II.A.1 Hydrogen Pathways Analysis for Solid Oxide Fuel Cell (SOFC) and Dark Fermentation

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Overall Objectives

The objectives of this project are to:

- Analyze hydrogen production and delivery (P&D) pathways to determine the most economical, environmentally benign and societally feasible paths for the P&D of hydrogen fuel for fuel cell electric vehicles (FCEVs).
- Identify key technical and economic barriers to the success of these pathways, primary cost drivers, and remaining R&D challenges.
- Assess technical progress, benefits and limitations, levelized hydrogen costs, and potential to meet U.S. DOE P&D cost goals of <$4 per gasoline gallon equivalent (gge) (dispensed, untaxed) by 2020.
- Provide analyses that assist DOE in setting research priorities.
- Apply the Hydrogen Analysis (H2A) production model as the primary analysis tool for projection of levelized hydrogen costs (U.S. dollars per kilogram of hydrogen [$/kg H_2]) and cost sensitivities.

Fiscal Year (FY) 2015 Objectives

In 2014–2015, these overall project objectives were applied to:

- Develop hydrogen pathway case studies for hydrogen generation via:
  - Dark fermentation of bio-feedstocks.
  - High temperature electrolysis using solid oxide electrolysis cells (SOEC).
- Select additional hydrogen pathways, gather information on those hydrogen pathways, and define those hydrogen pathways for future case study development.

Technical Barriers

This project addresses the following technical barriers from the Hydrogen Production section of the Fuel Cell Technologies Office Multi-Year Research, Development, and Demonstration Plan:

Hydrogen Generation by Water Electrolysis

(F) Capital Cost

(G) System Efficiency and Electricity Cost

(K) Manufacturing

Fermentative Hydrogen Production

(AX) Hydrogen Molar Yield

(AY) Feedstock Costs

(AZ) Systems Engineering

Technical Target

This project conducts cost modeling to attain realistic cost estimates for the production and delivery of hydrogen fuel for FCEVs. These values can help inform future technical targets.

- U.S. DOE P&D cost goals <$4/gge of H_2 (dispensed, untaxed) by 2020

FY 2015 Accomplishments

- Completed hydrogen pathway cases to determine the projected cost of hydrogen generated via high temperature SOEC.
  - Solicited and analyzed data from industry and research organizations on likely current and future SOEC technology and plant configurations.
  - Developed SOEC case studies representing current and future cases of a central plant producing 50,000 kg H_2/day. Case studies prepared using H2A Production Model (Version 3.1).
  - Validated the case studies through performance modeling, vetting with industry, and written supporting documentation. Made H2A cases

and documentation publicly available at http://www.hydrogen.energy.gov/h2a_prod_studies.html.

- Projected hydrogen cost via SOEC:
  - Current case: \$4.21/kg H_2 (\$3.21 to \$5.06/kg H_2 with 90% confidence)
  - Future case: \$3.68/kg H_2 (\$2.76 to \$4.57/kg H_2 with 90% confidence)
- Quantitatively demonstrated that the three main cost drivers for the levelized hydrogen cost from SOEC are (1) electricity price, (2) electrolyzer capital cost, and (3) heat price.

- Completed hydrogen pathway cases to determine the projected cost of hydrogen generated via dark fermentation of biomass.
  - Completed literature review for dark fermentation of corn stover for hydrogen production. Data was drawn heavily from past related reports [1,2] design and capital cost data.
  - Work closely with National Renewable Energy Laboratory (NREL) researchers to analyze and project fermentation performance and reaction kinetics.
  - Developed fermentation case studies representing current and future cases of a central plant producing 50,000 kg H_2/day. Case studies prepared using H2A Production Model (Version 3.1).
  - Validated the case studies through performance modeling, heat and energy balances, analysis of potential byproduct sales, and written supporting documentation. Made H2A cases and documentation publicly available at http://www.hydrogen.energy.gov/h2a_prod_studies.html.
  - Projected hydrogen cost via fermentation:
    - Current case: ~\$578/kg H_2 (due to non-economical fermentation broth concentration)
    - Future case: \$3.78 to \$5.47/kg H_2
  - Quantitatively demonstrated that the three main cost drivers for the levelized hydrogen cost from fermentation are (1) fermentation broth concentration, (2) feedstock cost, and (3) capital cost.
- Initiated case studies for the monolithic piston reactor and molten carbonate electrolysis reformer pathways.

