VIII.6 Hydrogen Quality Issues for Fuel Cell Vehicles

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Objectives

- Develop a process to determine hydrogen quality requirements for fuel cell vehicles, based on life-cycle costs.
  - Identify how fuel quality influences the life-cycle costs of the various components of the overall "hydrogen system".
  - Develop models to evaluate the effects of fuel quality on the costs of the hydrogen system components.
- Identify information gaps and the research and development (R&D) needed to fill those gaps (along with who/how best to conduct that R&D).

Technical Barriers

This project addresses the following technical barriers from the Systems Analysis section of the Hydrogen, Fuel Cells and Infrastructure Technologies Program Multi-Year Research, Development and Demonstration Plan:

(B) Stove-Piped/Siloed Analytical Capability

(D) Suite of Models and Tools

Contribution to Achievement of DOE Systems Analysis Milestones

This project will contribute to achieving the following DOE Systems Analysis milestones from the Systems Analysis section of the Hydrogen, Fuel Cells and Infrastructure Technologies Program Multi-Year Research, Development and Demonstration Plan:

- **Milestone 5: Complete analysis and studies of resource/feedstock, production/delivery and existing infrastructure for various hydrogen scenarios. (4Q, 2009)** Different hydrogen production and dispensing scenarios potentially entail different contaminants at different concentrations. In the current phase of our analyses, we will identify and quantify these fuel contaminants in three distributed hydrogen production scenarios.
- **Milestone 6: Complete analysis of the impact of hydrogen quality on the hydrogen production cost and the fuel cell performance. (4Q, 2010)** We are developing models for the effects of contaminants on the performance and costs of hydrogen production and purification, and for the degradation in the performance and durability of fuel cell systems. These models will permit trade-off and sensitivity analyses of these effects on a life-cycle cost basis.
- **Milestone 9: Complete analysis of the impact of hydrogen quality on the hydrogen production cost and the fuel cell performance for the long range technologies and technology readiness. (2Q, 2015)** Analyses similar to the ones described here will be extended to longer term technologies for hydrogen production, purification, use in the fuel cells, and hydrogen analysis and quality verification as those technologies reach a suitable stage of development for such analyses.

Accomplishments

- Developed an initial "framework" document to help define the work of the DOE Hydrogen Quality Working Group (H2QWG), which was conducted by holding in-person meetings three to four times a year and interim discussions, with input from experts in the fields of fuel cells, hydrogen gas production and purification, gas analysis technologies, and costing methodologies.
- Prepared a comprehensive draft roadmap that has been reviewed by the H2QWG and is presently being reviewed by DOE Technology Development Managers. The appendices to the roadmap contain species-specific discussions on test data, effects on fuel cell performance and durability, effectiveness of H_2 purification methods, modeling, and R&D needs for the individual species.
- Worked with model developers at Argonne and elsewhere to initiate the development and validation of performance and life-cycle cost models of the effects of fuel impurities on hydrogen production, purification, and use in fuel cells.

- Determined preliminary R&D needs and recommendations:
  - Need better quantification of the cost and performance of pressure-swing adsorption (PSA) vs. H_2 quality.
  - Need better quantification of the cost and performance of fuel cells vs. nature and level of contaminant, and of the costs of overcoming the deleterious effects of specific contaminants.
  - Need low-cost methods for hydrogen sampling and analysis for certification and on-line quality control.
- Provided briefings and updates to various DOE/FreedomCAR Technical Teams.

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Introduction

Developing and implementing fuel quality specifications for hydrogen are a prerequisite to the widespread deployment of hydrogen-fueled fuel cell vehicles. Several organizations are addressing this fuel quality issue, including, among others, the International Standards Organization (ISO), the Society of Automotive Engineers (SAE), the California Fuel Cell Partnership (CaFCP), and the New Energy and Industrial Technology Development Organization (NEDO)/Japan Automobile Research Institute (JARI). All of these activities, however, have focused on the deleterious effects of different potential contaminants on the automotive fuel cell or on-board hydrogen storage systems. While it is possible for the energy industry to provide extremely pure hydrogen, such hydrogen could entail excessive costs. It is the objective of this task to develop a process whereby the hydrogen quality requirements may be determined based on life-cycle costs of the complete hydrogen fuel cell vehicle "system." To accomplish this objective, the influence of different contaminants and their concentrations in fuel hydrogen on the life-cycle costs of hydrogen production, purification, use in fuel cells, and hydrogen analysis and quality verification must be assessed.

