Life Cycle Analysis of Microwave-Assisted Catalytic Conversion of CO_2 To Value –Added Chemicals

Solutions for Today | Options for Tomorrow

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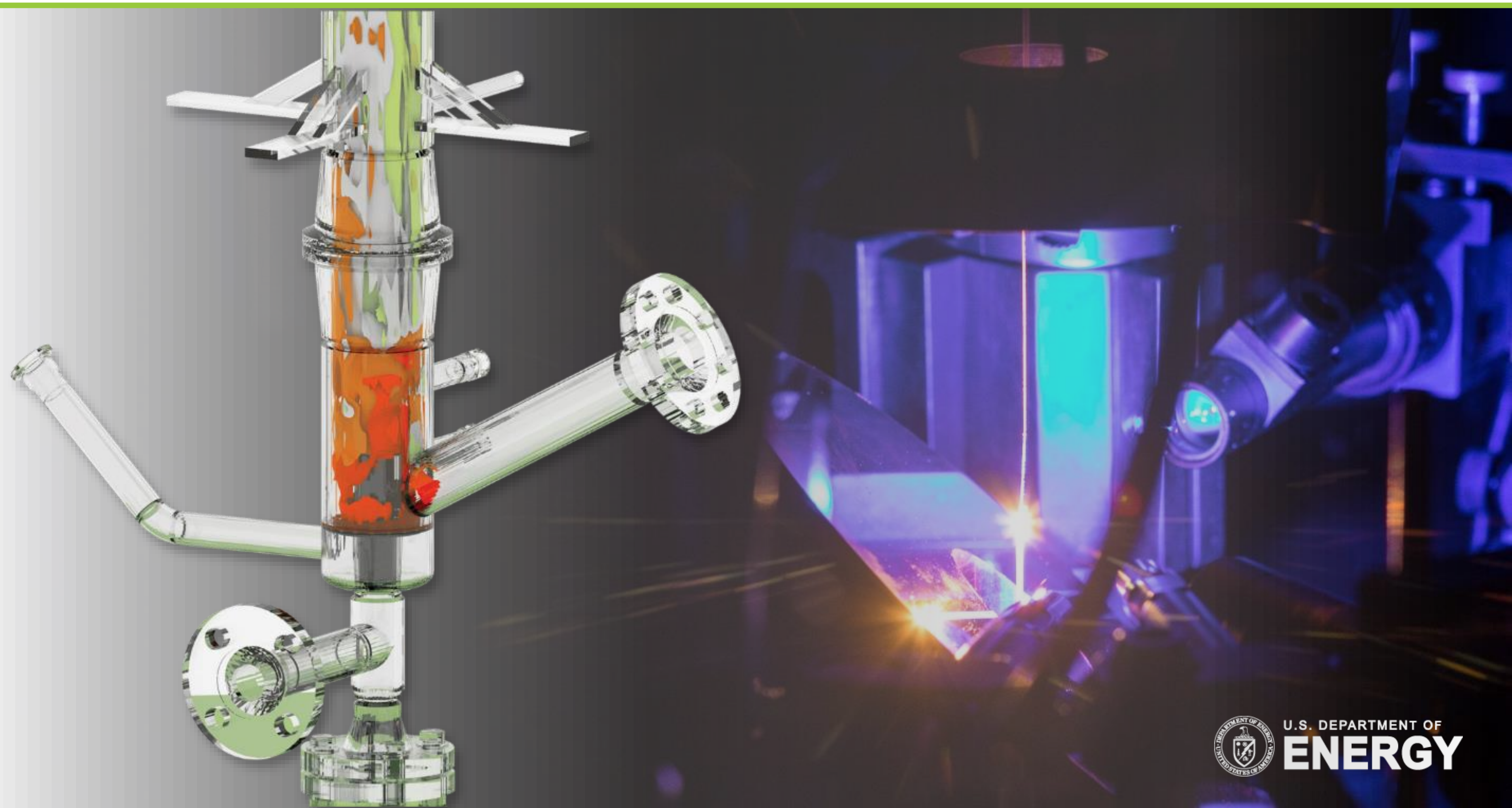


ACLCA 2022 Conference

Nov. 7–11, 2022

U.S. DEPARTMENT OF ENERGY

How Do We Use LCA?

Depends on the Question of Interest….

- Establish National Baselines
- Assess Emerging and Existing Technologies
- A|B Compare Technology and Scenario Tradeoffs
- Plan for the Future and Look Ahead

