2020 DOE Hydrogen and Fuel Cells Program Annual Merit Review





AMGAD ELGOWAINY (PI), PINGPING SUN, GUIYAN ZANG, KRISHNA REDDI, ADARSH BAFANA, YAN ZHOU, THOMAS STEPHENS

Argonne National Laboratory

May 30, 2020



This presentation does not contain any proprietary, confidential, or otherwise restricted information

Overview

Timeline

- Start: October 2018
- End: Determined by DOE
- % complete (FY20): 80%

Budget

• Funding for FY20: \$100K

Barriers to Address

- A: Future Market Behavior
 - Potential market for low value energy and potential hydrogen markets beyond transportation
- D: Insufficient Suite of Models & Tools
- E: Unplanned Studies and Analysis →H2@Scale is a new concept and requires analysis of its potential impacts

Partners/Collaborators

- NREL, INL, PNNL, SNL, LLNL, LBNL
- DOE NE Office
- Industry partners (utilities, energy companies and OEMs)



TODAY, MORE THAN 10M METRIC TONS OF HYDROGEN ARE PRODUCED IN THE U.S. ANNUALLY – Relevance/Impact

1600 mi. of H₂ pipeline; **10** Liquefaction plants in North America



H2@SCALE EXPANDS HYDROGEN UTILIZATION BEYOND CURRENT MARKETS – Relevance/Impact



COLLECT PERFORMANCE, ENERGY, MARKET DATA FOR CURRENT AND POTENTIAL FUTURE MARKETS – Approach



POTENTIAL HYDROGEN DEMAND BY FUEL CELL ELECTRIC VEHICLES (FCEVS)



POTENTIAL HYDROGEN DEMAND FOR LIGHT-DUTY FCEVS – Approach/Accomplishment

ORNL vehicle choice model (Ma3T) and VISION model for FCEV stock scenarios

FCEV Market Penetration					
Car	17.8%				
LDT	26.4%				
FCEV Stock (000)					
Car	28,400 ARM				
LDT	40,100				
Total LDV	68,500				

> Assumed H₂ at the pump declines from a high volume cost of \$8/kg to a target cost of \$5.0/kg (4/kg in 2007\$, inflated to 2015\$, plus \$0.5/kg taxes)

Hydrogen consumption at market equilibrium (18% of car and 26% of light truck stocks) is <u>11.7 MMT/yr</u> (4.3MMT for cars and 7.4MMT for light trucks)

POTENTIAL HYDROGEN DEMAND FOR MEDIUM- AND HEAVY-DUTY FCEVS – Approach/Accomplishment

- Estimated 12M medium-duty vehicles (MDVs) and 5.7M heavy-duty vehicles (HDVs) total stock in 2050 (VISION 2016)
- Assumed 22% stock penetration for both MD and HD FCEVs (the weighted average of the cars and light truck FCEVs at equilibrium)
 Conservatively, since FCEVs are assumed to be more attractive in
 - MDV and HDV markets compared to LDV market
- Assumed H₂ price at pump similar to FCTO target for light-duty FCEVs
 \$5/kg (2015\$)
- Estimated total VMT by all MDVs and HDVs at 212B and 252B, respectively in 2050 (VISION 2016)
- Estimated average fuel economy at 33 and 14.7 mi/kg for MD and HD FCEVs, respectively
- Estimated hydrogen consumption at market equilibrium at 1.4MMT and 3.8MMT for MD and HD FCEVs, respectively
 - ✓ a total of 5.2 MMT



POTENTIAL HYDROGEN DEMAND FOR E-FUEL (SYNFUEL) AND SYNTHETIC METHANOL PRODUCTION

$(H_2 + CO_2 \rightarrow LIQUID HYDROCARBON)$



MAJOR CO₂ AND ZERO-CARBON ELECTRICITY SOURCES TO CONSIDER – Relevance

Carbon Sources

Considered high purity CO₂ sources

Bio-derived CO₂

- Ethanol plants
- Waste streams (MSW, residues, etc.)