Approach

We have assembled a DOE H2QWG to obtain input from a broad spectrum of involved groups and organizations. Members of the H2QWG include DOE Hydrogen Program technology development managers from the Fuel Cell, Hydrogen Storage, Hydrogen Production, Delivery, Systems Analysis, Codes and Standards, and Cross-Cutting teams; U. S. automobile companies and fuel cell developers (DaimlerChrysler, Ford, General Motors, UTC Power); energy companies (BP, Chevron, ConocoPhillips, ExxonMobil, Shell); and DOE national laboratories (Argonne, Los Alamos, National Renewable Energy Laboratory). Argonne is helping to coordinate the activities of the H2QWG.

To develop the process for assessing the effects of hydrogen quality specifications on costs and energy usage of the fuel cell vehicle over its life-cycle, we have:

- developed a framework document to help define the work of the group;
- held in-person meetings three to four times a year to obtain input from developers of fuel cells, hydrogen purifiers, gas analysis technologies, and H2A costing methodologies;
- initiated a database of critically assessed relevant literature;
- worked with model developers at Argonne and other organizations to help develop and validate performance and life-cycle cost models; and
- provided briefings and updates to various FreedomCAR Technical Teams and other groups involved in related work.

Results

We have defined the overall hydrogen-fueled fuel cell vehicle system in terms of four major components, as shown in Figure 1. During FY 2007, we have identified the influence of the desired hydrogen quality on the costs and performance of these four components, hydrogen production and infrastructure, hydrogen purification, its use in the automotive fuel cell system, and fuel quality analysis and verification. Hydrogen

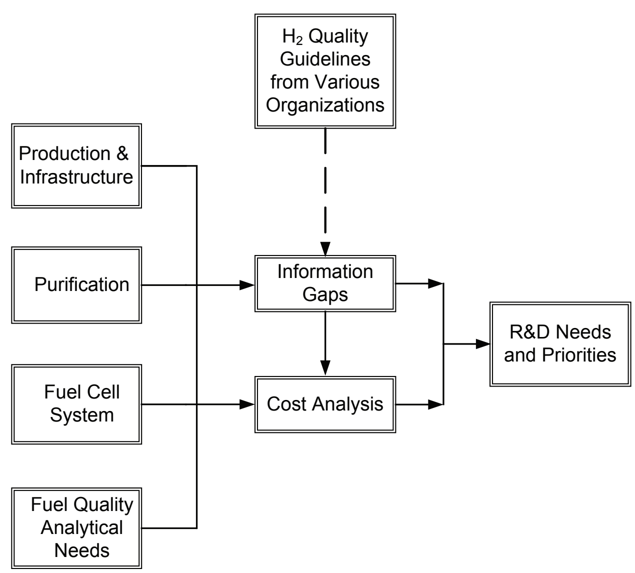

FIGURE 1. The Four Components of the Hydrogen System Analyzed in this Project to Determine R&D Needs and Priorities

quality guidelines are also being discussed by various other organizations, but there are still information and data gaps that the H2QWG has identified. Along with cost analyses, we are developing a prioritized list of R&D needs.

The focus of our current analyses is on the near- to mid-term, i.e., to the year 2015. Thus, we are considering only distributed (forecourt) hydrogen production by autothermal or steam reforming of natural gas, reforming of renewable fuels such as ethanol, and electrolysis by polymer electrolyte or alkaline electrolyzers. The hydrogen purification technologies considered include PSA and hydrogen-permeable membrane separators. Only compressed gas storage was considered as the on-board hydrogen storage system.

