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Title: ANALYSIS OF PEM ELECTROLYZERS

Author(s): M. W. Knobbe

MASTER

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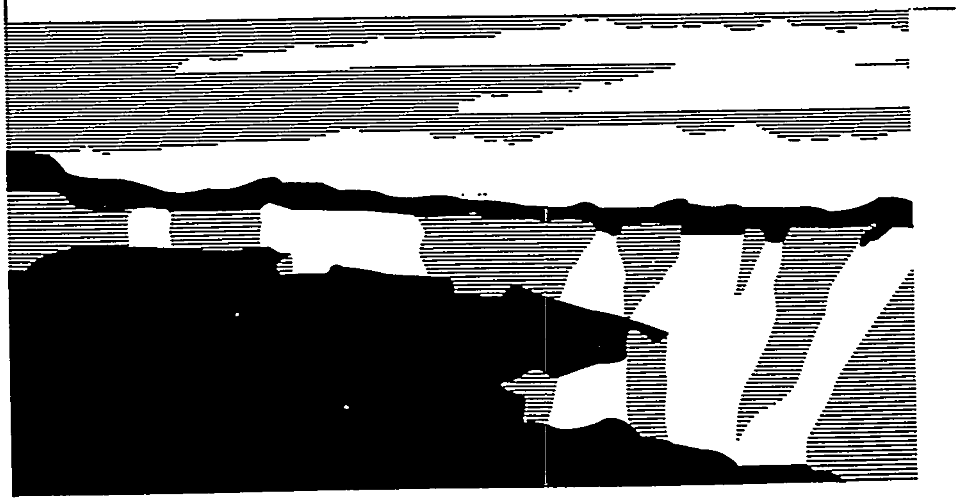

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ANALYSIS OF PEM ELECTROLYZERS

PART I: **Analysis of PEM Electrolyzers and Hydrogen Storage systems**

PART II: **Automotive Design of PEM Electrolyzers For Reduced Start-Up Emissions**

PART III: **Modeling Method For PEM Electrolyzers**

Prepared by
Mack W. Knobbe
Summer Undergraduate Intern
ESA-EPE
Fuel Cell Team
Los Alamos National Laboratory

Prepared for
Dr. Nick Vanderborgh
Fuel Cell Team leader
ESA-EPE
7/24/98

Part I: Analysis of PEM Electrolyzers and Hydrogen Storage Systems

INTRODUCTION:

Hydrogen and oxygen can be produced using a PEM electrolyzer. A PEM electrolyzer operates like a fuel cell in reverse. On the anode side of the electrolyzer, electrons are removed from water to form protons and oxygen molecules. The protons are then transported across the membrane. The protons then rejoin with electrons to form hydrogen molecules. In this way water is electrolyzed. Both half reactions are shown below.

$$H_2O \leftrightarrow 2H^+ + \tfrac{1}{2}O_2 + 2e^-$$

$$2H^+ + 2e^- \leftrightarrow H_2$$

ANALYSIS:

Two systems of storing hydrogen gas were analyzed. One system is to run the PEM electrolyzer at high pressure so the gaseous hydrogen is already compressed for storage. The other system examined is to operate the cell at low pressure and then pressurize the hydrogen and oxygen for storage using a compressor. Schematics of both systems are attached in Appendix A, pp 3-4.

The advantage of the high pressure system is that it does not require additional energy input to store the hydrogen. A drawback of this system is that the high pressures can produce a large amount of hydrogen crossover due to higher gas solubility. The gas crossover represents a loss in work. When the hydrogen flows back across the membrane, it will either react with the oxygen to form more water or mix with the gaseous oxygen being produced. In addition to a loss in work, this mixture of hydrogen with oxygen represents a safety hazard because it is an explosive mixture. Another requirement is a system of injecting liquid water at high pressure. The pump used to inject the water represents an energy consuming device.

Another drawback to the high pressure system is that it is less efficient than operating at low pressure. As the pressure of the cell increases, the potential needed to electrolyze the water increases. Only one reliable source of data were found (Int. J. Hydrogen Energy, Vol. 19, No. 5, Ledjeff, K.). This source contained data of current versus potential for electrolysis at 1 bar and 15 bars. These data were fit to a model using a non-linear least squares optimization routine. The objective function can be seen below. An explanation of the model can be seen in PART III. Four parameters were used to fit the data, i_0, α, γ, and R. The calculated values for these parameters were 7.36×10^{-3}, 0.511, 2.83, and 0.190, respectively. The equation was then extrapolated up to 200 bar. The formula used to model the electrolyzer behavior can be seen below. Graphs of the least squares fitted data and the extrapolated predictions can be seen in Figures 1 and 2 in Appendix A, pp 5-6.

$$F_{obj} = \sum_{k=1}^{n} [E_{\exp}(k) - E_{\text{model}}(k)]^2 = 0$$

The equations used to model the potential as a function of pressure, temperature, resistance, and current are:

$$E_{\text{model}} = E_{eq} + IR + \frac{R_G T}{\alpha F} \ln\left(\frac{I}{i_o}\right)$$

$$E_{eq} = E^{o} + 0.85 \times 10^{-4} (T - 298) + \frac{R_G T}{nF} \ln\left(\frac{a_{H_2}^{\gamma} a_{H_2}^{(\gamma/2)}}{a_{H_2O}}\right)$$

E^0 = standard potential, V
T = temperature, K
I = current density, A/cm^2
R = resistance, Ω

R_G = gas constant, 8.314 J/mol/K
F = Faraday's constant, 96487 C/mol e^-
n = moles of electrons exchanged
a = activity

The equations used for the diffusion of hydrogen through liquid water are:

$$N_{H_2} \equiv D_{H_2} \frac{C_{H_2}}{z}$$

$$D_{H_2} \equiv 7.4 \times 10^{-8} \frac{T (\varphi M_{H_2O})^{\frac{1}{2}}}{\mu V^{(0.6)}}$$

T = Temperature, K
M = Molecular weight, g/mol
μ = viscosity of liquid in centipoise
V = molar volume of gas, cm^3/mole
ψ = an association factor (2.26 for water)
C = concentration, mol/cm^3
z = thickness of water diffusion layer, cm
D = diffusion coefficient, cm/s

