Design, Integration, and Trade-Off Analyses of Gasoline-Fueled Polymer Electrolyte Fuel Cell Systems for Transportation

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INTRODUCTION

Prototype fuel-cell-powered vehicles have recently been demonstrated in Japan, Europe, and North America. Conceptual designs and simulations of fuel-cell-powered vehicles have also been published [1–3]. Many of these simulations include detailed vehicle performance models, but they use relatively simplistic fuel-cell power system models. We have developed a comprehensive model of a polymer electrolyte fuel cell (PEFC) power system for automotive propulsion. This system simulation has been used to design and analyze fuel-cell systems and vehicles with gasoline (or other hydrocarbons) as the on-board fuel. The major objective of this analysis is to examine the influence of design parameters on system efficiency and performance, and component sizes.

THE MODEL

We have developed an efficient, versatile system design and analysis code, GCtool [4]. The code includes component models (reactors, heat exchangers, etc.), mathematical utilities, property utilities, thermodynamic data, chemical kinetics, and multiphase equilibria. The model can be used to perform parameter sweeps, constrained optimizations, and time integrations (for dynamic

simulations). In this paper, we discuss simulation results for a reference system design and options to increase the system efficiency, thermal and water management, rapid cold start, influence of high design ambient temperatures, and atmospheric pressure systems vs. pressurized systems.

ANALYSIS OF A "PERFECT" SYSTEM

A preliminary analysis was conducted for a "perfect" fuel-cell system. This perfect system was assumed to have thermodynamically ideal partial-oxidation reforming at 25°C with stoichiometric amounts of air and water, 100% fuel utilization, no energy loss at the reformer, and no parasitic power consumption. For such a perfect system, the system efficiency depends only on the operating cell voltage; the results are shown as the top curve in Fig. 1. As the actual process inefficiencies are taken into account, however, the system efficiency decreases substantially. The lower curves in Fig. 1 show the cumulative effects of (a) 30% excess water use in the fuel processor, (b) fuel utilization decrease to 90%, (c) reformer heat loss of 10% of the input energy, and (d) parasitic power consumption of 5% of the gross power generated by the fuel cell. Thus, for example, an operating cell voltage of ≥0.8 V would be needed for a 45% efficient system that accounts for items (a)–(d).

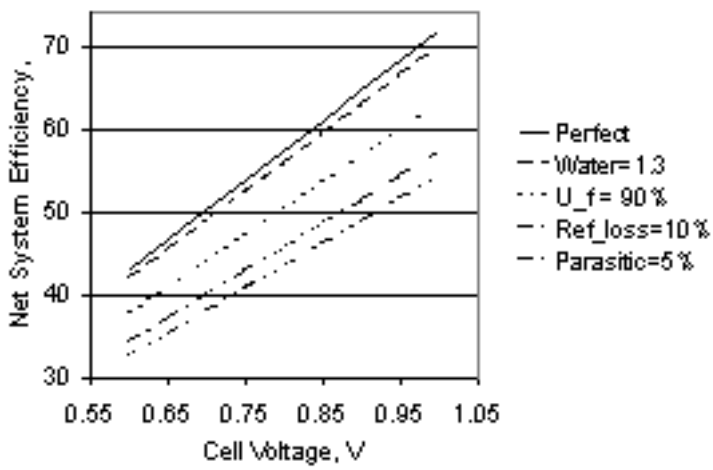

Fig. 1. Effect of Cell Voltage on Net Efficiency for a Perfect Gasoline-Fueled PEFC System: Base Case Analysis of a Reference System Design

GCtool was used to develop a detailed model of a pressurized, partial-oxidation (POX) reformed, gasoline-fueled PEFC system (for this analysis, the fuel was taken to be iso-octane). The model includes every system component that has an energy or material transport or balance aspect. For example, since there is less than 100% fuel utilization in the PEFC, the system includes a catalytic burner to handle the spent anode gas, as well as a gas-turbine bottoming cycle to recover the pressure and thermal energy in the exhaust from the catalytic burner. Process water is used in the reformer, and for water-gas shift and reformate quenching. Therefore, an exhaust cooler/condenser is included to recover enough water to be self-sufficient in water. A significant system integration issue is the mismatch between the temperatures of the POX reactor, the water-gas shift reactors,

and the fuel cell stack. Thermal integration is achieved by the use of a steam generator and an air preheater. The key design conditions and the controlling system variables are given in Table 1.

