II.I.6 Design, Optimization and Fabrication of a Home Hydrogen Fueling System

Mahesh M. Waje (Primary Contact), Jeremy Lange, Koray Ozdemir, Ashwin Balasubramanian, Brian Hennings Lynntech, Inc. 7610 Eastmark Drive College Station, TX 77840 Phone: (979) 693-0017 E-mail: mahesh.waje@lynntech.com

DOE Technology Development Manager: Monterey Gardiner Phone: (202) 586-1758 E-mail: Monterey.Gardiner@ee.doe.gov

Contract Number: DE-SC0001615

Project Start Date: July 20, 2009 Project End Date: April 19, 2010

Objectives

- Construct a multivariate system optimization model for a reformer-based home hydrogen fueling appliance that:
 - Provides system selection guidance for optimal system integration.
 - Determines the cost, energy requirement and CO₂ emissions for the selected system integration route.
 - Provides sensitivity analysis for the selected system integration routes with respect to critical cost and energy parameters such as natural gas price, electricity price, hydrogen production rate and bulk production volume.
- Determine the safety issues with the optimal system of choice for a hydrogen production rate of 0.5 kg/day to 3 kg/day. The safety of operation has to be evaluated for the operation of the appliance for a home owner or a person completely unskilled from technical and safety points of view.

Technical Barriers

This project addresses the following technical barriers from the Production section of DOE's Multi-Year Research, Development and Demonstration Plan:

- (A) Reformer Capital Costs
- (E) Greenhouse Gas Emissions
- (G) Capital Cost

Technical Targets

The technical target of the project is to develop an affordable and safe home hydrogen fueling appliance for a daily consumer that speeds up commercialization and general awareness of fuel cell technology. Insights gained from this project will be applied toward the design and fabrication of a home hydrogen fueling appliance in Phase II of the project. The target of the Phase I project was to design a system that meets average home-owner requirements for a fuel cell vehicle application. The specific targets are:

- H₂ production rate: 0.5-5 kg per day
- Fueling time: 2-8 hrs
- $H_2 \text{ cost: }$ \$2.00 to \$3.00 per kg H_2 for distributed H_2 production
- Fuel cell grade H₂ quality (SAE J2719 standard)
- H_2 delivery pressure: \geq 5,000 psig
- H₂ delivery temperature: 25-40°C

Accomplishments

- Identified safety codes and standards and developed operating guidelines.
- Constructed a user-friendly multivariate model that can perform sensitivity analyses and identified best options for a home fueling station for low H₂ production rates based on cost, CO₂ emissions and electricity consumption.
- Completed preliminary system design calculations for a Phase II prototype system for 0.5 kg/day H₂ production.
- Identified Go/No-Go milestones for Phase II for the optimized system fabrication.



Introduction

Cost, safety and energy requirement are the critical barriers for realizing the concept of home hydrogen fueling for widespread recognition and commercialization of fuel cells in automotive use. Reformation of hydrocarbon fuels such as natural gas and electrolysis of water are the two best options available for hydrogen production. For fuel cell vehicle application, hydrogen at high purity and pressure (>5,000 psig) is required. This presents a system integration problem, where individual processes of hydrogen generation, purification (only for reformation route) and compression have to be integrated together efficiently in order to produce an affordable device. Though there have been significant efforts in advancing and optimizing individual systems for centralized and distributed hydrogen generation, there is no effort made on the understanding and optimization of system integration strategies for very low hydrogen production rates (<5 kg/day, 8 hour operation) for a typical home fueling application.

Approach

The target of Phase I was to identify, select and integrate the individual subsystems (desulfurizer, reformer, hydrogen purifier and compressor) for a reformer-based home hydrogen generation unit, utilizing natural gas as the fuel feed. The selection criteria were to be based on optimization of critical parameters identified for successful commercial home fueling appliance through a multivariate analysis of the system. The chosen parameters for evaluation of the system were cost, safety and in particular, the electrical energy requirement of the appliance. Lynntech approached the system optimization problem in the following steps:

- Identify and qualify the subsystem or component options and weigh them qualitatively from cost, safety and operability standpoints. This is done by creating weighting factors for each criteria (cost, safety, etc.) and determining the overall system or component score.
- Select appropriate systems for integration from the weighting parameter analysis.
- Construct a quantitative multivariate model to estimate the cost, energy requirement and CO₂ emissions for selected system integration routes.
- Conduct the sensitivity analysis with the model for cost with respect to the variation in natural gas cost, electricity cost and bulk production volume.
- Design the most optimum system from the model results for fabrication of a Phase II prototype for 0.5 kg/day H₂ production.

Results

In accordance with the objectives of Phase I, Lynntech developed a multivariate system optimization tool to determine the cost, CO₂ emissions and energy requirement for different system integration strategies for natural gas reformation as well as the water electrolyzer route. The significant findings for a H_a production rate of 0.5 kg/day to 5 kg/day from the project was that a combination of natural gas reformation for H₂ production with electrochemical purification and compression offers the most economical system design. The competitive system analyzed was a low-pressure electrolyzer with a compressor. The cost of H₂ per kg, electricity requirements and CO₂ emissions are found to be less than the electrolyzer route. The results for H₂ production rate of 0.5 kg/day with 8 hours of operation per day are summarized in Figure 1.

The target of the system optimization was to develop a user-friendly system analysis tool, which allows user inputs for hydrogen production rate, selection of individual system components and their key operating or cost parameters and creates output of cost of hydrogen, CO_2 emission and electricity requirements. A weighting factor analysis procedure was formulated for comparing individual system components for initial screening of the system components for integration. The system components are scored for cost, safety, technology maturity, ease of operation, ease of integration and maintenance. A typical output from the program for comparing different system components is shown in Figure 2.