The flux expression above is a simplified form of general flux equation for this system, assuming that the hydrogen concentration on anode side is zero. These diffusion equations were obtained from Perry's Chemical Engineering Handbook. Solubilities for hydrogen were obtained from IUPAC Solubility Data Series. The data used was from Wiebe, R. and Gaddy, V.L. Using the equations above, the system was analyzed at 3000 psi (200 bar) and 50 °C, operating at 1.0 A/cm^2. According to the model, a potential of 2.03 V will be required to electrolyze the water at the operating conditions. The resulting back-diffusion loss calculated was 1.927×10^{-7} $mol/cm^2/sec$. This is equivalent to 0.0755 W/cm^2 of lost work at 2.03 V (see spreadsheets in Appendix A, pp 1-2, for calculation data). Also, if the hydrogen does not react with the oxygen at the catalyst to form water, it will create a mixture that is about 3.8 % hydrogen (mole percent). This represents a safety problem because of the combustibility of hydrogen and oxygen. Another power loss is to the pump used to inject the water into the electrolyzer. At 50% efficiency the pump will consume 0.037 W/cm^2. Operating at 1.0 A/cm^2 and 200 bar produces 2.33x10^{-6} moles of compressed hydrogen per Joule of energy input or 8.40 mole H_2/kWh. The efficiency of this system is 55%.

Another system is to run the electrolyzer at ambient pressure and then use a compressor to store the hydrogen and oxygen. The drawback of this system is that the compressor is an energy consuming device with moving parts. However, this system does not have high hydrogen crossover problems or the increased inefficiency due to high pressure. According to the model created it will take a 1.7 V potential to electrolyze the water at ambient pressure, 50 °C, and 1.0 A/cm^2. The back-diffusion rate for operating at ambient pressure is 1.1316x10^{-9} mol/cm^2/sec. This corresponds to a work loss of only 3.78x10^{-4} W/cm^2 at 1.7 V.

Another source of energy consumption is the compression of the hydrogen produced. The enthalpy change for hydrogen going from ambient pressure to 3000 psi at 25 °C is approximately 206.46 J/mol. However, there is also water vapor in the hydrogen and oxygen gas, which must be compressed. Assuming that heat exchangers can be used to bring the temperature to around 308 K and a compressor efficiency of 35%, this leads to a power requirement of 0.070 W/cm^2. This low pressure system should produce 2.923x10^{-6} moles of compressed hydrogen per Joule of energy input or 10.5 mole H_2/kWh. This represents an efficiency of 69%. Again, higher efficiency on the compressors will lead to lower power requirements. A brief summary of both systems can be seen in Table 1 in Appendix A, pg. 3.

The equation used to define compressor work is:

$$Work \equiv \frac{I * \Delta h}{2 * F * \eta}$$

I = current density, A/cm^2
Δh = enthalpy change, J/mol
F = Faraday's constant, C/mol e$^-$
η = compressor efficiency

THERMAL MANAGEMENT:

Another aspect which needs to be addressed is the thermal management. The electrolyzer will generate heat due to the internal resistance of the cell and the overvoltage of the electrode reactions. The overvoltage is the difference between the equilibrium potential and the actual potential. This difference is a heat loss due to inefficiency. The overall equations for the heat generation can be seen below. The overvoltage of the electrolyzer was found not to change with increasing pressure. According to the model developed, the overvoltage is primarily a function of current in the cell. The heat generated at 50 °C and 1.0 A/cm^2 is about 0.185 W/cm^2. This waste heat must be removed to prevent the cell from heating up.

The water being electrolyzed is the simplest way of cooling the electrolyzer. If water is injected at room temperature, 25 °C, it should sufficiently cool the cell. Due to the heating and evaporations of the water that is not electrolyzed, the electrolyzer will reach a steady state temperature. For the low pressure system, this steady state temperature is about 72 °C. For the high pressure system, the steady state temperature is about 84 °C. Operating at these elevated temperatures has little effect on the efficiencies of the overall systems. The biggest change will be in the heat exchanger requirement for the low pressure system. These heat exchangers will be required to condense the large amounts of water vapor in the hydrogen gas. This must be done in order to make the compression feasible because of the high amounts of energy required to condense water mechanically. Since the electrolyzers reach steady state, there is no need for heat exchangers on the electrolyzer itself. If operation at a cooler temperature is desired, the flow rate of water to the electrolyzer could be increased.

The equations used to describe the heat generation are:

$$q = q_{rev} + q_{irrev}$$

$$q_{rev} = T \Delta S$$

$$q_{irrev} = E_{\mathrm{mod}} - E_{eq}$$

CONCLUSIONS:

After analyzing both systems, the low pressure system is favored over the high pressure system on an energy basis. As shown in this report, there is an energy benefit and a safety benefit with the low pressure system. With the low pressure system, less energy is lost to hydrogen crossover and inefficiency. The low pressure system is 12% more energy efficient, neglecting the heat exchanger power requirement. This leads to producing about 17% less hydrogen per Joule of energy input. Also, with reduced crossover there is less chance of creating a hydrogen and oxygen mixture, which represents a safety hazard. Another advantage of the low pressure system is that there are fewer high pressure components. With the high pressure system, a compromise to any part of the system could damage the membrane and become a safety hazard. For the low pressure system, the storage tank is the only high pressure component. However, the high pressure system is mechanically simple. It has few, if any, moving parts. To make a final recommendation, an economic analysis must be performed. The capital cost and repair cost of the compressors and heat exchangers needed for the low pressure system must be analyzed and compared to the cost of the entire system.

PART II: Automotive Design of PEM Electrolyzers For Reduced Start-Up Emissions

INTRODUCTION:

In automobiles, the majority of pollutant emissions occur during the start-up of the vehicle. This is due to the fact that the emission reduction systems are not operational yet. In order to be effective, most emission reduction systems need to be hot. The system for a fuel cell driven vehicle being worked on at LANL has the same problem. During start-up there are increased emissions due to the fact that the Reformer and PROX are at low temperature. The Reformer and PROX must be at high temperatures to operate properly and reduce the pollutant emissions from the reformate hydrogen. In order to reduce these harmful emissions, a burner will be placed at the end of process to burn off the hydrocarbon emissions. However, this burner must also be hot to completely burn the harmful pollutants. One method of heating this burner quickly is to burn hydrogen before start-up. The burning of the hydrogen will not produce any pollutants. The only products of hydrogen combustion are water and heat. For this reason, a theoretical design of an electrolyzer/burner system was developed.

