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MULTI-FUEL REFORMERS FOR FUEL CELLS USED IN TRANSPORTATION

MULTI-FUEL REFORMERS

PHASE I. FINAL REPORT

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FOREWORD

This report documents a portion of the work performed by Arthur D. Little, Inc. under contract DE-AC02-92-CE50343, Multi-fuel Reformers for Fuel Cells Used in Transportation. One objective of this program is to develop advanced fuel processing systems to reform methanol, ethanol, natural gas, and other hydrocarbons into hydrogen for use in transportation fuel cell systems, while a second objective is to develop better systems for on-board hydrogen storage.

The objective of this program is to develop a prototype multi-fuel reformer system for a fuel cell-powered vehicle. The Phase I work reported here evaluated the feasibility of multi-fuel reformer concepts and selected a reforming technology for further development in Phase II. The ultimate goal of this program is the integration of the reformer technology demonstrated in this program with a DOE-designated fuel cell and vehicle configuration.

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I. Executive Summary

The Department of Energy (DOE) has identified fuel cells as a promising technology for solving the nation's air quality problems and foreign fuel dependence. Consequently, DOE has established the goal, through the Fuel Cells in Transportation Program, of fostering the rapid development and commercialization of fuel cells as economic competitors for the internal combustion engine. Central to this goal is a safe feasible means of supplying hydrogen of the required purity to the vehicular fuel cell system. Two basic strategies are being considered: (1) on-board fuel processing whereby alternative fuels such as methanol, ethanol or natural gas stored on the vehicle undergo reformation and subsequent processing to produce hydrogen, and (2) on-board storage of pure hydrogen provided by stationary fuel processing plants. This report analyzes fuel processor technologies, types of fuel and fuel cell options for on-board reformation.

The availability of a reformer technology capable of demonstrating fuel flexibility, ease of integration with currently available fuel cells, and rapid transient response and cold start-up could accelerate the acceptance of fuel cell powered vehicles. As the Phase I of a multi-phased program to develop a prototype multi-fuel reformer system for a fuel cell powered vehicle, the objective of this program was to evaluate the feasibility of a multi-fuel reformer concept and to select a reforming technology for further development in the Phase II program, with the ultimate goal of integration with a DOE-designated fuel cell and vehicle configuration.

The basic reformer processes examined in this study included catalytic steam reforming (SR), non-catalytic partial oxidation (POX) and catalytic partial oxidation (also known as Autothermal Reforming, or ATR). Fuels under consideration in this study included methanol, ethanol, and natural gas. A systematic evaluation of reforming technologies, fuels, and transportation fuel cell applications was conducted for the purpose of selecting a suitable multi-fuel processor for further development and demonstration in a transportation application. Generic fuel cell models were used, and no attempt was made to directly compare the suitability of one fuel cell technology over another.

For a given fuel cell technology, the efficiencies of reformer systems correlate with the fuel processor operating temperature and system operating pressure. Reformer temperature depends on the type of fuel and reformer technology. Lower reforming temperatures yield higher system efficiencies. Steam reforming systems require lower reforming temperature than either ATR or POX. ATR, which uses a catalyst, requires a lower reforming temperature than the non-catalytic POX. As a result, ATR enjoys a slight efficiency advantage over the POX technology.

For a given fuel processor, methanol requires by far the lowest reforming temperature and ethanol requires the highest reforming temperature. The reforming temperature required for methane is slightly lower than ethanol. Consequently, for any given fuel processor, methanol fuel will yield the highest efficiency, and ethanol will yield the lowest efficiency.

Net system efficiency improvements depend on fuel cell stack waste heat utilization and energy recovery. Opportunities for pure thermal integration are minimal when a high-temperature reformer is integrated with a low-temperature fuel cell; however, an expander can be used for energy recovery in fuel cell systems operating at above ambient pressure. In pressurized proton exchange membrane (PEM) systems analyzed steam reformers were found to be marginally more efficient than ATR or POX (1%-2% net system efficiency). For phosphoric acid fuel cells (PAFC) steam availability from the fuel cell integrates well with steam demand in a fuel processor based on the steam reforming technology. Considering the high weight and volume and long start-up time requirement dictated by the PAFC and SR, such a combination is perceived to be more applicable in heavy duty transportation applications such as locomotives, long-haul trucks and perhaps buses.

The combination of non-catalytic partial oxidation and PEM fuel cell, even though slightly lower in efficiency than other fuel processors, offers an attractive alternative over others due to its quick start-up and relative fuel insensitivity. Advanced concepts such as oxygen enrichment and power recovery can be applied to boost system performance and efficiency. However, the hardware components required to implement these advanced concepts will increase system complexity and development effort. Based on consumer expectations of quick start-up and transient response, the combination of PEM and POX is thought to be suitable for passenger car applications.

The state of development of fuel processor technology varies depending on technology, fuel and application. Methane steam reforming has been widely used for decades in large-scale stationary hydrogen production, but mobile applications have not been demonstrated yet. Mobile fuel processors have been developed using steam reforming technology with methanol as a fuel. However, steam reformer designs with ethanol as a fuel do not currently exist. Autothermal reformer development has been limited to catalysts research with the focus on distillate fuels such as diesel. Research on POX for fuel cell applications is embryonic, although industrial scale applications are well developed for hydrogen production.

In order to function acceptably for a multitude of fuels, the fuel processor would have to be designed to accommodate the most demanding operating conditions which would make it over-designed for all other conditions. Such a fuel processor design can not be optimal technically or economically. However, it may be attractive to develop the basic design for a selected fuel processor technology that will require minimal adaptation in hardware for different fuels and fuel cell stacks. Each of these designs can then be optimized for technical performance and production economics for a specific combination of fuel and fuel cell.

Considerable developmental experience has been accumulated for steam reforming of methane and methanol for fuel cell applications. However, a significant void exists for the use of ethanol as a fuel in steam reforming, autothermal or partial oxidation reforming. It is therefore appropriate to focus on ethanol as a fuel for fuel cell applications as an intermediate step towards the ultimate DOE objective of developing a multi-fuel processor.

With the exception of the reformer reactor, both ATR and POX fuel processors share a large number of common components. To maximize the benefit of development effort and to reduce the development risk, we recommend a simultaneous development of ATR and POX in the Phase II program. We believe this path is most beneficial to the advancement of DOE's fuel cell vehicle program.

II. Introduction

II.1. Background

Fuel cell powered vehicles are perceived to be more energy efficient and environmentally benign than those based on internal combustion engines. Most fuel cells under consideration for vehicle applications, such as phosphoric acid fuel cells (PAFC), proton exchange membrane (PEM) or most solid oxide fuel cells, require the external reformation of hydrocarbon fuels into hydrogen for use in the fuel cell. The reformation of hydrocarbon fuels into hydrogen can either be supplied from "gas stations" in stored form or generated on-board from stored hydrocarbon fuels. This study addresses issues related to fuel reformer technologies in the on-board vehicle application.

The availability of a reformer technology capable of demonstrating fuel flexibility, ease of integration with currently available fuel cells, and ability to meet vehicle power plant requirements in terms of transient response and cold start-up could accelerate the acceptance of fuel cell powered vehicles.

As the Phase I of a multi-phased program to develop a prototype multi-fuel reformer system for a fuel cell powered vehicle, the objective of this program was to evaluate the feasibility of a multi-fuel reformer concept and to select a reforming technology for further development in the Phase II program, with the ultimate goal of integration with a DOE-designated fuel cell and vehicle configuration.

The basic reformer processes examined in this study included catalytic steam reforming (SR), non-catalytic partial oxidation (POX), and catalytic partial oxidation (also known as Autothermal Reforming, or ATR). Fuels under consideration in this study included methanol, ethanol, and natural gas.

Many fuel processor systems are under advanced development or investigation. All of these systems are developed for specific combinations of fuel, reformer process, fuel cell technology and vehicle type. To compare various reforming technologies on a consistent basis with different choices of fuels and in the meantime to devise reasonable integration with the fuel cell technologies represented a major challenge of this program. To accomplish this task, process flow sheets for each reforming technology and fuel cell combination had to be modified from published prior development efforts or developed from process fundamentals to facilitate objective comparison. In addition, the study was hampered by a lack of reaction kinetics information on ethanol in the public domain: assumptions about reaction kinetics had to be made in order to perform process simulations with ethanol.

This study phase included thermodynamic analyses, process simulations of the three basic reforming processes with different fuels, design studies, and a comparison of reforming technologies with respect to fuel, energy efficiency, quality of reformate, reformer size and weight, transient response capability and other vehicle related performance issues.

This report addresses findings developed during the Phase I study.

II.2. Requirements for a Multi-Fuel Reformer for Fuel Cell Vehicles

On-board reformers face a number of challenges imposed by the performance requirements of vehicles. These vehicle performance imposed requirements include: start-up time, size and weight restrictions, fuel efficiency, fuel flexibility and load-following capability.

The start-up time for a fuel cell power plant in passenger cars is targeted to be less than 10 seconds for consumer acceptance. In heavy duty vehicles, such as trucks and buses, the start-up time is not a critical issue. Extrapolating from the current generation of fuel cell bus reformers, the volume and weight of an on-board reformer should aim to be less than 7 liter and 4 kg per kW of power output, respectively.

With regard to fuel efficiency, the overall system efficiency of a fuel cell vehicle needs to be comparable to or better than other advanced propulsion systems under development in order to be credible as an alternative vehicle power plant. As shown in Figure II-1, the fuel efficiency (defined as [Power to Wheels]/[LHV of Fuel]) of propulsion systems ranges from 14% in 1992 passenger cars to 35% in a Stirling-generator series hybrid system. The Stirling Engine-Generator Series Hybrid and the Internal Combustion (IC) Engine-Generator Series Hybrid are configurations that couple a constant-speed engine with an electric generator, use an electric motor to drive the wheels, and use batteries for electrical energy storage. Such a configuration allows the engine to always run at its most efficient operating point. The propulsion efficiency for fuel cell vehicles is currently estimated to fall between 30% and 45% (the "window" shown in Figure II-1).

To broadly penetrate the market, which requires achieving the economies of scale in the basic designs, tooling and manufacturing, it would be highly desirable to have a single basic fuel reformer design that can be readily modified for different types of fuels. The on-board reformer technologies must also be examined from the standpoint of load-following capability which is a critical requirement and unique to the vehicle application.

II.3. Fuels

Many hydrocarbons and alcohols can be considered as candidate fuels for vehicle fuel cells. The candidate fuels considered in this study were methane, methanol and ethanol. The different fuels were examined in this study for the primary purpose of identifying the impact of fuels on the fuel reforming process and their effect on the design of a multi-fuel reformer system. Conventional vehicle fuels including gasoline and diesel were not within the study scope.

Natural gas, with its proven indigenous reserve, and existing production and distribution infrastructure, is a clean, convenient alternative vehicle fuel. Its low storage density in comparison with diesel and gasoline has limited its widespread application in transportation.

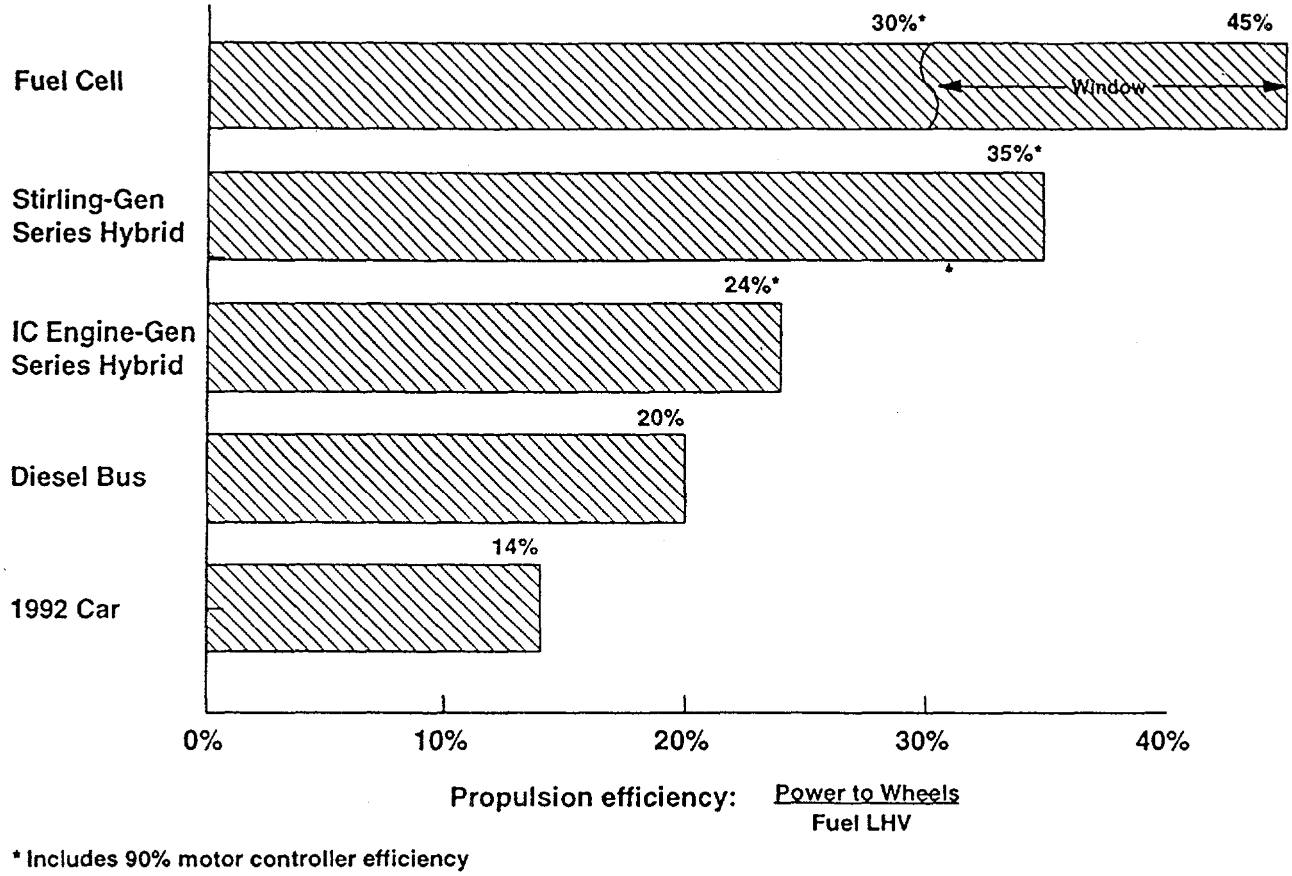


Figure II-1 Fuel Efficiency Targets for Alternative Vehicle Propulsion Systems

Natural gas is the most widely used feedstock in industrial hydrogen reformers. Methane is considered a refractory fuel which implies that high operating temperatures are required to reform methane into hydrogen.

Methanol is synthesized from hydrogen and carbon monoxide which, in turn, are generated by reforming natural gas or other hydrocarbon fuels. Methanol decomposes into hydrogen and CO at lower temperatures than methane. The production technology is highly developed. Currently the major use of methanol is as an intermediate for chemical synthesis and as a solvent. If methanol gains any acceptance as a motor fuel, the methanol production capacity would have to be significantly increased.

Ethanol, a transportable fuel producible from biomass, is regarded by many as an important indigenous future replacement of imported hydrocarbon fuels. Ethanol has been used as an additive to gasolines for octane enhancement. Ethanol, also considered a refractory fuel, has not been studied extensively as a reformer fuel.

II.4. Fuel Cell Integration

Fuel cell types under consideration for integration with the fuel processor in this study are the Proton Exchange Membrane (PEM) fuel cell and the Phosphoric Acid fuel cell (PAFC). The general characteristics and operating conditions of these two types of fuel cells are shown in Table II.1. As discussed in Section III.4, the fuel cell data used to calculate efficiencies were typical of current generation fuel cell technology and do not reflect the potential operating characteristics of more advanced fuel cells, such as the PEM data recently published by General Motors' Allison Gas Turbine Division.

Table II-1 General Characteristics and Operating Conditions for Fuel Cells

	PAFC	**PEM**
Electrolyte	Phosphoric Acid	Solid Polymer
Electrode (catalyst)	Platinum	Platinum
Anode Fuel	Hydrogen	Hydrogen
Cathode Oxidant	Oxygen (or Air)	Oxygen (or Air)
Operating Temperature, (C)	160 - 200 C	70 - 90 C
Operating Pressure, (atm)	1 - 4 atm	1 - 4 atm
Impurity Tolerance:		
CO_2	diluent	diluent
CH_4	diluent	diluent
N_2	diluent	diluent
CO	< 1% at 175 C < 2% at 190 C	< 10 ppm
H_2S, COS	< 100 ppm	< 5 ppm
NH_3	< 1 ppm	trace
Metal ions	nil	nil

PEM Fuel Cells

When a fuel reformer is operated with PEM fuel cells, the system integration must address the following PEM fuel cell characteristics:

- Low grade waste heat
- Sensitivity to carbon monoxide (CO)
- Quicker start-up
- Humidification requirement for anode and cathode streams
- Need for pressurized fuel cell stack

Low Grade Waste Heat

The PEM fuel cell typically operates at a relatively low temperature of about 80°C. The low grade waste heat available from the fuel cell is of limited use in the fuel processor aside from preheating feed streams. All reforming technologies under consideration generate waste heat at significantly higher temperature than that available from the PEM fuel cell.

Sensitivity to Carbon Monoxide

PEM fuel cells are sensitive to carbon monoxide poisoning of the platinum electrode catalyst. This CO sensitivity is inversely proportional to the fuel cell operating temperature. At 80°C, the allowable CO concentration in the anode gas is less than 10 parts per million (ppm). This low level of CO concentration is beyond the capability of conventional water shift reactors. A reformer integrated with a PEM fuel cell would require a reformate clean-up process module using, for example, selective oxidation of CO, to reduce the CO concentration to a trace level.

Sensitivity to Other Impurities

PEM fuel cells are extremely sensitive to sulfur compounds, such as COS and H_2S, which poison the electrodes. PEM fuel cells also have extremely low tolerance for ammonia. PEM fuel cell systems often require additional gas clean-up process modules to achieve the very low allowable concentrations of these impurities.

Quick Start-up Time

A PEM fuel cell can be started up relatively quickly due to its low operating temperature and ability to produce power at ambient temperatures. Therefore, the start-up characteristics of a reformer technology are relatively more critical in the integration with a PEM fuel cell than with other types of fuel cells.

Humidification Requirement for Anode and Cathode Streams

The electrolyte used in PEM fuel cells is a solid polymer membrane electrolyte. Dehydration of this membrane during operation causes it to cease functioning and can cause permanent damage to the membrane. The PEM anode and cathode streams need to be humidified with deionized water.

Need for Pressurized PEM Fuel Cell Stack

Currently, PEM fuel cells are typically designed to operate at pressurized conditions (approximately 3 atm). The high operating pressure in the cell stack is beneficial in maintaining a sufficiently high humidity without overly reducing the hydrogen and oxygen partial pressure, and therefore reducing the fuel cell efficiency.

Phosphoric Acid Fuel Cells (PAFC)

When a fuel reformer is operated with a phosphoric acid fuel cell, the system integration must address the fuel cell characteristics of PAFC:

- Higher potential (relative to PEM) for waste heat utilization,
- Higher tolerance to CO (relative to PEM),
- Inherent long start-up time,
- Chemical degradation of PA electrolyte, and
- Flexibility in fuel cell operating pressure.

Higher Potential (Relative to PEM) for Waste Heat Utilization

PAFCs typically operate at about 190°C. The waste heat available at this temperature is somewhat more feasible for utilization in the fuel processor than the 80°C waste heat available from a PEM fuel cell.

Higher Tolerance to CO (Relative to PEM)

In comparison with PEM fuel cells, PAFCs have a higher tolerance for CO without poisoning the electrode catalyst. At an operating temperature of 190°C, the allowable CO concentration in the anode inlet is about 2% on a dry basis which is achievable in a two-stage water-shift reactor without the complexity of a CO clean-up process module.

Inherently Long Start-Up Time

The start-up times for PAFCs are considerably longer than for PEM fuel cells due to the higher operating temperature and thermal mass of the electrolyte and pressure container. PAFCs cannot produce appreciable power until they are close to their operating temperature. This high inherent start-up time of the PAFC could allow additional start-up time for the fuel processor without creating a bottleneck in the start-up.

Chemical Degradation of PA Electrolyte

The phosphoric acid electrolyte is susceptible to chemical reactions with ammonia and sulphur. The effects of these reactions are cumulative as they deplete the concentration of phosphoric acid in the fuel cell. As shown in Table II.1, the allowable ammonia concentration in the inlet gas streams is less than 1 ppm. Therefore, when integrating a fuel processor technology with a PAFC, attention must be paid to preventing ammonia from entering the fuel cell.

Flexibility in Fuel Cell Operating Pressure

The operating pressure is not a limiting performance factor for PAFC technology. Various designs of PAFC stack exist, with operating pressures ranging from atmospheric to about 4 atm. However, a high operating pressure PAFC will add considerable weight to the stack which is not favored for vehicle applications.

Broadly speaking, the fuel reformer will need to integrate with the fuel cell stack for air supply, cooling, water management and waste heat utilization at the system design level.

II.5. Reformer Technologies

Major process technologies for reforming hydrocarbons and alcohols into hydrogen and carbon dioxide include:

- Catalytic steam reforming (SR),
- Non-catalytic partial oxidation (POX), and
- Catalytic autothermal reforming (ATR).

In vehicle fuel cell related applications, reformer research and development efforts have been focused on the steam reforming technology with methanol as the fuel. Prior effort on the development of ATR technology has been limited to catalyst research for diesel fuel, methanol, and methane. Non-catalytic partial oxidation technology has not been explored for fuel cell related programs, but it is used in large-scale hydrogen production from coal and naphtha. As ethanol has not been previously considered as a feedstock for hydrogen production, little fundamental information exists in the public domain on ethanol for any of the reforming technologies under consideration.

Steam Reforming

Steam reforming of hydrocarbons to produce hydrogen or synthesis gas is one of the oldest and most practiced processes in the chemical and refining industry. Common feedstocks for steam reforming include naphtha, natural gas, and other light hydrocarbons.

In this process, hydrocarbon feedstocks are catalytically converted to synthesis gas (H_2, CO, CO_2) by reaction with steam. This is an endothermic process where the heat of reaction is provided by the external combustion of fuel. The industrial process is typically carried out at 600-1000°C and 40-100 atm pressure, using nickel based catalysts which require protection from sulfur poisoning by removing sulfur species from contacting the catalyst or use of sulfur-resistant catalysts.

To increase the hydrogen concentration, the synthesis gas undergoes a water gas shift reaction where steam is reacted with CO to form H_2 and CO_2. The water gas shift reaction is usually carried out in two adiabatic shift reactors in series with an inter-cooler in between to remove the heat of reaction for the exothermic water gas shift reaction. The first-stage reactor typically operates at 350-450°C and is called the high-temperature shift (HTS) reactor. The HTS reactor uses a chromium-promoted iron oxide catalyst.

The second stage is a low-temperature shift (LTS) reactor which operates at 150-250°C, using a copper-zinc catalyst supported on alumina. The copper-based LTS catalysts are more susceptible to poisoning and sintering than the iron-based HTS catalysts. Steam condensation, sulfur poisoning, and sintering due to temperature excursions can considerably reduce the activity of the copper-based LTS catalysts. The LTS is capable of achieving a residual CO concentration on the order of 0.5-1.5 dry vol%. For integration with PEM fuel cells, the reformate needs to be processed in additional process modules to reduce the CO content to ppm level.

Standard nickel based steam reforming catalysts are suitable for reforming of methane and methanol. These catalysts require protection from sulfur poisoning. Limited data for steam reforming of ethanol using these catalysts have been reported in a patent by British Gas [3].

Partial Oxidation Reforming

Partial oxidation reforming is a non-catalytic process. The required heats of reaction are supplied *in-situ* by oxidizing a fraction of the feedstock. The extent of the oxidation reaction is regulated by the quantity of oxygen addition. Industrial partial oxidation processes typically use pure oxygen. Air can also be used as the source of oxygen if nitrogen dilution in the product stream is not a disadvantage. POX processes using air as the source of oxygen may produce trace quantities of ammonia.

Partial oxidation processes are typically used to reform heavy hydrocarbon feedstocks (such as heavy naphtha and refinery residues) or coal into synthesis gas. Without the benefit of catalysts, the POX process needs to operate at higher temperatures (1100-1500°C) than catalyst-assisted reforming processes.

The process effluent from the partial oxidation reactor requires the two-stage water-shift reaction and additional CO removal, similar to that in the steam reforming process, to convert most of the carbon monoxide into additional hydrogen production for use in fuel cells.

For integration with PAFC, any trace quantities of ammonia in the POX reformate will have to be removed to protect the phosphoric acid electrolyte.

Autothermal Reforming

Autothermal reforming technology (ATR) is a hybrid technology combining the catalytic aspect of the steam reforming technology with the *in-situ* oxidation feature of the POX technology. In the presence of oxidation catalysts, a portion of the hydrocarbon feed is oxidized with a controlled addition of oxygen. The control of oxygen is critical to prevent sintering of catalyst associated with temperature excursions.

The heat of oxidation provides the high temperature condition and heat requirement to reform the feedstock into hydrogen and carbon monoxide. For a given feedstock, the operating temperature of the autothermal reactor is lower than the POX reactor but higher than the steam reforming technology. Two different types of catalysts are employed in autothermal reactors. The first is usually a platinum based combustion catalyst which facilitates rich combustion. The second is the conventional nickel based steam reforming catalyst. Catalysts used in autothermal processes require protection from sulfur poisoning.

The process effluent from the autothermal reactor requires the two-stage water-shift reaction and additional CO removal, similar to those used in the steam reforming process, to convert most of the carbon monoxide into additional hydrogen production for uses in fuel cells.

III. Study Approach

The multi-fuel reformer concept for vehicular applications was analyzed in a systematic manner with the help of advanced computational tools. The general steps and tools used in the study are outlined below.

- Literature search to identify state of art on vehicle fuel cell reforming technologies
- Thermodynamics analysis of candidate fuels to develop plausible operating envelopes
- Development of process simulation model to allow quantification of equipment requirement and system performance
- Case studies for selected reforming technology, fuels and fuel cell combinations
- Sizing of major process components
- Comparison of reforming technologies on a consistent basis

The current state-of-the-art was assessed via an extensive literature search. The primary objectives of the literature search were to:

- Identify fuel reforming technologies available for hydrogen production,
- Determine prior effort and current status of fuel, fuel processor and fuel cell integration in stationary and vehicular applications,
- Review process flow schemes, process conditions and limitations, and
- Identify potential reforming catalysts used in the fuel processor for the various combinations of fuels and fuel reformers.

Based on this literature review, several potential fuel reforming technologies, process schemes and catalysts were identified and selected for further analysis.

Thermodynamic equilibrium analysis of all candidate fuels was studied to define the boundaries of plausible operating regions for all fuels and reforming technologies.
The purpose of equilibrium analysis was to:

- Establish carbon-free operating zone
- Understand the impact of operating conditions (temperature, pressure),
- Assess the impact of water-to-fuel ratio and air-to-fuel ratio, and
- Establish reformate quality at selected operating variables.

While equilibrium analysis is powerful in the interpretation of system behavior, it does not allow predictions of reaction mechanisms.

The chemical equilibrium problem in multi phase systems was computed by the minimization of the total Gibbs free energy method, using real gas effects. A computer model, developed at Arthur D. Little by Saini [7], was used to solve the constrained minimization problem of complex chemical equilibria. This computer model was also supplemented by NASA's equilibrium model and database (Gordon and McBride [4]).

Having analyzed the effects of several operating variables on the performance of the fuel reformers, system flow schemes integrating the fuel reformer with the fuel cell were developed, using industrial concepts or ADL conceived approaches. The flow schemes were developed keeping in mind the requirements for vehicular applications. Simulation studies were conducted on the flow diagrams to quantify the heat and mass balance and to evaluate system efficiencies. Several case studies for combinations of fuel type, reforming technology and fuel cell were selected and evaluated. These case studies were analyzed on a consistent basis so as to facilitate comparison across the different fuel types, reforming technologies and fuel cells.

Steady state simulation of the conceived flow diagrams was done on a commercial process simulator ChemCAD, from ChemStations, Inc. The simulation model allowed quantification of system performance.

Major process components for the selected technologies and case studies were sized to obtain weight and volume estimates. This essentially completed the matrix against which the several technologies could be analyzed on a consistent qualitative basis, viz. system efficiencies, weight and volume for combinations of fuel, reforming technology and fuel cells. Transient behavior, start-up issues, maintainability and safety were analyzed on a qualitative basis for the several competing technologies.

The results of this analysis were discussed with industry leaders for comment and verification. The results of our findings are presented in subsequent chapters.

III.1. Thermodynamics

Steam Reforming

In the steam reforming process, steam is reacted with hydrocarbons or alcohol in the presence of a suitable catalyst to produce hydrogen rich gas. Steam reforming is an endothermic process where one or more simultaneous reactions take place. Generally, steam reforming for hydrogen production is favored by high temperature and low pressures.

The major reactions taking place for methane steam reforming are:

$$\begin{array}{lc} & \Delta H_{298}\ KJ/mol \\ CH_4 + H_2O \rightleftharpoons CO + 3H_2 & +206.14 \\ \underline{CO + H_2O \rightleftharpoons CO_2 + H_2} & \underline{-41.17} \\ CH_4 + 2H_2O \rightleftharpoons CO_2 + 4H_2 & +164.97 \end{array} \qquad (1)$$

where, the first reaction is the endothermic methane reforming reaction and the second reaction is the mildly exothermic water gas shift reaction. The overall methane steam reforming reaction is endothermic, stoichiometrically requiring 2 moles of steam per mole of methane. Since there is an increase in the number of moles from 3 in the reactants to 5 in the products, the reaction is favored in the forward direction at low pressures.

The reactions involved during methanol steam reforming are:

$$\begin{array}{lr} & \Delta H_{298}\ KJ/mol \\ CH_3OH \rightleftharpoons CO + 2H_2 & +90.13 \\ CO + H_2O \rightleftharpoons CO_2 + H_2 & -41.17 \\ \hline CH_3OH + H_2O \rightleftharpoons CO_2 + 3H_2 & +48.96 \end{array} \tag{2}$$

where the first reaction is the methanol decomposition reaction and the second reaction is the water gas shift reaction. Stoichiometrically, an equimolar mixture of steam and methanol is required to form 4 moles of products, the forward reaction being favored at high temperatures and low pressures.

Similarly, ethanol steam reforming gives the following major reactions:

$$\begin{array}{lr} & \Delta H_{298}\ KJ/mol \\ C_2H_5OH \rightleftharpoons CO + H_2 + CH_4 & +49.05 \\ CH_4 + 2H_2O \rightleftharpoons CO_2 + 4H_2 & +164.97 \\ CO + H_2O \rightleftharpoons CO_2 + H_2 & -41.17 \\ \hline C_2H_5OH + 3H_2O \rightleftharpoons 2CO_2 + 6H_2 & +172.85 \end{array} \tag{3}$$

It is postulated that the ethanol decomposition reaction, given by the first reaction, forms methane, carbon monoxide and hydrogen. The methane further undergoes steam reforming as given by the overall reaction of Equation (1).

Some of the side reactions that take place during steam reforming are the coking reaction, methanation reaction and producer's gas reactions given by:

$$\begin{array}{rl} \textit{Coking}: & CO_2 + 2H_2 \rightarrow C + 2H_2O \\ \textit{Boudouard}: & 2CO \rightarrow C + CO_2 \\ \textit{Methanation}: & CO + 2H_2O \rightarrow CH_4 + H_2O \\ \textit{Methane Reforming}: & CH_4 + 2H_2O \rightarrow CO_2 + 4H_2 \\ \textit{Producer Gas Rxn.}: & C + 2H_2O \rightarrow CO_2 + 2H_2 \\ \textit{Producer Gas Rxn.}: & C + H_2O \rightarrow CO + H_2 \end{array} \tag{4}$$

Carbon Formation

The minimum amount of steam required for reforming is given by the carbon formation line. The carbon formation line is the point at which free carbon is formed by the coking reactions and defines the lower operating range for steam reforming. Coking is highly undesirable as it leads to clogging and deactivation of the catalyst and extreme care must be taken to prevent carbon formation. Carbon formation is a function of both the reforming temperature and steam to fuel ratio. The carbon formation lines for the three selected fuels are shown in Figure III-1. The region above the lines is carbon free, whereas carbon formation takes place at and below the lines. At a given temperature, carbon formation dictates the minimum steam to fuel ratio. Higher reforming temperatures and steam to fuel ratios prevent carbon formation.

Effect of Reformer Temperature on Reformate Quality

Steam reforming is an endothermic process requiring an external source of heat. The reformer is typically operated under isothermal conditions. The effect of reforming temperature on the reformate quality for a fixed steam to fuel ratio is shown in Figures III-2, III-3, and III-4 for methane, methanol and ethanol, respectively. At a given steam/fuel ratio, higher temperatures give better conversions and higher hydrogen yields. An operating temperature range between 700-800°C seems to be plausible for methane and ethanol steam reforming. The methanol curves shown in Figure III-3 were generated by assuming that methane is formed during the reforming process. However, this has not been observed in practice, and methanol reforming is typically carried out between 250-300°C.

Effect of Steam-to-Fuel Ratio

In steam reforming systems, higher steam-to-fuel ratios tend to produce higher hydrogen yield. Figure III.5 shows the effect of hydrogen yield at several steam-to-fuel ratios for the ethanol steaming reforming system in which the hydrogen yield is maximized at an operating temperature between 700-800°C.

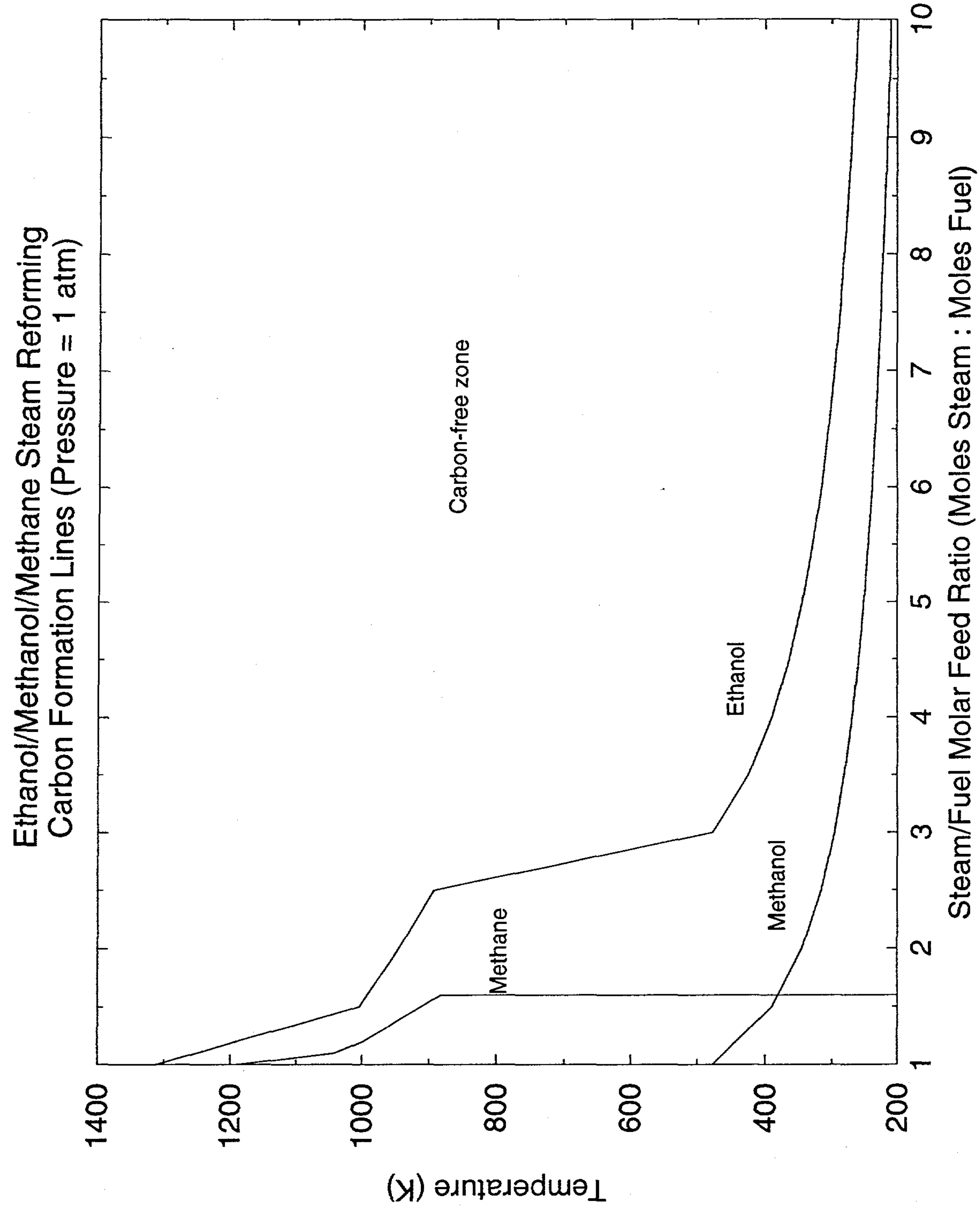


Figure III-1 Carbon Formation Lines for Methane/Methanol/Ethanol Steam Reforming

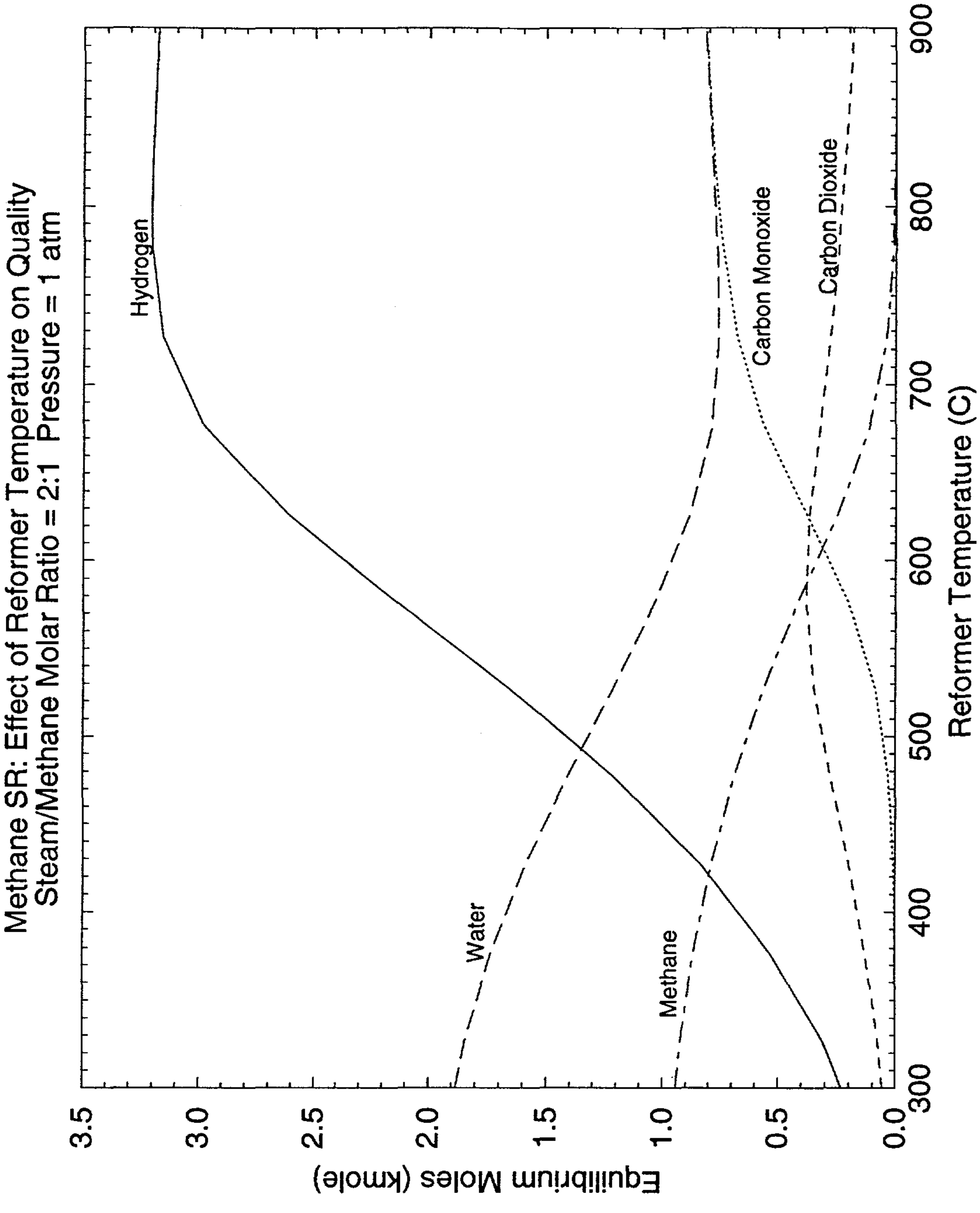


Figure III-2 Effect of Reformer Temperature on Methane Steam Reforming: Products From 1 kmole Methane

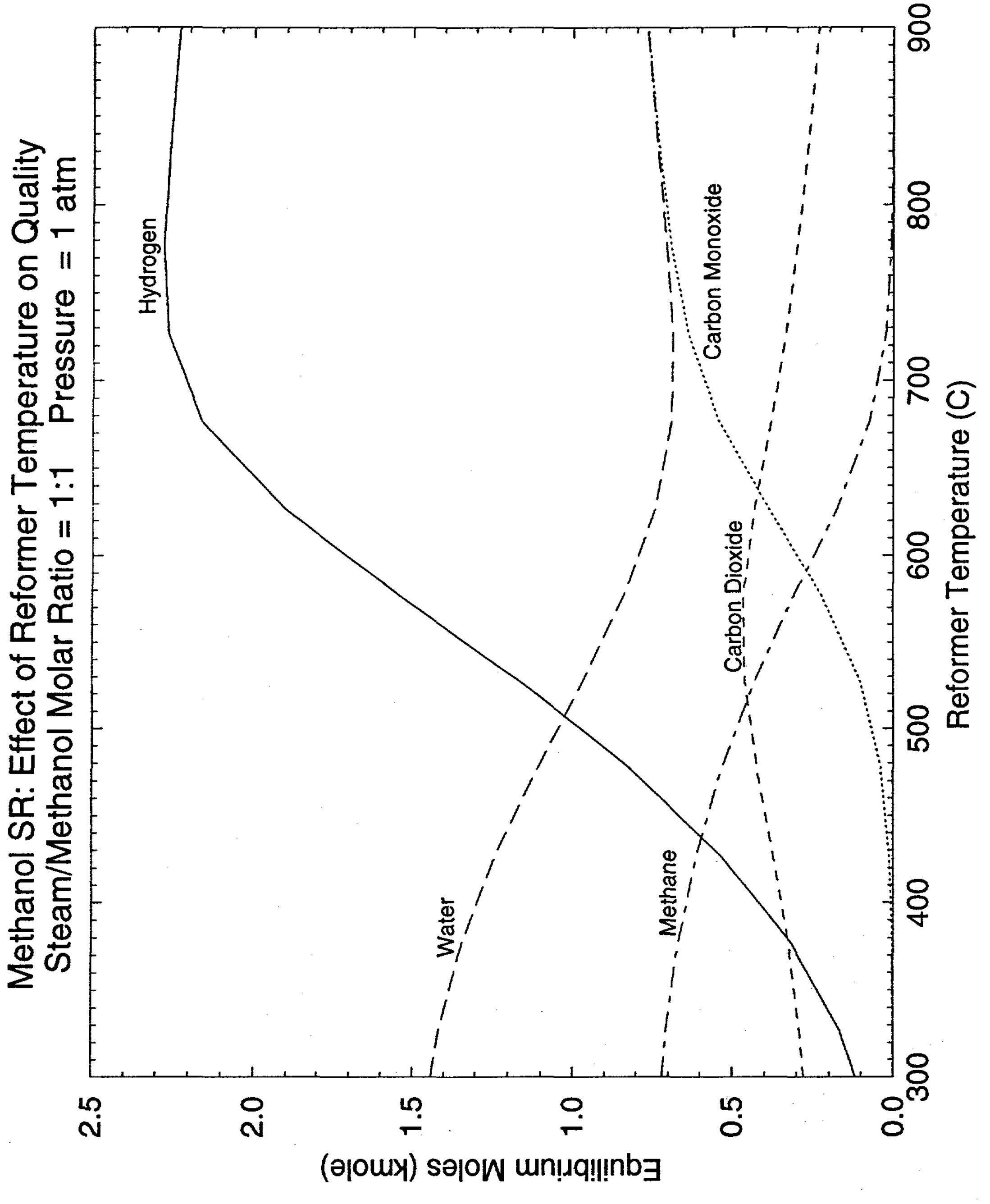


Figure III-3 Effect of Reformer Temperature on Methanol Steam Reforming: Products From 1 kmole Methanol

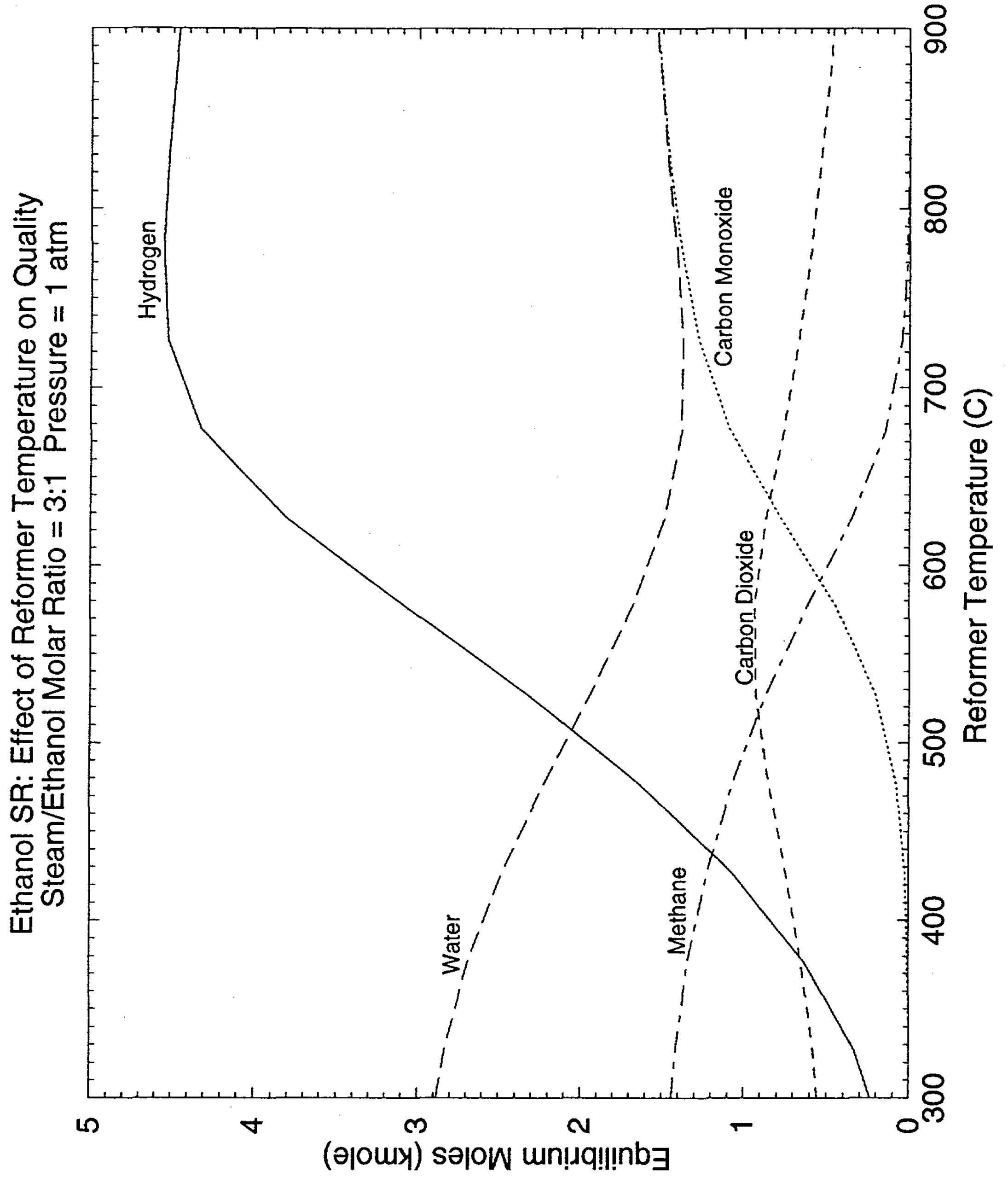


Figure III-4 Effect of Reformer Temperature on Ethanol Steam Reforming: Products From 1 kmole Ethanol

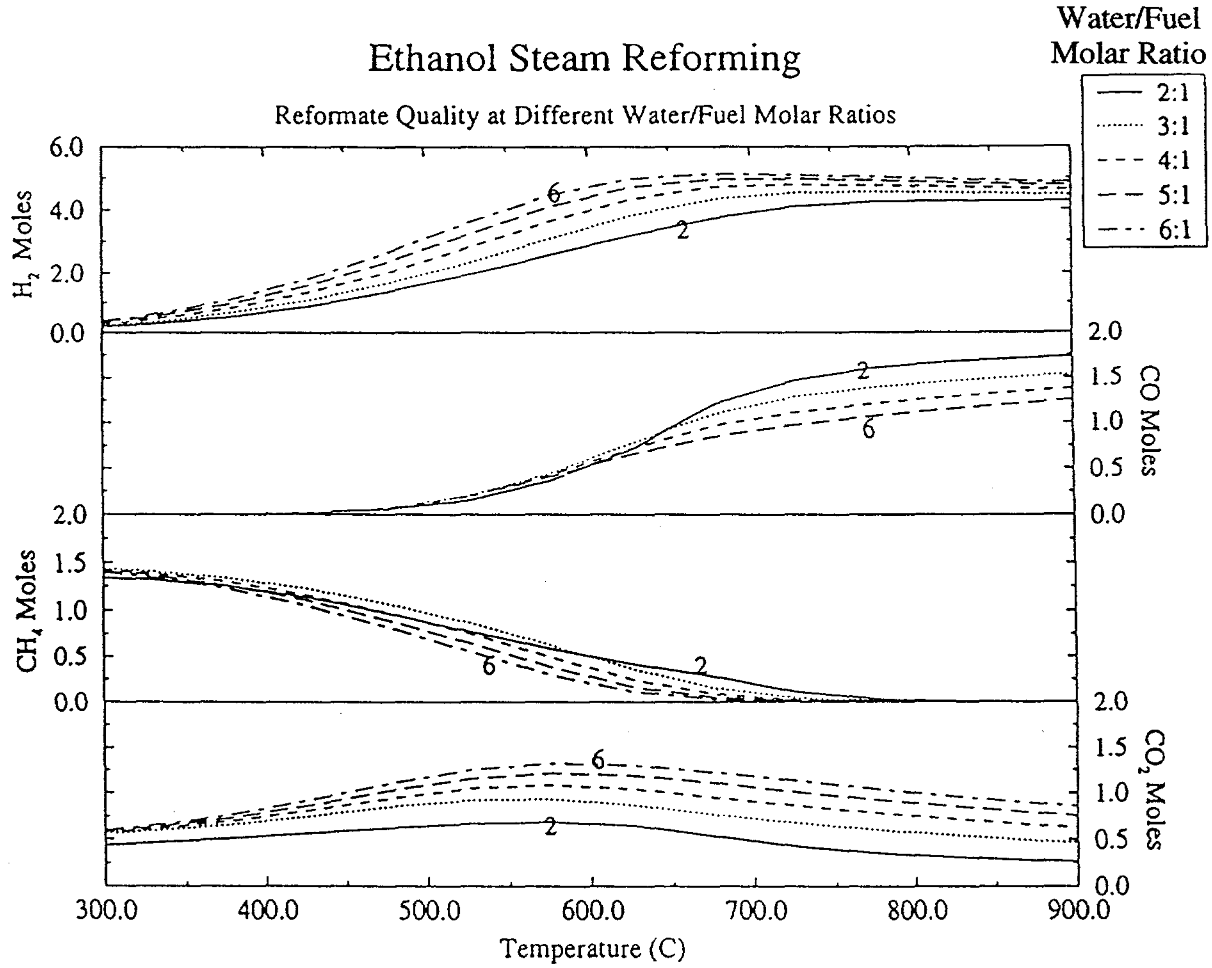


Figure III-5 Ethanol SR: Effect of Steam-to-Fuel Ratio on Reformate Quality: Products From 1 mole Ethanol

Autothermal and Partial Oxidation Reforming

Autothermal and partial oxidation reforming are similar to steam reforming except that part of the reactant fuel is burned *in-situ* to provide the heat of reaction for the endothermic reforming process. Partial oxidation is different from autothermal reforming in that little or no steam injection is used in partial oxidation reforming. Additionally, a catalyst is typically used in an ATR. Overall, ATR and POX are exothermic processes, the hydrogen yield being favored by low temperatures and low operating pressures.

