

PEM FUEL CELL SYSTEM OPTIMIZATION

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ABSTRACT

Fuel cells offer the potential of providing clean and efficient energy in a wide variety of applications. This paper presents a methodology for optimizing the fuel conversion efficiency and peak power of a direct-hydrogen proton-exchange-membrane (PEM) automotive fuel cell system over a wide range of power output. It is shown that optimal system operation can provide significant benefits in terms of both increased efficiency (especially in low power operation) and high peak power output from the system.

INTRODUCTION

Fuel cells offer the potential of providing clean and efficient energy in a wide variety of applications. Automotive applications are the most demanding because of the need for high peak power capability (vehicle acceleration and hill climbing performance), high energy conversion efficiency (fuel efficiency and range), and minimum space for the overall fuel cell power system (to provide adequate passenger and luggage). To achieve these simultaneous design requirements it is necessary to carefully optimize the overall fuel cell system.

This paper presents a methodology for optimizing the fuel conversion efficiency and peak power of a direct-hydrogen proton exchange membrane (PEM) automotive fuel cell system over a wide range of power output. The optimization process is based on the trade-off between the stack power and efficiency increases gained from operating at varying air pressures and air stoichiometric ratios, and the power losses required to provide the compressed air flow to the stack. This paper represents the further development and refinement of the concepts introduced by the authors in [1].

Emissions optimization is not included in this paper since a direct hydrogen fuel cell system produces only water and electricity. All of the emissions associated with a

direct-hydrogen PEM system are produced in creating the hydrogen, and therefore cannot be minimized through vehicle operation (other than to minimize fuel consumption). The tradeoffs associated with interior space are also not discussed in this paper.

The paper begins with a brief description of the UC Davis fuel cell system simulation and the associated component models that have been developed to analyze automotive fuel cell systems. Next, the optimization of the PEM system is contrasted with optimization of the PEM stack alone – to stress the need for optimizing system rather than stack performance. This highlights the importance of distinguishing between gross stack and net system power output. After the various components associated with the PEM system are briefly described, the emphasis is shifted to the system components that are the most significant for the direct hydrogen system optimization process (the stack and air supply).

Finally, the process of system optimization is described, and examples are provided to illustrate system performance under various operating conditions. The conditions typically used to represent fuel cell stack operation are presented and then contrasted with the system performance that can be achieved through an optimized control strategy. It is shown that optimal system control can provide significant benefits in terms of increased efficiency (especially in low power operation) and high peak power output from the system.

In closing, the limitations of the illustrative optimization curves are discussed. Key effects discussed are:

- Additional practical limitations associated with stack and compressor operation,
- Issues associated with the dynamic response of the air supply system,
- The added difficulties of optimizing a system that includes an expander for energy recovery.
- Complications associated with including a reformer system to supply hydrogen.

FUEL CELL SYSTEM MODEL

A realistic representation of each of the components in a fuel cell system is needed when evaluating the optimal system operating strategy. Through the support of the UC Davis Fuel Cell Modeling Program, a PEM fuel cell system simulation has been developed for automotive applications. The system simulation contains component models for each of the critical fuel cell system components. In turn, this system simulation is embedded in a fuel cell vehicle (FCV) simulation.

The overall FCV simulation is divided into two stages. The first stage models and then applies an optimization procedure for the key components where performance tradeoffs must be made (stack and air supply). The second stage incorporates the information from the first and simulates the performance of a complete fuel cell vehicle (FCV) over a second-by-second driving cycle. This paper focuses on the first stage of the model, the system simulation.

As noted above, the two components simulated and optimized in the first stage of the FCV model are the fuel cell stack and the air supply system. The PEM fuel cell stack model is based on analysis done by the Electronic Materials and Device Research Group at Los Alamos National Laboratory.^{2,3,4} The LANL analysis focuses on the mechanisms associated with the cathode (air side) reactions of a well-humidified direct-hydrogen PEM fuel cell.

The LANL cell analysis incorporates a physical understanding of the processes associated with:

- Interfacial kinetics at the interface between the cathode catalyst layer and the PEM membrane,
- Gas-transport and ionic conductivity limitations in the catalyst layer,
- Limitations associated with gas transport through the cathode backing layer.

Because of the physical basis of the model, it can also be used to predict the potential future performance of fuel cell stacks (as the characteristics of the cell and stack improve).

The air supply system model incorporates the ability to model compressors (high pressure and high flow) or blowers (low pressure, high flow). The compressor model used here to illustrate the optimization procedure is based on data supplied by Vairex Corporation for their variable displacement compressor (under development for fuel cell applications).

The simulation program has been developed within the Matlab programming environment, using both the Matlab programming language and Matlab's Simulink visual programming language. The use of Simulink allows for a simple modular design for the program and access to a vast library of mathematical functions and numerical calculation processes.

SYSTEMS VERSUS STACKS

For automotive fuel cell applications, an analysis must incorporate the complete systems that will be required to support the operation of the fuel cell. From the perspective of the fuel cell stack, it is provided with humidified fuel and air while

producing electricity and water that are either consumed or reused to continue the process of operating the vehicle.