The NETL CO2U LCA Guidance Toolkit

Overview

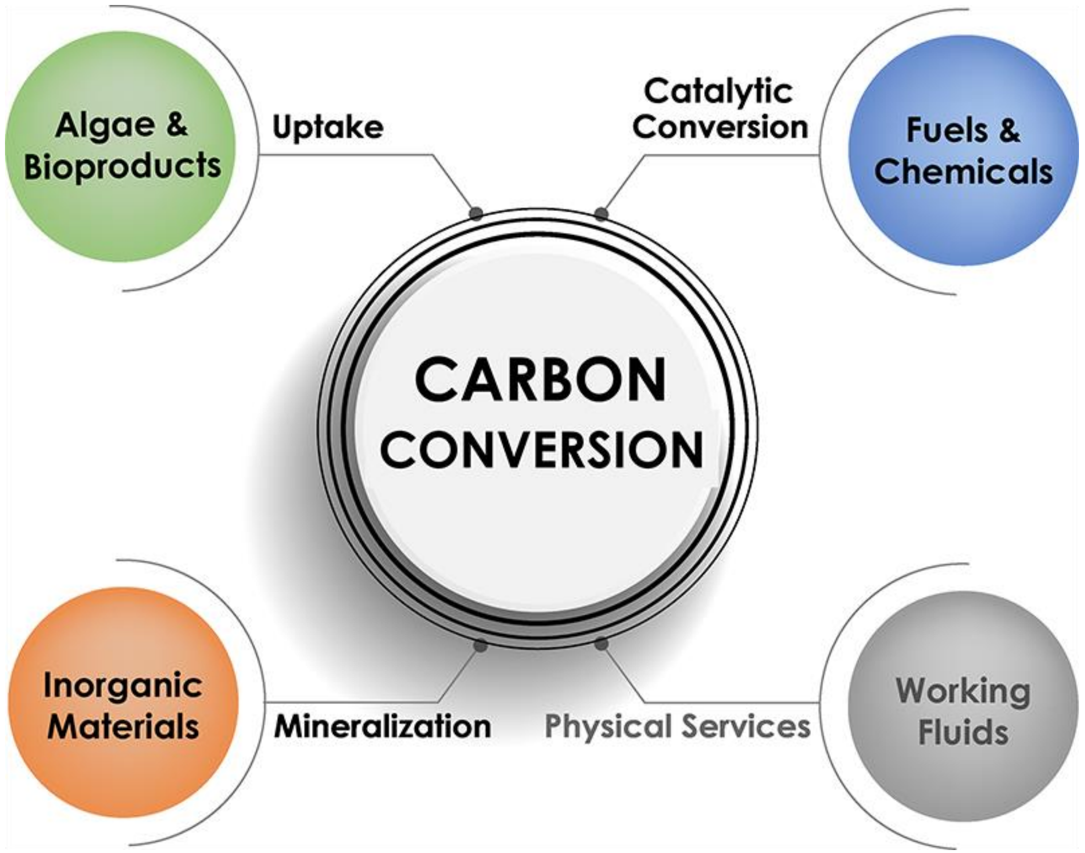
- Supports funding recipients with their LCA requirements.
- Fosters better decision-making for the U.S. DOE Carbon Conversion Program by providing a consistent and transparent analysis and reporting structure.
- Provides LCA guidance, data, and tools to LCA practitioners in the area of CO2U.
- Contributes to the global discussion on CO2U LCA and LCA methods.
- Toolkit site: netl.doe.gov/LCA/CO2U

NETL CO2U LCA GUIDANCE TOOLKIT V 2.0.0

LCA of CO2U Pathways

- **CO_2 conversion.**
  - Use of captured CO_2 from the air or point sources.
  - Conversion of CO_2 into economically valuable products.
  - Wide array of possible products and applications.

- **Catalytic conversion.**
  - CO_2 is transformed into fuels and chemicals.
  - Ranges from simple to complex and from feedstock to finished product.
    - e.g., syngas, ethylene.



Catalytic Conversion

Types

Microwave (MW):

- Two variations analyzed.
  - Dry reforming of methane (DRM).
  - Mixed reforming of methane (MRM).
- Quick response time.
- Rare materials not required for operation.
- Mild operating conditions.
  - i.e., low temperatures and pressures.
- Better energy performance.
  - i.e., high energy efficiency and power density.

Other types:

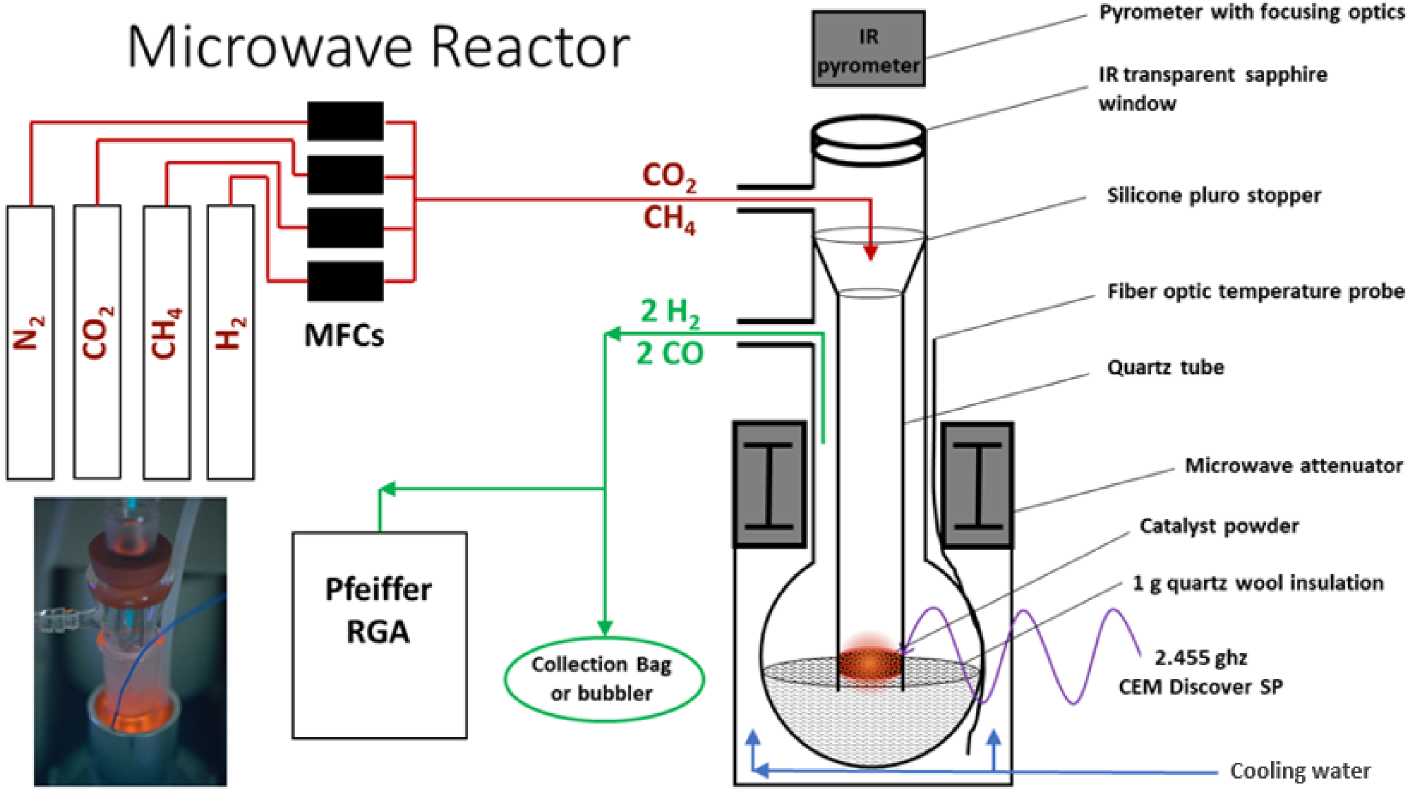
- Thermochemical.
- Electrochemical.
- Photochemical.
- Microbial.

