.71 MILLIONS ETU
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20 EXPand Shift (I) exit gas thruvgh poweh recovery tureine. TMIS STEP DESCHIHES A PROCESS GAS TUKGINE-EXPANUER

$$
\begin{array}{ccc} 
& \text { STREAM NUMGER } \\
\text { COMPONENT } \\
\text { NOLS }
\end{array}
$$

$$
\begin{array}{lrr}
\text { HC } & 22915.6 & 38.1 \\
\text { CH4 } & 3513.2 & 5.8 \\
\text { CU } & 4908.2 & 8.2 \\
\mathrm{CUZ} & 16607.8 & 27.6 \\
\mathrm{HLO} & 11495.3 & 19.1 \\
\mathrm{NL} & 200.5 & 0.3 \\
\mathrm{CRHG} & 0.0 & 0.0 \\
\mathrm{HRS} & 477.9 & 0.8 \\
\mathrm{NH3} & 0.0 & 0.0 \\
\mathrm{CUS} & 13.7 & 0.0
\end{array}
$$

$$
\text { TOIAL } 60132.3 \quad 100.0
$$

$$
\text { THE PHESSURE LET-DUMN RATIO IS } 0.422
$$

$$
\begin{aligned}
& \text { SHAFT ENEHGY DELIVERED, HORSEPOWER: } \\
& \text { KLLOWATTS: }
\end{aligned}
$$

ISENTROPIC GAS EXPANSION EFFICIENCY $1 S ~ 92.0 \%$. (SET BY USER)
MEGHANICAL EFFIGIENCY ASSUMEU IS Y
INLET PRESSURE IST
INLET VOLUME IS:

$$
28627.0
$$

$$
\text { UISCMARGE IS: } 57045.8 \text { ACFM }
$$



$$
\begin{aligned}
& \text { CASE AIRG•16n } \\
& \text { STFN } 23 \\
& 14 \text { JAN } 83 \quad 9821: 14
\end{aligned}
$$

23 H23T35 LOOL SHIFIEIS GAS IU WAKM SWEET FUEL 35.



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28 COUL TU AMRIENTI URUP CUNUENSAIEI DUAK HEAT TU AIH 6 CW.

This step cools dhe gas ip 100.0 F and subthacts condensate. | EXIT STREAM 28 |  |
| ---: | ---: |
| MOLS | 9 |
| 24963.3 | 49.0 |
| 3513.2 | 6.9 |
| 2860.6 | 5.6 |
| 14668.8 | 36.6 |
| 280.2 | 0.5 |
| 200.5 | 0.4 |
| 0.0 | 0.0 |
| 491.2 | 1.0 |
| 0.0 | 0.0 |
| 0.5 | 0.0 |
| 50978.1 | 100.0 |

> 100.0
173.0
FsIA
100.0 F
9154.2 MOLS
107.551 MILLIONS BTU
171.093 MILLIONS BTU
270.644 MILLIONS BTU FEEO STHEAM 27
 5.8
4.8
11.0
15.7
0.3
0.0
0.8
0.0
0.0 4963.3
351.3 .2
2880.6
8688.8
9434.4
200.5
0.0
491.2
0.0
0.5
0.0nt E*2E109
320.0 F
177.0 PSIA GAS DEW PUINT WATEH SUUTRACTED 244.8 F

CUMPONENT
HC
CH4
CO
CUZ
H2O
HL
CLHG
HLS
NH3
CUS

TUTAL
TEMPERAIIURE
PKESSLLRE
sailnn 39nvisx
GATER CONDENSING

## total

 EXIT STREAM 28

$$
\begin{array}{lll}
\text { CASE } & \text { AIR4. } 160 \\
\text { STFE } & 30 & \\
14 \text { JAN } & 83 & 9: 21: 14
\end{array}
$$

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$$
\begin{aligned}
& \text { CASt AIR4.160 } \\
& \text { STFN } 34 \\
& 14 \text { JAN } 83 \quad 9121114
\end{aligned}
$$

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Exit -


|  |  | COMPONENT | STREAM NUM MULS | $\triangle \text { EH }{ }_{8}^{34}$ |
| :---: | :---: | :---: | :---: | :---: |
|  |  | Hï | 23090.6 | 51.9 |
|  |  | CH4 | 324.7 .6 | 7.3 |
|  |  | CO | 2645.9 | 5.9 |
|  |  | CO 2 | 15331.7 | 34.5 |
|  |  | HCO | 0.3 | 0.0 |
|  |  | Ne | 185.5 | 0.4 |
|  |  | C2H6 | 0.0 | 0.0 |
|  |  | H25 | 0.0 | 0.0 |
|  |  | NH3 | 0.0 | 0.0 |
|  |  | cus | 0.3 | 0.0 |
|  |  | TOIAL. | 44502.0 | 100.0 |
| PROCESS | GAS | TEMPERATUPE* | FEED= | 385.4 |
| PRUCESS | GAS | ENITHALPY. | FEED: | 111.39 |