Fossil- derived CO₂

- Ammonia plants
- NG SMR plants
- NG processing plants
- Cement plants
- Iron & Steel mills
- Fossil power plants





POTENTIAL H₂ DEMAND FOR SYNTHETIC HYDROCARBON PRODUCTION FROM CONCENTRATED CO₂ SOURCES – Approach

- Considered 100 million MT of concentrated CO₂ sources (out of total~ 5 GT CO₂)
 - 44 million MT from ethanol plants
 - ✓ Current CO_2 supply capacity of 14 MMT, and market demand of 11 MMT
 - Remainder from hydrogen SMR (refineries) and ammonia plants



Source: Supekar and Skerlos, ES&T (2014)

MODELED H₂ DEMAND FOR SYNTHETIC FISCHER-TROPSCH (FT) PRODUCTION – Accomplishment Preliminary



- CO₂/H₂ mole ratio 1:2.4 for synthetic FT fuel production
 Carbon conversion efficiency ~ 46%
- Argonne

DEVELOPED LIFE CYCLE INVENTORY FOR PRODUCTION OF ETHANOL AND FT FUEL – Accomplishment



Well to wheel (WTW) boundary of FT fuel production from electrolysis hydrogen and ethanol plant by-product CO₂

Life cycle emissions



MODELED H₂ DEMAND FOR SYNTHETIC METHANOL PRODUCTION – Accomplishment

Preliminary



- CO₂/H₂ mole ratio 1:2.7 for synthetic methanol production
- Carbon conversion efficiency ~ 83%



DEVELOPED LIFE CYCLE INVENTORY FOR PRODUCTION OF ETHANOL AND METHANOL – Accomplishment





Well to wheel (WTW) boundary of methanol production from electrolysis hydrogen and ethanol plant by-product CO₂ Life





14 MMT POTENTIAL H₂ DEMAND WITH 100MMT CONCENTRATED CO₂ ANNULAY – Accomplishment

*Assumption: stoichiometric CO₂/H₂ mole ratio of 1:3







Preliminary

Installed nuclear plants



Wind electricity potential



Solar electricity potential





POTENTIAL HYDROGEN DEMAND FOR BIOFUEL PRODUCTION AND INJECTION INTO NATURAL GAS PIPELINES



UPDATED POTENTIAL HYDROGEN DEMAND ESTIMATES FOR BIOFUELS AND INJECTION INTO NATURAL GAS PIPELINE – Accomplishment Preliminary

- Assumed 50% of total AEO projected jet fuel demand in 2050 (38.6 billion gal/yr) to be bio-based
 - 1.8 billion gal/yr is from fats, waste oils & greases
 - 17.5 billion gal/yr from catalytic fast pyrolysis of biomass
- Calculated potential H₂ demand for biofuel production:
 - Hydroprocessing of fats and oils requires 76 g_{H2} /gal or 0.14 MMT/yr
 - Catalytic fast pyrolysis of biomass requires 490 g_{H2} /gal or 8.6 MMT/yr
 - Total potential hydrogen demand: <u>8.7 MMT/yr</u>
- Assumed 20% of total AEO projected natural gas consumption (by volume) in 2050 can be displaced with hydrogen
 - potential hydrogen injection into natural gas pipeline: <u>16 MMT/yr</u>
 - To breakeven with natural gas on Btu basis (\$5.88/MMBtu), hydrogen price is estimated at <u>\$0.80/kg_{H2}</u>



SERVICEABLE HYDROGEN CONSUMPTION POTENTIAL – Accomplishment

Application	Target H ₂ Price [\$/kg]	Potential H ₂ Demand [MMT]	Notes
Light-Duty FCEV (cars)	5	4.3	Vehicle choice model (Ma3T)
Light-Duty FCEV (trucks)	5	7.4	Vehicle choice model (Ma3T)
Medium-Duty FCEV	5	1.4	Assuming same average market penetration of light-duty FCEVs (22%)
Heavy-Duty FCEV	5	3.8	
Petroleum Refining	inelastic demand	7.5	No substitute for H_2 in refining process
Biofuels	inelastic demand	8.7	To meet 50% of jet demand in 2050
Ammonia	inelastic demand	2.5	Demand for current NH ₃
Ammonia	2	1.1	Competitive with imported NH ₃
Synthetic Methanol	1.73	6	Competitive with imported methanol
Methanol-to-gasoline	<1	8	Competitive with conventional gasoline
Injection to NG Infrastructure	0.8	16	Competitive with NG HHV
Iron Reduction and Steelmaking	1.7	4	To generate positive NPV
Iron Reduction and Steelmaking	0.8	8	Competitive with NG for DRI

✓ <u>Note:</u> that the assessed scenarios for potential H_2 demand by various applications may be exclusive of one another (i.e., the H_2 demand by different scenarios may not be additive) ¹⁹