Figure 1 presents a simplified block diagram of the major components required within an automotive fuel cell system. To provide for the proper operation of the fuel cell stack and to interface with the power requirements of the vehicle, four major subsystem components are integrated together with the fuel cell stack: hydrogen supply, air supply, water and thermal management, and power electronics. Each of these subsystems are discussed separately below. In addition, the overall system incorporates computer-based control to optimize the interactions within the system. This is, of course, analogous to an electronic control module for an internal combustion engine. Each of these subsystems can interact with one another and with the fuel cell stack to impact the performance of both the stack and the overall system.

Hydrogen Supply

The hydrogen supply subsystem for a direct-hydrogen FCV generally uses high pressure storage tanks for compressed hydrogen gas. From the perspective of the fuel cell stack, the compressed hydrogen gas (CHG) storage is the simplest and most efficient option. The hydrogen is stored at pressures significantly higher than needed for the stack (3000 to 5000 psi), so a simple pressure regulating system and mass flow control are all that are needed to ensure that the stack receives hydrogen at the necessary pressure and flow rate. Further, because the gas is essentially 100% hydrogen there are no performance losses in the anode side of the fuel cell associated with either diluted or CO poisoned input gases. In addition, the purity of the hydrogen allows any excess hydrogen fed through the anode to be recirculated (thereby essentially eliminating any significant losses from exhausting the excess hydrogen). Because of these characteristics, there is no optimization required between the stack and the CHG hydrogen supply – the CHG will essentially always be able to supply the optimal hydrogen input.

Air Supply

The two main choices for the air supply subsystem are either a blower or a compressor, each of which must be powered by an electric motor. The blower supplies near ambient pressure air to the fuel cell stack but can vary the mass flow rate supplied to the stack in order to achieve variable air stoichiometric ratios. In contrast, a compressor can provide either relatively fixed pressure air to the fuel cell stack at varying mass flow rates, or supply both variable air pressure and variable air mass flow.

These two basic types of air supply systems provide highly diluted oxygen (humidified air) to the fuel cell cathode. The strong dilution of the oxygen feed stream dramatically effects the oxygen partial pressure at the cathode catalyst layer, and, in turn,

this leads to the need for high overpotentials on the cathode. The interaction of the air supply subsystem with the fuel cell stack is the focus of this paper and is discussed in more detail in the System Optimization section.

Water and Thermal Management

Two extremes that can seriously impact the operation of PEM fuel cell stacks are the flooding of the cathode and anode backing layers due to excess water, and the drying out of the membranes when the water supply is inadequate. Flooding occurs when the combination of the water carried into the anode and cathode by the humidified gases plus the water produced in the reaction between hydrogen and oxygen is not removed efficiently from the respective backing layers.

Flooding impairs the ability of the reactant gases (primarily the oxygen) to diffuse through the backing layers to the catalytic reaction sites. This effect significantly increases the cathode overpotential required to generate high cell current, and ultimately limits the peak power output of the stack. At the other extreme, insufficient supply of water can dry out the anode side of the PEM membrane, causing a significant rise in stack resistance and reduced membrane durability.

To ensure that the stack remains properly humidified and does not flood, a water management system humidifies the incoming feed gasses and removes the excess water from the cathode and anode exhaust streams. This excess water can be re-used for gas humidification.

To ensure operation at the design point temperature, a thermal management system maintains the fuel cell stack operating temperature within a narrow range under widely varying power demands. This thermal management system is also necessary for quick warm-up and safe cool-down of the stack during off-and-on daily operating conditions of the FCV.

Various techniques have been pursued to achieve optimal thermal and water management. These focus on internal stack humidification and cooling along with external water supply pumps, heat exchangers and other ancillary equipment. These systems have to be carefully designed to minimize their power requirements while ensuring that the stack remains at its optimal temperature and humidification levels. The design and optimization of these systems is beyond the scope of this paper.

Power Electronics

The final major subsystem is the power electronics which is the interface of the PEM system with the vehicle drivetrain and vehicle hotel loads (heating, air conditioning and various vehicle accessories). For optimal efficiency, the vehicle electric drive motor

will probably operate around 300 volts, while many of the accessories for the fuel cell stack and vehicle may operate around 12 volts.

To accommodate these varying voltage requirements, a power electronics subsystem must be incorporated to either step up or step down the output voltage of the fuel cell stack. This system will have some associated efficiency penalties, but overall does not represent a significant loss in the system.

SYSTEM OPTIMIZATION

Based on the above discussion, it becomes clear that the major optimization for a direct-hydrogen fuel cell system involves the interaction of the stack with the air supply sub-system. The first step in this optimization process is understanding the characteristics of the fuel cell stack and the air supply system. Each of these components must be realistically modeled in order to ensure that the key operating characteristics and associated variables are included. Then the operation of the two components must be integrated to understand in detail where the tradeoffs occur.

PEM Fuel Cell Stack Characteristics

The performance of a direct-hydrogen fuel cell stack is typically illustrated by a polarization curve, which shows the relationship between voltage and current as variable power is drawn from the stack. This curve can vary significantly and depends on a number of factors, including the design and construction of the stack, the design of the membrane-electrode-assembly, and the operating temperature for the stack.

However, once the design of a direct-hydrogen stack, and its operating temperature, are fixed, two key external variables have a major impact on the shape of the polarization curve. These variables are the operating air pressure and the air stoichiometric ratio provided to the stack by the air supply. Together these two inputs control the oxygen partial pressure at the cathode catalyst layer, which in turn determines the cathode polarization (and conversion efficiency) for a specific cathode catalyst layer.

