

2000 National Student Design Competition

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Please read the rules on the following pages carefully before submitting a solution to AIChE

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2000 AICHE NATIONAL STUDENT DESIGN COMPETITION

Process Synthesis and Design of the Power Generation System for Automobiles: A Fuel Cell Approach

DEADLINE FOR MAILING

Solutions must be postmarked no later than midnight, June 4, 2000.

RULES OF THE CONTEST

Solutions will be graded on (a) substantial correctness of results and soundness of conclusions, (b) ingenuity and logic employed, (c) accuracy of computations, and (d) form of presentation. Accuracy of computations is intended to mean primarily freedom from mistakes; extreme precision is not necessary.

It is to be assumed that the statement of the problem contains all the pertinent data for those available in handbooks and literature references. The use of textbooks, handbooks, journal articles, and lecture notes is permitted.

Students may use any available commercial or library computer programs in preparing their solutions. Students are warned, however, that physical property data built into such programs may differ from data given in the problem statement. In such cases, as with data from other literature sources, values given in the problem statement are most applicable. Students using commercial or library computer programs or other solution aids should so state in their reports and include proper references and documentation. Judging, however, will be based on the overall suitability of the solutions, not on skills in manipulating computer programs.

The 2000 National Student Design Competition is designed to be solved either by an individual chemical engineering student working entirely alone, or a group of no more than three students working together. Solution will be judged in two categories: individual and team. There are, however, other academically sound approaches to using the problem, and it is expected that some Advisors will use the problem as classroom material. The following confidentiality rules therefore apply:

- 1. For individual students or teams whose solutions may be considered for the contest:

 The problem may not be discussed with anyone (students, faculty, or others, in or out of class) before or during the period allowed for solutions. Discussion with faculty and students at that college or university is permitted only after complete final reports have been submitted to the Chapter Advisor.
- 2. For students whose solutions are not intended for the contest:

 Discussion with faculty and with other students at that college or university who are not participating in the contest is permitted.
- 3. For all students:

The problem may not be discussed with students or faculty from other colleges or universities, or with individuals in the same institution who are still working on the problem for the contest, until after June 4, 2000. This is particularly important in cases where neighboring institutions may be using different schedules.

Submission of a solution for the competition implies strict adherence to the following conditions:

(Failure to comply will result in solutions being returned to the appropriate Faculty Advisor for revision. Revised submissions must meet the original deadline.)

ELIGIBILITY

- Sound on the National Student Members May Submit a Solution. Non-member entries will not be considered.
- Entries may be submitted either by individuals or by teams of no more than three students. Each team member must meet all eligibility requirements.
- Each Faculty Advisor should select the best solution or solutions, not to exceed two from each category (individual and team), from his or her chapter and send these by registered mail, as per the below instructions, to the Institute.

TIMELINE FOR COMPLETING THE SOLUTION

- A period of no more than thirty days is allowed for completion of the solution. This period may be selected at the discretion of the individual advisor, but in order to be eligible for an award, a solution must be postmarked no later than midnight, June 4, 2000.
- THE FINISHED REPORT SHOULD BE SUBMITTED TO THE FACULTY ADVISOR WITHIN THE 30-DAY PERIOD.

REPORT FORMAT

- The body of the report must be suitable for reproduction, that is, typewritten or computergenerated. Tables may be written in ink. Supporting calculations and other appendix material may be in pencil.
- The solution itself must bear no reference to the students' names or institution by which it might be identified. In this connection, graph paper bearing the name of the institution should not be used.

SENDING THE SOLUTION TO AICHE

- Two copies of each of the solution(s) must be sent to the address below; original manuscript(s) must remain in the possession of the Student Chapter Advisor, or Faculty Advisor, sponsoring the student(s)
- There should not be any variation in form of content between the solution submitted to the Faculty Advisor and that sent to the AIChE office.
- Each copy must be accompanied by the enclosed ENTRY FORM giving each contestant's name, AIChE membership number, college or university, Faculty Advisor name, address, home address, home telephone number, and student chapter, lightly attached to the report. This form will be retained for identification by the executive director of the Institute.
- DEADLINE: Entries must be postmarked no later than <u>midnight</u>, June 4, 2000. As soon as the winners have been notified, original manuscripts must be forwarded to the office of the executive director as soon as possible.

