WBS 2.1.0.506 and WBS 2.1.0.507

CO_2 Reduction and Upgrading for e-Fuels Consortium

U.S. DEPARTMENT OF ENERGY

Economics and Sustainability of CO_2 Utilization Technologies with TEA and LCA

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Project Overview

- This project performs techno-economic analysis (TEA), life cycle analysis (LCA), and water analysis of CO2 utilization (CO2U) technologies to address their costs and energy/environmental sustainability implications and to present economic and environmental value proposition of the technologies
- We develop analytic capabilities by leveraging two labs' existing expertise
  - **NREL's TEA:** leverage decades of TEA expertise on biomass conversion pathways to identify key cost drivers of CO2U technologies and to examine economic viability and trade-offs with sustainability performance
  - **ANL's LCA:** expand the GREET model that developed since mid-1990s with substantial datasets to examine energy and environmental impacts of CO2U technologies
  - **ANL's Water Analyses:** Adapt the WATER and AWARE-US models for CO2U technologies to simulate geospatial-explicit water resource availability, water footprint, and resulting water stress at U.S. county level

A dedicated Project Team to Address Costs and Sustainability

Michael Wang

- PI
- Overall project
- LCA task

Ling Tao

- Co-PI
- Overall project
- TEA Task

Uisung Lee

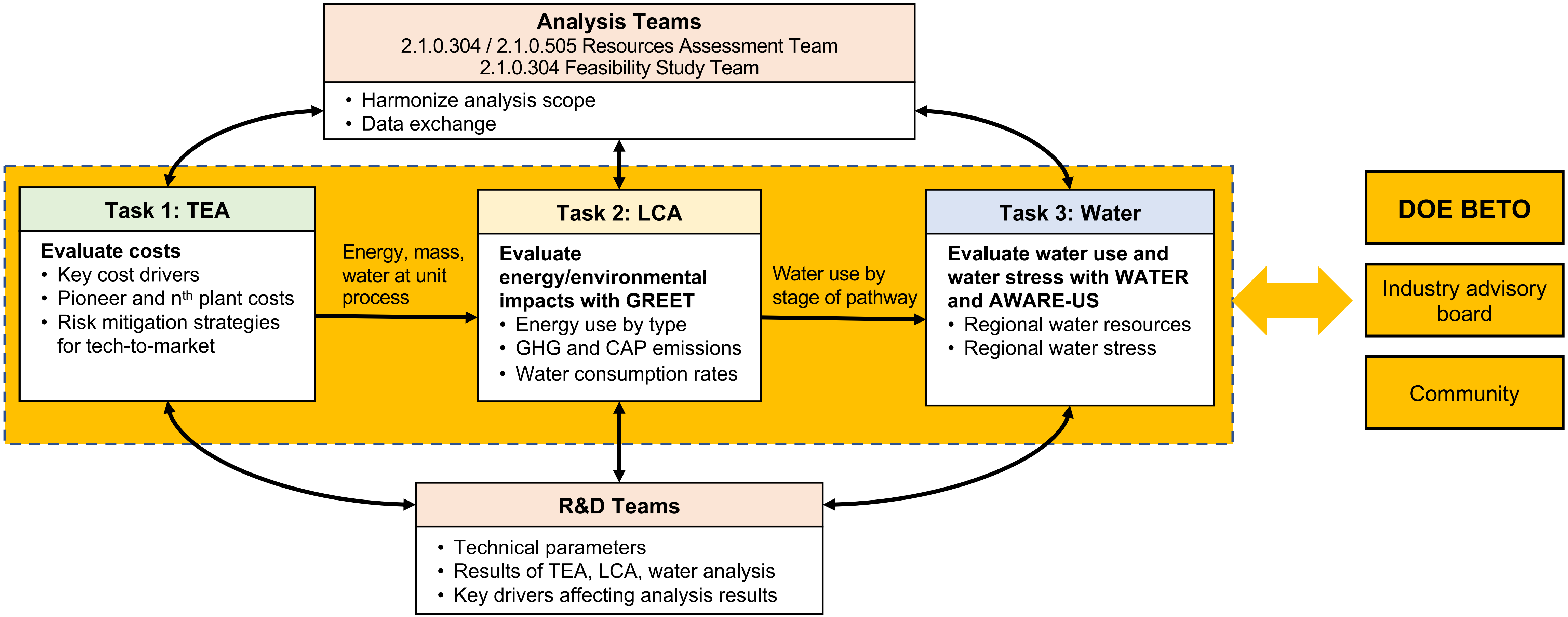
- LCA Task

May Wu

- Water task

1. Approach: Intra-Relationships of Project Tasks and Inter-Relationships with Other Projects

Internal task linkage of the project; project interactions with the R&D teams and the two other analysis teams; and outputs for BETO and community



1. Approach: CO2U Pathways to Evaluate

Six general low- and high-TRL CO2U pathways to explore the major near-to-mid term routes for CO2U and to understand the pros and cons between different approaches

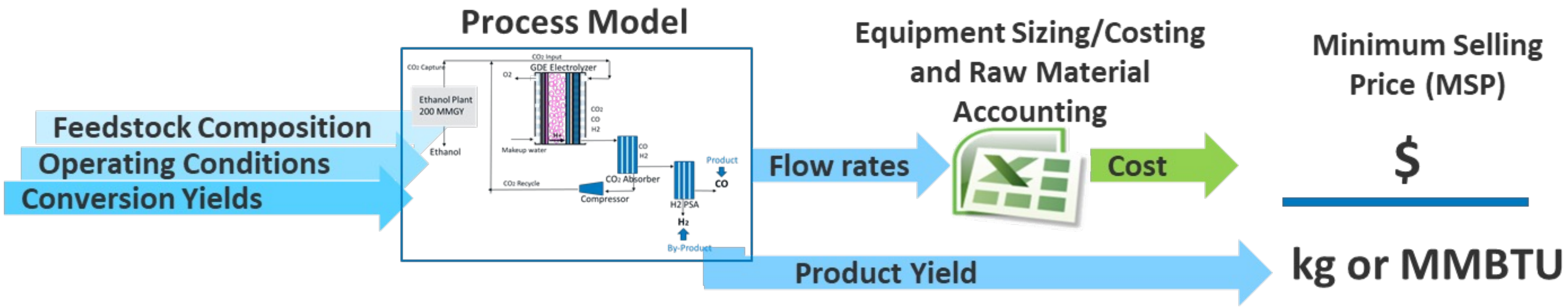
- Pathway 1: Electrolysis + Gas fermentation + ETJ
- Pathway 2: Electrolysis + FT
- Pathway 3: RWGS + FT (high TRL)
- Pathway 4: RWGS + Gas fermentation + ETJ (high TRL)
- Pathway 5: Direct CO2-to-MeOH (high TRL)
- Pathway 6: Direct CO2-to-EtOH + ETJ