Catalytic Conversion

Microwave Plasma

- **Inflow gas is heated in a high-temperature reactor until plasma is generated.**
  - Strontium-doped lanthanum cobaltite (LSC) catalyst.
    - Chemical selectivity and microwave absorptivity.

- **CO_2 and CH_4 inflow gas are reformed into syngas.**
  - Syngas is a key chemical building block.



Objectives

Preliminary LCA performed to understand:

- What are the life cycle environmental impacts associated with catalytic CO_2 conversion to other compounds?
- How does the life cycle environmental impacts of products made via catalytic CO_2 conversion compare to those made by more conventional means?
- Does catalytic CO_2 conversion as a utilization pathway have the potential to contribute to significant CO_2 reduction?
  - What processes contribute the most to environmental impacts?
  - How do we best remedy those hotspots?
  - How does performance change based on the future grid mix?

Background

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- **MeOH is chosen as a key product.**
  - Value in direct use and/or conversion into other chemicals.
  - Autothermal Reformer (ATR) MeOH is the conventional pathway for comparison.
  - Total global annual production.
    - MeOH: 98 million tons.[2]

[2]International Renewable Energy Agency (2021). *Innovation Outlook : Renewable Methanol*

- **For all pathways.**
  - Products identical in output ratios and conditions.
    - e.g., temperature, pressure.
    - MW-DRM syngas needs to be supplemented by H_2.
  - Multiple production scales considered.
  - Detailed contribution analysis.
    - Consider system breakdown of energy and material feeds and emissions.

Technical Specifications

- **No excess electricity generated for export to grid.**
  - Some internal heat recovery and use.
- **90% capture rate of CO_2 and unreacted hydrocarbons from production.**
- **ATR uses residual CO_2 in syngas to convert in MeOH synthesis.**
  - Emits a light gas mixture containing mostly N_2 and some H_2O.
- **Utilized NETL hydrogen baseline results for steam methane reforming (SMR), ATR, and polymer electrolyte membrane (PEM).**[1,2]

[1]INETL (2022). *Comparison of Commercial, State-of-the-Art, Fossil-Based Hydrogen Production Technologies*
[2]NETL (2022). *Life Cycle Greenhouse Gas Emissions and Water Consumption From Existing and Emerging Hydrogen Pathways*

Background

LCA Assumptions

- **Main CO_2 source is an SCPC plant.**
  - Electricity is a co-product.
  - Natural dome and ammonia plants are also explored.
- **Limited sensitivity and uncertainty ranges.**
  - Data from preliminary empirical experiments and TEA model.
    - Material and energy needs.
    - Production scaling effects.
- **For MW-DRM, additional H_2 is supplied from PEM electrolysis.**
  - Also, MW-MRM has an option of heating via an electric boiler.