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42 ade stean via turbine f phevent cakbon ukot in fuel cell.
THIS IS A HOWER RECOVEHY TURGINE WHICH EAHANDS B015. MOLS UF HIGH PRESSURE
SUPEHHEATEU STEAM INTO PKUCESS STREAM NUMGER 42 $\begin{array}{rr}\text { EXIT STREAM } & 42 \\ \text { MOLS } & \% \\ 23090.6 & 44.0 \\ 3247.6 & 6.2 \\ 2645.9 & 5.0 \\ 15331.7 & 29.2 \\ 8015.1 & 15.3 \\ 185.5 & 0.4 \\ 0.0 & 0.0 \\ 0.0 & 0.0 \\ 0.0 & 0.0 \\ 0.0 & 0.0\end{array}$
52516.4100 .0
FEED STKLAM 37
 COMPONENT THE STEAM PRESSURE LET-DOWN RAT10 IS 0.102
FRUM 1500.0 PSIA TU 153.0 PSIA
JALET STEAM TEMPERATURE AT THROTTLE IS: 1000.0 DEGREES F.
 MECHANICAL ESFICIENCY ASSUMEU IS $98.0 \%$
SHAFT ENERGY DELIVERED. HORSEPUWERE 14310.
KILUWATTS: 10668.




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43 Feev ain at 160.0\% uf Stuichiumetric. (including scalex).
this introuuces a secunu uk suhseguent feed gas as stur
$152057.2 \quad 300.0$
total

[^8]

SIEI 3 wolmoinis


46 R46G62 - WARM COMHUSTIUIN AIK FKOM CATHULIE RECYCLE W6R.
IHE UUTY OF IHIS PHOCESS HEATER 1S: 219.06 MILLIONS OTU PER HUUK.



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$$
\begin{array}{cc}
\text { EXIT STREAM } 48 \\
\text { MOLS } & 9 \\
13915.9 & 5.0 \\
30870.5 & 11.1 \\
194347.0 & 70.0 \\
38611.5 & 13.9 \\
277744.8 & 100.0 \\
823.9 \\
156.0
\end{array}
$$

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49 BUKN ANUUE EXHAUST GAS M57 WITH DILUTEU ABR \#48.

WI
IHIS IS A CATALYTIC RUKNEK FUR FUEL GAS 57, WITH AIRNUXYGEN SUPPLY 48. THE FLUE GAS IS 49.


[^9]
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 $\begin{array}{cc}52516.4 & 100.0 \\ \text { EXIT STREAM } & 50 \\ \text { MOLS } & 0 \\ 68059.0 & 18.6 \\ 68471.4 & 18.7 \\ 194532.5 & 53.0 \\ 35706.9 & 9.7\end{array}$

| no |
| :--- |
| $\vdots 0$ |
| 00 |
| -1 |

 $0.0 \quad 0.0$
 $366769.9 \quad 100.0$
1046.4
152.0

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CASt $A 1 R 4.160$
STEF 51
14 JAN $83 \quad 9821114$


SEPAKATE ANODE EXIT GAS, WBZ. FHUM CATHUUL EXIT GAS, MS3.
THIS STEP SEPAKATES HYRHID SIREAM BI 1 NTO FUEL GAS COMPONENTS: STREAM 52
AND OXIULZING GAS COMPONENTS: SIREAM B3.

$$
\begin{aligned}
& \text { PHODUCT GAS SITEAM ST2 } \\
& \begin{array}{r}
5.2 \\
0.0 \\
3.0 \\
81.6 \\
54.0 \\
0.3 \\
0.0 \\
0.0 \\
0.0
\end{array} \\
& 91904.7 \quad 100.0 \quad 145.0
\end{aligned}
$$

$$
\begin{aligned}
& 145.0
\end{aligned}
$$

$$
\begin{aligned}
& \begin{array}{r}
3326.2 \\
12.4 \\
2433.1 \\
51697.6 \\
34249.9 \\
185.5 \\
0.0 \\
0.0 \\
0.0 \\
0.0
\end{array} \\
& \text { Dinoduct Gas stream } \\
& \begin{array}{rr}
35141.1 & 11.1 \\
68471.4 & 21.6 \\
194532.5 & 61.3 \\
14248.0 & 6.1 \\
317393.0 & 100.0
\end{array} \\
& \begin{array}{l}
\text { MEMPERATURE }=1239.6 \text { UEGREES } F \\
\text { MRESSUKE } z \\
145.0 \text { PSIA }
\end{array}
\end{aligned}
$$