HEATING REQUIREMENTS:

In order to be convenient, the burner must heat very quickly. For this analysis, a 5 seconds start-up time was used. An existing burner was used for the basis of the analysis (see Appendix B, pp 3-4, for schematics of Electrolyzer and Burner). This burner is cylindrical with monolithic type square tubes in the center. It is assumed that the burner must be heated from 25 °C to 800 °C. Assuming the Ceramic burner is made of Cordierite, the process will require 500 kJ of energy for the 500 gram burner. It is assumed that 50% of the energy from the combusted hydrogen was transferred to the burner. This means it will require about 6.0 moles of hydrogen per start. Because of the very thin interior walls of the burner, the amount of hydrogen burned is the limiting step, not the heat transfer rate between the heated gas and the ceramic. These calculations were made using properties of cordierite for the burner and 5 times excess air for complete combustion of the hydrogen. The heat transfer calculation data can be seen in Appendix B, pp. 1-2.

DESIGN AND DISCUSSIONS:

A PEM electrolyzer can be use to produce the hydrogen required. The electrolyzer will be operated while the car is being operated. The electrolyzer will fill a storage vessel with hydrogen while the vehicle is running, store the hydrogen while the vehicle is dormant, and heat the burner immediately before start-up. The design for the electrolyzer system can be seen in Appendix B, pg. 4. The electrolyzer will be placed inside cylindrical tank. The tank will be used for storage of both the hydrogen and water. The electrolyzer will be submerged in water in order to provide the water needed for electrolysis and as a cooling media for the electrolyzer. The water surrounding the electrolyzer will eliminate the problem of the electrolyzer heating up. The electrolyzer will only produce around 0.18 W/cm^2 of heat. Using the 8.0 liters of water specified, the system would heat at a rate of 0.70 °C/min, if it were operated adiabaticly. Even if the electrolyzer is operated for extended periods of time, the excess heat may be removed by flowing air from the surroundings over the exterior of the tank. The hydrogen produced will be store in the space above the water level. The oxygen must be removed from the system. The oxygen may either be vented out of the system, or it may be sent to the cathode of the fuel cell stack.

In order to produce the hydrogen in a short period of time, around two thousand square centimeters of membrane will be required. For operation at 1.0 A/cm^2, 2000 cm^2 of membrane will produce 6.0 moles of hydrogen in about 10 minutes. For the design presented here, a fifteen cell stack will be used. Each membrane and electrode assembly will be 12 cm by 12 cm (144 cm^2). The potential needed to produce 1.0 A/cm^2 at 1000 psia and 308 K is around 1.92 V. For a series set up, the electrolyzer will require 28.8 V and 144 Amps. A larger membrane size will decrease the potential and increase the current required, and vice versa for decreasing the membrane size. The energy requirement will be around 4 kW. This work requirement is not out of reach of conventional lead acid automobile batteries. However, it makes more sense to run the electrolyzer directly off the electric power being produced by the fuel cell stack.

The estimated size of the tank is 16.4 liters (4.3 gallons). The tank will be 25 cm in diameter and 34 cm tall. Five liters of space is reserved for the hydrogen. This is enough space to store 14 moles of hydrogen at 1000 psia and 308 K. This allows the tank to store excess hydrogen in case the vehicle is not operated for a long enough period of time to replenish all of the hydrogen used in one start-up. The electrolyzer stack will have an estimated displacement of 3.4 liters. This volume is a rough estimate based on 0.25 inch flow field plates and 0.5 inch end plates. Eight liters of water will be used for this system. This is enough water to completely submerge the electrolyzer. This will assist in the heat removal from the electrolyzer as discussed earlier. This will also provide the hydraulic pressure needed keep the electrolyzer filled with water. One more reason for having the excess water is to separate the hydrogen from the electrolyzer. In case of any kind of compromise to the electrolyzer, the water may prevent the ignition of the hydrogen being stored in the tank.

The material of the tank must be strong enough to hold at least 1000 psia and be corrosion resistant. A stainless steel alloy could be used. It is estimated that the wall thickness will be approximately 0.25 inches. This will correspond to a tank weight of 21 kg. If an aluminum alloy is used, the tank will be 0.5 inches thick and weigh about 17 kg. The water in the system will weigh 8 kg. The electrolyzer weight is estimated at 10 kg. The total weight of the system will be between 30 and 40 kg.

The efficiency of the burner/electrolyzer system is estimated at 23%. This efficiency is in terms of enthalpy change of the ceramic burner divided by the energy used to produce the hydrogen burned. The efficiency of the electrolyzer is 64%. This is based on the standard state potential needed for electrolysis divided by the actual potential required. Note that these potentials are based on a membrane thickness of 0.0254 centimeters. The spreadsheet data for both the electrolyzer efficiency and the heat transfer data can be seen in Appendix B, pp 1-2.

CONCLUSIONS:

One drawback to the electrolyzer system is the high storage pressures. The 1000 psia storage pressure represents a safety hazard. In order to reduce the pressure, the tank must be made larger. However, the tank is already very big for portable applications. If a burner with a lower specific heat is used, less hydrogen will be required for the heating. This will lead to a smaller tank size. If space is not an issue, the hydrogen can be stored at lower pressures to reduce the safety hazard. Another difficulty will be the low temperature effects. Since the electrolyzer is submersed in water, freezing represents a major problem. In cold weather environments, a way of keeping the water from freezing must be designed. One more difficulty is the high temperature the burner must be heated to. Since methane is one of the emissions that must be burned, the heater must be heated to 800 °C. If methane is not present, the burner can be operated at around 400 °C. This will cut the size of the electrolyzer in half.

The system presented above is clearly capable of producing hydrogen and heating a ceramic burner very quickly. The electrolyzer system could be easily integrated into the entire fuel cell system. It will be a convenient way to heat the burner very quickly. One concern is the cost of the PEM electrolyzer. However, the cost of this electrolyzer should be small when compared to the cost of the fuel cell stack used to power the vehicle. The PEM electrolyzer will use electric energy being produced by the fuel cell. Assuming that the fuel cell will operate around 40-50 kW, the electrolyzer will only consume a small fraction of this energy and store it indefinitely. This means the energy requirement for the electrolyzer will not be a major concern. Clearly the electrolyzer design presented here is an effective and convenient way to heat the burner in order to reduce start-up emissions.

PART III: Modeling Method For PEM Electrolyzers

Data for PEM electrolyzers was found for 1 and 15 bars. The data was found in the International Journal of Hydrogen Energy, Vol 19, No. 5, pp 453-455, 1994. The report was authored by Ledjeff, K., Heinzel, A., Peinecke, V., and Mahlendorf, F. The electrolysis of water was modeled based on the Butler-Volmer equation for electro-kinetics. The overall reaction rate equals the forward rate of reaction minus the backward rate of reaction. The overall equation can be seen in Eq. 1.