The overall reactions taking place during autothermal reforming of methane are:

$$\begin{array}{llll} & & & \Delta H_{298}\ KJ/mol \\ CH_4 + \frac{1}{2}O_2 & \rightarrow & CO + 2H_2 & -35.68 \\ CH_4 + O_2 & \rightarrow & CO_2 + 2H_2 & -318.67 \\ CH_4 + 2H_2O & \rightleftharpoons & CO_2 + 4H_2 & +164.97 \\ CO + H_2O & \rightleftharpoons & CO_2 + H_2 & -41.17 \\ \hline CH_4 + \frac{1}{2}O_2 + H_2O & \rightleftharpoons & CO_2 + 3H_2 & -76.85 \end{array} \qquad (5)$$

Under partial oxidation reforming of methane only the first two reactions shown in the above equations take place. Stoichiometrically, methane ATR requires an equimolar feed of steam and methane and 0.5 moles of oxygen per mole of methane.

The overall reactions taking place during methanol autothermal and partial oxidation reforming are:

$$\begin{array}{llll} & & & \Delta H_{298}\ KJ/mol \\ CH_3OH + \frac{1}{2}O_2 & \rightleftharpoons & CO_2 + 2H_2 & -192.86 \\ CH_3OH + H_2O & \rightleftharpoons & CO_2 + 3H_2 & +48.96 \\ \hline CH_3OH + \frac{1}{4}O_2 + \frac{1}{2}H_2O & \rightleftharpoons & CO_2 + \frac{5}{2}H_2 & -71.95 \end{array} \qquad (6)$$

Methanol ATR/POX requires 0.5 mole of steam per mole of methanol and 0.25 mole of oxygen per mole of methanol.

Similarly, the overall ethanol autothermal and partial oxidation reforming reactions are:

$$\begin{array}{lr}
 & \Delta H_{298}\ KJ/mol \\
C_2H_5OH + \frac{1}{2}O_2 \rightarrow 2CO + 3H_2 & +13.37 \\
C_2H_5OH + \frac{3}{2}O_2 \rightarrow 2CO_2 + 3H_2 & -552.61 \\
C_2H_5OH + 3H_2O \rightleftharpoons 2CO_2 + 6H_2 & +172.85 \\
2CO + 2H_2O \rightleftharpoons 2CO_2 + 2H_2 & -82.34 \\
\hline
C_2H_5OH + \frac{2}{3}O_2 + \frac{5}{3}H_2O \rightleftharpoons 2CO_2 + \frac{14}{3}H_2 & -149.58
\end{array} \tag{7}$$

Establishing Operating Envelopes

Catalytic and non-catalytic partial oxidation is an exothermic process where the heat of reaction is provided by oxidizing a portion of the fuel *in situ* of the reformer as an adiabatic reactor. The reformer temperature (adiabatic reactor temperature) is controlled by the amount of fuel oxidized or equivalently by the amount of oxygen consumed. Higher ratios of oxygen-to-fuel produce higher adiabatic temperatures. The minimum oxygen-to-fuel ratio is determined by carbon formation, and the ability of the fuel to maintain stable combustion.

The effect of temperature on the reformate quality for ethanol autothermal reforming is shown in Figure III-6. Figure III-7 shows the corresponding oxygen to fuel ratios used to achieve these reformer temperatures. The oxygen is supplied as air. The ethanol ATR analysis used a steam to fuel ratio of 5:3 molar. High hydrogen yields are obtained at temperatures of 650-700°C which correspond to an oxygen to fuel ratio of 0.75-0.85 molar.

Figure III-8 shows the effect of reformer temperature on quality for methane autothermal reforming and Figure III-9 for methanol ATR.

Steam plays a dual role in autothermal reforming. It prevents carbon formation and also helps in the reforming of the fuel via the steam reforming route. This is possible in ATR since it is a catalytic process. Typically in non-catalytic partial oxidation little or no steam is used. Additionally, POX reformers operate at higher temperatures (higher oxygen/fuel ratios) since it is a non-catalytic process. This effect is shown in Figure III-10 for ethanol partial oxidation.

Potential for ammonia formation exists in an air-feed partial oxidation reformer. Figure III-11 shows the effect of pressure and oxygen enrichment on ammonia production for ethanol POX. Higher pressures and temperatures favor ammonia production which can be reduced by using oxygen-enriched air.

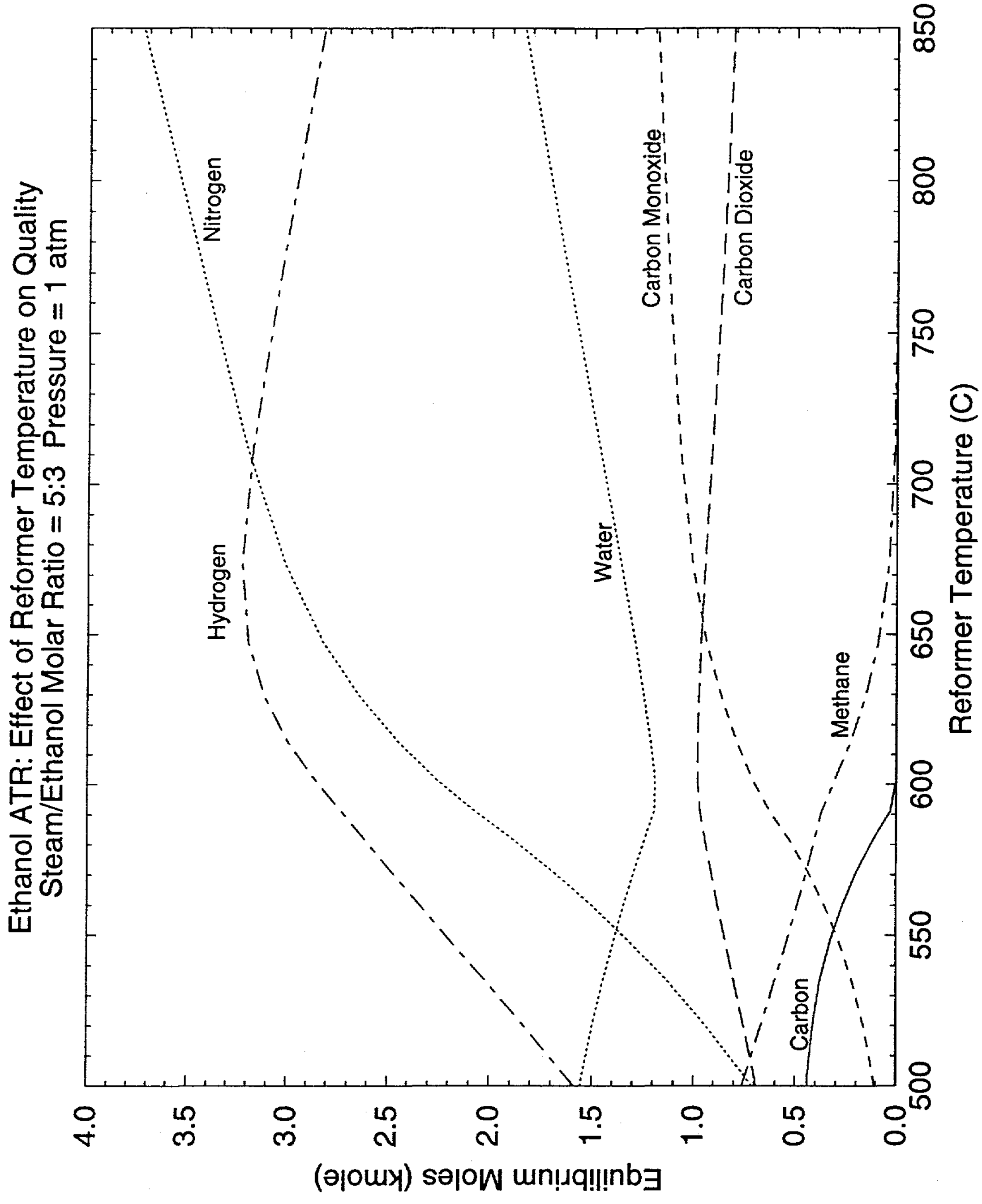


Figure III-6 Effect of Reformer Temperature on Reformate Quality in Ethanol ATR: Products from 1 kmole Ethanol.

Air feed is varied (as shown in Figure III-7) to achieve the reformer temperatures shown.

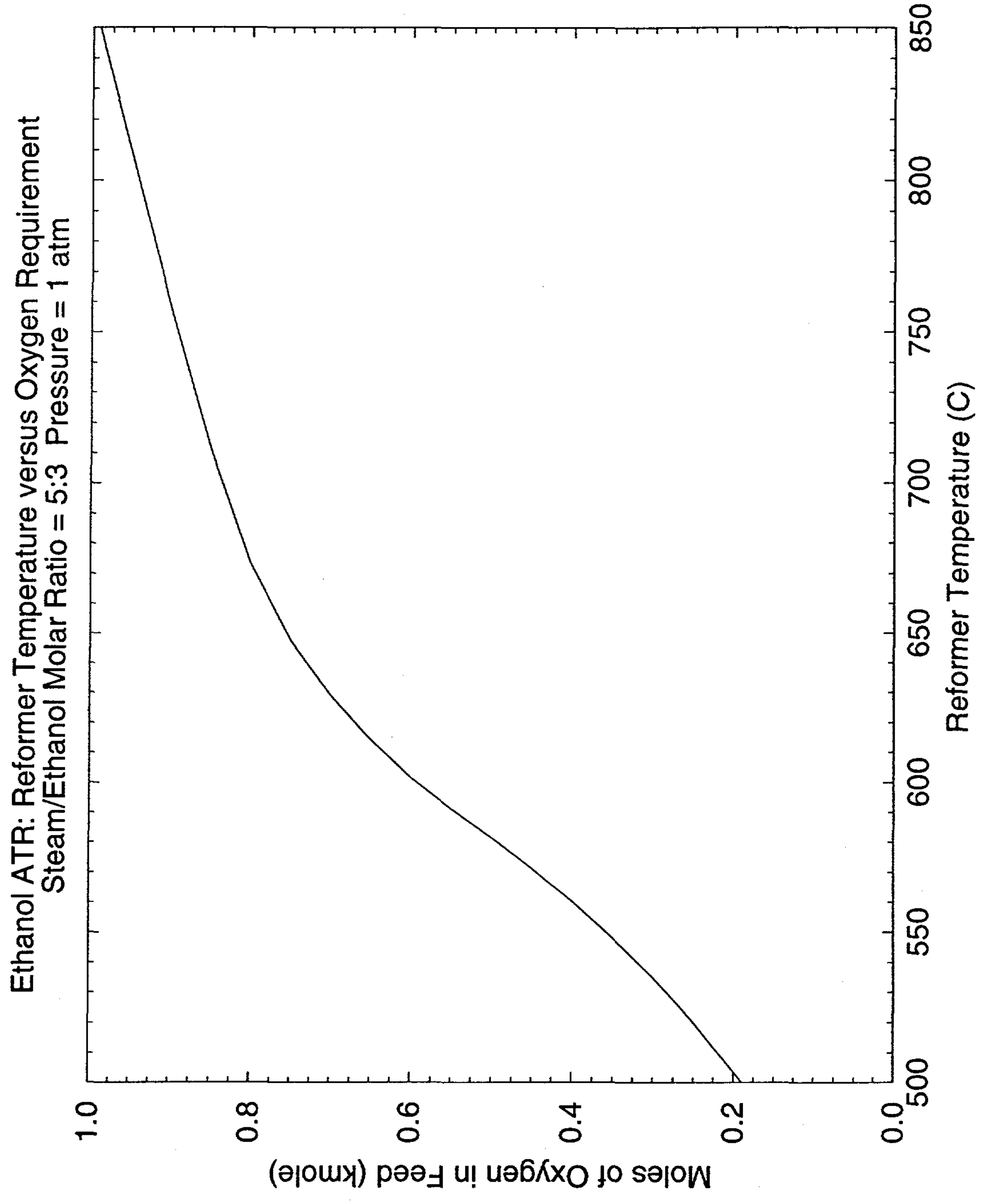


Figure III-7 Oxygen Required to Achieve a Given Reformer Temperature in Ethanol ATR: kmole Oxygen per kmole Ethanol.

Oxygen is supplied as air. The resulting reformate composition is shown in Figure III-6.

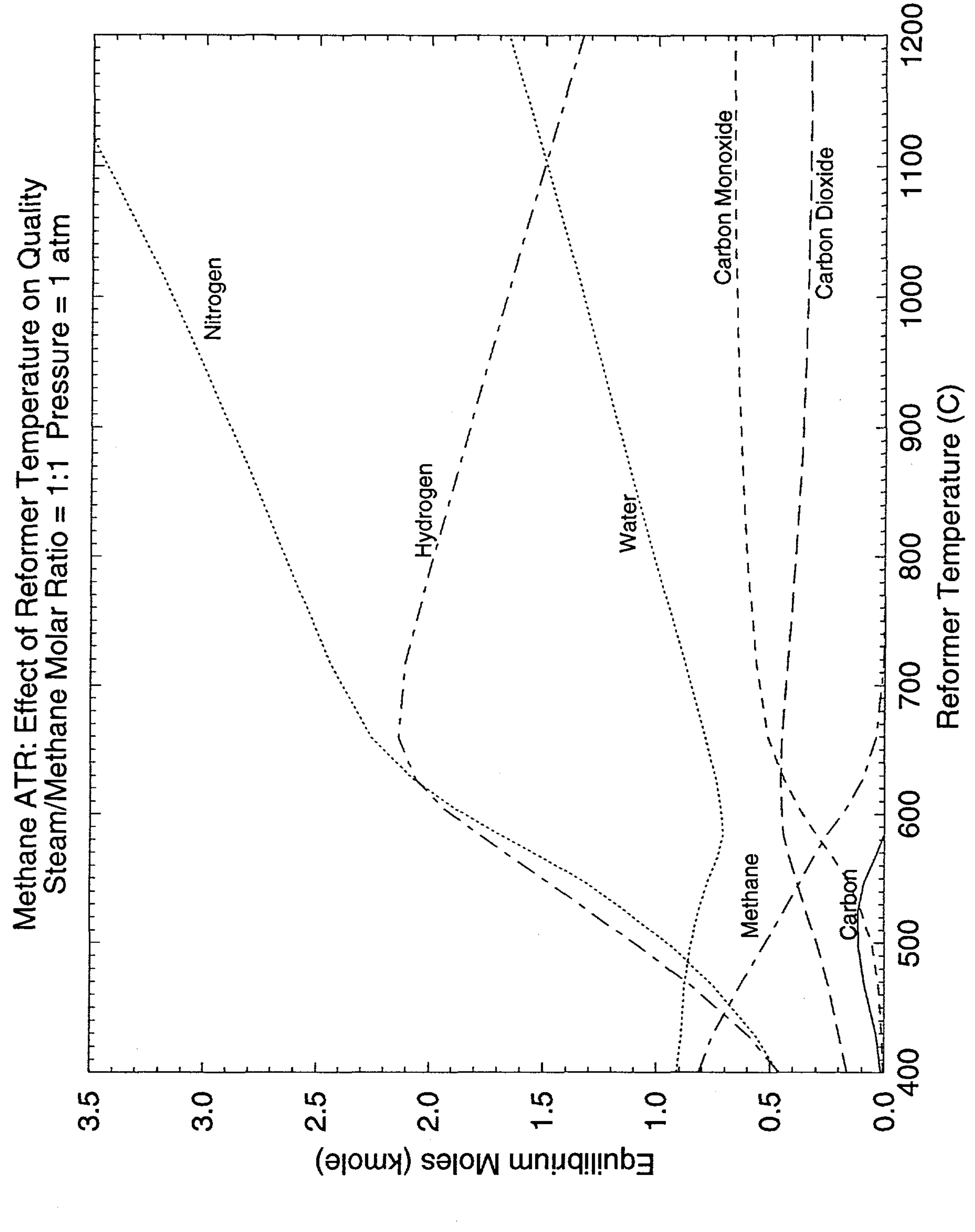


Figure III-8 Effect of Reformer Temperature on Reformate Quality in Methane ATR: Products From 1 kmole Methane.

Air feed is varied to achieve the reformer temperatures shown.

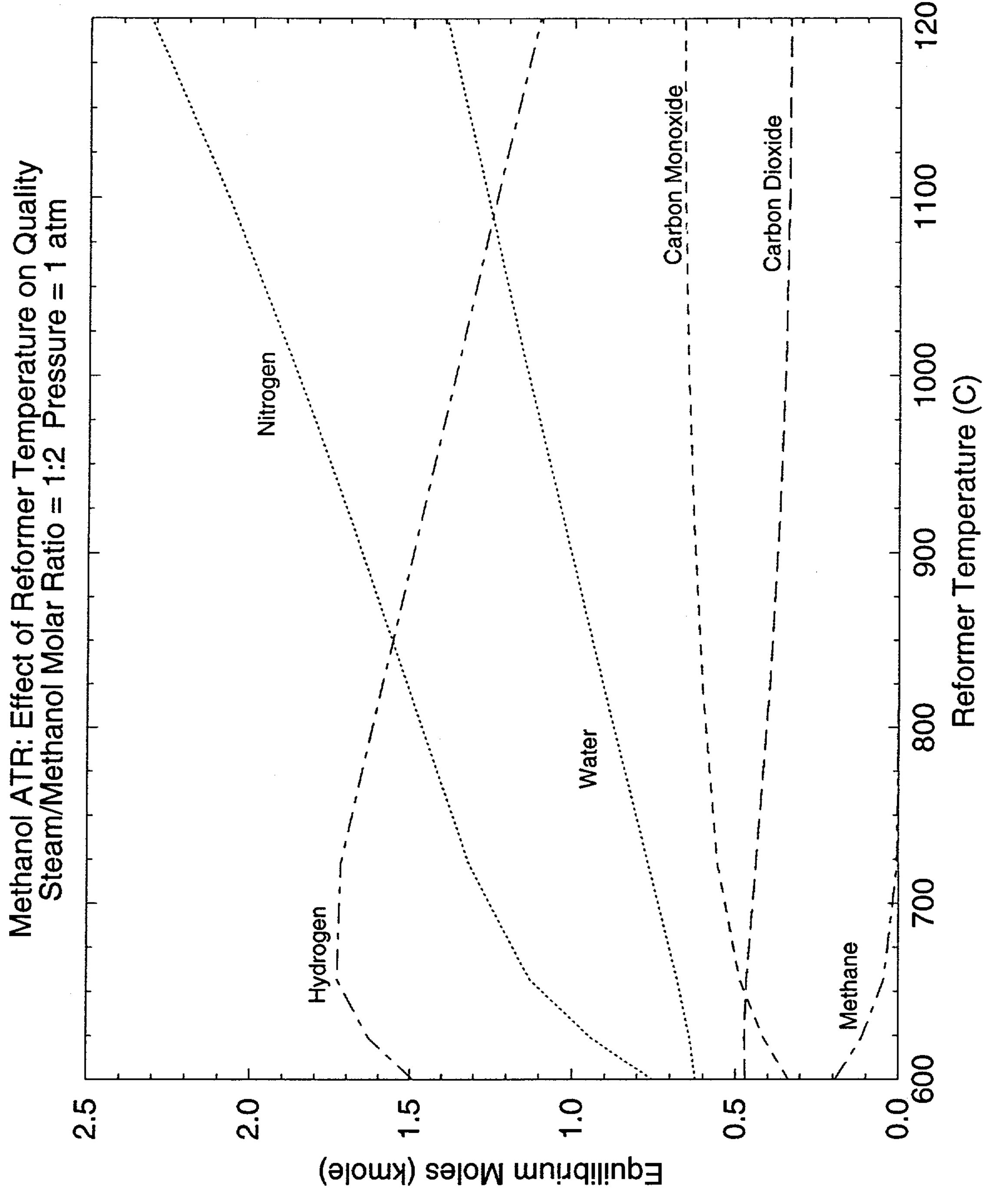


Figure III-9 Effect of Reformer Temperature on Reformate Quality in Methanol ATR: Products From 1 kmole Methanol.

Air feed is varied to achieve the reformer temperatures shown.

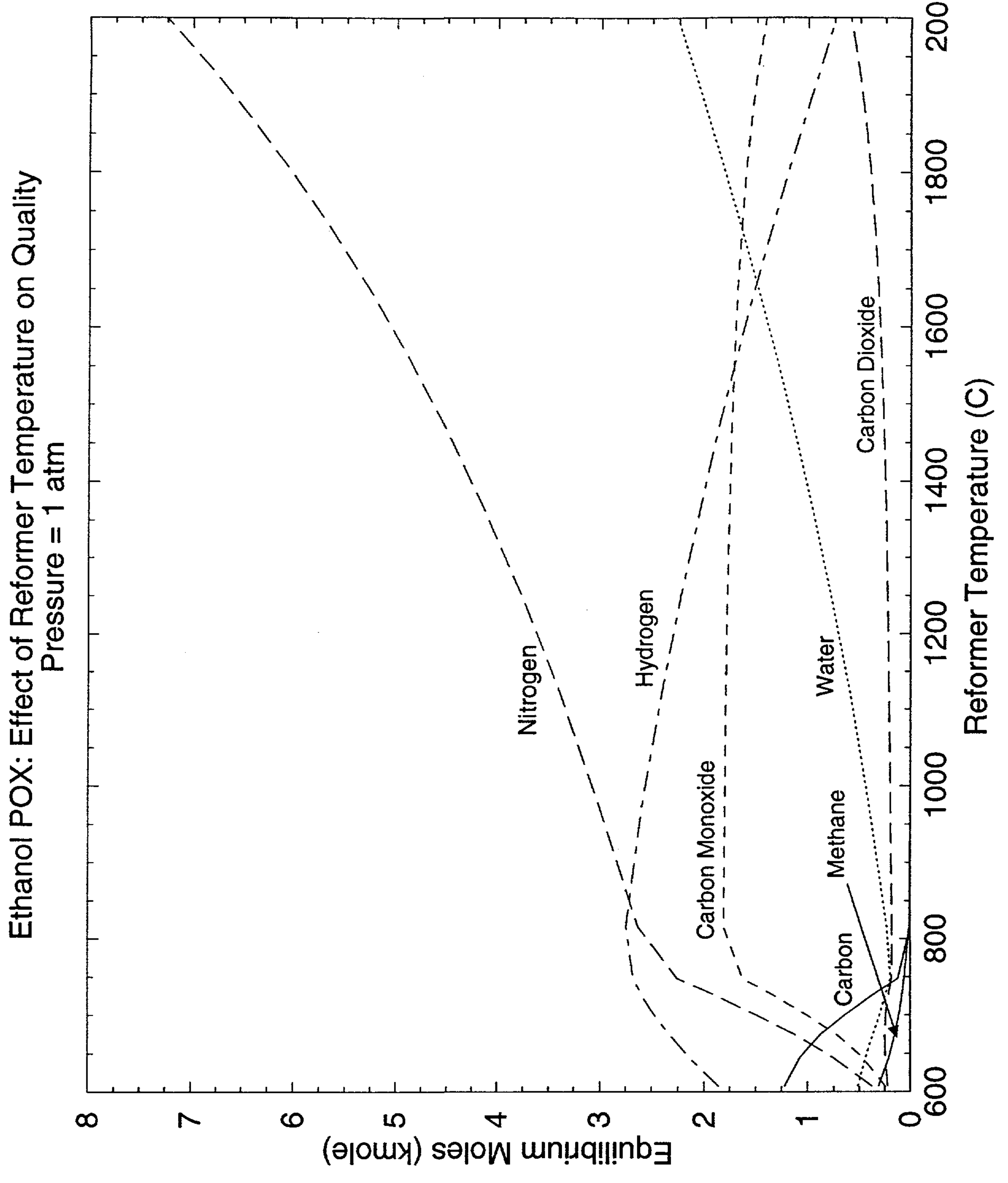


Figure III-10 Effect of Reformer Temperature on Reformate Quality in Ethanol POX: Products From 1 kmole Ethanol.

Air feed is varied to achieve the reformer temperatures shown.

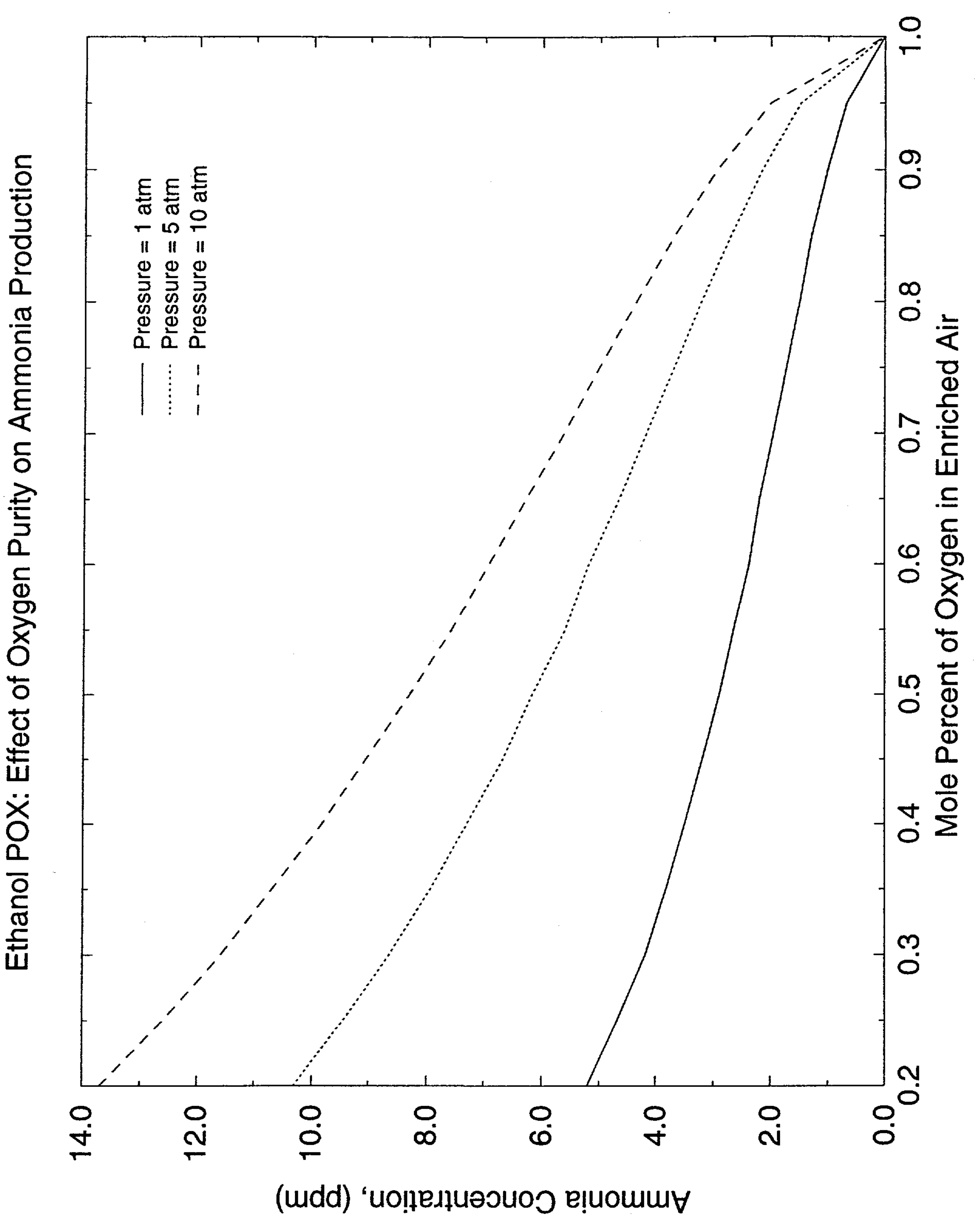


Figure III-11 Effect of Pressure and Oxygen Purity on Ammonia Production in Ethanol POX for POX with Oxygen-to-Ethanol Ratio of 0.67, Followed by Shift Reaction with Water-to-Fuel Ratio of 1.67

III.2. Efficiency Definitions

The efficiencies of a fuel cell and fuel processor and the overall system efficiency depend on the type of fuel cell, its operating characteristics and integration with the fuel processor. The efficiency definitions for the phosphoric acid and proton exchange membrane fuel cells are described below (these definitions are from "Handbook of Fuel Cell Performance", by T. G. Benjamin, et. al. [2]).

The overall electrochemical reaction in a PAFC is given by:

$$H_2(g) + \frac{1}{2}O_2(g) = H_2O(g) \tag{8}$$

and for a PEM the reaction is:

$$H_2(g) + \frac{1}{2}O_2(g) = H_2O\ (l) \tag{9}$$

The difference between these two reactions is the final form in which water is produced. In the high temperature PAFC water is produced in gaseous form and in the low temperature PEM it is in liquid form. Because of this difference, the definitions of several of the intermediate efficiencies (thermodynamic, heating value, fuel cell, and fuel processing efficiencies) for PEM fuel cells involve the higher heating value of the fuel, while the corresponding definitions for PAFCs involve the lower heating value. However, the Net System Efficiency is defined the same way for both PEM and PAFC systems and uses the higher heating value of the fuel.

There is not a fuel cell industry standard for the basis for system efficiency numbers. In general, in the internal combustion engine industry, it is common practice to use the lower heating value in calculating efficiency. In the heating and power generation industries, it is common practice to use the higher heating value. While the higher heating value is used here, the case-by-case results in the appendix also include the net system efficiencies as calculated on a lower heating value basis for comparison.

The various efficiency definitions for the fuel cell, fuel processor and overall system are given below.

Thermodynamic Efficiency
The fuel cell thermodynamic efficiency or maximum fuel cell efficiency is given by:

$$\eta_{Th} = \frac{\Delta G_r}{\Delta H_r} = \frac{Gibbs\ Free\ Energy\ of\ the\ Electrochemical\ Reaction}{Heating\ Value\ of\ Hydrogen\ in\ Anode\ Gas} \tag{10}$$

Voltage Efficiency

The voltage efficiency of the fuel cell is defined as the fraction of actual load voltage to the open circuit voltage:

$$\eta_V = \frac{V}{\varepsilon} = \frac{Actual\ Load\ Voltage}{Open\ Circuit\ Voltage} \tag{11}$$

The voltage under load conditions (V) can be estimated from the performance curve characteristics of the fuel cell. The performance curve characteristics for the PAFC were obtained from Benjamin, et. al. [2], and for the PEM fuel cell from Amphlett et. al. [1].

Current Efficiency

The current efficiency is given by:

$$\eta_I = \frac{I}{I_F} = U_f = (H_2\ utilization) = \frac{Actual\ Fuel\ Cell\ Current}{Current\ Predicted\ by\ Faraday' s\ Law} \tag{12}$$

This is equivalent to the amount of fuel utilized in the fuel cell (i.e. hydrogen utilization).

Electrochemical Efficiency

The electrochemical efficiency is defined as the product of thermodynamic, voltage and current efficiencies:

$$\eta_E = \eta_{Th} \cdot \eta_V \cdot \eta_I \tag{13}$$

Heating Value Efficiency

The anode feed gas contains, in addition to inert species (CO_2, N_2, H_2O) and electrochemically active species (H_2), some conventionally combustible species (unconverted CO, CH_4, etc.) that cannot be directly utilized by the fuel cell. The heating value efficiency takes this into account and is defined as the ratio of the heating value of hydrogen in the anode feed gas to the heating value of all combustibles in the anode feed gas:

For PAFC the heat content is the lower or net heating value and for PEM fuel cells it is the higher or gross heating value (to take into account the heat of condensation of product water

$$\begin{aligned}\eta_H &= \frac{\Delta H_r}{\Delta H_c}\\ &= \frac{Heating\ Value\ of\ H_2 \in Anode\ Gas}{Heating\ Value\ of\ Total\ Anode\ Gas}\end{aligned} \tag{14}$$

in a PEM fuel cell).

Fuel Cell Efficiency
The fuel cell efficiency is described as the amount of chemical energy available in the anode feed gas that is converted to DC power. It is given by:

$$\begin{aligned}\eta_{FC} &= \eta_E \cdot \eta_H\\ &= (\eta_{Th} \cdot \eta_V \cdot \eta_I) \cdot \eta_H\\ &= \frac{DC\ Power\ Produced}{Heating\ Value\ of\ Total\ Anode\ Gas}\end{aligned} \tag{15}$$

Fuel Processor Efficiency
The fuel processor efficiency is defined as the ratio of the heating value of the anode feed gas to the heating value of the total fuel to the fuel processor:

$$\begin{aligned}\eta_{FP} &= \frac{\Delta H_{Anode}}{\Delta H_{fuel}}\\ &= \frac{Heating\ Value\ of\ Total\ Anode\ Gas}{Heating\ Value\ of\ Total\ Fuel\ into\ FP}\end{aligned} \tag{16}$$

Gross System Efficiency
This is defined as the ratio of DC power produced to the heating value of the total fuel to the fuel processor. This is given by the product of the fuel cell and fuel processor efficiency:

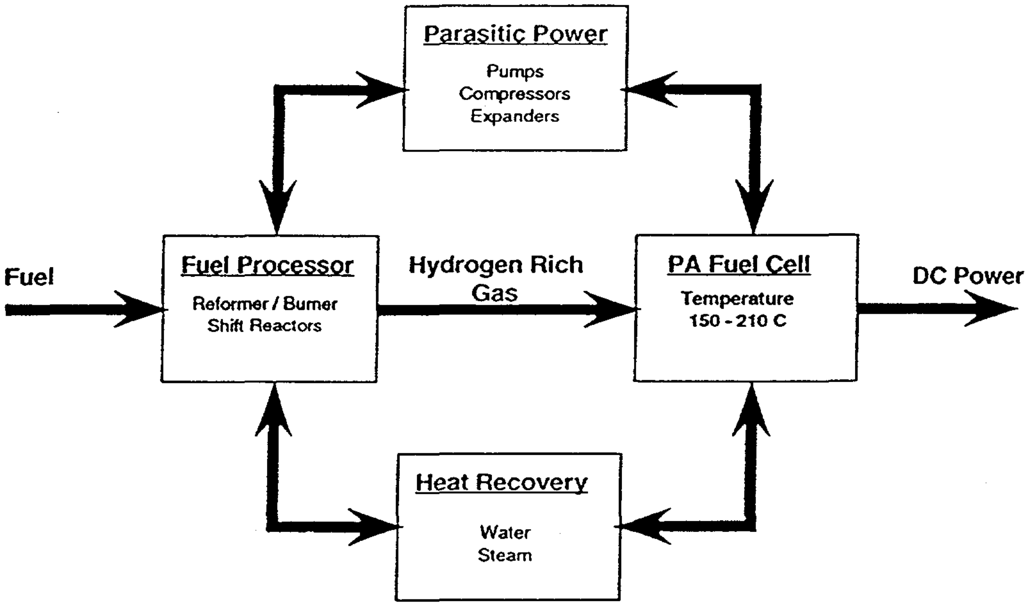
$$\begin{aligned}\eta_{Gross} &= \eta_{FC} \cdot \eta_{FP}\\ &= \frac{DC\ Power\ Produced}{Heating\ Value\ of\ Total\ Fuel\ into\ FP}\end{aligned} \tag{17}$$

Net System Efficiency
The net system efficiency is defined as the ratio of DC power produced less parasitic power to the heating value of the total fuel to fuel processor:

$$\eta_{Net} = \frac{(DC\ Power\ Produced) - (Parasitic\ Power)}{Heating\ Value\ of\ Total\ Fuel\ into\ FP} \qquad (18)$$

The efficiency definitions for phosphoric acid and proton exchange membrane fuel cells are summarized in Figure III-12 and Figure III-13, respectively.

Phosphoric Acid Fuel Cell
(PAFC)
Efficiency Definitions



$$H_2(g) + \frac{1}{2}O_2(g) = H_2O(g)$$

Thermodynamic Efficiency $\eta_{Th} = \frac{\Delta G_{rT,P}}{\Delta H_{rT}} = \frac{-n\mathcal{F}\mathcal{E}_{T H_2}}{\text{LHV of H2 in Anode Feed Gas}}$

Voltage Efficiency $\eta_V = \frac{V}{\mathcal{E}} = \frac{\text{Actual Load Voltage}}{\text{Open Circuit Voltage}}$

Current Efficiency $\eta_I = \frac{I}{I_F} = U_f$ (H2 utilization in fuel cell)

Electrochemical Efficiency $\eta_E = \eta_{Th} \cdot \eta_V \cdot \eta_I$

Heating Value Efficiency $\eta_H = \frac{\Delta H_{rT}}{\Delta H_{c_T}} = \frac{\text{LHV of H2 in Anode Feed Gas}}{\text{LHV of Anode Feed Gas}}$

Fuel Cell Efficiency $\eta_{FC} = \eta_E \cdot \eta_H = \frac{\text{DC Power Produced}}{\text{LHV of Anode Feed Gas}}$

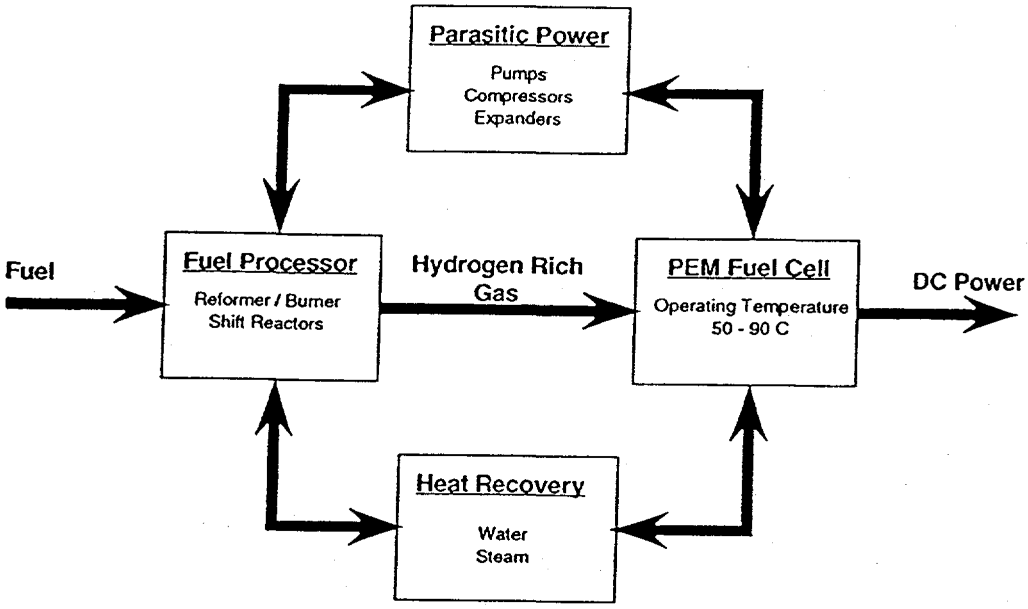
Fuel Processing Efficiency $\eta_{FP} = \frac{\text{LHV of Anode Feed Gas}}{\text{HHV of Total Fuel to Fuel Processor}}$

Gross System Efficiency $\eta_{Gross} = \eta_{FC} \cdot \eta_{FP} = \frac{\text{DC Power Produced}}{\text{HHV of Total Fuel to Fuel Processor}}$

Net System Efficiency $\eta_{Net} = \frac{\text{(DC Power Produced)-(Parasitic Power)}}{\text{HHV of Total Fuel to Fuel Processor}}$

Figure III-12 Efficiency Definitions for Phosphoric Acid Fuel Cells

Proton Exchange Membrane Fuel Cell
(PEMFC)
Efficiency Definitions



$$H_2(g) + \frac{1}{2}O_2(g) = H_2O(l)$$

Thermodynamic Efficiency	η_{Th}	$= \frac{\Delta G_{rT,P}}{\Delta H_{rT}} = \frac{-n\mathcal{F}\mathcal{E}x_{H2}}{\text{HHV of H2 in Anode Feed Gas}}$
Voltage Efficiency	η_V	$= \frac{V}{\mathcal{E}} = \frac{\text{Actual Load Voltage}}{\text{Open Circuit Voltage}}$
Current Efficiency	η_I	$= \frac{I}{I_r} = U_f$ (H2 utilization in fuel cell)
Electrochemical Efficiency	η_E	$= \eta_{Th} \cdot \eta_V \cdot \eta_I$
Heating Value Efficiency	η_H	$= \frac{\Delta H_{rT}}{\Delta H_{cT}} = \frac{\text{HHV of H2 in Anode Feed Gas}}{\text{HHV of Anode Feed Gas}}$
Fuel Cell Efficiency	η_{FC}	$= \eta_E \cdot \eta_H = \frac{\text{DC Power Produced}}{\text{HHV of Anode Feed Gas}}$
Fuel Processing Efficiency	η_{FP}	$= \frac{\text{HHV of Anode Feed Gas}}{\text{HHV of Total Fuel to Fuel Processor}}$
Gross System Efficiency	η_{Gross}	$= \eta_{FC} \cdot \eta_{FP} = \frac{\text{DC Power Produced}}{\text{HHV of Total Fuel to Fuel Processor}}$
Net System Efficiency	η_{Net}	$= \frac{\text{(DC Power Produced)-(Parasitic Power)}}{\text{HHV of Total Fuel to Fuel Processor}}$

Figure III-13 Efficiency Definitions for Proton Exchange Membrane Fuel Cells

III.3. Flowsheet Development

All reforming technologies require a similar set of unit process steps to convert the feedstock, such as methane, methanol or ethanol to hydrogen, and for the electrochemical conversion of hydrogen into electricity via a fuel cell. The key unit processing steps are shown graphically in Figure III-14.

Feed Preparation Section

The feed preparation step may include the preheating, vaporization and superheating of fuel and other reactants such as water and air, as required by the specific reforming technology prior to entering the reforming reactor. When fuels that contain sulfur are used with a reformer that uses sulfur-sensitive catalysts, additional pretreatment steps will have to be inserted for the sulfur removal function.

Reforming Section

Reforming the vaporized feed into hydrogen and carbon monoxide is carried out in this section. Supply of heat for the endothermic reforming reactions, via either the external combustion of fuel as in the steam reforming case or internal combustion of fuel as in the ATR or POX case, is performed in this section.

Post Reforming Section

In this section, the hot reformate is quenched with water to lower its temperature and to provide excess water (i.e., a water-to-CO ratio higher than stoichiometric) to promote the subsequent shift reactions. The quenched reformate would undergo typically a two-stage water-shift reaction to convert CO to hydrogen. A high temperature shift reactor is followed by an intercooler to remove the heat of shift reactions and finally a low temperature shift reactor.

Trace CO Removal and Anode Gas Conditioning

Depending on the type of fuel cell, the reformate gas may undergo additional removal of species detrimental to the fuel cell operation. This may include the selective oxidation of CO using air, removal of ammonia in a guard-bed, additional sulfur removal, anode gas humidification, etc. All of the PEM fuel cell system flow diagrams show a preferential oxidation (PROX) reactor. This reactor performs a selective catalytic oxidation of the trace amount of carbon monoxide to carbon dioxide, without oxidation of the hydrogen that is also present.

Fuel Cell Section

The hydrogen rich gas is introduced into the anode of the fuel cell, and air is supplied to the fuel cell cathode.

Anode Exhaust Utilization Section

The hydrogen depleted anode exhaust together with some supplemental fuel is used in the fuel processor to provide heat required in feed preparation or reaction in the reforming reactor.

Exhaust Energy Recovery Section

For pressurized systems, both the pressure energy and the waste heat energy can be recovered in expansion devises such as a turbo-expander or a rotary positive scroll expander. A rotary positive scroll expander may have the advantage of being able to handle a condensing stream which is expected for this application. The recovered power from the expander may be used directly to supplement the compressor power requirement through a common shaft, or may be used to generate electricity for use by the vehicle.

Based on these basic processing steps, conceptual flow diagrams showing major process components to support these basic process steps are developed for the three reforming technologies under consideration for integration with a PAFC or a PEM fuel cell.

The process flow diagrams for a steam reformer, autothermal reformer, and partial oxidation reformer integrated with a PEM fuel cell stack are shown in Figures III-15, III-16, and III-17, respectively. All three concepts are for a pressurized fuel processor and fuel cell stack.

Figure III-18 shows the process flow diagram for a pressurized steam reformer integrated with a pressurized, water-cooled phosphoric acid fuel cell.

