2024 DOE Hydrogen and Fuel Cells Program
Annual Merit Review

H_2 Delivery Technologies Analysis

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IN025

Overview

Timeline

- Start: October 2005
- End: Determined by DOE
- % complete (FY24): 70%

Barriers to Address

- Inconsistent data, assumptions and guidelines
- Insufficient suite of models and tools
- Stove-piped/Siloed analytical capability for evaluating sustainability

Budget

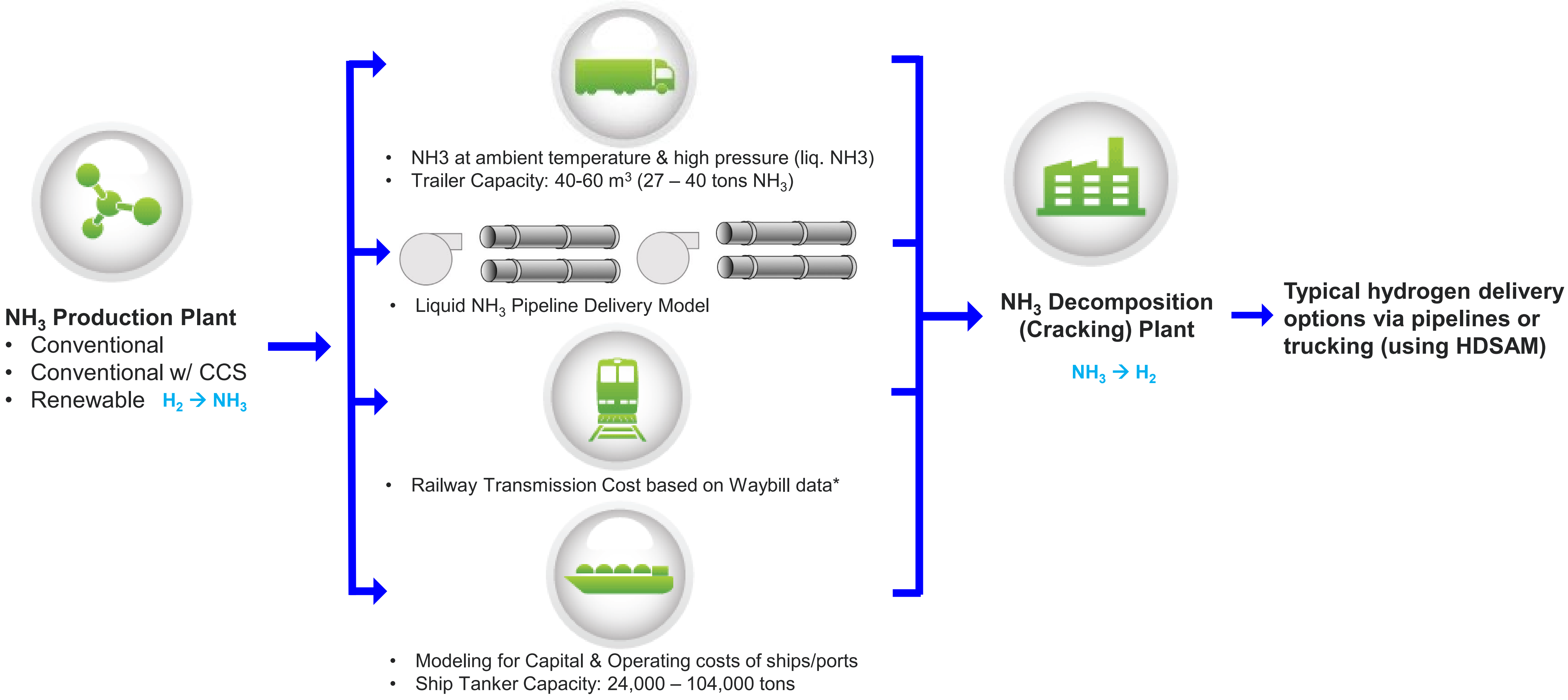
- Funding for FY24: $500K

Partners/Collaborators

- Industry partners
- D. Papadias and R. Ahluwalia, Argonne
- Daryl Brown, Energy Technology Analysis

Evaluate alternative hydrogen delivery options via ammonia as a carrier

- ➢ Cover entire supply chain pathways starting with ammonia production and ending with ammonia cracking
- ➢ Develop standalone Hydrogen Carrier Scenario Analysis Model (HCSAM)



NH_3 Production Plant

- Conventional
- Conventional w/ CCS
- Renewable $H_2 \rightarrow NH_3$

- NH3 at ambient temperature & high pressure (liq. NH3)
- Trailer Capacity: 40-60 m^3 (27 – 40 tons NH_3)

- Liquid NH_3 Pipeline Delivery Model

- Railway Transmission Cost based on Waybill data*

- Modeling for Capital & Operating costs of ships/ports
- Ship Tanker Capacity: 24,000 – 104,000 tons

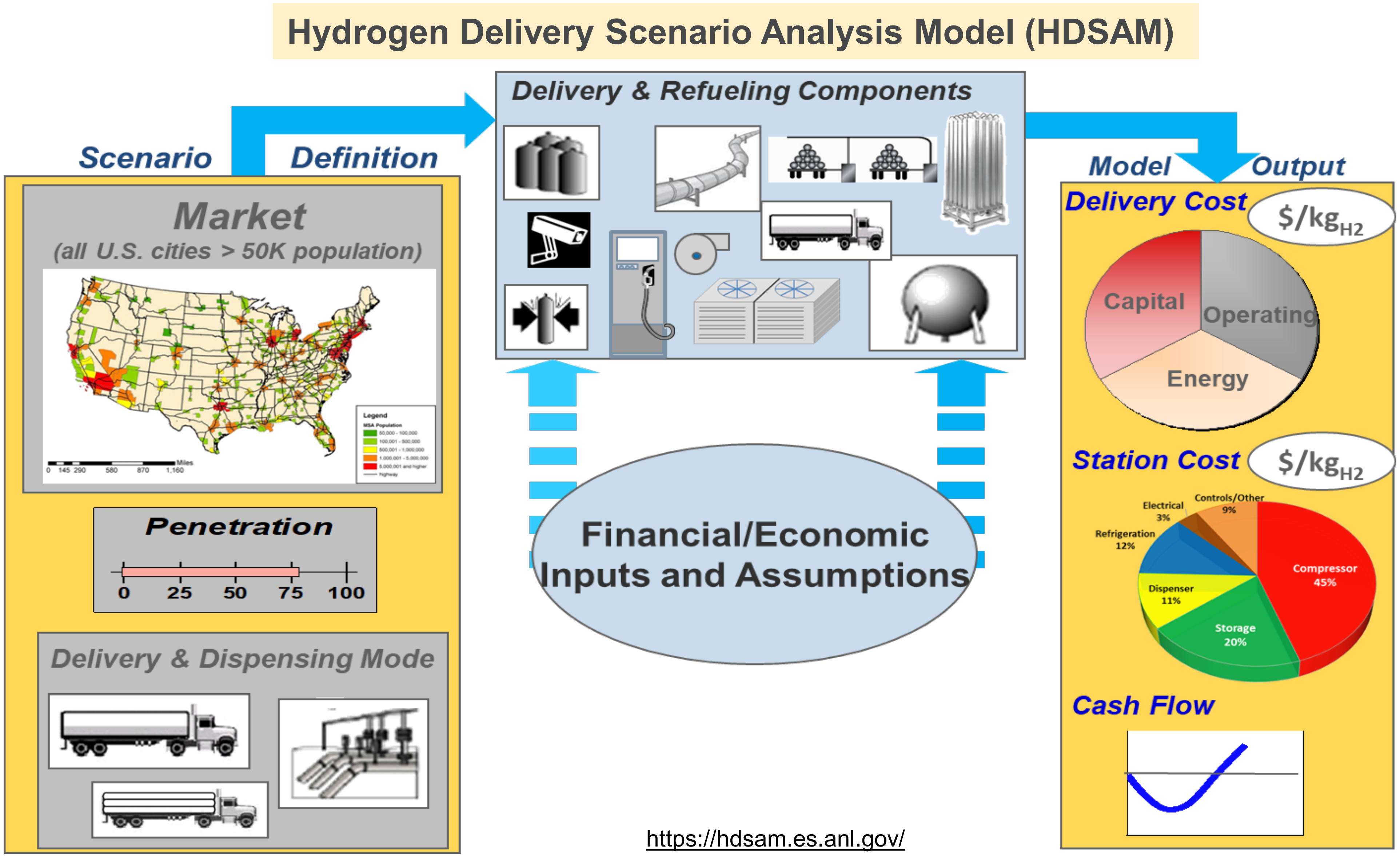
NH_3 Decomposition (Cracking) Plant

$NH_3 \rightarrow H_2$

Typical hydrogen delivery options via pipelines or trucking (using HDSAM)