Eight specific pathways by CO2U R&D Teams

WBS	Lab	Title
2.1.0.304	NREL	Feasibility Study of Utilizing Electricity to Produce Intermediates from CO2 and Biomass
2.1.0.504 2.1.0.505	NREL ANL	Markets, Resources, and Environmental and Energy Justice of CO2-to-Fuels Technologies
2.1.0.506 2.1.0.507	ANL NREL	Economics and Sustainability of CO2 Utilization Technologies with TEA and LCA
2.3.2.106	NREL	CO2 Valorization via Rewiring Carbon Metabolic Network
2.3.1.316	NREL	Electrocatalytic CO2 Utilization (ChemCatBio)
2.3.2.116 2.3.2.117	NREL ORNL	Integration of CO2 Electrolysis with Microbial Syngas Upgrading
2.3.2.118 2.3.2.119 2.3.2.120	LBNL LLNL ORNL	Bioconversion of Syngas from Electrochemical CO2 Reduction to Sustainable Aviation Fuels
2.3.2.121	NREL	Biological Conversion of Formic Acid for CO2-to-Fuels
2.3.4.301 2.3.4.302 2.3.4.303	NREL ANL ORNL	An Efficient and Scalable Process for the Electrochemical Reduction of CO2 to Formate
2.3.4.304 2.3.4.305	ANL NREL	Electrode and Membrane Materials for CO2 Electrolyzers: A Molecular Approach
2.4.1.102	NREL	Multiphysics CFD for Design and Scale-Up of Gas Bioreactors That Utilize CO2
2.6.3.502	NREL	CO2 Consortium Project Management

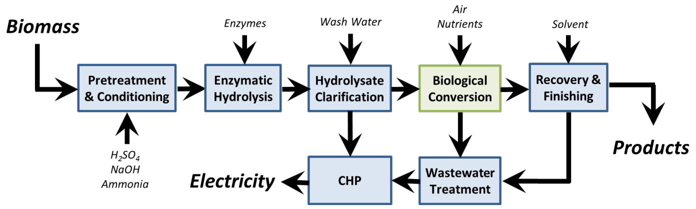
1. Approach: Task 1 TEA Methodology

- Collaborate with R&D Teams and the Resources Assessment Team to understand process concept; and establish consistent representation of feedstocks, CO2U conversion processes, and system boundaries for TEA
- Perform TEA (with interactive interaction of the LCA and the Water Tasks) on cost competitiveness of the integrated conversion technologies and future commercialization strategies
- Communicate TEA results routinely with subject matter experts to ensure credibility and to ensure industrial relevance

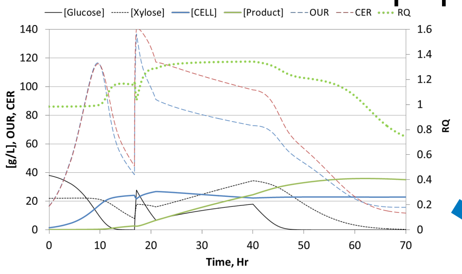


1. Approach: Task 1 TEA Methodology

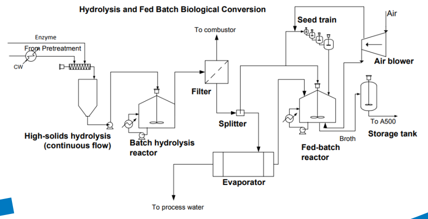
1) Conceptual process is **formulated/refined based on current research** with expected chemical transformations. Process flow diagram is synthesized.



2) Individual unit operations are **designed and modeled using experimental data**. Process model outputs are used to size and cost equipment.

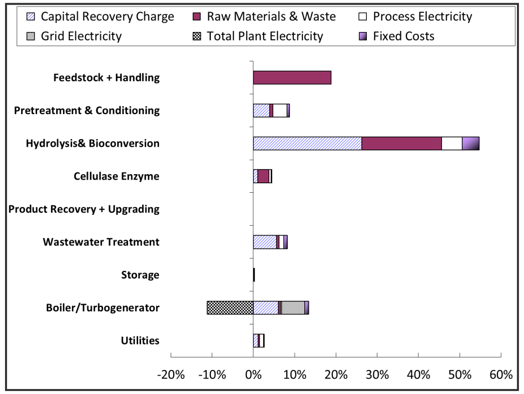


3a) Capital and operating costs are inputted into an economic model to **identify major cost drivers**.



3b) Material and energy flows are outputs to Task 2 to **identify the major sustainability drivers**.

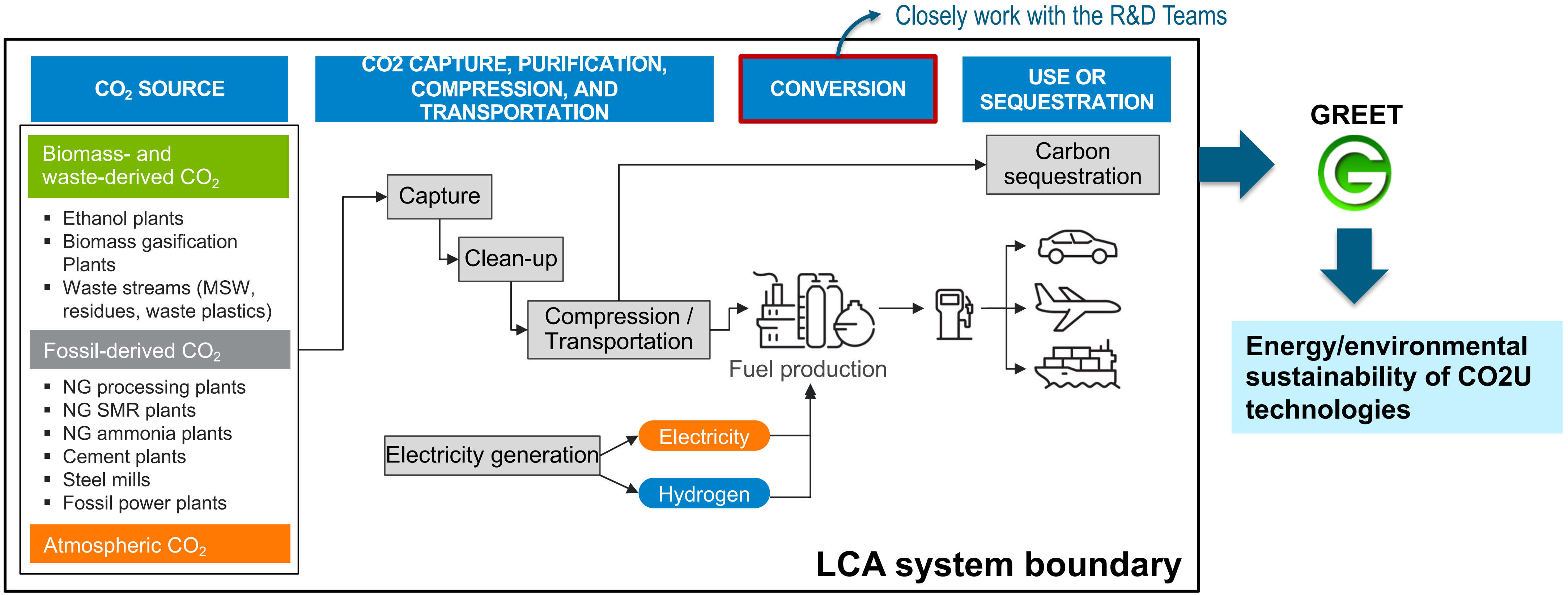
4) Results and **new understanding is fed back** into step 1) for iterative process modeling.