SEND TO:

Awards Administrator
American Institute of Chemical Engineers
3 Park Avenue
New York, New York 10016-5991

DEADLINE: JUNE 4, 2000

Process Synthesis and Design of the Power Generation System for Automobiles: A Fuel Cell Approach

"By the year 2015, fuel cells could be the primary source of power on vehicles and achieve levels of fuel economy and emissions performance only dreamed of today." (Chrysler Corporation)

Introduction

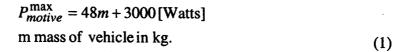
Fuel cells - used extensively on spacecraft - are potential long-term successors to the internal combustion engine. They operate with system efficiencies that are better than those of the conventional internal combustion engine and have lower emissions from the vehicle. The most likely choice of fuel cell for vehicles is the Proton Exchange Membrane, (PEM), design. These fuel cells would receive power from hydrogen, which could be either stored on-board the vehicle, or produced on-board by extracting hydrogen out of gasoline or methanol. Each fuel cell module in the stack generates electricity directly from a chemical reaction between hydrogen and oxygen, from ambient air, over platinum catalysts. The electrical energy generated from the process is then applied to power a traction motor - or motors - that drive the vehicle wheels.

Although hydrogen storage is possible, it does not seem feasible for vehicles intended for long range operation (ca. 600 kilometers), such as personal transportation. Hydrogen is difficult to distribute, has low energy density and the cost of on-board storage systems is currently very high. This leaves the option of generating the hydrogen on-board via a *fuel processing system* (see Figure 1). The effective design of the fuel processing system will be critical to the overall success of fuel cell vehicles. Your assignment is to make a preliminary design assessment of the most economic fuel processing system from among the choices described below. This cannot be carried out in isolation from the fuel cell design and hence a preliminary specification of this sub-system must also be made.

Vehicle Performance

The starting point of the problem is the power required to provide acceptable performance for the vehicle. To simplify the problem you are to consider designs where the fuel cell provides all the power necessary for the vehicle during all phases of its driving, except at start-up where additional energy storage will be supplied. You can assume that this small amount of energy will be generated during operation, either from electrical energy storage (batteries) or compressed hydrogen storage, and you do NOT need to consider its design. The maximum motive power required, power to enable the car to accelerate and cruise, is a function of the mass of the vehicle, its acceleration and road conditions. This can be approximated by Equation 1. The mass of the vehicle, including passengers and luggage but without the fuel processing system, is 1250 kg. Additional power is required for other functions, such as air conditioning, lighting, windshield wipers, etc, and totals 7 kW. This does not include any power required for the fuel processing system itself. The power demand is defined as the sum of the motive, auxiliary and fuel processing power requirements. The cruising range of the vehicle should be 600 kilometers and you should

assume that the average power demand is 35% of the maximum power demand. The annual distance that the vehicle is driven 20,000 kilometers. The life of the vehicle should be 5 years with a scrap value equal to 30% of its initial cost. Other non-fuel operating costs will be the same for each type of vehicle and all options.



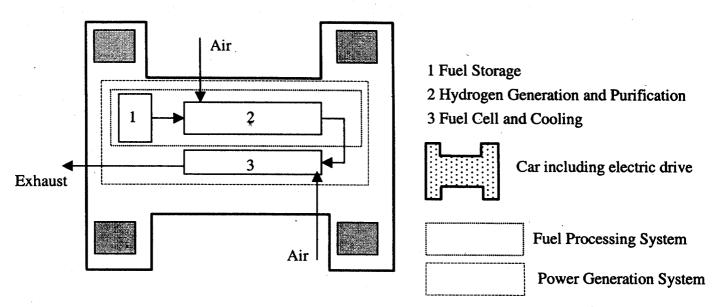


Figure 1 Overall Schematic of a Vehicle (Not to Scale)

The Fuels

The PEM fuel cell is extremely sensitive to poisoning with sulphur, thus it is expected that for both gasoline and methanol the sulphur content will be reduced to negligible levels by treatment at the processing plant. Gasoline is a mixture of many compounds and a surrogate formula of $C_{7.14}H_{14.25}$ should be used throughout; the table below gives the properties from Adler [1986].

	Fuel	Molecular Formula	Molecular Weight	Lower Heating Value kJ/mol	Boiling point, °C	Heat of Vaporization kJ/mol	Heat Capacity of vapor J/mol/K	Liquid Density Kg/m³
-	Gasoline	$C_{7.14}H_{14.25}$	100	4270	100	31	180	720.83

The cost at the pump for both gasoline and methanol is assumed to be equal to \$1.00 per U.S. gallon. This assumption avoids complex issues on recouping the investment costs of building the infrastructure necessary to provide methanol on a national basis, and the differences in taxation that currently exist between gasoline and methanol.

Fuel Processing System - Base Case Design

Figure 2 gives the basic schematic of the conversion of gasoline to hydrogen. The gasoline is first converted into a mixture of hydrogen, water, carbon monoxide and carbon dioxide in an auto-reformer. A particular version of autoreforming is the HotSpot Reactor [Edwards 98] described in the reactor design section. The composition of the mixture is governed by the oxygen in the air, insufficient for complete oxidation, which is 100% converted, and the water-gas-shift (WGS) equilibrium at the outlet temperature of the oxidizer. For the gasoline auto-reformer the temperature of the exiting gases is given as 750 °C; this must be maintained in all your gasoline system designs. To raise the efficiency of the overall system the energy value of the carbon monoxide is further converted to hydrogen by the addition of water in a two-stage WGS reactor system, one at high temperature and one at low temperature. The gas exiting the low temperature WGS must then be "polished" to remove the remaining carbon monoxide down to 100ppm to avoid poisoning the fuel cell anode catalyst. This is done by selective oxidation of the carbon monoxide at low temperature over a platinum catalyst in the preferential oxidation reactor or PROX. This gas is then fed to the fuel cell stack.

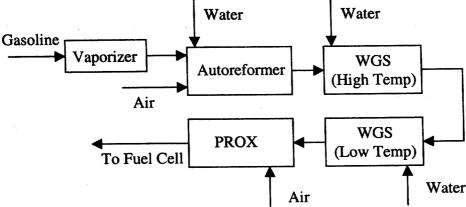


Figure 2 Schematic of Base Case Design Process

For methanol conversion the same base case design can be used. However, there is one variant to the above design that might be used in addition to the base case. The gasoline cannot be reformed to carbon dioxide and hydrogen by the direct addition of steam because of high temperatures required to—drive the reaction. However, methanol can be reformed in two ways. First, it can be auto-reformed as in the base case. Second, it can be directly reformed, but due to the endothermic nature of the reaction, this requires addition of heat that cannot be carried out quickly enough to enable transient operation, thus it will not be considered any further in this project. You are only to consider auto reforming of gasoline or methanol.

Thus, the fuel processing system has three major components: the reactor system, the fuel cell, and the auxiliaries (pumps, compressors, vaporizers, heat exchangers etc.). The design models, weights and costs for these components are given below. You should use these models in your design and any constraints on performance (such as limits of T and P) should be strictly adhered to.

Fuel Cell Performance and Operation

Principles of Operation

The fuel cell stack operates by the oxidation of hydrogen at the anodes of individual cells as:

$$H_2 = 2H^{\dagger} + 2e^{-} \tag{2}$$

The protons produced in this oxidation are transported through the PEM to the cathode side of each cell. Here oxygen from ambient air reacts with protons transferred through the PEM to produce water:

$$\frac{1}{2}O_{2} + 2H^{2} + 2e^{2} = H_{2}O$$
 (3)

Because the electrons produced in reaction (2) are at a voltage around 1 V more negative than are needed in reaction (3), electrical energy can be extracted in the external circuit. The individual cells are connected internally in series to provide the required power.