Scope and System Boundary

Cradle-to-gate

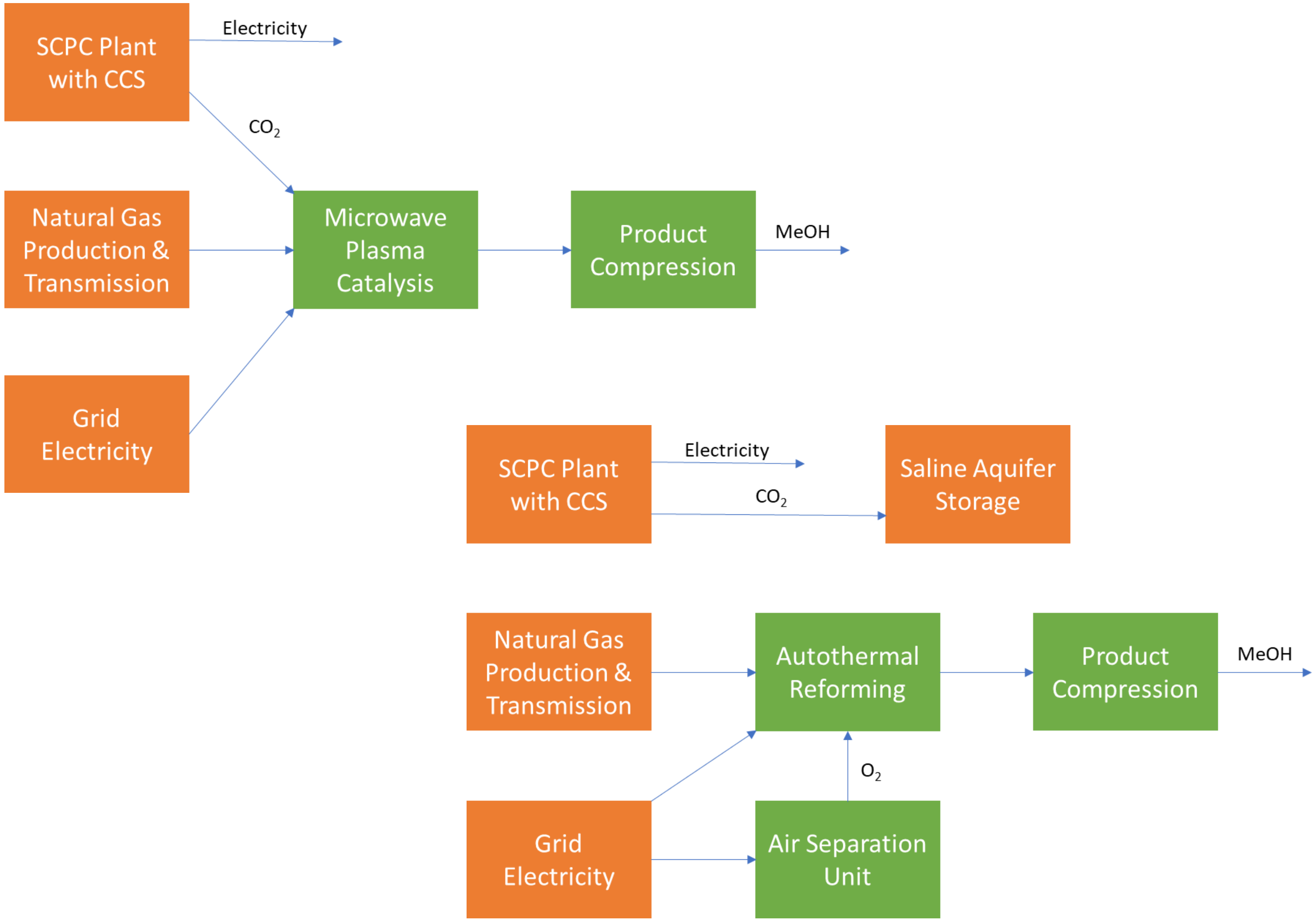
- Ends at production gate.

Functional units

- 1 kg of MeOH.

TEA model generates the system I/O

- NETL MW system empirical data.
  - Reaction temperature.
  - Energy efficiency.
  - Conversion efficiency.
  - Gas flow rate.
  - Gas compositions.



Methods

Data and Tools

Inventory

- Electricity.
  - Use is tracked for each system component.
  - 2020 U.S. average consumption mix.
  - 2020 marginal capacity grid mix.
  - 100% wind.
- Natural gas.
  - Used as both feedstock and thermal energy source.
  - 2018 U.S. average consumption mix.
- CO_2 source.
- Water.

Tools

- LCA.
  - openLCA.
  - Impact method – TRACI 2.1
- Uncertainty and sensitivity analysis.
- Based on TEA work using Aspen Model.

Methods

Inventory

Scenario	Electricity (kWh)	Natural Gas (kg)		CO_2 Feedstock (kg)	O_2 Feedstock (kg)	Water (kg)
per kg of product		feedstock	combusted			
MW assisted MeOH						
DRM	6.23	0.012	-	0.032	-	0.046
MRM	3.93	0.020	1.23E-3	0.015	-	0.017
MRM-electrified	4.17	0.019	-	0.015	-	0.017
ATR methanol	0.23	0.57	-	-	0.67	0.54
Supporting Processes						
SMR H_2	0.63	3.54	0.22	-	-	16.4
PEM H_2	55	-	-	-	-	8.94