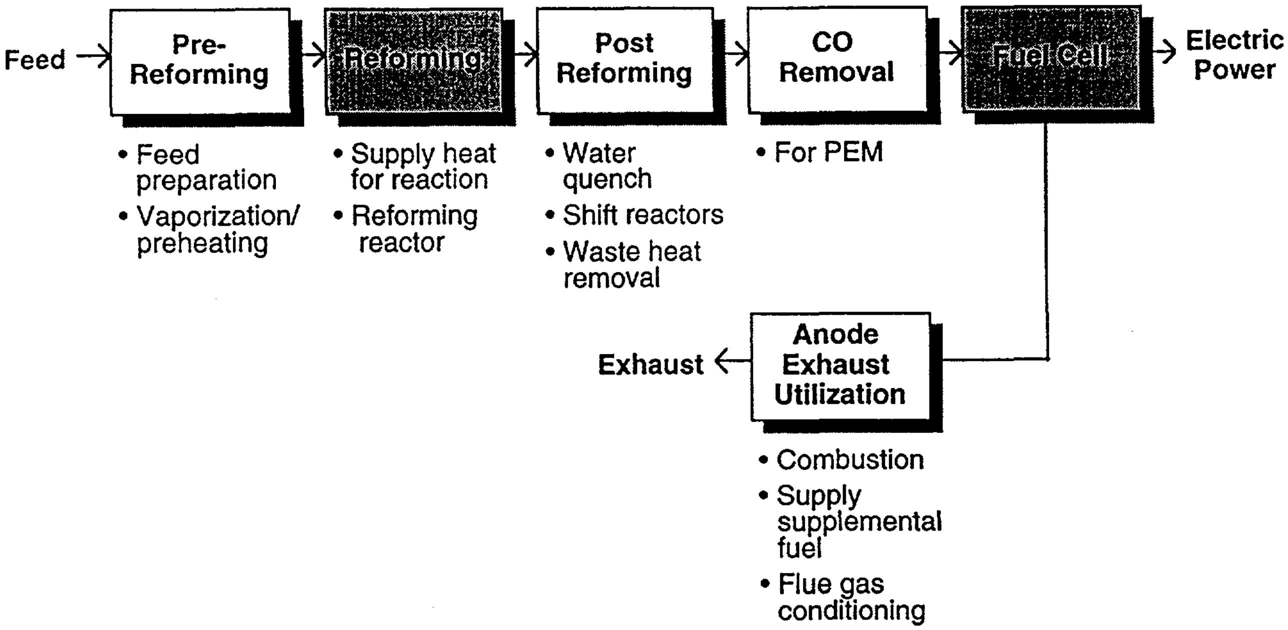


Figure III-14 Key Unit Processing Steps for all Reforming Technologies

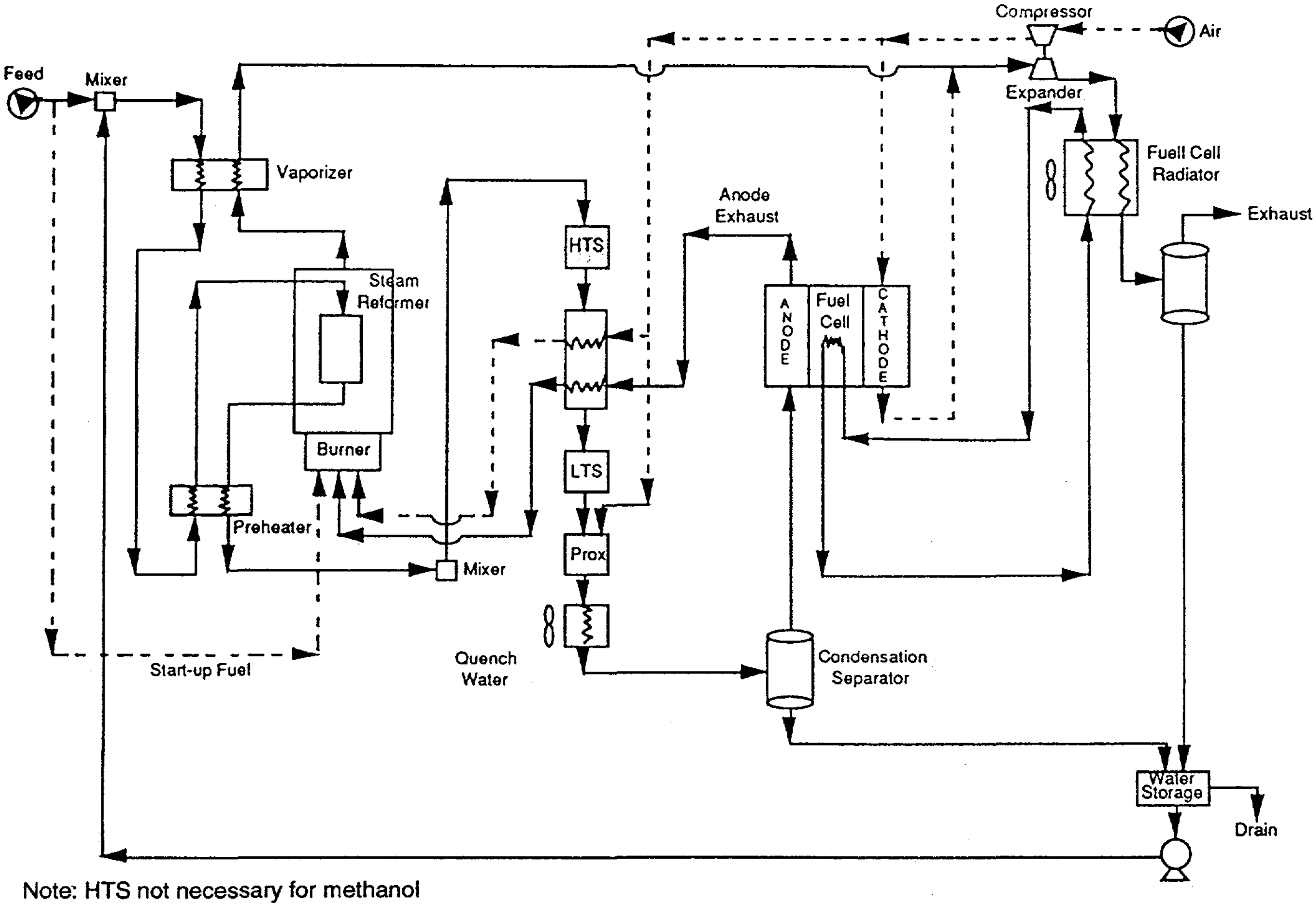


Figure III-15 Process Flow Diagram for Steam Reformer Integrated with a PEM Fuel Cell

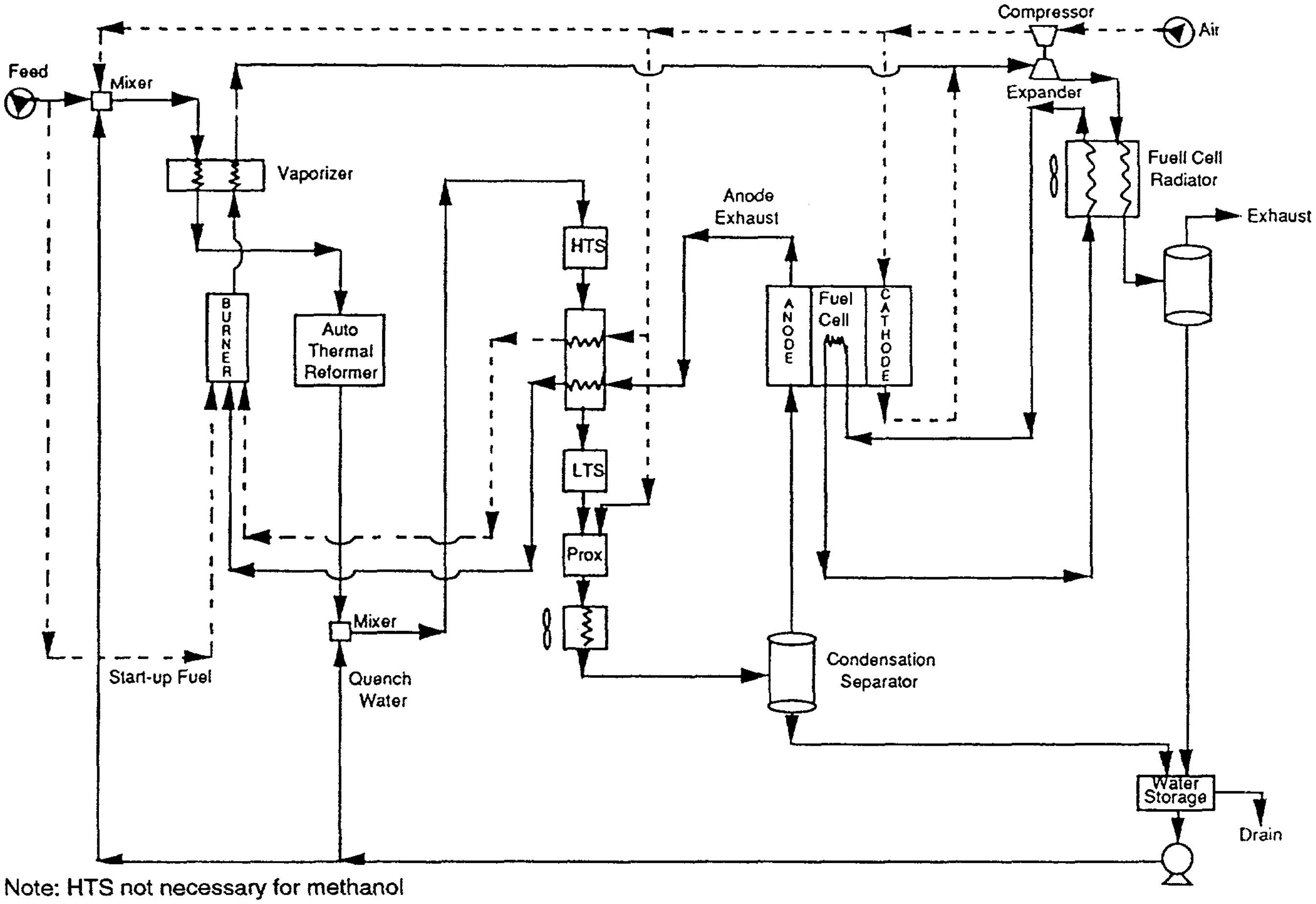
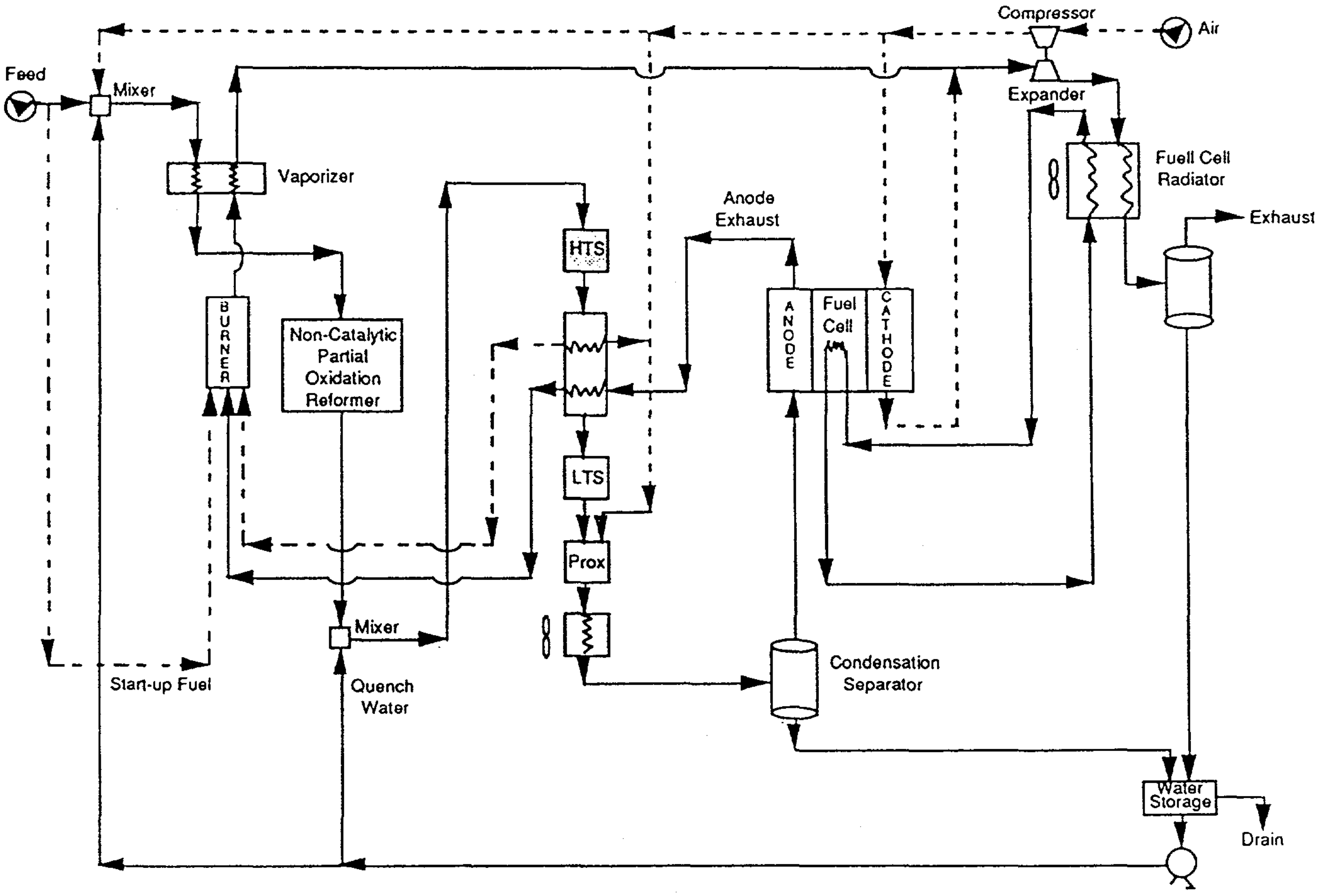
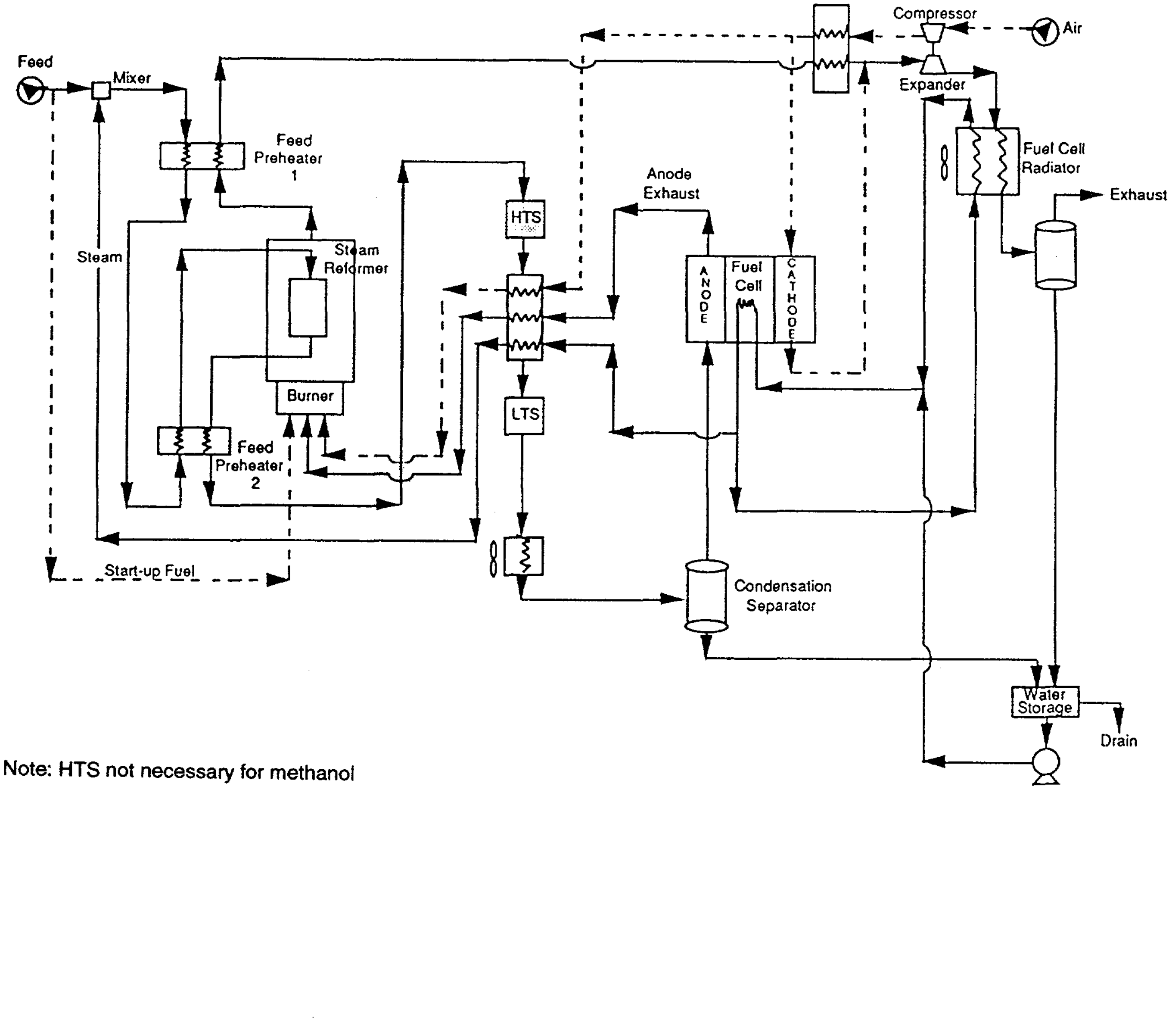


Figure III-16 Process Flow Diagram for Autothermal Reformer Integrated with PEM Fuel Cell



Note: HTS not necessary for methanol

Figure III-17 Process Flow Diagram for Partial Oxidation Reformer Integrated with PEM Fuel Cell



Note: HTS not necessary for methanol

Figure III-18 Process Flow Diagram for Steam Reformer Integrated with PAFC

III.4. Case Studies

Cases Studied

A number of design case studies were performed to quantify mass and energy balance so as to assess the impact of fuel, reforming technology and fuel cell integration. The variables under consideration are:

- *Fuel:* methane, methanol, ethanol
- *Reforming Technology:* steam reforming, autothermal reforming, partial oxidation
- *Fuel Cell:* phosphoric acid fuel cell, proton exchange membrane fuel cell

While the emphasis of this study is on the evaluation of reforming technologies as opposed to judgments on fuel or fuel cell technologies, one must address the impact of fuels and fuel cells on the reforming technologies. To fully analyze the combinations of the above variables, one will need to examine a matrix of 18 combinations. This was not possible under the constraints on this study in terms of schedule and allocated effort. In order to assess the impact of fuel and fuel cell type on reforming technology, nine selected cases were studied. These cases were selected by fixing two of these variables and varying the third.

Table III-1 Case Studies Analyzed

Case	1	2	3	4	5	6	7	8	9
Fuel Cell Type	PEM	PEM	PEM	PEM	PEM	PAFC	PAFC	PAFC	PAFC
Reformer Technology	SR	ATR	POX	SR	SR	SR	SR	ATR	POX
Fuel	Methane	Methane	Methane	Methanol	Ethanol	Methane	Methane	Methane	Methane
Anode Exhaust Utilization	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes
Power Recovery	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes
Pressure, atm	3	3	3	3	3	3	1	1	1

Table III-1 shows the nine cases and the combinations that were analyzed in this study. The first three cases compare the three (3) reforming technologies for a fixed type of fuel (methane) and a fixed type of fuel cell (PEM). Cases 4 and 5 analyze the effect of methanol and ethanol for a given reforming technology (SR) and fuel cell type (PEM). Case 6 analyzes the effect of methane as a fuel for SR technology and PAFC. The Cases 7, 8 and 9 compare the three reforming technologies for methane and PAFC, which, together with the first three cases, provide a basis for comparing the three reforming technologies against the two fuel cells for a fixed fuel.

The combination of Cases 1, 4 and 5 analyze the effect of the three fuels for a fixed reforming technology (SR) and fuel cell (PEM). Cases 1 and 6 analyze the effect of the two fuel cells for a fixed fuel (methane) and reforming technology (SR). In this manner, these 9 case studies provided a basis for meaningful assessment of reforming technologies and impacts of fuels and fuel cell type on the reforming technologies.

A consistent design basis was selected to facilitate a true comparison across the different fuels, reforming technologies and fuel cells:

Gross System DC Output:	25 kW		
Assumed Fuel Cell Conditions:	**PEM**	**PAFC**	**PAFC**
Current Density (ampere/ft^2):	400	300	300
Temperature (°C):	80	190	190
Pressure (atm):	3	3	1
Anode Hydrogen Utilization:	80%	80%	80%
Cathode Oxygen Utilization:	50%	50%	50%
Component Efficiency in Power Recovery System:			
Pumps:	70% (adiabatic)		
Compressors:	70% (adiabatic)		
Expanders:	70% (adiabatic)		

The design conditions for the last three case studies (Cases 7, 8 and 9) were different from the others in the system operating pressure. The first six cases were analyzed assuming the fuel processor and fuel cell stack to be pressurized to 3 atm. The last three cases were analyzed for an atmospheric fuel processor and phosphoric acid fuel cell.

Table III-2 shows the fuel processor operating conditions selected for the nine cases. This selection was based on either reported parameters by system developers or those estimated by ADL from thermodynamic and kinetic analysis.

The methane steam reformer (Cases 1, 6 and 7) operates at an isothermal temperature of 700°C and a steam-to-methane molar ratio of 3. The operating conditions for the methane steam reformer were based on those reported by KTI. The methanol steam reformer (Case 4) operates isothermally at 260°C and a steam to methanol molar ratio of 1.5 (conditions selected based on the work by GM/LANL [5]). The ethanol steam reformer (Case 5) operates at a fixed temperature of 750°C and a steam to fuel molar ratio of 4 (based in part on British Gas patent [3] and ADL analysis).

For the steam reformers, the heat of reaction is provided by oxidizing the anode exhaust and supplemental fuel external to the reformer. The autothermal methane reformer (Cases 2 and 8) operates adiabatically with an inlet temperature of 500°C and an outlet temperature of 890°C. The methane ATR employs a steam-to-fuel molar ratio of 1 and an oxygen to fuel molar ratio of 0.6 (the oxygen being obtained from air). The partial oxidation reformer (cases 3 and 9) operates adiabatically with an inlet gas temperature of 500°C and outlet temperature of

1105°C, employing an oxygen to fuel molar ratio of 0.67 and no steam addition. The total inlet flow rates are also given in Table III-2.

The outlet gas compositions from the fuel reformer along with the high and low temperature shift reactor conditions for all of the cases are given in the Appendix. The Appendix, which constitutes the second volume of this report, shows the results of the process simulation calculations for each of the nine cases.

Table III-2 Case Studies: Reforming Process Conditions

Case		**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**
Fuel Cell Type		**PEM**	**PEM**	**PEM**	**PEM**	**PEM**	**PAFC**	**PAFC**	**PAFC**	**PAFC**
Reformer Technology		**SR**	**ATR**	**POX**	**SR**	**SR**	**SR**	**SR**	**ATR**	**POX**
Fuel		**Methane**	**Methane**	**Methane**	**Methanol**	**Ethanol**	**Methane**	**Methane**	**Methane**	**Methane**
Fuel Reformer Conditions										
Inlet Temperature,	C	700	500	500	260	750	700	700	500	500
Outlet Temperature,	C	700	891	1105	260	750	700	700	890	1105
Pressure,	atm	3	3	3	3	3	3	1	1	1
Steam/Fuel Ratio,	molar	3.00	1.00	0.00	1.50	4.00	3.00	3.00	1.00	0.00
Oxygen/Fuel Ratio,	molar	NA	0.60	0.67	NA	NA	NA	NA	0.60	0.67
Air/Fuel Ratio,	molar	NA	2.86	3.19	NA	NA	NA	NA	2.86	3.19
Oxygen Content in Air,	mol%	NA	21.0%	21.0%	NA	NA	NA	NA	21.0%	21.0%
Total Inlet Flow,	kmol/hr	0.98	1.50	1.36	0.73	0.81	1.02	1.00	1.67	1.51
	kg/hr	17.17	36.03	35.18	17.28	19.11	17.93	17.60	40.00	38.97
Sources of Process Conditions		KTI	ADL	ADL	GM/LANL	ADL	KTI	KTI	ADL	ADL

Sizing of Major Components

Major components of a 25 kW system were sized for the SR, ATR and POX fuel processor systems using methane as the common fuel. The following describes the approaches for sizing each of those components.

The sizing of the catalytic steam reformer was based on the published space velocity of 50,000 per hour for a reduced nickel catalyst and the heat flux for controlling heat transfer as reported by IHI [9]. The methane ATR reactor was sized on the basis of a space velocity of 40,000 per hour as reported by British Gas on a reduced nickel catalyst (CRG F). The high temperature shift reactor sizing was based on a reduced Fe_2O_3 catalyst promoted with chromium oxide (e.g. the United Catalyst G-3). The low temperature shift reactor sizing was based on the published space velocity of 2,000 per hour for a catalyst with copper dispersed on a silica substrate. The selective oxidation reactor was based on the assumption that the Hopcalite type of catalyst, which is a mixture of copper, cobalt, manganese and silver, is effective for the operating environment. Heat exchanger sizing was based on compact heat exchanger correlations.

Sizing of POX Burner

Currently, there is no established methodology in the literature for sizing a POX burner/reactor. We fashioned the POX reaction mechanism after a staged combustion model which assumes near stoichiometric combustion of a portion of the feed dictated by the required POX reactor temperature, and non-catalytic reforming after mixing with additional hydrocarbon fuel.

We used the Chemkin program [6], a combustion kinetics model published by Sandia National Laboratories, to facilitate predictions of the residence time and performance which are needed to size the POX reactor. For the design basis, the predicted internal dimensions of the POX burner/reactor are 16 cm in diameter and 100 cm in length. Other design bases and performance characteristics of the POX reactor are as follows:

- Preheating of feed: 500°C
- O_2/CH_4 Ratio: 0.67
- Oxygen concentration: 21 dry vol%
- POX burner Pressure: 3 atm
- Residence time: 641 seconds
- Equilibrium H_2 concentration: 31.7 dry vol%
- Approach to equilibrium: 78.8%
- Predicted H_2 concentration: 25.0 dry vol%
- Predicted CO concentration: 13.3 dry vol%
- Predicted CH_4 concentration: 1.06 dry vol%

IV. Discussion of Results

IV.1. Anode Gas Conditions

The anode inlet gas conditions and composition of the various species for the cases analyzed are given in Table IV-1. This table indicates that steam reforming, among the three reforming technologies analyzed, gives the highest hydrogen concentrations (70-80% by volume on a dry basis) in the anode feed gas, irrespective of the type of fuel. The lower hydrogen concentrations in the ATR and POX cases (40-50% by volume on a dry basis) are due to the dilution caused by the presence of nitrogen in air.

The presence of nitrogen is also responsible for the formation of ammonia in the ATR and POX cases (Cases 2, 3, 8 and 9). Presence of ammonia in the anode feed gas can cause degradation over time of the phosphoric acid electrolyte in PAFC. The trace quantities of ammonia in the anode gas can be eliminated by passing the anode gas through a phosphoric acid "guard-bed" prior to entering the PAFC.

The small amounts of nitrogen in the anode feed gas in cases involving the combination of steam reforming and PEM (Cases 1, 4 and 5) are caused by the introduction of air into the selective CO oxidation module for carbon monoxide removal.

IV.2. Parasitic Power Requirements

Parasitic power includes power requirements for both the fuel processor and the fuel cell stack. Specific components include fuel pumps, air compressors (cathode air supply and reformer air requirements), fuel cell cooling water pumps and water feed pumps. The recovered power from an expander, if used in the flow arrangement, is credited to the compressor power requirement. An adiabatic efficiency of 70% is assumed for all pumps, compressors and expanders. The parasitic power requirements for the cases analyzed is summarized in Table IV-2.

It is observed that the variation of parasitic power requirement among different reforming technologies and fuel cell types is small. However, the overall system operating pressure has a large effect on the parasitic power requirements.

For pressurized systems (3 atm; cases 1 through 6), the parasitic power requirements amount to about 9-11% of the gross DC power produced. This is primarily because of air compression requirements. Part of the pressure energy in the these cases was recovered in turbo-expanders.

Systems operated under atmospheric pressure (cases 7, 8 and 9) have a parasitic power requirement of about 2.5% of the gross DC power produced.

IV.3. System Efficiency

The various efficiencies for the cases analyzed are summarized in Table IV-3. Figure IV-1 graphically displays the efficiencies for the fuel processor, fuel cell, gross system and net system for the nine cases analyzed. As previously defined in Section III.2, the gross system efficiency is the product of the fuel processor efficiency and the fuel cell efficiency. The difference between gross system efficiency and net system efficiency is the heating value of feed consumed to supply the parasitic power for both the fuel processor and the fuel cell. The detailed results of the case studies are summarized in the Appendix.

The factors affecting the fuel processor, fuel cell and overall system efficiency are discussed below. It should be noted that the observations made below are limited to the process flow schemes, operating conditions and design basis investigated. However, these observations would not be affected if a different set of operating conditions or design basis were selected as long as they are applied consistently across all cases.

Effect of Reforming Technology

Among the three reforming technologies (steam reforming, ATR, and POX), there was not a clear winner for all cases. The relative advantages of one reforming technology over another depended on the fuel, fuel cell, and system pressurization level. In general, the steam reformer offered a significant advantage over ATR or POX in an atmospheric-pressure PAFC system (Cases 7-9), but its advantage was insignificant in the 3-atmosphere PEM system (Cases 1-3).

In comparing reformer technologies, it is important to compare the net system efficiencies. Comparisons of fuel processing efficiencies can be confusing. Fuel processing efficiency can be greater than 100% because of the way it is defined. It is the ratio of the heating value of the anode gas (the output of the fuel processor) divided by the heating value of the fuel input (fuel to the reformer, plus supplemental fuel to the burner, if any). Fuel processing efficiency does not account for the energy inputs to the fuel processor other than the fuel input, i.e., the heat from the anode burner exhaust, and the heat recovered from the PAFC cooling loop. Thus, the fuel processing efficiency reflects not only the reformer technology, but also how effectively it integrates with the chosen fuel cell.

For example, Cases 1 and 6 are both for steam reforming, with methane as fuel, and at 3 atm pressure. The difference is that Case 1 is for a PEM fuel cell, and Case 6 is for a PAFC. The LHV/LHV fuel processing efficiency for Case 1 is 94.2%, while for Case 6 it is 118.4% (as shown in Table IV-3). The higher fuel processing efficiency for the PAFC case is due to the use of the waste heat from the PAFC to raise steam, which is used in the steam reformer. In ATR and POX systems, the fuel processing efficiencies are not as much affected by the choice of fuel cell because the ATR and POX reformers cannot effectively use the waste heat from the fuel cell.

For any given fuel, ATR and POX require higher reforming temperatures than does steam reforming. These high temperatures are achieved by preheating the reactants and by the heat that is released by the ATR and POX reactions which is, in effect, the *in-situ* burning of a fraction of the fuel. For greatest efficiency, this fraction should be minimized which means minimizing the oxygen-to-fuel molar ratio.

As an example, the sensitivity of efficiency to the oxygen-to-fuel molar ratio for POX was investigated using variations of Case 3. In Case 3 (PEM, POX, methane, 3 atm), which uses an oxygen-to-fuel ratio of 0.67, the LHV/LHV fuel processor efficiency is 79.5%, and the net system efficiency is 28.6%. If the oxygen-to-fuel ratio is increased to 1.1, the LHV/LHV fuel processing efficiency drops to 54.4%, and the net system efficiency drops to 18.2%. The additional oxygen causes a greater fraction of the fuel to be burned, resulting in a higher temperature in the POX reactor (1759°C vs. 1105°C) and a smaller amount of hydrogen produced.

The oxygen-to-fuel ratios used here (in the cases presented in Tables IV-1 to IV-3) for the ATR cases are the theoretical minimum values that can be used without soot formation. For the POX cases, the slightly higher oxygen-to-fuel ratios used are the minimum values required to maintain flame stability.

Effect of Fuel

The effect of fuel on net system efficiency is shown by Cases 1, 4, and 5 (Table IV-3). These cases use methane, methanol, and ethanol, respectively, in a 3-atmosphere PEM system with steam reforming. The net system efficiency is significantly higher with methanol (37.5%) than with ethanol (29.7%) or methane (30.7%).

Methanol is an easy fuel to reform requiring low reforming temperatures. On the other hand, methane is considered a "refractory" fuel which means it is difficult to reform and requires higher reforming temperatures. Ethanol reforms partially into methane, carbon monoxide and hydrogen. In the case of the fuel cell application in which it is desirable to minimize the methane content and maximize the hydrogen yield, a reforming temperature greater than that of methane is required for ethanol reforming. Fuels that could be reformed at low temperatures with high hydrogen yield will give high efficiencies.

Effect of Fuel Cell Type

As discussed previously, the type of fuel cell (PAFC or PEM) has a significant effect on the net system efficiency for systems with steam reforming, as illustrated by Cases 1 and 6 (both for methane, 3 atm). Net system efficiencies are 37.0% for PAFC and 30.7% for PEM. The difference is due to fuel cell waste heat utilization in the PAFC system. Heat recovered from the high temperature (190°C) fuel cell is used in the steam reformer, reducing the required amount of supplemental fuel.

For ATR and POX systems, the effect of fuel cell type is minor because adequate heat is already available in the PEM systems; the ATR and POX reformers have no need for the additional waste heat that the higher temperature PAFC can provide.

Effect of Pressure

The effect of pressurization of both the fuel processor and the fuel cell stack on the overall system efficiencies is illustrated by examining cases 6 and 7 in Table IV-3. Both cases utilize methane as the fuel in a steam reformer integrated with a phosphoric acid fuel cell. Case 7 operates at 1 atm pressure and shows a net system efficiency of 35.5%. Case 6 is pressurized to 3 atm and yields a higher net system efficiency of 37%.

Increasing both the fuel processor and fuel cell stack operating pressure raises the partial pressure of hydrogen in the anode feed gas, which boosts the fuel cell's electrochemical efficiency from 38.6% at 1 atm to 43.0% at 3 atm. However, increasing the operating pressure in the fuel processor is accompanied by a reduction in reformer effectiveness as evident by the increased methane slip in the reformate (or anode feed gas). The methane concentration increases from 0.7 dry vol% in the 1 atm case (case 7) to 3.5 dry vol% in the 3 atm case (case 6). In contrast, the hydrogen concentration decreases from 79.2 dry vol% in the 1 atm case to 77.0 dry vol% in the 3 atm case. Consequently, increasing the system operating pressure reduces the heating value efficiency of the fuel cell from 95.6% at 1 atm to 86.3% at 3 atm.

Overall, the net effect of system pressurization is an increase in the fuel cell efficiency from 36.9% at 1 atm to 37.1% at 3 atm, since the fuel cell efficiency is defined as the product of electrochemical efficiency and the heating value efficiency. However, this increase in fuel cell efficiency with further pressurization is expected to level out and eventually decrease.

Pressurization of the steam reformer also has two opposing effects. The heat of reaction for the endothermic steam reforming process is provided by combustion of the hydrogen depleted anode exhaust gas together with supplemental fuel. An increase in system pressure increases methane slip and decreases the amount of hydrogen produced in the reformer. However, on the combustion side, an increase in system pressure improves combustion efficiency and, benefitted by the additional methane from the reduced steam reforming, results in a decreasing supplemental fuel requirement.

The net effect is an improvement in the fuel processing efficiency with increasing pressure (98.2% at 1 atm to 106.7% at 3 atm) up to the point of zero supplemental fuel requirement. Further pressure increase beyond this point would lower the fuel processing efficiency due to decreasing steam reforming effectiveness and lower hydrogen concentrations.

The consequences of system pressurization will be slightly different for systems with POX reformers, as increasing reformer pressure will decrease the methane slip in POX (rather than increase it as in steam reforming). Thus, POX systems are expected to show a much greater benefit from increased system pressure.

Overall System Efficiency

Comparison of the fuel processor, fuel cell, gross system and net system efficiencies as a function of reformer temperature for systems integrated with PEM (Cases 1, 2, and 3) indicates that for a PEM fuel cell using methane as the fuel, the steam reforming technology has an appreciable efficiency advantage over both autothermal and partial oxidation at the fuel processor level. However, the net system efficiency differences among the three competing technologies are less dramatic, with the maximum difference being about 1.5%. Note that the fuel cell efficiency is nearly constant across all fuels and reforming technologies.

IV.4. Weight and Volume

A series of conceptual layout studies were conducted to compare the reforming technology for weight and volume using natural gas as the common fuel:

Figure	IV-2	IV-3	IV-4	IV-5	IV-6	IV-7
Design	#1	#2	#3	#4	#5	#6
Reforming Technology	SR	SR	SR	ATR	POX-1	POX-2
Concept Number	1	2	3	-	1	2
Burner Location	Center	External	External	Top	Center	Center
Reforming Reactor	Packed Annular	Packed Annular	Packed Annular	Packed Torus	Packed Annular	Packed Annular
Shift Reactors	External Annular	Internal Torus	Internal Cylindrical	Internal Cylindrical	Separate Cylindrical	External Annular

Estimates of weight and volume for selected designs, as shown in Table IV-4, were based on preliminary designs which did not have the benefit of detailed thermal analysis, or design optimization in either process design or packaging engineering. It is, however, noticeable that shift reactors and insulation contribute significantly to the weight of the total system in the cases studied. Table IV-5 summarizes the weight and volume power density for the cases studied. It is observed that either the ATR or the POX reforming technology offers the potential for being more compact in weight and volume than the steam reforming technology. However, a significant amount of additional developmental and engineering effort is required to verify this tentative conclusion.

Table IV-6 compiles the weight and volume performance data from prior design or study efforts on small scale fuel processors in fuel cell applications. It should be noted that not all designs have been optimized or integrated for vehicular applications.

Figure IV-8 compares the specific weight and volume for five of the design cases with a Fuji steam methanol reformer in a bus configuration, a Rolls-Royce (R-R) natural gas ATR design for a stationary application and an Analytic Power diesel ATR design. Both the Fuji and R-R designs are for nominal 50 kW, the Analytical Power design is for nominal 10 kW and the Arthur D. Little designs are for nominal 25 kW. The weight estimate in this study for the ATR system is bracketed by the independent Analytical Power and R-R estimates. The R-R and Analytical Power designs indicate a higher specific volume probably because these designs are for applications that are relatively insensitive to the weight and volume of the reformer. The Fuji methanol steam reformer shows the lowest specific weight which is primarily due to the low methanol reforming temperature and the absence of a high temperature shift reactor. The relatively high specific volume of the Fuji design is likely due to the low volume sensitivity of the bus application.

In comparison with these other independent sources, the weight and volume estimates performed in this study appear to be reasonable.

IV.5. Cold Start and Transient Response

Start-up from Cold Conditions

The start-up time required for a given reformer system is determined by the thermal mass of the system. Thermal mass is the product of mass times specific heat which determines the amount of energy input necessary for the system to reach a given design temperature from a given starting temperature. A lower thermal mass will allow a quicker start-up. The thermal mass critical to start-up is the portion of the reformer that has to reach the design temperature in order to initiate the reforming process.

In a steam reformer, the critical thermal mass includes preheaters, catalytic reformer and external reformer burner. For autothermal reforming, this includes preheaters and the catalytic ATR reactor. For partial oxidation reforming, the mass critical for start-up includes the preheaters only. The thermal mass of refractory material and downstream fuel processing equipment is less important to start-up. The POX system will have the lowest start-up time due to its low critical thermal mass, the ATR system is a close second, and the SR system is expected to be the slowest.

Transient Response

The up-transient response of any system depends on how fast fuel can be processed to reach the reforming conditions, how fast the reformate can be delivered to the fuel cell anode and the availability of auxiliary energy storage capacity in the vehicle design.

The fuel delivery time to the reformer is approximately the same for all technologies if additional fuel from storage is used to supplement the anode exhaust. The residence time within the fuel processor subsystem is estimated to be on the order of 0.05-0.2 seconds. This is not likely to noticeably affect the up-transient response.

The down-transient of the fuel processor can be managed by unloading excess power to auxiliary energy storage devices. These storage devices, either ultra-capacitors or batteries, can also be used to enhance the up-transient. The transient response needs to be managed in the vehicle system design. While the POX technology has the potential of being "pedal responsive," we feel that transient response is not a differentiating issue for reforming technologies.

Turndown Capability

The turndown capability of a reformer system is defined as the ratio of the maximum power to the minimum controllable power. In the design of conventional chemical systems, a design capacity based on the most likely demand load is selected for performance optimization. Capacity turn-up or turn-down is generally managed by component design and process controls. Sub-optimal performance will be expected in all capacity levels away from the design point.

The minimum operating capacity is dictated by maintaining acceptable temperature for the critical thermal mass and supplying the minimum required power to the vehicle system. The turndown requirement for either the PAFC bus (2:1) or the PEM passenger car (3:1) is not difficult from the design standpoint for all reforming technologies.

IV.6. Maintainability

Maintainability and life of the fuel processor depend on the complexity of the system. Catalytic systems experience inherent performance degradation even under the carefully controlled conditions in the chemical industry. Catalysts can be permanently damaged due to thermal cycling, poisoning and sintering caused by temperature excursions. Many commonly used reforming and shift catalysts need to be maintained in a reduced state to retain catalytic activity. Exposure to atmospheric oxygen would require regeneration of the catalyst. To prevent moisture condensation the system will need to be purged with an inert gas.

A POX reformer enjoys an advantage over the catalytic steam reformer and the autothermal reforming system because it does not use catalysts. However, catalytic shift reactor systems required in all reforming technologies.

The maintainability issue is common to all reforming technologies and needs to be managed through careful engineering and well-thought out maintenance programs.

IV.7. Safety

Vehicular applications present a potential for a modest safety risk. The presence of hydrogen in an accident scenario could be a major safety concern. This concern is common to all reforming technologies (as well as to on-board hydrogen storage designs).

Any reforming technology integration with PEM fuel cell requires the removal of CO to trace level. The current technology to achieve low CO concentration in the reformate is by selective oxidation which involves the injection of a controlled amount of oxygen into the hydrogen-rich reformate. The introduction of oxygen considerably increases the hazard potential of a PEM fuel cell system integrated with a reformer.

The introduction of oxidant into the ATR or POX reactor incurs a degree of safety risk similar to that of internal combustion systems, unless an excessive amount of oxygen remains in the system.

A rigorous Hazard and Operability (HAZOP) study must be conducted for any selected system to fully quantify the safety and risk implications.

Table IV-1 Case Studies: Anode Gas Conditions

Case		1	2	3	4	5	6	7	8	9
Fuel Cell Type		**PEM**	**PEM**	**PEM**	**PEM**	**PEM**	**PAFC**	**PAFC**	**PAFC**	**PAFC**
Reformer Technology		**SR**	**ATR**	**POX**	**SR**	**SR**	**SR**	**SR**	**ATR**	**POX**
Fuel		**Methane**	**Methane**	**Methane**	**Methanol**	**Ethanol**	**Methane**	**Methane**	**Methane**	**Methane**
Anode Gas Conditions										
Temperature,	C	80	80	80	80	80	190	190	190	190
Pressure,	atm	3	3	3	3	3	3	1	1	1
Total Anode Flow,	kmol/hr	1.27	2.19	2.35	1.38	1.48	1.16	1.33	2.30	2.46
	kg/hr	15.26	40.72	45.56	19.71	22.16	12.52	14.82	42.69	47.46
Inlet Gas Composition (Dry):										
Methane,	ppm	34,429	222	19	0	13,532	34,978	7,432	31	3
Carbon Monoxide,	ppm	0	0	0	88	0	6,116	10,199	585	708
Carbon Dioxide,	mol%	19.1%	16.5%	16.1%	24.3%	24.1%	18.8%	19.0%	16.5%	16.1%
Hydrogen,	mol%	75.4%	45.9%	42.4%	70.1%	66.5%	77.1%	79.2%	46.2%	43.0%
Oxygen,	mol%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
Nitrogen,	mol%	2.0%	37.6%	41.5%	5.5%	8.1%	0.0%	0.0%	37.3%	40.8%
Nitric Oxide,	ppm	0	0	0	0	0	0	0	0	0
Nitrogen Dioxide,	ppm	0	0	0	0	0	0	0	0	0
Nitrous Oxide,	ppm	0	0	0	0	0	0	0	0	0
Ammonia,	ppm	0	74	28	0	0	0	0	27	10
Total,	*mol%*	*100.0%*	*100.0%*	*100.0%*	*100.0%*	*100.0%*	*100.0%*	*100.0%*	*100.0%*	*100.0%*

Table IV-2 Case Studies: Parasitic Power Requirements

Case		**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**
Fuel Cell Type		**PEM**	**PEM**	**PEM**	**PEM**	**PEM**	**PAFC**	**PAFC**	**PAFC**	**PAFC**
Reformer Technology		**SR**	**ATR**	**POX**	**SR**	**SR**	**SR**	**SR**	**ATR**	**POX**
Fuel		**Methane**	**Methane**	**Methane**	**Methanol**	**Ethanol**	**Methane**	**Methane**	**Methane**	**Methane**
Parasitic Power										
Water Feed Pump,	kW	0.001	0.001	0.001	0.001	0.001	0.001	0.000	0.000	0.000
Fuel Feed Pump,	kW	0.000	0.000	0.000	0.001	0.001	0.000	0.000	0.000	0.000
F/C Cooling Water Pump,	kW	0.152	0.179	0.178	0.167	0.171	0.069	0.101	0.102	0.102
Air Compressor/Blower,	kW	5.938	5.900	6.097	4.688	5.963	5.436	0.441	0.494	0.516
Expander,	kW	-4.189	-3.575	-4.471	-2.001	-3.868	-3.836	-	-	-
Total Parasitic Power,	kW	1.9	2.5	1.8	2.9	2.3	1.7	0.5	0.6	0.6
% of Gross DC Power		7.6%	10.0%	7.3%	11.4%	9.1%	6.7%	2.2%	2.4%	2.5%

Table IV-3 Case Studies: Efficiencies

Case		**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**
Fuel Cell Type		**PEM**	**PEM**	**PEM**	**PEM**	**PEM**	**PAFC**	**PAFC**	**PAFC**	**PAFC**
Reformer Technology		**SR**	**ATR**	**POX**	**SR**	**SR**	**SR**	**SR**	**ATR**	**POX**
Fuel		**Methane**	**Methane**	**Methane**	**Methanol**	**Ethanol**	**Methane**	**Methane**	**Methane**	**Methane**
Fuel Reformer Conditions										
Inlet Temperature,	C	700	500	500	260	750	700	700	500	500
Outlet Temperature,	C	700	891	1105	260	750	700	700	890	1105
Pressure,	atm	3	3	3	3	3	3	1	1	1
Steam/Fuel Ratio,	molar	3.00	1.00	0.00	1.50	4.00	3.00	3.00	1.00	0.00
Oxygen/Fuel Ratio,	molar	NA	0.60	0.67	NA	NA	NA	NA	0.60	0.67
Air/Fuel Ratio,	molar	NA	2.86	3.19	NA	NA	NA	NA	2.86	3.19
Oxygen Content in Air,	mol%	NA	0.21	0.21	NA	NA	NA	NA	0.21	0.21
Total Inlet Flow,	kmol/hr	0.98	1.50	1.36	0.73	0.81	1.02	1.00	1.67	1.51
	kg/hr	17.17	36.03	35.13	17.28	19.11	17.93	17.60	40.00	38.97
Efficiencies										
Thermodynamic Efficiency,	E(Th)	81.7%	81.2%	81.1%	81.7%	81.5%	95.2%	92.7%	91.8%	91.7%
Voltage Efficiency,	E(V)	58.9%	57.0%	56.7%	57.5%	57.3%	56.5%	52.1%	52.6%	52.6%
Current Efficiency,	E(I)	80.0%	80.0%	80.0%	80.0%	80.0%	80.0%	80.0%	80.0%	80.0%
Electrochemical Efficiency,	E(E)	38.5%	37.0%	36.8%	37.6%	37.4%	43.0%	38.6%	38.7%	38.6%
Heating Value Efficiency,	E(H)	87.5%	99.8%	100.0%	100.0%	94.0%	86.3%	95.6%	99.8%	99.8%
Fuel Cell Efficiency,	E(FC)	33.7%	36.9%	36.8%	37.6%	35.2%	37.1%	36.9%	38.6%	38.5%
Fuel Processing Efficiency,	E(FP)	98.7%	89.0%	84.0%	112.7%	92.8%	106.7%	98.2%	76.7%	72.8%
Gross System Efficiency,	E(Gross)	33.3%	32.9%	30.9%	42.3%	32.6%	39.6%	36.3%	29.6%	28.1%
Net System Efficiency,	E(Net)	30.7%	29.6%	28.6%	37.5%	29.7%	37.0%	35.5%	28.9%	27.4%
Fuel Processing Efficiency (LHV/LHV)		94.2%	84.2%	79.5%	109.3%	87.9%	118.4%	109.0%	85.0%	80.8%
Power Output										
Gross DC Power,	kW	24.9	25.1	24.9	25.0	25.0	25.0	25.0	25.1	25.0
Net DC Power,	kW	23.0	22.6	23.0	22.1	22.7	23.4	24.5	24.5	24.4
Parasitic Power,	kW	1.9	2.5	1.8	2.9	2.3	1.7	0.5	0.6	0.6

Table IV-4 Case Studies: Weight and Volume for Major Components

Preliminary Fuel Processor Packaging Design Study

Design Number		1	2	3	4	5
Reforming Technolgoy		SR	SR	SR	ATR	POX-1
Fuel		Methane	Methane	Methane	Methane	Methane
Gross DC Power,	kW	24.9	24.9	24.9	25.1	24.9
Net DC Power,	kW	23.0	23.0	23.0	22.6	23.0
Component Weights:						
Pumps,	lb	1	1	1	1	1
Vaporizer/Feed Preheater,	lb	5	5	5	5	5
Anode Exhaust Burner,	lb	25	25	25	20	20
Reforming Reactor:						
Catalyst,	lb	16	16	16	4.5	-
Shell,	lb	25	31	42	1.5	36
HX-8,	lb	1.5	1.5	1.5	-	-
HTS Reactor:						
Catalyst,	lb	30	30	30	52	52
Shell,	lb	20	11	9	15	15
HX-11,	lb	1.5	1.5	1.5	1.5	1.5
HX-10,	lb	-	-	-	1.5	1.5
LTS Reactor:						
Catalyst,	lb	22	22	22	39	39
Shell,	lb	20	11	9	15	13
Prox Reactor:						
Catalyst,	lb	1	1	1	1.5	1.5
Shell,	lb	1	2	2	2.5	2.5
HX-17,	lb	1.5	1.5	1.5	1.5	1.5
Compressor/Expander/Motor,	lb	40	40	40	40	40
Subtotal,	lb	171	160	167	162	190
Misc.(Piping,Controls,etc),	lb	34	32	33	32	38
Refractory,	lb	17	16	17	50	74
Total Estimated F-P Weight,	lb	222	207	216	244	301
	kg	101	94	98	111	137
Total Estimated F-P Volume,*	ft3	3.99	5.08	2.30	2.12	2.51
	liter	113	144	65	60	71

Table IV-5 Weight and Volume Power Density for Design Cases

Preliminary Fuel Processor Packaging Design Study

Design Number		**1**	**2**	**3**	**4**	**5**
Reforming Technolgoy		**SR**	**SR**	**SR**	**ATR**	**POX-1**
Fuel		**Methane**	**Methane**	**Methane**	**Methane**	**Methane**
Gross DC Power,	kW	24.9	24.9	24.9	25.1	24.9
Net DC Power,	kW	23.0	23.0	23.0	22.6	23.0
Total Estimated F-P Weight,	lb	222	207	216	244	301
	kg	101	94	98	111	137
Total Estimated F-P Volume,	ft3	3.99	5.08	2.30	2.12	2.51
	liter	113	144	65	60	71
Specific Weight (Net),	kg/kW	4.37	4.09	4.27	4.89	5.94
Specific Volume (Net),	liter/kW	4.91	6.26	2.83	2.65	3.09
Power Density (Net),	kW/kg	0.23	0.24	0.23	0.20	0.17
Power Density (Net),	kW/liter	0.20	0.16	0.35	0.38	0.32

Table IV-6 Weight and Volume Comparisons of Available Small Scale Fuel Processor Designs

	Fuel	Reformer Type	FC Net Output (kW)	Net Electrical Efficiency (LHV)	Fuel Processor Weight (kg)	Overall Dimensions (cm)	Reformer Volume (liters)	Power Density (kW/kg)	Power Density (kW/liter)	Comments
Fuji Bus	Methanol	Steam Annular Packed Bed	55	38%	200	70D x 100L	384	0.25	0.14	
ERC Bus	Methanol	Steam Annular Packed Bed	28	31%	225	35D x 100L	100	0.12	0.28	Without Shift
GM/LANL	Methanol	Steam Recirc. Bed	60	45-55%	NA	NA	NA	NA	NA	
ERC Army	Methanol	Steam Annular Packed Bed	5	NA	21	23D x 90L	37	0.24	0.13	
Analytic Power	Diesel	Autothermal with cathode regeneration	10	32%	43	25D x 26L	38	0.23	0.26	
Rolls-Royce	Methane	Autothermal	50	28%	350	NA	500	0.14	0.10	Stationary
Hydrogen Burner Technology, Inc.	Methane	POX Burner	4	NA	NA	15D x 20L	3.5	NA	1.10	Reactor Only

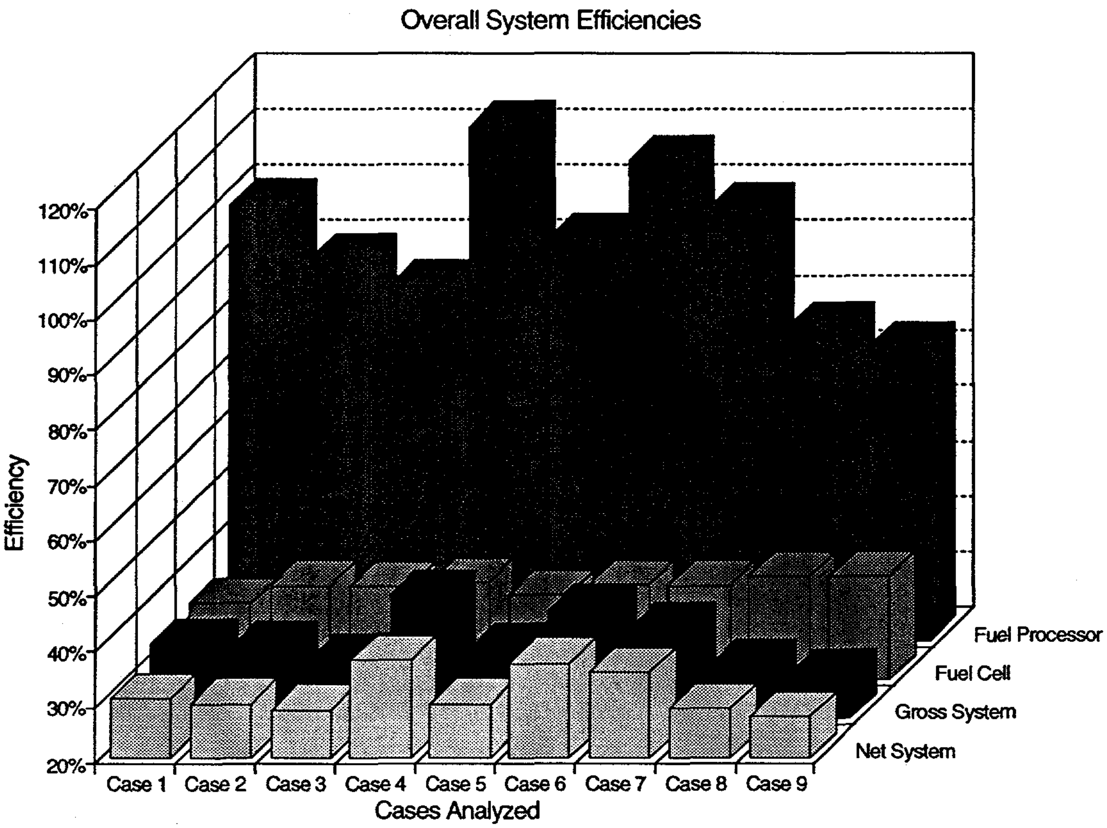


Figure IV-1 Case Studies: Overall System Efficiencies

STEAM REFORMER CONCEPT

(Concept 1)

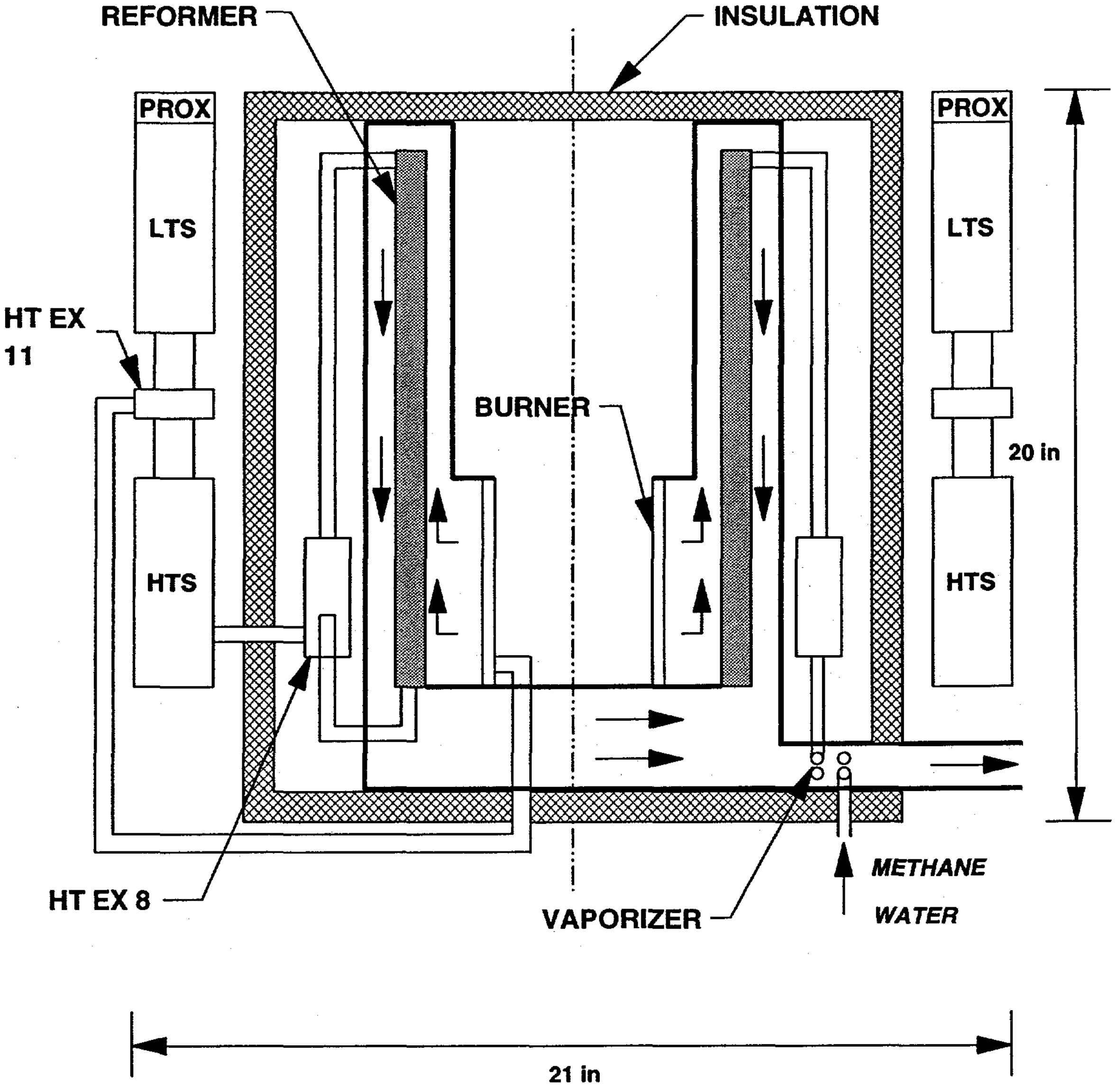


Figure IV-2 Steam Reformer Concept 1

STEAM REFORMING CONCEPT

(Concept 2)