The selected system components were then linked with each other to create complete system integration strategies. The assumptions for electricity and natural gas cost are taken from H2A analysis. Capital cost is the primary cost driver in the hydrogen production range under consideration. Figure 3 compares the capital costs of only the reactor-purifier systems under consideration, e.g. the two combinations for the reformer systems, steam methane reformer with electrochemical purifier (SMR-ECM) and steam methane reformer with pressure

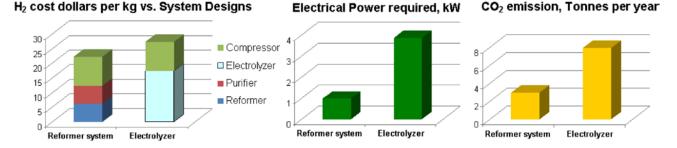


FIGURE 1. Comparison of system optimization results for 0.5 kg/day H₂ (8 hour per day operation) production for Lynntech's proposed reformer system and a low-pressure water electrolyzer.

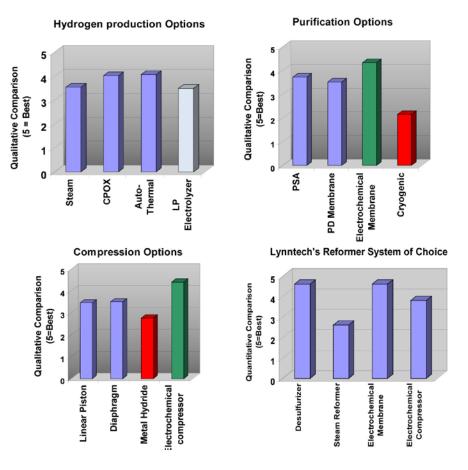


FIGURE 2. Scoring comparison for different systems and Lynntech's reformer system of choice. CPOX - catalytic partial oxidation; PD - palladium; LP - low pressure

swing adsorption (SMR-PSA). The cost numbers are based on material requirements only and do not take labor into account. It is assumed that the labor cost will become negligible with bulk production practice. Compressor cost is not included in the cost data in Figure 3. The cost for the low-pressure electrolyzer option is compared with the reformer systems. It is found that the combination of electrochemical purification with reformer is the best system from the capital cost perspective. Electrolyzer does come close to be competitive with the SMR-ECM system at lower production rates.

After deducing the capital and operating costs for the systems under consideration, the cost of hydrogen was determined by amortizing the capital cost over a period of 10 years. The rate of return on investment for this period was assumed to be 10%. Figure 4 shows a comparison of hydrogen cost for different production rates for the four system integration options considered under the project. System 1, a SMR-ECM was found to be the best choice among the systems analyzed. It was inferred from the bar plots that for purification and compression, the mechanical systems, PSA and mechanical compression become competitive with electrochemical systems at hydrogen production rates of 5 kg/day, but below that electrochemical systems are the preferred choice. Sensitivity analysis was then

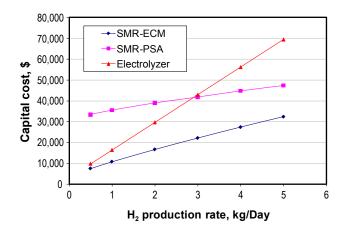


FIGURE 3. Capital costs for the reformer systems and electrolyzer as a function of H₂ production (assuming 8 hour per day operation).

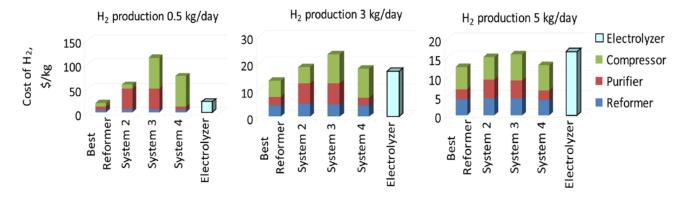


FIGURE 4. Comparison of system optimization results for H_2 cost at H_2 production rates of 0.5 kg/day, 3 kg/day and 5 kg/day for the reformer systems and low-pressure water electrolyzer. The results indicated System 1 to be the best reformer system for the hydrogen production rates under consideration.

conducted to determine the dependence of H_2 cost on the cost of electricity and natural gas feedstock.

Based on the optimal system integration strategy, preliminary plant design for the complete hydrogen production plant was developed for 5,000 psig H_2 output as per SAE J2719 quality standard. Safety analysis was then conducted as per ISO 16110, to identify critical failure modes and control strategies or equipment needed. A cheap and effective control strategy was developed to reduce the complexity and cost of the sensor and control equipments used.

Conclusions and Future Directions

- A multivariate model was developed for system optimization and sensitivity analyses of home hydrogen fueling systems.
- Model results for 0.5 to 5 kg/day hydrogen production rate:
 - Reformation of natural gas is the cost-effective way to produce hydrogen gas as compared to water electrolyzers.

- Capital cost of purification and compression are the critical cost drivers for the reformer-based hydrogen production systems.
- Electrochemical purification and compression technologies offer the most cost-effective route as compared to conventional PSA and mechanical compression technologies.
- Combination of reformation for H₂ production with electrochemical purification and compression offers the most economical system design.
- The commercial benefits are multiple and include:
 - Small-scale hydrogen refueling stations offering significant cost and process advantages over existing designs.
 - Modeling and simulation tools for implementation of future hydrogen economy equipment items and infrastructure.
- The future task will be to refine the model and convert it into a user-friendly program that can be used as a tool for selection of subsystems for a home hydrogen fueling system.
- Lynntech plans to use the model results to develop and demonstrate a cheap (low capital cost) home hydrogen fueling appliance for 0.5 kg/day H₂ production in Phase II.