*Based on NETL LCA and TEA data

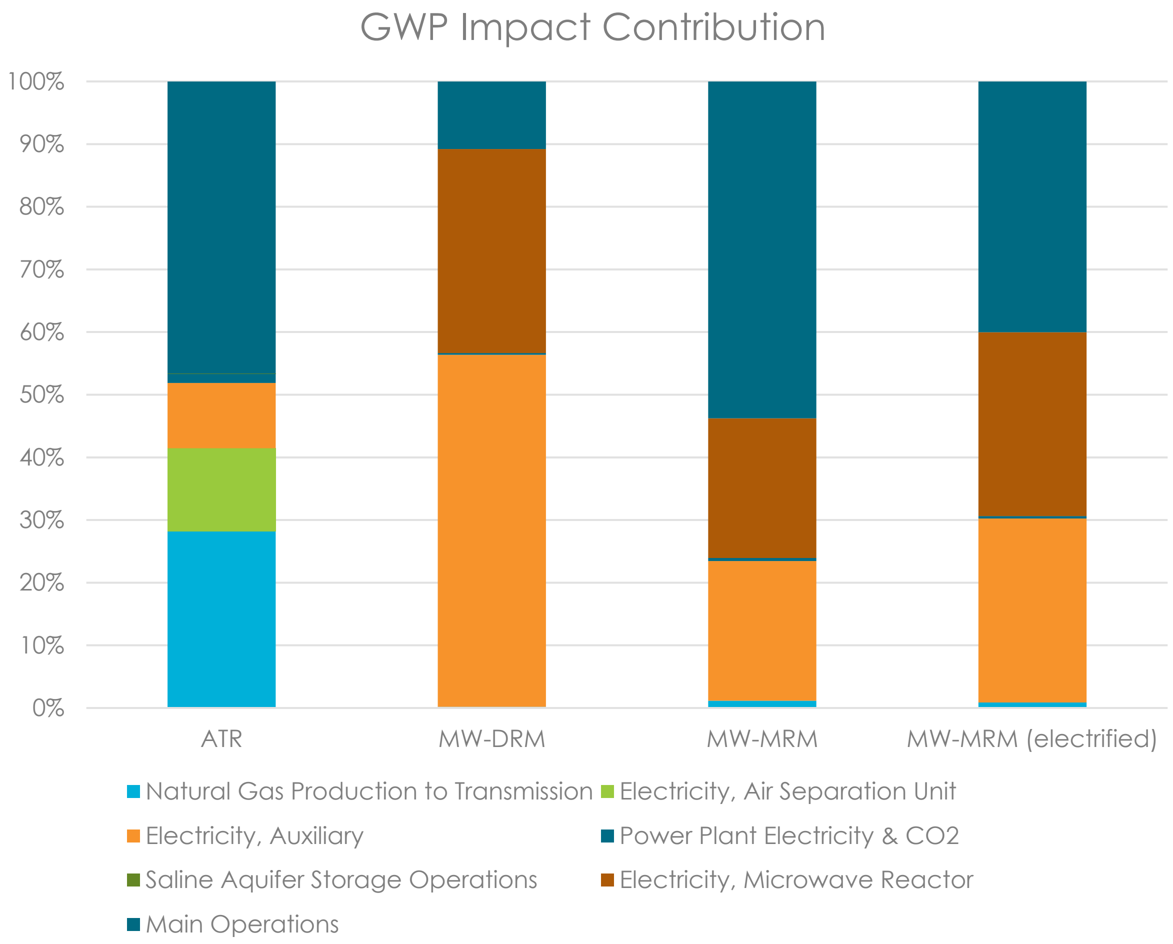
Contribution Analysis

Conventional

- Besides main operations, significant global warming potential (GWP) share is upstream natural gas.
  - ATR MeOH: ~28%.