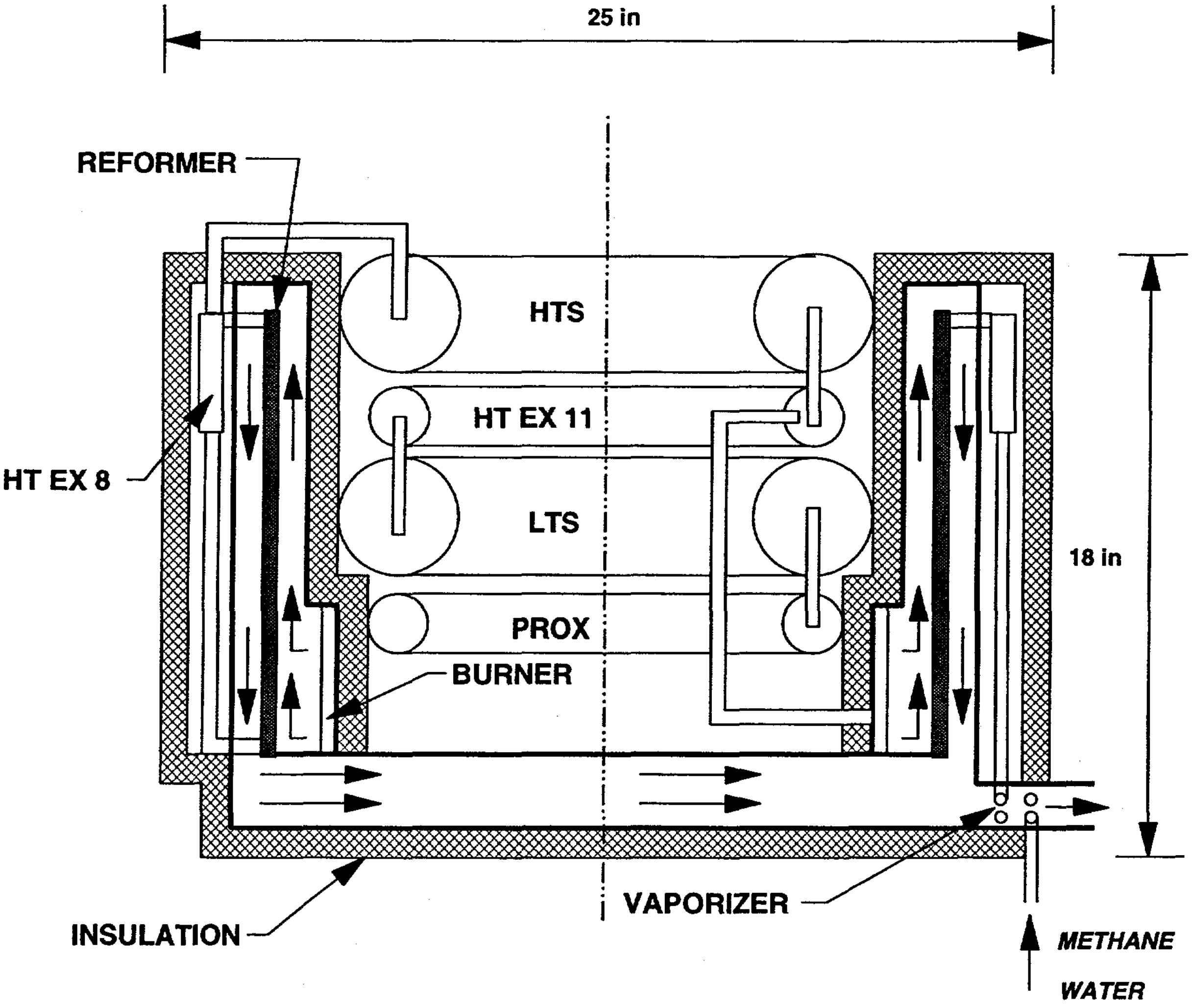


Figure IV-3 Steam Reformer Concept 2

STEAM REFORMING CONCEPT

(Concept 3)

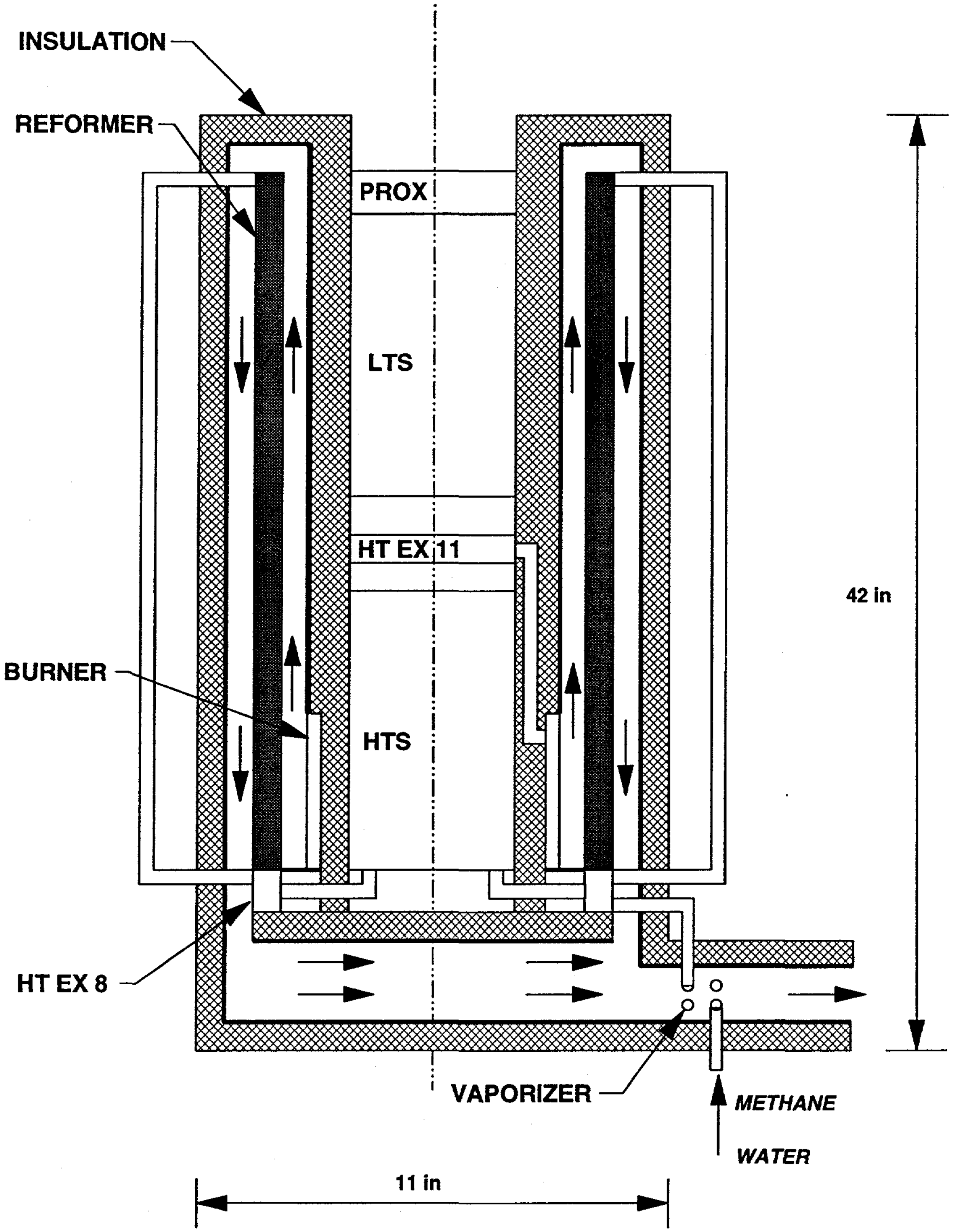


Figure IV-4 Steam Reformer Concept 3

ATR CONCEPT

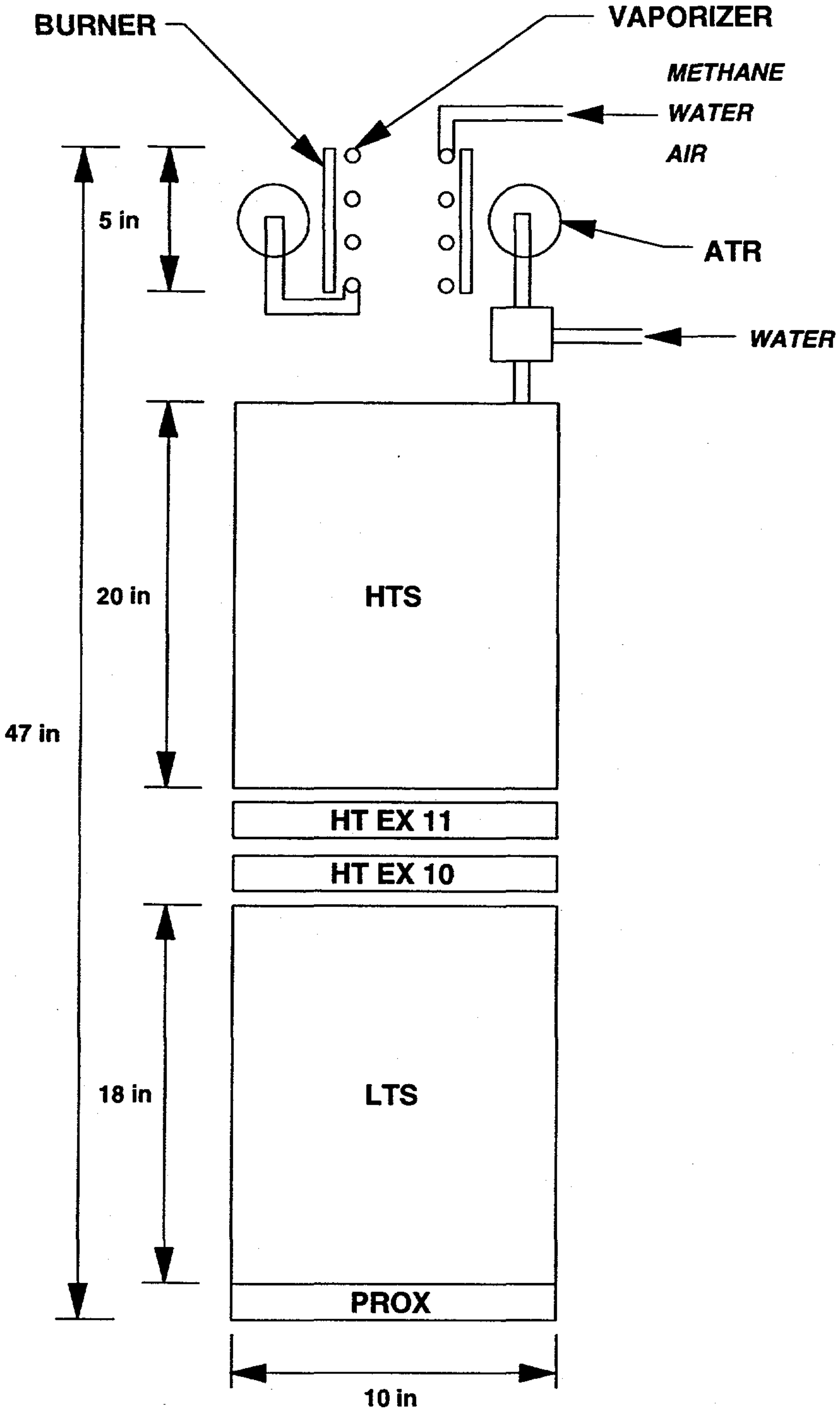


Figure IV-5 Autothermal Reformer Concept

POX CONCEPT 1

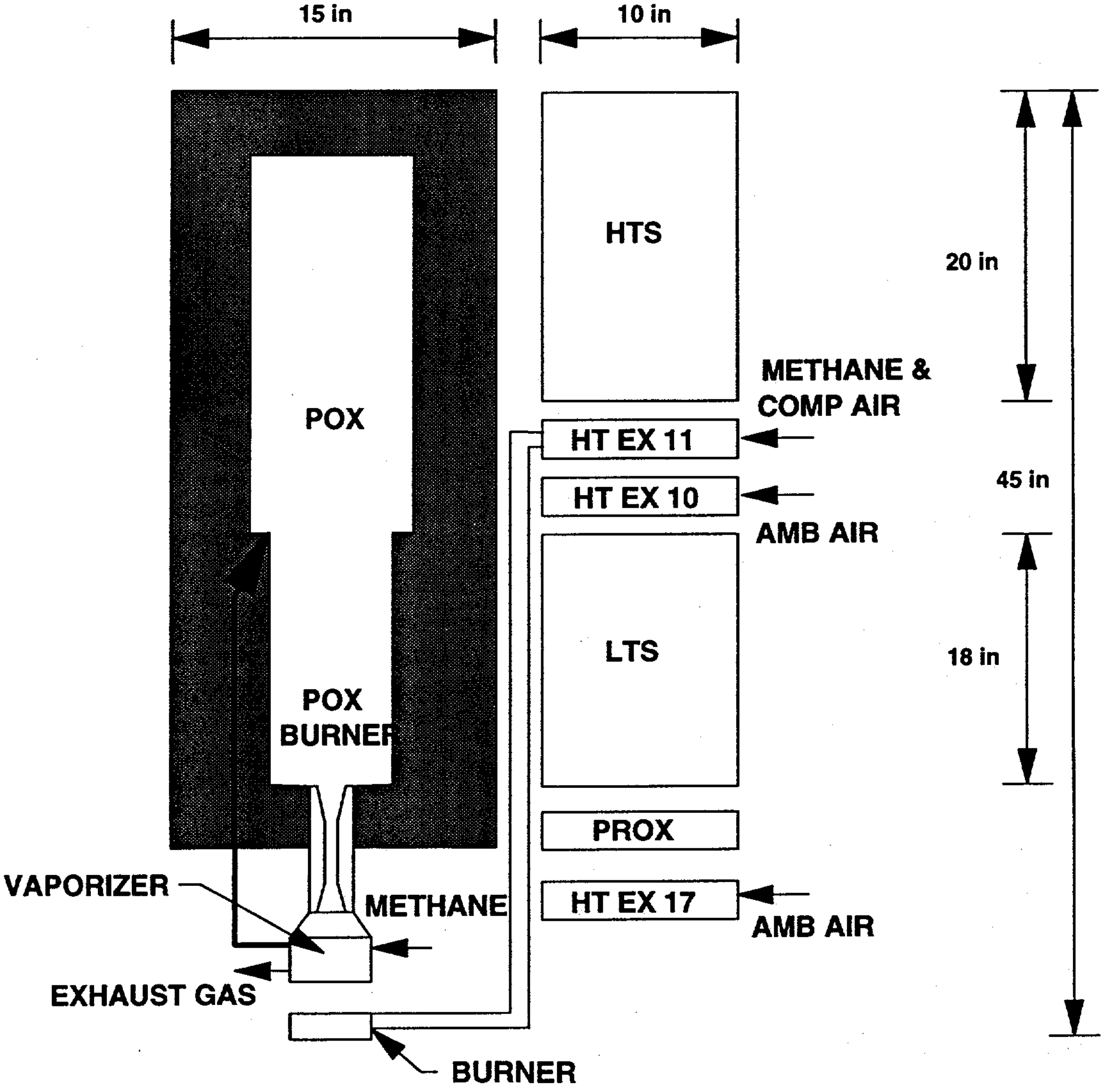


Figure IV-6 Partial Oxidation Reformer Concept 1

POX CONCEPT 2

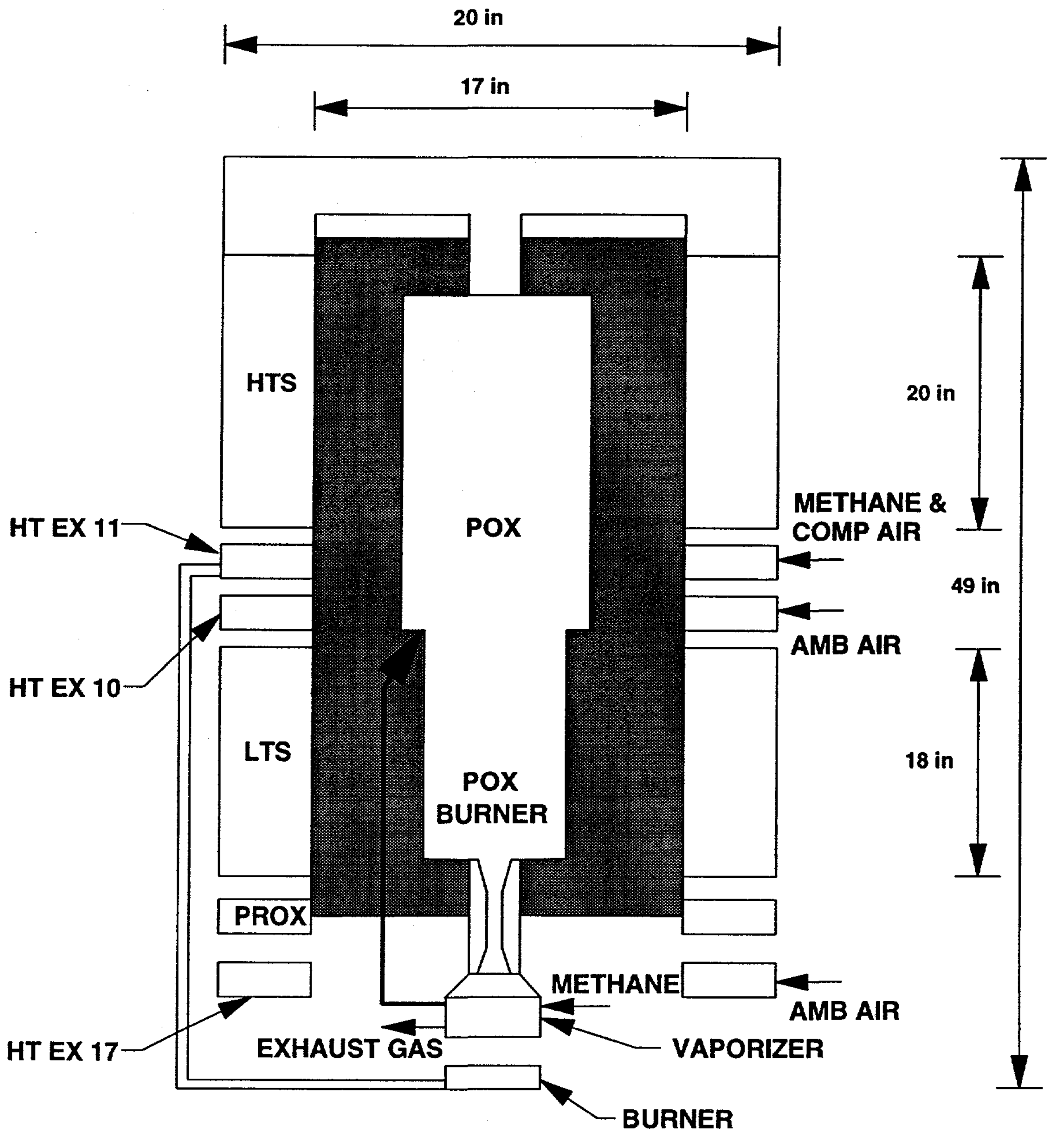


Figure IV-7 Partial Oxidation Reformer Concept 2

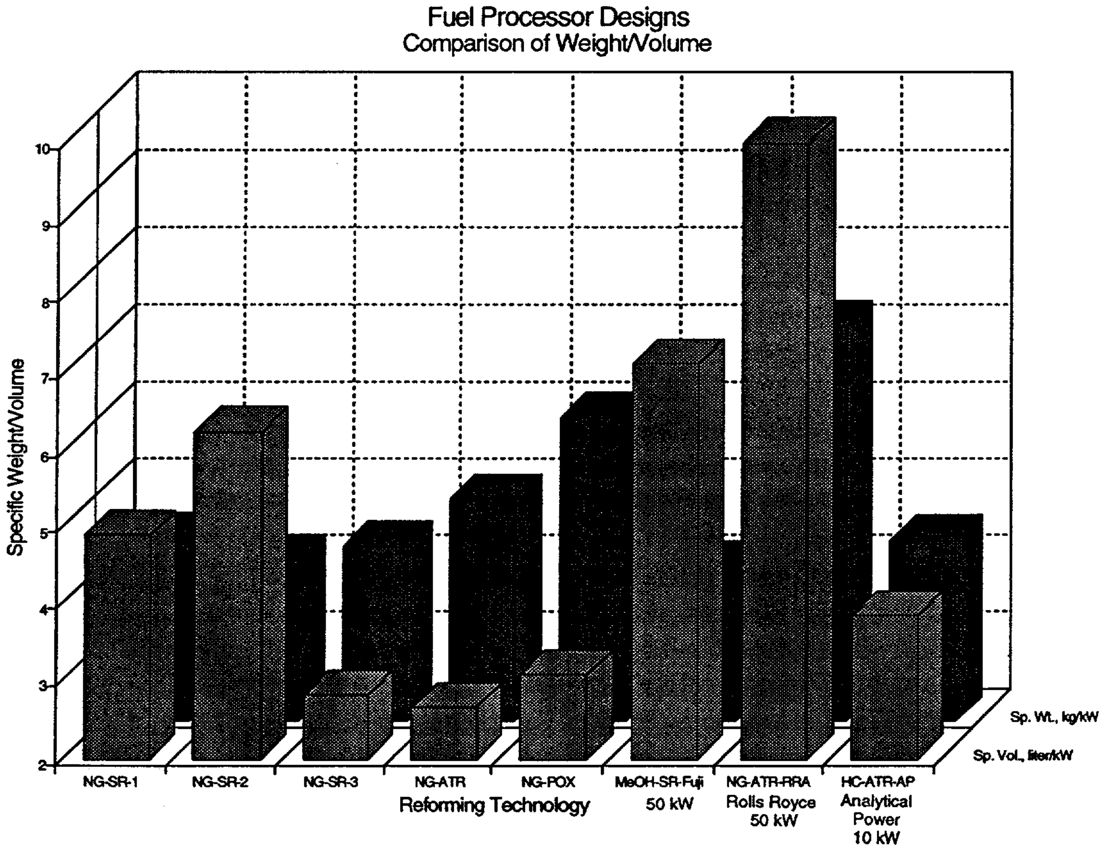


Figure IV-8 Comparison of Weight and Volume in Available Fuel Processor Design

V. Conclusions

A systematic evaluation of reforming technologies for fuel cell systems in transportation applications was conducted in this study. The objective of this study is to evaluate available reformer technologies for the purpose of selecting a suitable multifuel processor for further development and demonstration in fuel cell transportation applications.

The reformer process technologies examined in this study included catalytic steam reforming, non-catalytic partial oxidation (POX) and catalytic partial oxidation (also known as autothermal reforming). Each reforming technology was analyzed as part of an integrated system designed for a specific fuel (methanol, ethanol, or natural gas) and a specific fuel cell: proton exchange membrane (PEM) or phosphoric acid fuel cell (PAFC).

Reforming Technologies

In addition to the inherent differences among reforming technologies, the selection of a multifuel reformer for further development requires the consideration of a myriad of factors which include fuel characteristics, fuel cell type, vehicle application, and development risk.

All reforming technologies require the same set of unit processing steps and share approximately the same level of system complexity. The major technological difference between steam reforming and ATR or POX is the mechanism of providing heat required for the endothermic reforming reactions. In the steam reforming technology, the heat of reaction is supplied through heat transfer surface by an external furnace. In the cases of ATR or POX, the heat of reaction is supplied *in-situ* by oxidizing a portion of the reactant and thus eliminating the requirements for heat transfer surface.

This difference in the heat supply mechanism is suggestive of the potential advantages in weight, volume and start-up time of ATR or POX over the steam reforming technology. The weight, volume and transient responses for the systems examined in this study were assessed qualitatively. The transient response for the steam reforming technology may be the slowest due to the amount of thermal mass that has to be brought to the required reformer condition. The POX technology possesses the potential of being "pedal responsive." However, the transient response can be influenced more effectively by such measures as energy storage devices. It is our opinion that the transient response consideration is not a major differentiating factor for the selection of reforming technology.

Systems using catalysts in the reforming section, including steam reforming and ATR, are slightly more vulnerable to catalyst degradation due to poisoning and thermal or mechanical shocks than the non-catalytic POX technology. However, all systems require the use of catalysts in the water-shift reaction steps. The low temperature shift reactor (LTS) catalyst is particularly susceptible to poisoning by sulfur compounds. Systems using catalysts in the key fuel processing section obviously increase considerably the vehicle maintenance requirement. Relatively speaking, this catalyst maintenance consideration is less severe for POX technology than for either steam reforming or autothermal reforming.

The efficiencies of reformer systems correlate with the fuel processor operating temperature. In turn, the reformer temperature depends on the type of fuel and reformer technology. Lower reforming temperatures yield higher system efficiencies. Steam reforming systems require lower reforming temperature than either ATR or POX. ATR, which uses a catalyst, requires a lower reforming temperature than the non-catalytic POX. As a result, ATR enjoys a slight efficiency advantage over the POX technology. The difference in net system efficiency between ATR, POX, and SR also depends on fuel cell system thermal integration and energy recovery as discussed below.

Fuel Considerations

Methanol is considered an easy fuel to reform whereas methane is considered a "refractory" fuel due to the inherent differences in their thermo-chemical properties. Ethanol is more of a refractory fuel than methane based on the hypothesis that it is reformed to hydrogen and CO via methane as the intermediate product.

For a given fuel processor, methanol requires by far the lowest reforming temperature and ethanol requires the highest reforming temperature. The reforming temperature required for methane is slightly lower than ethanol. Consequently, for any given fuel processor, methanol fuel will yield the highest efficiency, and ethanol will yield the lowest efficiency.

A considerable amount of application know-how exists for natural gas reforming by either SR, ATR or POX technology because it has been the most widely used feedstock in industrial hydrogen production. Methanol has also been investigated as a fuel in steam reforming technology but not for autothermal reforming. Limited experimental data exists for the use of ethanol for any of the reforming technologies. For the steam reforming, and to a lesser extent for autothermal technology, additional catalyst research has to be performed to identify a universal reforming catalyst. Consequently, the non-catalytic POX reformer possesses a lower developmental risk.

Fuel Cell Integration

Net system efficiency depends on fuel cell and fuel processor efficiencies and on fuel cell stack waste heat and anode tail gas utilization and energy recovery. Opportunities for thermal integration are minimal when a high temperature reformer is integrated with a low temperature fuel cell. Therefore, steam reformers will be marginally more efficient than ATR or POX (1%-2% net system efficiency) with pressurized systems such as those using PEM fuel cells. Because of the synergy of steam availability in PAFC and steam demand in a fuel processor based on the steam reforming technology, this combination is more energy efficient. Considering the high weight and volume and long start-up time requirement dictated by the PAFC and SR, such a combination is perceived to be more applicable in heavy duty transportation applications such as locomotive, long-haul trucks and perhaps buses. The system efficiency advantage of steam reforming over POX is considerably larger (about 8 percentage points) in atmospheric systems such as the PAFC system modeled in this analysis.

The combination of non-catalytic partial oxidation and PEM fuel cell, even though lower in efficiency, offers an attractive alternative over others due to its quick start-up and relative fuel insensitivity. Advanced concepts such as oxygen enrichment and power recovery can be applied to boost system performance and efficiency. However, the hardware components required to implement these advanced concepts will increase system complexity and development effort. Based on consumer expectations of quick start-up and transient response, the combination of PEM and POX is thought to be suitable for passenger car applications.

Integration of either a PAFC or PEM fuel cell with an autothermal reformer has the potential of achieving the quick start-up and fuel flexibility of POX and the high efficiency of steam reforming. However, the effort required to identify a suitable multifuel ATR catalyst is uncertain.

Fuel Processor Development Status

Methane steam reforming has been widely used in large-scale industrial hydrogen production. Fuel processor designs using steam reforming technology with methanol as a fuel have been developed by GM/LANL [5] for integration with a PEM powered passenger vehicle and by H-Power for a PAFC powered bus. Steam reformer designs with ethanol as a fuel do not currently exist.

JPL [9] has conducted autothermal reactor design and catalyst studies without fuel cell integration. Analytical Power is developing an ATR system integrated with a PEM fuel cell for small scale applications. Both efforts are focused on distillate fuels such as diesel. In addition, research for ATR catalysts has been reported for methanol and ethanol.

Research on POX for fuel cell application is embryonic. Hydrogen Burner Technology Inc. claims that a proof-of-concept POX burner has been shown to be operable on methane at oxygen-to-fuel ratios between 0.8 and 1, but the design has not been integrated with a fuel cell. For methane POX technology to be practical in fuel cell vehicle applications, the ratio of oxygen-to-fuel must be reduced to 0.6 to 0.7. This improvement of POX technology could be achieved through staged combustion and/or oxygen enrichment in accordance with established combustion theory which reduces the risk associated with POX reformer development.

VI. Recommendations

In order to function acceptably for a multitude of fuels, the fuel processor would have to be designed to accommodate the most demanding operating conditions which would make it over-designed for all other conditions. Such a fuel processor design can not be optimal technically or economically. However, it may be attractive to develop the basic design for a selected fuel processor technology that will require minimal adaptation in hardware for different fuels and fuel cell stacks. Each of these designs can then be optimized for technical performance and production economics for a specific combination of fuel and fuel cell.

Considerable developmental experience has been accumulated for steam reforming of methane and methanol for fuel cell applications. However, a significant void exists for the use of ethanol as a fuel in steam, autothermal or partial oxidation reforming and in development of small-scale methane reformers. Because ethanol represents the greatest challenge of the fuels studied, it is, therefore, appropriate to focus on ethanol as a fuel for fuel cell applications as an intermediate step towards the ultimate DOE objective of developing a multifuel processor. Expanding the resulting fuel processor design to include methane and methanol would be a relatively straightforward task once a working ethanol fuel processor has been demonstrated.

With the exception of the reformer reactor, both ATR and POX fuel processors share a large number of common components. To maximize the benefit of development effort and to reduce the development risk, we recommend a simultaneous development of ATR and POX in the Phase II program, with a high-temperature fuel (ethanol or natural gas) as most beneficial to the advancement of DOE's fuel cell vehicle program.

Bibliography

1. Amphlett, J. C., et. al., "The Operation of a Solid Polymer Fuel Cell: A Parametric Model", Royal Military College of Canada, Kingston Ontario, 1991. Published in Proceedings of the 26th IECEC 2, pp. 624-629, August 1991.

2. Benjamin, T. G., "Handbook of Fuel Cell Performance", Institute of Gas Technology, 1980.

3. British Gas Corporation, "Process for the Manufacture of Methane Containing Gas from Ethanol", European Patent No. 0034407, 1981.

4. Gordon, S., McBride, B. J., "Computer Program for Calculation of Complex Chemical Equilibrium Compositions, Rocket Performance, Incident and Reflected Shocks, and Chapman-Jouguet Detonations", NASA Lewis Research Center, 1976, NASA SP-273.

5. Helms, H. E., Haley, P. J., "Development of a PEM Fuel Cell System for Vehicular Application", SAE International, Future Transportation Technology Conference, California, 1992.

6. Kee, R. J., Rupley, F. M., Miller, J. A., "Chemkin: A FORTRAN Chemical Kinetics Package for the Analysis of Gas-Phase Chemical Kinetics", Sandia Report, 1991. SAND89-800 9B.UC-706.

7. Saini, R., "Computation of Complex Equilibria by the Direct Minimization of the Gibbs Free Energy", M.S. Thesis, Northeastern University, 1989.

8. Voecks, G. E., Flytzani-Stephanopoulos, M., "Conversion of Hydrocarbons for Fuel Cell Applications", Jet Propulsion Laboratory, JPL Publication 82-37, 1981.

9. Watanabe, T., et. al., "Development of Reformer for Fuel Cell System", IHI Engineering Review, Vol. 21 No. 4, October 1988.

Glossary

Fuel Processor	An integrated system of components for producing hydrogen; includes a reformer, shift reactors, and heat exchangers
Preferential Oxidation	Selective catalytic oxidation of trace amounts of carbon monoxide to carbon dioxide, without oxidation of the hydrogen that is also present
Reformate	Hydrogen-rich gas produced by a reformer or fuel processor
Reformer	A reactor for converting a fuel to a hydrogen-rich gas
Shift Reaction	Conversion of carbon monoxide plus water to hydrogen plus carbon dioxide
Stack	The fuel cell physical assembly, consisting of the individual electrochemical cells as well as gas flow distribution manifolds, electrical interconnections, and internal support structures

Abbreviations

ADL	Arthur D. Little, Inc.
ATR	Autothermal Reformer
HHV	Higher Heating Value
HTS	High Temperature Shift
KTI	Kinetics Technology International B.V.
LHV	Lower Heating Value
LTS	Low Temperature Shift
NG	Natural Gas
PAFC	Phosphoric Acid Fuel Cell
PEM	Proton Exchange Membrane
POX	(non-catalytic) Partial Oxidation
PROX	Preferential Oxidation
R-R	Rolls-Royce
SR	Steam Reformer

Symbols

ΔG_r	Free energy change of electrochemical reaction
ΔH_{298}	Enthalpy change of reaction at 298 K
ΔH_c	Heating value of anode gas
ΔH_r	Heating value of hydrogen in anode gas
η	Efficiency
η_E	Electrochemical efficiency (see page 31)
η_{FC}	Fuel cell efficiency (see page 32)
η_{FP}	Fuel processor efficiency (see page 32)
η_{Gross}	Gross efficiency (see page 32)
η_H	Heating value efficiency (see page 31)
η_I	Current efficiency (see page 31)
η_{Net}	Net system efficiency (see page 32)
η_{Th}	Thermodynamic efficiency (see page 30)
η_V	Voltage efficiency (see page 31)
U_f	Fuel utilization: mole percent of the hydrogen in the anode feed that is used in the fuel cell (the rest is exhausted in the hydrogen-depleted anode exhaust stream)
U_o	Oxygen utilization: mole percent of the oxygen entering the cathode that is used in the fuel cell (the rest is exhausted in the oxygen-depleted cathode exhaust stream)

DOE/CE/50343-2

MULTI-FUEL REFORMERS FOR FUEL CELLS USED IN TRANSPORTATION

MULTI-FUEL REFORMERS

PHASE I. FINAL REPORT

Appendix

May 1994

Prepared for

U.S. Department of Energy
Office of Transportation Technologies

Contract No. DE-AC02-92-CE50343

Arthur D Little

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Explanatory Note

As described in pages 30-33 of the main report, the definitions of several of the intermediate efficiencies (thermodynamic, heating value, fuel cell, and fuel processing efficiencies) for PEM fuel cell systems involve the higher heating value of the fuel, while the corresponding definitions for PAFC systems involve the lower heating value. However, the Net System Efficiency is defined the same way for both PEM and PAFC systems, and uses the higher heating value of the fuel.

There is not a fuel cell industry standard for the basis for system efficiency numbers. In general, in the internal combustion engine industry, it is common practice to use the lower heating value in calculating efficiency. In the heating and power generation industries, it is common practice to use the higher heating value. While the higher heating value is used as a common basis in the main report, the case-by-case results presented here also include the net system efficiencies as calculated on a lower heating value basis.

Additional Symbols Used in Appendix

Page number references indicate where terms are defined in the main report.

ASF	Amps per square foot
E(E)	Electrochemical efficiency (see page 31)
E(FC)	Fuel cell efficiency (see page 32)
E(FP)	Fuel processor efficiency (see page 32)
E(Gross)	Gross efficiency (see page 32)
E(H)	Heating value efficiency (see page 31)
E(I)	Current efficiency (see page 31)
E(Net)	Net system efficiency (see page 32)
E(Th)	Thermodynamic efficiency (see page 30)
E(V)	Voltage efficiency (see page 31)

Case 1: Steam Reforming - Methane - PEM

Case 1: Steam Reforming - Methane - PEMFC

Methane Steam Reformer Integrated with PEMFC Design Basis

1. Proton Exchange Membrane Fuel Cell Conditions

Gross DC Power	kW	25
Current Density	ASF	400
Current Density	mA/cm2	431
Temperature	C	80
	K	353
Pressure	atm	3
H2 Utilization	Uf	80%
O2 Utilization	Uo	50%

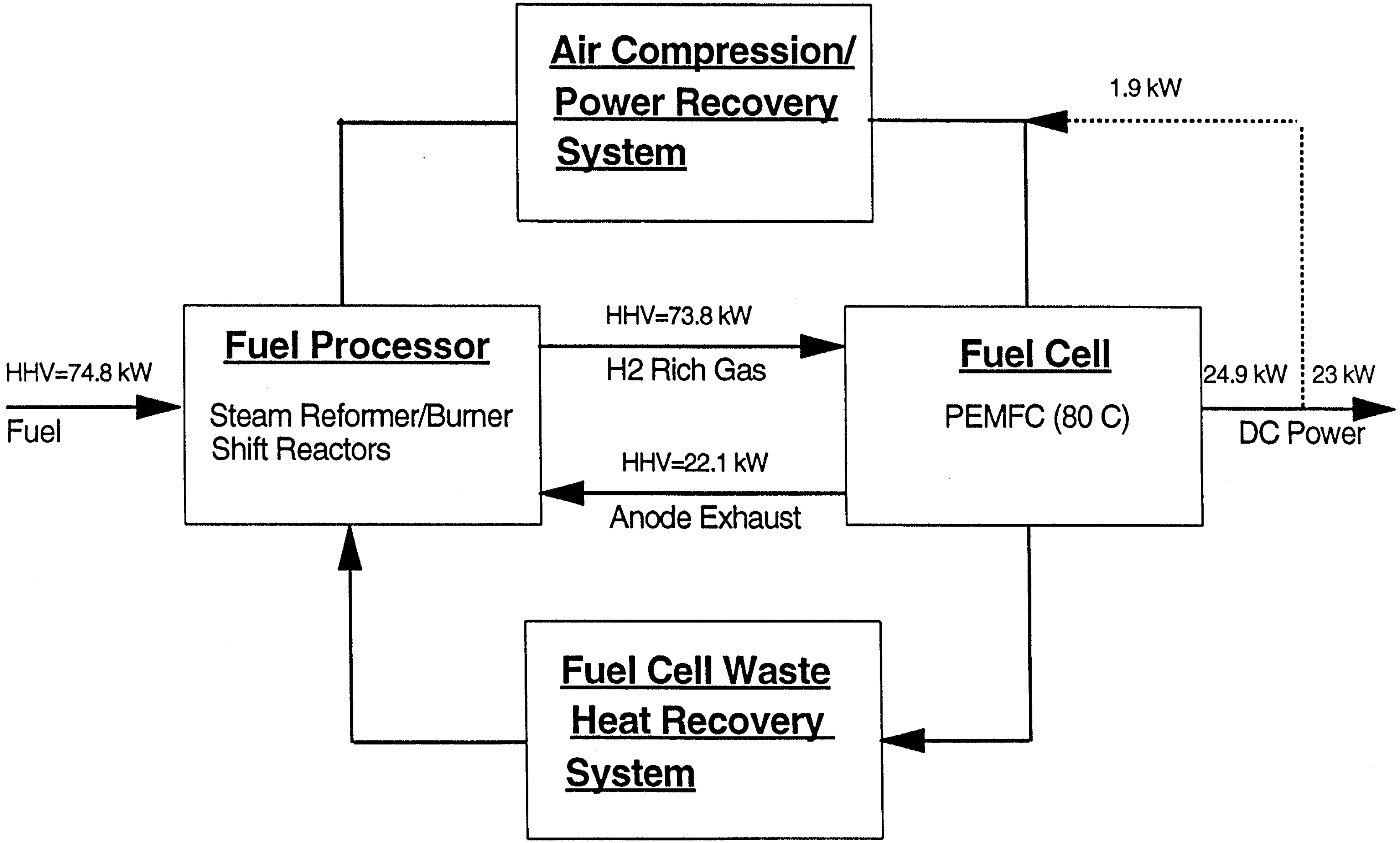
2. Reformer Conditions

Temperature	C	700
	K	973
Pressure	atm	3
Steam/Fuel Ratio	molar	3

3. Air Compression/Power Recovery System Assumptions

Pump Efficiency	70.0%
Compressor Efficiency	70.0%
Expander Efficiency	70.0%

Methane Steam Reformer Integrated with PEMFC: Overall Block Diagram



Air Compression/ Power Recovery System

1.9 kW

HHV=74.8 kW

Fuel

Fuel Processor

Steam Reformer/Burner
Shift Reactors

HHV=73.8 kW

H2 Rich Gas

HHV=22.1 kW

Anode Exhaust

Fuel Cell

PEMFC (80 C)

24.9 kW

23 kW

DC Power

Fuel Cell Waste Heat Recovery System

Fuel Processing Efficiency E(FP) = 98.7 % (94.2 % LHV/LHV)
Gross System Efficiency E(Gross) = 33.3 %
Net System Efficiency E(Net) = 30.7 %

Methane Steam Reformer Integrated with PEMFC

Overall Balance:

Total Fuel to FP	kmol/hr	0.303
	kg/hr	4.853
HHV of Total Fuel to FP	J/hr	-2.7E+08
	kW	74.8
LHV of Total Fuel to FP	J/hr	-2.4E+08
		67.4

Total Flow Into Anode	kmol/hr	1.266
	kg/hr	15.257
HHV of Anode Feed	J/hr	-2.7E+08
	kW	73.8
Flow of Anode Exhaust	kmol/hr	0.611
	kg/hr	13.937
HHV of Anode Exhaust	J/hr	-8.0E+07
	kW	22.1

Gross DC Power	kW	24.9
Net DC Power	kW	23.0
Parsitic Power	kW	1.9

Efficiencies based on HHV of Fuel:

		HHV/HHV	LHV/HHV
Fuel Processing Efficiency	E(FP)	98.7%	84.9%
Gross System Efficiency	E(Gross)	33.3%	
Net System Efficiency	E(Net)	30.7%	

Efficiencies based on LHV of Fuel:

		HHV/LHV	LHV/LHV
Fuel Processing Efficiency	E(FP)	109.6%	94.2%
Gross System Efficiency	E(Gross)	36.9%	
Net System Efficiency	E(Net)	34.1%	

Methane Steam Reformer Integrated with PEMFC Fuel Processor Conditions

A. Reformer

Temperature	C	700
	K	973
Pressure	atm	3
Steam/Fuel Ratio	molar	3
Total Inlet Flow	kmol/hr	0.980
	kg/hr	17.171

Inlet Composition:	***kmol/hr***	***mol%***
Water	0.735	75.0%
Methane	0.245	25.0%
Total	*0.980*	*100.0%*

Outlet Composition:	***kmol/hr***	***mol%***	***mol%(Dry)***
Water	0.430	30.8%	0.0%
Methane	0.037	2.7%	3.9%
Carbon Monoxide	0.110	7.9%	11.4%
Carbon Dioxide	0.098	7.0%	10.1%
Hydrogen	0.720	51.6%	74.6%
Total	*1.395*	*100.0%*	*100.0%*

Methane Steam Reformer Integrated with PEMFC Fuel Processor Conditions

B. Burner:

Inlet Temperature	C	302
Outlet Temperature	C	547
Pressure	atm	3
Supplemental Fuel	kmol/hr	0.058
	kg/hr	0.922
Air Flow	kmol/hr	1.550
	kg/hr	44.718
Total Inlet Flow	kmol/hr	2.219
	kg/hr	59.577

Inlet Composition:	***kmol/hr***	***mol%***	***mol%(Dry)***
Water	0.180	8.1%	0.0%
Methane	0.095	4.3%	4.7%
Carbon Monoxide	0.000	0.0%	0.0%
Carbon Dioxide	0.208	9.4%	10.2%
Hydrogen	0.164	7.4%	8.0%
Oxygen	0.326	14.7%	16.0%
Nitrogen	1.247	56.2%	61.2%
Nitric Oxide	0.000	0.0%	0.0%
Nitrogen Dioxide	0.000	0.0%	0.0%
Nitrous Oxide	0.000	0.0%	0.0%
Total	*2.219*	*100.0%*	*100.0%*

Outlet Composition:	***kmol/hr***	***mol%***	***mol%(Dry)***
Water	0.534	25.0%	0.0%
Methane	0.000	0.0%	0.0%
Carbon Monoxide	0.000	0.0%	0.0%
Carbon Dioxide	0.302	14.2%	18.9%
Hydrogen	0.000	0.0%	0.0%
Oxygen	0.054	2.5%	3.4%
Nitrogen	1.247	58.3%	77.8%
Nitric Oxide	0.000	0.0%	0.0%
Nitrogen Dioxide	0.000	0.0%	0.0%
Nitrous Oxide	0.000	0.0%	0.0%
Total	*2.137*	*100.0%*	*100.0%*

Methane Steam Reformer Integrated with PEMFC Fuel Processor Conditions

C. High Temperature Shift (HTS) Reactor:

Inlet Temperature	C	500
Outlet Temperature	C	531
Pressure	atm	3
Total Inlet Flow	kmol/hr	1.395
	kg/hr	17.172

Outlet Composition:	***kmol/hr***	***mol%***	***mol%(Dry)***
Water	0.389	27.9%	0.0%
Methane	0.037	2.7%	3.7%
Carbon Monoxide	0.069	5.0%	6.9%
Carbon Dioxide	0.138	9.9%	13.7%
Hydrogen	0.761	54.5%	75.6%
Total	*1.395*	*100.0%*	*100.0%*

D. Low Temperature Shift (LTS) Reactor:

Inlet Temperature	C	150
Outlet Temperature	C	209
Pressure	atm	3
Total Inlet Flow	kmol/hr	1.395
	kg/hr	17.172

Outlet Composition:	***kmol/hr***	***mol%***	***mol%(Dry)***
Water	0.323	23.1%	0.0%
Methane	0.037	2.7%	3.5%
Carbon Monoxide	0.003	0.2%	0.3%
Carbon Dioxide	0.205	14.7%	19.1%
Hydrogen	0.827	59.3%	77.2%
Total	*1.395*	*100.0%*	*100.0%*

Methane Steam Reformer Integrated with PEMFC Fuel Processor Conditions

E. PROX Reactor:

Inlet Temperature	C	207
Outlet Temperature	C	270
Pressure	atm	3
Air Flow	kmol/hr	0.028
	kg/hr	0.813
Total Inlet Flow	kmol/hr	1.423
	kg/hr	17.985

Inlet Composition:	*kmol/hr*	*mol%*	*mol%(Dry)*
Water	0.323	22.7%	0.0%
Methane	0.037	2.6%	3.4%
Carbon Monoxide	0.003	0.2%	0.3%
Carbon Dioxide	0.205	14.4%	18.6%
Hydrogen	0.827	58.1%	75.2%
Oxygen	0.006	0.4%	0.5%
Nitrogen	0.022	1.6%	2.0%
Nitric Oxide	0.000	0.0%	0.0%
Nitrogen Dioxide	0.000	0.0%	0.0%
Nitrous Oxide	0.000	0.0%	0.0%
Total	*1.423*	*100.0%*	*100.0%*

Outlet Composition:	*kmol/hr*	*mol%*	*mol%(Dry)*
Water	0.332	23.4%	0.0%
Methane	0.037	2.6%	3.4%
Carbon Monoxide	0.000	0.0%	0.0%
Carbon Dioxide	0.208	14.6%	19.1%
Hydrogen	0.819	57.8%	75.4%
Oxygen	0.000	0.0%	0.0%
Nitrogen	0.022	1.6%	2.0%
Nitric Oxide	0.000	0.0%	0.0%
Nitrogen Dioxide	0.000	0.0%	0.0%
Nitrous Oxide	0.000	0.0%	0.0%
Total	*1.417*	*100.0%*	*100.0%*

Methane Steam Reformer Integrated with PEMFC Fuel Cell Conditions (Proton Exchange Membrane)

Anode:

Temperature	C	80
Pressure	atm	3
Total Anode Flow	kmol/hr	1.266
	kg/hr	15.257

Inlet Composition:	*kmol/hr*	*mol%*	*mol%(Dry)*
Water	0.180	14.2%	0.0%
Methane	0.037	3.0%	3.4%
Carbon Monoxide	0.000	0.0%	0.0%
Carbon Dioxide	0.208	16.4%	19.1%
Hydrogen	0.819	64.7%	75.4%
Oxygen	0.000	0.0%	0.0%
Nitrogen	0.022	1.8%	2.0%
Nitric Oxide	0.000	0.0%	0.0%
Nitrogen Dioxide	0.000	0.0%	0.0%
Nitrous Oxide	0.000	0.0%	0.0%
Total	*1.266*	*100.0%*	*100.0%*

Cathode:

Temperature	C	80
Pressure	atm	3
Total Cathode Flow	kmol/hr	3.237
	kg/hr	92.096

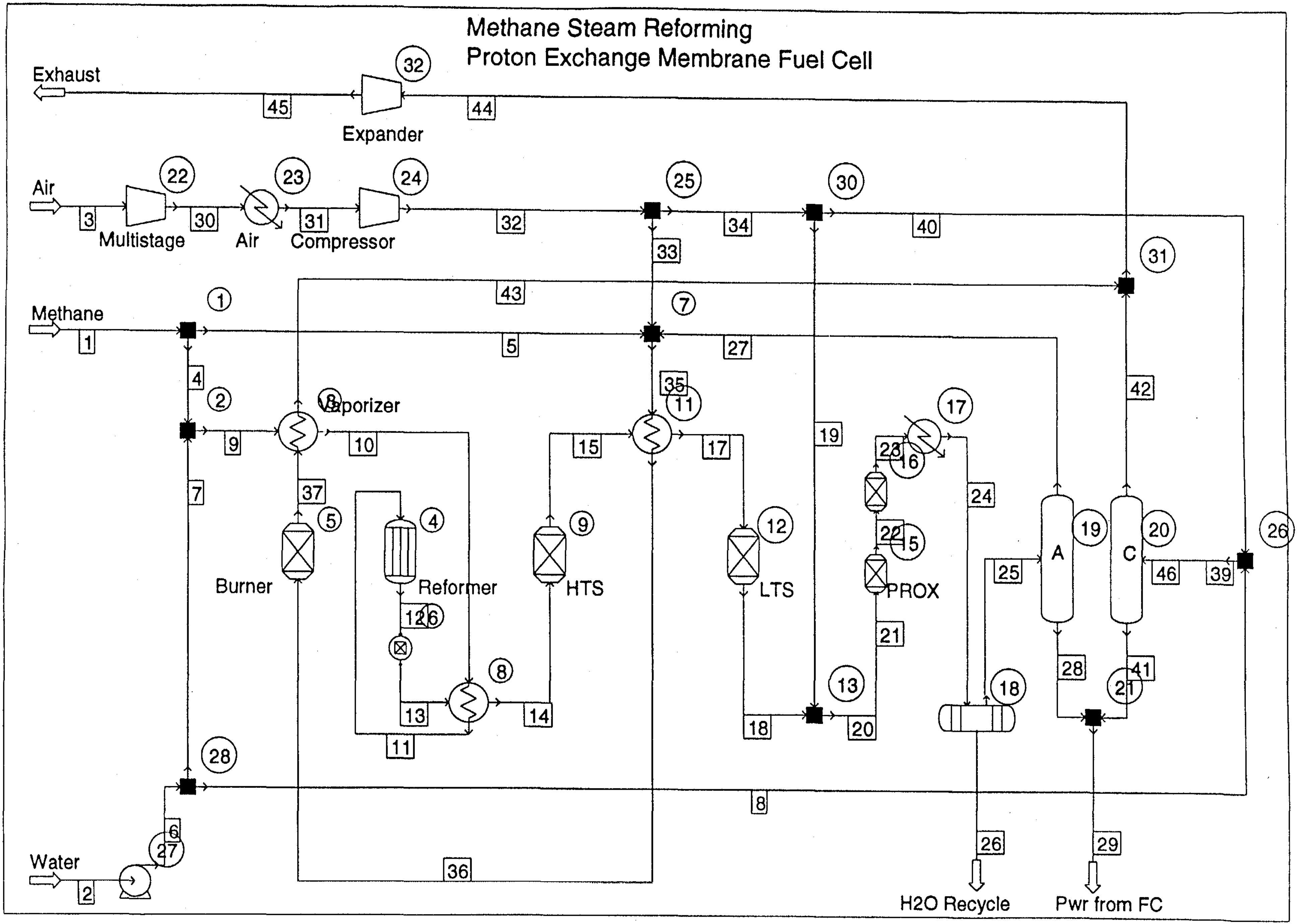
Inlet Composition:	*kmol/hr*	*mol%*
Oxygen	0.655	20.2%
Nitrogen	2.464	76.1%
Water	0.118	3.7%
Total	*3.237*	*100.0%*