GREET LIFE-CYCLE MODEL

1. Approach: Task 2 LCA Methodology

- Interact with the TEA Task, the R&D Teams, and the Resources Assessment Team to configure CO2U technology LCA in GREET
- Conduct LCA for pathways to identify key drivers affecting sustainability performance for improvements
- Pathways cover various CO2 feedstocks, production of intermediates, and conversion to final products



1. Approach: Task 2 LCA Methodology

2. CO2 sources

1.1) CO2 capture & transportation

1.1.1) CO2 sources

CO2 source	1	1 -- Ethanol plant 2 -- Ammonia plant 3 -- NG processing 4 -- Hydrogen (SM 5 -- Cement plant 6 -- Iron/steel palnt 7 -- NGCC power p 8 -- Coal power pl 9 -- DAC
Location of CO2 capturing facility	1	0--on-site, 1--off-site

Energy requirements for CO2 capture and transportation

Energy uses (Btu/kg CO2)	Selected: Ethanol	Ethanol	Ammonia	NG process	Hydrogen	Cement	Iron/steel	NGCC power	Coal fired power	DAC
Electricity for CO2 capture	0.0	0	0	0	131	149	150	806	955	1,361
Natural gas for CO2 capture	0.0	0	0	0	4,218	4,208	4,227	0	0	0
Electricity for CO2 compression for transportation,off-site	393.3	393	366	327	393	336	336			

Energy Sources for CO2 capture & transportation

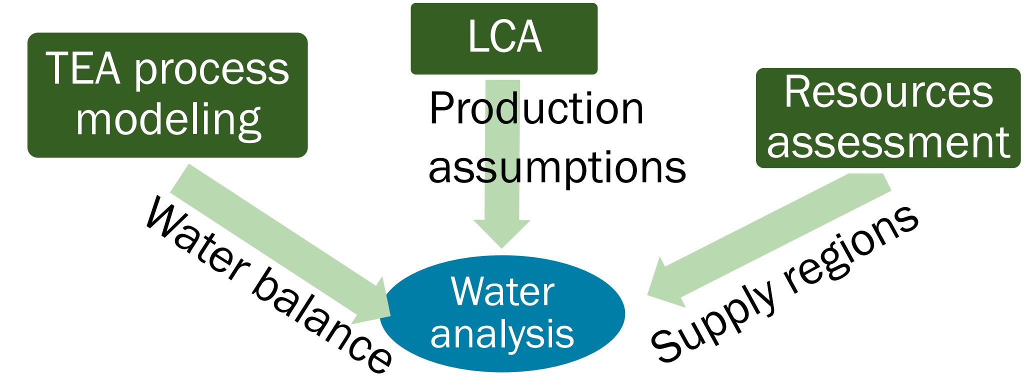
Electricity Sources for CO2 capture	5	1--US mix, 2--NGCC electricity, 3--Coal IGCC electricity, 4--Biomass IGCC electricity, 5--Renewable (Wind), 6-Nuclear
NG Sources for CO2 capture	1	1--North American NG, 2--Non-North Amerian NG, 3--RNG, 4--Waste heat
Electricity Sources for CO2 transportation	1	1--US mix, 2--NGCC electricity, 3--Coal IGCC electricity, 4--Biomass IGCC electricity, 5--Renewable (Wind), 6-Nuclear

- GREET is being expanded to include the six general (done) and eight specific CO2U pathways (to be completed).
- GREET allows changes in energy/material inputs of individual LCA stages to show interactive LCA results of CO2U technology improvements; source of CO2; source of hydrogen; and source of electricity.
- Embodied emissions associated with renewable electricity (e.g., manufacture of solar PV and wind turbine) are optionally included in CO2U LCA.
- The GREET CO2U LCA module will be available to individual R&D Teams

	CO2 to SAF (three step)					
	CO2 to syngas	Syngas to EtOH	EtOH to jet	FT Fuel Transportation and Distribution	FT Fuel Storage	CO2 capture
Share of feedstock input as feed (the remaining in						
Energy efficiency						
Urban emission share				67.00%	70.00%	
Loss factor				1.000	1.000	
Steam exported: Btu/mmBtu of fuel produced						
Electricity exported: KWh/mmBtu of fuel produced	-6.5					
CO2 input: grams per mmBtu FT fuel product	87,008					
Shares of hydrogen as process fuels	0.00%					
Natural gas	0.00%					
Hydrogen	64.44%					
Electricity	35.56%					
Natural gas						0.00
Feed loss	0.00%					
Energy use: Btu/mmBtu of fuel throughput (except						
Hydrogen	1,080,093		43,426			
Electricity	596,104	60,457				128,724
Natural gas		540,774	13,477			
Diesel						
Fuel gas						
Feedstock loss				46	0	
Material use: g/mmBtu of fuel throughput (except						
Catalyst-Oligomerization			7			
Hydrogenation Catalyst			0			
C4 Catalyst			2			
KH2PO4		62				
NaCl		625				
CaCl2		12				
MgSO4		72				
NH4Cl		1,059				
Yeast Extract		94				
NH3		266				
Catalyst-hydroisomerization						
Zinc Oxide (ZnO) Catalyst						
FT Synthesis Catalyst (Co based)						
Hydrotreating Catalyst (sulfided CoMo or NiMo)						
Amine Make-Up						
Boiler Chemicals						
Cooling Tower Chems						
Total energy	3,195,380	648,836	117,858	3,898	0	135,305
Fossil fuels	767	581,582	14,560	3,603	0	0
Coal	293	5,364	135	349	0	0
Natural gas	460	568,065	14,322	803	0	0
Petroleum	13	8,152	104	2,450		0
Water consumption, gallons/mmBtu of fuel throughput	28	14.916	1	0.152		0
Total emissions: grams/mmBtu of fuel throughput						
VOC	0.007	-13.219	-0.358	1.141		0.000

1. Approach: Task 3 Water Analysis Methodology

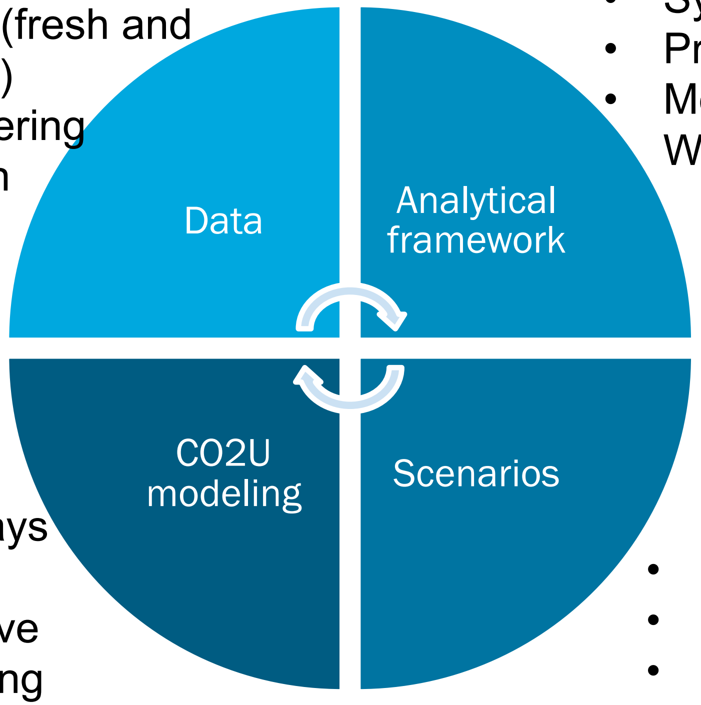
Inputs from Two Project Tasks and Resource Assessment Team



Four Interactive Aspects of The Task

- Water resource (fresh and reclaimed water)
- Process engineering
- Electricity region

- System boundary
- Production assumptions
- Modeling platforms: WATER, AWARE-US



- Multiple pathways and scenarios
- Online interactive
- CO2U plant siting comparison