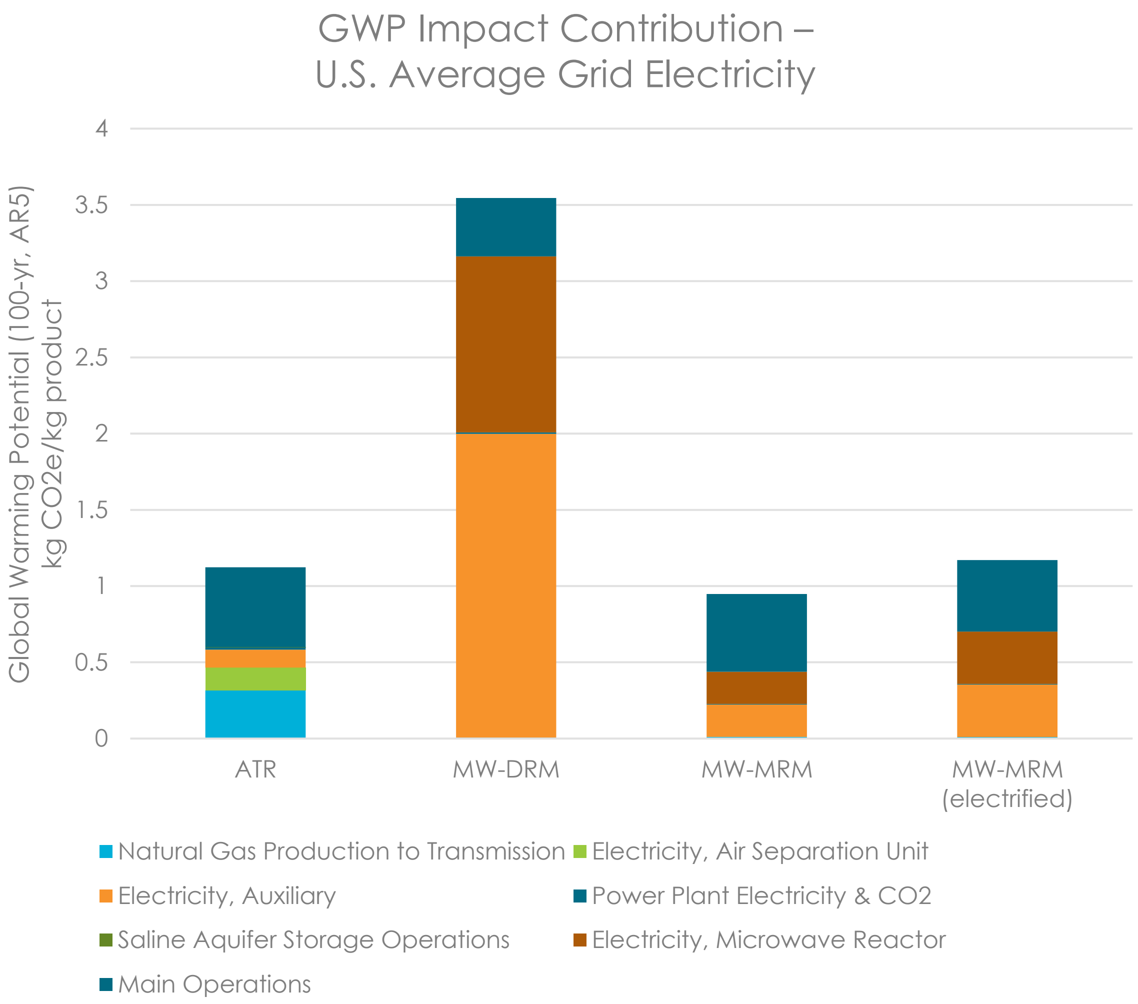
Microwave

- Significant GWP share is MW reactor and auxiliary loads.
  - MW DRM: 33%, 56%.
  - MW MRM: 22 – 29% each.



Results

- **MW has greater resource requirement.**
  - Electricity.
    - MRM: +180 to 290%
    - DRM: +1700%
- **MW-DRM has significant GWP decrease with cleaner grid mix.**
  - 100% wind.
  - Marginal grid mix.
    - NG: 51%
    - Solar: 21%
    - Wind: 27%



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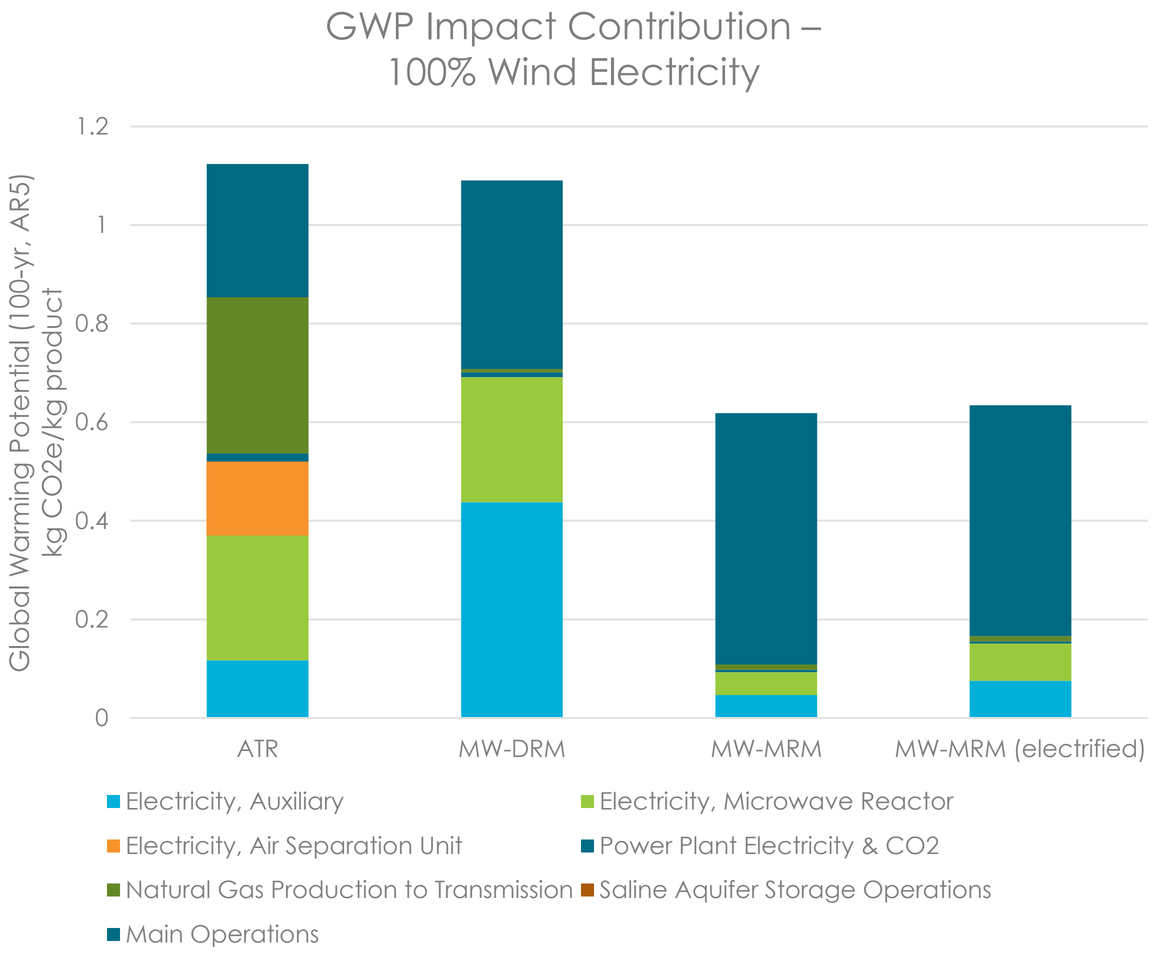