Methane Steam Reformer Integrated with PEMFC Air Compression/Power Recovery System

Water Feed Pump	kW	0.001
FC Cooling Water Pump	kW	0.152
Air Compressor	kW	5.938
Expander	kW	-4.189
Total Parasitic Power	kW	1.9
% of Gross DC Power		7.6%

Methane Steam Reformer Integrated with PEMFC Efficiencies

Thermodynamic Efficiency	E(Th)	81.7%
Voltage Efficiency	E(V)	58.9%
Current Efficiency	E(I)	80.0%
Electrochemical Efficiency	E(E)	38.5%
Heating Value Efficiency	E(H)	87.5%
Fuel Cell Efficiency	E(FC)	33.7%
Fuel Processing Efficiency	E(FP)	98.7%
Gross System Efficiency	E(Gross)	33.3%
Net System Efficiency	E(Net)	30.7%
Gross DC Power	kW	24.9
Net DC Power	kW	23.0
Parasitic Power	kW	1.9

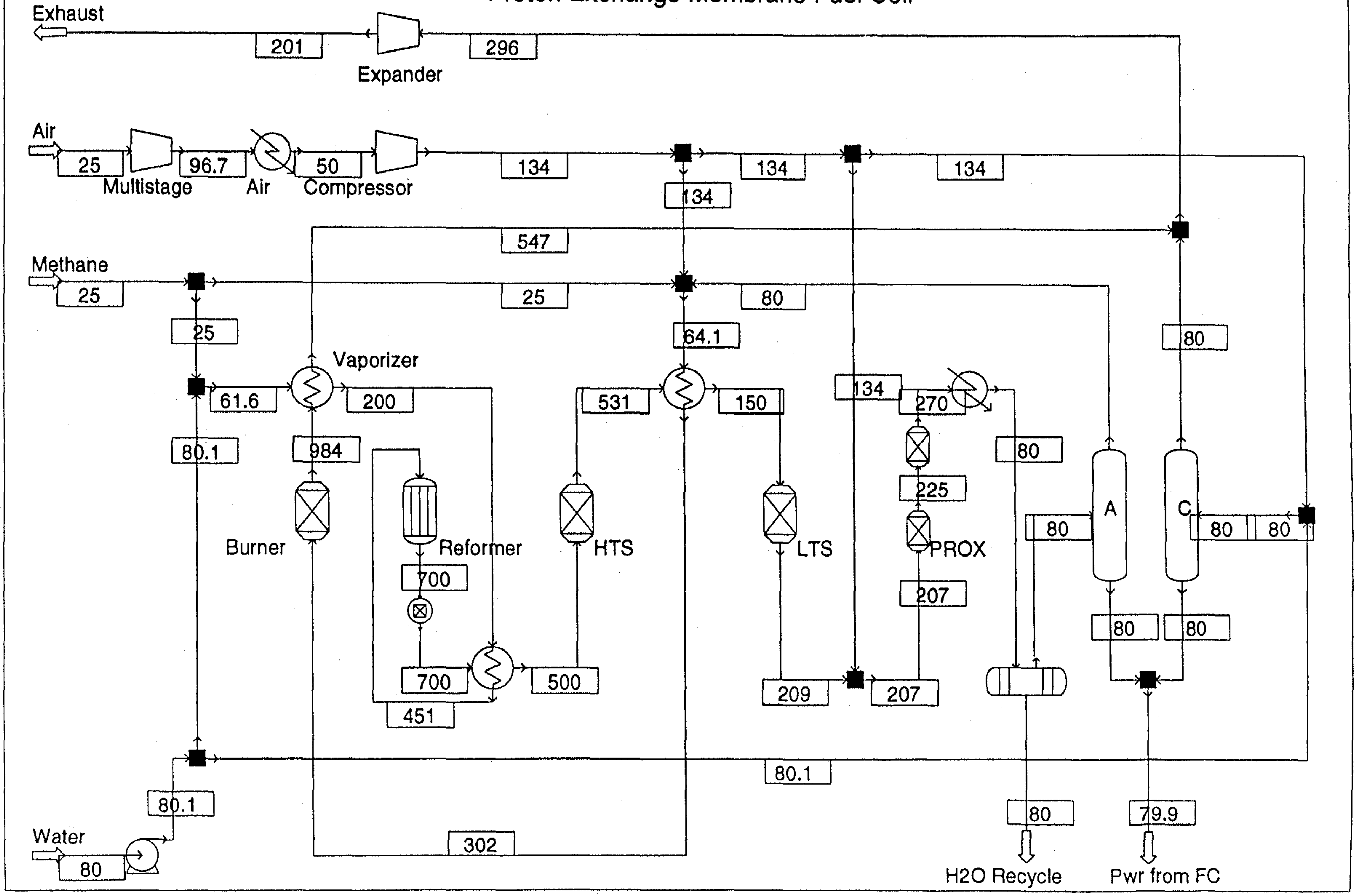


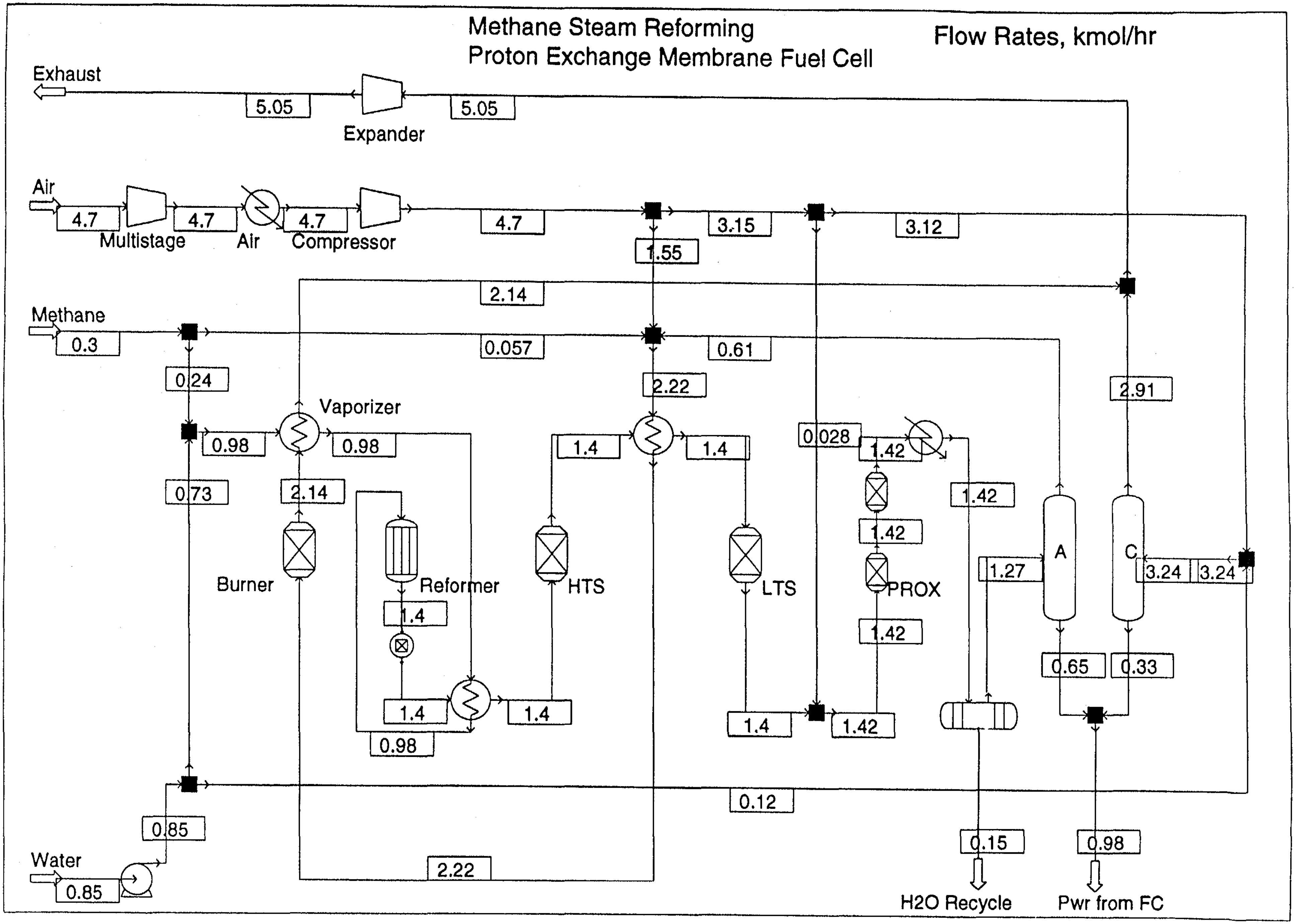
Methane Steam Reforming
Proton Exchange Membrane Fuel Cell

For simulation: numbers in boxes are stream numbers
numbers in circles are component numbers

Methane Steam Reforming
Proton Exchange Membrane Fuel Cell

Temperatures, C




Methane Steam Reforming
Proton Exchange Membrane Fuel Cell
Flow Rates, kmol/hr
Exhaust
5.05
Expander
5.05
Air
4.7
Multistage
4.7
Air
4.7
Compressor
4.7
3.15
1.55
3.12
2.14
Methane
0.3
0.057
0.61
0.24
2.22
2.91
Vaporizer
0.98
0.98
1.4
1.4
0.028
1.42
1.42
0.73
2.14
Burner
Reformer
HTS
LTS
1.42
PROX
A
C
1.27
3.24
3.24
1.4
1.4
1.4
1.4
1.42
1.42
0.65
0.33
0.98
0.12
0.85
Water
0.85
2.22
0.15
0.98
H2O Recycle
Pwr from FC

Case 2: Autothermal Reforming - Methane - PEM

Case 2: Autothermal Reforming - Methane - PEMFC

Methane Autothermal Reforming Integrated with PEMFC Design Basis

1. Proton Exchange Membrane Fuel Cell Conditions

Gross DC Power	kW	25
Current Density	ASF	400
Current Density	mA/cm2	431
Temperature	C	80
	K	353
Pressure	atm	3
H2 Utilization	Uf	80%
O2 Utilization	Uo	50%

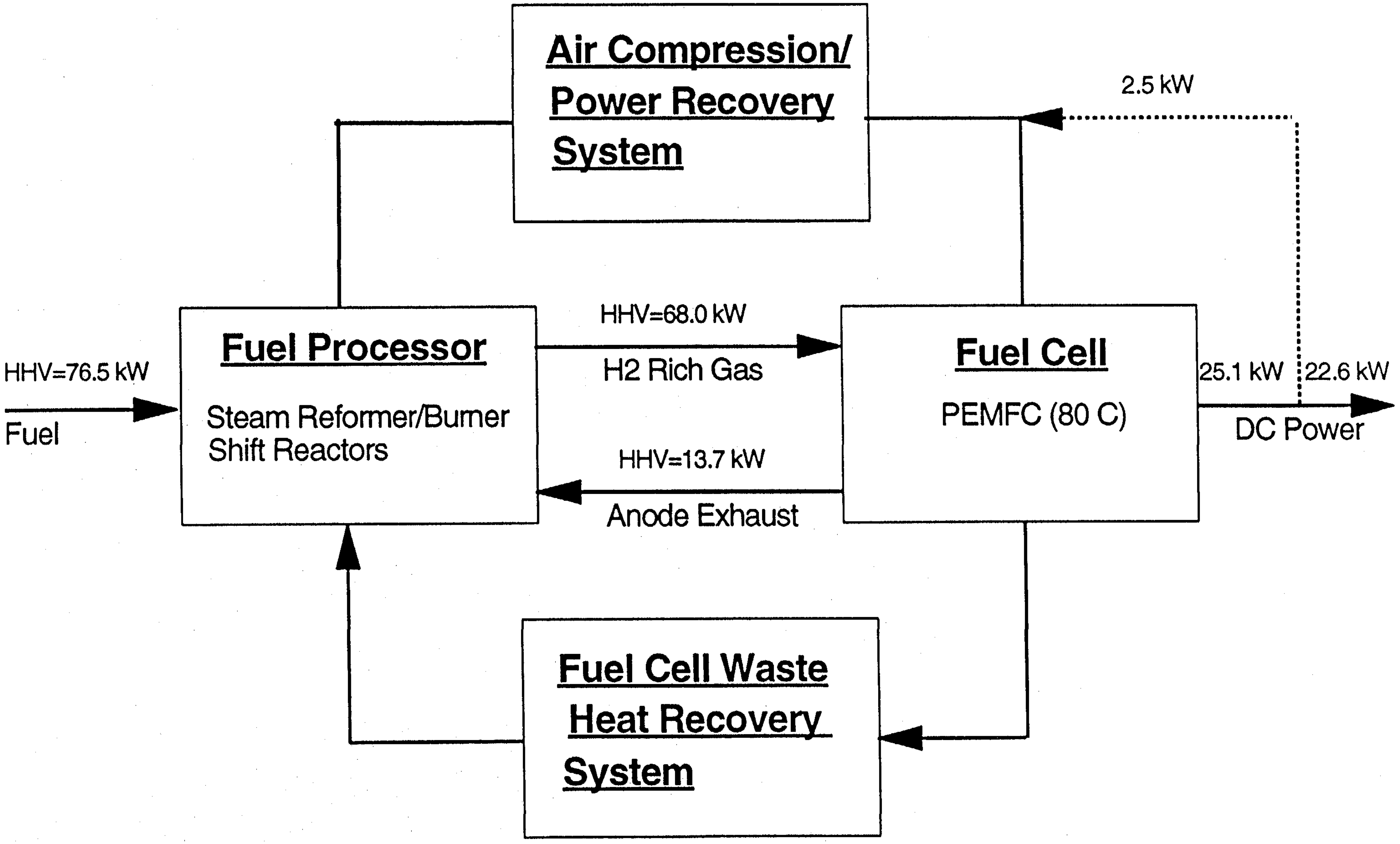
2. Autothermal Reforming Conditions

Temperature	C	Adiabatic Reactor
Pressure	atm	3
Steam/Fuel Ratio	molar	1
Oxygen/Fuel Ratio	molar	0.6

3. Air Compression/Power Recovery System Assumptions

Pump Efficiency	70.0%
Compressor Efficiency	70.0%
Expander Efficiency	70.0%

Methane Autothermal Reforming Integrated with PEMFC



Air Compression/ Power Recovery System

2.5 kW

HHV=76.5 kW

Fuel

Fuel Processor

Steam Reformer/Burner
Shift Reactors

HHV=68.0 kW

H2 Rich Gas

HHV=13.7 kW

Anode Exhaust

Fuel Cell

PEMFC (80 C)

25.1 kW

22.6 kW

DC Power

Fuel Cell Waste Heat Recovery System

Fuel Processing Efficiency E(FP) = 89.0 % (84.2 % LHV/LHV)
Gross System Efficiency E(Gross) = 32.9 %
Net System Efficiency E(Net) = 29.6 %

Methane Autothermal Reforming Integrated with PEMFC

Overall Balance:

Total Fuel to FP	kmol/hr	0.309
	kg/hr	4.962
HHV of Total Fuel to FP	J/hr	-2.8E+08
	kW	76.5
LHV of Total Fuel to FP	J/hr	-2.5E+08
		68.9
Total Flow Into Anode	kmol/hr	2.186
	kg/hr	40.715
HHV of Anode Feed	J/hr	-2.4E+08
	kW	68.0
Flow of Anode Exhaust	kmol/hr	1.498
	kg/hr	39.328
HHV of Anode Exhaust	J/hr	-4.9E+07
	kW	13.7
Gross DC Power	kW	25.1
Net DC Power	kW	22.6
Parasitic Power	kW	2.5

Efficiencies based on HHV of Fuel:

		HHV/HHV	LHV/HHV
Fuel Processing Efficiency	E(FP)	89.0%	75.9%
Gross System Efficiency	E(Gross)	32.9%	
Net System Efficiency	E(Net)	29.6%	

Efficiencies based on LHV of Fuel:

		HHV/LHV	LHV/LHV
Fuel Processing Efficiency	E(FP)	98.7%	84.2%
Gross System Efficiency	E(Gross)	36.4%	
Net System Efficiency	E(Net)	32.8%	

Methane Autothermal Reforming Integrated with PEMFC Fuel Processor Conditions

A. Autothermal Reforming Reactor

Inlet Temperature	C	500
Outlet Temperature	C	891
Pressure	atm	3
Steam/Fuel Ratio	molar	1.0
Oxygen/Fuel Ratio	molar	0.6
Air/Fuel Ratio	molar	2.9
Oxygen Content in Air	mol%	21%
Total Inlet Flow	kmol/hr	1.502
	kg/hr	36.029

Inlet Composition:	*kmol/hr*	*mol%*
Water	0.309	20.6%
Methane	0.309	20.6%
Oxygen	0.186	12.4%
Nitrogen	0.698	46.5%
Total	1.502	100.0%

Outlet Composition:	*kmol/hr*	*mol%*	*mol%(Dry)*	*ppm (Dry)*
Water	0.293	15.1%	0.0%	-
Methane	0.000	0.0%	0.0%	253
Carbon Monoxide	0.230	11.9%	14.0%	-
Carbon Dioxide	0.079	4.1%	4.8%	-
Hydrogen	0.634	32.8%	38.6%	-
Oxygen	0.000	0.0%	0.0%	-
Nitrogen	0.698	36.1%	42.5%	-
Nitric Oxide	0.000	0.0%	0.0%	0
Nitrogen Dioxide	0.000	0.0%	0.0%	0
Nitrous Oxide	0.000	0.0%	0.0%	0
Ammonia	0.000	0.0%	0.0%	89
Total	1.934	100.0%	100.0%	

Methane Autothermal Reforming Integrated with PEMFC Fuel Processor Conditions

B. Burner:

Inlet Temperature	C	303
Outlet Temperature	C	904
Pressure	atm	3
Supplemental Fuel	kmol/hr	0.000
	kg/hr	0.000
Air Flow	kmol/hr	0.497
	kg/hr	14.341
Total Inlet Flow	kmol/hr	1.996
	kg/hr	53.670

Inlet Composition:	*kmol/hr*	*mol%*	*mol%(Dry)*	*ppm (Dry)*
Water	0.311	15.6%	0.0%	-
Methane	0.000	0.0%	0.0%	247
Carbon Monoxide	0.000	0.0%	0.0%	0
Carbon Dioxide	0.309	15.5%	18.3%	-
Hydrogen	0.172	8.6%	10.2%	-
Oxygen	0.104	5.2%	6.2%	-
Nitrogen	1.099	55.1%	65.2%	-
Nitric Oxide	0.000	0.0%	0.0%	0
Nitrogen Dioxide	0.000	0.0%	0.0%	0
Nitrous Oxide	0.000	0.0%	0.0%	0
Ammonia	0.000	0.0%	0.0%	82
Total	1.996	100.0%	100.0%	

Outlet Composition:	*kmol/hr*	*mol%*	*mol%(Dry)*	*ppm (Dry)*
Water	0.484	25.4%	0.0%	-
Methane	0.000	0.0%	0.0%	0
Carbon Monoxide	0.000	0.0%	0.0%	0
Carbon Dioxide	0.309	16.2%	21.7%	-
Hydrogen	0.000	0.0%	0.0%	0
Oxygen	0.017	0.9%	1.2%	-
Nitrogen	1.099	57.5%	77.1%	-
Nitric Oxide	0.000	0.0%	0.0%	42
Nitrogen Dioxide	0.000	0.0%	0.0%	0
Nitrous Oxide	0.000	0.0%	0.0%	0
Ammonia	0.000	0.0%	0.0%	0
Total	1.910	100.0%	100.0%	

Methane Autothermal Reforming Integrated with PEMFC Fuel Processor Conditions

C. High Temperature Shift (HTS) Reactor:

Inlet Temperature	C	450
Outlet Temperature	C	522
Pressure	atm	3
Total Inlet Flow	kmol/hr	2.460
	kg/hr	45.495

Outlet Composition:	*kmol/hr*	*mol%*	*mol%(Dry)*	*ppm (Dry)*
Water	0.658	26.7%	0.0%	-
Methane	0.000	0.0%	0.0%	231
Carbon Monoxide	0.070	2.8%	3.9%	38,693
Carbon Dioxide	0.239	9.7%	13.3%	-
Hydrogen	0.794	32.3%	44.1%	-
Oxygen	0.000	0.0%	0.0%	-
Nitrogen	0.698	28.4%	38.7%	-
Nitric Oxide	0.000	0.0%	0.0%	0
Nitrogen Dioxide	0.000	0.0%	0.0%	0
Nitrous Oxide	0.000	0.0%	0.0%	0
Ammonia	0.000	0.0%	0.0%	81
Total	2.460	100.0%	100.0%	

D. Low Temperature Shift (LTS) Reactor:

Inlet Temperature	C	150
Outlet Temperature	C	185
Pressure	atm	3
Total Inlet Flow	kmol/hr	2.460
	kg/hr	45.495

Outlet Composition:	*kmol/hr*	*mol%*	*mol%(Dry)*	*ppm (Dry)*
Water	0.589	24.0%	0.0%	-
Methane	0.000	0.0%	0.0%	222
Carbon Monoxide	0.001	0.0%	0.1%	557
Carbon Dioxide	0.308	12.5%	16.5%	-
Hydrogen	0.863	35.1%	46.1%	-
Oxygen	0.000	0.0%	0.0%	-
Nitrogen	0.698	28.4%	37.3%	-
Nitric Oxide	0.000	0.0%	0.0%	0
Nitrogen Dioxide	0.000	0.0%	0.0%	0
Nitrous Oxide	0.000	0.0%	0.0%	0
Ammonia	0.000	0.0%	0.0%	78
Total	2.460	100.0%	100.0%	

Methane Autothermal Reforming Integrated with PEMFC Fuel Processor Conditions

E. PROX Reactor:

Inlet Temperature	C	185
Outlet Temperature	C	198
Pressure	atm	3
Air Flow	kmol/hr	0.010
	kg/hr	0.286
Total Inlet Flow	kmol/hr	2.470
	kg/hr	45.782

Outlet Composition:	*kmol/hr*	*mol%*	*mol%(Dry)*	*ppm (Dry)*
Water	0.592	24.0%	0.0%	-
Methane	0.000	0.0%	0.0%	222
Carbon Monoxide	0.000	0.0%	0.0%	0
Carbon Dioxide	0.309	12.5%	16.5%	-
Hydrogen	0.860	34.9%	45.9%	-
Oxygen	0.000	0.0%	0.0%	-
Nitrogen	0.706	28.6%	37.6%	-
Nitric Oxide	0.000	0.0%	0.0%	0
Nitrogen Dioxide	0.000	0.0%	0.0%	0
Nitrous Oxide	0.000	0.0%	0.0%	0
Ammonia	0.000	0.0%	0.0%	78
Total	2.468	100.0%	100.0%	

Methane Autothermal Reforming Integrated with PEMFC Fuel Cell Conditions (Proton Exchange Membrane)

Anode:

Temperature	C	80
Pressure	atm	3
Total Anode Flow	kmol/hr	2.186
	kg/hr	40.715

Inlet Composition:	*kmol/hr*	*mol%*	*mol%(Dry)*	*ppm (Dry)*
Water	0.311	14.2%	0.0%	-
Methane	0.000	0.0%	0.0%	222
Carbon Monoxide	0.000	0.0%	0.0%	0
Carbon Dioxide	0.309	14.1%	16.5%	-
Hydrogen	0.860	39.3%	45.9%	-
Oxygen	0.000	0.0%	0.0%	-
Nitrogen	0.706	32.3%	37.6%	-
Nitric Oxide	0.000	0.0%	0.0%	0
Nitrogen Dioxide	0.000	0.0%	0.0%	0
Nitrous Oxide	0.000	0.0%	0.0%	0
Ammonia	0.000	0.0%	0.0%	74
Total	2.186	100.0%	100.0%	

Cathode:

Temperature	C	80
Pressure	atm	3
Total Cathode Flow	kmol/hr	3.400
	kg/hr	96.754

Inlet Composition:	*kmol/hr*	*mol%*
Oxygen	0.688	20.2%
Nitrogen	2.588	76.1%
Water	0.124	3.7%
Total	3.400	100.0%

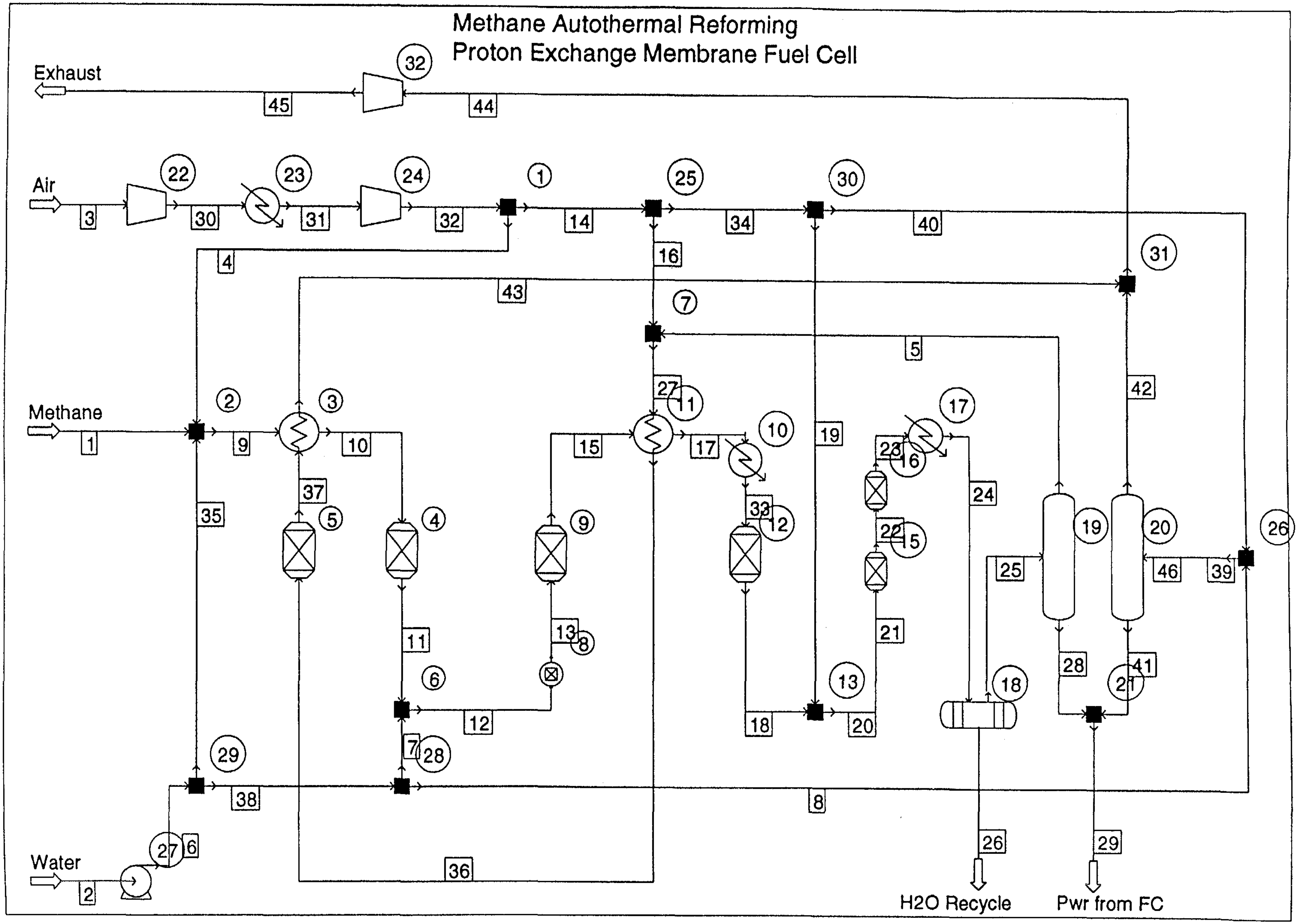
Methane Autothermal Reforming Integrated with PEMFC Air Compression/Power Recovery System

Water Feed Pump	kW	0.001
FC Cooling Water Pump	kW	0.179
Air Compressor	kW	5.900
Expander	kW	-3.575
Total Parasitic Power	kW	2.5
% of Gross DC Power		10.0%

Methane Autothermal Reforming Integrated with PEMFC Efficiencies

Thermodynamic Efficiency	E(Th)	81.2%
Voltage Efficiency	E(V)	57.0%
Current Efficiency	E(I)	80.0%
Electrochemical Efficiency	E(E)	37.0%
Heating Value Efficiency	E(H)	99.8%
Fuel Cell Efficiency	E(FC)	36.9%
Fuel Processing Efficiency	E(FP)	89.0%
Gross System Efficiency	E(Gross)	32.9%
Net System Efficiency	E(Net)	29.6%
Gross DC Power	kW	25.1
Net DC Power	kW	22.6
Parasitic Power	kW	2.5

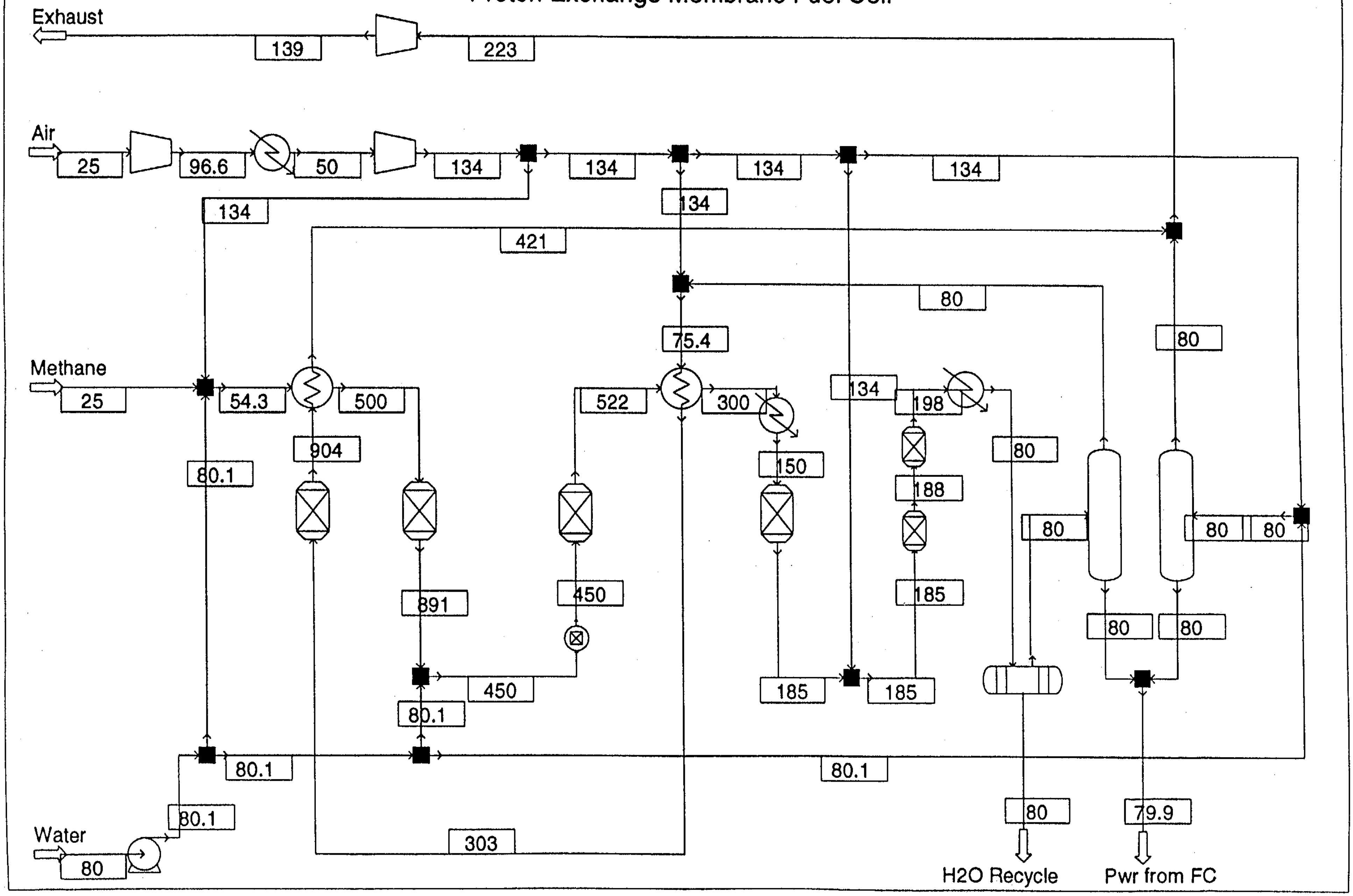
Methane Autothermal Reforming
Proton Exchange Membrane Fuel Cell



For simulation: numbers in boxes are stream numbers
numbers in circles are component numbers

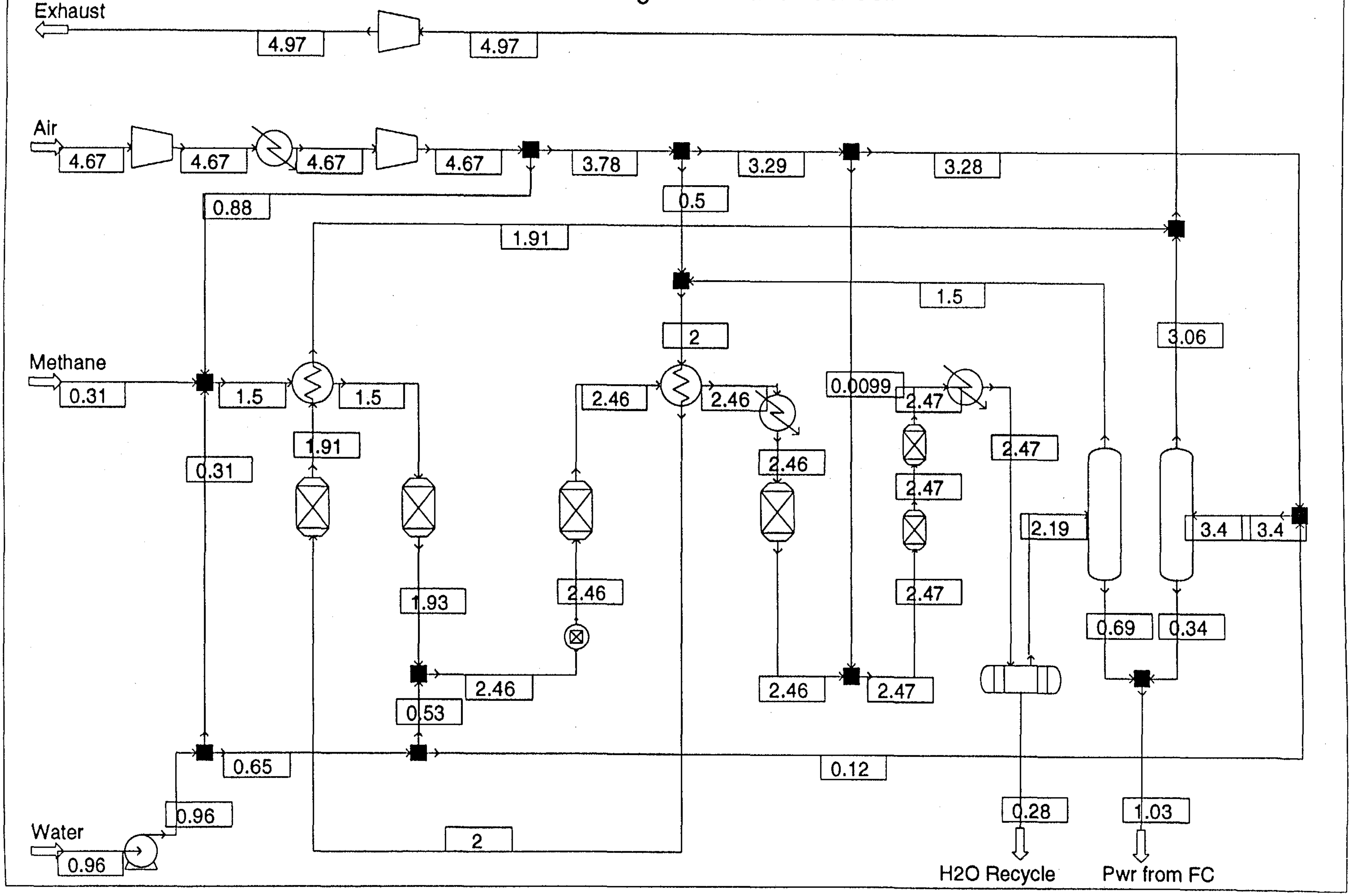
Methane Autothermal Reforming
Proton Exchange Membrane Fuel Cell

Temperatures, C



Methane Autothermal Reforming
Proton Exchange Membrane Fuel Cell

Flow Rates, kmol/hr



Case 3: Partial Oxidation Reforming - Methane - PEM

Case 3: Partial Oxidation - Methane - PEMFC

Methane Partial Oxidation (non-catalytic) Integrated with PEMFC Design Basis

1. Proton Exchange Membrane Fuel Cell Conditions

Gross DC Power	kW	25
Current Density	ASF	400
Current Density	mA/cm2	431
Temperature	C	80
	K	353
Pressure	atm	3
H2 Utilization	Uf	80%
O2 Utilization	Uo	50%

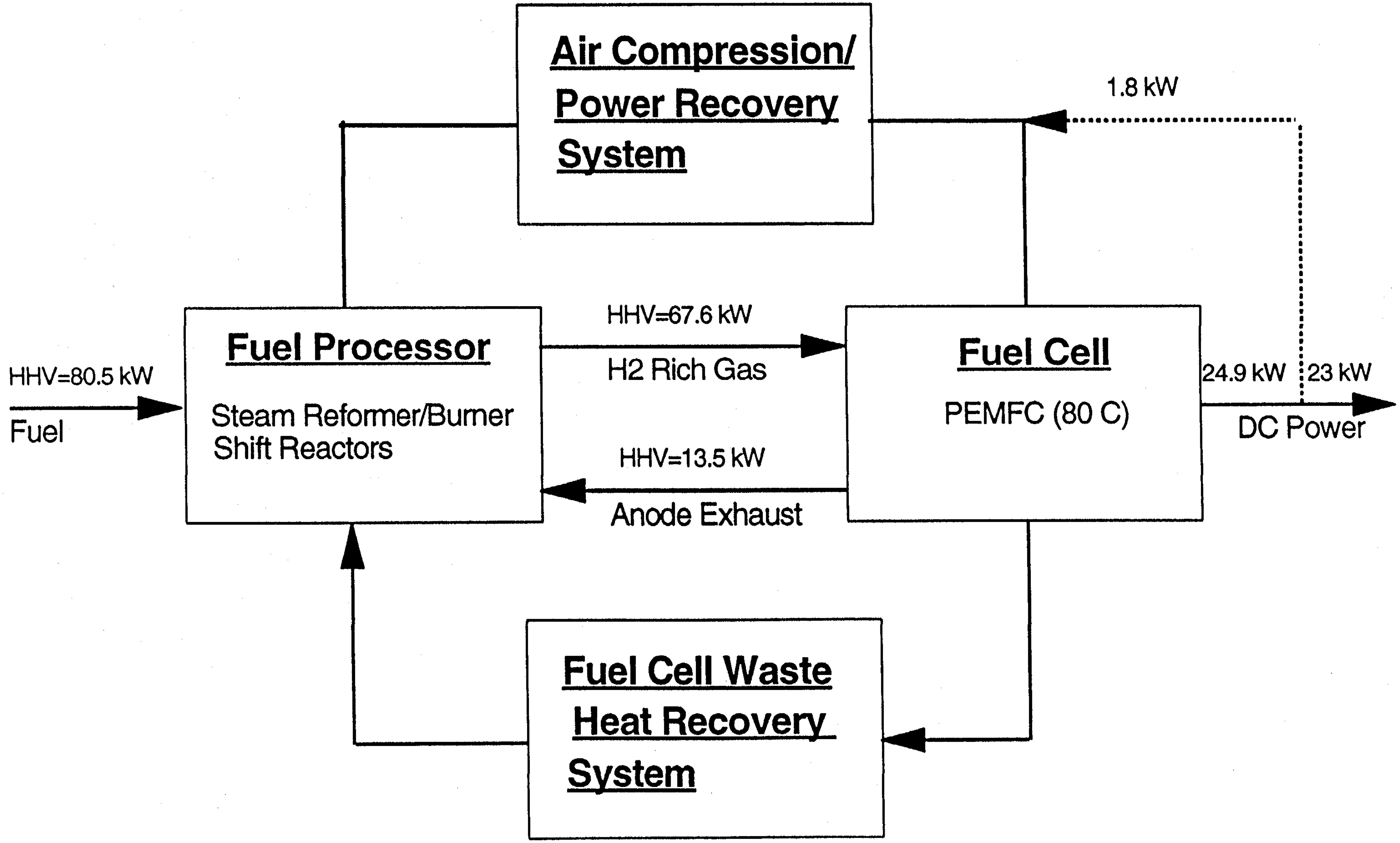
2. Partial Oxidation (non-catalytic) Conditions

Temperature	C	Adiabatic Reactor
Pressure	atm	3
Oxygen/Fuel Ratio	molar	0.67

3. Air Compression/Power Recovery System Assumptions

Pump Efficiency	70.0%
Compressor Efficiency	70.0%
Expander Efficiency	70.0%

Methane Partial Oxidation (non-catalytic) Integrated with PEMFC



HHV=80.5 kW
Fuel

Fuel Processor
Steam Reformer/Burner
Shift Reactors

HHV=67.6 kW
H2 Rich Gas

HHV=13.5 kW
Anode Exhaust

Fuel Cell
PEMFC (80 C)

24.9 kW
23 kW
DC Power

1.8 kW

Air Compression/ Power Recovery System

Fuel Cell Waste Heat Recovery System

Fuel Processing Efficiency E(FP) = 84.0% (79.5% LHV/LHV)
Gross System Efficiency E(Gross) = 30.9%
Net System Efficiency E(Net) = 28.6%

Methane Partial Oxidation (non-catalytic) Integrated with PEMFC

Overall Balance:

Total Fuel to FP	kmol/hr	0.325
	kg/hr	5.221
HHV of Total Fuel to FP	J/hr	-2.9E+08
	kW	80.5
LHV of Total Fuel to FP	J/hr	-2.6E+08
		72.5
Total Flow Into Anode	kmol/hr	2.355
	kg/hr	45.562
HHV of Anode Feed	J/hr	-2.4E+08
	kW	67.6
Flow of Anode Exhaust	kmol/hr	1.670
	kg/hr	44.181
HHV of Anode Exhaust	J/hr	-4.9E+07
	kW	13.5
Gross DC Power	kW	24.9
Net DC Power	kW	23.0
Parsitic Power	kW	1.8

Efficiencies based on HHV of Fuel:

		HHV/HHV	LHV/HHV
Fuel Processing Efficiency	E(FP)	84.0%	71.7%
Gross System Efficiency	E(Gross)	30.9%	
Net System Efficiency	E(Net)	28.6%	

Efficiencies based on LHV of Fuel:

		HHV/LHV	LHV/LHV
Fuel Processing Efficiency	E(FP)	93.2%	79.5%
Gross System Efficiency	E(Gross)	34.3%	
Net System Efficiency	E(Net)	31.8%	

Methane Partial Oxidation (non-catalytic) Integrated with PEMFC Fuel Processor Conditions

A. Partial Oxidation (non-catalytic) Reactor

Inlet Temperature	C	500
Outlet Temperature	C	1105
Pressure	atm	3
Steam/Fuel Ratio	molar	0.00
Oxygen/Fuel Ratio	molar	0.67
Air/Fuel Ratio	molar	3.19
Oxygen Content in Air	mol%	21%
Total Inlet Flow	kmol/hr	1.364
	kg/hr	35.180

Inlet Composition:	*kmol/hr*	*mol%*
Water	0.000	0.0%
Methane	0.325	23.9%
Oxygen	0.218	16.0%
Nitrogen	0.820	60.1%
Total	1.364	100.0%

Outlet Composition:	*kmol/hr*	*mol%*	*mol%(Dry)*	*ppm (Dry)*
Water	0.089	5.0%	0.0%	-
Methane	0.000	0.0%	0.0%	-
Carbon Monoxide	0.304	16.9%	17.8%	-
Carbon Dioxide	0.021	1.2%	1.3%	-
Hydrogen	0.561	31.3%	32.9%	-
Oxygen	0.000	0.0%	0.0%	-
Nitrogen	0.820	45.7%	48.0%	-
Nitric Oxide	0.000	0.0%	0.0%	0
Nitrogen Dioxide	0.000	0.0%	0.0%	0
Nitrous Oxide	0.000	0.0%	0.0%	0
Ammonia	0.000	0.0%	0.0%	34
Total	1.797	100.0%	100.0%	

Methane Partial Oxidation (non-catalytic) Integrated with PEMFC Fuel Processor Conditions

B. Burner:

Inlet Temperature	C	316
Outlet Temperature	C	865
Pressure	atm	3
Supplemental Fuel	kmol/hr	0.000
	kg/hr	0.000
Air Flow	kmol/hr	0.500
	kg/hr	14.425
Total Inlet Flow	kmol/hr	2.170
	kg/hr	58.606

Inlet Composition:	*kmol/hr*	*mol%*	*mol%(Dry)*	*ppm (Dry)*
Water	0.335	15.4%	0.0%	-
Methane	0.000	0.0%	0.0%	-
Carbon Monoxide	0.000	0.0%	0.0%	-
Carbon Dioxide	0.325	15.0%	17.7%	-
Hydrogen	0.171	7.9%	9.3%	-
Oxygen	0.105	4.8%	5.7%	-
Nitrogen	1.233	56.8%	67.2%	-
Nitric Oxide	0.000	0.0%	0.0%	0
Nitrogen Dioxide	0.000	0.0%	0.0%	0
Nitrous Oxide	0.000	0.0%	0.0%	0
Ammonia	0.000	0.0%	0.0%	31
Total	2.170	100.0%	100.0%	

Outlet Composition:	*kmol/hr*	*mol%*	*mol%(Dry)*	*ppm (Dry)*
Water	0.506	24.3%	0.0%	-
Methane	0.000	0.0%	0.0%	-
Carbon Monoxide	0.000	0.0%	0.0%	-
Carbon Dioxide	0.325	15.6%	20.6%	-
Hydrogen	0.000	0.0%	0.0%	-
Oxygen	0.019	0.9%	1.2%	-
Nitrogen	1.233	59.2%	78.1%	-
Nitric Oxide	0.000	0.0%	0.0%	31
Nitrogen Dioxide	0.000	0.0%	0.0%	0
Nitrous Oxide	0.000	0.0%	0.0%	0
Ammonia	0.000	0.0%	0.0%	0
Total	2.084	100.0%	100.0%	

Methane Partial Oxidation (non-catalytic) Integrated with PEMFC Fuel Processor Conditions

C. High Temperature Shift (HTS) Reactor:

Inlet Temperature	C	450
Outlet Temperature	C	545
Pressure	atm	3
Total Inlet Flow	kmol/hr	2.502
	kg/hr	47.885

Outlet Composition:	*kmol/hr*	*mol%*	*mol%(Dry)*	*ppm (Dry)*
Water	0.580	23.2%	0.0%	-
Methane	0.000	0.0%	0.0%	-
Carbon Monoxide	0.090	3.6%	4.7%	46,636
Carbon Dioxide	0.236	9.4%	12.3%	-
Hydrogen	0.776	31.0%	40.4%	-
Oxygen	0.000	0.0%	0.0%	-
Nitrogen	0.820	32.8%	42.7%	-
Nitric Oxide	0.000	0.0%	0.0%	0
Nitrogen Dioxide	0.000	0.0%	0.0%	0
Nitrous Oxide	0.000	0.0%	0.0%	0
Ammonia	0.000	0.0%	0.0%	30
Total	2.502	100.0%	100.0%	

D. Low Temperature Shift (LTS) Reactor:

Inlet Temperature	C	150
Outlet Temperature	C	194
Pressure	atm	3
Total Inlet Flow	kmol/hr	2.502
	kg/hr	47.885

Outlet Composition:	*kmol/hr*	*mol%*	*mol%(Dry)*	*ppm (Dry)*
Water	0.493	19.7%	0.0%	-
Methane	0.000	0.0%	0.0%	-
Carbon Monoxide	0.002	0.1%	0.1%	1,173
Carbon Dioxide	0.323	12.9%	16.1%	-
Hydrogen	0.863	34.5%	43.0%	-
Oxygen	0.000	0.0%	0.0%	-
Nitrogen	0.820	32.8%	40.8%	-
Nitric Oxide	0.000	0.0%	0.0%	0
Nitrogen Dioxide	0.000	0.0%	0.0%	0
Nitrous Oxide	0.000	0.0%	0.0%	0
Ammonia	0.000	0.0%	0.0%	29
Total	2.502	100.0%	100.0%	

Methane Partial Oxidation (non-catalytic) Integrated with PEMFC Fuel Processor Conditions

E. PROX Reactor:

Inlet Temperature	C	193
Outlet Temperature	C	223
Pressure	atm	3
Air Flow	kmol/hr	0.022
	kg/hr	0.648
Total Inlet Flow	kmol/hr	2.524
	kg/hr	48.533

Outlet Composition:	*kmol/hr*	*mol%*	*mol%(Dry)*	*ppm (Dry)*
Water	0.500	19.8%	0.0%	-
Methane	0.000	0.0%	0.0%	-
Carbon Monoxide	0.000	0.0%	0.0%	0
Carbon Dioxide	0.325	12.9%	16.1%	-
Hydrogen	0.856	34.0%	42.4%	-
Oxygen	0.000	0.0%	0.0%	-
Nitrogen	0.838	33.3%	41.5%	-
Nitric Oxide	0.000	0.0%	0.0%	0
Nitrogen Dioxide	0.000	0.0%	0.0%	0
Nitrous Oxide	0.000	0.0%	0.0%	0
Ammonia	0.000	0.0%	0.0%	29
Total	2.520	100.0%	100.0%	

Methane Partial Oxidation (non-catalytic) Integrated with PEMFC Fuel Cell Conditions (Proton Exchange Membrane)

Anode:

Temperature	C	80
Pressure	atm	3
Total Anode Flow	kmol/hr	2.355
	kg/hr	45.562

Inlet Composition:	*kmol/hr*	*mol%*	*mol%(Dry)*	*ppm (Dry)*
Water	0.335	14.2%	0.0%	-
Methane	0.000	0.0%	0.0%	19
Carbon Monoxide	0.000	0.0%	0.0%	0
Carbon Dioxide	0.325	13.8%	16.1%	-
Hydrogen	0.856	36.4%	42.4%	-
Oxygen	0.000	0.0%	0.0%	-
Nitrogen	0.838	35.6%	41.5%	-
Nitric Oxide	0.000	0.0%	0.0%	0
Nitrogen Dioxide	0.000	0.0%	0.0%	0
Nitrous Oxide	0.000	0.0%	0.0%	0
Ammonia	0.000	0.0%	0.0%	28
Total	2.355	100.0%	100.0%	

Cathode:

Temperature	C	80
Pressure	atm	3
Total Cathode Flow	kmol/hr	3.385
	kg/hr	96.315

Inlet Composition:	*kmol/hr*	*mol%*
Oxygen	0.685	20.2%
Nitrogen	2.576	76.1%
Water	0.124	3.7%
Total	3.385	100.0%

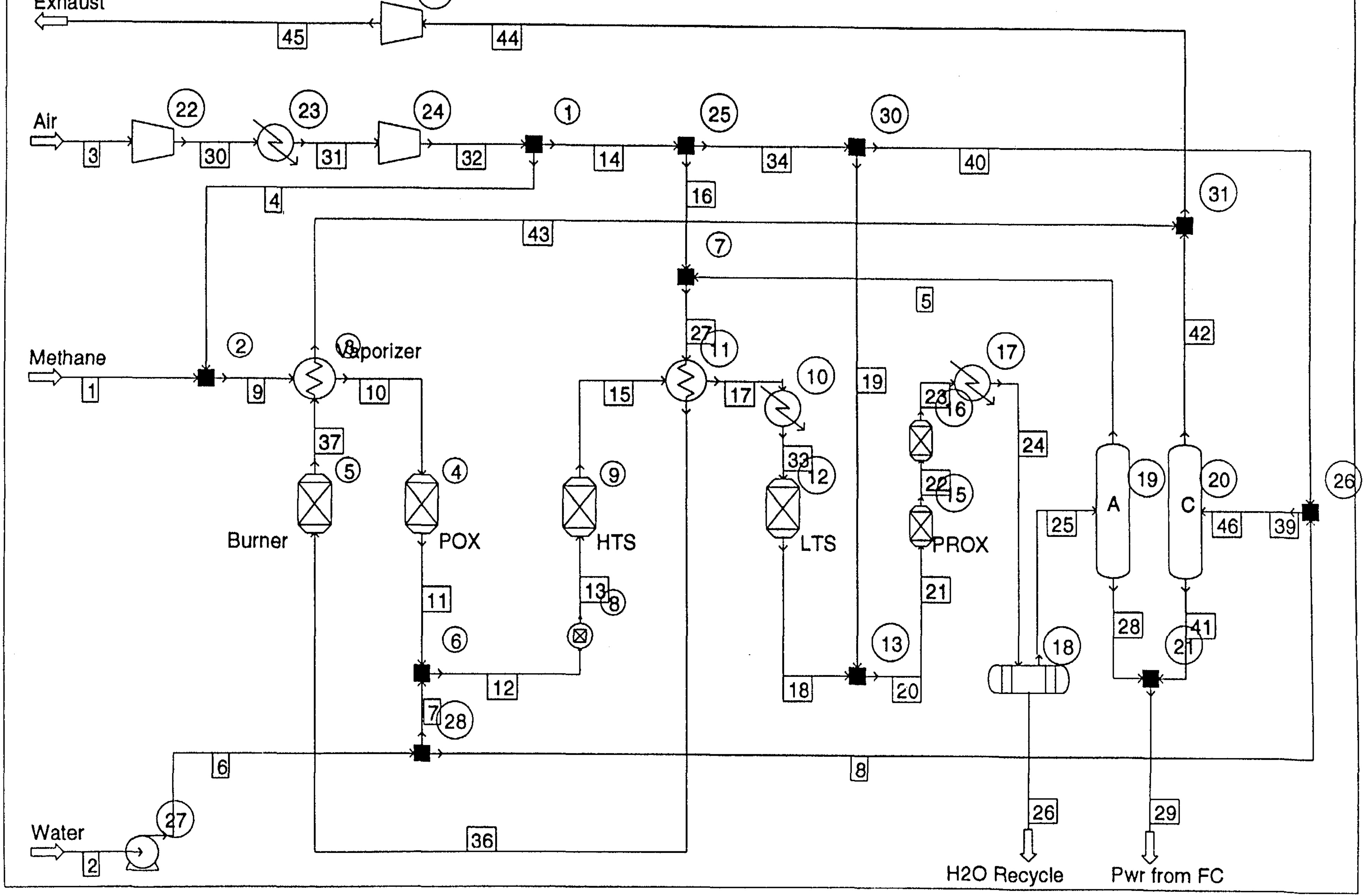
Methane Partial Oxidation (non-catalytic) Integrated with PEMFC Air Compression/Power Recovery System

Water Feed Pump	kW	0.001
FC Cooling Water Pump	kW	0.178
Air Compressor	kW	6.097
Expander	kW	-4.471
Total Parasitic Power	kW	1.8
% of Gross DC Power		7.3%

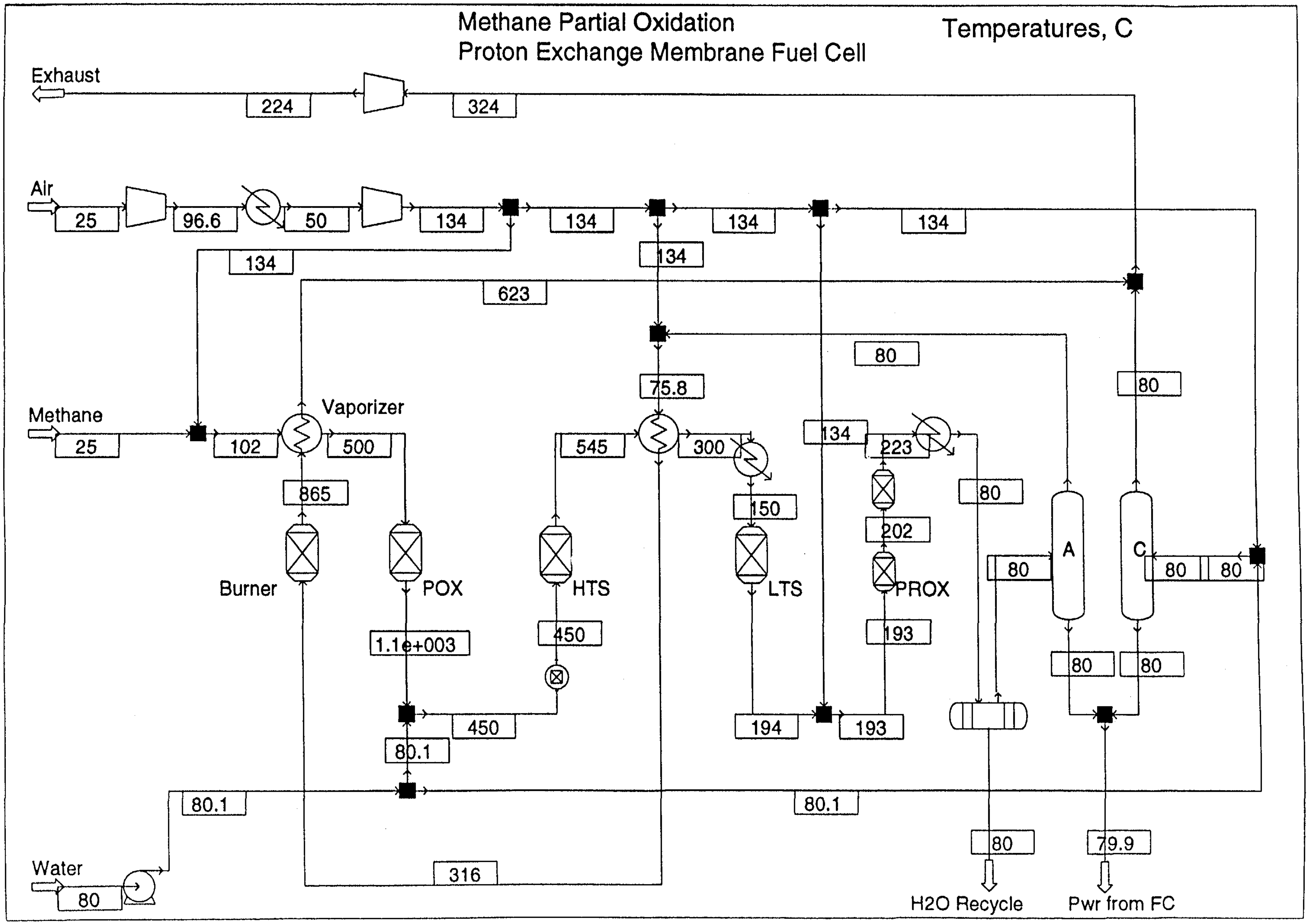
Methane Partial Oxidation (non-catalytic) Integrated with PEMFC Efficiencies

Thermodynamic Efficiency	E(Th)	81.1%
Voltage Efficiency	E(V)	56.7%
Current Efficiency	E(I)	80.0%
Electrochemical Efficiency	E(E)	36.8%
Heating Value Efficiency	E(H)	100.0%
Fuel Cell Efficiency	E(FC)	36.8%
Fuel Processing Efficiency	E(FP)	84.0%
Gross System Efficiency	E(Gross)	30.9%
Net System Efficiency	E(Net)	28.6%
Gross DC Power	kW	24.9
Net DC Power	kW	23.0
Parasitic Power	kW	1.8

Methane Partial Oxidation
Proton Exchange Membrane Fuel Cell

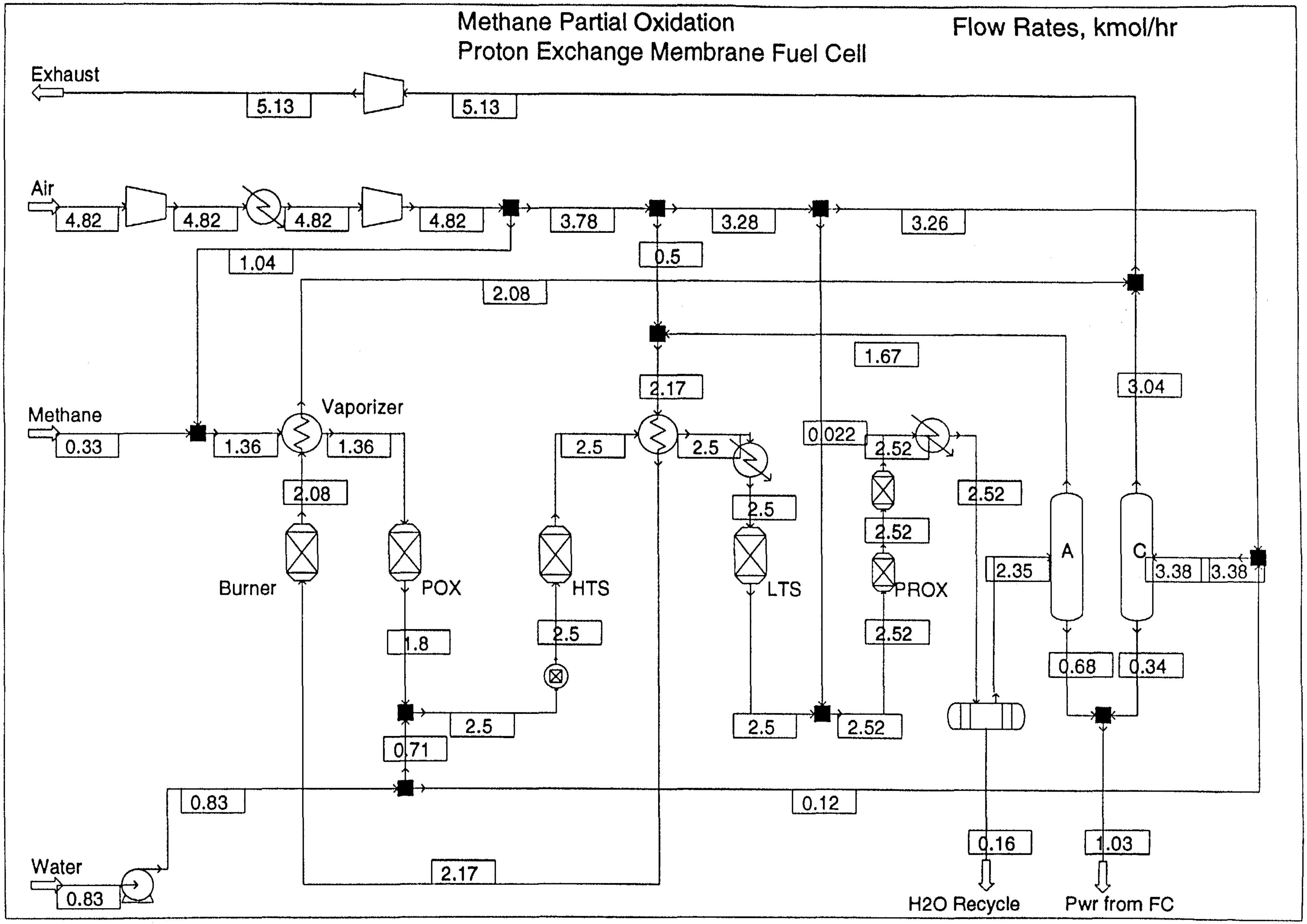


For simulation: numbers in boxes are stream numbers
numbers in circles are component numbers



Methane Partial Oxidation
Proton Exchange Membrane Fuel Cell

Temperatures, C



Methane Partial Oxidation
Proton Exchange Membrane Fuel Cell

Flow Rates, kmol/hr

Case 4: Steam Reforming - Methanol - PEM

Case 4: Steam Reforming - Methanol - PEMFC

Methanol Steam Reformer Integrated with PEMFC Design Basis

1. Proton Exchange Membrane Fuel Cell Conditions

Gross DC Power	kW	25
Current Density	ASF	400
Current Density	mA/cm2	431
Temperature	C	80
	K	353
Pressure	atm	3
H2 Utilization	Uf	80%
O2 Utilization	Uo	50%

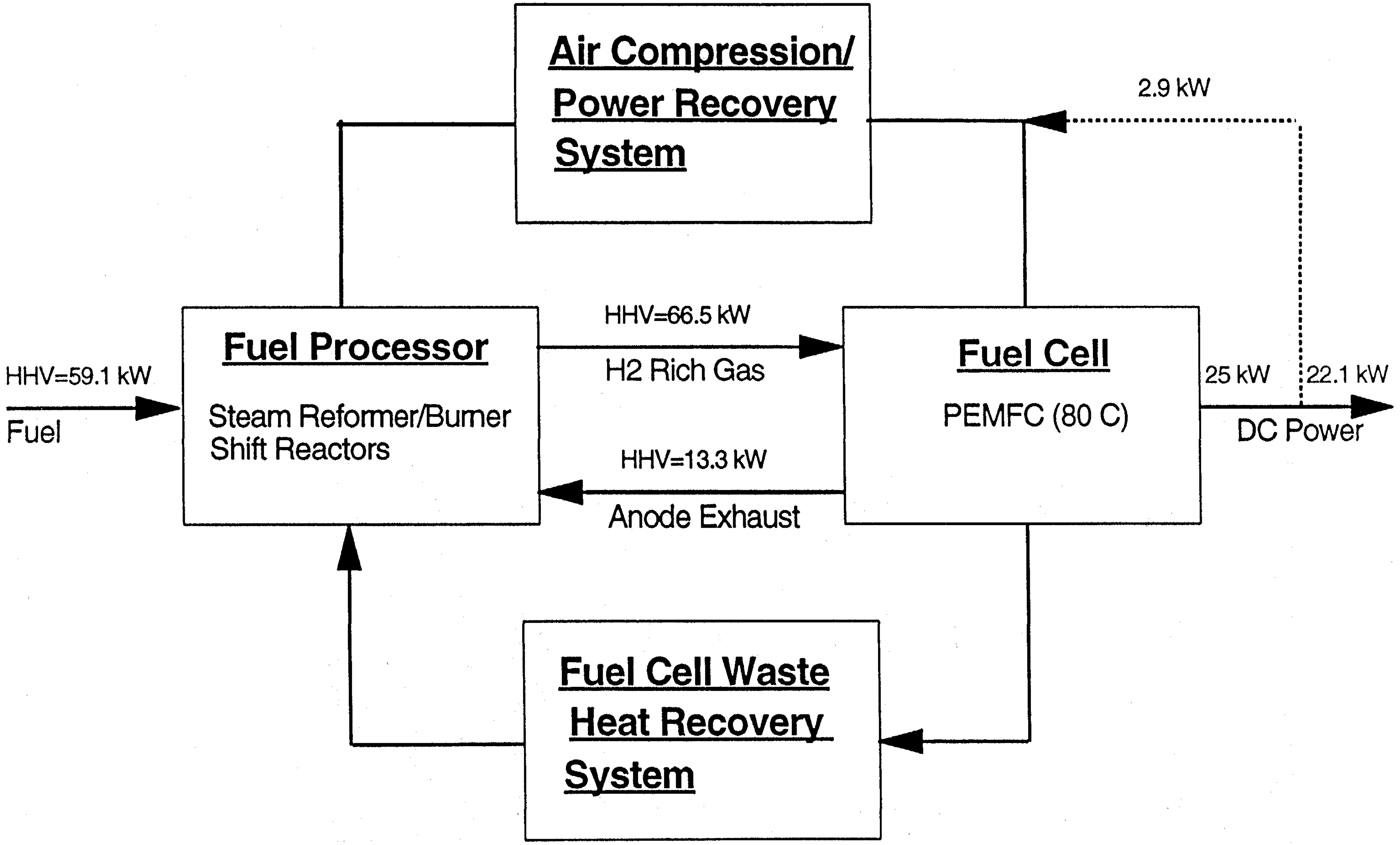
2. Reformer Conditions

Temperature	C	260
	K	533
Pressure	atm	3
Steam/Fuel Ratio	molar	1.5

3. Air Compression/Power Recovery System Assumptions

Pump Efficiency	70.0%
Compressor Efficiency	70.0%
Expander Efficiency	70.0%

Methanol Steam Reformer Integrated with PEMFC: Overall Block Diagram



Fuel Processing Efficiency E(FP) = 112.7% (109.3% LHV/LHV)
Gross System Efficiency E(Gross) = 42.3%
Net System Efficiency E(Net) = 37.5%

Methanol Steam Reformer Integrated with PEMFC

Overall Balance:

Total Fuel to FP	kmol/hr	0.293
	kg/hr	9.377
HHV of Total Fuel to FP	J/hr	-2.1E+08
	kW	59.1
LHV of Total Fuel to FP	J/hr	-1.9E+08
		51.9

Total Flow Into Anode	kmol/hr	1.383
	kg/hr	19.715
HHV of Anode Feed	J/hr	-2.4E+08
	kW	66.5
Flow of Anode Exhaust	kmol/hr	0.709
	kg/hr	18.357
HHV of Anode Exhaust	J/hr	-4.8E+07
	kW	13.3

Gross DC Power	kW	25.0
Net DC Power	kW	22.1
Parsitic Power	kW	2.9

Efficiencies based on HHV of Fuel:

		HHV/HHV	LHV/HHV
Fuel Processing Efficiency	E(FP)	112.7%	96.1%
Gross System Efficiency	E(Gross)	42.3%	
Net System Efficiency	E(Net)	37.5%	

Efficiencies based on LHV of Fuel:

		HHV/LHV	LHV/LHV
Fuel Processing Efficiency	E(FP)	128.2%	109.3%
Gross System Efficiency	E(Gross)	48.2%	
Net System Efficiency	E(Net)	42.7%	

Methanol Steam Reformer Integrated with PEMFC Fuel Processor Conditions

A. Reformer

Temperature	C	260
	K	533
Pressure	atm	3
Steam/Fuel Ratio	molar	1.5
Total Inlet Flow	kmol/hr	0.732
	kg/hr	17.284

Inlet Composition:	*kmol/hr*	*mol%*
Water	0.439	60.0%
Methanol	0.293	40.0%
Total	0.732	100.0%

Outlet Composition:	*kmol/hr*	*mol%*	*mol%(Dry)*
Water	0.166	12.6%	0.0%
Methanol	0.000	0.0%	0.0%
Carbon Monoxide	0.020	1.5%	1.7%
Carbon Dioxide	0.273	20.7%	23.7%
Hydrogen	0.858	65.2%	74.6%
Methane	0.000	0.0%	0.0%
Total	1.317	100.0%	100.0%

Methanol Steam Reformer Integrated with PEMFC Fuel Processor Conditions

B. Burner:

Inlet Temperature	C	351
Outlet Temperature	C	825
Pressure	atm	3
Supplemental Fuel	kmol/hr	0.000
	kg/hr	0.000
Air Flow	kmol/hr	0.415
	kg/hr	11.973
Total Inlet Flow	kmol/hr	1.124
	kg/hr	30.330

Inlet Composition:	*kmol/hr*	*mol%*	*mol%(Dry)*
Water	0.182	16.2%	0.0%
Methanol	0.000	0.0%	0.0%
Carbon Monoxide	0.000	0.0%	0.0%
Carbon Dioxide	0.293	26.0%	31.0%
Hydrogen	0.168	15.0%	17.9%
Oxygen	0.087	7.8%	9.2%
Nitrogen	0.394	35.1%	41.8%
Nitric Oxide	0.000	0.0%	0.0%
Nitrogen Dioxide	0.000	0.0%	0.0%
Nitrous Oxide	0.000	0.0%	0.0%
Methane	0.000	0.0%	0.0%
Total	1.124	100.0%	100.0%

Outlet Composition:	*kmol/hr*	*mol%*	*mol%(Dry)*
Water	0.350	33.7%	0.0%
Methanol	0.000	0.0%	0.0%
Carbon Monoxide	0.000	0.0%	0.0%
Carbon Dioxide	0.293	28.1%	42.4%
Hydrogen	0.000	0.0%	0.0%
Oxygen	0.003	0.3%	0.4%
Nitrogen	0.394	37.9%	57.2%
Nitric Oxide	0.000	0.0%	0.0%
Nitrogen Dioxide	0.000	0.0%	0.0%
Nitrous Oxide	0.000	0.0%	0.0%
Methane	0.000	0.0%	0.0%
Total	1.040	100.0%	100.0%

Methanol Steam Reformer Integrated with PEMFC Fuel Processor Conditions

C. Low Temperature Shift (LTS) Reactor:

Inlet Temperature	C	200
Outlet Temperature	C	210
Pressure	atm	3
Total Inlet Flow	kmol/hr	1.317
	kg/hr	17.285

Outlet Composition:	*kmol/hr*	*mol%*	*mol%(Dry)*
Water	0.155	11.8%	0.0%
Methanol	0.000	0.0%	0.0%
Carbon Monoxide	0.009	0.7%	0.8%
Carbon Dioxide	0.284	21.5%	24.4%
Hydrogen	0.869	66.0%	74.8%
Methane	0.000	0.0%	0.0%
Total	1.317	100.0%	100.0%

Methanol Steam Reformer Integrated with PEMFC Fuel Processor Conditions

D. PROX Reactor:

Inlet Temperature	C	206
Outlet Temperature	C	397
Pressure	atm	3
Air Flow	kmol/hr	0.084
	kg/hr	2.430
Total Inlet Flow	kmol/hr	1.401
	kg/hr	19.715

Inlet Composition:	*kmol/hr*	*mol%*	*mol%(Dry)*
Water	0.155	11.1%	0.0%
Methanol	0.000	0.0%	0.0%
Carbon Monoxide	0.009	0.6%	0.7%
Carbon Dioxide	0.284	20.3%	22.8%
Hydrogen	0.869	62.0%	69.7%
Oxygen	0.018	1.3%	1.4%
Nitrogen	0.067	4.8%	5.3%
Nitric Oxide	0.000	0.0%	0.0%
Nitrogen Dioxide	0.000	0.0%	0.0%
Nitrous Oxide	0.000	0.0%	0.0%
Methane	0.000	0.0%	0.0%
Total	1.401	100.0%	100.0%

Outlet Composition:	*kmol/hr*	*mol%*	*mol%(Dry)*
Water	0.182	13.1%	0.0%
Methanol	0.000	0.0%	0.0%
Carbon Monoxide	0.000	0.0%	0.0%
Carbon Dioxide	0.293	21.1%	24.3%
Hydrogen	0.842	60.9%	70.1%
Oxygen	0.000	0.0%	0.0%
Nitrogen	0.067	4.8%	5.5%
Nitric Oxide	0.000	0.0%	0.0%
Nitrogen Dioxide	0.000	0.0%	0.0%
Nitrous Oxide	0.000	0.0%	0.0%
Methane	0.000	0.0%	0.0%
Total	1.383	100.0%	100.0%

Methanol Steam Reformer Integrated with PEMFC Fuel Cell Conditions (Proton Exchange Membrane)

Anode:

Temperature	C	80
Pressure	atm	3
Total Anode Flow	kmol/hr	1.383
	kg/hr	19.715

Inlet Composition:	*kmol/hr*	*mol%*	*mol%(Dry)*
Water	0.182	13.1%	0.0%
Methanol	0.000	0.0%	0.0%
Carbon Monoxide	0.000	0.0%	0.0%
Carbon Dioxide	0.293	21.1%	24.3%
Hydrogen	0.842	60.9%	70.1%
Oxygen	0.000	0.0%	0.0%
Nitrogen	0.067	4.8%	5.5%
Nitric Oxide	0.000	0.0%	0.0%
Nitrogen Dioxide	0.000	0.0%	0.0%
Nitrous Oxide	0.000	0.0%	0.0%
Methane	0.000	0.0%	0.0%
Total	1.383	100.0%	100.0%

Cathode:

Temperature	C	80
Pressure	atm	3
Total Cathode Flow	kmol/hr	3.330
	kg/hr	94.756

Inlet Composition:	*kmol/hr*	*mol%*
Oxygen	0.202	20.2%
Nitrogen	0.761	76.1%
Water	0.037	3.7%
Total	1.000	100.0%

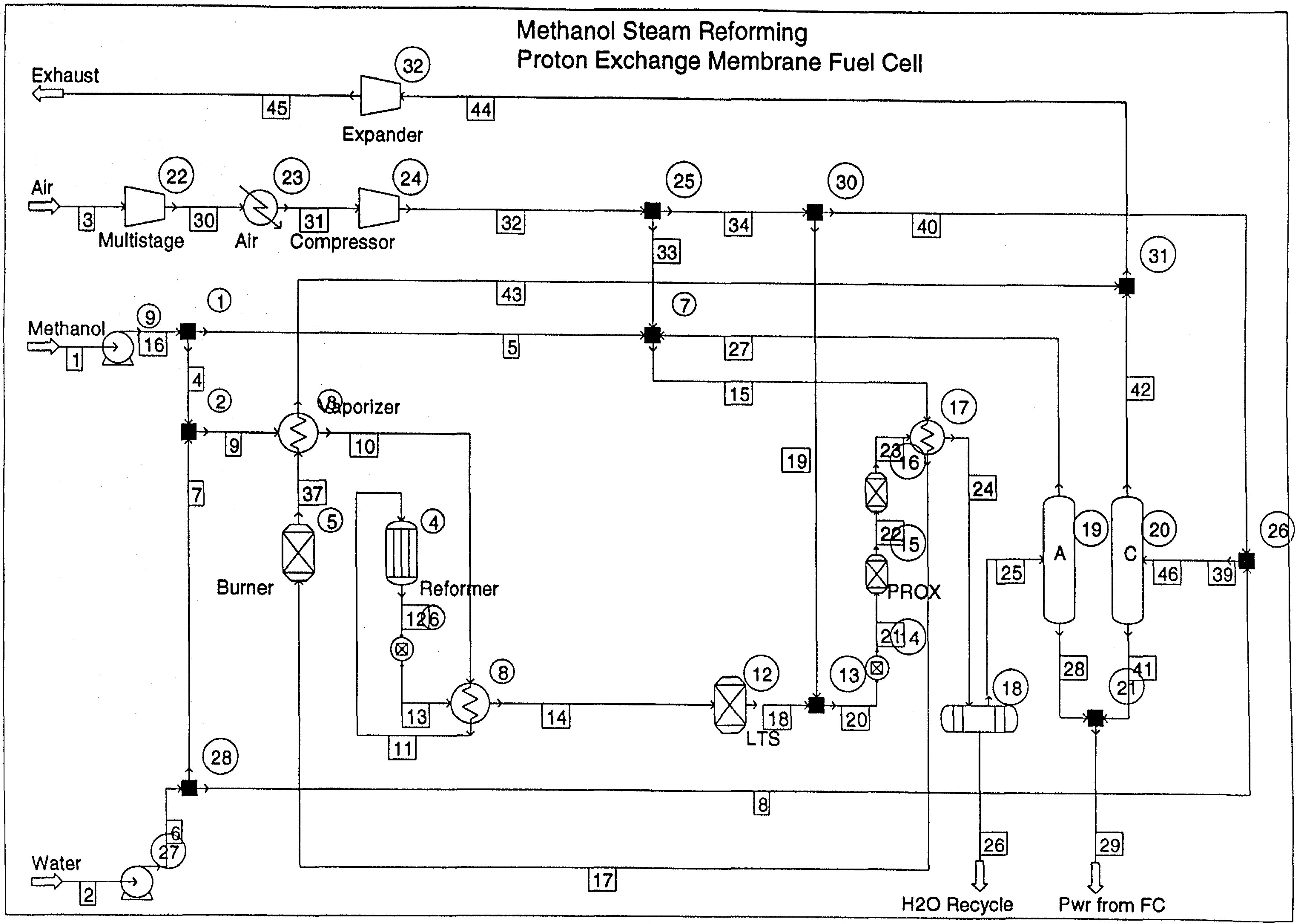
Methanol Steam Reformer Integrated with PEMFC Air Compression/Power Recovery System

Water Feed Pump	kW	0.001
Methanol Feed Pump	kW	0.001
FC Cooling Water Pump	kW	0.167
Air Compressor	kW	4.688
Expander	kW	-2.001
Total Parasitic Power	kW	2.9
% of Gross DC Power		11.4%

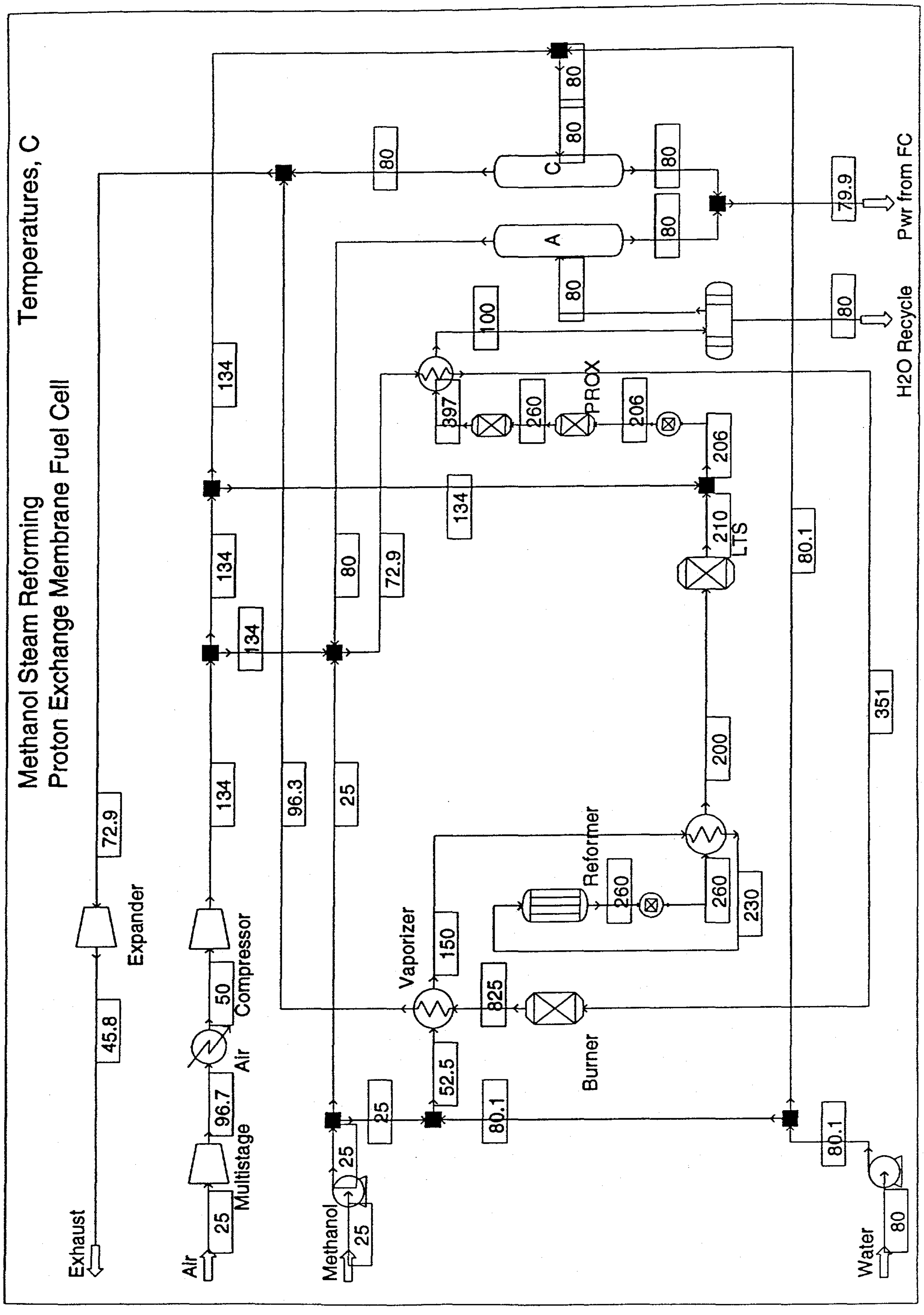
Methanol Steam Reformer Integrated with PEMFC Efficiencies

Thermodynamic Efficiency	E(Th)	81.7%
Voltage Efficiency	E(V)	57.5%
Current Efficiency	E(I)	80.0%
Electrochemical Efficiency	E(E)	37.6%
Heating Value Efficiency	E(H)	100.0%
Fuel Cell Efficiency	E(FC)	37.6%
Fuel Processing Efficiency	E(FP)	112.7%
Gross System Efficiency	E(Gross)	42.3%
Net System Efficiency	E(Net)	37.5%
Gross DC Power	kW	25.0
Net DC Power	kW	22.1
Parasitic Power	kW	2.9

Methanol Steam Reforming
Proton Exchange Membrane Fuel Cell



For simulation: numbers in boxes are stream numbers
numbers in circles are component numbers


Methanol Steam Reforming
Proton Exchange Membrane Fuel Cell
Temperatures, C
Exhaust
Air
Methanol
Water
Multistage
Air
Compressor
Expander
Vaporizer
Burner
Reformer
LTS
PROX
A
C
H2O Recycle
Pwr from FC
45.8
72.9
25
96.7
50
134
134
134
134
134
134
134
25
25
25
25
52.5
80.1
80.1
80.1
80
150
825
260
260
230
200
210
206
206
260
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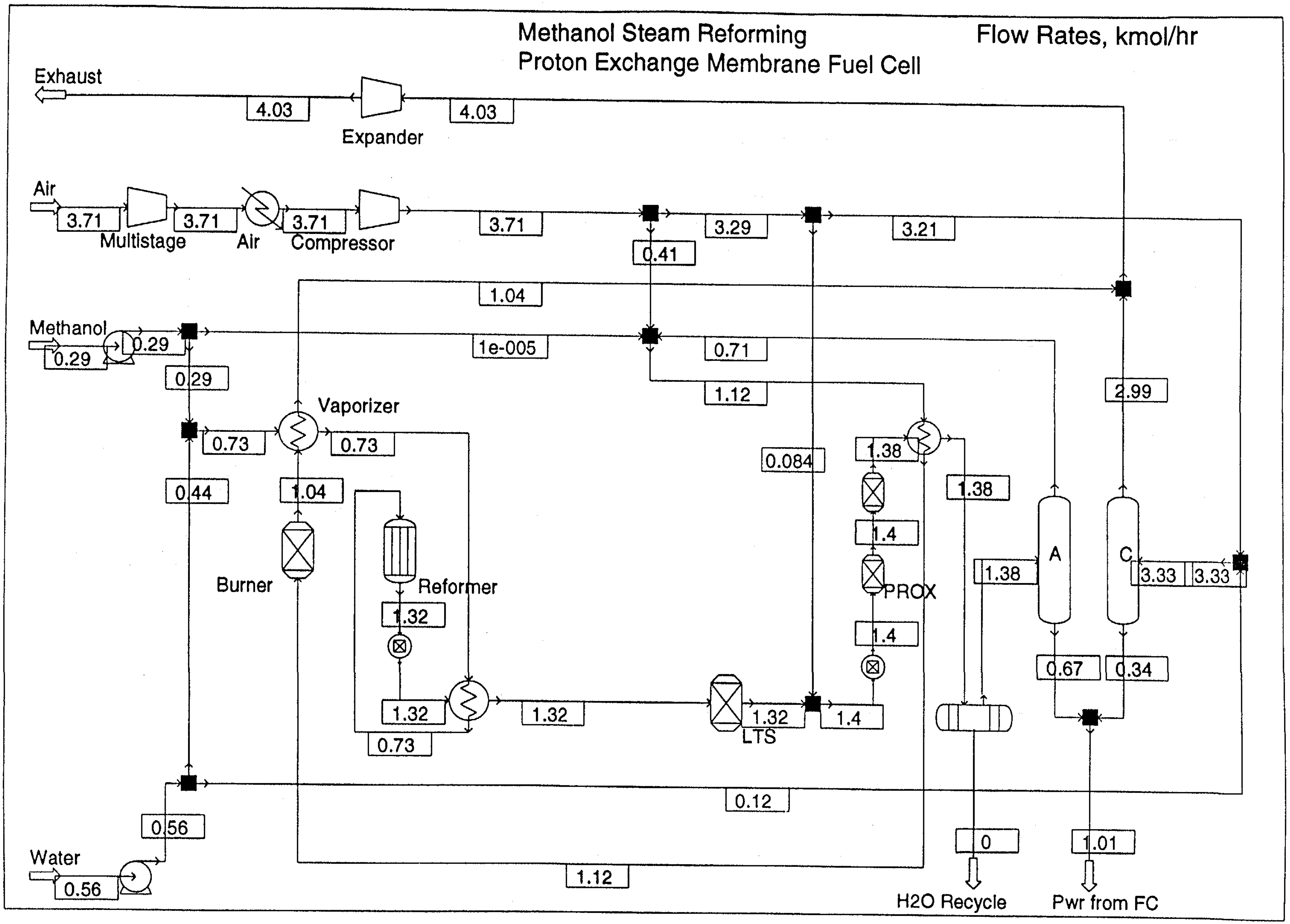
79.9
80
96.3
80
72.9
351


Methanol Steam Reforming
Proton Exchange Membrane Fuel Cell
Flow Rates, kmol/hr

Case 5: Steam Reforming - Ethanol - PEM

Case 5: Steam Reforming - Ethanol - PEMFC

Ethanol Steam Reformer Integrated with PEMFC Design Basis

1. Proton Exchange Membrane Fuel Cell Conditions

Gross DC Power	kW	25
Current Density	ASF	400
Current Density	mA/cm2	431
Temperature	C	80
	K	353
Pressure	atm	3
H2 Utilization	Uf	80%
O2 Utilization	Uo	50%

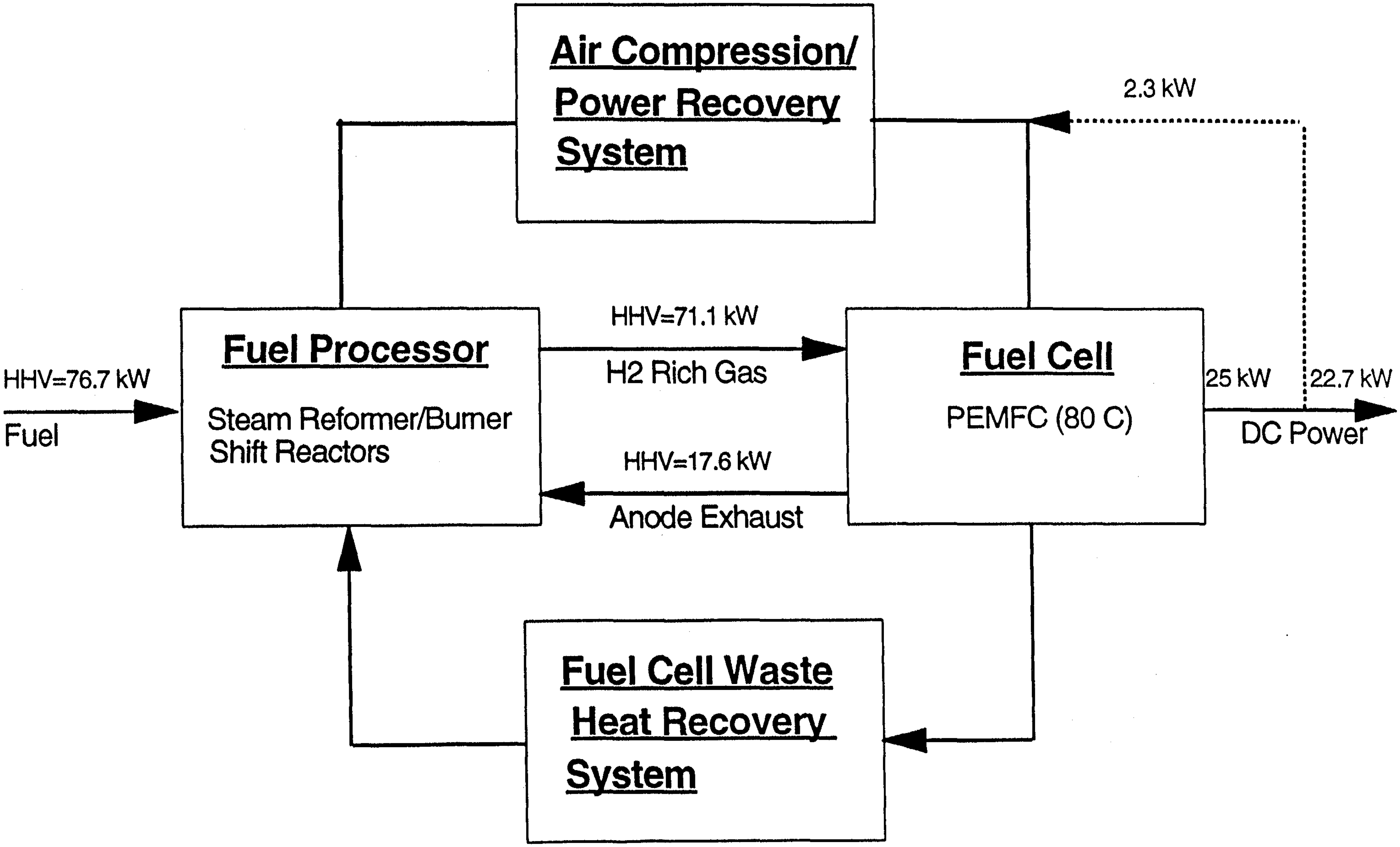
2. Reformer Conditions

Temperature	C	750
	K	1023
Pressure	atm	3
Steam/Fuel Ratio	molar	4

3. Air Compression/Power Recovery System Assumptions

Pump Efficiency	70.0%
Compressor Efficiency	70.0%
Expander Efficiency	70.0%

Ethanol Steam Reformer integrated with PEMFC: Overall Block Diagram



Air Compression/ Power Recovery System

2.3 kW

HHV=76.7 kW

Fuel

Fuel Processor

Steam Reformer/Burner
Shift Reactors

HHV=71.1 kW

H2 Rich Gas

HHV=17.6 kW

Anode Exhaust

Fuel Cell

PEMFC (80 C)

25 kW

22.7 kW

DC Power

Fuel Cell Waste Heat Recovery System

Fuel Processing Efficiency E(FP) = 92.8% (87.9% LHV/LHV)
Gross System Efficiency E(Gross) = 32.6%
Net System Efficiency E(Net) = 29.7%

Ethanol Steam Reformer Integrated with PEMFC

Overall Balance:

Total Fuel to FP	kmol/hr	0.202
	kg/hr	3.237
HHV of Total Fuel to FP	J/hr	-2.8E+08
	kW	76.7
LHV of Total Fuel to FP	J/hr	-2.5E+08
		69.3
Total Flow Into Anode	kmol/hr	1.485
	kg/hr	22.161
HHV of Anode Feed	J/hr	-2.6E+08
	kW	71.1
Flow of Anode Exhaust	kmol/hr	0.807
	kg/hr	20.795
HHV of Anode Exhaust	J/hr	-6.3E+07
	kW	17.6
Gross DC Power	kW	25.0
Net DC Power	kW	22.7
Parasitic Power	kW	2.3

Efficiencies based on HHV of Fuel:

		HHV/HHV	LHV/HHV
Fuel Processing Efficiency	E(FP)	92.8%	79.4%
Gross System Efficiency	E(Gross)	32.6%	
Net System Efficiency	E(Net)	29.7%	

Efficiencies based on LHV of Fuel:

		HHV/LHV	LHV/LHV
Fuel Processing Efficiency	E(FP)	102.6%	87.9%
Gross System Efficiency	E(Gross)	36.1%	
Net System Efficiency	E(Net)	32.8%	

Ethanol Steam Reformer Integrated with PEMFC Fuel Processor Conditions

A. Reformer

Temperature	C	750
	K	1023
Pressure	atm	3
Steam/Fuel Ratio	molar	4
Total Inlet Flow	kmol/hr	0.809
	kg/hr	19.108

Inlet Composition:	*kmol/hr*	*mol%*
Water	0.647	80.0%
Ethanol	0.162	20.0%
Total	0.809	100.0%

Outlet Composition:	*kmol/hr*	*mol%*	*mol%(Dry)*
Water	0.382	26.9%	0.0%
Ethanol	0.000	0.0%	0.0%
Carbon Monoxide	0.186	13.1%	17.9%
Carbon Dioxide	0.120	8.4%	11.6%
Hydrogen	0.715	50.3%	68.9%
Methane	0.017	1.2%	1.7%
Total	1.421	100.0%	100.0%

Ethanol Steam Reformer Integrated with PEMFC Fuel Processor Conditions

B. Burner:

Inlet Temperature	C	278
Outlet Temperature	C	904
Pressure	atm	3
Supplemental Fuel	kmol/hr	0.040
	kg/hr	1.843
Air Flow	kmol/hr	1.360
	kg/hr	39.236
Total Inlet Flow	kmol/hr	2.207
	kg/hr	61.874

Inlet Composition:	*kmol/hr*	*mol%*	*mol%(Dry)*
Water	0.212	9.6%	0.0%
Ethanol	0.040	1.8%	2.0%
Carbon Monoxide	0.000	0.0%	0.0%
Carbon Dioxide	0.306	13.9%	15.3%
Hydrogen	0.169	7.7%	8.5%
Oxygen	0.286	12.9%	14.3%
Nitrogen	1.177	53.3%	59.0%
Nitric Oxide	0.000	0.0%	0.0%
Nitrogen Dioxide	0.000	0.0%	0.0%
Nitrous Oxide	0.000	0.0%	0.0%
Methane	0.017	0.8%	0.9%
Total	2.207	100.0%	100.0%

Outlet Composition:	*kmol/hr*	*mol%*	*mol%(Dry)*
Water	0.535	24.8%	0.0%
Ethanol	0.000	0.0%	0.0%
Carbon Monoxide	0.000	0.0%	0.0%
Carbon Dioxide	0.404	18.7%	24.8%
Hydrogen	0.000	0.0%	0.0%
Oxygen	0.046	2.1%	2.9%
Nitrogen	1.177	54.4%	72.3%
Nitric Oxide	0.000	0.0%	0.0%
Nitrogen Dioxide	0.000	0.0%	0.0%
Nitrous Oxide	0.000	0.0%	0.0%
Methane	0.000	0.0%	0.0%
Total	2.163	100.0%	100.0%

Ethanol Steam Reformer Integrated with PEMFC Fuel Processor Conditions

C. High Temperature Shift (HTS) Reactor:

Inlet Temperature	C	500
Outlet Temperature	C	546
Pressure	atm	3
Total Inlet Flow	kmol/hr	1.421
	kg/hr	19.108

Outlet Composition:	*kmol/hr*	*mol%*	*mol%(Dry)*
Water	0.321	22.6%	0.0%
Ethanol	0.000	0.0%	0.0%
Carbon Monoxide	0.125	8.8%	11.4%
Carbon Dioxide	0.181	12.7%	16.5%
Hydrogen	0.777	54.6%	70.6%
Methane	0.017	1.2%	1.6%
Total	1.421	100.0%	100.0%

D. Low Temperature Shift (LTS) Reactor:

Inlet Temperature	C	150
Outlet Temperature	C	245
Pressure	atm	3
Total Inlet Flow	kmol/hr	1.421
	kg/hr	19.108

Outlet Composition:	*kmol/hr*	*mol%*	*mol%(Dry)*
Water	0.210	14.8%	0.0%
Ethanol	0.000	0.0%	0.0%
Carbon Monoxide	0.014	1.0%	1.1%
Carbon Dioxide	0.293	20.6%	24.2%
Hydrogen	0.888	62.5%	73.3%
Methane	0.017	1.2%	1.4%
Total	1.421	100.0%	100.0%

Ethanol Steam Reformer Integrated with PEMFC Fuel Processor Conditions

E. PROX Reactor:

Inlet Temperature	C	237
Outlet Temperature	C	500
Pressure	atm	3
Air Flow	kmol/hr	0.130
	kg/hr	3.765
Total Inlet Flow	kmol/hr	1.552
	kg/hr	22.873

Inlet Composition:	*kmol/hr*	*mol%*	*mol%(Dry)*
Water	0.210	13.5%	0.0%
Ethanol	0.000	0.0%	0.0%
Carbon Monoxide	0.014	0.9%	1.0%
Carbon Dioxide	0.293	18.9%	21.8%
Hydrogen	0.888	57.2%	66.2%
Oxygen	0.027	1.8%	2.0%
Nitrogen	0.103	6.6%	7.7%
Nitric Oxide	0.000	0.0%	0.0%
Nitrogen Dioxide	0.000	0.0%	0.0%
Nitrous Oxide	0.000	0.0%	0.0%
Methane	0.017	1.1%	1.3%
Total	1.552	100.0%	100.0%

Outlet Composition:	*kmol/hr*	*mol%*	*mol%(Dry)*
Water	0.251	16.5%	0.0%
Ethanol	0.000	0.0%	0.0%
Carbon Monoxide	0.000	0.0%	0.0%
Carbon Dioxide	0.306	20.1%	24.1%
Hydrogen	0.847	55.5%	66.5%
Oxygen	0.000	0.0%	0.0%
Nitrogen	0.103	6.8%	8.1%
Nitric Oxide	0.000	0.0%	0.0%
Nitrogen Dioxide	0.000	0.0%	0.0%
Nitrous Oxide	0.000	0.0%	0.0%
Methane	0.017	1.1%	1.4%
Total	1.524	100.0%	100.0%

Ethanol Steam Reformer Integrated with PEMFC Fuel Cell Conditions (Proton Exchange Membrane)

Anode:

Temperature	C	80
Pressure	atm	3
Total Anode Flow	kmol/hr	1.485
	kg/hr	22.161

Inlet Composition:	*kmol/hr*	*mol%*	*mol%(Dry)*
Water	0.212	14.2%	0.0%
Ethanol	0.000	0.0%	0.0%
Carbon Monoxide	0.000	0.0%	0.0%
Carbon Dioxide	0.306	20.6%	24.1%
Hydrogen	0.847	57.0%	66.5%
Oxygen	0.000	0.0%	0.0%
Nitrogen	0.103	6.9%	8.1%
Nitric Oxide	0.000	0.0%	0.0%
Nitrogen Dioxide	0.000	0.0%	0.0%
Nitrous Oxide	0.000	0.0%	0.0%
Methane	0.017	1.2%	1.4%
Total	1.485	100.0%	100.0%

Cathode:

Temperature	C	80
Pressure	atm	3
Total Cathode Flow	kmol/hr	3.348
	kg/hr	95.261

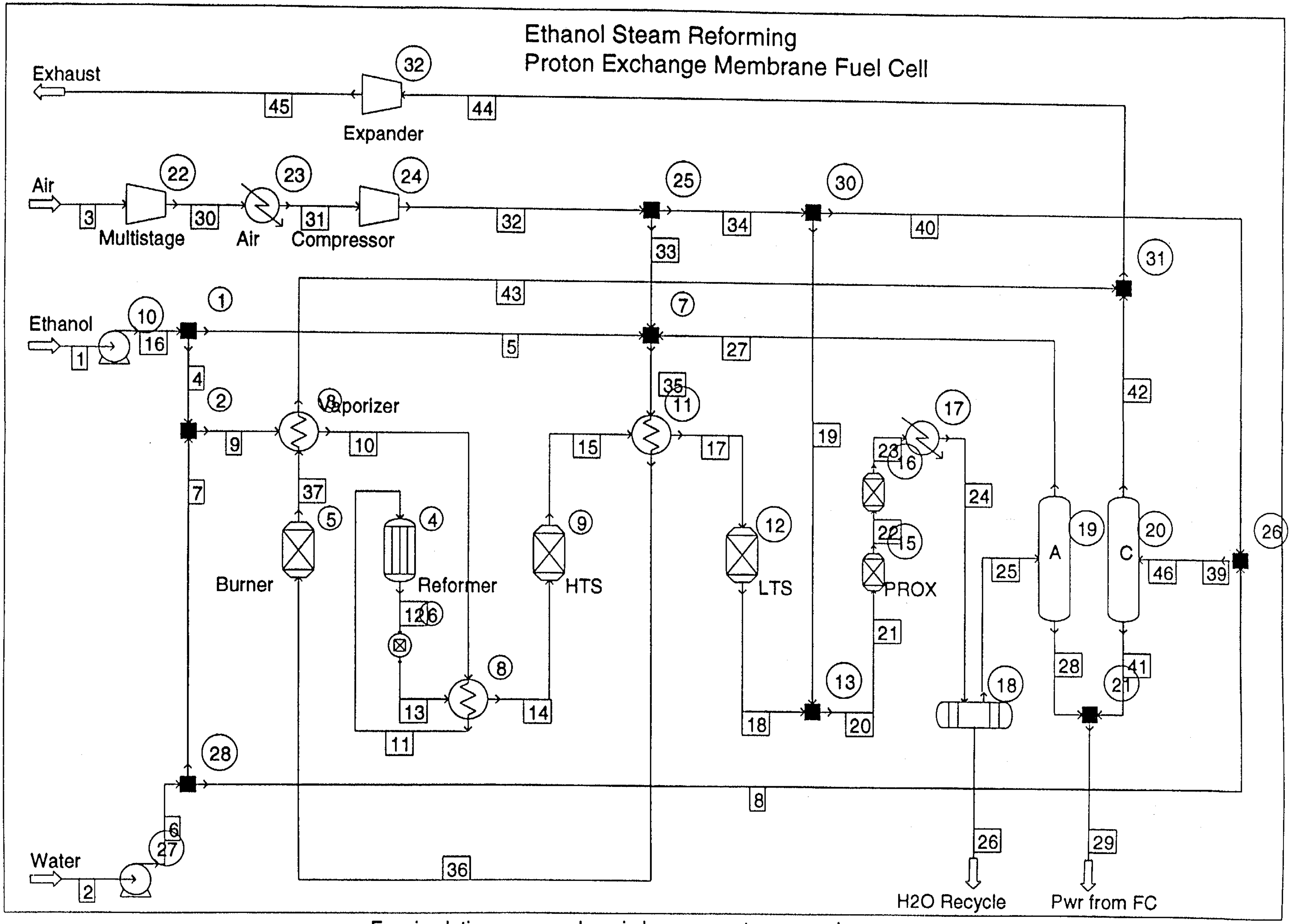
Inlet Composition:	*kmol/hr*	*mol%*
Oxygen	0.202	20.2%
Nitrogen	0.761	76.1%
Water	0.037	3.7%
Total	1.000	100.0%

Ethanol Steam Reformer Integrated with PEMFC Air Compression/Power Recovery System

Water Feed Pump	kW	0.001
Ethanol Feed Pump	kW	0.001
FC Cooling Water Pump	kW	0.171
Air Compressor	kW	5.963
Expander	kW	-3.868
Total Parasitic Power	kW	2.3
% of Gross DC Power		9.1%

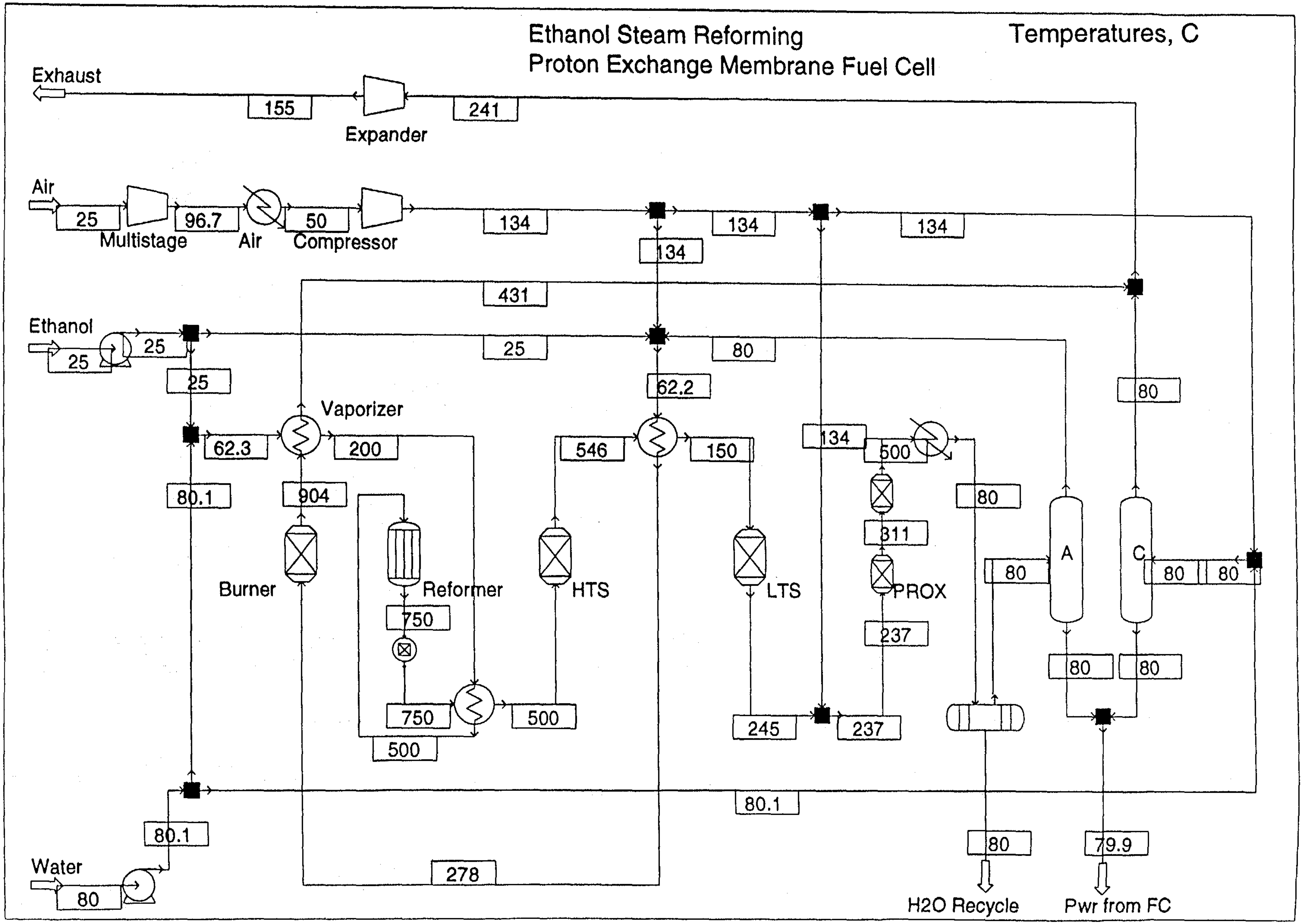
Ethanol Steam Reformer Integrated with PEMFC Efficiencies

Thermodynamic Efficiency	E(Th)	81.5%
Voltage Efficiency	E(V)	57.3%
Current Efficiency	E(I)	80.0%
Electrochemical Efficiency	E(E)	37.4%
Heating Value Efficiency	E(H)	94.0%
Fuel Cell Efficiency	E(FC)	35.2%
Fuel Processing Efficiency	E(FP)	92.8%
Gross System Efficiency	E(Gross)	32.6%
Net System Efficiency	E(Net)	29.7%
Gross DC Power	kW	25.0
Net DC Power	kW	22.7
Parasitic Power	kW	2.3



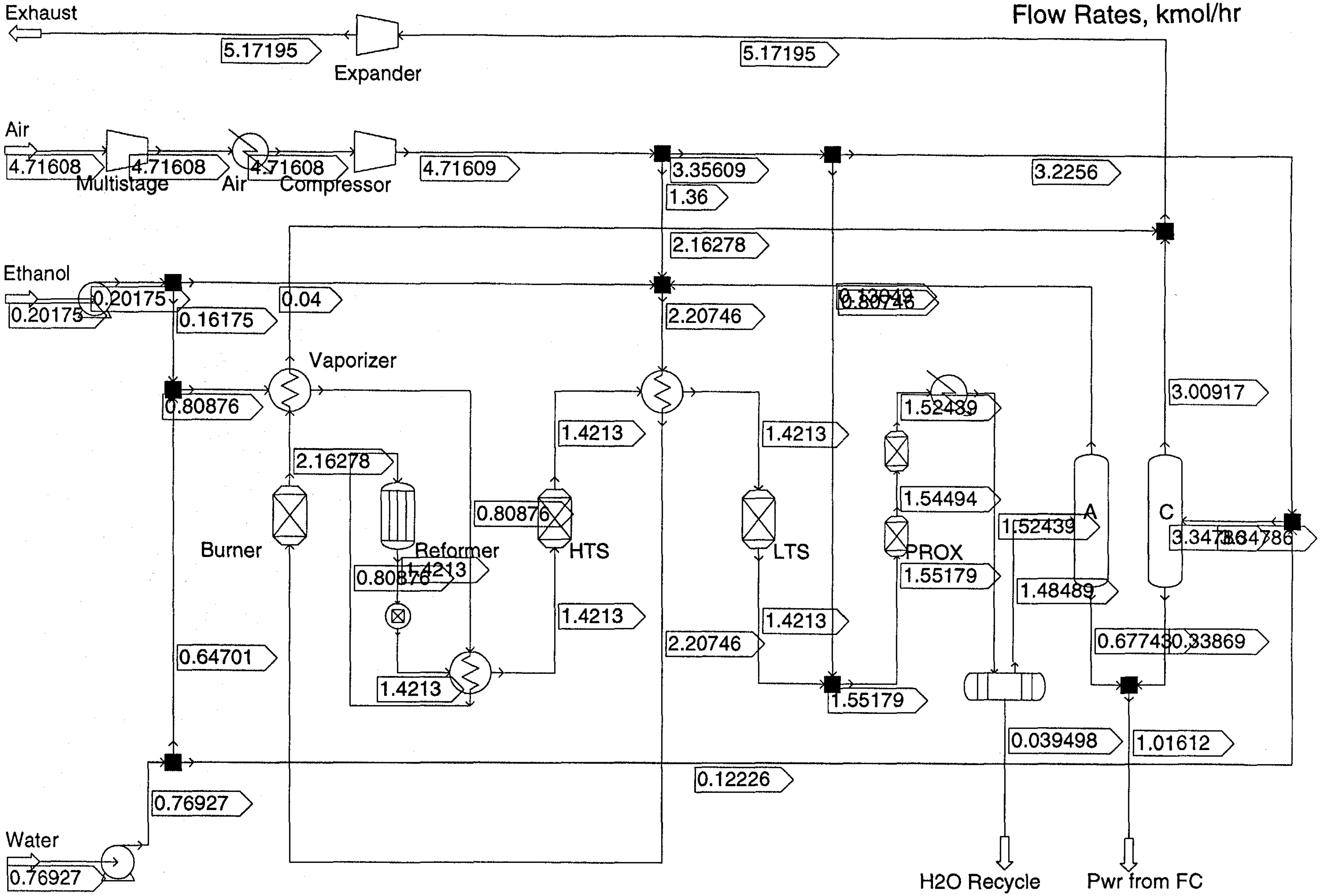
Ethanol Steam Reforming
Proton Exchange Membrane Fuel Cell

For simulation: numbers in boxes are stream numbers
numbers in circles are component numbers



Ethanol Steam Reforming
Proton Exchange Membrane Fuel Cell

Temperatures, C



Ethanol Steam Reforming
Proton Exchange Membrane Fuel Cell

Case 6: Steam Reforming - Methane - PAFC (3 atm)

Case 6: Steam Reforming - Methane - PAFC

Methane Steam Reformer Integrated with PAFC Design Basis

1. Phosphoric Acid Fuel Cell Conditions

Gross DC Power	kW	25
Current Density	mA/cm2	323
Temperature	C	190
	K	463
Pressure	atm	3
H2 Utilization	Uf	80%
O2 Utilization	Uo	50%

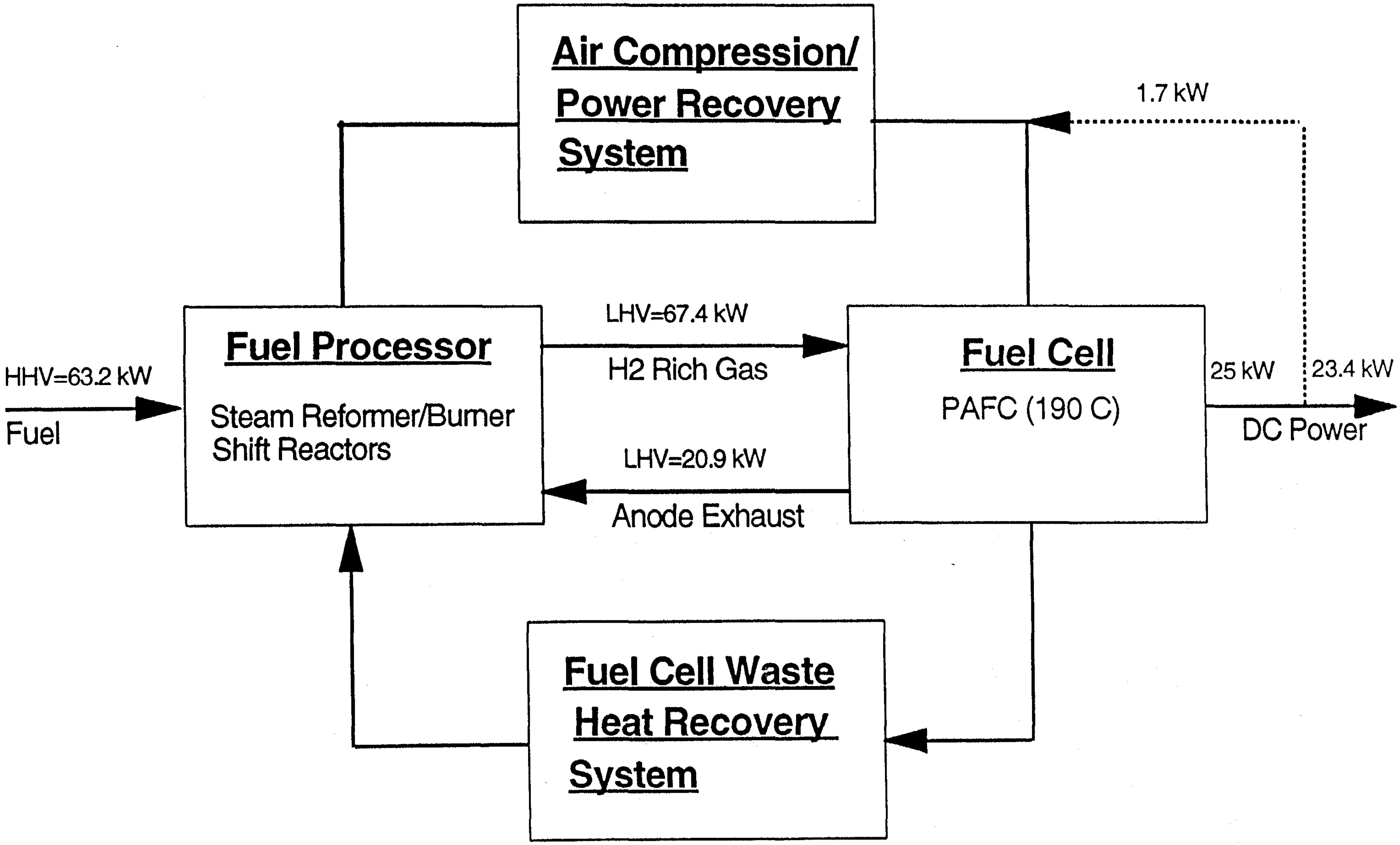
2. Reformer Conditions

Temperature	C	700
	K	973
Pressure	atm	3
Steam/Fuel Ratio	molar	3

3. Air Compression/Power Recovery System Assumptions

Pump Efficiency	70.0%
Compressor Efficiency	70.0%
Expander Efficiency	70.0%

Methane Steam Reformer Integrated with PAFC: Overall Block Diagram



Fuel Processing Efficiency E(FP) = 106.7 % (118.4 % LHV/LHV)
Gross System Efficiency E(Gross) = 39.6 %
Net System Efficiency E(Net) = 37.0 %

Methane Steam Reformer Integrated with PAFC

Overall Balance:

Total Fuel to FP	kmol/hr	0.256
	kg/hr	4.103
HHV of Total Fuel to FP	J/hr	-2.3E+08
	kW	63.2
LHV of Total Fuel to FP	J/hr	-2.1E+08
		57.0
Total Flow Into Anode	kmol/hr	1.157
	kg/hr	12.523
LHV of Anode Feed	J/hr	-2.4E+08
	kW	67.4
Flow of Anode Exhaust	kmol/hr	0.469
	kg/hr	11.136
LHV of Anode Exhaust	J/hr	-7.5E+07
	kW	20.9
Gross DC Power	kW	25.0
Net DC Power	kW	23.4
Parasitic Power	kW	1.7

Efficiencies based on HHV of Fuel:

		LHV/HHV
Fuel Processing Efficienc	E(FP)	106.7%
Gross System Efficiency	E(Gross)	39.6%
Net System Efficiency	E(Net)	37.0%

Efficiencies based on LHV of Fuel:

		LHV/LHV
Fuel Processing Efficienc	E(FP)	118.4%
Gross System Efficiency	E(Gross)	44.0%
Net System Efficiency	E(Net)	41.0%

Methane Steam Reformer Integrated with PAFC Fuel Processor Conditions

A. Reformer

Temperature	C	700
	K	973
Pressure	atm	3
Steam/Fuel Ratio	molar	3
Total Inlet Flow	kmol/hr	1.023
	kg/hr	17.925

Inlet Composition:	*kmol/hr*	*mol%*
Water	0.767	75.0%
Methane	0.256	25.0%
Total	1.023	100.0%

Outlet Composition:	*kmol/hr*	*mol%*	*mol%(Dry)*
Water	0.449	30.8%	0.0%
Methane	0.039	2.7%	3.9%
Carbon Monoxide	0.115	7.9%	11.4%
Carbon Dioxide	0.102	7.0%	10.1%
Hydrogen	0.752	51.6%	74.6%
Total	1.456	100.0%	100.0%

Methane Steam Reformer Integrated with PAFC Fuel Processor Conditions

B. Burner:

Inlet Temperature	C	283
Outlet Temperature	C	539
Pressure	atm	3
Supplemental Fuel	kmol/hr	0.000
	kg/hr	0.000
Air Flow	kmol/hr	1.023
	kg/hr	29.515
Total Inlet Flow	kmol/hr	1.492
	kg/hr	40.651

Inlet Composition:	*kmol/hr*	*mol%*	*mol%(Dry)*
Water	0.041	2.7%	0.0%
Methane	0.039	2.6%	2.7%
Carbon Monoxide	0.007	0.5%	0.5%
Carbon Dioxide	0.210	14.1%	14.5%
Hydrogen	0.172	11.5%	11.9%
Oxygen	0.215	14.4%	14.8%
Nitrogen	0.808	54.2%	55.7%
Nitric Oxide	0.000	0.0%	0.0%
Nitrogen Dioxide	0.000	0.0%	0.0%
Nitrous Oxide	0.000	0.0%	0.0%
Total	1.492	100.0%	100.0%

Outlet Composition:	*kmol/hr*	*mol%*	*mol%(Dry)*
Water	0.291	20.7%	0.0%
Methane	0.000	0.0%	0.0%
Carbon Monoxide	0.000	0.0%	0.0%
Carbon Dioxide	0.256	18.2%	23.0%
Hydrogen	0.000	0.0%	0.0%
Oxygen	0.047	3.4%	4.3%
Nitrogen	0.808	57.6%	72.7%
Nitric Oxide	0.000	0.0%	0.0%
Nitrogen Dioxide	0.000	0.0%	0.0%
Nitrous Oxide	0.000	0.0%	0.0%
Total	1.402	100.0%	100.0%

Methane Steam Reformer Integrated with PAFC Fuel Processor Conditions

C. High Temperature Shift (HTS) Reactor:

Inlet Temperature	C	500
Outlet Temperature	C	531
Pressure	atm	3
Total Inlet Flow	kmol/hr	1.456
	kg/hr	17.926

Outlet Composition:	*kmol/hr*	*mol%*	*mol%(Dry)*
Water	0.406	27.9%	0.0%
Methane	0.039	2.7%	3.7%
Carbon Monoxide	0.072	5.0%	6.9%
Carbon Dioxide	0.144	9.9%	13.7%
Hydrogen	0.794	54.5%	75.6%
Total	1.456	100.0%	100.0%

D. Low Temperature Shift (LTS) Reactor:

Inlet Temperature	C	200
Outlet Temperature	C	255
Pressure	atm	3
Total Inlet Flow	kmol/hr	1.456
	kg/hr	17.926

Outlet Composition:	*kmol/hr*	*mol%*	*mol%(Dry)*
Water	0.341	23.4%	0.0%
Methane	0.039	2.7%	3.5%
Carbon Monoxide	0.007	0.5%	0.6%
Carbon Dioxide	0.210	14.4%	18.8%
Hydrogen	0.860	59.1%	77.1%
Total	1.456	100.0%	100.0%

Methane Steam Reformer Integrated with PAFC Fuel Cell Conditions (Phosphoric Acid)

Anode:

Temperature	C	190
Pressure	atm	3
Total Anode Flow	kmol/hr	1.157
	kg/hr	12.523

Inlet Composition:	*kmol/hr*	*mol%*	*mol%(Dry)*
Water	0.041	3.5%	0.0%
Methane	0.039	3.4%	3.5%
Carbon Monoxide	0.007	0.6%	0.6%
Carbon Dioxide	0.210	18.1%	18.8%
Hydrogen	0.860	74.4%	77.1%
Total	1.157	100.0%	100.0%

Cathode:

Temperature	C	190
Pressure	atm	3
Total Cathode Flow	kmol/hr	3.276
	kg/hr	94.526

Inlet Composition:	*kmol/hr*	*mol%*
Oxygen	0.688	21.0%
Nitrogen	2.588	79.0%
Total	3.276	100.0%

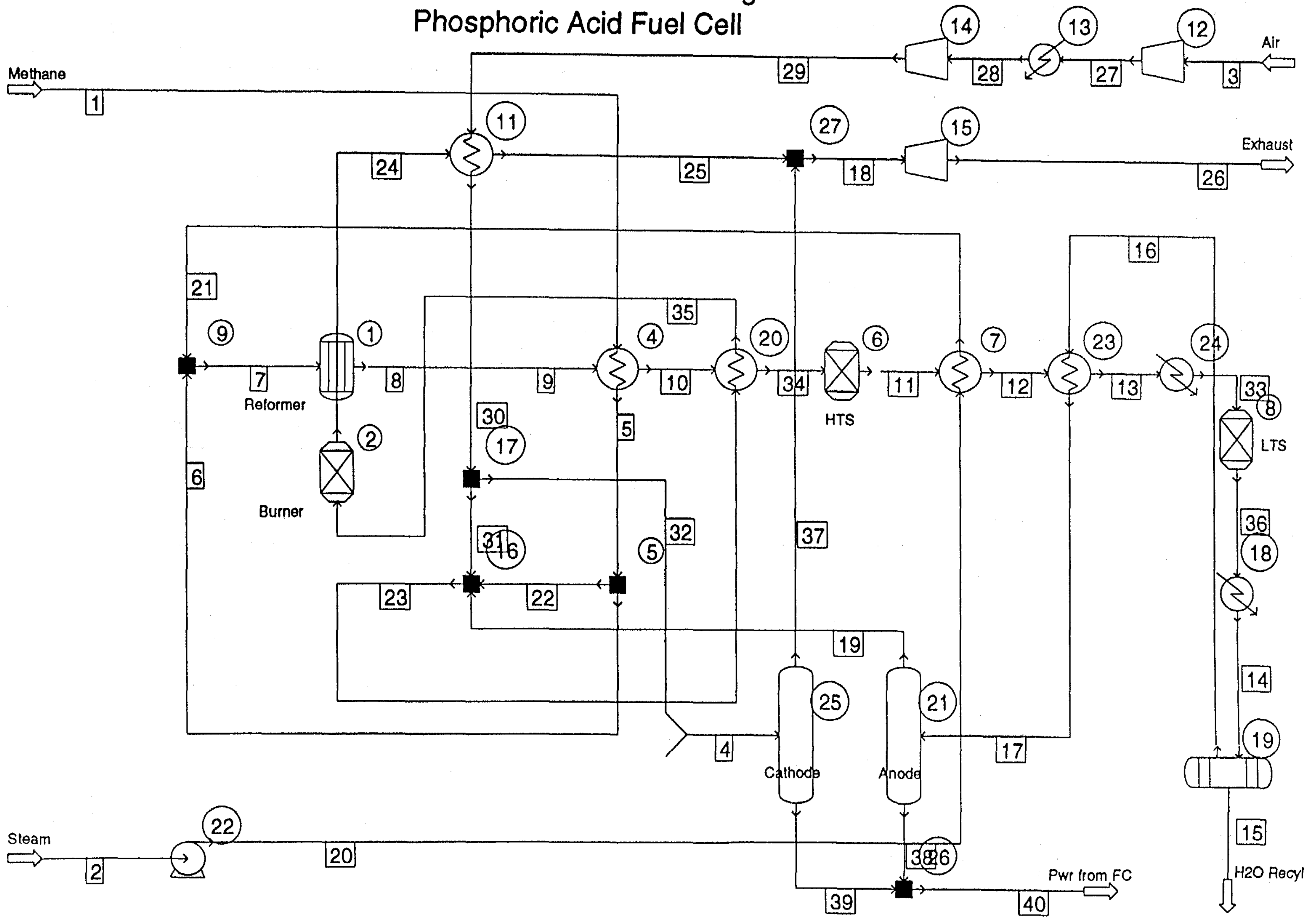
Methane Steam Reformer Integrated with PAFC Air Compression/Power Recovery System

Water Feed Pump	kW	0.001
FC Cooling Water Pump	kW	0.069
Air Compressor	kW	5.436
Expander	kW	-3.836
Total Parasitic Power	kW	1.7
% of Gross DC Power		6.7%

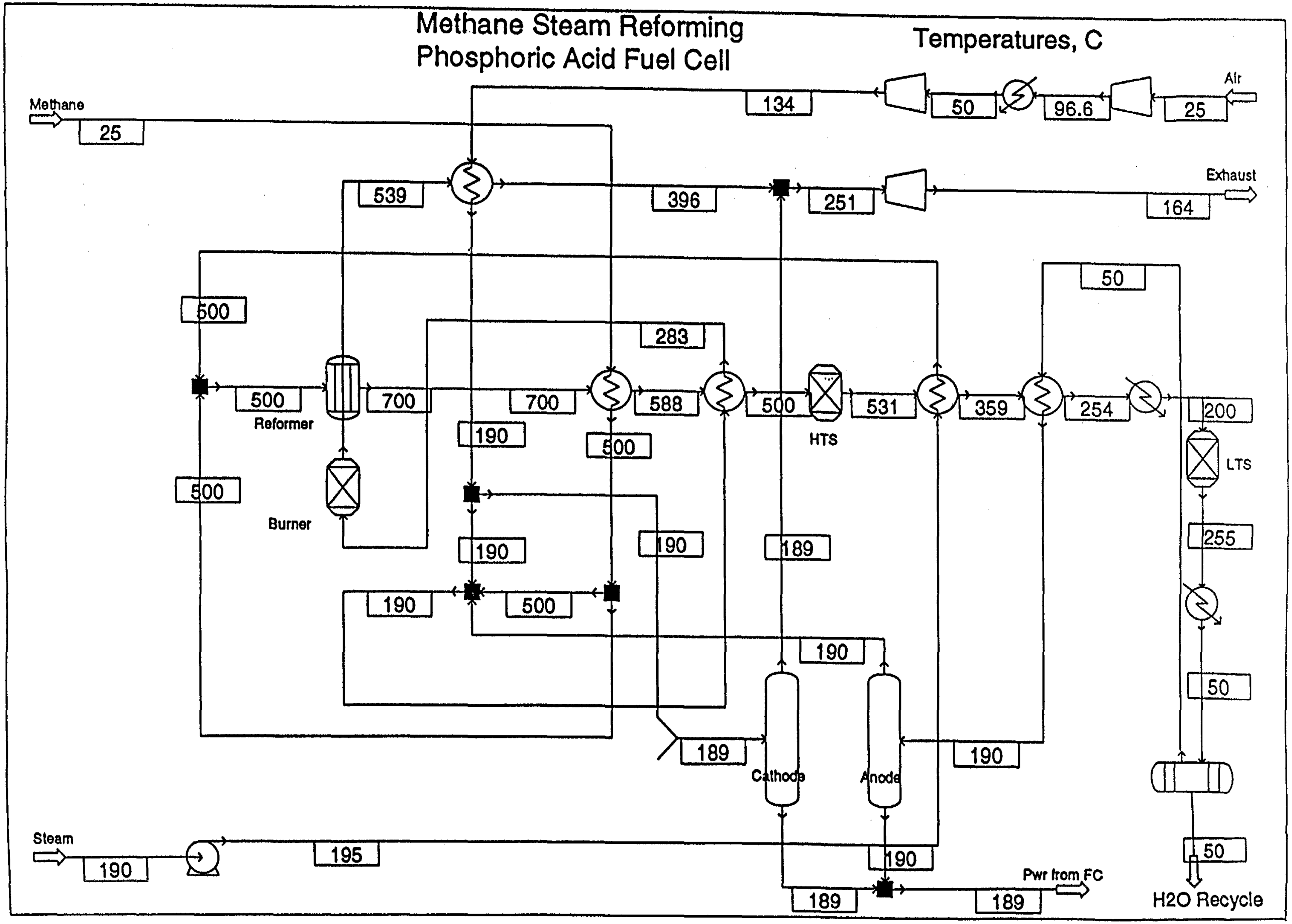
Methane Steam Reformer Integrated with PAFC Efficiencies

Thermodynamic Efficienc	E(Th)	95.2%
Voltage Efficiency	E(V)	56.5%
Current Efficiency	E(I)	80.0%
Electrochemical Efficienc	E(E)	43.0%
Heating Value Efficiency	E(H)	86.3%
Fuel Cell Efficiency	E(FC)	37.1%
Fuel Processing Efficienc	E(FP)	106.7%
Gross System Efficiency	E(Gross)	39.6%
Net System Efficiency	E(Net)	37.0%
Gross DC Power	kW	25.0
Net DC Power	kW	23.4
Parasitic Power	kW	1.7

Methane Steam Reforming
Phosphoric Acid Fuel Cell



For simulation: numbers in boxes are stream numbers
numbers in circles are component numbers

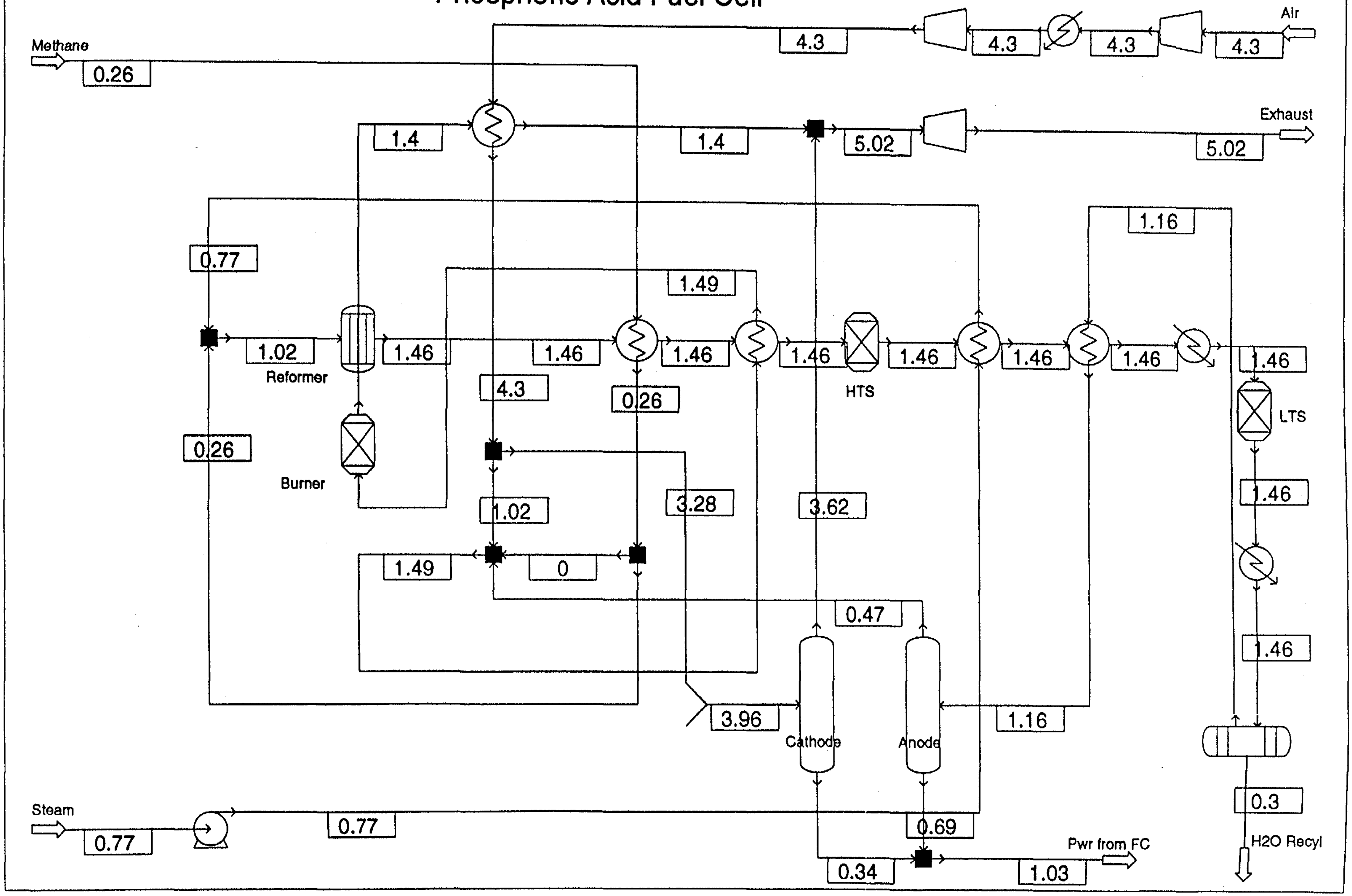


Methane Steam Reforming
Phosphoric Acid Fuel Cell

Temperatures, C

Methane Steam Reforming
Phosphoric Acid Fuel Cell

Flow Rates, kmol/hr



Case 7: Steam Reforming - Methane - PAFC (1 atm)

Case 7: Steam Reforming - Methane - PAFC (1 atm)

Methane Steam Reformer Integrated with PAFC Design Basis

1. Phosphoric Acid Fuel Cell Conditions

Gross DC Power	kW	25
Current Density	mA/cm2	323
Temperature	C	190
	K	463
Pressure	atm	1
H2 Utilization	Uf	80%
O2 Utilization	Uo	50%

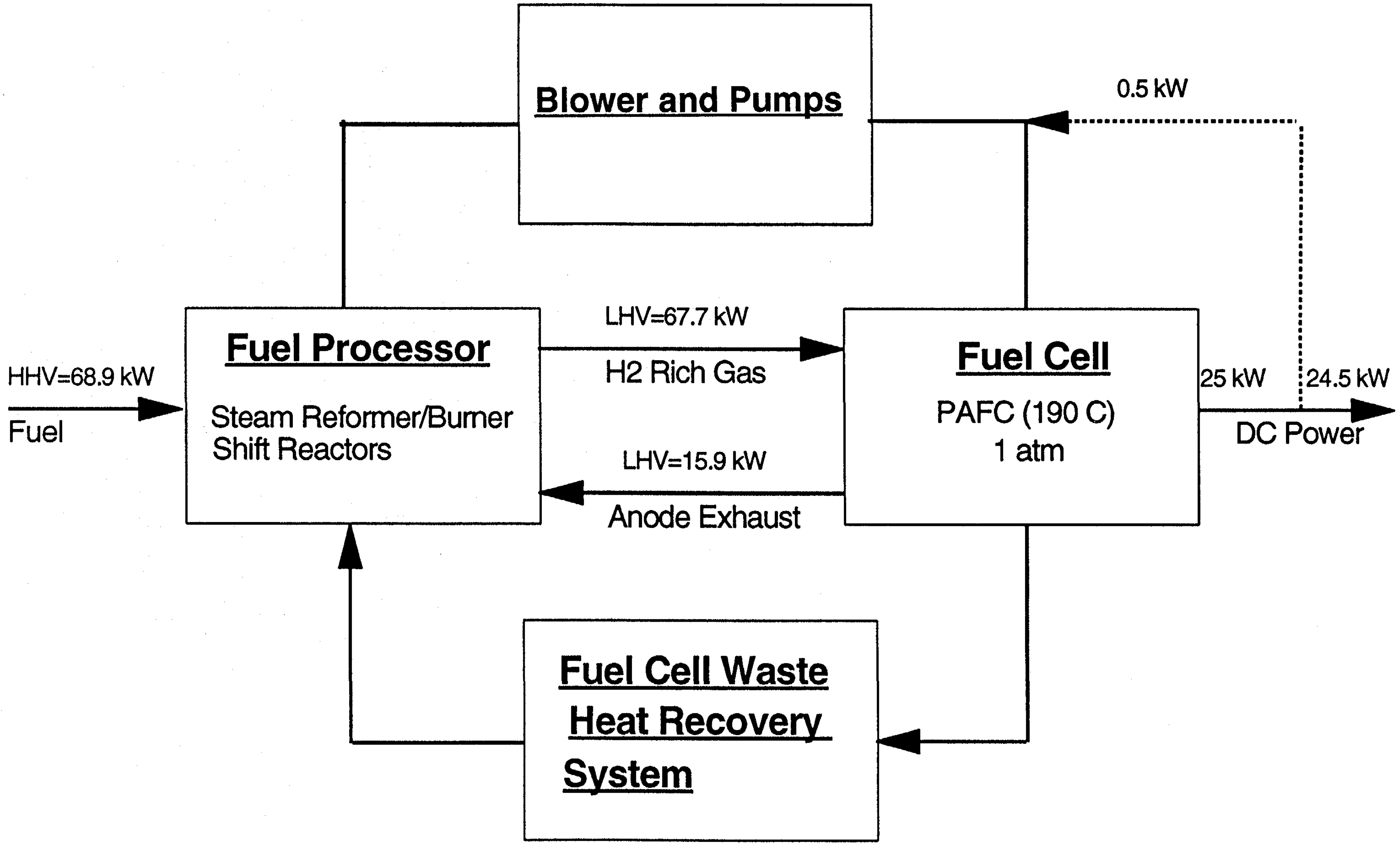
2. Reformer Conditions

Temperature	C	700
	K	973
Pressure	atm	1
Steam/Fuel Ratio	molar	3

3. Parasitic System Assumptions

Pump Efficiency	70.0%
Blower Efficiency	70.0%

Methane Steam Reformer Integrated with PAFC: Overall Block Diagram



Fuel Processing Efficiency E(FP) = 98.2% (109.0% LHV/LHV)
Gross System Efficiency E(Gross) = 36.3%
Net System Efficiency E(Net) = 35.5 %

Methane Steam Reformer Integrated with PAFC

Overall Balance:

Total Fuel to FP	kmol/hr	0.279
	kg/hr	4.471
HHV of Total Fuel to FP	J/hr	-2.5E+08
	kW	68.9
LHV of Total Fuel to FP	J/hr	-2.2E+08
		62.1
Total Flow Into Anode	kmol/hr	1.334
	kg/hr	14.822
LHV of Anode Feed	J/hr	-2.4E+08
	kW	67.7
Flow of Anode Exhaust	kmol/hr	0.570
	kg/hr	13.280
LHV of Anode Exhaust	J/hr	-5.7E+07
	kW	15.9
Gross DC Power	kW	25.0
Net DC Power	kW	24.5
Parasitic Power	kW	0.5

Efficiencies based on HHV of Fuel:

		LHV/HHV
Fuel Processing Efficiency	E(FP)	98.2%
Gross System Efficiency	E(Gross)	36.3%
Net System Efficiency	E(Net)	35.5%

Efficiencies based on LHV of Fuel:

		LHV/LHV
Fuel Processing Efficiency	E(FP)	109.0%
Gross System Efficiency	E(Gross)	40.3%
Net System Efficiency	E(Net)	39.4%

Methane Steam Reformer Integrated with PAFC Fuel Processor Conditions

A. Reformer

Temperature	C	700
	K	973
Pressure	atm	1
Steam/Fuel Ratio	molar	3
Total Inlet Flow	kmol/hr	1.004
	kg/hr	17.597

Inlet Composition:	*kmol/hr*	*mol%*
Water	0.753	75.0%
Methane	0.251	25.0%
Total	1.004	100.0%

Outlet Composition:	*kmol/hr*	*mol%*	*mol%(Dry)*
Water	0.409	27.4%	0.0%
Methane	0.009	0.6%	0.8%
Carbon Monoxide	0.140	9.4%	12.9%
Carbon Dioxide	0.103	6.9%	9.5%
Hydrogen	0.829	55.7%	76.8%
Total	1.488	100.0%	100.0%

Methane Steam Reformer Integrated with PAFC Fuel Processor Conditions

B. Burner:

Inlet Temperature	C	411
Outlet Temperature	C	570
Pressure	atm	1
Supplemental Fuel	kmol/hr	0.028
	kg/hr	0.443
Air Flow	kmol/hr	0.999
	kg/hr	28.827
Total Inlet Flow	kmol/hr	1.596
	kg/hr	42.550

Inlet Composition:	*kmol/hr*	*mol%*	*mol%(Dry)*
Water	0.127	8.0%	0.0%
Methane	0.037	2.3%	2.5%
Carbon Monoxide	0.012	0.8%	0.8%
Carbon Dioxide	0.230	14.4%	15.6%
Hydrogen	0.191	12.0%	13.0%
Oxygen	0.210	13.1%	14.3%
Nitrogen	0.789	49.4%	53.7%
Nitric Oxide	0.000	0.0%	0.0%
Nitrogen Dioxide	0.000	0.0%	0.0%
Nitrous Oxide	0.000	0.0%	0.0%
Total	1.596	100.0%	100.0%

Outlet Composition:	*kmol/hr*	*mol%*	*mol%(Dry)*
Water	0.392	26.2%	0.0%
Methane	0.000	0.0%	0.0%
Carbon Monoxide	0.000	0.0%	0.0%
Carbon Dioxide	0.279	18.6%	25.3%
Hydrogen	0.000	0.0%	0.0%
Oxygen	0.035	2.3%	3.2%
Nitrogen	0.789	52.8%	71.6%
Nitric Oxide	0.000	0.0%	0.0%
Nitrogen Dioxide	0.000	0.0%	0.0%
Nitrous Oxide	0.000	0.0%	0.0%
Total	1.495	100.0%	100.0%

Methane Steam Reformer Integrated with PAFC Fuel Processor Conditions

C. High Temperature Shift (HTS) Reactor:

Inlet Temperature	C	500
Outlet Temperature	C	534
Pressure	atm	1
Total Inlet Flow	kmol/hr	1.488
	kg/hr	17.597

Outlet Composition:	*kmol/hr*	*mol%*	*mol%(Dry)*
Water	0.363	24.4%	0.0%
Methane	0.009	0.6%	0.8%
Carbon Monoxide	0.094	6.3%	8.3%
Carbon Dioxide	0.148	10.0%	13.2%
Hydrogen	0.875	58.8%	77.7%
Total	1.488	100.0%	100.0%

D. Low Temperature Shift (LTS) Reactor:

Inlet Temperature	C	200
Outlet Temperature	C	267
Pressure	atm	1
Total Inlet Flow	kmol/hr	1.488
	kg/hr	17.597

Outlet Composition:	*kmol/hr*	*mol%*	*mol%(Dry)*
Water	0.281	18.9%	0.0%
Methane	0.009	0.6%	0.7%
Carbon Monoxide	0.012	0.8%	1.0%
Carbon Dioxide	0.230	15.4%	19.0%
Hydrogen	0.956	64.2%	79.2%
Total	1.488	100.0%	100.0%

Methane Steam Reformer Integrated with PAFC Fuel Cell Conditions (Phosphoric Acid)

Anode:

Temperature	C	190
Pressure	atm	1
Total Anode Flow	kmol/hr	1.334
	kg/hr	14.822

Inlet Composition:	*kmol/hr*	*mol%*	*mol%(Dry)*
Water	0.127	9.5%	0.0%
Methane	0.009	0.7%	0.7%
Carbon Monoxide	0.012	0.9%	1.0%
Carbon Dioxide	0.230	17.2%	19.0%
Hydrogen	0.956	71.6%	79.2%
Total	1.334	100.0%	100.0%

Cathode:

Temperature	C	190
Pressure	atm	1
Total Cathode Flow	kmol/hr	3.642
	kg/hr	105.081

Inlet Composition:	*kmol/hr*	*mol%*
Oxygen	0.765	21.0%
Nitrogen	2.877	79.0%
Total	3.642	100.0%

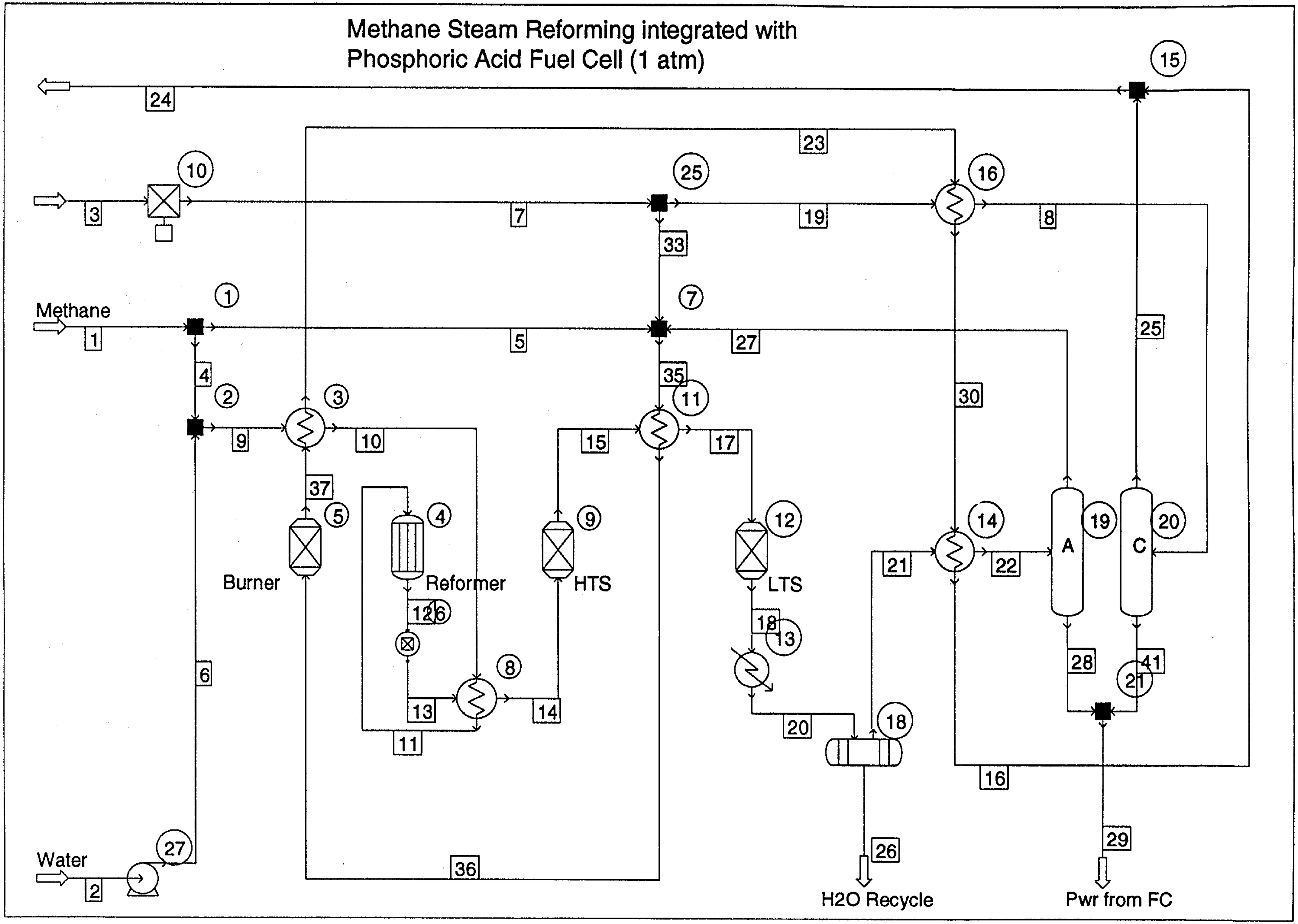
Methane Steam Reformer Integrated with PAFC Air Compression/Power Recovery System

Water Feed Pump	kW	0.000
FC Cooling Water Pump	kW	0.101
Air Blower	kW	0.441
Total Parasitic Power	kW	0.5
% of Gross DC Power		2.2%

Methane Steam Reformer Integrated with PAFC Efficiencies

Thermodynamic Efficiency	E(Th)	92.7%
Voltage Efficiency	E(V)	52.1%
Current Efficiency	E(I)	80.0%
Electrochemical Efficiency	E(E)	38.6%
Heating Value Efficiency	E(H)	95.6%
Fuel Cell Efficiency	E(FC)	36.9%
Fuel Processing Efficiency	E(FP)	98.2%
Gross System Efficiency	E(Gross)	36.3%
Net System Efficiency	E(Net)	35.5%
Gross DC Power	kW	25.0
Net DC Power	kW	24.5
Parasitic Power	kW	0.5

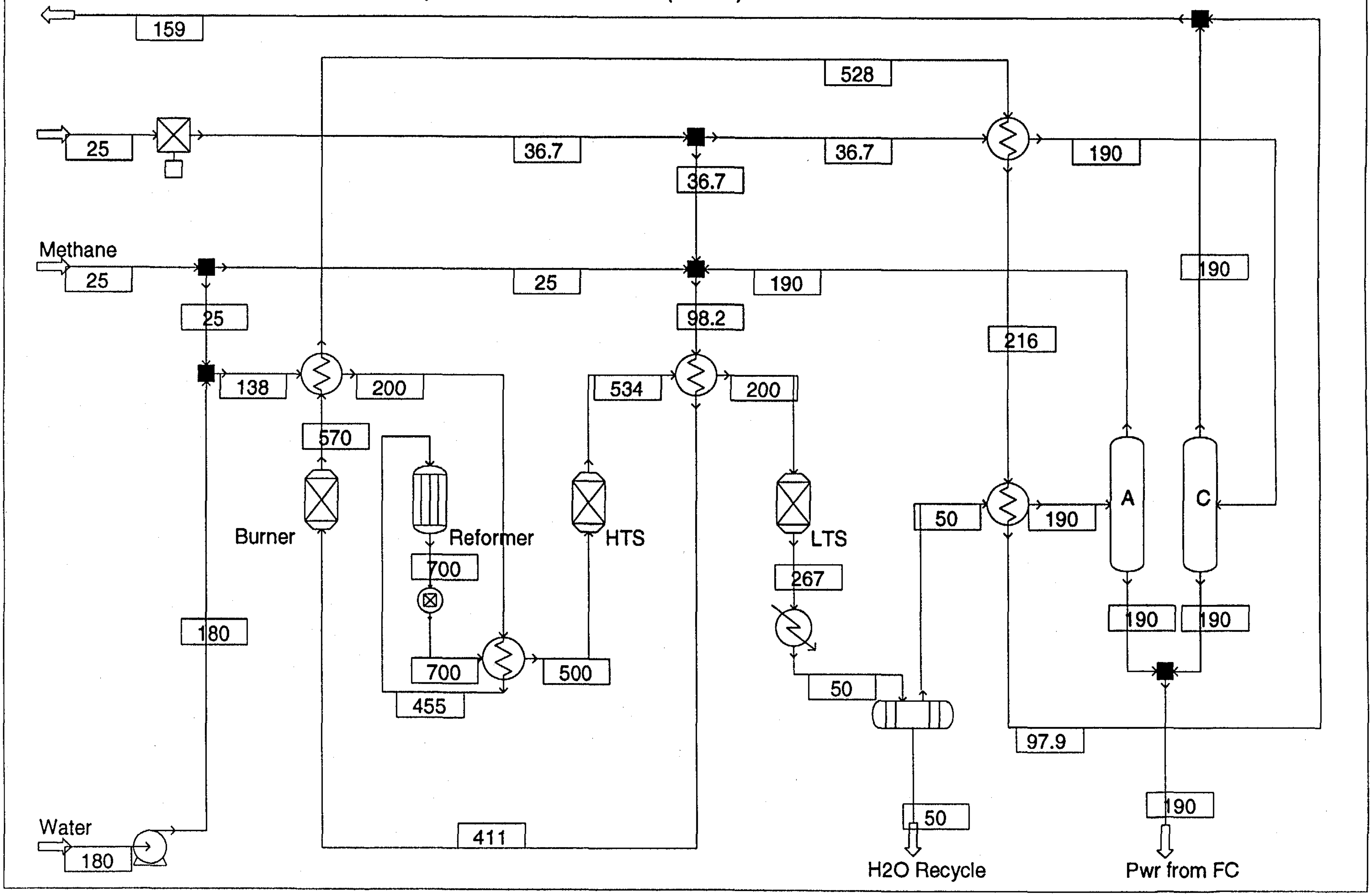
Methane Steam Reforming integrated with Phosphoric Acid Fuel Cell (1 atm)



For simulation: numbers in boxes are stream numbers
numbers in circles are component numbers

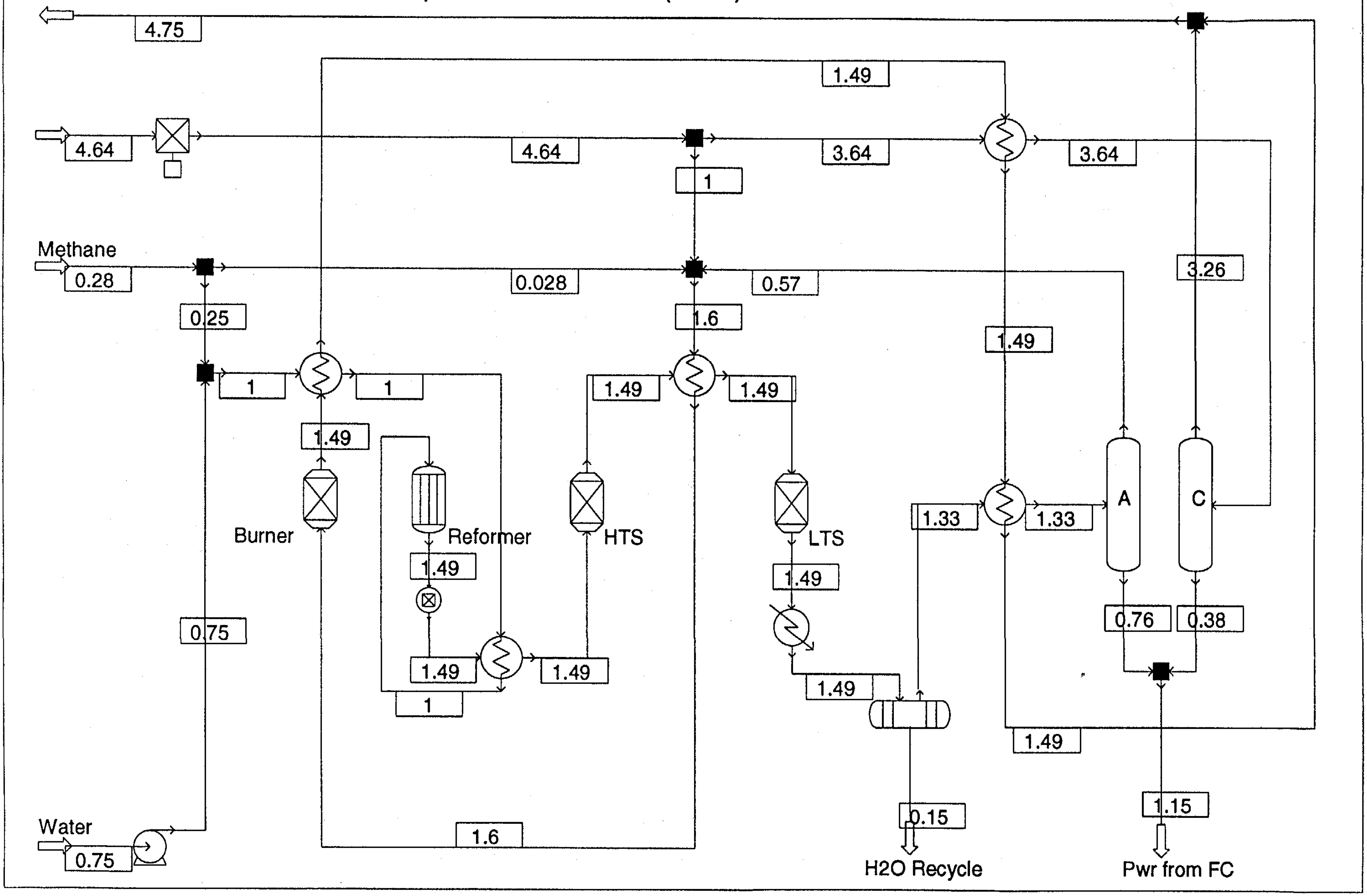
Methane Steam Reforming integrated with Phosphoric Acid Fuel Cell (1 atm)

Temperatures, C



Methane Steam Reforming integrated with Phosphoric Acid Fuel Cell (1 atm)

Flow Rates, kmol/hr



Case 8: Autothermal Reforming - Methane - PAFC (1 atm)

Case 8: Autothermal Reforming - Methane - PAFC (1 atm)

Methane Autothermal Reformer Integrated with PAFC Design Basis

1. Phosphoric Acid Fuel Cell Conditions

Gross DC Power	kW	25
Current Density	mA/cm2	323
Temperature	C	190
	K	463
Pressure	atm	1
H2 Utilization	Uf	80%
O2 Utilization	Uo	50%

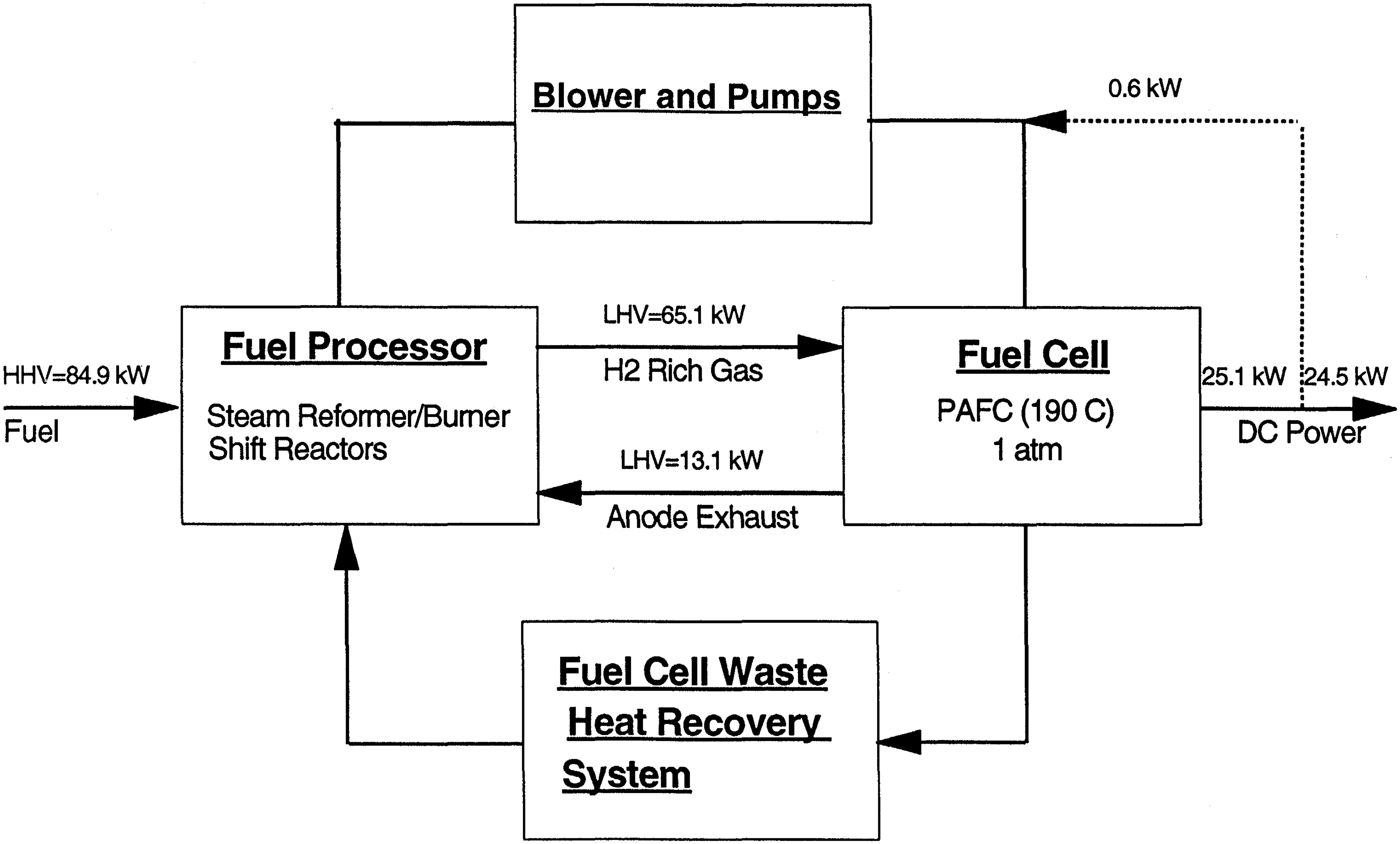
2. Reformer Conditions

Temperature	C	Adiabatic Reactor
Pressure	atm	1
Steam/Fuel Ratio	molar	1
Oxygen/Fuel Ratio	molar	0.6

3. Parasitic System Assumptions

Pump Efficiency	70.0%
Blower Efficiency	70.0%

Methane Autothermal Reformer integrated with PAFC: Overall Block Diagram



Fuel Processing Efficiency E(FP) = 76.7% (85.0% LHV/LHV)
Gross System Efficiency E(Gross) = 29.6%
Net System Efficiency E(Net) = 28.9%

Methane Autothermal Reformer Integrated with PAFC

Overall Balance:

Total Fuel to FP	kmol/hr	0.343
	kg/hr	5.509
HHV of Total Fuel to FP	J/hr	-3.1E+08
	kW	84.9
LHV of Total Fuel to FP	J/hr	-2.8E+08
		76.5
Total Flow Into Anode	kmol/hr	2.298
	kg/hr	42.688
LHV of Anode Feed	J/hr	-2.3E+08
	kW	65.1
Flow of Anode Exhaust	kmol/hr	1.530
	kg/hr	41.140
LHV of Anode Exhaust	J/hr	-4.7E+07
	kW	13.1
Gross DC Power	kW	25.1
Net DC Power	kW	24.5
Parasitic Power	kW	0.6

Efficiencies based on HHV of Fuel:

		LHV/HHV
Fuel Processing Efficiency	E(FP)	76.7%
Gross System Efficiency	E(Gross)	29.6%
Net System Efficiency	E(Net)	28.9%

Efficiencies based on LHV of Fuel:

		LHV/LHV
Fuel Processing Efficiency	E(FP)	85.0%
Gross System Efficiency	E(Gross)	32.8%
Net System Efficiency	E(Net)	32.0%

Methane Autothermal Reformer Integrated with PAFC Fuel Processor Conditions

A. Reformer

Inlet Temperature		500
Outlet Temperature	C	890
Pressure	atm	1
Steam/Fuel Ratio	molar	1
Oxygen/Fuel Ratio	molar	0.6
Air/Fuel Ratio	molar	2.9
Oxygen Content in Air	molar	21%
Total Inlet Flow	kmol/hr	1.668
	kg/hr	40.002

Inlet Composition:	*kmol/hr*	*mol%*
Water	0.343	20.6%
Methane	0.343	20.6%
Oxygen	0.206	12.4%
Nitrogen	0.775	46.5%
Total	1.668	100.0%

Outlet Composition:	*kmol/hr*	*mol%*	*mol%(Dry)*
Water	0.325	15.1%	0.0%
Methane	0.000	0.0%	0.0%
Carbon Monoxide	0.256	11.9%	14.0%
Carbon Dioxide	0.088	4.1%	4.8%
Hydrogen	0.705	32.8%	38.7%
Oxygen	0.000	0.0%	0.0%
Nitrogen	0.775	36.1%	42.5%
Nitric Oxide	0.000	0.0%	0.0%
Nitrogen Dioxide	0.000	0.0%	0.0%
Nitrous Oxide	0.000	0.0%	0.0%
Ammonia	0.000	0.0%	0.0%
Total	2.149	100.0%	100.0%

Methane Autothermal Reformer Integrated with PAFC Fuel Processor Conditions

B. Burner:

Inlet Temperature	C	444
Outlet Temperature	C	1075
Pressure	atm	1
Supplemental Fuel	kmol/hr	0.000
	kg/hr	0.000
Air Flow	kmol/hr	0.558
	kg/hr	16.089
Total Inlet Flow	kmol/hr	2.087
	kg/hr	57.230

Inlet Composition:	*kmol/hr*	*mol%*	*mol%(Dry)*
Water	0.219	10.5%	0.0%
Methane	0.000	0.0%	0.0%
Carbon Monoxide	0.001	0.1%	0.1%
Carbon Dioxide	0.342	16.4%	18.3%
Hydrogen	0.192	9.2%	10.3%
Oxygen	0.117	5.6%	6.3%
Nitrogen	1.216	58.2%	65.1%
Nitric Oxide	0.000	0.0%	0.0%
Nitrogen Dioxide	0.000	0.0%	0.0%
Nitrous Oxide	0.000	0.0%	0.0%
Ammonia	0.000	0.0%	0.0%
Total	2.087	100.0%	100.0%

Outlet Composition:	*kmol/hr*	*mol%*	*mol%(Dry)*
Water	0.411	20.7%	0.0%
Methane	0.000	0.0%	0.0%
Carbon Monoxide	0.000	0.0%	0.0%
Carbon Dioxide	0.343	17.3%	21.7%
Hydrogen	0.000	0.0%	0.0%
Oxygen	0.020	1.0%	1.3%
Nitrogen	1.216	61.1%	77.0%
Nitric Oxide	0.000	0.0%	0.0%
Nitrogen Dioxide	0.000	0.0%	0.0%
Nitrous Oxide	0.000	0.0%	0.0%
Ammonia	0.000	0.0%	0.0%
Total	1.991	100.0%	100.0%

Methane Autothermal Reformer Integrated with PAFC Fuel Processor Conditions

C. High Temperature Shift (HTS) Reactor:

Inlet Temperature	C	450
Outlet Temperature	C	522
Pressure	atm	1
Total Inlet Flow	kmol/hr	2.707
	kg/hr	50.071

Outlet Composition:	*kmol/hr*	*mol%*	*mol%(Dry)*
Water	0.707	26.1%	0.0%
Methane	0.000	0.0%	0.0%
Carbon Monoxide	0.079	2.9%	4.0%
Carbon Dioxide	0.264	9.7%	13.2%
Hydrogen	0.882	32.6%	44.1%
Oxygen	0.000	0.0%	0.0%
Nitrogen	0.775	28.6%	38.7%
Nitric Oxide	0.000	0.0%	0.0%
Nitrogen Dioxide	0.000	0.0%	0.0%
Nitrous Oxide	0.000	0.0%	0.0%
Ammonia	0.000	0.0%	0.0%
Total	2.707	100.0%	100.0%

D. Low Temperature Shift (LTS) Reactor:

Inlet Temperature	C	150
Outlet Temperature	C	187
Pressure	atm	1
Total Inlet Flow	kmol/hr	2.707
	kg/hr	50.071

Outlet Composition:	*kmol/hr*	*mol%*	*mol%(Dry)*
Water	0.629	23.2%	0.0%
Methane	0.000	0.0%	0.0%
Carbon Monoxide	0.001	0.0%	0.1%
Carbon Dioxide	0.342	12.6%	16.5%
Hydrogen	0.960	35.5%	46.2%
Oxygen	0.000	0.0%	0.0%
Nitrogen	0.775	28.6%	37.3%
Nitric Oxide	0.000	0.0%	0.0%
Nitrogen Dioxide	0.000	0.0%	0.0%
Nitrous Oxide	0.000	0.0%	0.0%
Ammonia	0.000	0.0%	0.0%
Total	2.707	100.0%	100.0%

Methane Autothermal Reformer Integrated with PAFC Fuel Cell Conditions (Phosphoric Acid)

Anode:

Temperature	C	190
Pressure	atm	1.1
Total Anode Flow	kmol/hr	2.298
	kg/hr	42.688

Inlet Composition:	*kmol/hr*	*mol%*	*mol%(Dry)*
Water	0.219	9.5%	0.0%
Methane	0.000	0.0%	0.0%
Carbon Monoxide	0.001	0.1%	0.1%
Carbon Dioxide	0.342	14.9%	16.5%
Hydrogen	0.960	41.8%	46.2%
Oxygen	0.000	0.0%	0.0%
Nitrogen	0.775	33.7%	37.3%
Nitric Oxide	0.000	0.0%	0.0%
Nitrogen Dioxide	0.000	0.0%	0.0%
Nitrous Oxide	0.000	0.0%	0.0%
Ammonia	0.000	0.0%	0.0%
Total	2.298	100.0%	100.0%

Cathode:

Temperature	C	190
Pressure	atm	1
Total Cathode Flow	kmol/hr	3.657
	kg/hr	105.505

Inlet Composition:	*kmol/hr*	*mol%*
Oxygen	0.768	21.0%
Nitrogen	2.889	79.0%
Total	3.657	100.0%

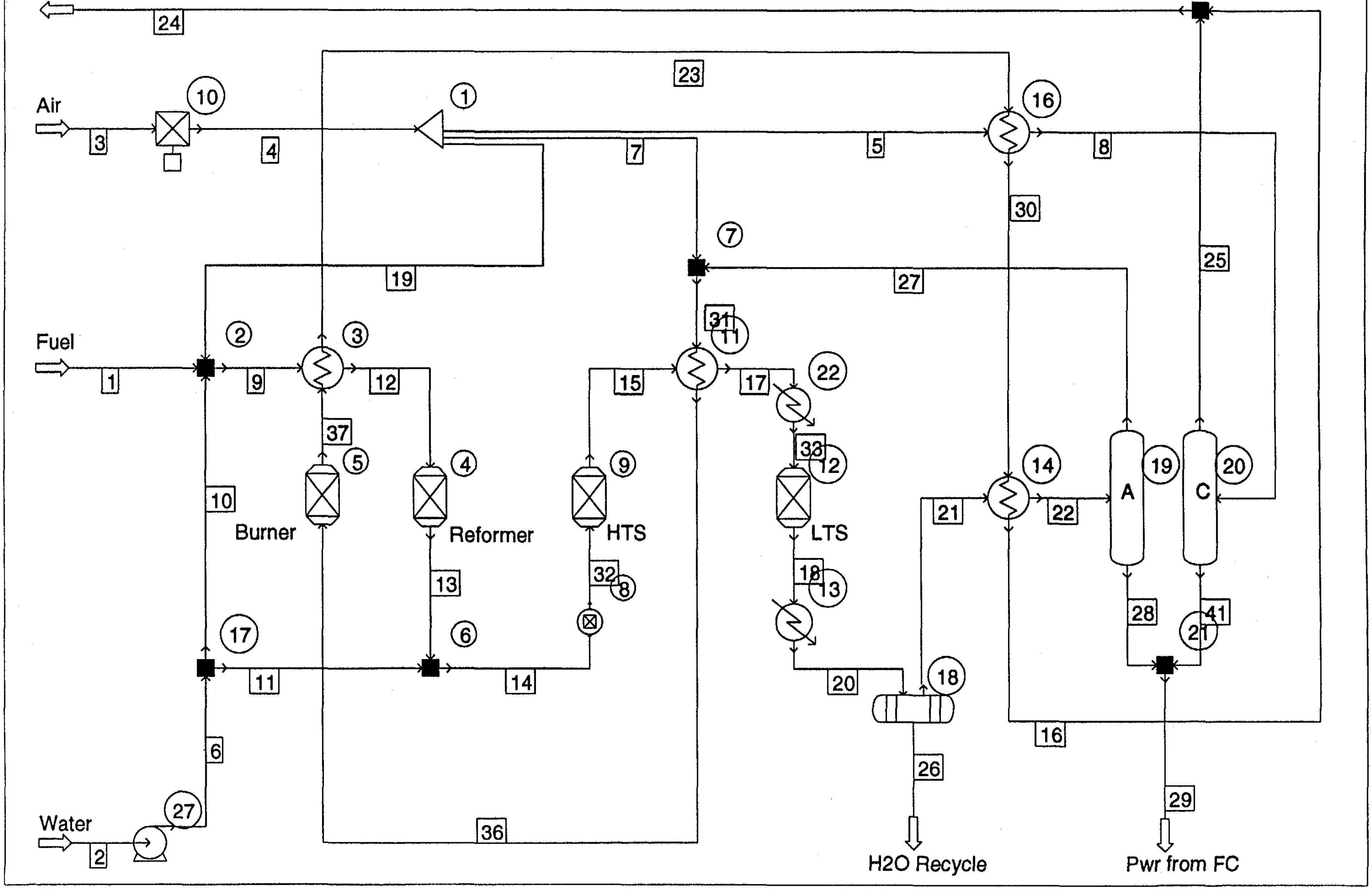
Methane Autothermal Reformer Integrated with PAFC Air Compression/Power Recovery System

Water Feed Pump	kW	0.000
FC Cooling Water Pump	kW	0.102
Air Blower	kW	0.494
Total Parasitic Power	kW	0.6
% of Gross DC Power		2.4%

Methane Autothermal Reformer Integrated with PAFC Efficiencies

Thermodynamic Efficiency	E(Th)	91.8%
Voltage Efficiency	E(V)	52.6%
Current Efficiency	E(I)	80.0%
Electrochemical Efficiency	E(E)	38.7%
Heating Value Efficiency	E(H)	99.8%
Fuel Cell Efficiency	E(FC)	38.6%
Fuel Processing Efficiency	E(FP)	76.7%
Gross System Efficiency	E(Gross)	29.6%
Net System Efficiency	E(Net)	28.9%
Gross DC Power	kW	25.1
Net DC Power	kW	24.5
Parasitic Power	kW	0.6

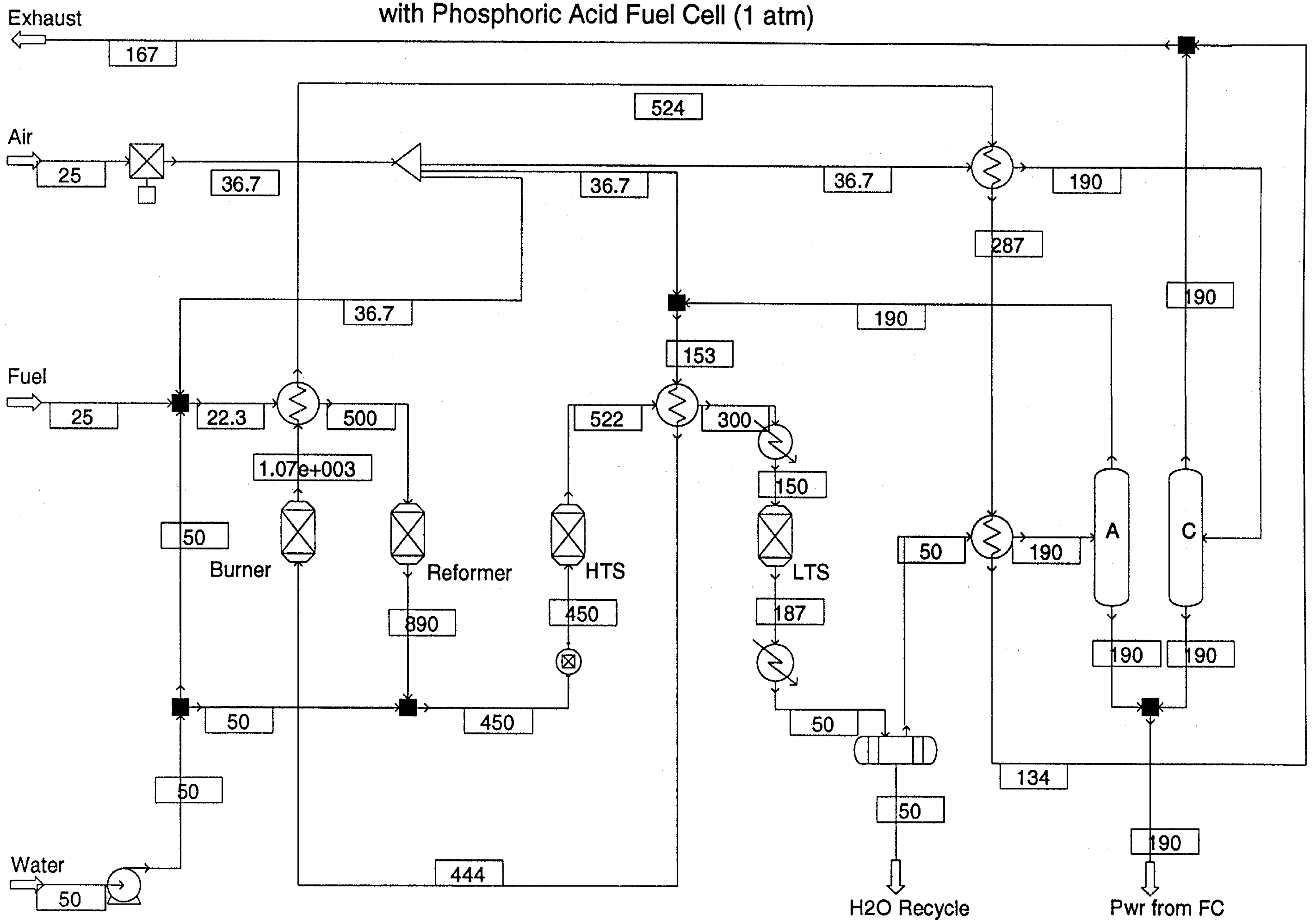
Methane Autothermal Reforming integrated with Phosphoric Acid Fuel Cell (1 atm)

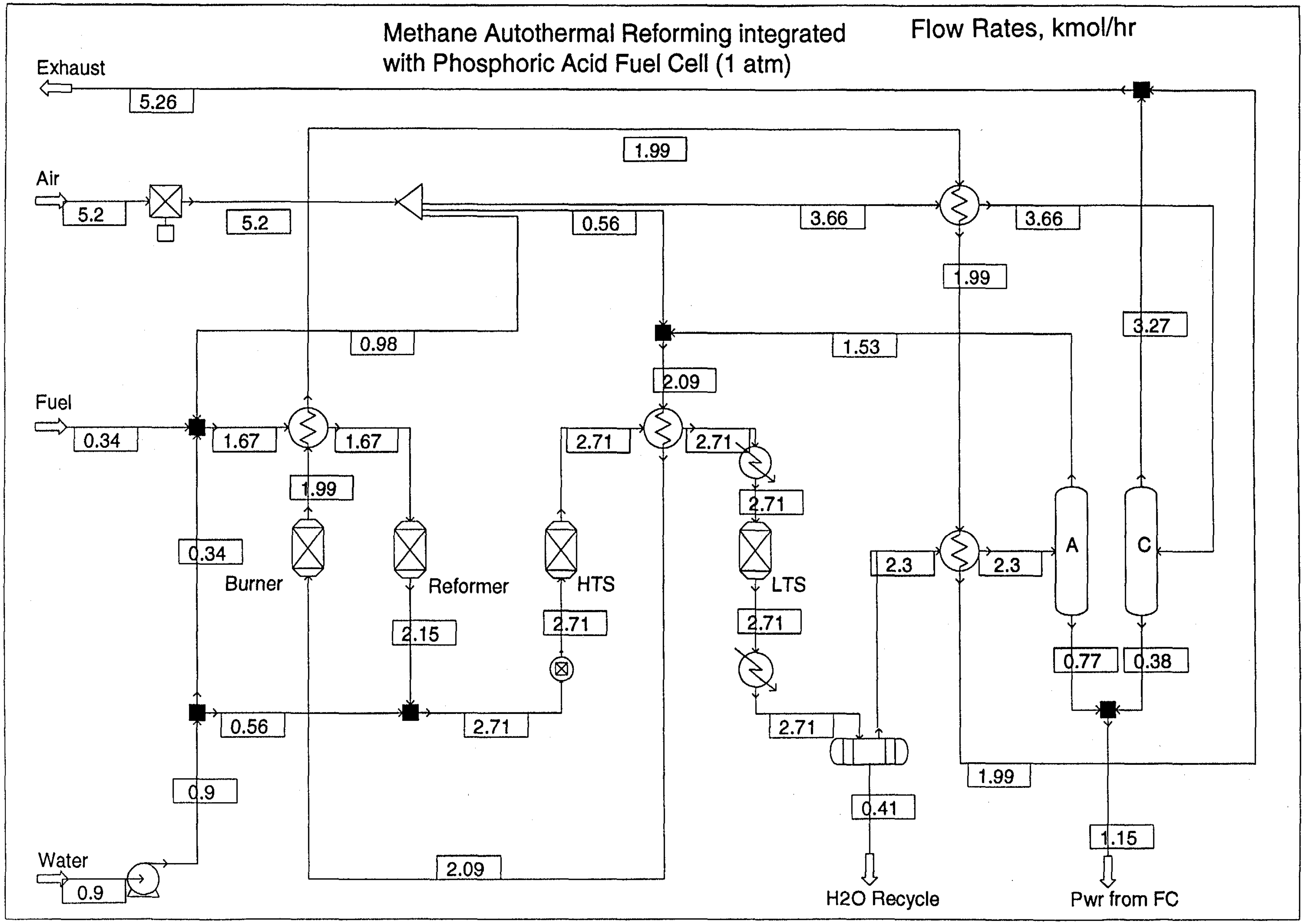


For simulation: numbers in boxes are stream numbers
numbers in circles are component numbers

Methane Autothermal Reforming integrated with Phosphoric Acid Fuel Cell (1 atm)

Temperatures, C





Methane Autothermal Reforming integrated with Phosphoric Acid Fuel Cell (1 atm)

Flow Rates, kmol/hr

Case 9: Partial Oxidation Reforming - Methane - PAFC (1 atm)

Case 9: Partial Oxidation Reforming - Methane - PAFC (1 atm)

Methane Partial Oxidation Reformer Integrated with PAFC Design Basis

1. Phosphoric Acid Fuel Cell Conditions

Gross DC Power	kW	25
Current Density	mA/cm2	323
Temperature	C	190
	K	463
Pressure	atm	1
H2 Utilization	Uf	80%
O2 Utilization	Uo	50%

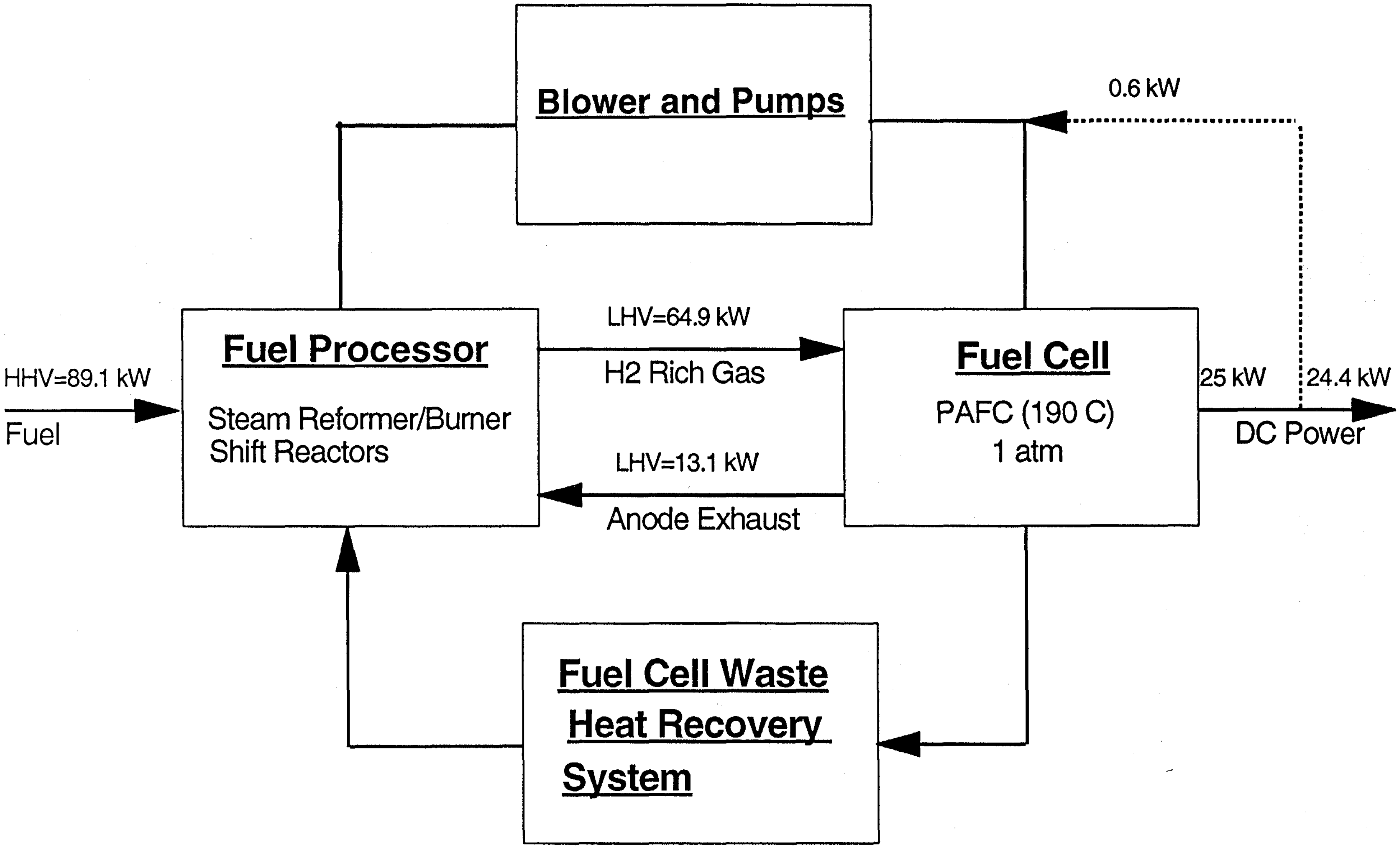
2. Reformer Conditions

Temperature	C	Adiabatic Reactor
Pressure	atm	1
Steam/Fuel Ratio	molar	0
Oxygen/Fuel Ratio	molar	0.67

3. Parasitic System Assumptions

Pump Efficiency	70.0%
Blower Efficiency	70.0%

Methane Partial Oxidation Reformer Integrated with PAFC: Block Diagram



Blower and Pumps

0.6 kW

HHV=89.1 kW

Fuel

Fuel Processor

Steam Reformer/Burner
Shift Reactors

LHV=64.9 kW

H2 Rich Gas

LHV=13.1 kW

Anode Exhaust

Fuel Cell

PAFC (190 C)
1 atm

25 kW

24.4 kW

DC Power

Fuel Cell Waste Heat Recovery System

Fuel Processing Efficiency E(FP) = 72.8% (80.8% LHV/LHV)
Gross System Efficiency E(Gross) = 28.1%
Net System Efficiency E(Net) = 27.4%

Methane Partial Oxidation Reformer Integrated with PAFC

Overall Balance:

Total Fuel to FP	kmol/hr	0.361
	kg/hr	5.785
HHV of Total Fuel to FP	J/hr	-3.2E+08
	kW	89.1
LHV of Total Fuel to FP	J/hr	-2.9E+08
		80.3
Total Flow Into Anode	kmol/hr	2.462
	kg/hr	47.461
LHV of Anode Feed	J/hr	-2.3E+08
	kW	64.9
Flow of Anode Exhaust	kmol/hr	1.696
	kg/hr	45.917
LHV of Anode Exhaust	J/hr	-4.7E+07
	kW	13.1
Gross DC Power	kW	25.0
Net DC Power	kW	24.4
Parasitic Power	kW	0.6

Efficiencies based on HHV of Fuel:

		LHV/HHV
Fuel Processing Efficiency	E(FP)	72.8%
Gross System Efficiency	E(Gross)	28.1%
Net System Efficiency	E(Net)	27.4%

Efficiencies based on LHV of Fuel:

		LHV/LHV
Fuel Processing Efficiency	E(FP)	80.8%
Gross System Efficiency	E(Gross)	31.1%
Net System Efficiency	E(Net)	30.4%

Methane Partial Oxidation Reformer Integrated with PAFC Fuel Processor Conditions

A. Reformer

Inlet Temperature		500
Outlet Temperature	C	1105
Pressure	atm	1
Steam/Fuel Ratio	molar	0
Oxygen/Fuel Ratio	molar	0.67
Air/Fuel Ratio	molar	3.19
Oxygen Content in Air	molar	21%
Total Inlet Flow	kmol/hr	1.511
	kg/hr	38.973

Inlet Composition:	*kmol/hr*	*mol%*
Water	0.000	0.0%
Methane	0.361	23.9%
Oxygen	0.242	16.0%
Nitrogen	0.909	60.1%
Total	1.511	100.0%

Outlet Composition:	*kmol/hr*	*mol%*	*mol%(Dry)*
Water	0.099	5.0%	0.0%
Methane	0.000	0.0%	0.0%
Carbon Monoxide	0.337	16.9%	17.8%
Carbon Dioxide	0.024	1.2%	1.3%
Hydrogen	0.622	31.3%	32.9%
Oxygen	0.000	0.0%	0.0%
Nitrogen	0.909	45.7%	48.0%
Nitric Oxide	0.000	0.0%	0.0%
Nitrogen Dioxide	0.000	0.0%	0.0%
Nitrous Oxide	0.000	0.0%	0.0%
Ammonia	0.000	0.0%	0.0%
Total	1.991	100.0%	100.0%

Methane Partial Oxidation Reformer Integrated with PAFC Fuel Processor Conditions

B. Burner:

Inlet Temperature	C	445
Outlet Temperature	C	1015
Pressure	atm	1
Supplemental Fuel	kmol/hr	0.000
	kg/hr	0.000
Air Flow	kmol/hr	0.630
	kg/hr	18.176
Total Inlet Flow	kmol/hr	2.326
	kg/hr	64.093

Inlet Composition:	*kmol/hr*	*mol%*	*mol%(Dry)*
Water	0.235	10.1%	0.0%
Methane	0.000	0.0%	0.0%
Carbon Monoxide	0.002	0.1%	0.1%
Carbon Dioxide	0.359	15.4%	17.2%
Hydrogen	0.191	8.2%	9.2%
Oxygen	0.132	5.7%	6.3%
Nitrogen	1.407	60.5%	67.3%
Nitric Oxide	0.000	0.0%	0.0%
Nitrogen Dioxide	0.000	0.0%	0.0%
Nitrous Oxide	0.000	0.0%	0.0%
Ammonia	0.000	0.0%	0.0%
Total	2.326	100.0%	100.0%

Outlet Composition:	*kmol/hr*	*mol%*	*mol%(Dry)*
Water	0.426	19.1%	0.0%
Methane	0.000	0.0%	0.0%
Carbon Monoxide	0.000	0.0%	0.0%
Carbon Dioxide	0.361	16.2%	20.0%
Hydrogen	0.000	0.0%	0.0%
Oxygen	0.036	1.6%	2.0%
Nitrogen	1.406	63.1%	78.0%
Nitric Oxide	0.000	0.0%	0.0%
Nitrogen Dioxide	0.000	0.0%	0.0%
Nitrous Oxide	0.000	0.0%	0.0%
Ammonia	0.000	0.0%	0.0%
Total	2.229	100.0%	100.0%

Methane Partial Oxidation Reformer Integrated with PAFC Fuel Processor Conditions

C. High Temperature Shift (HTS) Reactor:

Inlet Temperature	C	450
Outlet Temperature	C	546
Pressure	atm	1
Total Inlet Flow	kmol/hr	2.740
	kg/hr	52.473

Outlet Composition:	*kmol/hr*	*mol%*	*mol%(Dry)*
Water	0.614	22.4%	0.0%
Methane	0.000	0.0%	0.0%
Carbon Monoxide	0.103	3.7%	4.8%
Carbon Dioxide	0.258	9.4%	12.1%
Hydrogen	0.857	31.3%	40.3%
Oxygen	0.000	0.0%	0.0%
Nitrogen	0.909	33.2%	42.7%
Nitric Oxide	0.000	0.0%	0.0%
Nitrogen Dioxide	0.000	0.0%	0.0%
Nitrous Oxide	0.000	0.0%	0.0%
Ammonia	0.000	0.0%	0.0%
Total	2.740	100.0%	100.0%

D. Low Temperature Shift (LTS) Reactor:

Inlet Temperature	C	150
Outlet Temperature	C	197
Pressure	atm	1
Total Inlet Flow	kmol/hr	2.740
	kg/hr	52.473

Outlet Composition:	*kmol/hr*	*mol%*	*mol%(Dry)*
Water	0.513	18.7%	0.0%
Methane	0.000	0.0%	0.0%
Carbon Monoxide	0.002	0.1%	0.1%
Carbon Dioxide	0.359	13.1%	16.1%
Hydrogen	0.957	34.9%	43.0%
Oxygen	0.000	0.0%	0.0%
Nitrogen	0.909	33.2%	40.8%
Nitric Oxide	0.000	0.0%	0.0%
Nitrogen Dioxide	0.000	0.0%	0.0%
Nitrous Oxide	0.000	0.0%	0.0%
Ammonia	0.000	0.0%	0.0%
Total	2.740	100.0%	100.0%

Methane Partial Oxidation Reformer Integrated with PAFC Fuel Cell Conditions (Phosphoric Acid)

Anode:

Temperature	C	190
Pressure	atm	1.1
Total Anode Flow	kmol/hr	2.462
	kg/hr	47.461

Inlet Composition:	*kmol/hr*	*mol%*	*mol%(Dry)*
Water	0.235	9.5%	0.0%
Methane	0.000	0.0%	0.0%
Carbon Monoxide	0.002	0.1%	0.1%
Carbon Dioxide	0.359	14.6%	16.1%
Hydrogen	0.957	38.9%	43.0%
Oxygen	0.000	0.0%	0.0%
Nitrogen	0.909	36.9%	40.8%
Nitric Oxide	0.000	0.0%	0.0%
Nitrogen Dioxide	0.000	0.0%	0.0%
Nitrous Oxide	0.000	0.0%	0.0%
Ammonia	0.000	0.0%	0.0%
Total	2.462	100.0%	100.0%

Cathode:

Temperature	C	190
Pressure	atm	1
Total Cathode Flow	kmol/hr	3.648
	kg/hr	105.234

Inlet Composition:	*kmol/hr*	*mol%*
Oxygen	0.766	21.0%
Nitrogen	2.882	79.0%
Total	3.648	100.0%

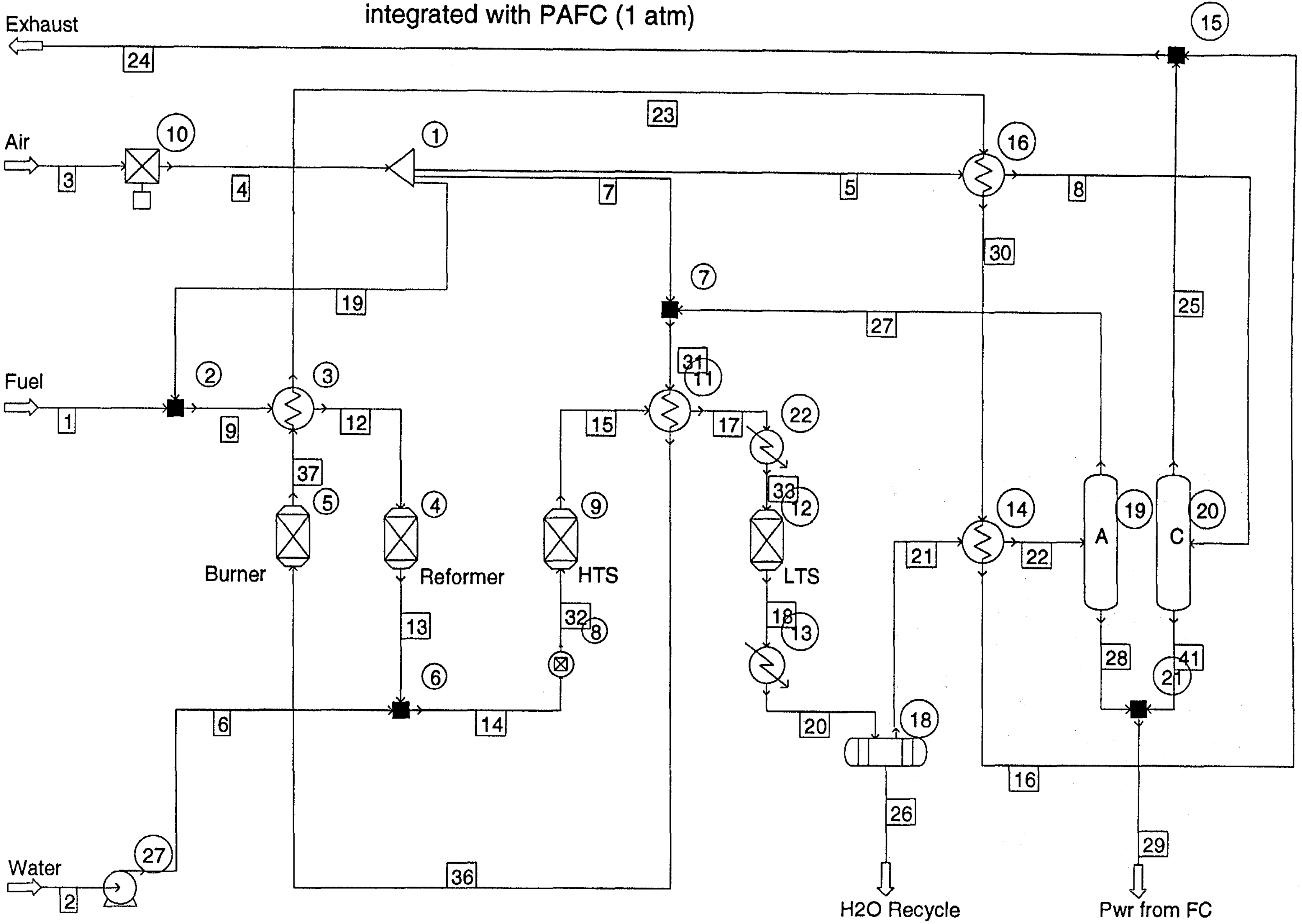
Methane Partial Oxidation Reformer Integrated with PAFC Air Compression/Power Recovery System

Water Feed Pump	kW	0.000
FC Cooling Water Pump	kW	0.102
Air Blower	kW	0.516
Total Parasitic Power	kW	0.6
% of Gross DC Power		2.5%

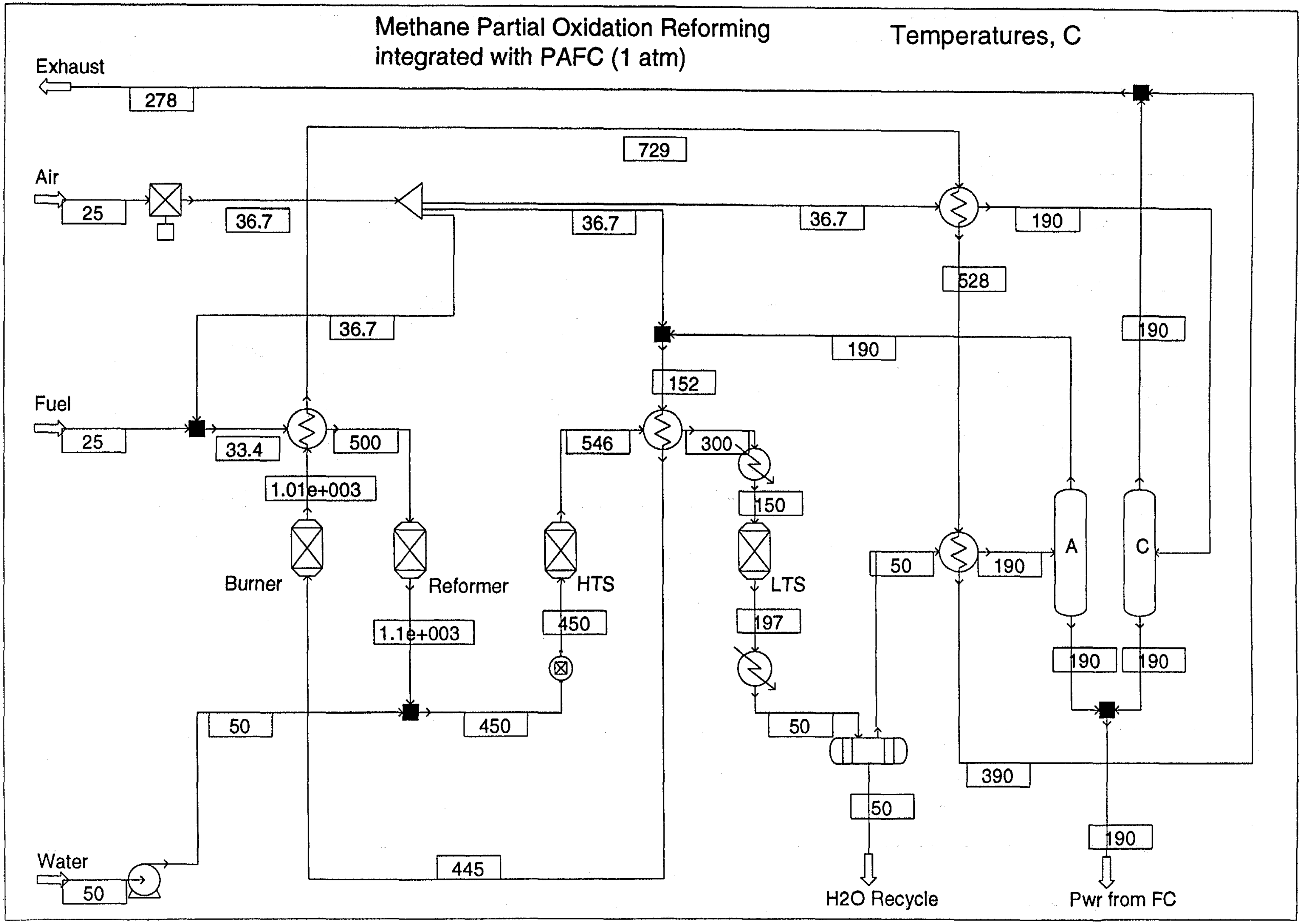
Methane Partial Oxidation Reformer Integrated with PAFC Efficiencies

Thermodynamic Efficiency	E(Th)	91.7%
Voltage Efficiency	E(V)	52.6%
Current Efficiency	E(I)	80.0%
Electrochemical Efficiency	E(E)	38.6%
Heating Value Efficiency	E(H)	99.8%
Fuel Cell Efficiency	E(FC)	38.5%
Fuel Processing Efficiency	E(FP)	72.8%
Gross System Efficiency	E(Gross)	28.1%
Net System Efficiency	E(Net)	27.4%
Gross DC Power	kW	25.0
Net DC Power	kW	24.4
Parasitic Power	kW	0.6

Methane Partial Oxidation Reforming integrated with PAFC (1 atm)



For simulation: numbers in boxes are stream numbers
numbers in circles are component numbers



Methane Partial Oxidation Reforming integrated with PAFC (1 atm)

Temperatures, C

Methane Partial Oxidation Reforming integrated with PAFC (1 atm)

Flow Rates, kmol/hr