TABLE 1 IMPORTANT SYSTEM DESIGN PARAMETERS AND CONTROL VARIABLES

Design Parameter	Variable
Partial-oxidation temperature: 1300 K	Fuel-to-air ratio
High-temperature shift reaction: 700 K	Water-to-fuel ratio
Low-temperature shift reaction: 450 K	Water flow to LTS
Oxygen utilization: 50%	Air-to-fuel ratio
Net power output: 50 kWe	Fuel feed rate

Other base-case design values were based on near-term PEFC performance and are given in Table 2. The resulting power generation and power requirements by the various components for a 50-kW electric (net) system are shown in Table 3. The calculated efficiency for this base case system is 35.1%.

TABLE 2 ADDITIONAL BASE-CASE (NEAR-TERM) DESIGN PARAMETER VALUES

Design Parameter	Value
Fuel utilization in PEFC	85%
Cell voltage, current density	0.685 V @ 0.7 A/cm^2
Air-mover efficiencies	80%
Pump efficiencies	75%

TABLE 3. COMPONENT POWER GENERATION AND CONSUMPTION AT FULL LOAD (50 kWE)	
Component	**Power (kW)**
Fuel-cell stack	52.5
Expander	9.2
Compressor	9.3
Radiator fan	1.5
Condenser fan	0.6
Water pump	0.1
Fuel pump	<5 W

The base-case analysis showed the following:

- Water-to-fuel ratio in fuel processor = 3.6 (g/g), 22.8 (mol/mol)
- Overall air-to-fuel ratio in system = 22.3 (g/g) (i.e., 1.33 times stoichiometric)
- Coolant water circulation rate = 0.5 kg/s (for a 25ºC temperature rise across fuel-cell stack)
- Cooling air flow rates: radiator = 2.7 kg/s, 2.3 m^3/s; condenser = 1.2 kg/s, 1 m^3/s

Water Balance in the System
Relative to the fuel feed rate, m_f, the various process water flows are

- Water in reformer feed / m_f = 3.6 (g/g), 22.5 (mol/mol)
- In-cell production of water / m_f = 2.2 (g/g), 14.2 (mol/mol)

- Water recovered in cathode exhaust separator / m_f = 2.3 (g/g)
- Water recovered in condenser / m_f = 1.2 (g/g)

Heating/Cooling Loads in the System
Component heat duties and the corresponding log-mean temperature differences (LMTDs) are shown in Table 4. Half of the condenser heat load is in the form of phase change heat transfer.

TABLE 4 COMPONENT HEAT DUTIES AND TEMPERATURE DIFFERENCE DRIVING FORCES

Component	Heating/Cooling Duty (kW)	LMTD (K)
Fuel-cell stack	52.7	14.3
Radiator	66.6	25.4
Condenser	17.2	49.4
Steam generator	1.0	226.9
Air preheater	5.6	675.8
Reformate cooler	14.4	31.8
Compressor intercooler	4.3	14.4
Fuel vaporizer	2.7	79.4

DESIGNING A HIGH-PERFORMANCE SYSTEM

A high-performance system was designed based on the effects of varying several key design and operating parameters. As the POX temperature is raised, the system efficiency decreases, as shown in Fig. 2. The system efficiency is increased by increasing the cell voltage, which also decreases the heat duties at the fuel-cell stack, radiator, and condenser, as indicated in Table 5. Increasing the fuel utilization also results in a small improvement in system efficiency. On the basis of these

analyses, reducing the POX temperature from 1300 K to 1000 K, increasing the fuel utilization from 85% to 90%, and increasing the cell voltage from 0.685 V to 0.8 V would increase the system efficiency from 35.1% to 46.9%. In addition, the component cooling loads would decrease substantially: fuel cell stack, from 52.7 kW to 36.8 kW; radiator, from 66.6 kW to 40.1 kW; and condenser, from 17.2 kW to 10.1 kW.