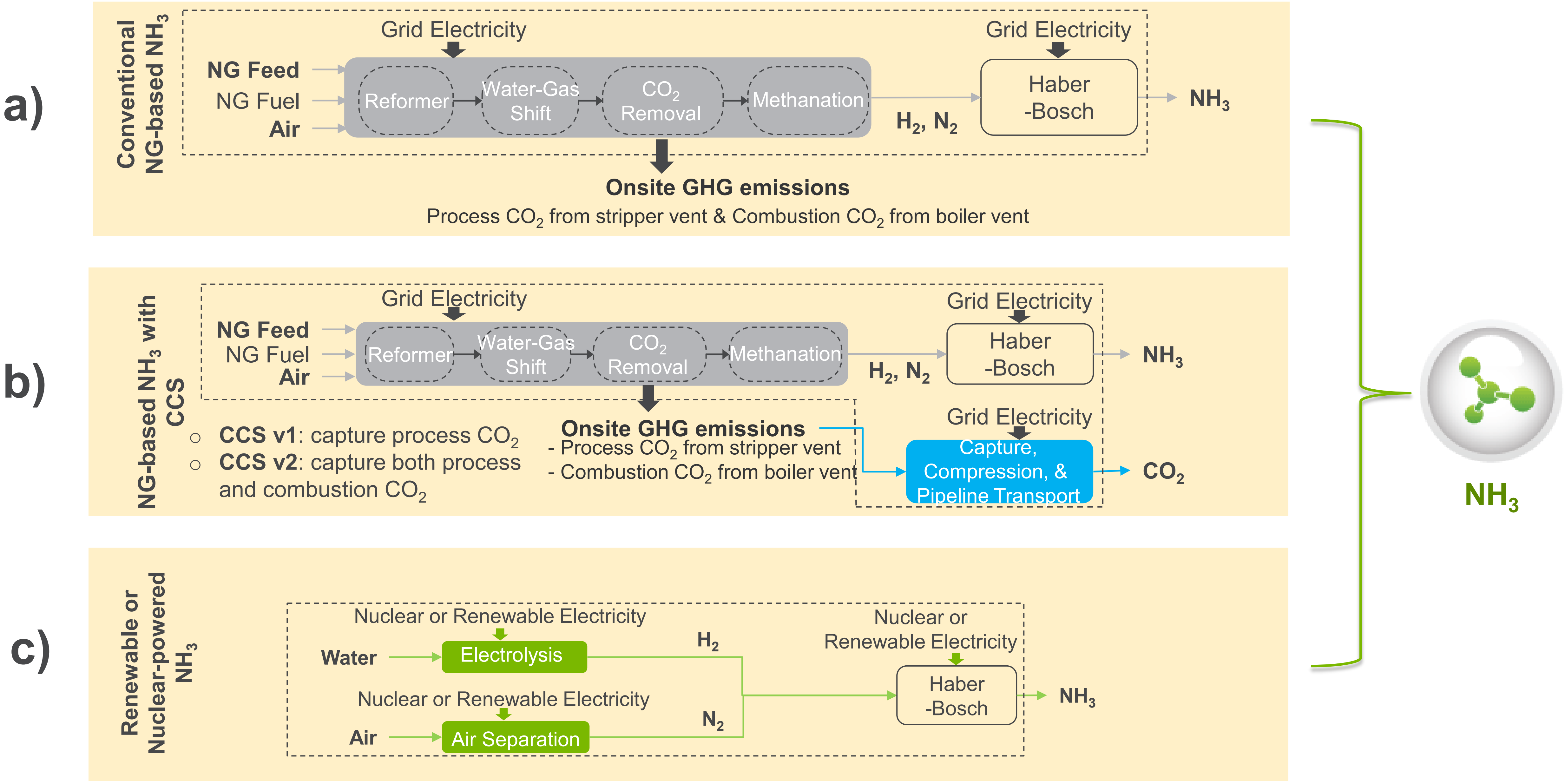
*Surface Transportation Board – Carload Waybill Sample: https:// prod.stb.gov/reports-data/waybill/

Develop techno-economic modeling for evaluating cost of ammonia delivery technologies on HDSAM platform



https://hdsam.es.anl.gov/

[1] Three Production Pathways for NH_3 implemented in HCSAM



a)

Conventional NG-based NH_3

Grid Electricity

NG Feed
NG Fuel
Air

Reformer → Water-Gas Shift → CO_2 Removal → Methanation

H_2, N_2

Grid Electricity

Haber -Bosch

NH_3

Onsite GHG emissions

Process CO_2 from stripper vent & Combustion CO_2 from boiler vent

b)

NG-based NH_3 with CCS

Grid Electricity

NG Feed
NG Fuel
Air

Reformer → Water-Gas Shift → CO_2 Removal → Methanation

H_2, N_2

Grid Electricity

Haber -Bosch

NH_3

- ○ **CCS v1**: capture process CO_2
- ○ **CCS v2**: capture both process and combustion CO_2

Onsite GHG emissions
- Process CO_2 from stripper vent
- Combustion CO_2 from boiler vent

Grid Electricity

Capture, Compression, & Pipeline Transport

CO_2

c)

Renewable or Nuclear-powered NH_3

Nuclear or Renewable Electricity

Water → Electrolysis → **H_2**

Nuclear or Renewable Electricity

Air → Air Separation → **N_2**

Nuclear or Renewable Electricity

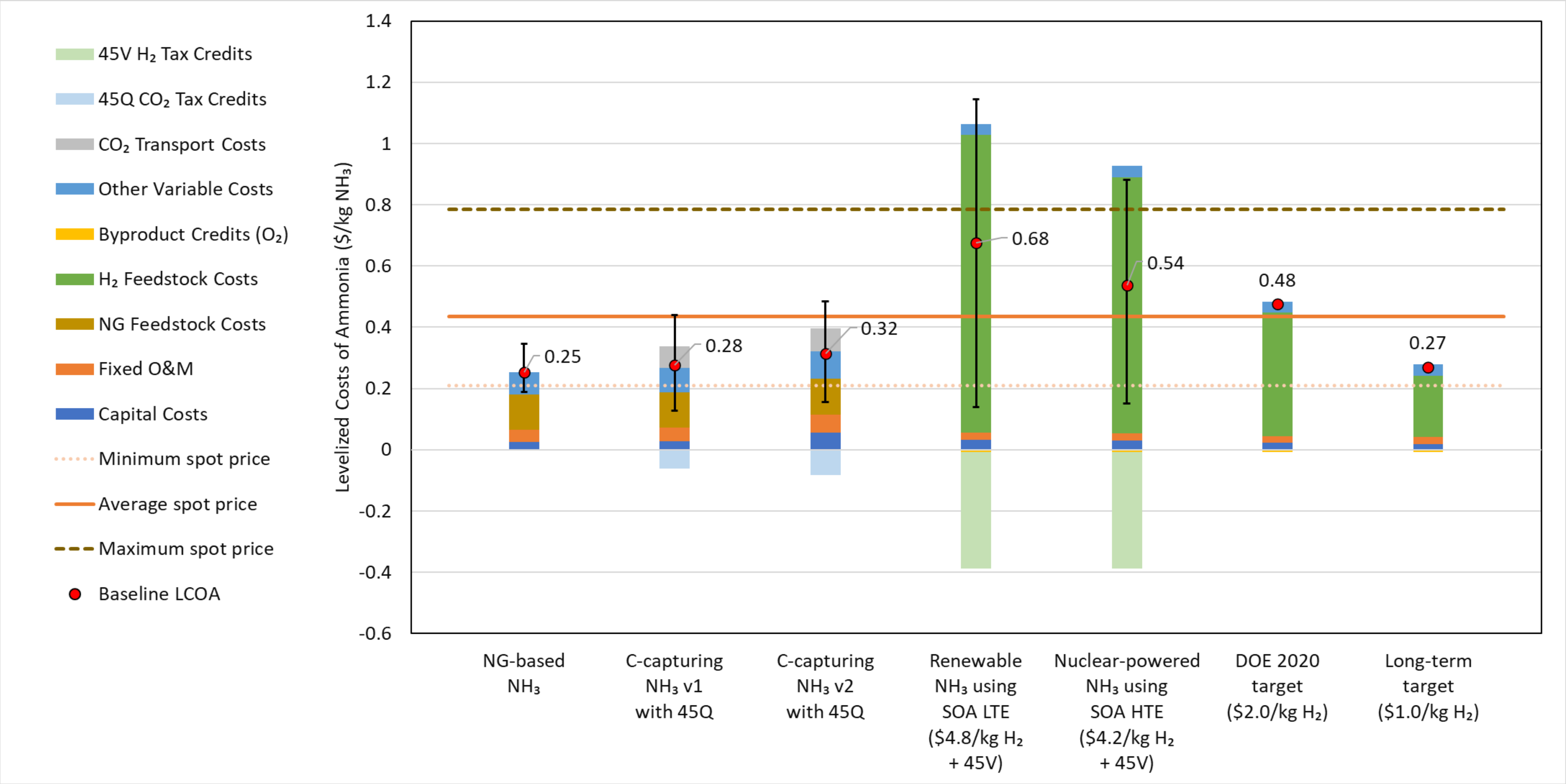
Haber -Bosch

NH_3

NH_3

NH_3 Production Cost Varies by Technology and Feedstock options

Accomplishment



Lee , X. Liu , P. Vyawahare , P. Sun , A. Elgowainy and M. Wang , *Green Chem.*, 2022, **24** , 4830 —4844