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INTRODUCTION

This report reflects work conducted in the second year of a three year project to analyze innovative hydrogen production and delivery pathways and their potential to meet the U.S. DOE hydrogen P&D cost goal of <\$4/gge by 2020. Work in the first year of the project concentrated on hydrogen production from proton exchange membrane electrolysis. Work in the second year has focused on SOEC technology and dark fermentation. The analysis methodology utilizes DOE's H2A Distributed and Central Hydrogen Production models [3]. Those models provide a transparent modeling framework and apply standard mass, energy, and economic analysis methods agreed upon by DOE's Hydrogen and Fuel Cell technology teams.

APPROACH

The following steps summarize the analysis methodology applied to each of the hydrogen production pathways examined in the project.

- Conduct literature review
- Develop, circulate, and analyze results from an industry survey covering the targeted technology
- Define generalized cases for systems of different sizes and technology readiness levels
- Run H2A models with general case input data to calculate the levelized cost of hydrogen (\$/kg H_2)
- Perform sensitivity analyses (including tornado and waterfall charts) to identify key cost drivers
- Document case study results
- Vet case study results with DOE, industry, and team partners
- Repeat these steps until agreement attained among project partners

Specific Approach to SOEC Analysis

A questionnaire spreadsheet was circulated to six research and industrial groups to gather data on SOEC performance and cost. Collected data included H2A model input parameters necessary for developing cases and covered engineering system definition, stack and balance of plant (BOP) capital costs, and other economic parameters. The data was analyzed and used to synthesize generalized cases reflecting realistic parameters and a representative production scenario while protecting proprietary technical information.

Two public generalized cases were developed:

- Current Central
- Future Central

Both cases are based on "Central" production at 50,000 kg H_2/day. Two technology development time horizons are considered: "Current" representing a Year 2015 technology and "Future" representing a Year 2025 technology. Current Central cases assume a short-term technology readiness projection from technology that has been demonstrated already in the lab. Future Central cases assume an advanced development of the technology via better materials, capabilities, efficiencies, lifetimes, and/or costs. Both Current and Future cases are based on projected system capital costs for mature, developed markets (i.e., not one-of-a-kind plant pricing).

The SOEC cases are based on high temperature (800°C) SOECs splitting steam into H_2 and O_2. The H_2 is separated from the steam and captured for transport. The O_2 is vented (and thus is not assumed to generate any byproduct sales revenue). The stacks operate near the thermo-dynamic neutral point: 1.34 volts/cell for the Current case and 1.28 volts/cell for the Future case. Heat is added to the system to maintain the 800°C reactants stack entry temperature. Heat price is based on burning of natural gas but the analysis is meant to be heat agnostic, i.e., the results are not tightly tied to the source of heat. Primary differences between the Current and Future cases are: slightly lower electrical usage, higher pressure operation allowing electrical generation from exhaust gases, and a higher current density. Further details of the two cases appear in Table 1.

Data from the two generalized cases were used to populate the H2A Model (Version 3.1) and to generate estimates of the levelized hydrogen cost. The electrolyzer

TABLE 1. SOEC Input Parameters

Parameter	Current Central	Future Central	Cost Basis
Plant Capacity (kg/day)	50,000	50,000	H2A
Total Uninstalled Capital (2012$/kW)	$820	$430	Ind. Questionnaire
Stack Capital Cost (2012$/kW)	$287	$99	Ind. Questionnaire
Balance of Plant (BOP) Capital Cost (2012$/kW)	$533	$331	Ind. Questionnaire
Total Energy Usage (kWh/kg)	50.9	46.6	Ind. Questionnaire
Stack Voltage (V)	1.34	1.28	Ind. Questionnaire
Current Density[1] (mA/cm^2)	1000	1500	Ind. Questionnaire
Net System Energy Efficiency[2]	66%	72%	Ind. Questionnaire
Stack Electrical Usage (kWh/kg)	33.49	34.05	Ind. Questionnaire
System Electrical Usage (kWh/kg) (% LHV H_2)	36.8 91%	35.1 95%	Ind. Questionnaire
System Heat Usage (kWh/kg)	14.1	11.5	Ind. Questionnaire
Electrolyzer Power Consumption (MW)	76.6	73.1	Eng. Calculation
Average Electricity Price over Life of Plant[3] (2007¢/kWh)	6.24	6.89	AEO/Eng. Calc.
Electricity Price in Startup Year (H2A Default Values)[4] (2007¢/kWh)	5.74	6.59	AEO/Eng. Calc.
Thermal Energy Cost (2007$/GJ)[5] (2007¢/kWh)	10.1 3.64	11.5 4.13	AEO/Eng. Calc.
Hydrogen Outlet Pressure (MPa)	2.1 (300 psi)	4.8 (700 psi)	Ind. Questionnaire
Installation Cost (% of uninstalled capital cost)	12%	10%	H2A
Replacement Interval (years) [Stack/BOP]	4/10	7/12	Ind. Questionnaire
Replacement Cost of Major Components (% of installed capital cost)	15%	12%	Ind. Questionnaire

