

Toluene-Methylcyclohexane as Two-Way Carrier for Hydrogen Transmission and Storage

Final CRADA Report

Energy Systems Division

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Non Proprietary Final CRADA Report

For the Office of Scientific and Technical Information (OSTI)

CRADA Number: 19122

CRADA Title: Toluene-Methylcyclohexane as Two-Way Carrier for Hydrogen Transmission and Storage

CRADA Start Date 11/2/2021 – **End Date** [Click or tap here to enter end date](#)

DOE Program or Other Government Support

Program office: Energy Efficiency & Renewable Energy – Hydrogen & Fuel Cell Technologies

Program manager name: Zeric Hulvey

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Participant(s)

Participant 1 name: Argonne National Laboratory

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Participant 2 name: Chiyoda International Corporation

Complete address: 2050 W Sam Houston Pkwy S, Houston, TX 77042, U.S.A.

Participant 3 name: [Click or tap here to enter text.](#)

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Argonne National Laboratory

Argonne PI(s): Rajesh, K. Ahuwalla and Dionissios, D. Papadias

Funding Table

To add rows, right-click in bottom row and select "Insert" "rows above".

	Planned Funding	Actual Funding	In-Kind
Government	50,000 \$	50,000\$	
Argonne National Laboratory	\$	\$	\$
Chiyoda Int. Corporation	50,000\$	50,000\$	\$
Click or tap here to enter text.	\$	\$	\$
Total	100,000\$	100,000\$	\$

Nature of Work

Describe the research (summary of Scope of Work and principal objectives of the CRADA):

Investigate the performance, regulated/unregulated greenhouse gas (GHG) emissions and cost advantages of using a two-way toluene-methylcyclohexane (MCH) carrier for hydrogen transmission and storage.

Develop and analyze specific hydrogen supply and demand scenarios that are particularly favorable for toluene-MCH carrier.

DOE mission area(s):

Energy and Environmental Science and Technology

Choose an item.

Choose an item.

Conclusions drawn from this CRADA; include any major accomplishments:

The performance, regulated/unregulated greenhouse gas (GHG) emissions and cost advantages of using a two-way toluene-methylcyclohexane (MCH) carrier for hydrogen transmission and end use was analyzed for different scenarios.

- By-product H₂ incurs the lowest cost among the pathways analyzed. Using ships as transmission mode, the cost, reflected by NG substitution only, could potentially be below \$2/kg (\$1.88/kg S₁/T₂)
- By-product H₂ pathway could reduce GHG by ~58% relative to H₂ produced by SMR if emissions are mass-allocated to all co-products (5.05 kg-CO₂/kg-H₂ vs 11.84 kg-CO₂/kg-H₂). Potentially, GHG emissions could be reduced by a total of 71% with biogas available for dehydrogenation.
- Transmission of MCH/toluene by large product tankers (115,000 DWT) is 50% less expensive than transmission by rail (\$0.7/kg vs \$1.53/kg). Emissions utilizing ships for transmission are reduced by half relative to rail.

Technology Transfer-Intellectual Property

Argonne National Laboratory background IP:

None

Participant(s) background IP:

None

Identify any new Subject Inventions as a result of this CRADA:

None

Summary of technology transfer benefits to industry and, if applicable, path forward/anticipated next steps towards commercialization:

None

Other information/results (papers, inventions, software, etc.):

Presented at the U.S. DOE Hydrogen and Fuel Cells Program 2020 Annual Merit Review and Peer Evaluation Meeting Washington, D.C. 30 May 2020. Project ID: H2058

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We used actual cost data for transmission of toluene/MCH by rail. U.S. rail carriers shipping over 4,000 carloads annually are mandated to supply a sample of the waybill for carloads and commodities shipped. We used the 2018 waybill data⁶ and correlated the transmission cost in terms of \$/ton-mile as a function of shipping distance. The freight revenue in \$/ton-mile generally decreases with distance and number of freight cars per train. The limiting rail transmission cost is related to the fuel consumption, about 380 ton-mile/gal, fuel cost, perceived hazard in transporting material, and for distances greater than 1,000 miles is 0.044/ton-mile for toluene.

For ships, we consider chemical tankers up to 115,000 deadweight ton (DWT). The capital cost of the ship as function of size (DWT) is estimated using statistical data from global shipyards. Additional cost of 20% is included to account for U.S. maritime commerce regulation requiring ships to be produced domestically if sailing from two U.S. ports. Panama Canal fees per roundtrip are estimated on laden conditions and additional port fees are included at \$0.52/DWT-day. The crew complement consists of 2 deck officers, 4 engineers, and 24 deckhands for a total crew of 30. Infrastructure costs are included to account for the costs of constructing and operating railyards for loading and unloading MCH/toluene to and from the railcars, jetty system which allows the ships to anchor away from the shore, and pipelines to transfer the MCH/toluene to the shore.

Shown in Fig. 4 are the transmission costs for rail and ships as function of daily demand. Transmission costs by rail do not show any significant cost reduction with capacity and total to about 1.53-1.64 \$/kg-H₂. The main cost is due to fuel and delivery charges incurred by the railroad.

Despite a longer route, 4,950 miles compared to 1,950 miles by rail, transmitting by ships is more economical. As the demand increases, the ships get bigger and more economical. The transmission cost at the lowest demand (50 tpd) is close to that by rail, \$1.42/kg-H₂, but decreases to \$0.70/kg-H₂ for a demand of 650 tpd, which is less than half the transmission cost by rail.

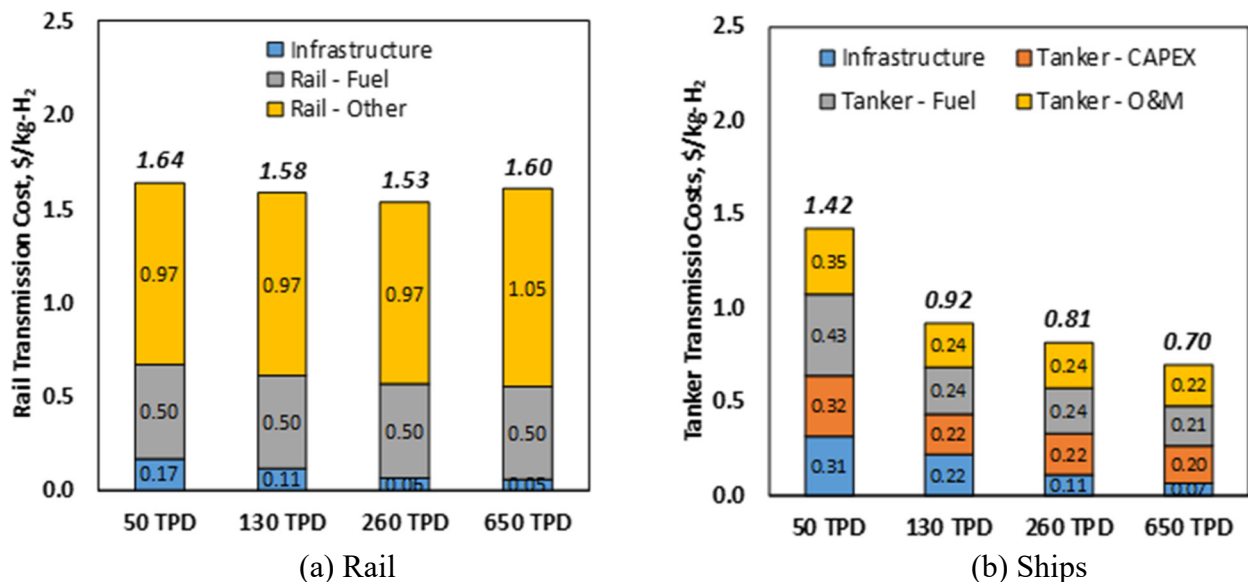


Figure 4 Transmission costs from TX to CA by rail and by chemical tankers

⁶ <https://prod.stb.gov/>

Cost and GHG Emissions

Figure 5a presents the breakdown of the levelized costs in terms of the individual process steps for hydrogen production, toluene hydrogenation, transmission and MCH dehydrogenation. The byproduct hydrogen cost is calculated from the calorific value of replacement NG data in Fig. 2 and the assumed \$2.65/million-Btu 2018 NG cost for TX. Renewable hydrogen production cost was estimated from the capital and operating costs of PEM electrolysis and wind or solar farms. GHG emissions were estimated from energy use and well to point of use metrics according to latest GREET model 2019⁷. Byproduct H₂ emissions were compared on the bases of NG substitution and mass-allocation (i.e., CO₂ emissions split to all co-products).