[2] Four Delivery Pathways for NH_3 implemented in HCSAM

a. Trucking

b. Pipeline

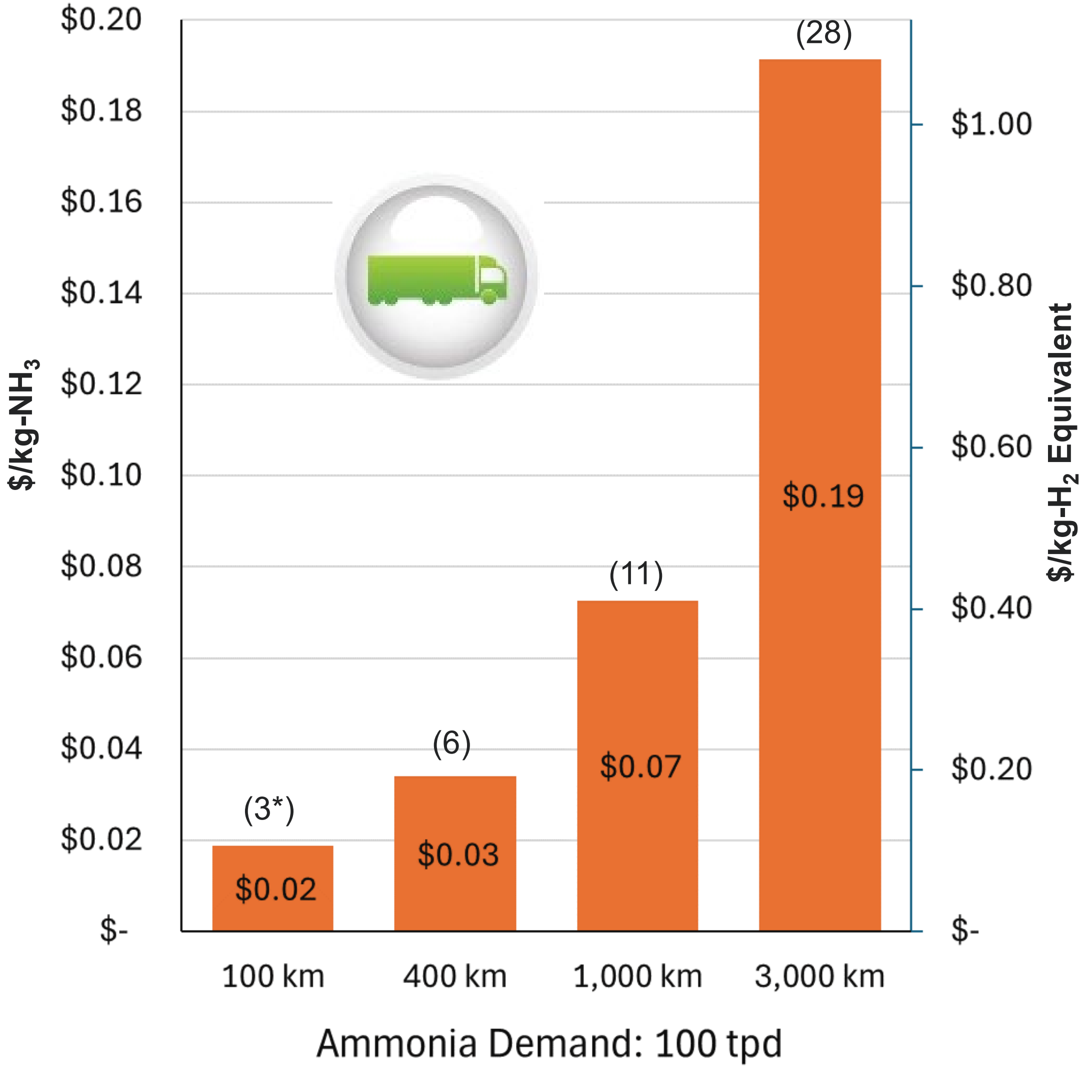
c. Rail

d. Ocean tankers

[2] a. NH_3 Transport by Truck-Trailer

Assumptions for Truck-Trailer Transport (can be changed in HCSAM):

- NH_3 Demand: 100 tons/day
- Transport Distance: 100 – 3,000 km
- Ammonia Trailer Capacity: 40 m^3 (27.3 tons NH_3 → 4.82 tons H_2 equivalent, based on stoichiometry)
- Truck-Trailer Operation: 18 hrs/day
- Trailer Usable Capacity: 87.5%



Right-vertical axis is shown for cost based on stoichiometric equivalent of H_2;
*Numbers at top of bars shows the number of truck-trailers required for transport

Truck-Trailer Transport of NH_3 is lower cost compared to H_2 Trucking

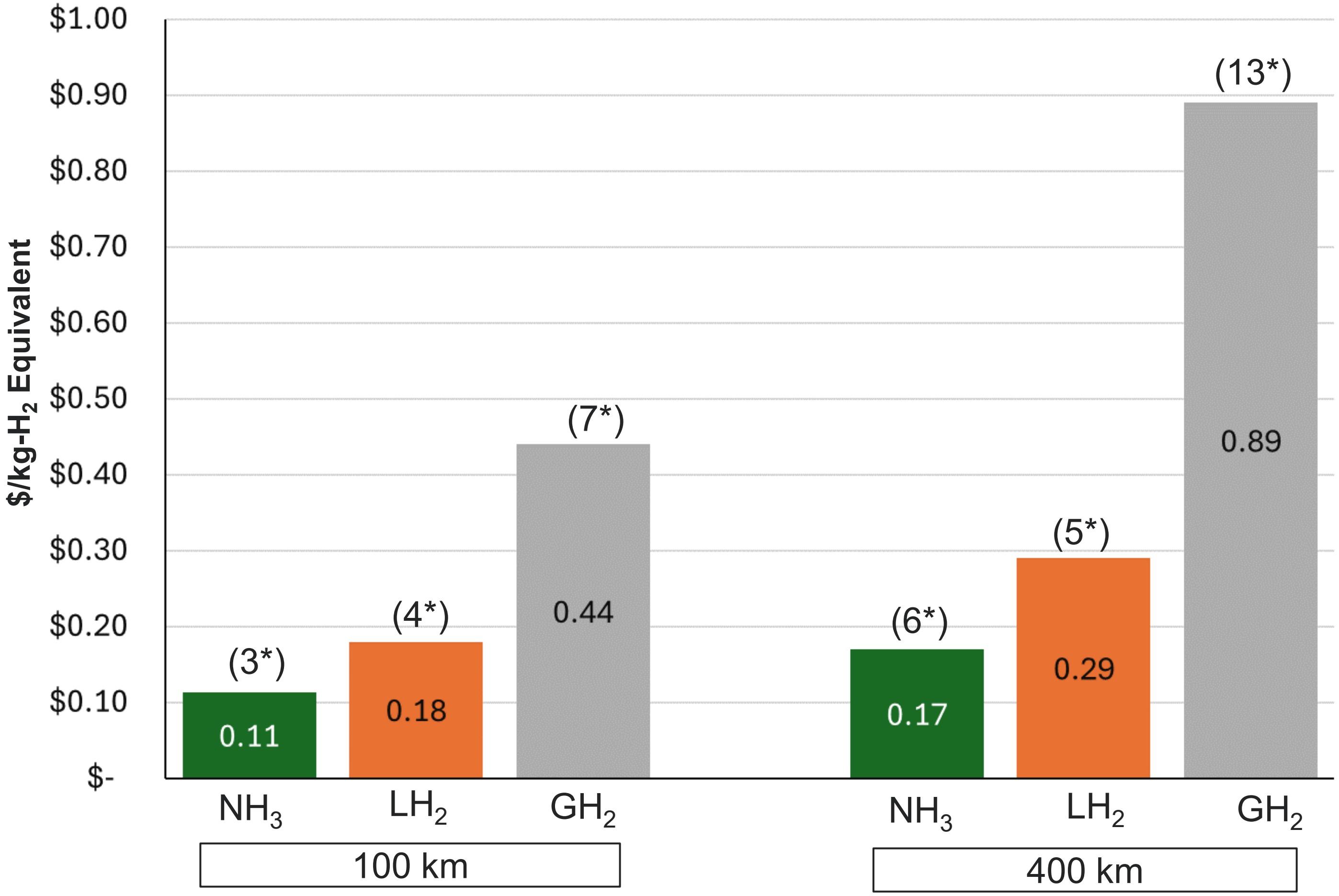
Accomplishment

- Mainly because of higher hydrogen payload carrying capacity of NH_3 trucks
- But NH_3 production is additional overhead

Assumptions for Truck-Trailer Transport:

- NH_3 Demand: 100 tons/day
- Transport Distance: 100 – 400 km

Mode	Capacity
NH_3 Truck-Trailer	27.3 tons NH_3 (40 m^3) (Equivalent H_2: 4.82 tons based on stoichiometry) NH_3 Pressure = 16 bar
LH_2 Tanker	3.8 tons H_2 (56 m^3) LH_2 Pressure = 3 bar
GH_2 Tube-Trailer	800 kg H_2 (41 m^3) GH_2 Pressure = 350 bar



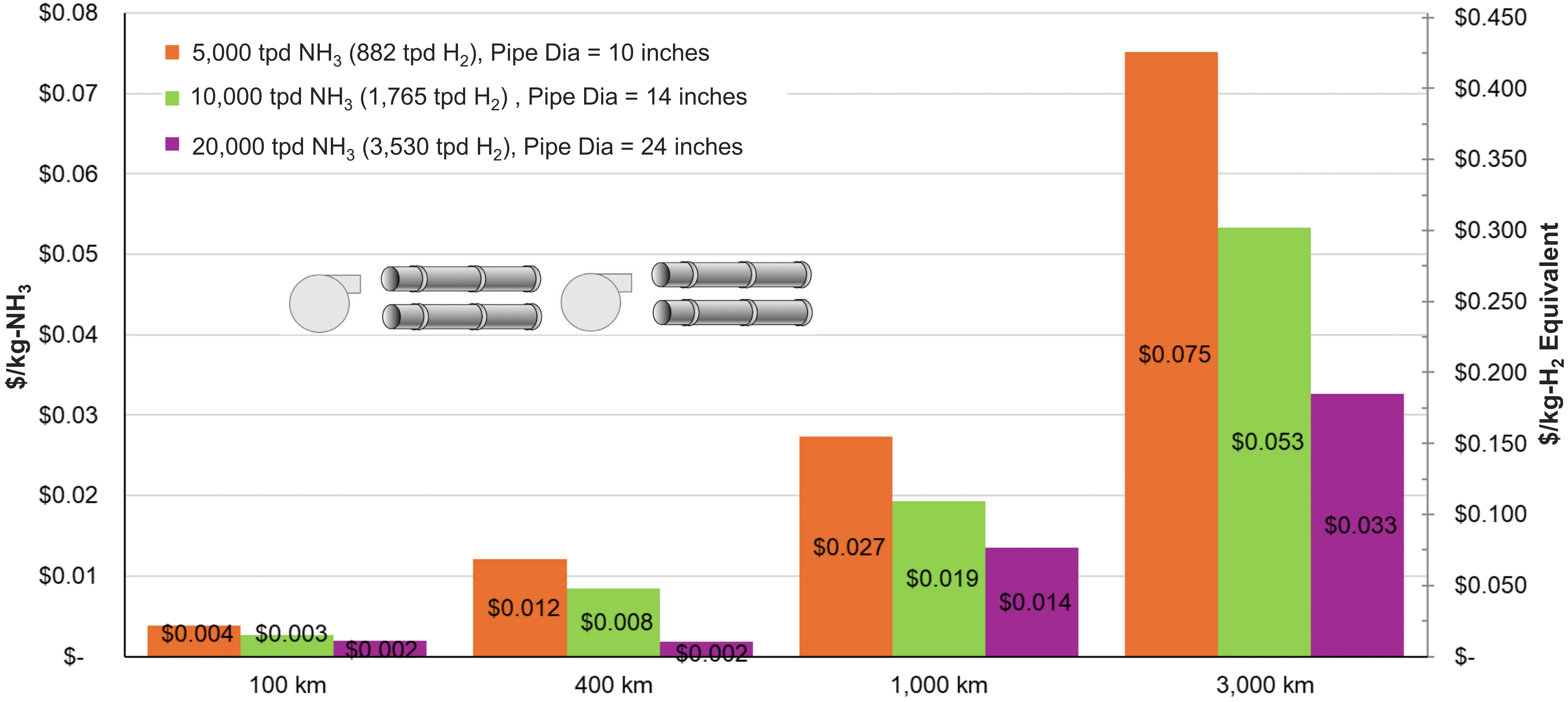
*Indicates the number of trucks required for transporting 100 tons of NH_3 or equivalent H_2 per day