[1]Current density is not used directly within the H2A analysis but is included here as a representative value to allow comparison between the Current and Future cases.
[2]Efficiency is defined as H_2 product output energy/input electrical and heat energy. H_2 product energy is based on the lower heating value (LHV) of H_2.
[3]Average electricity price over life of plant (40 years for Central cases).
[4]H2A Default Values from Energy Information Administration (EIA) Annual Energy Outlook (AEO) data.
[5]The thermal energy cost is based on the average EIA's AEO 2009 reference case costs for natural gas over the plant life, a combustion efficiency of 85.7%, and burner capital costs over the plant lifetime of ~$0.01/GJ.

companies vetted the generalized cases, H2A model results, sensitivity limit parameters and results, and resulting documentation.

Specific Approach to Fermentation Analysis

A questionnaire spreadsheet was circulated to various research and industrial groups to gather data on dark fermentation performance and cost. Unfortunately, industry response was limited and the academic group responses reflected both the low technology maturity of the systems as well as diversity of feedstock and organism approach. Consequently, it was decided to focus on dark fermentation of corn stover based primarily on the approach and experimental results from researchers at the NREL. NREL data sources were used to develop detailed mass and energy balance which provided input parameters for H2A analysis.

Two public generalized cases were developed:

- Current Central
- Future Central

Data from the two generalized cases were used to populate the H2A Model (Version 3.1) and to generate estimates of the levelized hydrogen cost. The fermentation questionnaire respondents vetted the generalized cases, H2A model results, sensitivity limit parameters and results, and resulting documentation.

The fermentation cases are based on a corn stover feedstock, hemicellulous pre-treatment, fermentation reaction using a *Clostridium thermocellum* consortium, pressure-swing adsorption for hydrogen gas purification, and waste water treatment of the liquid effluent. Data for the *C. thermocellum* bacteria was provided by NREL. The fermentation capacity for the Current case is taken from existing NREL lab results. The Future case data is extrapolated from similar NREL data and has a higher fermentation capacity (producing more hydrogen for each molecule of sugar) than the Current case. Undigested solids (primarily lignin) are combusted to generate process heat. Biogas (methane) generated in the waste water treatment facility is combusted for process heat in the Current case or is fed to a turbine generator to produce electricity for byproduct sale in the Future case.

The primary differences between the Current and Future cases are (1) higher feedstock-to-hydrogen conversion, (2) higher fermentation broth concentration, and (3) generation of byproduct electricity. Further details of the two cases appear in Figure 1.

RESULTS

All cases studied demonstrate a production price between approximately \$3/kg H_2 to \$5/kg H_2 with the exception of the fermentation Current case, which has a cost of approximately \$577/kg H_2. Figure 2 details the cost breakdown of both SOEC cases and the fermentation Future case. From Figure 2, the SOEC cost drivers are seen to be variable costs such as electrical price and thermal energy price or the fixed installed capital cost. In Figure 3, these cost drivers are further identified to be electricity price, thermal energy price, and the capital cost. The electricity price averages 6.8¢/kWh and 6.97¢/kWh for the Current and Future cases, respectively. Results of a Monte Carlo analysis for the SOEC technology indicate a probable H_2 cost range of \$3.21/kg H_2 to \$5.02/kg H_2 for the Current case and \$2.76/kg H_2 to \$4.57/kg H_2 for the Future case. These ranges represent 90% confidence, i.e., the middle 90% of possible outcomes.