The impacts on the polarization plot of varying the air pressure and air side stoichiometric ratio (SRa) are illustrated in Figure 2 and Figure 3, respectively. To simplify the illustration of the impact of air pressure and stoichiometry, these plots do not include the effects associated with limited gas transport or limited proton conductivity in the catalyst layer. If present, these effects will alter the shape of the curves, but for the purpose of discerning the gross impacts of altering pressure and SRa it is not necessary to include them.

Figure 2 shows that the primary effect of increasing the air pressure in the fuel cell cathode is to raise the cell voltage relatively uniformly for each value of current density. Since raising the voltage directly increases the gross cell efficiency, this is generally viewed as a positive effect. The increased air pressure also produces a marginal increase in the cell limiting current density.

Figure 3 shows that the two primary impacts of increasing SRa are: a slower rate of decrease in cell voltage with increasing current, and an increase in the limiting current density. The slower voltage decrease increases the gross cell efficiency (similar to the effect of increasing pressure, but concentrated at higher current densities). The higher limiting current density allows the cell to reach higher peak power density.

Thus increasing either the air pressure or air flow will increase both the efficiency and the peak power density of a fuel cell. From this result, one might conclude that a direct-hydrogen stack should be operated at the highest pressure and highest SRa possible to achieve maximum efficiency and power density. However, the difficulty with this conclusion is that the energy required to compress and supply high pressure and high mass flow rates of air are substantial, and can overwhelm the gains illustrated in Figure 2 and Figure 3. Thus, the power demand characteristics of the compressor must also be included in the system optimization process.

Air Supply Characteristics

The more flexible of the two air supply options is the compressor, since it can be operated at both varying air pressures and varying air flow. This allows an investigation of the system optimization that is available over the full range from high pressure and high SRa to low pressure and low SRa.

There are many different types of compressors that are being investigated for use in fuel cell vehicles and each has different operating characteristics. Since the purpose of this paper is to present the principle of fuel cell system optimization, the most flexible compressor technology was chosen to demonstrate the trade-off that is available. This is the Vairex variable displacement compressor, a piston compressor that allows relatively independent alterations in the output pressure and mass flow rates.

For the fuel cell vehicle application, air supply system characteristics are best described in terms of the relationship between power demand and mass flow rate at various pressure ratios. Figure 4 presents experimental data (normalized) for the Vairex compressor. The trend towards increasing power requirements with increasing pressure and mass flow indicates that the apparent improvements in performance for the fuel cell stack may not be realized in a system.

At any particular pressure ratio, we can look at the effect of increasing mass flow. It can be seen that small increases from a low level will likely be beneficial to the fuel cell stack – since the power demand does not rise that steeply. But for an increase in air mass flow at higher SRa, the benefits are likely to disappear as the slope of the power curve rises significantly. Although it is difficult to see in Figure 4, the compression

power demand increases more sharply with increasing pressure at any specific mass flow rate. This suggests that there may be a point of optimization for the net power from the fuel cell system through a combination of both air pressure and air flow control.

Integrated System Characteristics and Optimization

To begin investigating the interaction between the compressor and the fuel cell stack, a simple case can be investigated based on operation at a single pressure and SRa. Typically, the idealized operation of a fuel cell stack is explained using a single polarization plot at high pressure and high air side stoichiometric ratios, as shown in Figure 5. This figure illustrates that both high stack voltages and high currents can be attained by using both high pressure and high air stoichiometry.

Another context for viewing the performance of a fuel cell stack (that is particularly useful for automotive applications) is the efficiency versus net power plot. Figure 6 illustrates this format for the same conditions as Figure 5. In Figure 6 it can be seen that the fuel cell stack operates at gross efficiencies on the order of 50 to 70 percent over the most of its power range.

However, Figure 6 also indicates that if the power required for high pressure and high air flow is subtracted from the gross stack power, then the operating characteristics of the fuel cell system are not as favorable. In fact both the net efficiency and the net peak power are significantly reduced for these operating conditions. Of course the net efficiency and net power characteristics are the actual determinants of the fuel cell system performance. The critical question is whether the net efficiency and net power characteristics of the fuel cell system can be optimized by operating the fuel cell stack at varying air pressure and/or air stoichiometry.

Varying the air pressure alone corresponds to the polarization plots in Figure 2, where SRa is kept constant and the pressure is varied. Figure 7 shows the impact on net stack efficiency for operation at a SRa of 2.5 with pressure varying from 1.1 to 3.25 atmospheres (assuming a compressor inlet pressure of 1.0 atm). In the low power region the most efficient operation is found at the lower pressures, where the compressor energy requirements are relatively low and very little benefit is achieved in the fuel cell stack from increased pressure. As the pressure increases, higher and higher powers can be maintained at higher efficiency until the extra energy required to compress the air outweighs the benefit of going to a higher stack operating pressure, shown in Figure 7 as occurring between 2.5 atm and 3.25 atm. It can also be seen that the benefit to going from a pressure of 1.5 atm to 2.5 atm is not very large, an increase in net peak power of only about 1 kW.

The location of this crossover point, where additional compression no longer benefits the net characteristics of the fuel cell system, is highly dependent on the SRa. Figure 8 represents a similar case as Figure 7, but at a lower SRa. When the SRa is fixed at 1.5, the increase in pressure from 1.5 to 2.5 atm results in a net peak power increase of over 2 kW, or about eight percent of the net power available at 1.5 atm, and twice the increase as when SRa was 2.5. The increased pressure crossover point is still between 2.5 and 3.25 atm, but in this case it is further from 2.5 than before. Thus, at lower SRa, the stack performance is more sensitive to variations in pressure.