During the initial estimations of the system, it was found that the term for the reverse reaction was far smaller than the forward reaction. This is due to the magnitude of Faraday's constant and the fact that there is a negative sign inside the exponential. For ease of calculation this term was canceled out. Also, the water concentration term was simplified to one, since the concentration of the liquid water phase is constant with respect to temperature and pressure. These cancellations left the defining equation as seen in Eq. 2.

Since the current appears in more than one term, the equation was rearranged to isolate E, see Eq. 3. In this equation, E_{eq} must have both a temperature and pressure dependence in order to be a useful model. To account for this, a term for both temperature and pressure change were added to E^0, see Eq. 4.

Data for the fugacity of both hydrogen and oxygen were correlated to accommodate the pressure variation. The pressure dependence of the fugacity for both hydrogen and oxygen were best described by a third order polynomial. Both were correlated from data at 120 ^{0}F (49 ^{0}C). Similar correlations could easily be made for any temperature desired. ΔS was considered constant for the analysis range. γ was added to account for the possibility that the reaction was not elementary. If the reaction were elementary, γ would go to one, but this was found not to be the case.

These equations were modeled using Fortran. The built-in IMSL function BCLSF was used to fit the experimental data against the model using the objective function see below, Eq. 5. Four parameters were necessary to fit the data given, i_0, α, γ, and R. The BCLSF uses a non-linear least squares method to fit the data. The algorithm uses a modified Levenberg-Marquardt method. The routine fit the four parameters in the theoretical equation to the given data. The best fit values are 7.36×10^{-3}, 0.511, 2.83, and 0.190 for i_0, α, γ, and R, respectively. The comparison between the experimental values and the theoretical fit can be seen in Figure 1, Appendix A, pg. 5. The trends of the extrapolated curves can be seen in Figure 2, Appendix A, pg. 6. It can be clearly seen that the magnitude of the pressure effect decreases as the pressure increases. The most dramatic increases in potential occur with the first 15 bar increase in pressure. The gradient between each pressure decreases as the pressure is continually increased. This trend is confirmed by experimental data provided by Jim McElroy of Hamilton Standard. Since the data provided by Jim McElroy is for a different electrode loading, the magnitude of the numbers is different, but the trends are the same as the theoretical data. This helps confirm the validity of the model. To truly confirm the validity of the model, experimental data for very high pressures must me obtained.

Eq. 1.

$$I = i_o\left\{\frac{C_{H_2O}}{C^o_{H_2O}}\exp\left(\frac{\alpha F}{R_G T}[E-E_{eq}-IR]\right)-\frac{C_{H_2}C^{0.5}_{O_2}}{C^o_{H_2}{C^o_{O_2}}^{0.5}}\exp\left(\frac{-\beta F}{R_G T}[E-E_{eq}-IR]\right)\right\}$$

Eq. 2.

$$I = i_o \exp\left(\frac{\alpha F}{R_G T} (E - E_{eq} - IR) \right)$$

Eq. 3.

$$E_{\text{model}} = E_{eq} + IR + \frac{R_G T}{\alpha F} \ln\left[\frac{I}{i_o} \right]$$

Eq. 4.

$$E_{eq} = E^0 - (T - T^0)\frac{\partial E}{\partial T} + \frac{R_G T}{nF} \ln\left[\frac{a_{H_2}^{\gamma} a_{O_2}^{(\gamma/2)}}{a_{H_20}} \right]$$

Eq. 5.

$$F_{obj} = \sum_{k=1}^{n} [E_{\exp}(k) - E_{\text{model}}(k)]^2 = 0$$

Substitutions for Eq. 4.

$a_{H_2O} = 1$

$a_{H_2} = f_{H_2}$

$a_{O_2} = f_{O_2}$

$\frac{\partial E}{\partial T} = \frac{\Delta S}{nF}$

$T^0 = 298K$

$\Delta S = -163.076 \frac{J}{mol*K}$

Equations for Fugacity

$$f_{H_2} = 2\times10^{-7}P^3 + 0.0006P^2 + P$$
$$f_{O_2} = 5\times10^{-7}P^3 - 0.0003P^2 + 1.0004P$$

Definition of Terms:

I = current density (A/cm^2)
R_G = Gas constant, 8.314 J/mol/K
F = Faraday's constant, 96487 C/mol e^-
E = cell potential (V)
E_{eq} = equilibrium potential (V)
E^0 = standard cell potential (V)
R = resistance (Ω)
T = temperature
n = mole of electrons per reaction, 2 mol e^-
a_i = activity of component i
f_i = fugacity of component i, (bar)
ΔS = entropy change of reaction, (J/mol/K)
i_0 = pre-exponential fitted parameter
α = fitted parameter inside exponential
γ = fitted parameter for non-elementary reaction

APPENDIX A

Crossover Loss In a PEM Electrolyzer and Parameter Results

Crossover @ 200 atm

Current Density	1.00	A/cm^2
P(Bar)	206	bar
T (K)	323	K
Ψ	2.26	
Mol. Weight	18.02	g/mol
μ	0.5463	centpoise
V (molal volum	26	cm^3/mol
Dh2	3.9532E-05	cm^2/s
xh2	0.0022305	*
ρ	55.5	mol/L
z (thickness)	0.0254	cm
N/A	1.9267E-07	mol/cm^2/sec
N/A	0.03718013	A/cm^2
Potential	2.03	volts
Lost Work	**0.07547567**	**Watts/cm^2**

Crossover @ 1 atm

Current Density	1.00	A/cm^2
P(Bar)	1.01325	bar
T (K)	323	K
Ψ	2.26	
Mol. Weight	18.02	g/mol
μ	0.5463	centpoise
V (molal volu	26	cm^3/mol
Dh2	3.95322E-05	cm^2/s
xh2	1.31E-05	
ρ	55.5	mol/L
z (thickness)	0.0254	cm
N/A	1.13157E-09	mol/cm^2/sec
N/A	0.000218363	A/cm^2
Potential	1.7	volts
Lost Work	**0.000371218**	**Watts/cm^2**