Fuel Cell Performance

The performance of the fuel cell can be represented by the curves given below [Kim 95]. Figure 3 shows the variation in cell potential with current density for two different pressures and Figure 4 plots the power density as a function of the current density. It is assumed that the oxygen is in 100% excess, and that any additional increase in excess oxygen will have negligible effect on the power output. The design decision is the current density at which to operate the fuel cell. The higher the current density the lower the area required for a given power, but the higher the rate of hydrogen consumption. The efficiency of the fuel cell is thus governed by the current density and is defined as the ratio of electrical power output to the higher heating value of the hydrogen fuel. Note that any energy not converted to electrical power must be removed from the fuel cell by cooling it.

The pressure of air on the cathode side of the fuel cell must balance that of the fuel gas on the anode side. The current density is also a function of the fuel cell temperature and can be assumed to be linear in temperature, increasing at 2.5 mA/cm²/°C over the range of 60 °C to 90 °C [Amphlett 91].

The fuel cell has a platinum-ruthenium anode catalyst that will tolerate concentrations of carbon monoxide up to 100 ppm; the fuel cell should be kept to a temperature below 85 °C. On the air (cathode) side, the catalyst can be assumed to be tolerant to all contaminants in ambient air. The maximum allowed consumption of hydrogen is such that the anode outlet gas has a minimum concentration of 8% by volume of hydrogen, calculated on a dry basis. Fuel cell costs are given in the cost section.

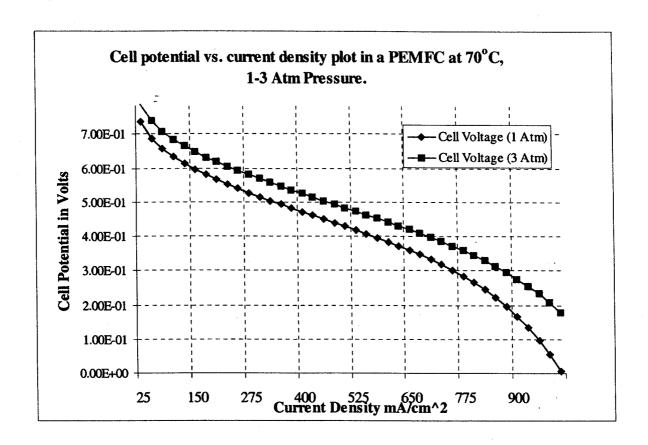


Figure 3 Fuel Cell Operation - Cell Potential as a function of Current Density

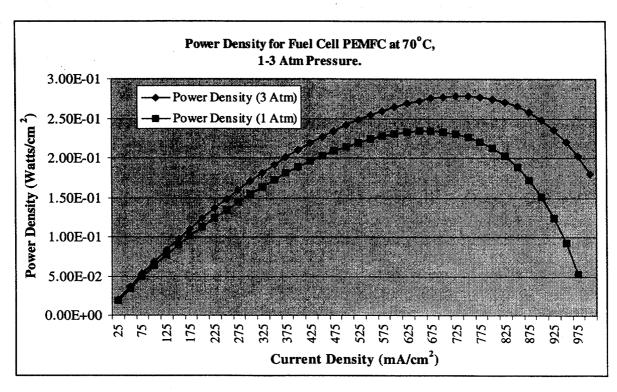


Figure 4 Fuel Cell Operation - Power Density as a function of Current Density

Reactor System Design and Operation

There are three different reactor systems that can be designed, sized and costed;

- the auto-reformer for both fuels,
- the water gas shift reactor(s) for both fuels,
- the PROX reactor for both fuels.

There are several tradeoffs in the design and operation of each reactor and in the reactor system integrated with the rest of the power conversion system. You should consider finding the best configuration, operating conditions and sizes of the reactors for your chosen system.

Auto-Reformer

An auto-reformer is a packed catalyst bed and is operated adiabatically. There do not exist publicly available models for the kinetics of the reactor, thus it should be sized based on the electrical power output of the fuel cell, at 0.34 Liters per kw¹ for methanol, and 0.51 liters per kw for gasoline. The catalyst is proprietary, and has a particle diameter of 4.76 mm, and bulk density of 0.8 kg l⁻¹. Fuel, air, and water are fed to the reactor. The air is fed at a quantity sufficient to combust a portion of the fuel, releasing heat that drives the endothermic steam reformation of the remaining fuel. The gas leaves the reactor with all species in water gas shift equilibrium, as well as steam reforming equilibrium. In order for the above correlations to hold the outlet temperature should be equal to 750 °C, for both the methanol and gasoline fuel case.

Water Gas Shift

A Water-Gas-Shift reactor is a packed catalyst bed. It can be assumed to be a PFR.

Reaction

$$CO + H_2O \iff CO_2 + H_2$$
 (reversible)

Kinetic model

$$-r_{co} = \eta k[CO] (1 - \beta)$$
, mol s⁻¹ kg cat⁻¹

where:

 η = effectiveness factor to account for intraparticle mass transport limitation, unitless.

$$\operatorname{Ln} k = \operatorname{Ln} k_0 - E/(RT)$$

¹ Kilowatts of electric power

[CO] = gas phase concentration of CO, mol 1⁻¹

 $\beta = [CO_2][H_2] / \{[H_2O][CO]K_T \}$

 $K_{_{T\,=}} \ equilibrium \ constant \ for \ the \ WGS \ reaction \ , = [CO_{_2}]_{_{eq}} \ [H_{_2}]_{_{eq}} \ / \ \{[H_{_2}O]_{_{eq}} \ [CO]_{_{eq}}\}$

 $Ln(K_T) = 4577.8 / T - 4.33$

T in Kelvin

	High Temperature Shift		Low Temperature Shift	
Range	300 to 420 °C		160 to 250 °C	
Catalyst	Fe ₃ O ₄ - Cr ₂ O ₃		Cu/ZnO/Al ₂ O ₃	
Ln k _o	15.38		13.39	
E/R, K	8437		5557	
Particle shape	Sphere		Sphere	
Particle diameter, mm	3.2		3.2	
Particle density, kg/l	1.25		1.36	
Bulk density, kg/l	0.75		0.82	
Effectiveness factor:				
	<u>T, ℃</u>	n	<u>T, °C</u>	<u>n</u>
	300	0.65	160	0.6
	370	0.35	200	0.4
	420	0.25	250	0.25

PROX Reactor

The PROX reactor is a packed catalyst bed run isothermally at 200 °C.

Catalyst: 0.5% wt Pt / •- alumina, with a particle diameter of 4.76 mm, and bulk density of 800 kg m⁻³. The purpose is to remove residual CO to 100 ppm or less, by combustion. It can be assumed to be a plug flow reactor (PFR). Reaction

$$H_2 + 1/2 O_2 -> H_2O$$
 (side reaction; irreversible)

The selectivity S is defined as mols O_2 consumed in combusting CO per total mols O_2 consumed in combusting CO and H_2 . At 200 °C, S = 0.4.

Reactor Model

$$X_{CO} = 1 - (1 - \eta * k_1 * k_2 / Q_{total})^{1.66}$$

where

X_{co} is Fractional Conversion

 η is effectiveness factor = 0.5

$$k_1 = 7.58 \times 10^8 \exp(-8552 / T [K]), \min^{-1}$$

$$k_2 = 26.2 * P^{0.4} y_{CO,in}^{-0.6} * \lambda^{0.82} * m_{Pt}, \text{ std cm}^3$$

where,

P is total pressure, Torr (absolute)

y_{co.in} is carbon monoxide mole fraction in feed to PROX

 $\lambda = 2 * [O_2]/[CO]$ (The air fed at the PROX inlet should be set at a rate such that λ does not vary throughout the PROX).

 $Q_{total} = std \text{ cm}^3 \text{ per minute of feed to the PROX.}$

Auxiliary System Design and Cost Equations

The auxiliary systems are: pumps, compressor/expander, piping, and heat exchangers

Compressor/Expander – as noted above in the description of the fuel cell operation, higher power densities can be obtained by operating at pressures up to 3 atmospheres. To do this will require compression of the feed gases, both air and fuel, to the fuel cells.

This could be accomplished by an electrically-driven compressor, but it may be advantageous to use the exhaust gases from the fuel cell to power the compression through a compressor-expander combination similar to a turbocompressor used in many automobiles. Note that it may be advantageous to combust the remaining fuel in the anode exhaust before such expansion. Current automobile compressor-expanders operate to about 18psig and have a weight of 9 kg for gas flows similar to those in this problem. Assume an overall efficiency of the unit of 50%.

For any heat exchangers assume the following overall heat transfer coefficients:

Exchanger System	Overall Heat Transfer Coefficient [Btu/(°F-ft²-hr)]		
Water(Shell)-Gas(tube)	40		
Water(Tube)-Gas(shell)	80		
Gas-Gas (plate and fin)	15		

Assume any exchangers that contact fuel gas to be corrosion-free.

Unit	Cost	Weight
Fuel Cell	\$27/Sq. ft	0.5 lb/kW
Auto Reformer (Methanol)	\$35/kg catalyst	800 kg/m³ catalyst
Auto Reformer (Gasoline)	\$53/ kg catalyst	800 kg/m³ catalyst
WGS (High Temp)	\$14/ kg catalyst	750 kg/m³ catalyst
WGS (Low Temp)	\$22/ kg catalyst	8200 kg/m³ catalyst
PROX	\$150/kg catalyst	8020 kg/m³ catalyst
Compressor/Expander	\$600¹	9 lbs ¹
Pump (Any fluid)	\$150	5 lbs
Heat Exchangers (gas/liquid)	\$1.80/lb	200 ft ² s.a./ft ³ 6.3 lb/ft ³
Heat Exchangers (gas/gas)	\$1.80/lb	400 ft ² s.a./ft ³ 12.6 lb/ft ³
Reactor Vessels	\$1.80/lb	$0.05 \text{ lb/ft}^2 \text{s.a}$
Piping	\$1.80/lb	0.04 lb/ft of pipe

Assume this as a base case and that cost and weight scale with pressure in psig

Cost/Weight Scaling of compressor/expander =
$$\left(\frac{P}{18}\right)^{0.6}$$

s.a. abbreviation for surface area

References

Adler, U. (ed in chief) Automotive Handbook, p216, Robert Bosch, Stuggart, 1986.

Amphlett, J.C., M. Farahani, R.F. Mann, B.A. Peppley, and P.R. Roberge, The Operation of a Solid Polymer Fuel Cell: A Parametric Model, *Proceedings of International Society*

Energy Conversion Engineering Conference (IECEC), American Chemical Society, 625-629, 1991.

Edwards, N., et al., On-board hydrogen generation for transport applications: the HotSpot methanol processor, Journal of Power Sources, 71, 123-128, 1998.

Kim, J., S. Lee, S. Srinivasan, C.E. Chamberlain, Modeling of Proton Exchange Membrane Fuel Cell Performance with an Empirical Equation, *Journal of the Electrochemical Society*, **142**, 2670-2674, 1995.

Reaction information was adapted from the following references:

- 1. M. J. Kahlich, H. A. Gasteiger, and T. J. Behm, "Kinetics of the Selective CO Oxidation in H₂ Rich Gas on Pt/Al₂O₃", J. Catalysis 171, 93, (1997)
- 2. N. Edwards, S. R. Ellis, J. C. Frost, S. E. Golunski, A. N. J. van Keulen, N. G. Lindewald, J. G. Reinkingh, "On-board Hydrogen Generation for Transport Applications: the HotSpot[™] Methanol Processor", J. Power Sources 71, 123, (1998)
- 3. R. L., Keiski, O. Despons, Y. -F. Chang, and G. A. Somorjai, "Kinetics of the Water Gas Shift Reaction Over Several Alkane Activation and Water Gas Catalysts", *Applied Catalysis A: General*, **101**, 317 (1993).