Similar shifts in the stack characteristics can be observed when the pressure is held constant and the air stoichiometric ratio is varied. Figure 9 shows an increase in peak net power with increasing SRa that is similar to that observed for increasing pressures. However, there is not the same increase in stack operating efficiency at lower power (Note: The power scale has been altered in Figure 9 to allow the details at high power to be more visible). This trend is a result of the fact that at these low currents, the air side stoichiometric ratio does not impact the partial pressure of oxygen at the cathode catalyst layer as directly as total pressure does. Under the conditions in Figure 9, the SRa crossover point seems to occur somewhere between 2.5 and 3.0, but closer to a SRa of 2.5. When operating at a lower pressure (not shown), this crossover point shifts out closer to 3.0, indicating that at lower pressures, the stack performance is more sensitive to variations in SRa.

All of this information can be brought together to develop an optimization process for the fuel cell stack and the air supply. In general, it has been shown that low air pressure operation is the best way to improve net system efficiency at low net powers. Further, it was shown that increasing SRa does not have a significant impact on stack efficiency at low powers. Therefore the most efficient low power operation of the fuel cell system will be at low pressure and low SRa.

In the higher power regions, it was shown that both an increased pressure and an increased SRa will improve peak net power achievable in the fuel cell system. Thus, the two should be increased together to achieve the maximum possible benefits. This improvement is eventually terminated by increased power demand for the compression process.

The application of this combination of pressure and flow control is illustrated in Figure 10, where the pressure and flow are both varied depending on the net power drawn from the system. The optimal operating curve for the fuel cell system is the envelope of the curves shown. This can be translated into an optimal operation strategy that achieves high efficiency at low power and also provides a high peak power capability.

This optimal operating strategy can be compared with the high pressure and high SRa operating strategy presented in Figure 6. Figure 11 indicates that the optimal control strategy achieves the same peak net power as that for fixed pressure and SRa, but shows significant efficiency improvement in the low power regions. The peak efficiency is increased by 6 percentage points, for a 15 percent overall improvement in peak efficiency. Further, this increase occurs in the lower power regions where the fuel cell would be expected to operate during normal driving. The efficiencies still do not reach the gross efficiencies as would be expected from compressor energy requirements.

ADDITIONAL CONSIDERATIONS

There are a number of additional stack and compressor limitations that can influence the choice of the optimum operating strategy for a particular direct hydrogen fuel cell system. Examples are:

- **Poor Cathode Catalyst Layer Performance:** For example because of high resistance to protonic transport, or poor oxygen diffusivity, in the catalyst layer.
- **Compressor Limitations:** The inability of a particular compressor type or technology to cover the full range of pressure and flow required for the optimization process.
- **Dynamic Response of the Air Supply:** The inability of the air compressor to follow the required pressure and flow profile during rapid changes in power demand for a vehicle driving cycle.
- **Expander Energy Recovery:** The need for a relatively high stack air exhaust pressure for energy recovery.

Most of these issues are already incorporated in the model and future work will continue to expand the breadth of complications that can be analyzed. However, even if these effects are present, the system optimization will proceed in the same method as discussed above, only the quantitative details will differ.

Finally, if the optimization of a reformat fuelled PEM system is considered, a similar optimization must be carried out for the reformat fuel supply and anode interaction. For reformat, the situation is more complicated because one must deal both with hydrogen dilution effects (analogous to the oxygen dilution in air), and with CO poisoning effects.

SUMMARY

The optimization procedure presented in this paper has been developed to account for the operation of a complete direct-hydrogen PEM fuel cell system. The focus is on the key limiting components, the fuel cell stack and the air supply. The fuel cell stack alone could be optimized by operation at high pressure and high-air side stoichiometric ratio, but in the system context, the power required for compression at low output power significantly reduces the efficiency advantage of the fuel cell system.

The combination of the operating characteristics of the fuel cell stack and air supply leads to an optimal operating strategy where low power operation is achieved using low pressure and low air-side stoichiometry. This allows the power associated with the air supply to be minimized, increasing the overall system efficiency at low power. Under high power conditions, both the pressure and air-side stoichiometry are

increased, but limited to the point where diminishing returns set in due to increasing compressor power requirements and minimal stack performance improvements.

Overall, this paper shows that a direct-hydrogen fuel cell system can be optimized to achieve high peak power and high efficiency over a broad range of output powers. The key to achieving this in a practical system is the flexibility of the air supply to provide air at varying pressures and mass flow rates. A balance must be found between the performance characteristics of the stack and the air supply systems. Additional components and practical limitations will alter the results of the optimization process, but the fundamental procedure remains the same and can account for the additional issues.