*valid between 25.33 and 1000 bar

Results for fitted parameters obtained from Fortran

Io = 7.36E-03
α = 0.5105316
γ = 2.827439
R = 0.1901832

Potential and Energy Balance Calculations For General Electrolyzer Use

T	323
P	1
Pv	0.1233663
io	7.36E-03
α	0.5105316
γ	2.827439
R	0.1901832

Pressure	1	1	5	10	15	50	100	150	200
current	voltage ex	Calculated							
0	1.23	1.243452	1.344808	1.38655	1.410814704	1.48286	1.5248	1.549764	1.5678
0.25	1.55	1.483187	1.584544	1.62628	1.650549993	1.72259	1.76453	1.789499	1.8075
0.51	1.62	1.571502	1.672858	1.7146	1.73886454	1.81091	1.85285	1.877814	1.8959
0.8	1.7	1.651198	1.752554	1.7943	1.818560663	1.8906	1.93255	1.95751	1.9756
1	1.73	1.701399	1.802756	1.8445	1.868762117	1.9408	1.98275	2.007711	2.0258
1.2	1.75	1.749375	1.850732	1.89247	1.916738133	1.98878	2.03072	2.055687	2.0737
1.5	1.8	1.818595	1.919952	1.96169	1.985957906	2.058	2.09994	2.124907	2.143
2	1.85	1.92937	2.030726	2.07247	2.096732679	2.16878	2.21072	2.235682	2.2537

Energy Balance

Pv	0.1233663	bar		
P	1	bar	200	bar
yh20	0.1233663		0.00062	
	qgen		qin	
	0.1850984	W/cm^2	0.1851	
	qcon	del q	qout	del q
	0.0565001	0.128598	0.07925	0.10585143

HXN duty

Tout	308	K
Pv	0.0562354	bar
yh20	0.0562354	
Δh	**-0.026434**	W/cm^2

Compressor Work (low pressure system)

Isothermal

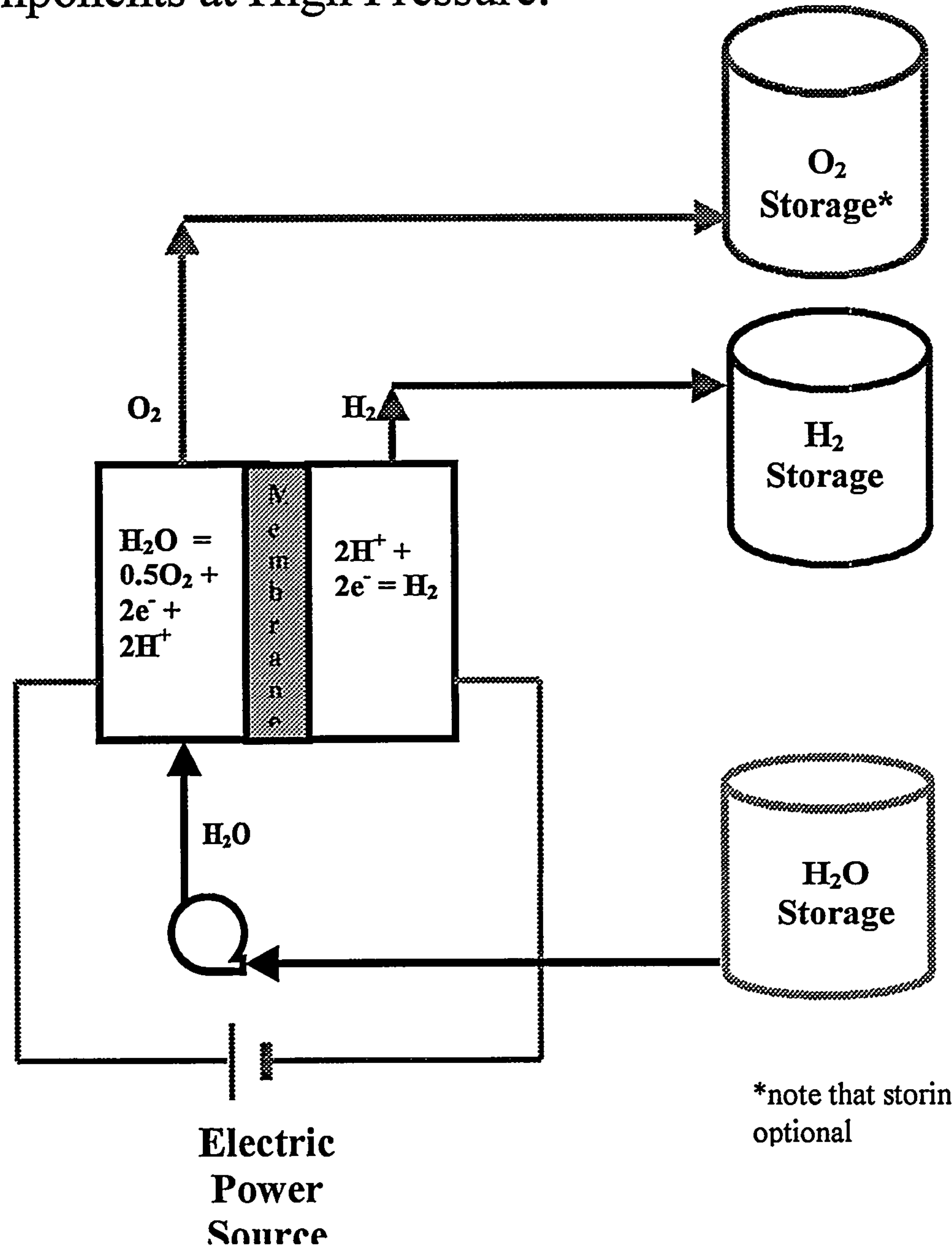
ΔH (h20)	43179.562	J/mol
ΔH (h2)	206	J/mol
ΔH (O2)	1386.5	J/mol
W ideal	0.0246591	W/cm^2
eff.	0.35	
actual W	**0.0704547**	W/cm^2

Pump Work (high pressure system)

mole H20	5.2E-06	mol/cm^2/sec
Pump work	0.01869	W/cm^2
eff	0.5	
Pump W(act)	**0.03739**	W/cm^2