Final Report Format

- 1. Title Page
- 2. Table of Contents
- 3. Executive Summary One (1) page (maximum) condensation of report
- 4. **Introduction** Orient the reader to the problem and the requirements of a solution, give sufficient background that a chemical engineer familiar with fuel cells would understand.
- 5. Summary summarize the results of the analysis, conclusions and recommendations. Briefly list the options that were considered and the advantages and disadvantages of each. At a minimum this should contain the summary information, given below, for each option considered in the main body of the report.
- 6. Conclusions Interpret your results. Structure your conclusions to place the most important ones first.
- 7. **Recommendations** What is the final design that you have chosen? What additional research and development should be a priority?
- 8. Project Premises & Assumptions The information upon which you based your design, be sure to distinguish between the information provided to you (premises) and the assumptions that you made. Be certain to provide references for any assumptions you have made. If you deviate from any unit performance assumptions given in the problem statement you must provide clear documentation of your reasons and explicit (page numbers and sources) for all such deviations.
- 9. **Process Flow Diagrams (PFDs)** Include all items of process equipment and streams. Do this for each alternative that you considered in detail. If you use a computer process simulator then be sure that the simulator process flow diagram stream and unit labels correspond to those you use on the PFD.
- 10. Stream Attributes For each of your PFDs, all streams labeled with total molar flow rates, component molar flow rates in mols/sec, temperatures in centigrade and compositions in mole percent. Each stream should have a label and a short title that is descriptive of its role in the flow sheet and the label should match that of the PFD.
- 11. **Process Description** Using your stream labels from the PFD walk through the process and describe each major unit's operation (design conditions) and purpose.
- 12. Equipment Information Summary Weights and costs of all major pieces of equipment in the power generation system and all specifications of unit parameters such as type and weight of catalysts, in kg, operating temperatures and pressures, in centigrade and bar and volumes/areas, in liters and cm².
- 13. Operating Information Summary Summarize the power consumption and generation of the system, the major losses of efficiency and fuel consumption.
- 14. Process Rationale & Optimization Summarize the major tradeoffs that were made to arrive at the unit designs for each of your PFDs. Be as precise and as quantitative as possible. Summarize the tradeoffs and decisions between design alternatives as well as within alternatives. Describe any innovations you made in the design and your reasons behind them.

15. Economic Analysis - An annualized cost of the power generation system for each alternative considered in detail including capital and fuel costs in dollars based on the assumptions in this problem statement. Any other assumptions you make in arriving at the cost should be clearly documented.

Appendix

- 16. **Hand Calculations** Include example calculations for any major calculation that you did by hand to arrive at any of your alternative designs.
- 17. Computer Input and Output Include input and output files for your recommended design. Make sure to detail the simulator type and version that you used. Try to keep the output to a reasonable level of detail for your alternatives. Ensure that the labels for equipment and streams are the same as items 9,10 and that the units are similarly consistent and the categories of information reported at least cover the same information.

Summary Information

A maximum power – give the maximum power that your fuel cell delivers and justify the value on the basis of the power requirements of the car.

A choice of fuel – either gasoline or methanol with a justification of why you chose the specific fuel.

Operating Pressure (1-3 Atm)

Overall system efficiency of the design, in terms of km/liter of fuel.

Overall fuel efficiency defined as: kW of electrical power

kW of HHV of fuel(methanol or gasoline)

Fuel cell efficiency defined as: $\frac{\text{kW of electrical power}}{\text{kW of HHV of H}_2 \text{ fed to fuel cell}}$



2000 National Student Design Competition ENTRY FORM

Student Name:	
AIChE Member #:	
University Address	
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Team Members*	
"Up to two additional persons may be entered. Each team :	member must submit a separate entry form.
ALL TEAM MEMBERS MUST BE AICHE NATIONAL MEMB	
WILL NOT BE CONSIDERED.	
This solution has been prepared in accordance with	contest rules.
Faculty/Advisor Signature	<u>an salah salah katalah salah </u>
Student Signature	

Lightly attach this form to your design entry; do not bind or staple the form, as it will be separated from your solution during the judging process. Send your solution with the entry form for each team member to:

Awards Administrator, AIChE
3 Park Avenue, New York, NY 10016-5991

DEADLINE FOR SUBMISSIONS: June 9, 2000