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Sム CUUL ANUUE EXIT GAS IN WHE KAISE STEAM.
THE UUTY UF THIS PROCESS COULER 1S: -334. 74 MILLIONS GTU PER HOUR.
 $\begin{array}{lll}\text { CASE AIR4.160 } \\ \text { STEN } & \text { A4 } & \\ 14 \text { JAN } 83 & 9: 21114\end{array}$先

CASE AIR4.160
STEN S7
14 IAN 43.21 .14
कllez6 fR NOF कt

AIR4. 1.60 JPL4, 2-STAGE AJIR COMPRESSUR, WITH AIR FEED $160.0 \%$ OF STUICHIOME IRIC
57 AIVOUE EXIT GAS ROUSIER FAN. TO FEED CATALYTIC GURNER.
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\text { THE COMPKESSION RAIIO (PER STAGE) IS } 1.11
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& \text { HER STAGE TUTAL. } \\
& \text { 111G7. } 11167 .
\end{aligned}
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\begin{array}{lcc}
\text { HCRSEPOWER } & \text { PER STAGE } & \text { TUTAL } \\
\text { KILUMATIS } & 1167 . & 11167 . \\
& \text { G325. } & \\
\hline
\end{array}
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\begin{aligned}
& \text { ISENTHOPIC GAS COMPRESSION EFFICIENCY IS } 88.0 \text { \%. (BY DEFAULT) } \\
& \text { MECHANICAL EFFICIENCY ASSUMEU IS 9d.0\% } \\
& \text { AT EACH STAGE SUCTION TEMPEHATULE IS: } 855.0 \text { DISCHARGE IS: } 883.5 \text { DEGREES F. } \\
& \text { PRESSURE IPSIAI: SUCTION DISCHARGE } \\
& \text { STAGE I VOLUME (ACFM): SUCTION DISCHARGE }
\end{aligned}
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\begin{aligned}
& \text { STREAM NUMUER ST } \\
& \begin{array}{lrr}
\text { HC } & 3326.2 & 3.0 \\
\text { CH4 } & 12.4 & 0.0 \\
\text { CU } & 2433.1 & 2.6 \\
\text { CU2 } & 51691.6 & 56.3 \\
\text { HEO } & 34249.9 & 37.3 \\
\text { NL } & 185.5 & 0.2 \\
\text { CCH6 } & 0.00 & 0.0 \\
\text { H2S } & 0.00 & 0.0 \\
\text { NH3 } & 0.0 & 0.0 \\
\text { CUS } & 0.0 & 0.0
\end{array} \\
& \text { TOIAL } 91904.7 \quad 100.0
\end{aligned}
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| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| C02 | 35141.1 | 11.1 | 13415.9 | 11.1 | 21225.21 | 11.1 |
| H20 | 68471.4 | 21.6 | 27114.7 | 21.6 | 41356.72 | 21.6 |
| N2 | 194532.5 | 61.3 | 77034.9 | 61.3 | 117497.6 | 61.3 |
| 02 | 1424R.0 | 6.1 | 7622.2 | 6.1 | 11625.8 | 6.1 |
| tutal | 311393.010 | 00.0 | 125687.610 | 00.0 | 191705.410 | 00.0 |
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& \text { EXIT= } 1044.35 \text { MILLIONS QTU. }
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OL H46FO2 COOL CATHUUE HELYGLE TO WAKM CUMBUSTIUN AIR. T46.


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HORSE.POMER
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AIR4. 160


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THIS STEP deschiges a process gas !ungine-expander $\begin{array}{rr}\text { STREAM NUMUEK } & 64 \\ \text { PULS } & \% \\ 21.225 .2 & 11.1 \\ 41356.1 & 21.6 \\ 117497.6 & 61.3 \\ 11625.8 & 6.1\end{array}$

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UISCHARGE ISI 2143494.8 ACFM
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65 \text { RUSF } 65 \text { COOL STACK GAS TU WAKM COMBUSTIUN AIR M45. }
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ot Read cunmusilin fel valut ef ran gas fhon gasifier.
$\begin{array}{rc}\text { SWEETENED GAS } \\ \text { MOLS } & \\ & \\ 13633.2 & 46.7 \\ 3249.8 & 11.1 \\ 21.03 .9 & 41.5 \\ & \\ 185.5 & 0.6 \\ 0.0 & 0.0\end{array}$ 0.0
29172.5100 .0


STEP IDENIfICATION * 66 SOURCE STKEAM" 2

| URIED FUEL GAS |  |
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| MOLS | 8 |
| 13633.2 | 36.2 |
| 3249.8 | 8.6 |
| 12403.9 | 32.2 |
| 7954.5 | 21.1 |