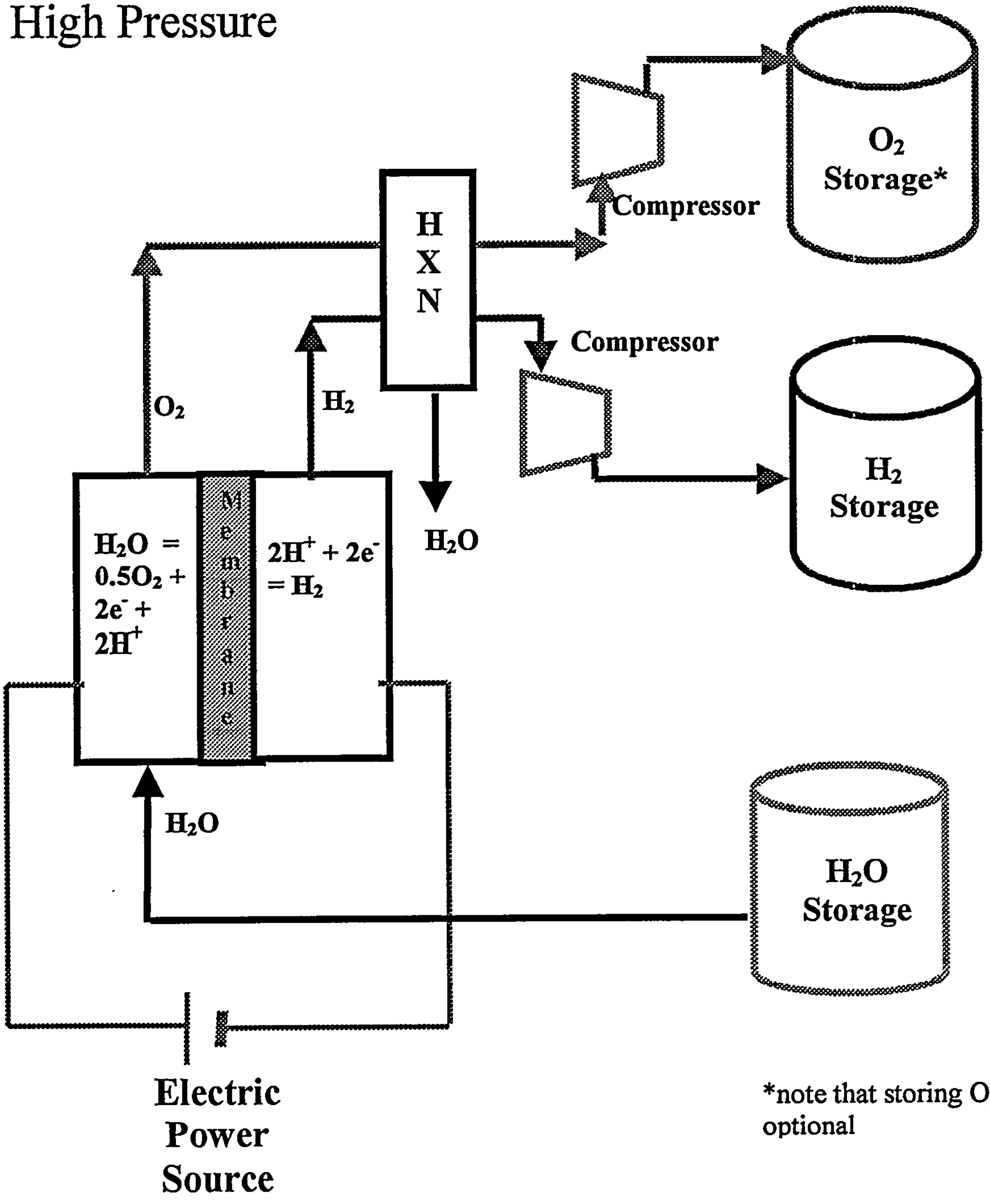
Table 1. Comparison of Calculations									
Pressure (atm)	Current (A/cm^2)	Potential (V)	Moles H2 Produced*	Moles Lost to Diffusion*	Compressor Work (W/cm^2)	Total Work (W/cm^2)	Moles of compressed H2 per Joule	Moles of comp. H2 per kWh	Efficiency
1	1.00	1.701	5.182E-06	1.132E-09	0.0705	1.772	2.923E-06	10.52	0.694
200	1.00	2.026	5.182E-06	1.927E-07	0.0374	2.138	2.333E-06	8.40	0.554
*moles/cm^2/s									

High Pressure System. All Components at High Pressure.