SUMMARY – Accomplishment

- Evaluated serviceable hydrogen consumption potential for various applications
 - FCEVs (LDV and M/HDV) \rightarrow 16.9 MMT
 - Synthetic Methanol (14 MMT)
 - Biofuels production \rightarrow 8.7 MMT
 - Injection into NG pipelines \rightarrow 16 MM
- Additional potential future H₂ market demands were previously evaluated
 - Petroleum refining (7.5 MMT)
 - Ammonia production (3.6 MMT)
 - Steel refining (12 MMT)
- Modeled hydrogen demand and product yield for synthetic FT and methanol production
- Documented data sources, assumptions, modeling approach and analysis in a report
 - Report has been peer reviewed
 - Pending publication



Collaborations and Acknowledgments

- Mark Ruth and Paige Jadun: NREL
- Richard Boardman: INL
- Jamie Holliday: PNNL
- Elizabeth Connelly: DOE
- George Parks: FuelScience



Future Work

- Conduct regional analysis considering proximity of supply and demand
 - Delivered H₂ vs. onsite production
 - Delivery mode / bulk storage requirement
 - As a function of volume, schedule, and pressure requirement
- Consider additional CO₂ sources for synthetic hydrocarbon production
- Conduct economic and environmental analysis of evaluated applications
 - To determine competitive cost of hydrogen for each application
 - To determine potential CO₂ reduction for each technology pathway compared to baseline current technologies
- Consider potential other markets (e.g., hythane for NG power generators)
- Consider non-physical materials for delivering and storing hydrogen (e.g., chemical carriers)
- Publish H2@Scale Demand Report

Any proposed future work is subject to change based on funding levels



Project Summary

- Relevance: Hydrogen from clean energy sources can serve energy sectors beyond transportation while enabling renewable and zero-carbon power production
- Approach: Evaluate potential hydrogen demand for existing and emerging applications
- Collaborations: H2@Scale is a multi-national laboratory effort with collaboration across DOE national lab complex

Technical accomplishments and progress:

- Evaluated serviceable hydrogen consumption potential for various applications
 - Biofuels production, FCEVs (LDV and M/HDV), Injection into NG pipelines, and synthetic hydrocarbon production from concentrated CO₂ sources
- Modeled hydrogen demand for synthetic FT and methanol production
- Documented all data sources, modeling approach and analysis in a report
 - Report was peer reviewed
 - Publication pending

• Future Research:

- Develop economic analysis to determine breakeven hydrogen cost
- Conduct regional analysis considering proximity of supply and demand
- Consider potential other markets (e.g., hythane for NG power generators)
- Consider additional CO_2 sources for synthetic hydrocarbon production
- Publish H2@Scale demand report

Response to Reviewers' Comments from 2019 AMR

The approach used to estimate the hydrogen demand from oil refineries, ammonia, and steel plants is laid out reasonably. However, the assumptions in the demand estimation for the e-fuels are unclear. For the three existing markets, the study does not seem to make a distinction as to whether the source of hydrogen is renewable, which is nice to know but not necessary for this analysis. However, for e-fuels, hydrocarbon combustion products CO2 and water are converted back to hydrocarbon products; if the process is to make sense, there needs to be a clear statement that the input energy (electricity and/or heat) can only be renewable. Otherwise, the conversion process will result in more emissions to the atmosphere. Note that the e-fuels concept is inherently a reverse combustion process. Therefore, the market demand estimates should reflect this reality.

We agree that the input energy to e-fuels must come from renewable sources. In this updated analysis, we explained in details the possible energy sources and pathways for near zero-carbon hydrogen production, and thus near-zero carbon synthetic fuel and chemical production using available CO₂ surces. We also conducted detailed Aspen Plus simulations to estimate the H₂/CO₂ ratio, the carbon conversion efficiency and the synthetic hydrocarbon yield. Finally, we estimated the available CO₂ from various sources to evaluate the potential synthetic fuel and chemical production volumes, as well as the corresponding hydrogen demand.

• The team did an excellent job in using historical data to estimate future hydrogen demand for the three existing markets. Obviously, there are more uncertainties for those early or non-existent markets, such as e-fuels, which needs to be reflected in the final results.

To address the uncertainties with potential (future) non-existing markets, we improved our analysis by conducting detailed process level simulations to evaluate the potential of such processes to produce synthetic fuels and chemicals. In particular, we conducted Aspen Plus simulations to estimate the possible yields of synthetic hydrocarbons from various process designs, and conducted preliminary techno-economic analysis to estimate the hydrogen price for breakeven with conventional hydrocarbon prices.