As a first performance and cost modeling effort, we are examining the costs of distributed hydrogen production by steam-methane reforming (SMR) and purification by PSA. The purification step is estimated to contribute approximately 5 to 20% of the cost of hydrogen. To quantify this cost more precisely and, in particular, to assess the effects of hydrogen quality specifications on this cost, we have initiated the development of a PSA model. The cost of the PSA is a function of the desired hydrogen recovery fraction, process parameters, scale of hydrogen production, reformate composition, and the required reduction in the concentrations of the different impurities. Some contaminant species, such as CH_4 and CO, are relatively easy to remove by PSA; others, such as O_2 and N_2, are more difficult to remove by PSA. Thus, the nature of the contaminant species and their permissible concentrations in the product gas have a direct bearing on the adsorption bed sizes, hydrogen recovery, and purification costs.

We have developed a preliminary model of the SMR/PSA production/purification pathway that currently includes the removal of CO, CO_2, CH_4, and H_2S. Figure 2 shows the results for a 4-bed PSA system, to which the 150 psig feed is the reformate from an SMR operated with a steam-to-carbon ratio of 3.0 and a gas composition corresponding to thermodynamic equilibrium at 435°C. The figure shows that as the permissible CO concentration in the product hydrogen varies from 0.01 ppm to 100 ppm, the hydrogen recovery increases from ~65% to ~80%; the cost of the hydrogen would decrease correspondingly. Additionally, Figure 3 shows that as the product hydrogen's CO specification is tightened over the same range, the sorption bed volume increases by ~60%. Figure 3 also shows that the removal of CO_2 and CH_4 is directly proportional to the removal of CO, and that for the proposed hydrogen quality guidelines of 0.2 ppm CO, 2 ppm CO_2, and up to 100 ppm CH_4, the CO is the controlling specification for sizing the PSA beds. We are currently adding N_2 to the list of contaminant species in the model, as well as

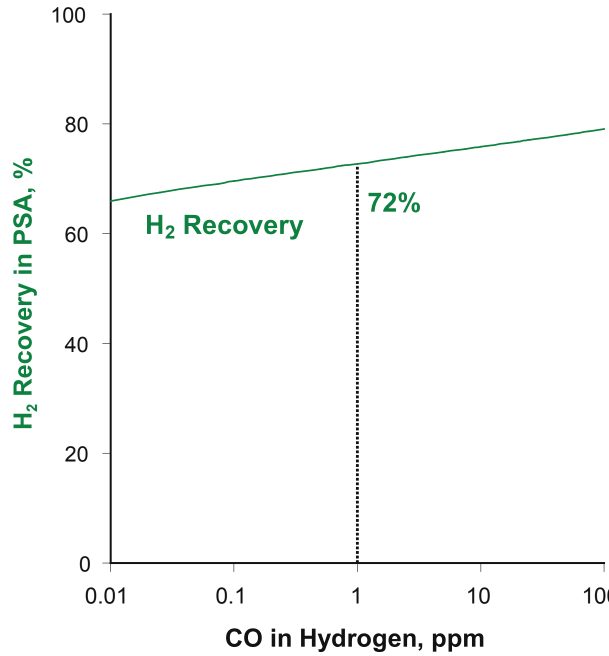

FIGURE 2. Hydrogen Recovery Fraction Increases as the Permissible Concentration in Product Hydrogen Increases from 0.01 ppm to 100 ppm

multi-bed capability (i.e., activated carbon plus zeolite beds) and heat effects in the PSA process.

As a result of the discussions of the H2QWG, we have prepared a comprehensive draft roadmap for the group's continuing activities. The appendices to this roadmap contain species-specific discussions of test data, effects on fuel cell performance and durability, effectiveness of hydrogen purification methods, modeling, and R&D needs for the individual species.