Costs for the fermentation cases are \$578/kg H_2 and \$4.62/kg H_2 for the Current and Future cases, respectively. The Current case cost is extremely high due to the fermentation reaction being carried out with a low concentration (5 g/L) fermentation broth, a concentration level more appropriate for lab scale research than commercial operation. The Future case, modeled with a fermentation broth concentration of 300 g/L (60 times greater than the Current case fermentation broth concentration), yields a more competitive H_2 cost of \$4.62/kg H_2. As shown in Figure 2, this cost is dependent on a byproduct credit received from converting excess lignin and biogas to thermal energy which is then converted to electrical energy and selling it back to the grid at industrial rates. Figure 4 identifies the primary cost drivers of the fermentation case as feed stock cost, capital cost, and broth concentration. In reality, broth concentration is a vital factor and is not the top parameter in Figure 4, only because it is bound between 100 g/L and 400 g/L. As the broth concentration decreases, it affects the cost of hydrogen production significantly more than any other cost driver. Molar yield is also a critical parameter but is not identified specifically as it is incorporated in several of the other parameters due to its use in the mass balance. Due to the extremely wide range of the various input parameters, as well as overlapping influences of the parameters on the cost model, a Monte Carlo analysis was not conducted as it would yield a final hydrogen cost range so wide that it would hold little meaning.

CONCLUSIONS AND FUTURE DIRECTIONS

In its second year, this project made key observations and important achievements.

- Representative pathway analysis cases were completed for hydrogen generation from SOEC and fermentation using the H2A Production Model (Version 3.1).
- Large capital cost reductions are predicted between Current and Future systems for both pathways.