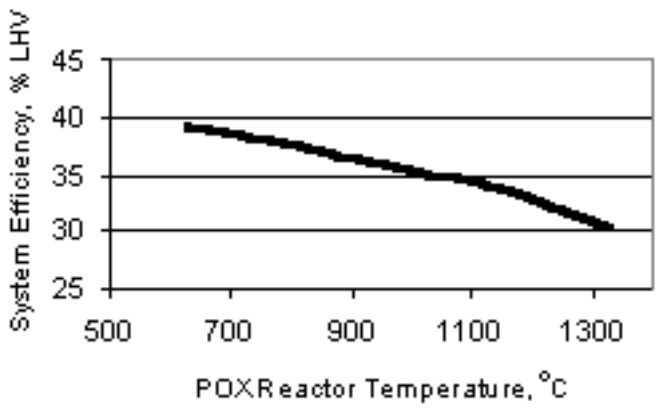

Fig. 2. System Efficiency Decreases with Increasing POX Temperature

OTHER ANALYSES

Elevated Design Ambient Temperatures

As the design ambient temperature is increased from 20°C to 47°C (68 to 117°F), the radiator size increases by a factor of five, as shown in Fig. 3. The condenser size also increases, but only by about 50%.

TABLE 5 EFFECT OF CELL VOLTAGE ON SYSTEM EFFICIENCY AND COMPONENT HEAT DUTIES

Cell Voltage (V)	System Efficiency (%)	Component Heat Duties (kW)		
		PEFC	Radiator	Condenser
0.685	35.1	52.7	66.6	17.2
0.700	35.9	50.5	64.0	16.8
0.750	38.7	43.4	55.9	15.6
0.800	41.4	37.3	49.0	14.6

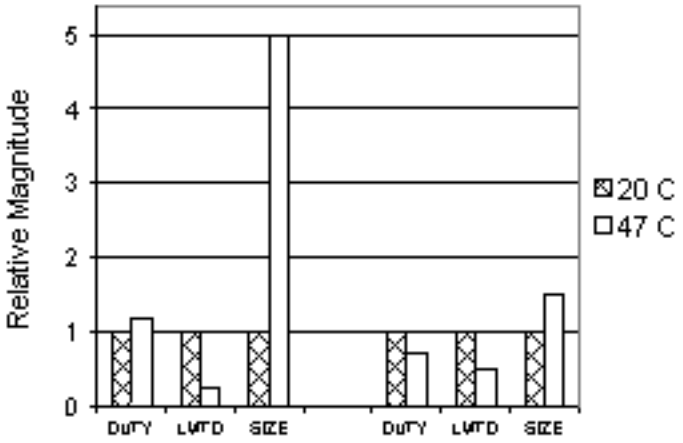

Fig. 3. Radiator and Condenser Design Parameters at Two Different Ambient Temperatures

Operating Requirements for Rapid Cold Start

With air, fuel, and water at the design feed rates (with 10% excess fuel to burner), the system can deliver 80% of full power in 130 s. With air and fuel feed rates at twice their design values, cold start time is reduced to 63 s. Cold start could be achieved in 36 s if fuel processor component masses were reduced to one-half their values in the present designs.

Atmospheric Pressure System

Such a system needs no compressor or expander, but it is difficult to recover the energy in the spent anode gas. There is a large heat load on the condenser for water recovery. The fuel-cell stack needs nearly twice the active cell area for system efficiency comparable to that of a pressurized system. Water management is a significant issue, particularly at elevated ambient temperatures.

ACKNOWLEDGMENT

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