Conclusions and Future Directions

- PSA technology can achieve most of the hydrogen impurity guidelines proposed by SAE/ISO, but it may add 5–20% to the cost of hydrogen.
- PSA is ineffective for removing helium, while the effectiveness of PSA for removing certain species has not been reported (e.g., for formic acid).
- The proposed levels for CO_2 and O_2 may be overly restrictive.
- Testing and analysis of hydrogen for contaminants may be a very significant cost factor, both for control of hydrogen quality and for its certification.
- If stringent quality specifications are necessary, we need better quantification of the cost and performance of PSA versus hydrogen quality to determine life-cycle costs.
- A better quantification is needed of the cost and performance impacts of impurities on fuel cells, and

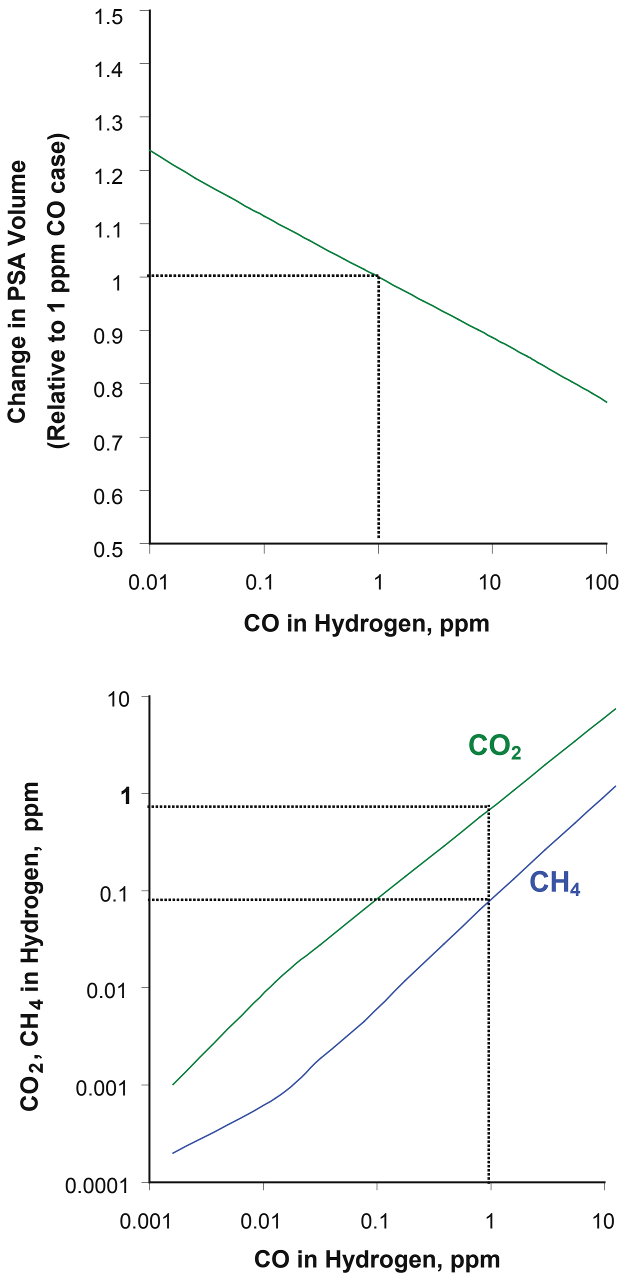

FIGURE 3. The PSA Sorption Bed Volume Increases with Tighter CO Specifications while the Removal of CO_2 and CH_4 is Directly Proportional to the Removal of CO

the costs of overcoming the deleterious effects of specific contaminants.

- Development of low-cost methods for gas sampling and analysis is needed for on-line quality control and certification (and for fuel quality regulation enforcement).

FY 2007 Publications/Presentations

1. FreedomCAR Technical Team briefings and updates:

– Fuel Pathways Integration Technical Team, March 22, 2007.

– DOE Fuel Quality Meeting: February 14, 2007.

– USCAR Technology Leadership Council, February 12, 2007.

– Delivery Technical Team/Hydrogen Production Technical Team, October 23, 2006.