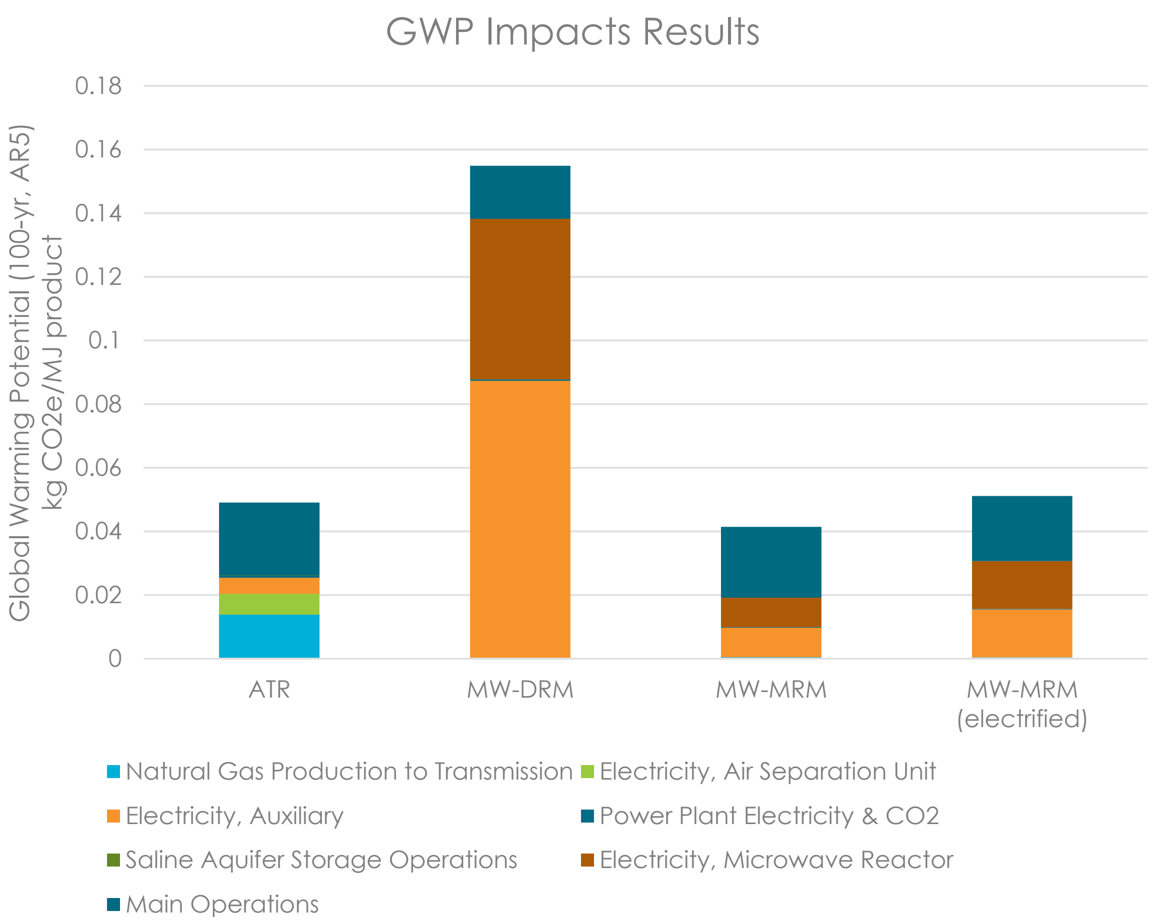
Results

Relative change in impacts

- Energy basis rather than mass basis.

Energy density

- MeOH: 23 MJ/kg.



Discussion and Future Work

- **MW-DRM is still at early TRL (3–4)**
  - Energy demands are 100 –1000 times greater at commercial scale.
  - Absence of energy-conserving effects is typical of industrial systems.

- **Literature sources did not focus on environmental performance.**
  - Technical improvements are mainly in energy and conversion efficiency.
  - One source studied nitric acid as the target product.

- **Inclusion of more pathways and construction stages for comparison.**
  - Conventional: coal-to-methanol, coke-to-methanol.
  - Novel: thermochemical, electrochemical, photochemical, microbial.

Conclusions and Future Work

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- **Converting captured CO_2 into value-added products such as methanol is a growing field of interest.**
  - Can help accelerate the widespread deployment of carbon capture systems.
  - More economically attractive than just saline aquifer CO_2 storage.
- **Potential GWP advantage of MW-DRM and MW-MRM in MeOH products.**
  - Conventional systems w/o CCS and MW systems with 100% renewable electricity.
  - Improvements need to focus on the energy and resource efficiency of the MW reactor.