*note that storing O_2 is optional

Low Pressure System.
Only Storage Tanks at High Pressure



*note that storing O_2 is optional

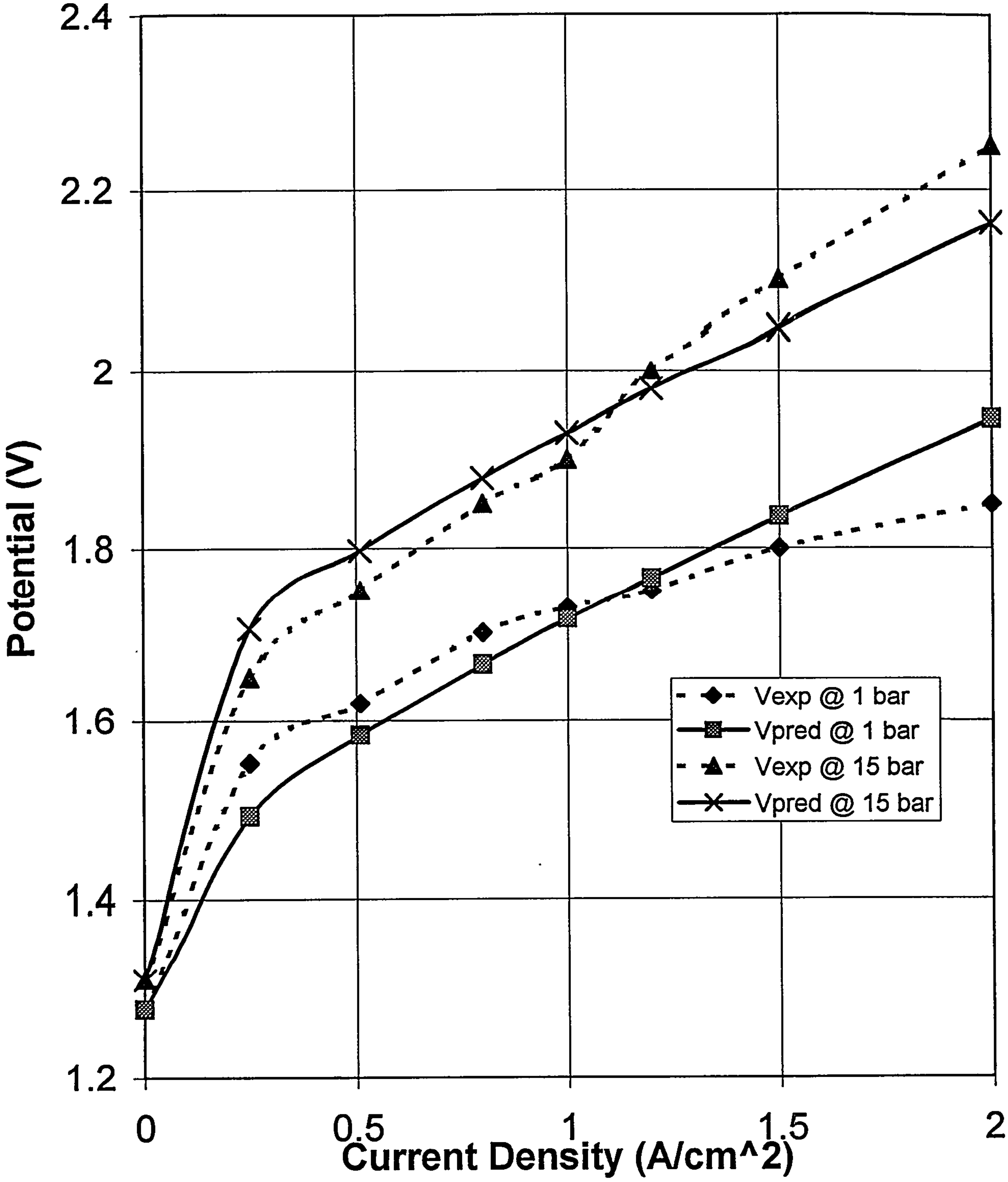


Figure 1. Data Fit With 4 Parameters

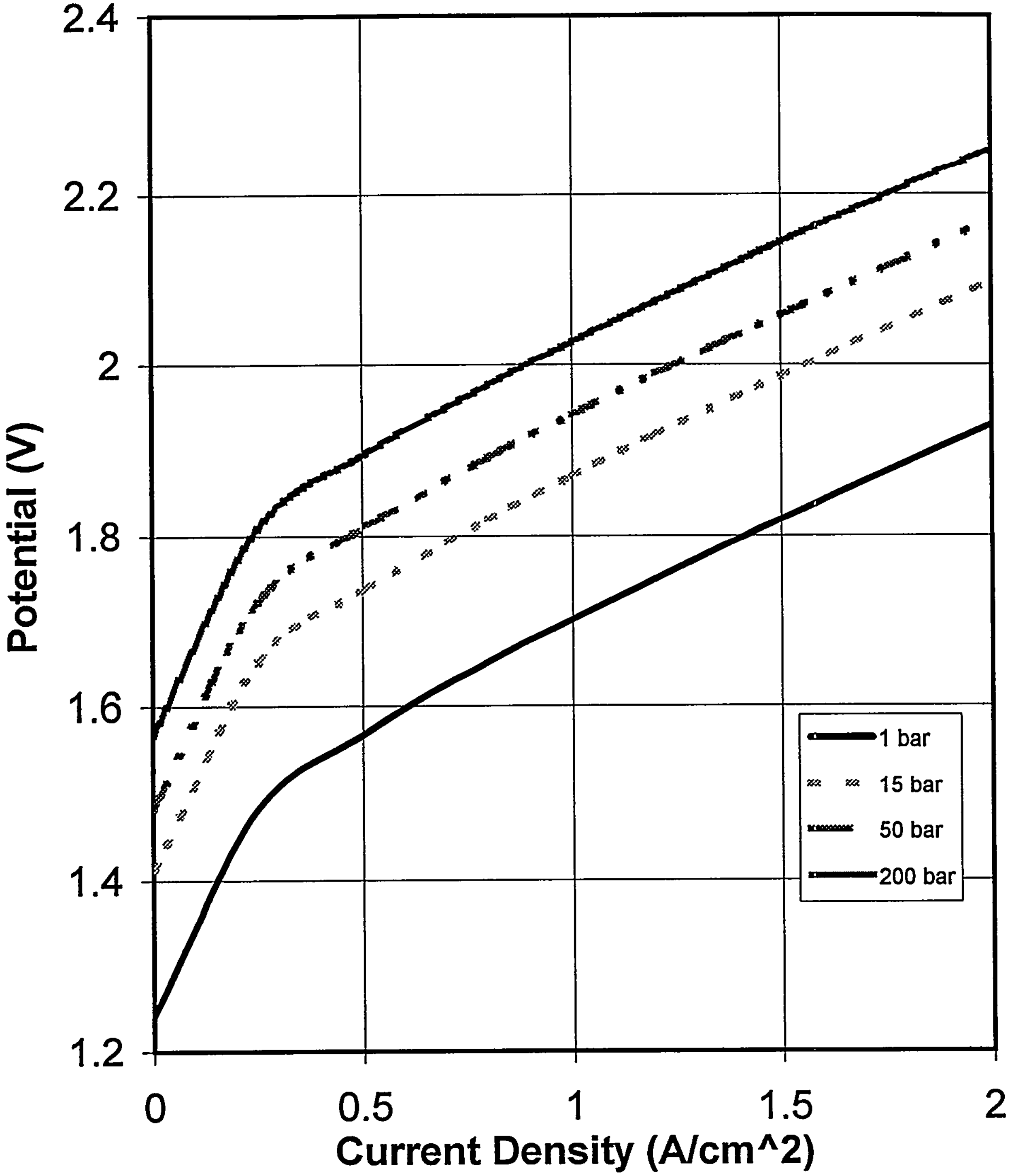


Figure 2. Model Predicted Curves

APPENDIX B

Heat Transfer Data and Calculations For Automobile Electrolyzer

burner T	1073	K	
P	68	atm	
Flame T	2318	K	
HHV	285.84	KJ/mol	
LHV	241.827	KJ/mol	
HV(Air)	166.911	KJ/mol	
Tout	1250	K	
Mass Cer	0.5	Kg	
del H Cer	505421.9	J	
Mol H2 req	3.028092	mole	
eff. Ass.	0.5		
Act. Mol	**6.056185**	**mole H2**	
Start Time	5	sec	
Flow Rate	1.211237	mole/sec	H2
Flow Rate	6.747223	mole/sec	N2,H20
ρ	0.006093	kmol/m^3	
ρ	0.150439	kg/m^3	
G	0.166589	Kg/s	
friction fact.	0.014267		
Gmax	11.37121	kg/s	
Tube D	0.00127	m	
Tube L	0.14605	m	
# of tubes	2500		
burn D	0.092075	m	
Heat ex A	0.00094	m^2	
cross A	1.61E-06	m^2	
k (flue gas)	0.02803	W/m/K	
Pr	0.060066		
Re	1121.448		
Gz	0.58575		
Nu	3.773512		
h	**83.2857**	W/m^2/K	
Efficiency	**0.227352**		