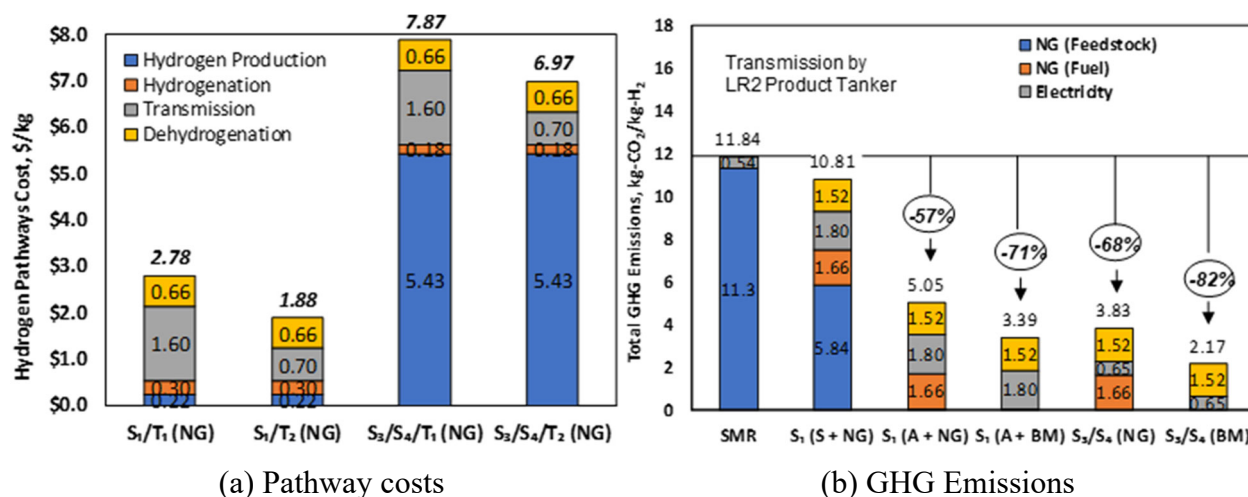


Figure 5 Pathway costs of hydrogen and GHG emissions at a daily production rate of 650 tpd. S: substitution; A: mass-allocation, NG: natural gas; BM: biomethane

The levelized cost of hydrogen for a few scenarios is shown in Fig. 5a. For brevity, costs are only presented for the large demand case, 650 tpd. Because the costs of byproduct hydrogen from chlor-alkali plants (S₁) and NGL steam cracking plants (S₂) are about the same, we only show results for the S₁ scenario. Similarly, because the costs of producing hydrogen by wind and solar are about the same, we group the pathway costs for S₃ and S₄ routes. By-product H₂ incurs the lowest cost among the pathways analyzed. Using ships (T₂) as transmission mode, the byproduct H₂ pathway cost can potentially be as low as \$1.88/kg-H₂. The \$0.22/kg cost of byproduct H₂ only reflects the cost of NG substitution for heat demand. For comparison, the cost of H₂ production by a large steam methane reformer (SMR) in CA is ~\$1.25/kg. The cost of renewable hydrogen pathway is \$6.97/kg-H₂ with ships as transmission mode. The \$5.43/kg cost of renewable H₂ is dominated by the estimated ϕ 7.9/kWh cost of electricity generation by solar and wind.

The equivalent GHG emissions in kg-CO₂/kg-H₂ are shown in Fig. 5b for S₁, S₃ and S₄ with chemical tankers as transmission mode. For comparison, we also show the GHG emissions from a large-scale SMR in CA. In case of NG substitution for by-product hydrogen, the GHG emissions are similar to the SMR case. By-product H₂ could reduce GHG by 57-71% relative to SMR if emissions are mass-allocated to all co-products and if bio-methane is available for dehydrogenation. In case of biomethane, hydrogen produced from wind and solar can reduce the

⁷ Argonne GREET Mode. <https://greet.es.anl.gov>

emission by up to 82% relative to the SMR. Transmission by ship accounts for the majority of GHG emissions (1.52 kg-CO₂/kg-H₂).

Summary and Conclusions

The performance, regulated/unregulated greenhouse gas (GHG) emissions and cost advantages of using a two-way toluene-methylcyclohexane (MCH) carrier for hydrogen transmission and end use was analyzed for different scenarios.

- By-product H₂ incurs the lowest cost among the pathways analyzed. Using ships as transmission mode, the cost, reflected by NG substitution only, could potentially be below \$2/kg (\$1.88/kg S₁/T₂)
- By-product H₂ pathway could reduce GHG by ~58% relative to H₂ produced by SMR if emissions are mass-allocated to all co-products (5.05 kg-CO₂/kg-H₂ vs 11.84 kg-CO₂/kg-H₂). Potentially, GHG emissions could be reduced by a total of 71% with biogas available for dehydrogenation.
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