[2] b. NH_3 Transport by Pipeline

Accomplishment

Assumptions for Pipeline Transport of NH_3 (can be changed in HCSAM):

- NH_3 Demand: 5,000 – 20,000 tons/day (Equivalent H_2 Demand: 882 – 3,530 tons/day)
- Distance: 100 – 3,000 km
- NH_3 pressure at origin: 90 bar, minimum NH_3 pressure at destination: 60 bar

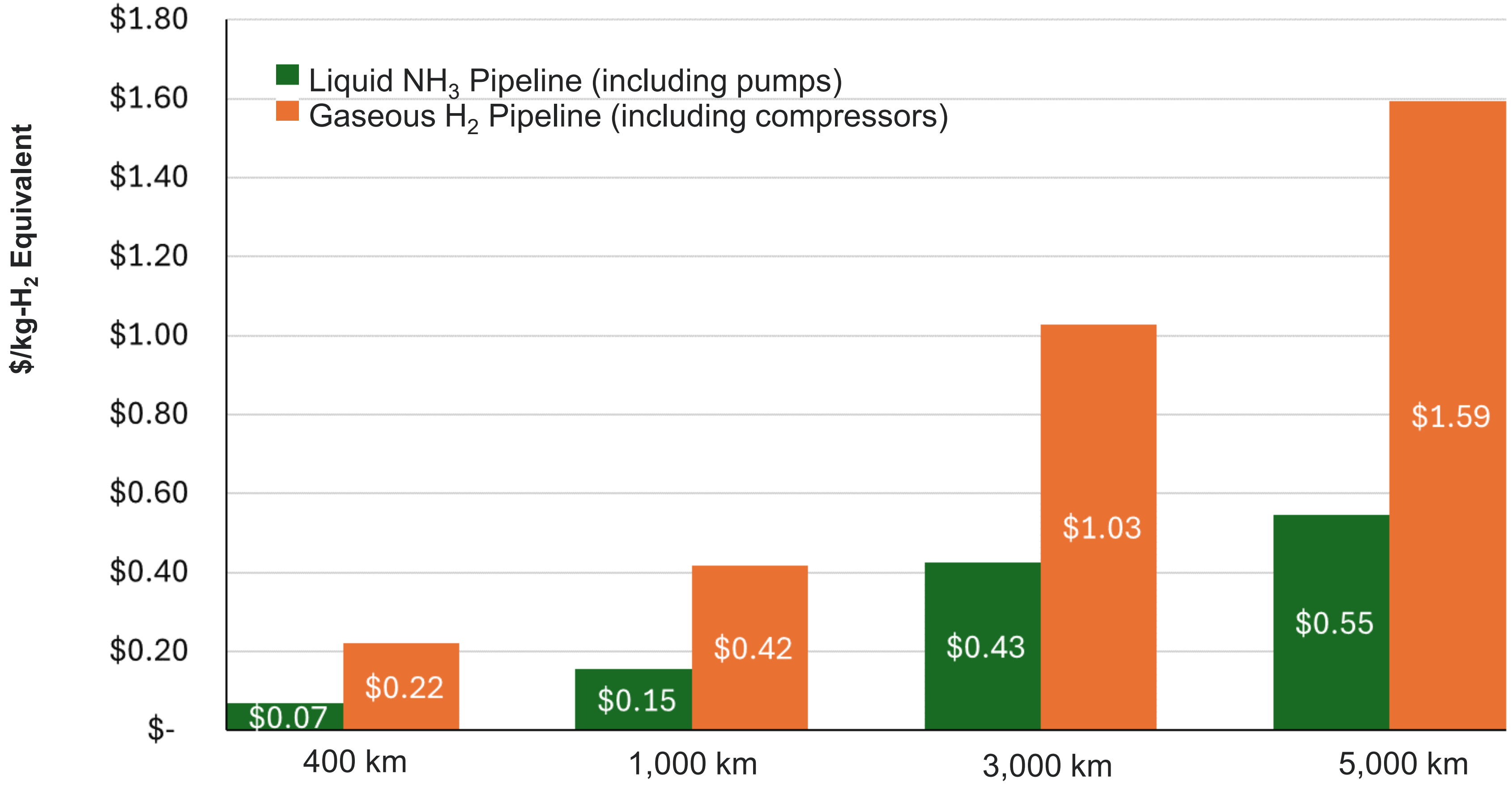


Pipeline Transport of NH_3 is lower cost compared to H_2

- Mainly because of higher energy density of liquid NH_3 compared to gaseous hydrogen
- But NH_3 production is additional an overhead

Assumptions for Pipeline Transport:

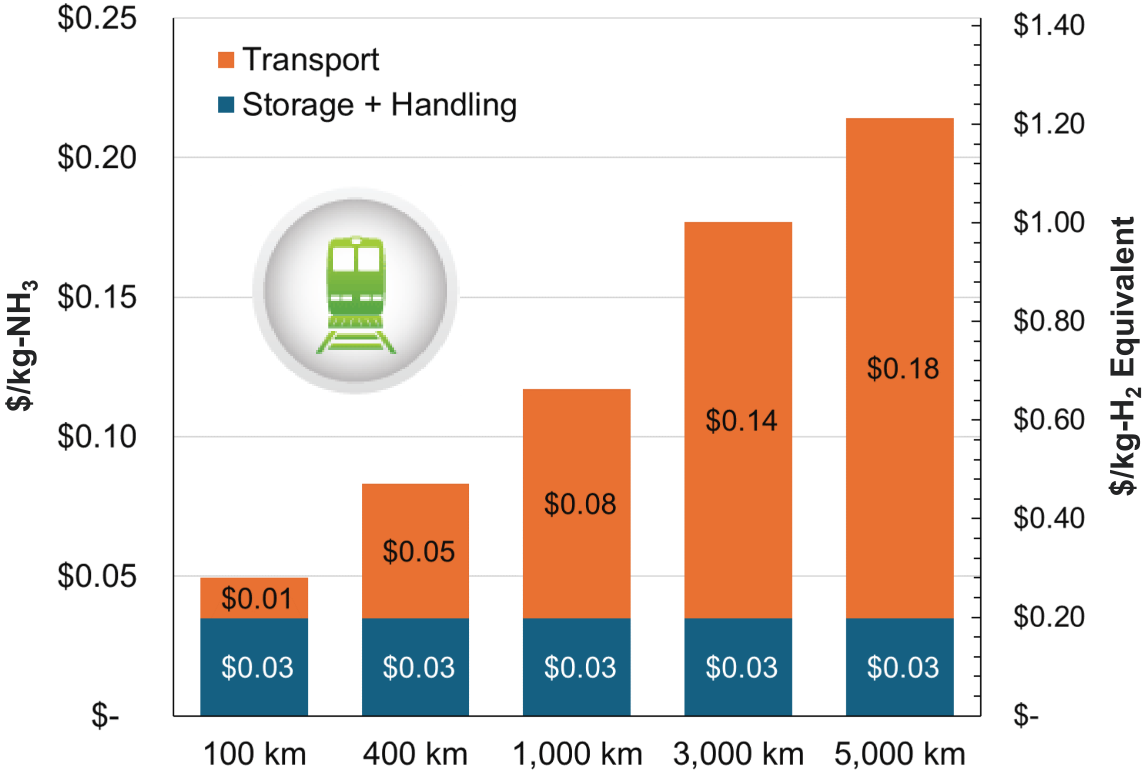
- NH_3 Demand: 5,000 tons/day (Equivalent H_2 Demand: 882 tons/day)
- Distance: 400 – 5,000 km



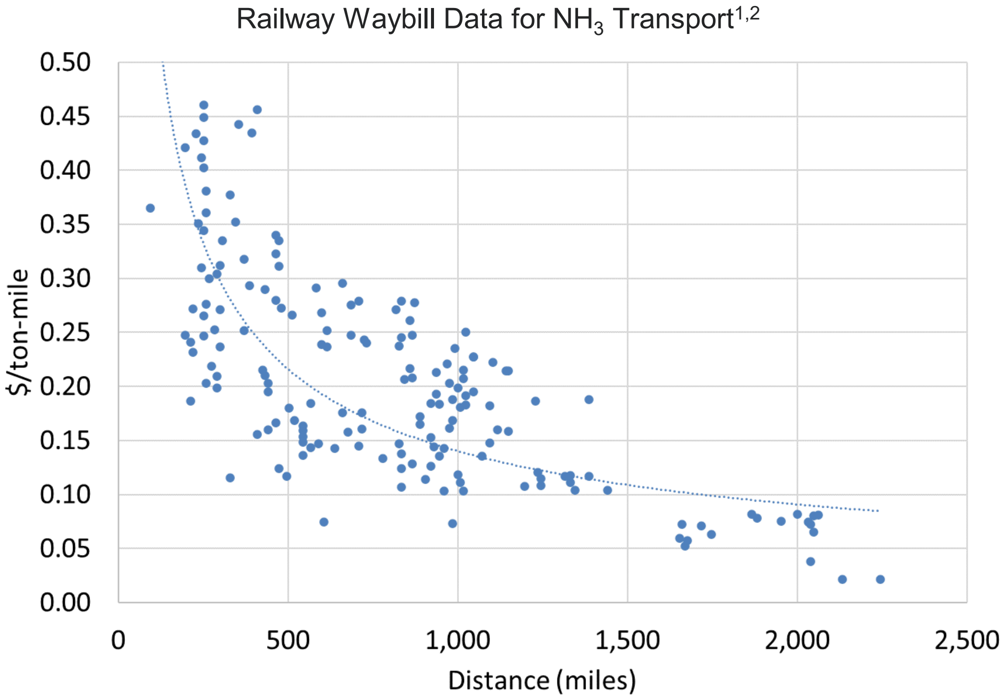
[2] c. NH_3 Transport by Rail

Assumptions for Railway Transport:

- Transport Distance: 100 – 5,000 km
- NH_3 transport cost based on Railway Waybill data[1,2]
- \$0.035/kg-NH_3 is charged by Railway for storage and handling[2]



Right-vertical axis shows the cost of NH_3 transport in terms of stoichiometric equivalent hydrogen \$/kg-H_2



- **Railway transport of NH_3 is based on Waybill data and is obtained for 4,000 carloads annual supply of NH_3**
- **4,000 carloads/year is equivalent to 500-700 tpd assuming 50 - 70 tons/carload**

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[1] *Surface Transportation Board – Carload Waybill Sample: https://prod.stb.gov/reports-data/waybill/*

[2] *Papadias et al. Int. J of Hydrogen Energy, 46(47), 24169-24189.*

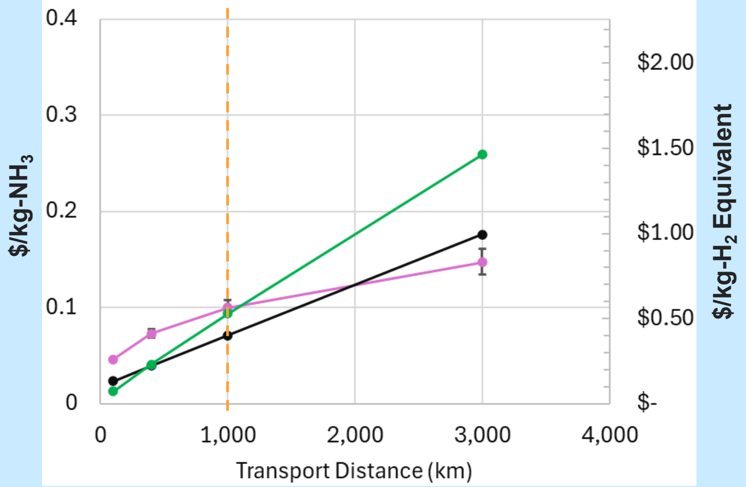
Comparison of Domestic Modes of NH_3 Transport Cost

Accomplishment

- Truck-Trailers are lower cost compared to rail modes NH_3 transport for shorter distances
- Pipeline transport of NH_3 is economic for higher throughput/demand and for longer transport distances

NH3 Demand: 1,000 tpd (Eq. H_2 Demand: 176 tpd)

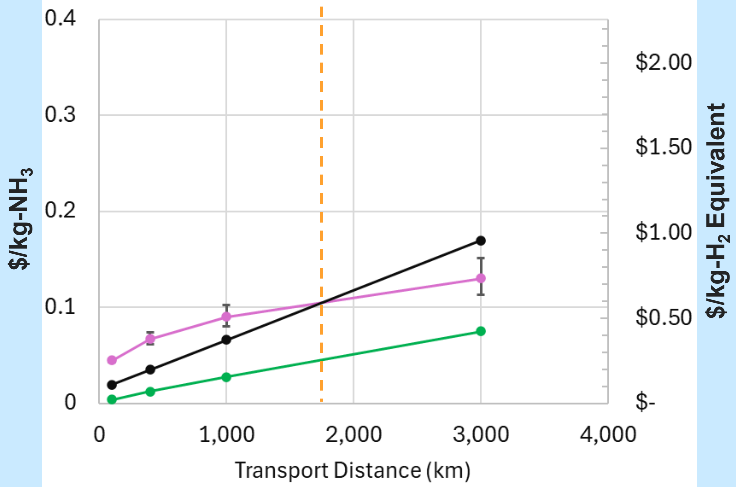
Truck-Trailer ~ Pipeline < Rail | Truck-Trailer ~ Rail < Pipeline



The upper and lower bounds for Rail transport cost indicate the lowering of transport cost for higher demand using the scale factor ranging between 0.85 – 0.95

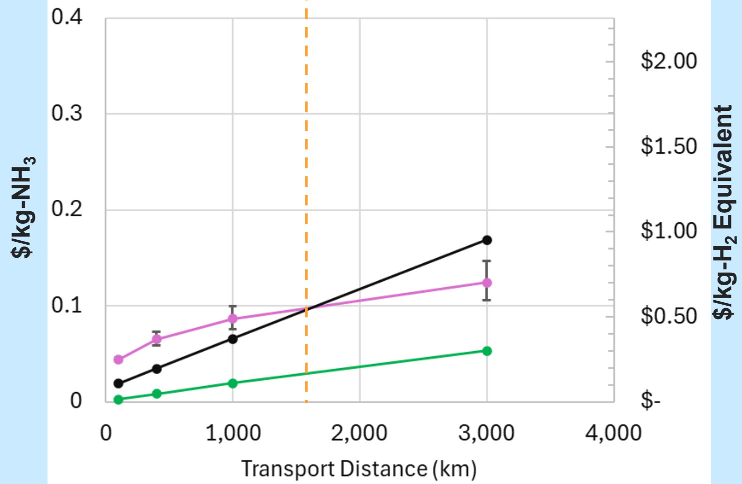
NH3 Demand: 5,000 tpd (Eq. H_2 Demand: 882 tpd)

Pipeline < Truck-Trailer < Rail | Pipeline < Rail < Truck-Trailer



NH3 Demand: 10,000 tpd (Eq. H_2 Demand: 1,765 tpd)

Pipeline < Truck-Trailer < Rail | Pipeline < Rail < Truck-Trailer



[2] d. NH_3 Transport by Ocean Tanker

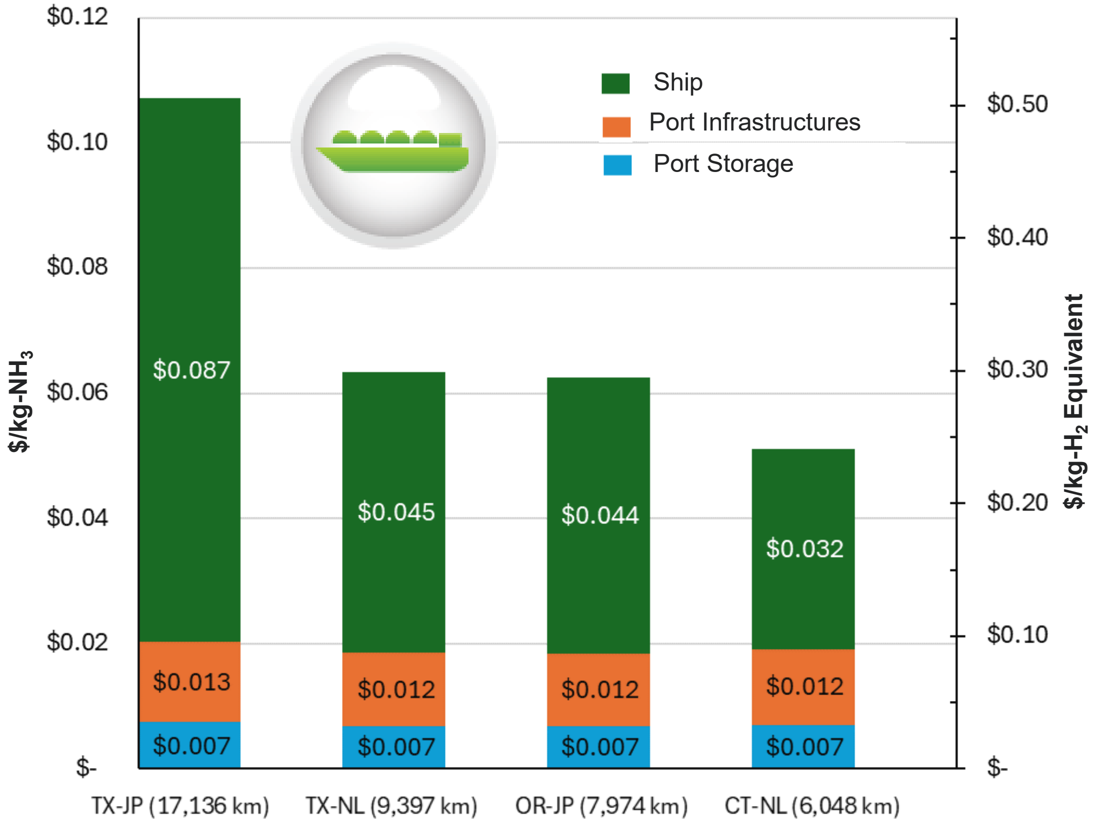
Accomplishment

HCSAM Parameters for Ship Tanker Transport of NH_3 (can be changed by user):

- 3 Options for Ship Tanker Capacity in HCSAM:
  → 38,000 m^3 (24,000 tons-NH_3) → 85,000 m^3 (52,000 tons-NH_3) → 160,000 m^3 (104,000 tons-NH_3)
- Cruise Speed, Fuel Cost, Applicable Port Fees and Canal Crossing Fees

Case study[1] of NH_3 transport:

- Transport Distance:
  Texas – Japan: 17,136 km
  Texas-Netherlands: 9,397 km
  Oregon-Japan: 7,974 km
  Connecticut-Netherlands: 6,048 km
- Max. Ship Capacity: 85,000 m^3 NH_3, (52,000 tons-NH_3)
- Max. Dead Weight Tonnage: 80,000
- Avg. Cruise Speed: 16 knots (30 km/hr)



Data label shows cost breakdown in $/kg-$NH_3$. Right-vertical axis shows the cost of NH_3 transport in terms of stoichiometric equivalent hydrogen $/kg-$H_2$

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[1] *Ahluwalia et al. 2023 DOE Hydrogen Program AMR. (2023)*

[3] NH_3 Decomposition (Cracking) to H_2

- ➢ Leveraged prior HFTO funded work by Dionissios Papadias

Parameters in Ammonia Decomposition Plant

1) Storage:

- Compressed gas cylinder (maximum size of 270 tonnes-NH_3)
- Refrigerated tank (4,500 tonnes-NH_3 to 50,000 tonnes-NH3)

2）Ammonia Cracker:

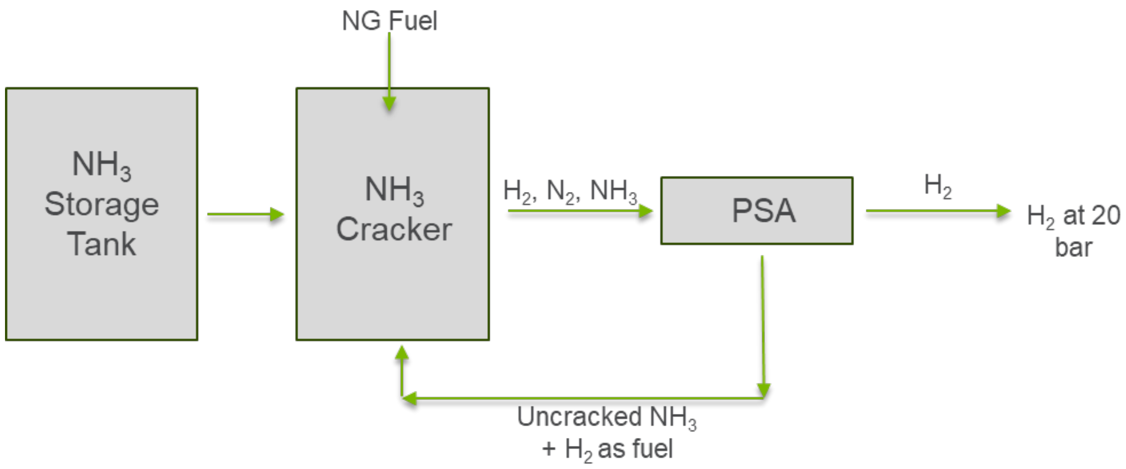
- 99% conversion rate by default*
  - (Option -1) Nickel – based (800°C)*
  - (Option -2) Ruthenium – based (550°C)+
- Cracker operating pressure: 20 bar
- Catalyst replaced once every 3 years

3) Separation:

- PSA (75% Purifying Efficiency)^

4) Burner:

- Use natural gas + unconverted ammonia + unpurified hydrogen as feedstock



Schematic of NH_3 Decomposition Plant. *Source: Papadias et al. International Journal of Hydrogen Energy, 2021.* ***46****(47): p. 24169-24189.*

- ➢ Other cracking technologies are currently being modeled in ASPEN-Plus for incorporation in HCSAM

^Note: 75% of hydrogen is recovered while 25% is returned to use as fuel for burner

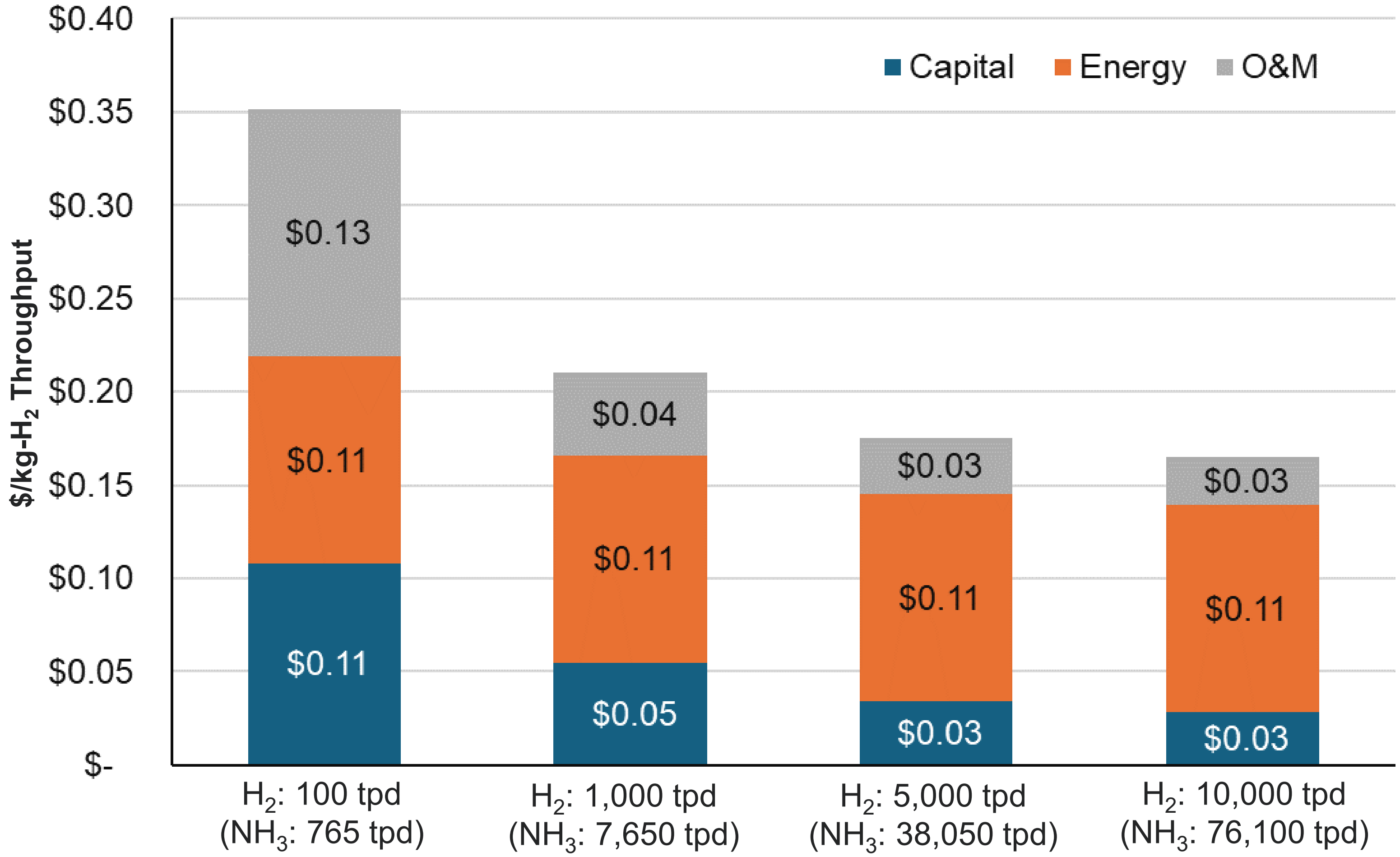
*Papadias et al. International Journal of Hydrogen Energy, 2021. **46**(47): p. 24169-24189

+Lamb et al. (2019). *International Journal of Hydrogen Energy*, *44*(7), 3580-3593

Cost of NH_3 Decomposition (Cracking) to H_2

Assumptions for decomposition plant:

- Decomposition Plant Capacity: hydrogen throughput of 100 - 10,000 tons/day
- Overall Decomposition Plant Efficiency: (Considering 99% Cracker efficiency and 75% PSA efficiency): 0.131 kg-H_2/kg-NH_3*
- PSA has 75% absorption efficiency where uncracked NH_3 as well as H_2 not separated by PSA are recycled back to furnace



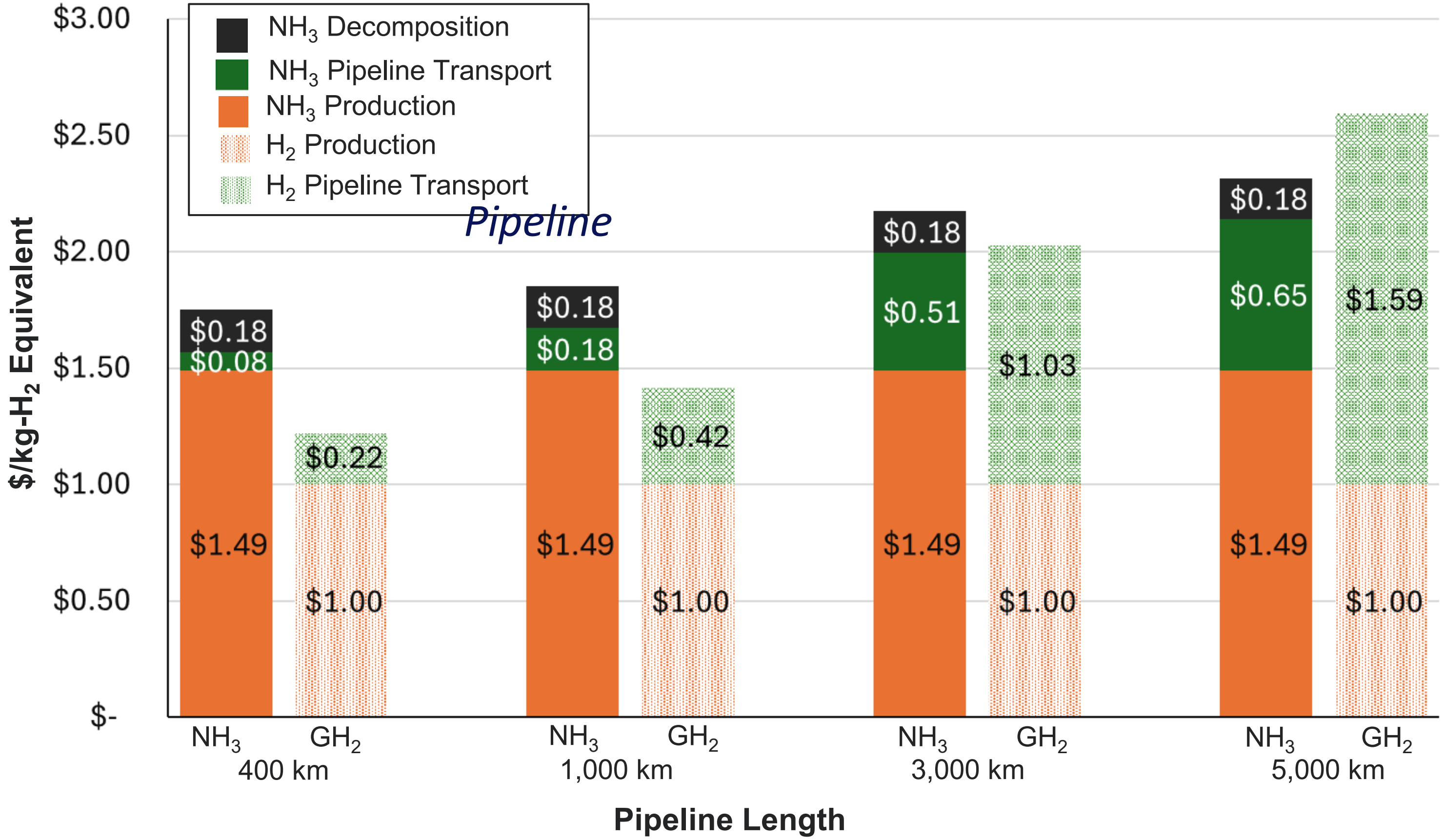
*NH_3 used for decomposition is implied in its upstream delivered cost

Total Cost of NH_3 Production, Transport and Decomposition, compared to Delivered H_2 Cost via Pipeline

Accomplishment

Assumptions for Pipeline Transport:

- NH_3 Demand: 5,000 tons/day (Equivalent H_2 Demand: 665 tons/day*)
- Distance: 400 – 5,000 km
- NH3 production pathway: Conventional (NG based, \$4.2/MMBtu NG for NH_3 cost)
- Hydrogen production cost assumed to be \$1/kg



✓ **For longer distance and higher throughput, transport of H_2 via NH_3 as carrier via pipeline can be lower cost compared to H_2 transport cost**

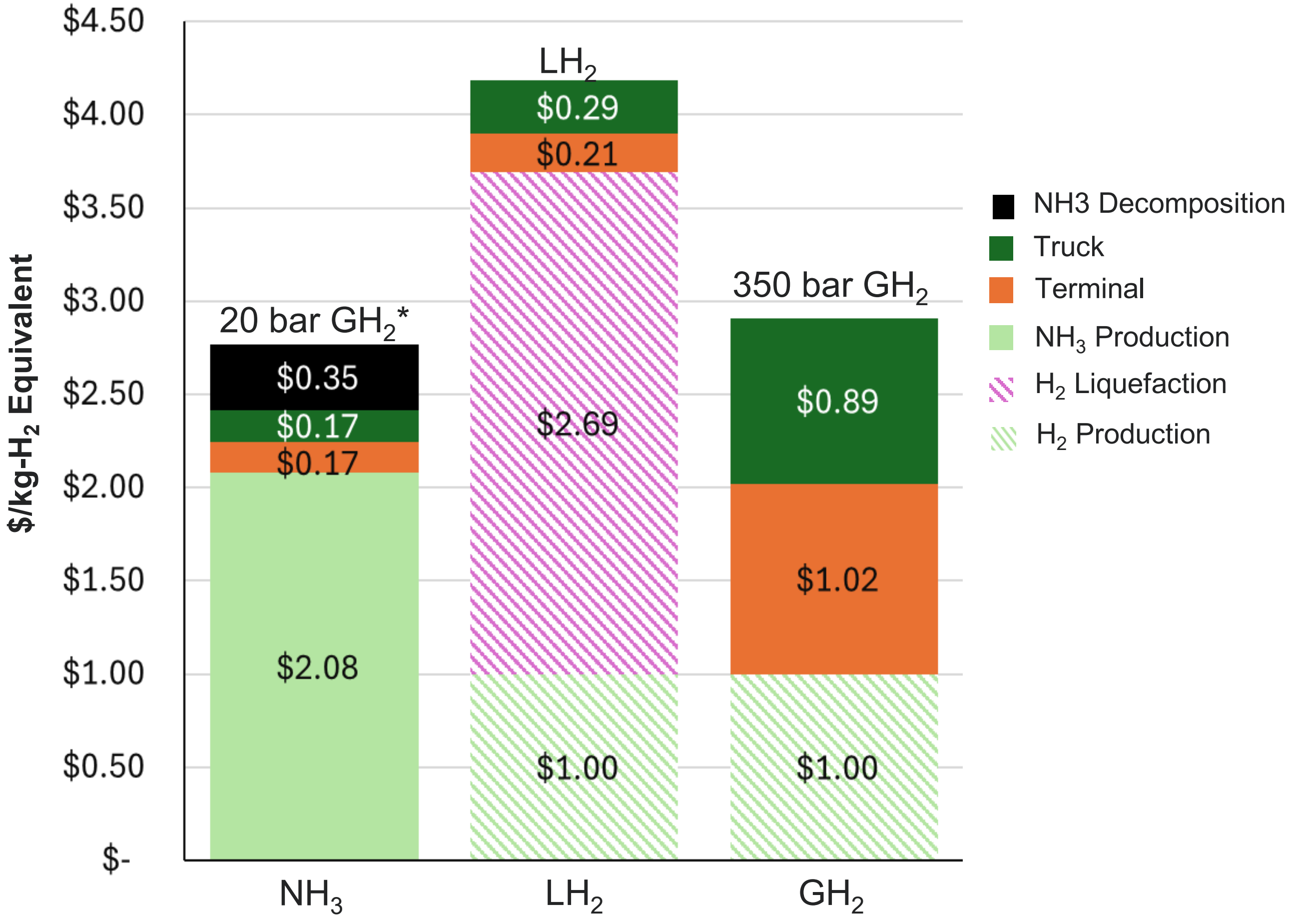
*Equivalent accounting for PSA absorption efficiency (75%) and NH3 cracker conversion efficiency (99%)

Total Cost of NH_3 Production, Transport and Decomposition, compared to Delivered H_2 Cost via Trucks

Assumptions for Truck-Trailer Transport:

- NH_3 Demand: 100 tons/day
- Transport Distance: 400 km
- NH_3 Production pathway: Conventional (NG based, $4.2 /MMBtu)
- H_2 production cost assumed to be $1/kg for LH_2 and GH_2 pathways

Mode	Capacity
NH_3 Truck-Trailer	27.3 tons NH_3 (40 m^3) (Equivalent H_2: 4.82 tons based on stoichiometry) NH_3 Pressure = 16 bar
LH_2 Tanker	3.8 tons H_2 (56 m^3) LH_2 Pressure = 3 bar
GH_2 Tube-Trailer	800 kg H_2 (41 m^3) GH_2 Pressure = 350 bar



*Shows the condition of H_2 after NH_3 cracking

Transmission Cost of NH_3: HCSAM
Liquefaction & Transmission Cost of LH_2: HDSAM

- ✓ **H_2 transport via NH_3 as carrier in trucks is lower cost compared to trucking GH_2 & LH_2**
- ✓ **LH_2 and compressed GH_2 have cost advantage for certain H_2 end use (e.g., FCEV refueling stations) compared to H_2 from cracked NH_3**

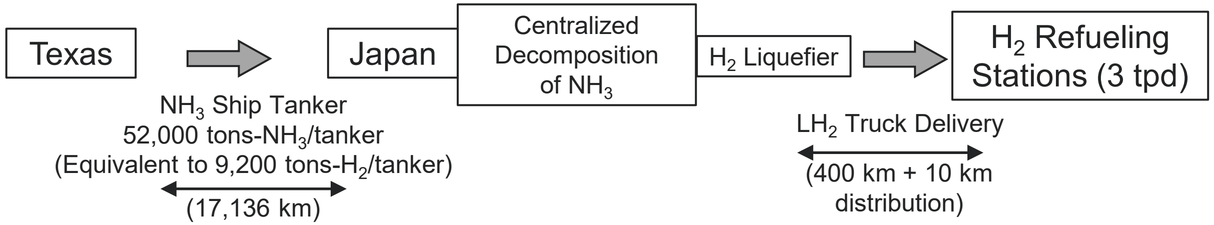
Comparison of Inter-continental transport of Liquid H_2 vs. NH_3 as H_2 Carrier vs. & impact on FCEV Refueling Cost at End Use

Accomplishment

Assumptions:

- Case studies of inter-continental hydrogen transport via LH_2* & NH_3
- H_2 liquefaction capacity: 650 tpd *(current H_2 Liquefaction < 50 tpd)*
- H_2 or NH_3 Production Pathway: Conventional w/ CCS

NH_3 shipping pathway:



Texas

NH_3 Ship Tanker
52,000 tons-NH_3/tanker
(Equivalent to 9,200 tons-H_2/tanker)
(17,136 km)

Japan

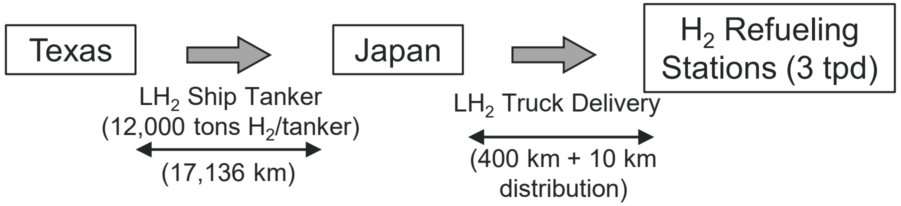
Centralized Decomposition of NH_3

H_2 Liquefier

LH_2 Truck Delivery
(400 km + 10 km distribution)

H_2 Refueling Stations (3 tpd)

Liquid H_2 shipping pathway:



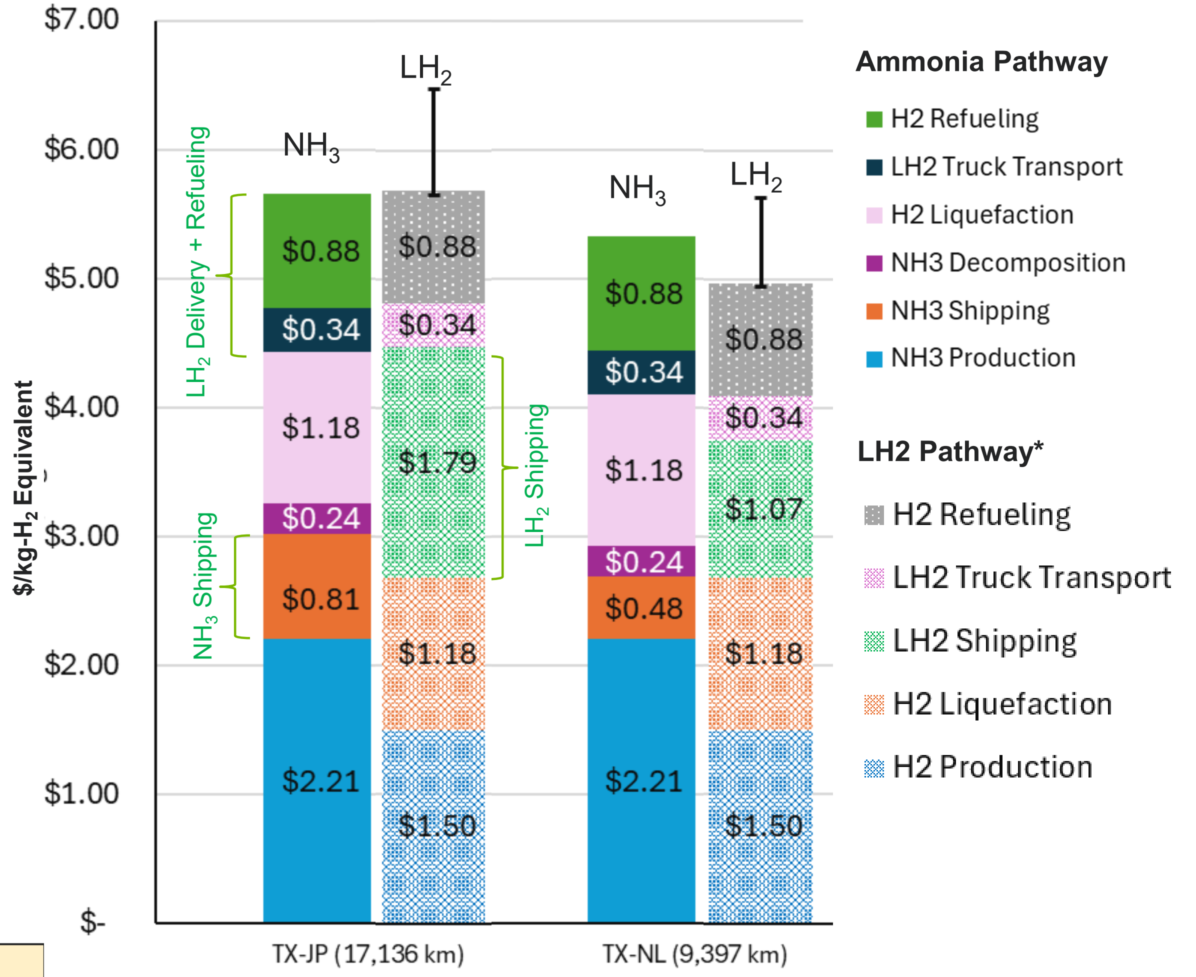
Texas

LH_2 Ship Tanker
(12,000 tons H_2/tanker)
(17,136 km)

Japan

LH_2 Truck Delivery
(400 km + 10 km distribution)

H_2 Refueling Stations (3 tpd)



- Upper and lower bounds for LH_2 pathway indicate variation due to boil-off loss (0% to 0.5% per day)⁺
- H_2 Delivery and Refueling cost estimated from HDSAM

✓ **Ship-tanker transport of NH_3 is lower cost compared to Liquid H_2**
✓ **Overall cost of NH_3 & LH_2 are comparable**
✓ **Improved PSA efficiency from 75% can improve economic benefit for NH_3 pathway**

**Ahluwalia et al. System Level Analysis of Hydrogen Storage Options. 2023 DOE Hydrogen Program AMR.*
⁺Petitpas, G. (2018). Boil-off losses along LH2 pathway. Lawrence Livermore National Lab.

Summary of Accomplishments, Challenges and Future Work

- **Summary of accomplishments and Findings**
  - Developed a comprehensive technoeconomic model (HCSAM) for NH_3 production, transport, and decomposition
  - Acquired data for entire ammonia value chain and implemented in HCSAM
  - The economics of physical H_2 delivery compared to its delivery in the form of NH_3 carrier depends on several factors:
    - Delivery amount and distance
    - Selected mode of delivery
    - End use of H_2 (e.g., industrial use vs. vehicle fueling)
- **Challenges and barriers**
  - Access to cost information for ammonia decomposition technologies
  - Uncertainties with boiloff for LH_2 shipping via ocean tankers
- **Future work**
  - Release the first version of model Hydrogen Carrier Scenario Analysis Model (HCSAM) by the end of fiscal year
  - Incorporate additional ammonia cracking technologies using ASPEN-Plus modeling for incorporation in HCSAM
  - Consider incorporating value chain for other H_2 carriers such as methanol and Methylcyclohexane (MCH) in HCSAM

Proposed future work is subject to DOE approval

Collaborations and Acknowledgments

- Industry experts provides general review of logistic details and cost information
- Energy Technology Analysis who supported review of techno-economic model and cash flow calculations
- Dennis Papadias and Rajesh Ahluwalia from ANL for providing ammonia shipping and cracking cost data from prior funded HFTO projects

Project Summary

- **Relevance**:
  - Techno-economic modeling and analysis is needed for evaluating cost of H_2 delivery via NH_3 as energy carrier
- **Approach**:
  - Bottom-up techno-economic modeling to evaluate production, delivery and decomposition costs of ammonia as a hydrogen carrier
- **Collaborations**:
  - Collaborated with consultants and experts from industries
- **Technical accomplishments and summary of findings**:
  - Developed a comprehensive model (HCSAM) for NH_3 production, transport, and decomposition
  - Acquired data for entire ammonia value chain and implemented in HCSAM
  - The economics of physical H_2 delivery compared to its delivery in the form of NH_3 carrier depends on:
    - Delivery amount and distance
    - Selected mode of delivery
    - End use of H_2 (e.g., industrial use vs. vehicle fueling)
- **Future Research**:
  - Release Hydrogen Carrier Scenario Analysis Model (HCSAM) in public domain by the end of fiscal year
  - Model NH_3 cracking technologies using ASPEN-Plus for incorporation in HCSAM
  - Consider additional H_2 carriers such as methanol and Methylcyclohexane (MCH) for incorporation in HCSAM

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ACCOMPLISHMENTS AND PROGRESS:
RESPONSES TO PREVIOUS YEAR REVIEWERS' COMMENTS

- ***Inclusion of NH_3 as hydrogen carrier is consistent with international efforts to transport hydrogen worldwide. The focus on delivered hydrogen cost is very timely and appropriate.***
- ***It would be good to see comparable data for the delivery of NH_3 and H_2 and costs to separate H_2 from both.***

Thank you for the insightful comments and recommendations. We agree that as hydrogen production and demand scales up in the United States and abroad, there is growing need to understand the trade off between various hydrogen packaging and delivery options as a function of scale, distance, delivery mode, and end use applications. In FY24, we used the valuable feedback comments to expand the model and analysis to cover entire ammonia supply chain, including production technologies, delivery modes, and ammonia decomposition. We also compared delivering hydrogen in physical forms versus delivering it via ammonia as hydrogen carrier. The model will be released in public domain for use by the global hydrogen community. We further proposed in future work to expand the model scope to include additional potential hydrogen carriers such as methanol and methylcyclohexane (MCH) by covering their entire value chain.