$\begin{array}{rr}185.5 & 0.5 \\ 0.0 & 0.0 \\ 477.9 & 1.3 \\ 13.7 & 0.0 \\ 37618.6 & 100.0\end{array}$
109633.
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STEP IDENILFICATIUN * 67 SUURCE SIREAM 31

| URIED FUEL GAS |  |
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68 READ COMBUSTION FUEL VALUE UF SWFET ANUDE FEED GAS.
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THIS HOUTIAE GIVES CUMBUSTION HEAT VALUES.


| SWEETENEU GAS |  |
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70 CUMPHESS RECYCLE GAS TU INJELT FEED CUAL TO GASIFIEN.
THIS STti dESCHIBES a phocess gas Cumblessor of 2 stages.
THE COMPKESSION RAIIO (PER STAGE) IS 1.84

## ENEHGY REQUIREMENTS


CUMPONENT
$\begin{array}{lrr}\text { MORSEPOWER } & 1206 . & 24110^{\circ} \\ \text { KILUWATIS } & 899 . & 1797 .\end{array}$

AT EACH STAGE SUCTION TEMPERATURE I5: 100.0 DISCHARGE IS: 205.2 DEGREES F.
$\begin{array}{lcccrrr}\text { URE (PSIA): SUCTION DISCHARGE } & \text { VOLUME (ACFM)I SUCTION DISCMARGE } \\ \text { STAGE } 1 & 168.0 & 309.6 & & 2072.4 & 1335.8 \\ \text { STAGE } 2 & 298.4 & 550.0 & & 1166.7 & 752.0\end{array}$
INTERSTAGE COOLING DUTY ISt 3.07 MILLIUNS BTU

AIR4. 160 JPL4. 2-SIAGE AIR COMHRESSUK, WITH AIH FEEU $160.0 \%$ OF STUICHIOME!RIC
 Non-Confidential Fluidized-Bed Cases


PRODUCT GAS EOMPOSITION,
PRQDUET GAS EOMPQSITION：HOLE PERCENT：CO
H2O ANR NH3 FREE： 25.127
MOLECULAR WEIGHT $=19.6355$（EAS UOLUME $=$
REEYCLE GAS COHPOSITIDN，HOLE PERCENT：CO
HOLECULAR WEIGHT $=20.0397$
TOTAL H2O：H2S，COS，NH3，HCN FREE PROLUCT GAS＝ 102.3170 MOLES（ 2050.387 LBS）

COMPOSITION：MOLE PERCENT
MOLECULAR ：HETGHT $\begin{array}{ll}\text { MOLECULAR UEIGHT } & =20.0395 \\ \text { HIGHER HEATING UALUE } & =293.206\end{array}$
$\begin{array}{ll}\text { NET GAS PRODUCTION } & =0.1052548 E+0 B \text { BTH } \\ \text { NET PRODUET GAS HHU／COAL HHV } & =0.8242\end{array}$

## $\pi$ 7

$11 \cdot 86=N$
$98^{\circ} \mathrm{G6}=N$

## KINETEC RATE CONSTANT

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=98.49 x
$$

267．711 BTU／SCF） 20.0395
293.206 BTU／SCF ILHV $=$
267．711 2TU．SCF

$\cdot$
$=96.49 \%$
$=96.88 \%$
$=98.76 \%$
$=97.48 \%$
$: \quad C=85.12$
$: \quad C=98.49$
$=1.50 \% 0 F$
$=1.44 \% 0 F$
$=1.79 \% 0 F$
$=1.44 \%$ OF FEED COAL（MAF）
$=1.29 \%$ OF FEEB COAL CARBON
$=1.0000$ HOL／HDL $1.4999 \mathrm{LB} / \mathrm{LB}$
CARBON GASIFICATION EFFICIENCY
CARBON UTILIZATION EFFICIENCY
MAF COAL GASIFICATION EFFICIENCY MAF EOAL UTILIZATION EFFICIENCY

CONUERSIONS IN FINES
CONUERSIONS IN AGGLOHERATES
OUERALL GONVERSIONS
FINES LOSS（KF）
FINES LOSS（MAF）
CARBON IN FINES LDSS
EXTERNAL STEAH／CARBON EXTERNAL STEAH／CBAL（AS FED）$\quad=1.0166 \mathrm{LH} / \mathrm{LB}$
$=1.15 \mathrm{BE}$ LB／LB $=1.0246 \mathrm{MOL} / \mathrm{HOL}$
$=1.0416 \mathrm{LB} / \mathrm{LB}$ $=1.0416 \mathrm{LB} / \mathrm{LB}$
$=1.0684 \mathrm{LB} / \mathrm{LB}$ $=1.1873 \mathrm{LB} / \mathrm{LB}$
$=0.3525 \mathrm{HOL} / \mathrm{HDL}$

$=37.31 \%$
$=38.81 \%$
$=38.81 \%$
$=8.33 \%$ DF FEED CARBON

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34．023 ATM： 34.472 BAR

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AGGLDMERATES

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| 0.0979 |
| 0.4112 |
| 8.1125 |
| 0.0000 |
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GASIFIER PRESSURE
GASIFIER HEAT LOSS COAL FEER（MOISTURE－FREE） FEEDSTUCK HEATING VALUE
FEEDSTOUK MOISTURE CONTENT N2 CONTENT IN OXIBANT FEED
PRODUET GAS SHIFT TEMF．

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& =\quad 0.500 \% \\
& =1725.0 \text { DEGREE }
\end{aligned}
$$



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APPENDIX Da. Analysis of Variations in Basic Assumptions

## analysis of vartations in basic assumptions

## General

During the course of the work effort, it became apparent that significant variations in the system efficiency could be achieved with relatively minor adjustments in the operating parameters. The systems analyst must use extreme care to be certain that two systems to be compared are identical in all respects except the variable being altered, fo avoid clouding the results by the effects of unwanted changes. In fact, many of the cases presented in Appendix Ca were reevaluated several times during the course of the program as the analyst became more familiar with the overall system and sought to ensure strictly comparable results for analysis. For that matter, the results presented in the body of the text, using essentially the same systems as employed in Appendix Ca, show slightly different efficiencies because one last iteration was used to ensure identical assumptions.

The above effect occurs because of the relative complexity of the system and the number of elements employed. At each step of the process, many hundreds of millions of Btu's per hour are being transferred or converted. The final efficiency is determined by sumining the power productions and consumptions in the overall system - the sums and differences of very large numbers. However, a difference of only 25,000 to $50,000 \mathrm{Btu} / \mathrm{hr}$, in recovered power, might be considered a significant change in efficiency. Only a small variation in certain of the operating parameters is sufficient to generate such an effect. This change might be as simple as the change in the initial assumptions on one of the subelements of the process.

The above effect raises concern about the comparability of results prepared by different organizations, or even different analysts, unless the bases for these results are clearly defined. For example, this analysis showed a much lower efficiency for the primary base case (using the entrainedbed gasifier) than had been developed by earier investigators. Similar discrepancies with the literature were also noted for other cases.

Consequently, a subprogram was undertaken to illustrate the apparent variation in overall system performance, employing essentially the same system, depending upon the assumptions selected by the analyst for various elements in the subsystem.

This appendix is a discussion of the results of that subinvestigation. Table Da-1 presents the result of 21 variations on the same system, yielding overall system efficiencies between $45.4 \%$ and $56.5 \%$, depending upon the inftial assumptions employed. The data of Table Da-1 were generated in a fashion consistent with the original efficiency analysis of Appendix Ca - a constant quantity of coal was fed to the system and variation in power output were analyzed. Summary printouts for the primary cases of this analysis are presented in Appendix Db.

The first analysis presented uses the same degree of conservatism that was employed throughout the majority of the program; somewhat less restrictive assumptions were then employed for each of the 20 orher variations upon the system. These assumptions, however, would not result in an inoperable system - a quench is used on the raw gas in each case to avoid carbon deposition and trains of crossflow heat exchangers are used for heat recovery, rather than the countercurrent heat exchange reported in many other designs. Fuel gas conversions was held constant at $85 \%$ in the fuel cell in each case. Also, the current density and, after initial evaluation, the quantity of air supplied to the cathode were held constant. Thus, the modifications employed are primarily variations in the assumptions of the operating conditions of the various elements of the system.

Case A - The Base Case

The basic system for this analysis was the combitiaiton of a methaneproducing, fluidized-bed gasifier integrated with an internally-reforming molten carbonate fuel cell as illustrated in Figure Da-l. This is the case labeled IV in Appendix Ca. This base case system had indicated significant promise in the earlier evaluations and appears to be a near-term process efficiency improvement that is currently undergoing evaluation in several fuel ce11 laboratories. Because all of the systems employed in this analysis are variations in the assumptions underlying this basic case, Figure Da-l is applicable for all of the cases reported in this appendix.

The major assumptions underlying this case have been outlined in the general discussion of this document. Because many of these assumptions are critical to understanding the overall impact of this evaluation of initial assumptions, they will be reviewed here.

[^10]
## ORiGINAL PEE OF POOR QUALITY

Table Da-1. sGEIISIS Of VARIATIONS IN INITIAL ASSUMPTIONS
© © and Feed - 4991 Tons/Day)




The gasifier operates in a fluidized-bed mode at approximately 500 psi using a steam/carbon molar ratio of 1.0 . Dust losees, carbon reporting to the ash, and the need for fuel injection gas are considered in the design. The gasifier is in thermal and mass balance and the off-gas is assumed to contain $13.5 \%$ of the feed carbon in the form of methane ( $6.1 \%$ methane in the raw, wet gas), based upon extrapolation of current pilot plant operating data.

After initial dust recovery to regasification, the raw gas is quenched with suffiaient liquid water to render the gas thermodynamically stable for carbon deposition, using a factor of safety in the water addition such that the resulting gas composition is midway between that required for stability when considering both amorphous and graphitic carbon. In other words, the minimum amount of water required for this system is that calculated for the deposition of carbon in the amorphous form, which has a higher thermodynamic activity than carbon in a graphitic form. This minimun water is required because carbon is anticipated to condense in the amorphous form. However, the factor of safety is employed by calculating the amount of water required for deposition of graphitic carbon and selecting the average quantity of water.

The quench gas is cooled in a recuperative heat exchange train so that it may be washed for final dust removal and then it is reheated in the same train. Much of the water content is converted to hydrogen by reaction over a water-gas shift catalyst with a temperature-of-approach to thermodynamic equilibrium of approximately $50^{\circ} \mathrm{F}$.

The heat of the exothermic shift reaction elevates the temperature of the gas. Power is then recovered by expansion of the gas to a pressure level consistent with the 150 psi fuel cell operating pressure (and intermediate pressure drops within the system). After heat recovery, the gas is passed through another shift reactor to take advantage of the improved shift equilibrium at lower tempieratures.

The gas is then cooled through a second recuperative heat exchange train. Midway within the train is a reactor to drive the carbonyl sulfide hydrolysis reaction toward completion at a preferred operating condition, thus minimizing the amount of $\operatorname{COS}$ that must be removed from the system. After final air- and water-cooling, the gas is scrubbed for selective sulfur removal In a selexol system. The acid-gas renoved from the system is assumed to contain $19 \% \mathrm{H}_{2} \mathrm{~S}$; $\operatorname{COS} 1 s$ distributed between the acid gas and the treated gas aceording to dàa from several designs.

The sweetened gas is reheated in the heat exchange train, finally passing over zinc oxide to remove the last traces of sulfur. Steam, after energy recovery in an expansion turbine, is added to the system to eliminate the potential for carbon deposition in the downstream fuel cell. Again, the quantity of steam added is taken as midway between that required for amorphous carbon deposition and graphitic carbon deposition.

The fuel cell system of Figure Da-1 incorporates significant heat exchange to alleviate operating conditions in the recycle blowers and to ensure operability of the catalytic combustor in the temperature range of commercially available catalysts. In most systems, the fuel cell off-gas temperature is $1260^{\circ} \mathrm{F}$. The air supply to the fuel cell employs a conservative compressor design of three stages. The final exhaust from the system is about $500^{\circ} \mathrm{F}$ to minimize plume formation from the very wet off-gas discharged from the atmosphere. Pressure drops throughout the system were identified in the body of this document, and the efficiency of recovery of waste heat to steam and power is assumed to be $35.2 \%$, as discussed elsewhere in this document. The overall power produced from this system, using the base amount of coal, was 706 MW for a system efficiency of $45.4 \%$.

## Case B - Modified Air Compressor

The first modification of the base case was to change the air compressor from three stages to two stages. For this modification, it is assumed that compressors are available with outboard bearings and seals that can withstand the higher off-gas temperature encountered. This approach minimizes the heat lost to interstage cooling and results in more heat present in the compressed cathode air. Note that not all of this gain was readily recoverable - the balancing of the heat exchange system required that the system off-gas temperature be increased to approximately $540^{\circ} \mathrm{F}$. Nevertheless, the addition of this modification increased the power output of the system to 710 MW and the efficiency to $45.6 \%$.

Case $C$ - Optimized Cathode Air Supply
Five cases were run at varying quantities of air flow to the fuel cell, to determine if significant improvement can be achieved. The initially assumed aiz flow was near optimum; modification raised the system output to 712 MW and a system efficiency of $45.8 \%$. This case became Case IVe of the
initial analysis and Case 5 in the body of the report. The complete system computer printout of this case is included in A'ppendix Cd.

## Case D - Add High-Temperature Heat Recovery

For this modification, high-temperature heat recovery was added. Heat is available both before and after the quench that can be recovered to more useful application that the initial assumption of converting it to steam or steam. superheat. Heat exchangers were added on the raw gas stream, both before and after the initial quench, to drive a greater quantity of heat into the shifted off-gas, prior to the expansion turbine. Caution was exercised to ensure that the raw gas was not cooled into the carbon-depositing regime before quench water was added. For this modificarion, the availability of high-temperature heat recuperation equipment was assumed. Incoloy 800 or Inconel 600 would probably be the preferred materials of construction. This modification increases the overall power output of the system to 728 MW and the systen efficiency increased to $46.8 \%$.

## Case E - Add Steam Expanders

This system modification included steam expanders for all the lowpressure steam used throughout the system. Prior examples had assumed that the steam employed in the gasifier and the acid-gas removal system was raised at the conditions necessary. For this case, it is assumed that all steam is raised at 1500 psi and superheated to $1000^{\circ} \mathrm{F}$. As is discussed elsewhere, the accurate steam balance cannot be projected in this effort because the total system of steam make and consumption is not defined (sulfur recovery, tail gas treatment, power water stripping, ammonia recovery, etc.). Therefore, the stedm system had been assumed to correspond to that required and the quantity of steam raised is assumed to correspond with the Btu's available.

Again, for this case the steam quantity corresponds to Btu's avallable; however, it is assumed that low-temperature heat is used for BFW heating, moderate-temperature heat is used for vaporization, and high-temperature heat is available for superheat. Thus all the steam is produced at higis pressure and superheat. For this option, the quantity of steam make decreases, but the quality is hlgher. Dellvered shaft horsepower inereased significantly as expanders were included between the steam header and the lower pressure steam consumers. The total system power increased to 764 MW and the efficiency climbed $49.1 \%$.

## Case F - Add Flue-Gas Economizer

Case $F$ includes an economizer on the cathode exhaust tall gas. In prioz examples, the tail gas was exhausted to the atmosphere at temperatures of about $500^{\circ} \mathrm{F}$ to avoid the political problems of plumes from the wet exhaust. Common power plant practice is to discharge the stack gas at about $320^{\circ}$ to $350^{\circ} \mathrm{F}$ to avoid a stack plume (except with cold ambient air.) With the very wet exhaust of this system, a higher stack-gas temperature of $500^{\circ}$ had been selected for the same reason.

For this option, it was assumed that such political objections would not be present and that the exhaust could be cooled to $250^{\circ} \mathrm{F}$. The heat is recovered into the boiler feedwater preheat and, eventually, into the highpressure steam system. The improved heat recovery results in more power recovered from the steam system, increasing the total system power to 798 MW and the system efficiency to $51.3 \%$.

Case G - Minimum Quench
For this option, the quantity of water used to quench the gas is reduced to the thermodynamic minimum. Thus, both the raw gas and the sweetened gas, which are unstable for carbon deposition in certain temperature ranges, are humidified only to the amorphous carbon limit. This effect improves the heat recovery from the system and, also, slightly improves the fuel cell power because the Nernst concentration polarization at the anode is reduced as the steam fed to the anode is minimized. The total system power increased to 805 MW and the efficiency increased to $51.7 \%$.

Case H - Optimistic Gasifier Design
Tie design of the fluidized-bed gasifier was optimized to miamize the factor of safety employed. The steam/carbon ratio was reduced to 0.75 and the operating pressure was increased to 600 psi , the limit of currently available lockhopper valves. Interestingly, the total system performance does not change significantly, on an overall basis. The altered gas composition required more quench water, thus negating the effect af the reduced gasifier steam consumption. The gas quality was somewhat improved, resulting in higher fuel cell output, but the total system power remained the assentially unchanged at 803 MW with a system efficiency of $51.6 \%$.

## Case I - Quench With Steam

The form of water used in the quench system was changed from liquid water (Case J) to steam for this modification. Liquid water had been used in the earlier analyses to minimize the size of BFW treatment system. Although the total moles of water (or water vapor) added are the same, the effect improves system efficiency because high-temperature heat is not used to provide the latent heat of water vaporization. Thus, the overall system improved to 822 MW and the system efficificy improved to $52.8 \%$.

## Case J-Remove More Carbon Dinside

For this option, the acid gas was removed from the sour gas at lower $\mathrm{H}_{2} \mathrm{~S}$ concentration. This approach removes more $\mathrm{CO}_{2}$ with the $\mathrm{H}_{2} \mathrm{~S}$ and permits reduced steam requirement for stabilization of the anode fuel. Operationally, it would be assumed that a Stretford process or the Ralph N. Parsons "Selectox" system would be used for sulfur recovery. Two cases were analyzed in this approach. The overall power from the facility declined because of greater cathode concentration polarization. Therefore, this option was not considered further. It should be noted, however, that system nerformance may well increase if the purified $\mathrm{CO}_{2}$, exiting from the Stretford process, were to be recompressed into the cathode feed.