ACKNOWLEDGMENTS

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FIGURES

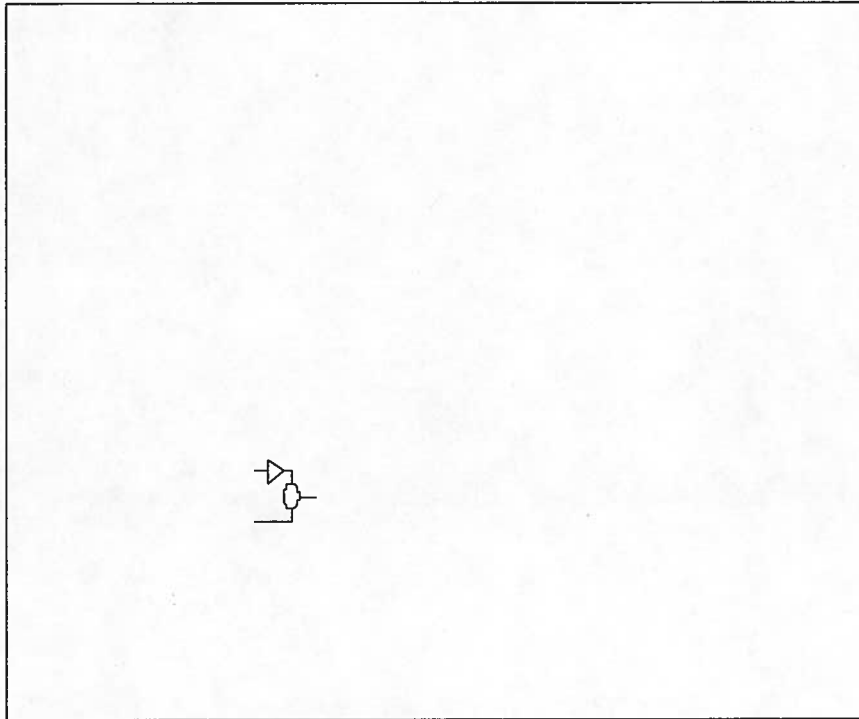


Figure 1. Simplified Schematic of an Automotive Fuel Cell System.

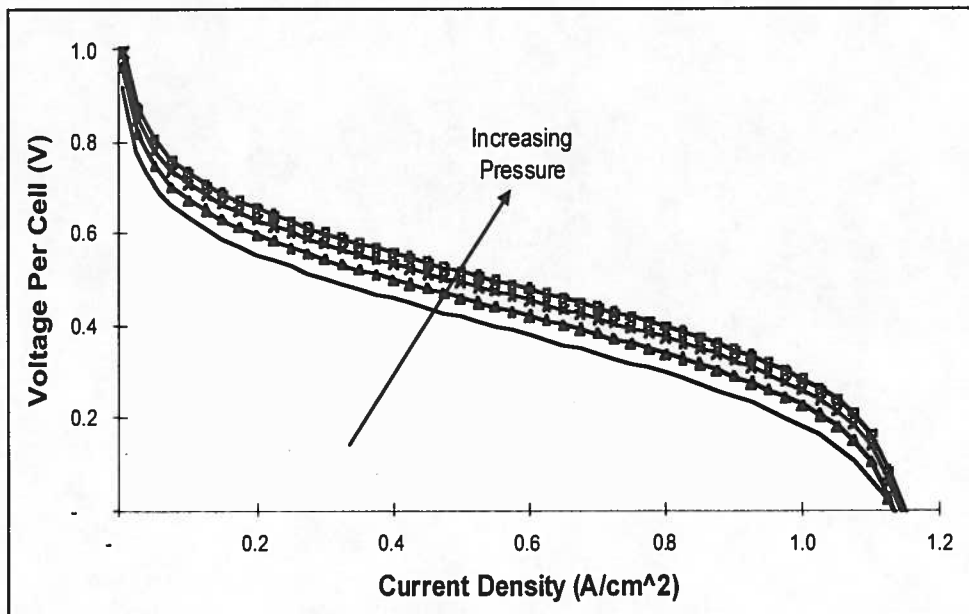


Figure 2. Polarization Plot for Varying Pressure.

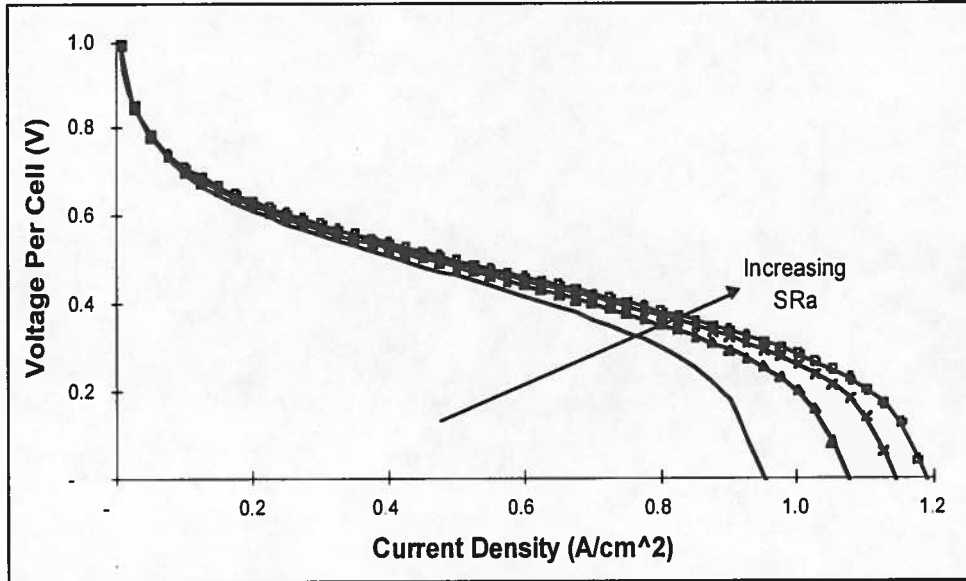


Figure 3. Polarization Plot for Varying Air Side Stoichiometric Ratio (SRa).

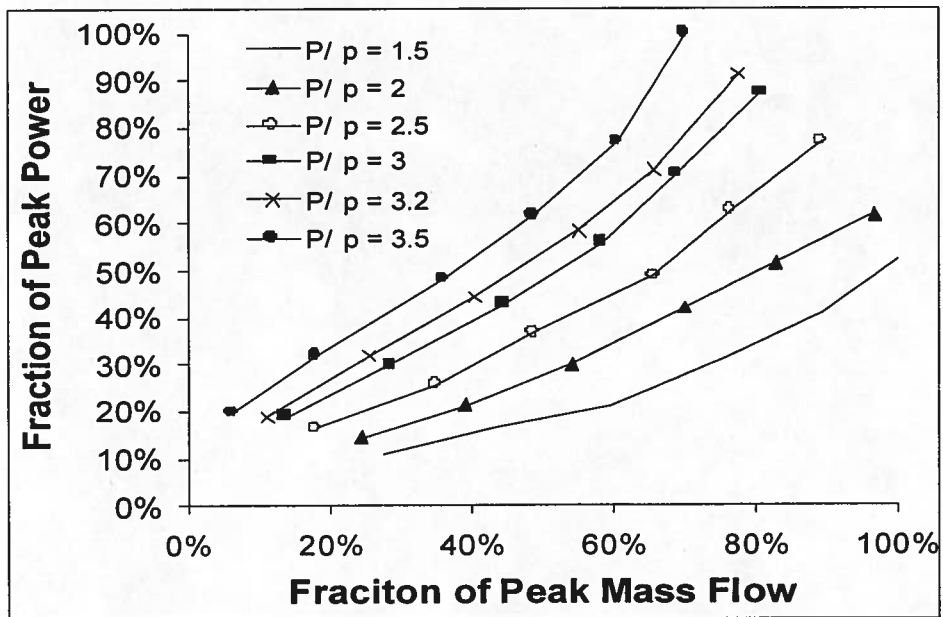


Figure 4. Power Characteristics of the Vairex Variable Displacement Piston Compressor. Source: Vairex Corporation.

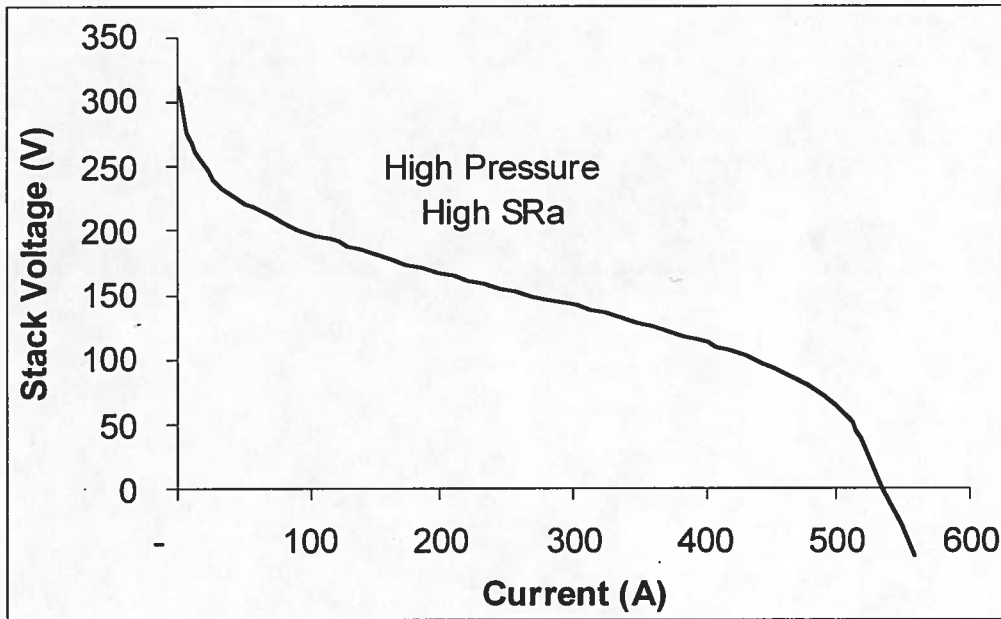
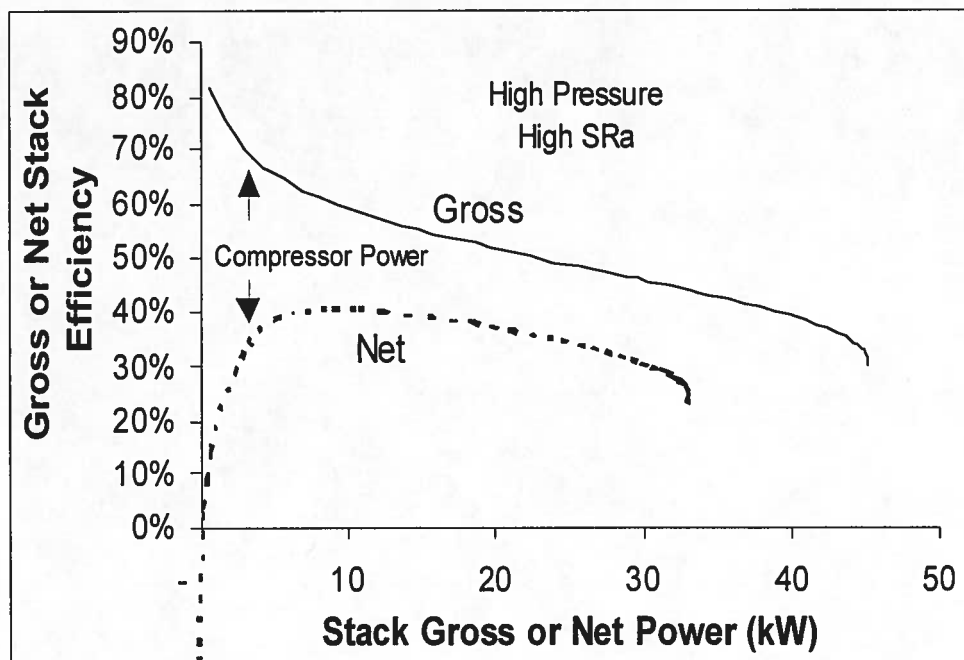


Figure 5. Polarization Plot for a Fuel Cell Operating at High Pressure and High SRa.



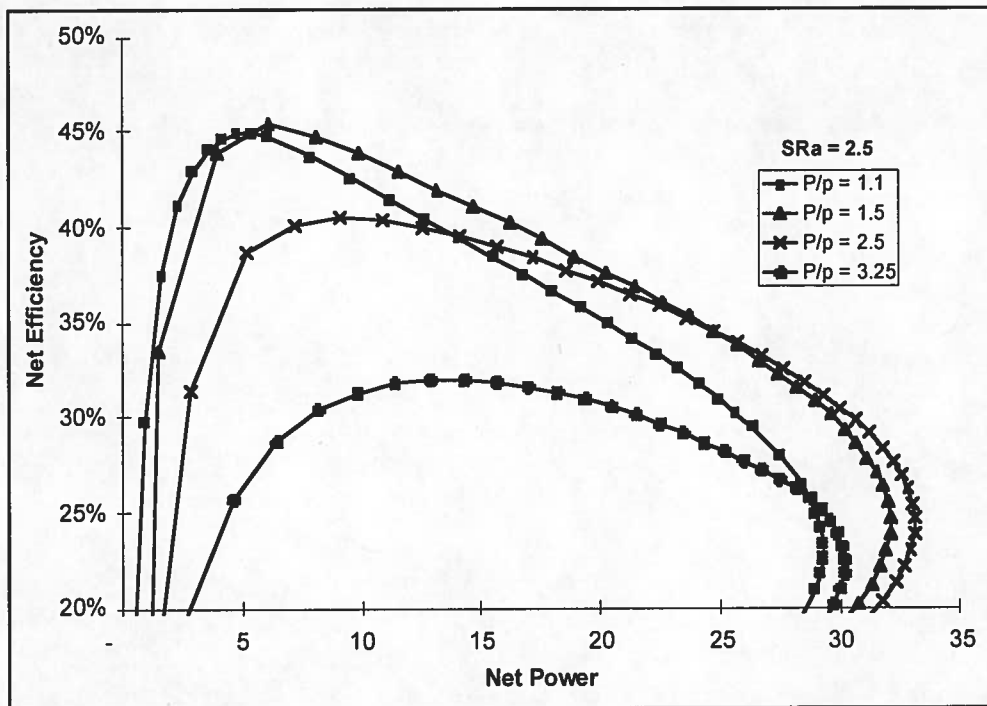
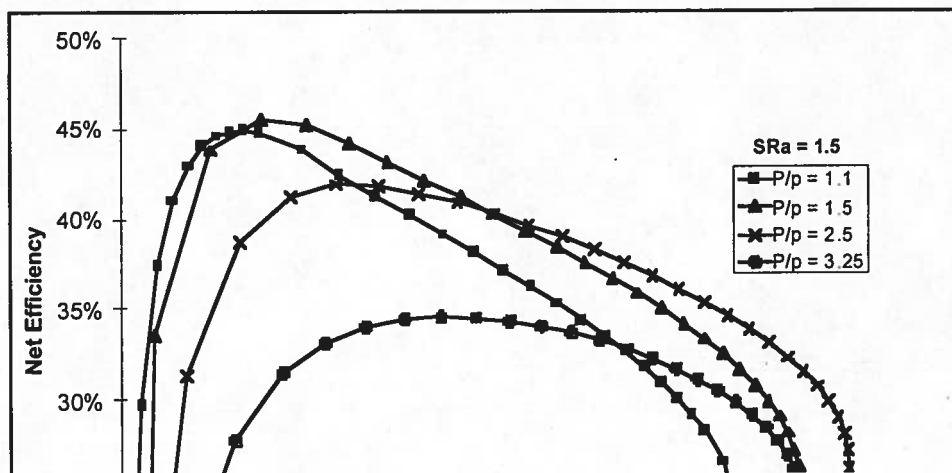


Figure 7. Net Efficiency Plot with SRa at 2.5 and Pressure Varying.



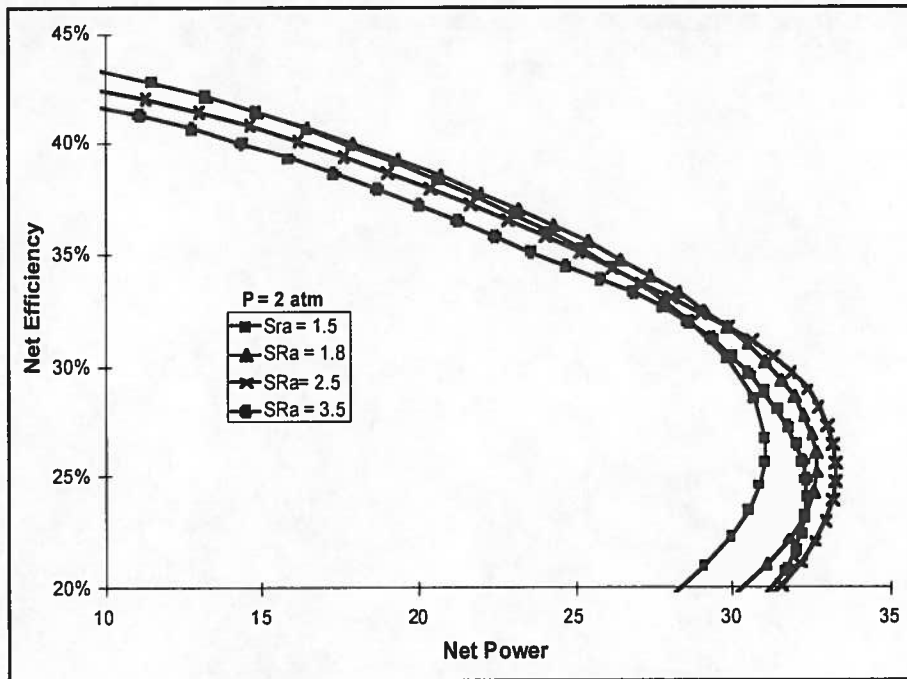
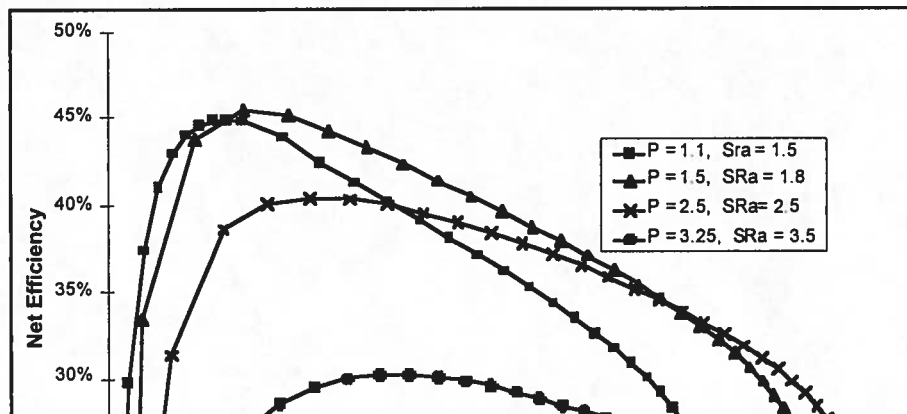


Figure 9. Net Efficiency Plot with P at 2 atm and SRa Varying.



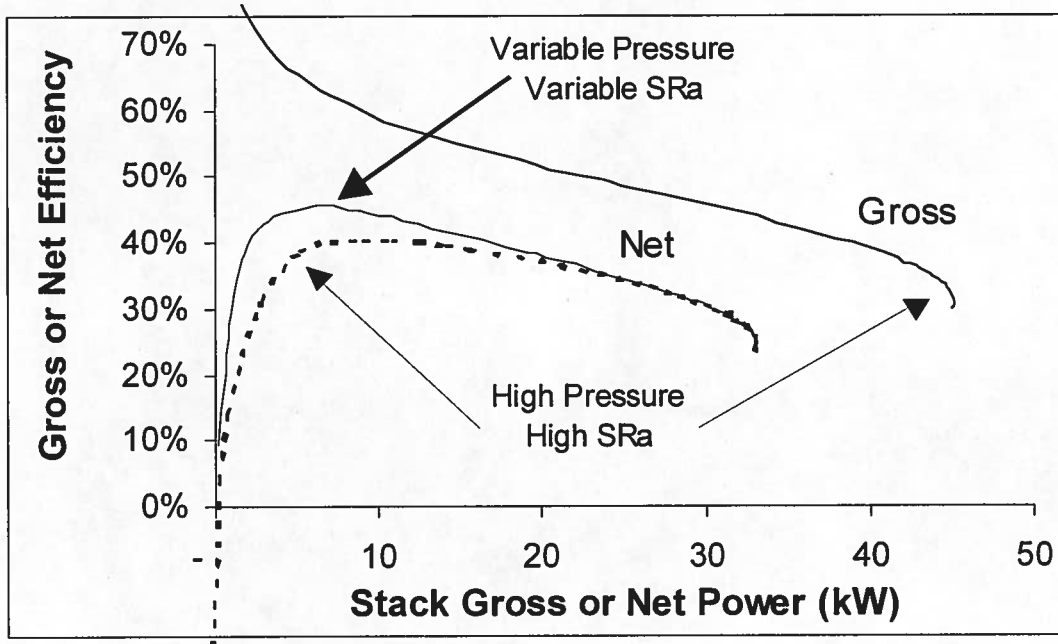


Figure 11. Comparison of Efficiencies Between the Optimized and Non-Optimized Systems.