$C_p = a+bT+c/T^2$

	a	b	c	del H
O2	8.27	0.000258	-187700	43900.5087
N2	6.5	0.001		36607.0241
H20	8.22	0.00015	0.00000134	46301.9446
Cordierite	612.19	0.10997		

Nmole of Air per mole of H2	4.57052285

μ	4.77979E-05	H20
μ	0.000046534	N2
μ	4.67868E-05	average
Cp (N2)	32.4477	J/molK
Cp (h20)	43.9666335	J/molK
Cv(n2)	24.3137	J/molK
Cv(H20)	35.8326335	J/molK
k(n2)	0.023828895	W/m/K
k(h20)	0.044836131	W/m/K
Pr(n2)	0.063365139	
Pr(h20)	0.046870966	

Cordierite Properties

Cp	1230	J/kg/K
ρ	2.53	g/cm^3
k*	1	W/m/K

*assumed value, actual value not know

** Cordierite Properties from Engineered Materials Handbook, Vol 4, Ceramics And Glasses

***All other data from Perry's Chemical Engineers' Handbook, 7th edition

Energy Balance Calculations For Automobile Electrolyzer

T	308
Pv	0.0562354
Model Parameters	
io	7.36E-03
α	0.5105316
γ	2.827439
R	0.1901832

Pressure	68 bar
current	Potential
0	1.4771414
0.25	1.7079514
0.51	1.794461
0.8	1.8730174
1	1.9226539
1.2	1.9701683
1.5	2.0388232
2	2.1488696

Energy Balance

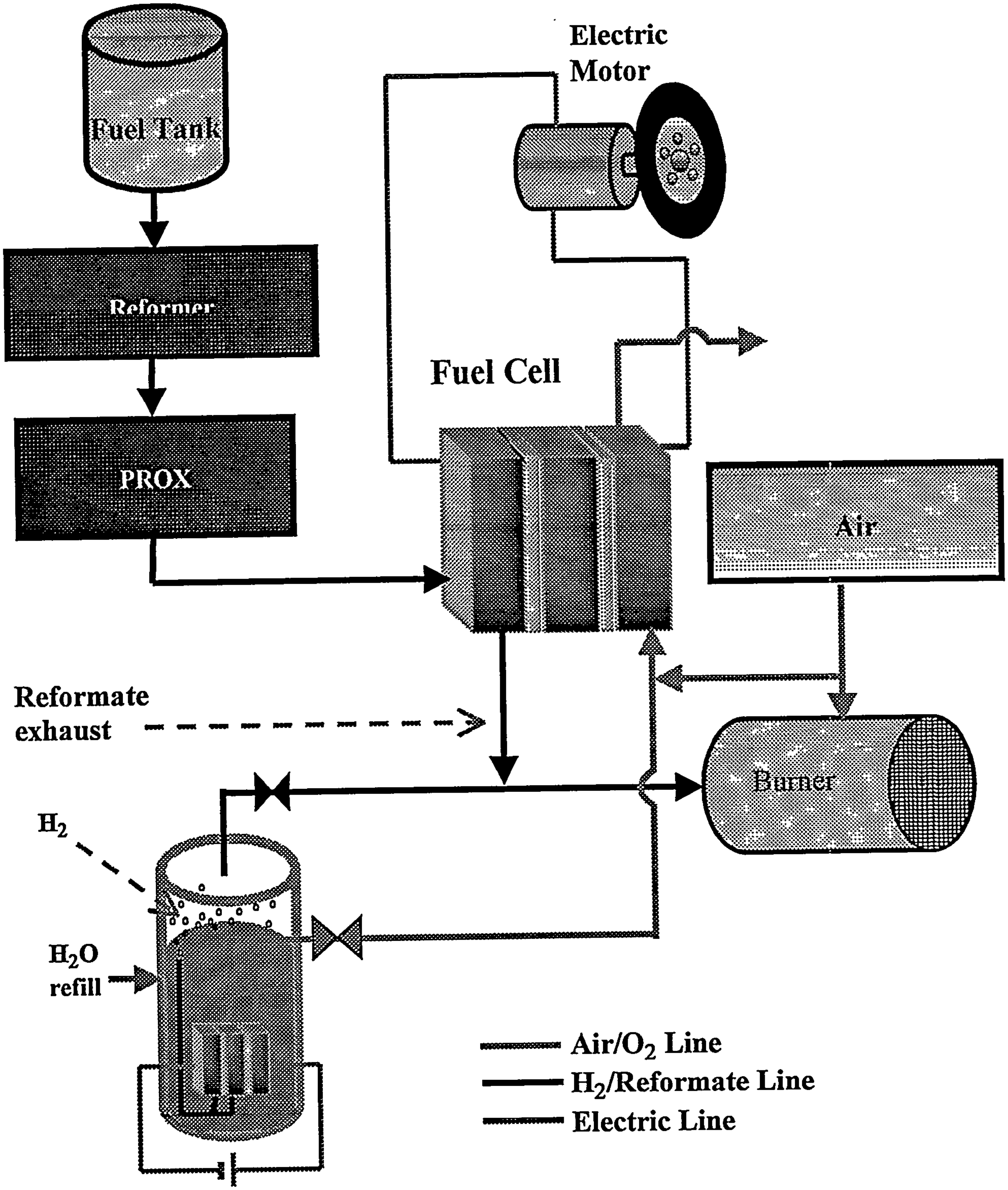
I	1	A/cm^2	I	2	
Pv	0.0562354	bar	Pv	0.0562354	
P	68	bar	P	68	bar
yh20	0.000827		yh20	0.000827	
qgen	0.1853346	W/cm^2	qgen	0.4115503	W/cm^2
qcon	0.0041846	W/cm^2	qcon	0.0041846	W/cm^2
del q	0.18115	W/cm^2	del q	0.4073657	W/cm^2

Table 2. Comparison of Calculations At 1 and 2 A/cm^2

Pressure (atm)	Current (A/cm^2)	Potential (V)	Moles H2 Produced*	Total Work (W/cm^2)	Moles of comp. H2 per kWh	Efficiency
68	1.00	1.923	5.182E-06	1.923	9.70	0.640
68	2.00	2.14887	1.036E-05	4.298	8.68	0.572

*moles/cm^2/s

Schematic of Automotive Fuel Cell System:



Electrolyzer Design: