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E-FUELS MODELING & TECHNOECONOMIC ANALYSIS



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E-fuels value chain study- Process modeling, TEA and LCA, supply & market



- We evaluate the full efuels value chain including CCUS and H2 value chains.
- H2 value chain includes production (with/without embodied emission), infrastructure (pure and H2/NG blend), refueling for vehicles and H2 for industrial use.
- CCUS value chain covers capture (from various sources and DAC), infrastructure, utilization for fuels/chemicals/materials, and storage.
- HDSAM for H2 infrastructure
- HCSAM and NH3 infrastructure

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

https://www.hydrogen.energy.gov/docs/hydrogenprogramlibr aries/pdfs/review24/in025_elgowainy_2024_o.pdf?sfvrsn=1 4b08ed8_3



E-FUELS STUDY TOOLS

Process and infrastructure modeling

Feedstock preparation Methanol/FT fuel production process simulated in Aspen Plus S1 RWGS reaction S2-1 FT fuel synthesis and purification CO₂ CO₂ CO₂ recycle pipeline Stationary CO2 sources $nCO+(2n+1)H_2 \longrightarrow C_nH_{2n+2}+nH_2O$ Wax+ $H_2 \longrightarrow C_n H_{2n+2}$ Water S2-2 Methanol synthesis and purification Solar/wind electricity H₂ storage Syngas $CO+2H_2 \leftrightarrow CH_3OH$ Electrolysis $CO_2+H_2 \leftrightarrow CO+H_2O$ $CO_2+3H_2 \leftrightarrow CH_3OH+H_2O$ H₂ production

Life cycle analysis (LCA) by using GREET model



Technoeconomic analysis (TEA) (cost \$\$)



Regional analysis with variation in technology, supply, storage and cost



INDUSTRIAL CO2 SOURCE LOCATIONS AND AMOUNTS

Industrial CO₂ Source Distribution in the U.S. (as of now)



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- Industrial sector is the second largest CO₂ emission source, after transportation sector.
- Industrial sector emission is sourced from both process and fuels combustion.
- The CO₂ capture energy demand and cost generally increases with decreasing purity.

Industrial CO₂ Source Data

Sector	Purity	# of Plants	Available CO ₂ [MMT/yr]
Ethanol	High	136	27
Ammonia	High	26	20
NG Processing	High	44	10
Hydrogen	Mid	74	40
Cement	Mid	89	64
Iron and Steel	Mid	18	37

COST OF CO₂ CAPTURE AND COMPRESSION



• The cost of CO2 capture and compression are greatly influenced by purity and process scale.





In-house CO2 pipeline model: to NPP for efuels



ESTABLISHED E-FUELS MODELING



SNG- PROCESS MODELING

Process modeling of SNG production

- SNG plant was scaled for a commercial capacity (20 MT/hr), validated in Europe.
- The plant generates 1,020 MMBtu-HHV/hr SNG, 3% of national average NG pipeline throughput, with energy
 efficiency of 77% (without steam byproduct) and 91% (with steam byproduct)



Techno-economic and life cycle analysis of synthetic natural gas production from low-carbon H2 and point-source or atmospheric CO2 in Window Construction States, K Lee, P Sun, A Elgowainy, KH Baek, P Bobba, Journal of CO2 Utilization 83, 102791

SNG-TECHNOECONOMIC ANALYSIS (TEA)



- H₂ production cost is based on DOE 2020 record, Fossil NG cost is based on EIA data, RNG cost is based on literature
- The SNG product cost with a lower electricity price and 45V H₂ credit could be comparable to Fossil NG and RNG cost depending on CO₂ source



FT FUELS PRODUCTION COST- BRAIDWOOD NUCLEAR



- Hydrogen cost is key cost driver for synfuels production, even with 45 V tax credit.
- The impact of 45Q is smaller than that of 45V using nuclear energy.

ENERGY Argonne National Laboratory is a U.S. Department of Energy laboratory managed by UChicago Argonne, LLC. Techno-economic analysis and life cycle analysis of e-fuel production using nuclear energy, HE Delgado, V Cappello, G Zang, P Sun, C Ng,, ...Journal of CO2 Utilization 72, 102481



E-fuels -methanol







SUMMARY

- We thank the great support from various DOE offices (HFTO, Nuclear office, ARPA-E, BETO)
- We evaluate various technologies through full value chain of e-fuels, with Aspen modeling of various production technologies (continuous and dynamic operation) and infrastructure modeling
- We develop in-house H₂ infrastructure, NH₃ infrastructure and CO₂ pipeline model.
- For e-fuels production, the key cost driver is H₂ cost. In U.S.A, IRA credit, e.g. 45V has a significant impact.





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Techno-economic and life cycle analysis of synthetic natural gas production from low-carbon $\rm H_2$ and point-source or atmospheric $\rm CO_2$ in the United States



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Techno-economic analysis and life cycle analysis of e-fuel production using nuclear energy

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Performance and cost analysis of liquid fuel production from $\rm H_2$ and $\rm CO_2$ based on the Fischer-Tropsch process

Guiyan Zang *, Pingping Sun, Amgad A. Elgowainy, Adarsh Bafana, Michael Wang

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Technoeconomic and Life Cycle Analysis of Synthetic Methanol Production from Hydrogen and Industrial Byproduct CO₂

Guivan Zang * Pinoning Sun, Amgad Floowainy, and Michael Wang



Plants in the United States

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Synthetic Methanol/Fischer-Tropsch Fuel Production Capacity, Cost, and Carbon Intensity Utilizing CO₂ from Industrial and Power

Guiyan Zang,* Pingping Sun, Eunji Yoo, Amgad Elgowainy, Adarsh Bafana, Uisung Lee, Michael Wang, and Sarang Supekar



Blending low-carbon hydrogen with natural gas: Impact on energy and life cycle emissions in natural gas pipelines



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THANK YOU! psun@anl.gov

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