Case K - Burn a Portion of Anode Exhaust Into Cathode Exhaust
For this modification, the system of Case $I$ was employed, but a rortion of the anode exhaust was combusted directly into the cathode exhaust, rather than all of the anode exhaust being combusted into the cathode feed. This modification was made because it had been noted that the power recovered fron the cathode exhaust turbine was very sensitive to the operating temperature; slightly increasing the temperature by combustion was attempted to improve the overall system power. However, the increased Nernst concentration voltage loss at the cathode, due to bypassing part of the carbon dioxide, caused a slight reduction in the system performance. Therefore, this system was not considered further.

Case L - Reduced Pressure Drops
For this modification, the basic system was the same as Case I but it was assumed that the pressure drop across each element of the system could be decreased by a factor of two. As was discussed in the body of this report,
the pressure drops assumed for the various elements in the system are relatively low, compared with normal chemical process industry practice. However, several designs appearing in the literature have assumed constructional characteristics that would further decrease the pressure drops significantly. Therefore, this case was developed to indicate the effect of lower pressure drop. The reduced pressure losses in the system permitted much greater shaft horsepower recovery, providing 841 MW from the base coal fed to the system and a system efficiency of $54.0 \%$.

## Case M - Higher-Temperature Cathode Exhaust

As was discussed under Case $K$, higher temperatures in the cathode exhaust system are desirabie. For this modification, the flow of the cathode recycle cooling gas around the fuel cell was controlled to result in a fuel cell offgas temperature of $1300^{\circ} \mathrm{F}$ - a value assumed to be operable without excessive electrolyte loss. The increase in the ruel ce? exhaust gas temperature of only $40^{\circ} \mathrm{F}$ improved the total system performance to 848 MW , with a total system efficiency of $54.5 \%$.

Case N - Higher Steam System Efficiency.
For this option, the efficiency of recovery of heat from waste steam into power is assumed to increase to $40 \%$. All earlier analyses had used an efficiency of $35.2 \%$, a value that includes penalties for boiler feedwater treatment and the cooling water systems. However, modern power plants operate near this efficiency and include penalties for $\mathrm{SO}_{2}$ scrubbing (not required here). Thus, an improvement of efficiency to $40 \%$ would be considered reasonable. For this presentation, the modification was estimated, rather than calculated on the system simulator. Such simulations had been made earlier in the program and the impact is the same as is estimated here. The total system power increased to 854 MW and the efficiency climbed to $54.9 \%$.

Case 0 - Correct Fuel Cell Voltage
As is discussed elsewhere in this document, the modified fuel cell simulator subpacket reported a fuel cell voltage that was somewhat lower than the current experimental performance. Consequently, the cell potential was increased by 55 mV with a corresponding refuction in the waste heat from the syster. This change resulted in a total system performance improvement to 879 MW with a system efficiency of $56.5 \%$. Again, the process simulator was not

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used for this comparison beegnge of the time required for simulator modification; rather, hand calculation was employed and the results are reported as estimated.

## Summary

The analysis above Indicates that a wide variation in the reported efficiency of the sasifier/fuel cell system can be obtained, depending upon the assumptions employed by the system analyst in setting the design conditions for each element within the system. It is therefore suggested that comparisons of systems derived by different analysts be evaluated carefully, because even minor variations in basic assumptions may cause an apparent system efficiency change of over 1 percentage point. Any such comparative analysis must be made with care to be certain that difterences in apparent system performance are real.

# APPENDIX Db. Summary Printouts for Cases in Appendix Da 

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CASE A
The Base Case

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CASE C
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NORMAL FUEL CELL. 1200 F I INPUT SETS VUL.IAGE, 1260 F FXIT.

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## CASE F

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## CASE G

## Employ Minimum Quenching to Amorphous Carbon




## CASE H

Change Gasifier to More Optimistic Design Point



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## CASE I

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## CASE J

## Remove More $\mathrm{CO}_{2}$ With $\mathrm{H}_{2} \mathrm{~S}$


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## CASE K

As Case I, but Burn Part of Anode Exhaust into Cathode Exhaust

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## CASE L

As Case I, Employ Low-Pressure Drops Throughout the System




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Case M

## Increase Fuel Cell Exhaust to $1300^{\circ} \mathrm{F}$


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[^0]:    * Because of the volume of the printouts, only the summary printouts of cases other than the one discussed here are appended to the report; others have been placed on file with the prime contractor.

[^1]:    * Three terms for heat capacity factors and three additional terms for correlating the heats and free energies of reactions.

[^2]:    See Appendix Cb for more complete discussion.

[^3]:    FThermal cycle efficiency, coal pile to busbar.

[^4]:    * Report published by Electric Power Research Institute, Palo Alto, California.

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