- Base and water reuse
- Stand-alone plant
- H2-co-located plant

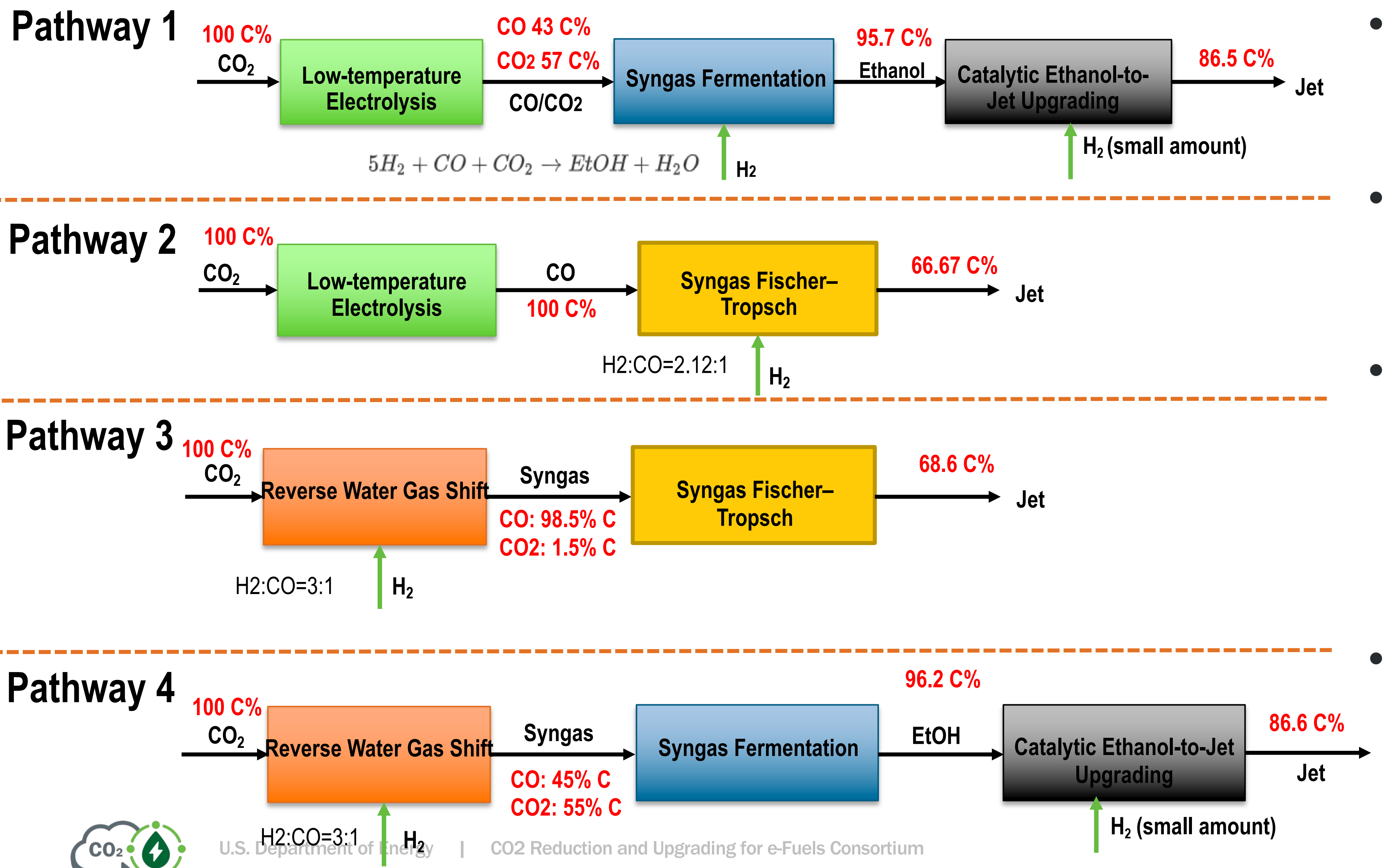
1. Approach: Milestones/Deliverables

Milestone Name/Description	Criteria	End Date	Type
Complete the first round integrated TEA and LCA	Perform TEA and LCA and report findings for the CO2U technologies with emphasis on key drivers for costs and environmental effects; conduct high-level water resource analysis using the updated data inventory for 1-2 CO2U technologies in the CO2 and electricity resource regions based on preliminary screening results from the Resource Assessment project.	12/31/2022	QPM
Joint with WBS#2.3.4.301 to complete baseline TEA and LCA for CO2 to formate (or formic acid) pathway	Perform TEA and LCA and report analysis findings to assist upcoming R&D activities.	3/31/2023	QPM
Joint with WBS#2.3.4.304 to complete baseline TEA from CO2 to methanol via electrochemical conversion	Perform TEA and LCA and report analysis findings to assist upcoming R&D activities.	3/31/2023	QPM
Joint with WBS#2.1.0.504-5 to perform iterative analysis with grid model and CO2U conversion pathways	The jointed project teams will report grid outputs (e.g., electricity mix, electricity costs, carbon emissions) and potential implications of electricity loads on approaching 35-billion-gallon SAF production goal by 2050.	6/30/2023	QPM
Document and report the first round TEA and LCA findings	Report TEA and LCA findings of the CO2U technologies with emphasis on key drivers for costs and environmental effects; Complete water resource availability and stress analysis with emphasis on water reuse for four CO2U pathways in the selected locations and report findings.	9/30/2023	Annual SMART
Deliver in-depth TEA packages and the GREET CO2U LCA module	Deliver TEA and LCA CO2U analysis tool packages, which provide detailed costs, sustainability, and water results for all studied CO2U technologies; Complete reports/papers on value proposition of BETO-selected CO2U technologies with integrated cost and sustainability results and water resource and stress results with key technical drivers for policy designs, business development, and public communications.	9/30/2024	End of Project Milestone

1. Approach: Additional Information

- **Go/No-go (6/30/2023)**
  - Determine CO2U technologies to be included in TEA/LCA modeling and the developed TEA and LCA tools.
- **Risk mitigation**
  - Data limitation: Maintaining engagement with the R&D teams within the BETO CO2U Consortium, external industrial stakeholders, and other collaborators.
  - Cost uncertainty on pioneer plants: Engaging with experts from industry, academia, and national labs who have expertise in scale-up commercialization.
- **Diversity, Equity, and Inclusion (DEI)**
  - Plan to hold seminars for the public, especially including under-represented students and researchers to disseminate the research findings.

2. Progress and Outcomes – TEA of Two Syngas Options with Two Syngas Conversions to SAF



- Implications for the consortium and industry
- Perform LCA and TEA interactively and iteratively
- De-risk strategies for commercializing and deploying CO2U technologies at scale and with regionality
- Sample results on the left show FT synthesis has ~30% carbon loss.