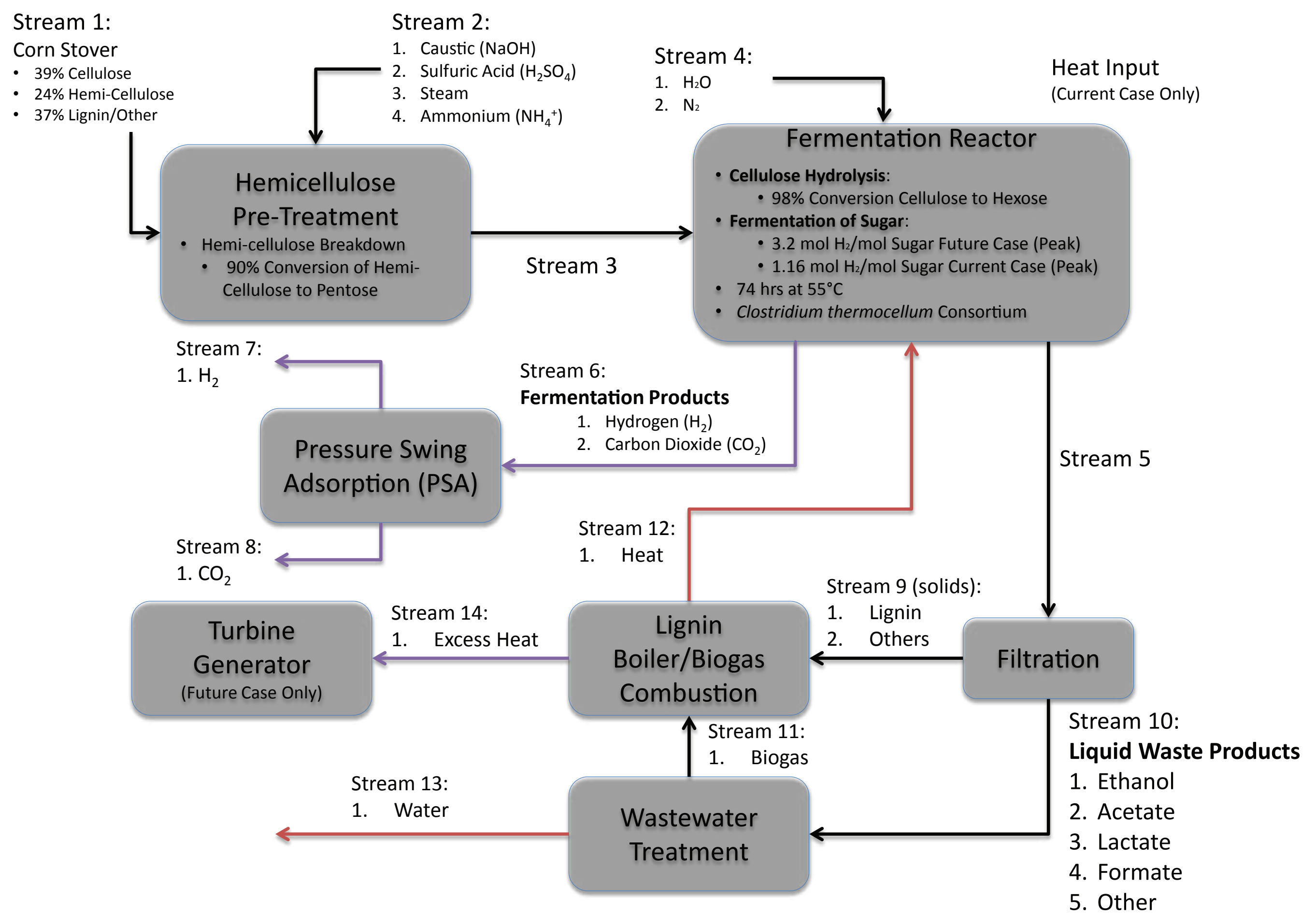

FIGURE 1. Dark fermentation process flow diagram

- Predicted SOEC hydrogen production costs are ~\$4.21/kg H_2 (Current case) and \$3.68/kg H_2 (Future case).
- Predicted fermentation hydrogen production costs are ~\$578/kg H_2 (Current case) and \$4.62 /kg H_2 (Future case). The Current cost is elevated due to use of a low concentration fermentation broth density.
- Further research is needed to demonstrate systems in which high molar yields (approaching 3.2 mol H_2/mol hexose) are possible with high broth concentrations (~300 g/L).

FY 2015 PUBLICATIONS/PRESENTATIONS

Presentations

1. James, B.D. DeSantis, D.A. Moton, J.M "*H_2 Pathways Project Update to DOE,"* Delivered remotely from Arlington, VA, 2015/02/27.

2. James, B.D., Moton, J.M, DeSantis, D.A., Houchins, C., "*Benchmarking Transformational Energy Technologies,"* Chicago, IL, 2015/5/28

3. James, B.D., DeSantis, D.A., Moton, J.M., "*Analysis of Advanced H_2 Production Pathways,"* 2015 DOE Hydrogen and Fuel Cells Program and Vehicle Technologies Office Annual Merit Review and Peer Evaluation Meeting, Arlington, VA, 2015/6/10.

4. Colella, W.G., James, B.D., Saur, G., "*Technical and Economic Performance of Next Generation Solid Oxide Electrolysis Cell (SOEC) Systems for Hydrogen Production,"* Hydrogen Production Technical Team Meeting, 1/6/2015.

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1. James, B.D., Baum, G.N., Perez, J., and Baum, K.N. *Technoeconomic Boundary Analysis of Biological Pathways to Hydrogen Production. Production* (2009). at http://www1.eere.energy.gov/hydrogenandfuelcells/pdfs/46674.pdf.

2. Davis, R. *et al. Process Design and Economics for the Conversion of Lignocellulosic Biomass to Hydrocarbons: Dilute-Acid and Enzymatic Deconstruction of Biomass to Sugars and Biological Conversion of Sugars to Hydrocarbons Process Design and Economics for the Conversion*. (2013). doi:10.2172/1107470.

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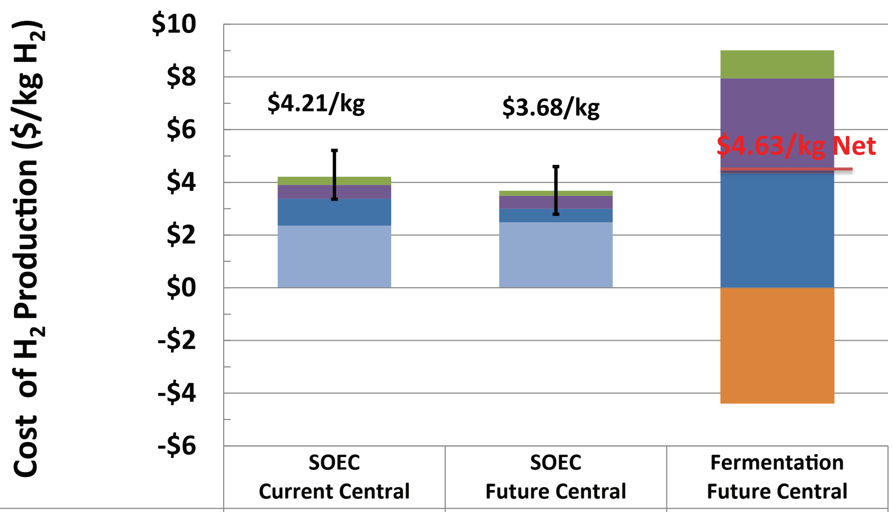