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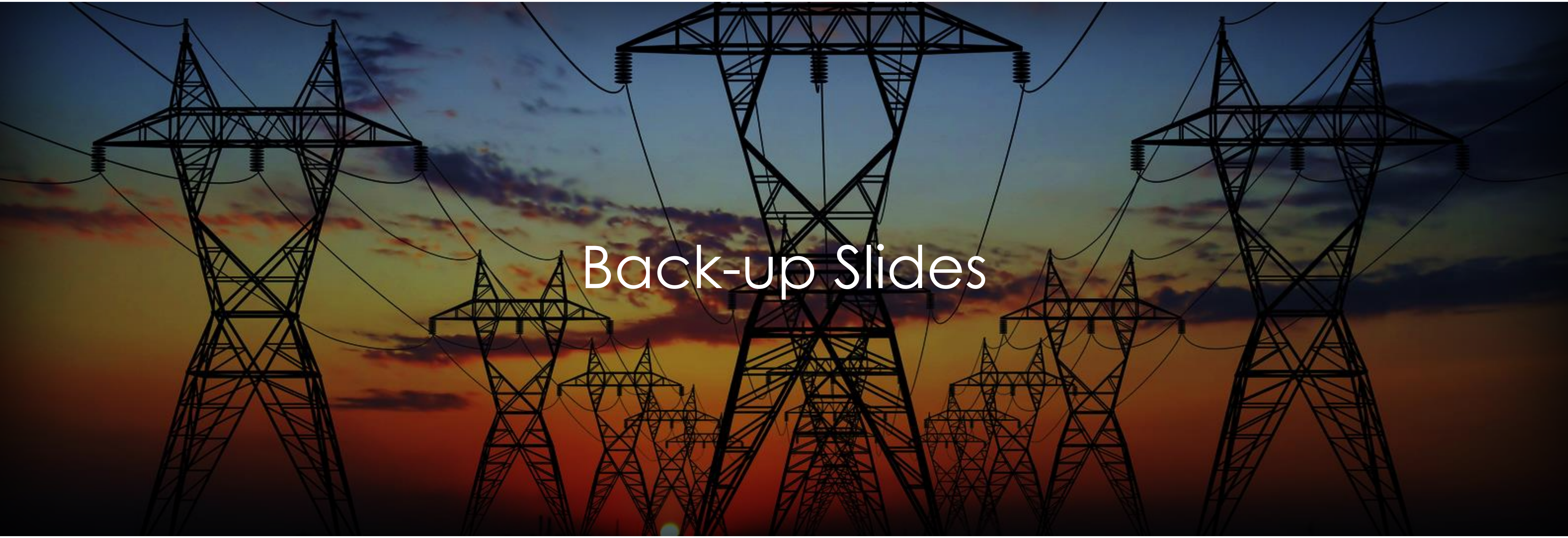
Questions?

Back-up Slides



Energy Life Cycle Analysis (LCA)

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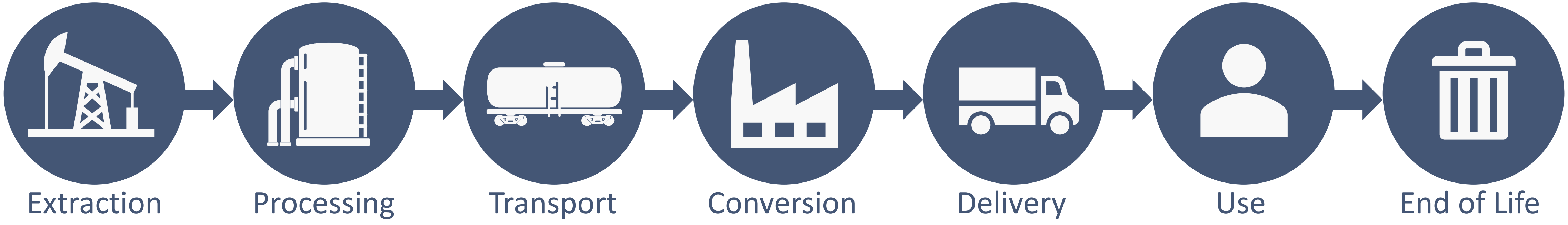
Cradle-to-Grave Environmental Footprint of Energy Systems



What is Life Cycle Assessment/Analysis (LCA)?

LCA is a technique that helps people make better decisions to improve and protect the environment by accounting for the potential impacts from raw material acquisition through production, use, end-of-life treatment, recycling, and final disposal (i.e., cradle-to-grave).

NETL CO2U Guidance Key Points

Comparative LCA

Goal is to compare the CO2U system to the long-run marginal competitor in the market (comparison system).

Guidance for comparison processes and system

Data quality and representativeness: Expectations based on TRL.

Multiproduct functional unit with system expansion

Improve comparability and results interpretation.

Three modeling options

1. openLCA with provided data.
2. Excel-based documentation sheet.
3. Other commercial LCA modeling software.

Default scenarios for CO_2 sources

Coal-fired power generation: flue gas, captured CO_2 greenfield, and retrofit.

Interpretation requirements

Specific data/figures to provide consistency to study comparisons.

Results and Discussion

Contribution Analysis

	ATR	SMR	MW	
	Methanol	Hydrogen	Methanol	Hydrogen
Natural Gas Production to Transmission	35%	38%	9%	5%
Combustion of Natural Gas		5%		
SCPC electricity and CO_2	36%	38%	12%	6%
CO_2 Storage Operations		2%		
Electricity				
ASU	8%			
Product Compression	5%	5%	12%	5%
Auxiliary	1%	4%	0.4%	8%
CCS		0.3%		<0.1%
MW Reactor			27%	31%
MDEA				<0.1%
WGS				<0.1%