2. Progress and Outcomes – TEA and LCA of Decarbonization Options for Four SAF Pathways

Pathway 1: Electrolysis + Gas fermentation + ETJ

Base 1.0	US mix electricity, H_2 from fossil NG SMR, CO_2 (biorefinery)
Pathway 1.1	+Renewable electricity @ $0.02/kWh
Pathway 1.2	+Renewable H_2 @ $1/kg
Pathway 1.3.1	+Renewable NG @ $10/MMBtu
Pathway 1.3.2	+Waste heat @ $0/MMBtu

Pathway 2: Electrolysis + FT

Base 2.0	US mix electricity, H_2 from fossil NG SMR, CO_2 (biorefinery)
Pathway 2.1	+Renewable electricity @ $0.02/kWh
Pathway 2.2	+Renewable H_2 @ $1/kg

Pathway 3: RWGS + FT

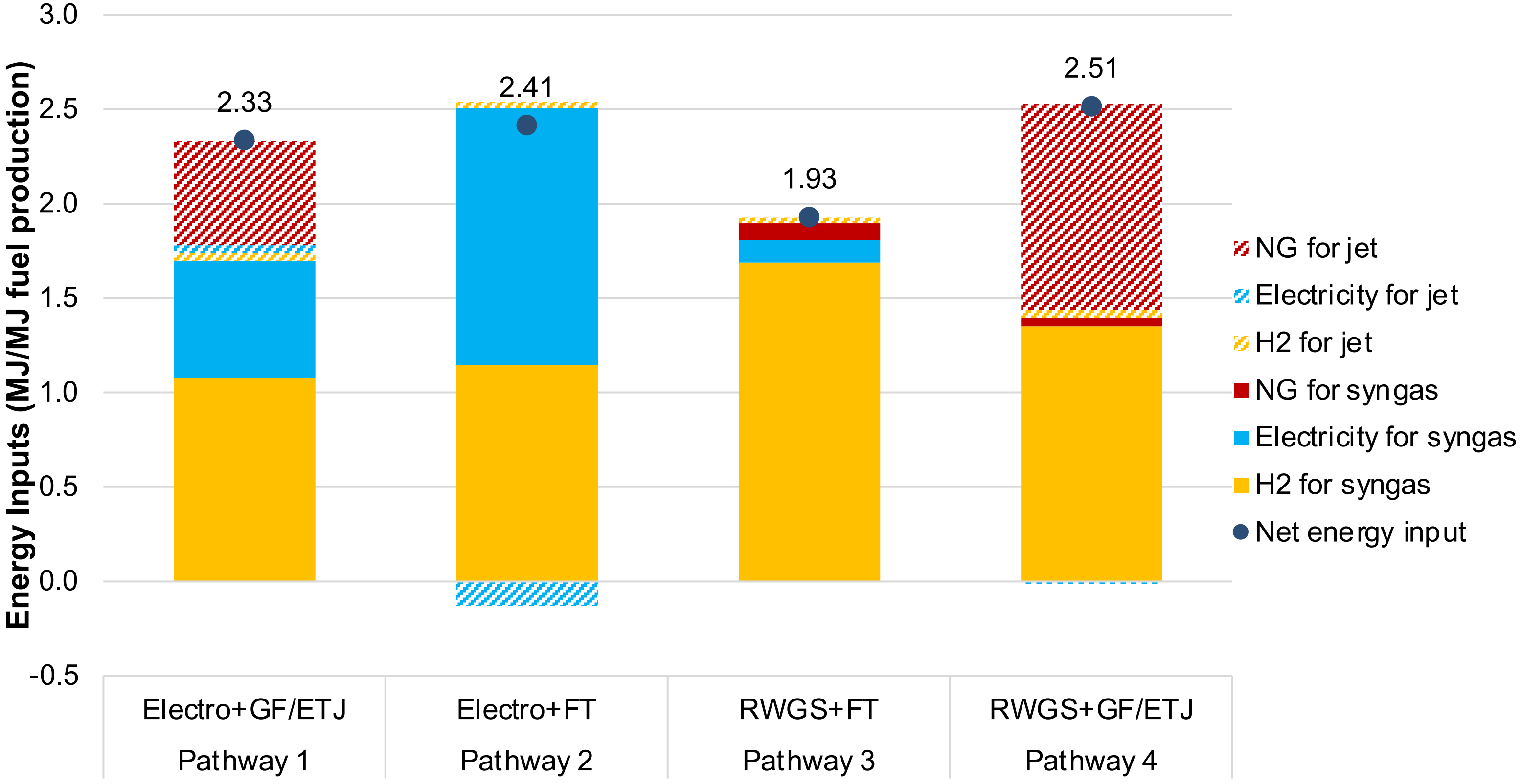
Base 3.0	US mix electricity, H_2 from fossil NG SMR, CO_2 (biorefinery)
Pathway 3.1	+Renewable electricity @ $0.02/kWh
Pathway 3.2	+Renewable H_2 @ $1/kg

Pathway 4: RWGS + Gas fermentation + ETJ

Base 4.0	US mix electricity, H_2 from fossil NG SMR, CO_2 (biorefinery)
Pathway 4.1	+Renewable H_2 @ $1/kg
Pathway 4.2.1	+Renewable NG @ $10/MMBtu
Pathway 4.2.2	+Waste heat @ $0/MMBtu

2. Progress and Outcomes– LCA Results of Four SAF Pathways

- GF/ETJ requires less CO_2-to-CO conversion (less energy intensive in syngas production) compared FT that requires full CO_2-to-CO conversion.
- FT requires much less energy to convert syngas to fuels compared to GF/ETJ
- GF/ETJ requires significant heat inputs mainly during ETJ conversion.

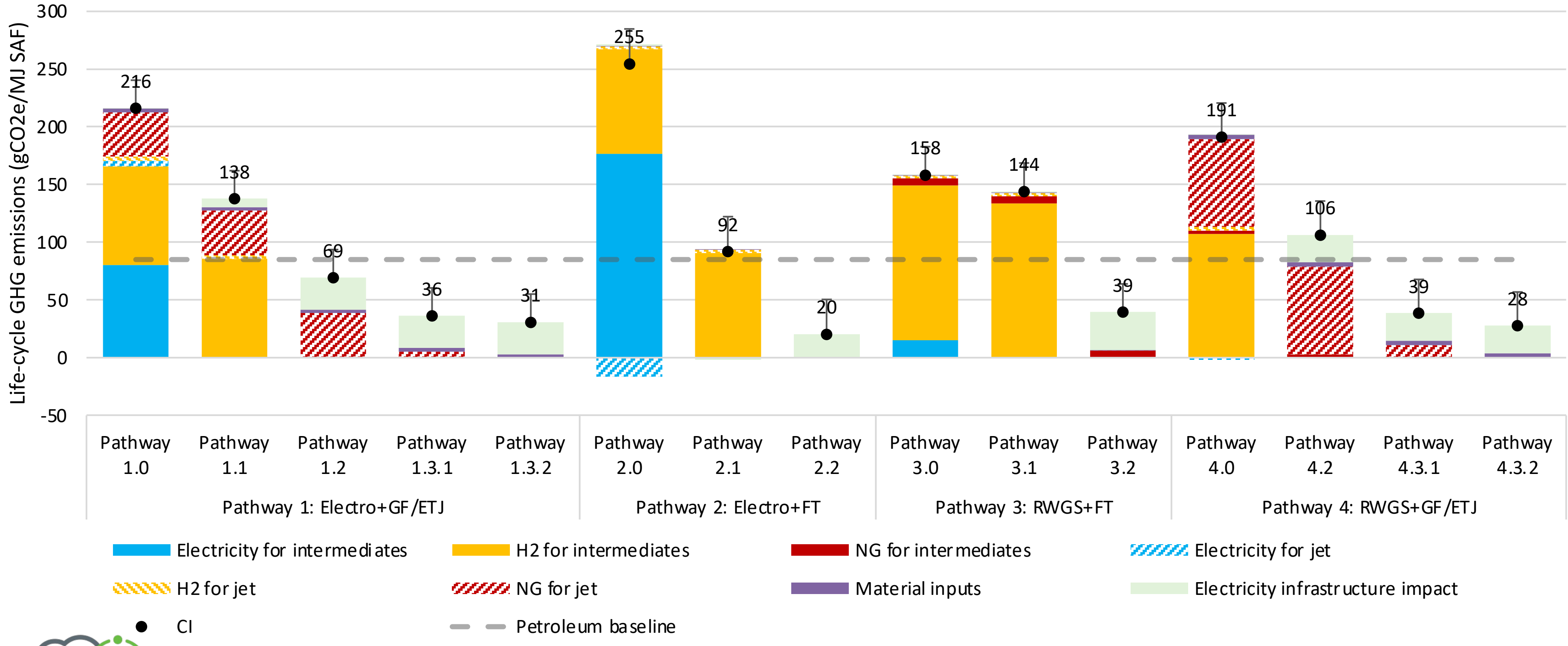


- For all pathways, H_2 input is significant (1.1–1.7 MJ H_2/MJ jet) because HC fuels need H_2, together with CO_2; RWGS requires more H_2 compared to electrolysis.
- Green H_2 production requires 1.4 MJ of electricity per MJ H_2 *
- For RWGS, electricity input is minor.

*** H_2 production using electrolysis with the efficiency of 72.6%**

2. Progress and Outcomes– LCA Results of Four SAF Pathways with Decarbonization Options

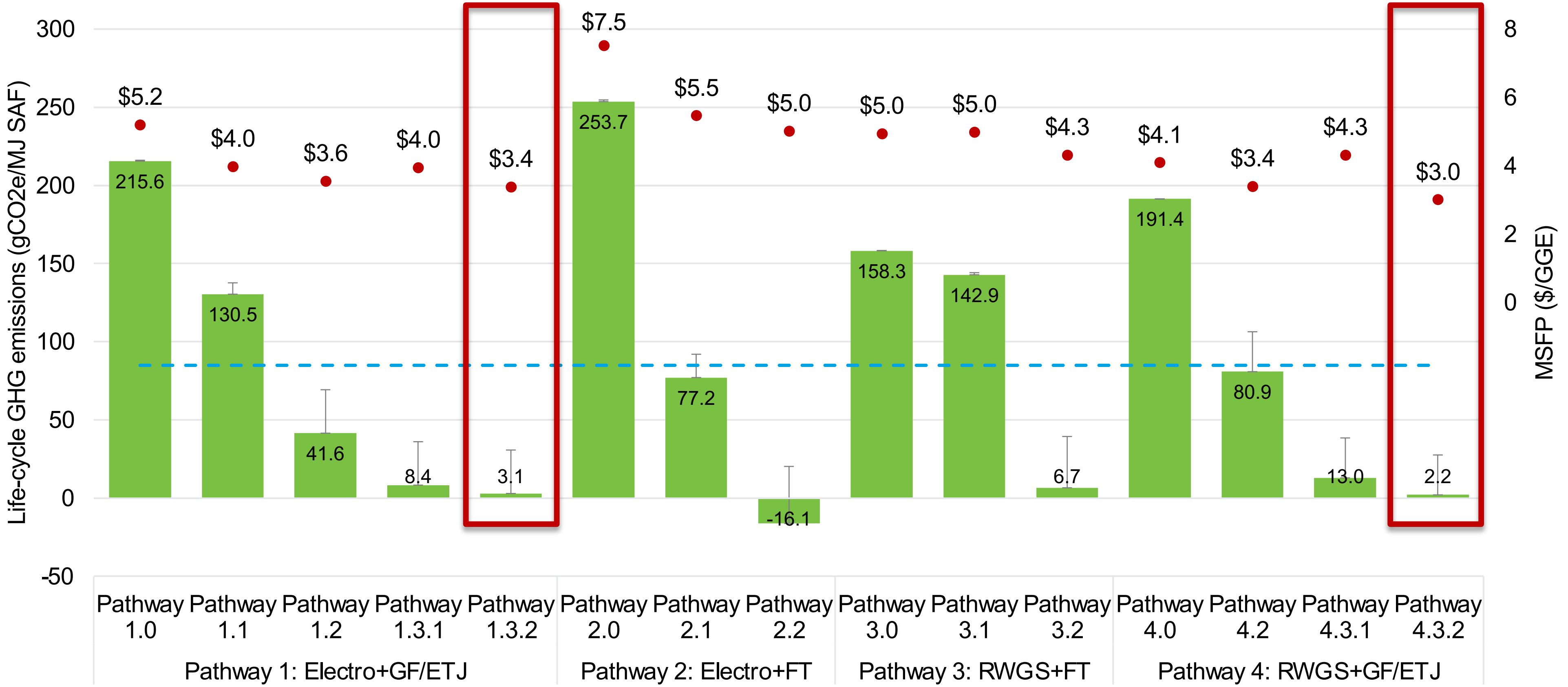
- Decarbonization options for each SAF CO2U pathway show significant GHG reductions.
- LCA results include the embodied impacts of solar PV production.
- Error bars present the variation of using different CO_2 sources with different CO_2 purity levels requiring additional energy inputs to purify.



Pathway 1.0	Baseline
Pathway 1.1	+Renewable electricity
Pathway 1.2	+Renewable H_2
Pathway 1.3.1	+Renewable NG
Pathway 1.3.2	+Waste heat
Pathway 2.0	Baseline
Pathway 2.1	+Renewable electricity
Pathway 2.2	+Renewable H_2
Pathway 3.0	Baseline
Pathway 3.1	+Renewable electricity
Pathway 3.2	+Renewable H_2
Pathway 4.0	Baseline
Pathway 4.2	+Renewable H_2
Pathway 4.3.1	+Renewable NG
Pathway 4.3.2	+Waste heat

2. Progress and Outcomes– Combined LCA/TEA Results of Four SAF Pathways

- TEA/LCA results show reductions in both MSFPs and CIs using low-cost renewable electricity/H2 ($0.02/kWh and $1/kg H2) vs. baseline costs ($0.068/kWh and $1.38/kg H2).
- With the maximum CI reduction (near net-zero SAFs), four cases present $3.0-$5.0/gal MSFP.



Pathway 1.0	Baseline
Pathway 1.1	+Renewable electricity
Pathway 1.2	+Renewable H_2
Pathway 1.3.1	+Renewable NG
Pathway 1.3.2	+Waste heat
Pathway 2.0	Baseline
Pathway 2.1	+Renewable electricity
Pathway 2.2	+Renewable H_2
Pathway 3.0	Baseline
Pathway 3.1	+Renewable electricity
Pathway 3.2	+Renewable H_2
Pathway 4.0	Baseline
Pathway 4.2	+Renewable H_2
Pathway 4.3.1	+Renewable NG
Pathway 4.3.2	+Waste heat

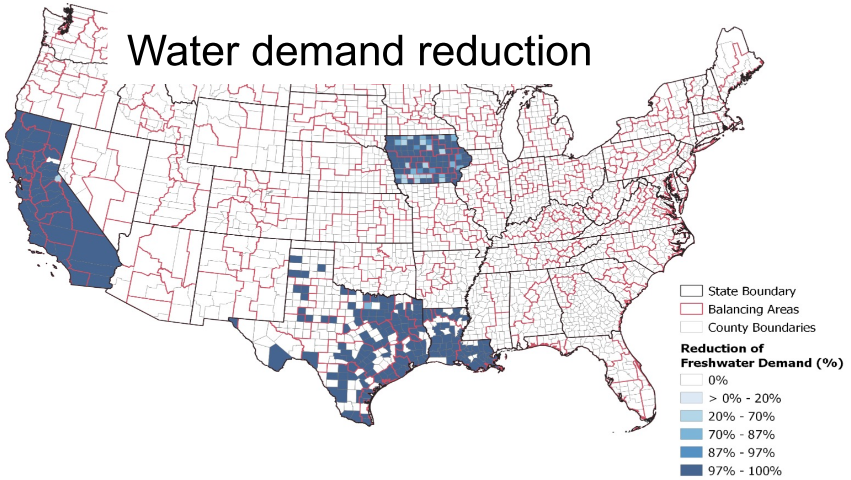
Error bars indicate the embodied solar PV production impact