	SOEC Current Central	SOEC Future Central	Fermentation Future Central
Byproduct Cost	$0.00	$0.00	-$4.38
Other Raw Material Cost	$0.00	$0.00	$0.00
Fixed O&M	$0.31	$0.19	$1.06
Feedstock Cost	$0.53	$0.49	$3.60
Decommissioning Cost	$0.00	$0.00	$0.01
Installed Capital Cost	$1.02	$0.52	$4.34
Other Variable Cost	$2.36	$2.48	$0.00

FIGURE 2. Cost breakdown of analyzed systems

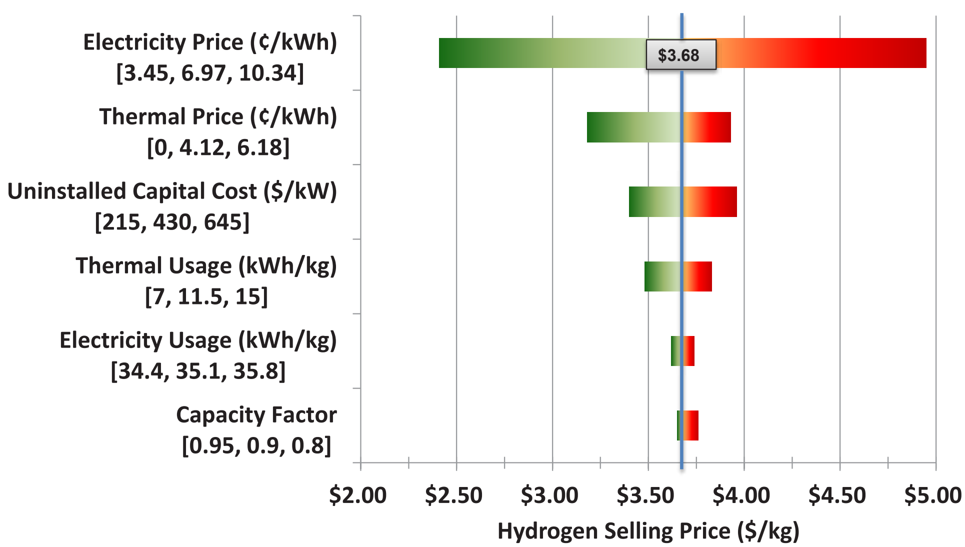

FIGURE 3. Tornado chart for SOEC future case sensitivity study

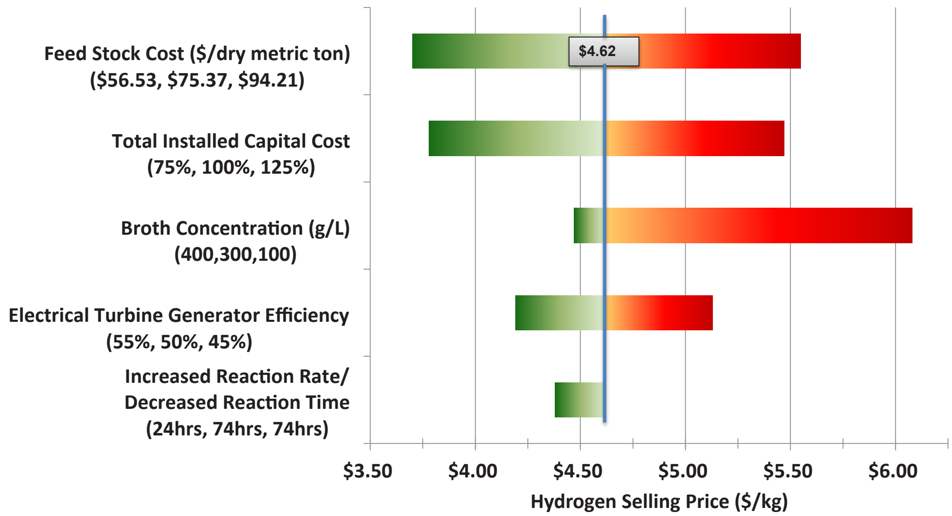

FIGURE 4. Tornado chart for fermentation future case sensitivity study