2. Progress and Outcomes: Water Analysis Results

Base case

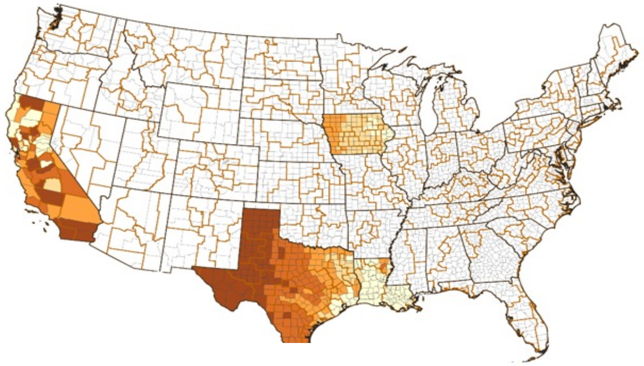
	Pathway 1	Pathway 2	Pathway 3
	LTE-GF-ETJ	LTE-FT-Jet	RWGS-FT-Jet
Fuel production (kg/y)	83,436,285	66,508,219	68,603,336
Water demand (fuel and H_2 prod) (MGY)	44.2	52.6	69.7
% of cooling	0%	31%	22%
Water consumption rate (Fuel, H_2) (gal/kg fuel)	0.53	0.79	1.02
Water consumption (fuel) (gal/kg fuel)	0.02	0.26	0.23

Reclaimed water for CO2U plants

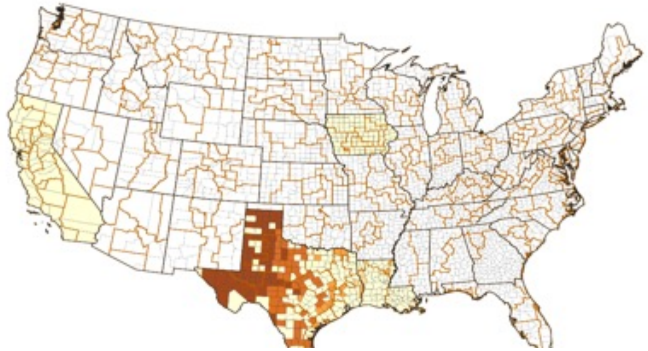


More counties are available for CO2U plants, meeting up to 100% water demand.

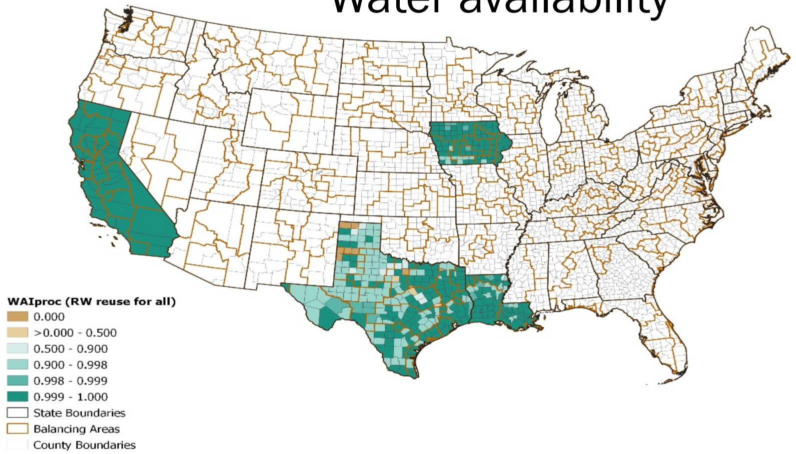
Impact of CO2U plants on water Stress



Fresh water



Fresh and reclaimed water



3. Impact: Integrated Results of Three Tasks

- Provide detailed TEA, LCA and water results addressing economic viabilities, energy/environmental sustainability, and water resource impacts of CO2U technologies
- Identify value proposition (opportunities) and bottlenecks/hot spots (challenges) of costs and sustainability of CO2U technologies to provide insights so that the CRU Consortium can improve technology performance
- Help reduce costs and investment risks and improve sustainability with analysis-driven decisions by BETO, other agencies, and industries
- Support federal government goals of 3 BGY SAF by 2030, 35 BGY by 2050 with 70% reduction of LCA GHG emissions

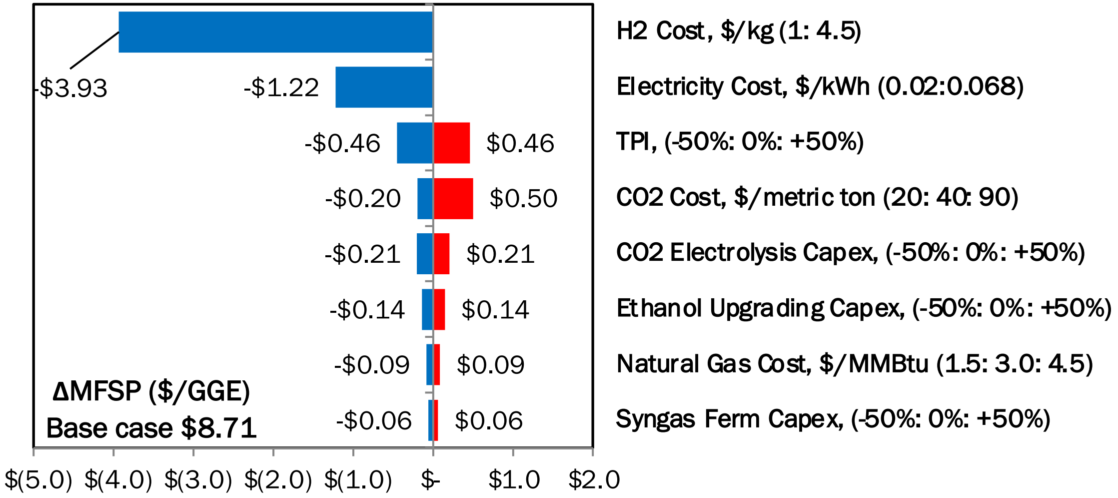
3. Impact: TEA

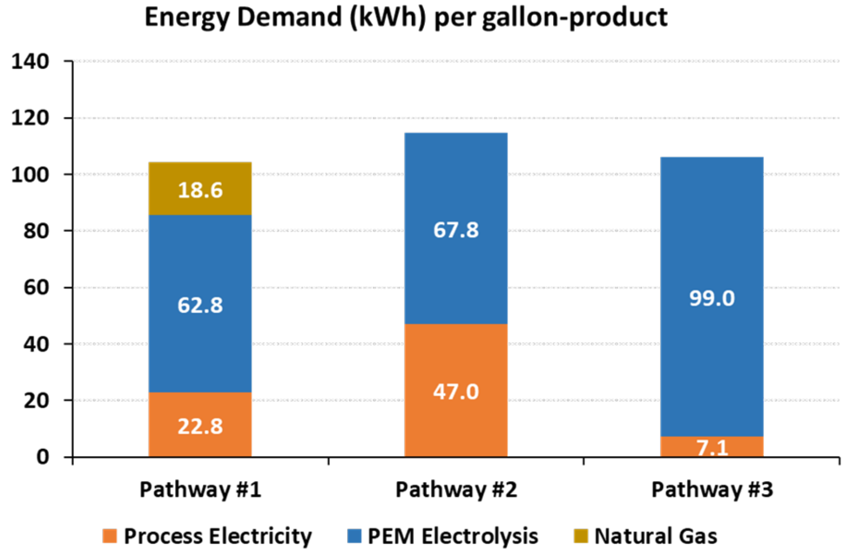
For R&D Teams:

- Identify key cost and environmental drivers to improve technologies
- Help R&D priorities and to present economic and environmental value proposition of technologies

For LCA Task and the Resources Assessment Team:

- Bridge pathway strategies with LCA and market analysis to understand renewable energy and renewable hydrogen demand





kWh per gallon product, result courtesy of WBS#2.1.0.505

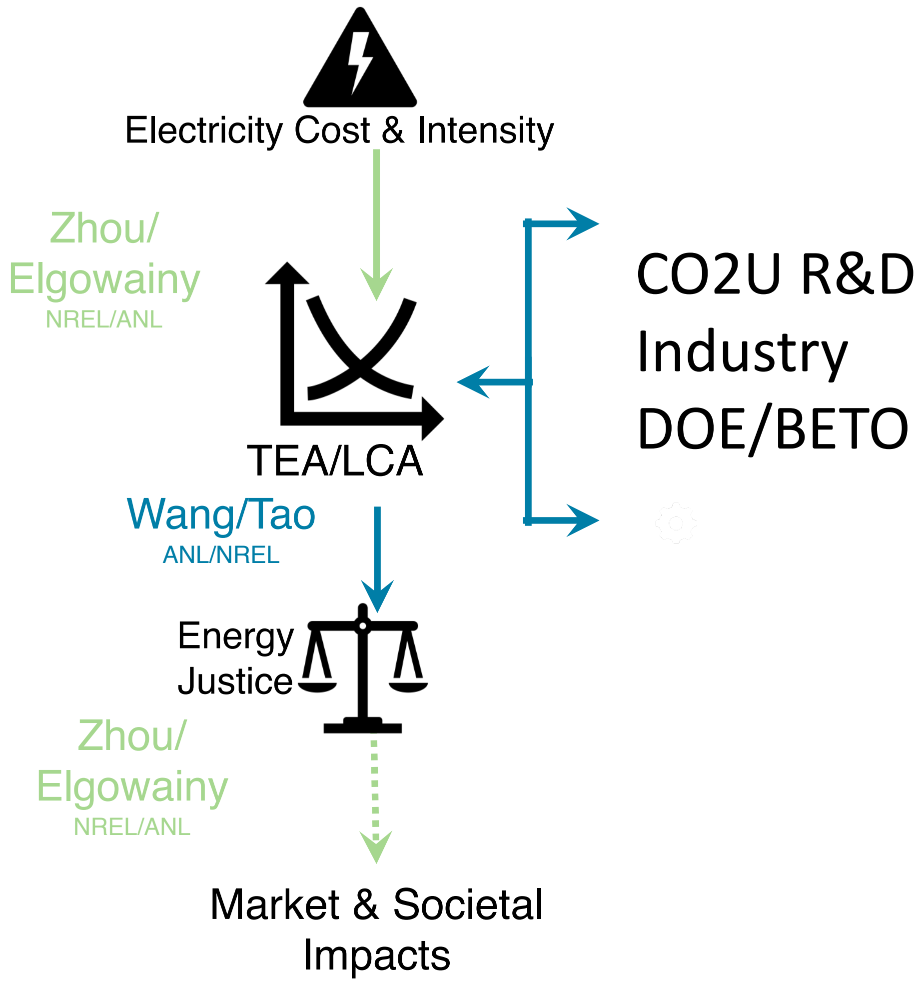
3. Impact: TEA

For DOE and BETO:

- Support R&D decision making with identified key cost drivers and with prioritized technology strategies
- Provide alternative decarbonization options

For Industry:

- Improve carbon conversion efficiency at CO2U plants
- Provide cost effective solutions
- De-risk technologies toward commercialization and deployment



3. Impact: LCA

For the R&D Teams:

- The GREET CO2U LCA module will include general CO2U pathways and specific pathways under consideration by R&D Teams
- LCA identify environmental hotspots for R&D to help improve environmental performance of the CO2U technologies

For the Two Analysis Teams (2.1.0.304, 2.1.0.504/2.1.0.505): The LCA results will identify decarbonization options by

- What CO2 source
- What electricity source/hydrogen source
- What end-use fuels
- In which regions for feasibility, planning, and regionalization of CO2U deployment

3. Impact: LCA

For DOE and BETO:

- Help DOE identify decarbonization opportunities for hard-to-abate transportation sectors
- Help BETO determine R&D direction in CO2U area
- Help the CRU Consortium prioritize R&D areas with identified key drivers for sustainability improvement of R&D progress

For industry stakeholders:

- Help industry quantify emission reduction benefits of CO2U technologies
- Provide insights by identifying environmental hot spots
- Identify key process drivers to help improve sustainability of CO2U technologies

For the CO2U community:

- Credible sustainability results will assist policy making and public support of CO2U technology deployment

3. Impact: Water Analysis

For the R&D Teams:

- Facilitate R&D priorities with water matric and water reuse in the early development stage

For the Two Analysis Teams:

- Support market analysis with the regionality of water resources aiding refinery location down-selection process
- Provide non-conventional water resource options for economic and carbon analyses
- Enhance pathway comparison at the facility level in the regional context with a CO2U water resource analysis tool

For DOE and BETO:

- Support decision-making by providing regional-specific water availability and water stress analysis of CO2U technologies while meeting BETO's goal of decarbonization of hard-to-abate transportation sectors

For Industry:

- Provide the most updated water data and analysis to support risk assessment in CO2U technology deployment

Summary

- **Approach:**
  - This project addresses costs and energy/environmental sustainability metrics of CO2U technologies for the CRU Consortium
- **Progress and Outcomes:**
  - Completed the analysis on four CO2-to-SAF pathways and provided insights to the R&D Teams
  - TEA/LCA results present value proposition of CO2U technologies in decarbonizing hard-to-abate transportation sectors cost-effectively
- **Impact:**
  - Present benefits of CO2U technologies and identify opportunities to further improve technology performance
  - The project is an integral part of the CRU Consortium with interacting with the R&D Teams to consider their technologies and technology progress and by interacting with the two Analysis Teams to benefit from spatial/temporal resource assessment results

Quad Chart Overview

Timeline

- *Project start date: 12/1/2021*
- *Project end date: 9/30/2024*

	FY22 Costed	Total Award
DOE Funding	*$700K ($400K ANL and $300K NREL) (10/01/2021 – 9/30/2022)*	*$2,100K*
Project Cost Share	*None*	

TRL at Project Start: *N/A*

TRL at Project End: *N/A*

Project Goal

Perform techno-economic analysis (TEA), life cycle analysis (LCA), and water analysis of CO2 utilization (CO2U) technologies to address their costs and environmental sustainability implications and to present economic and environmental value proposition of the technologies

End of Project Milestone

Deliver in-depth TEA packages and the GREET CO2U LCA module

Funding Mechanism

BETO Lab Call

Project Partners

- ANL, NREL, ORNL, LBNL, LLNL

Thank You

CO_2 Reduction and Upgrading for e-Fuels Consortium
U.S. DEPARTMENT OF ENERGY