February 19, 2025

Introducing Hydrogen in R&D GREET®

2:00-3:00 p.m. CT

Instructors

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Table of contents

Hydrogen Sector

Today, more than 10 million metric tons of hydrogen are produced in the U.S. per year

Most of the hydrogen is produced from steam methane reforming (SMR) of fossil natural gas (NG)

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What Does R&D GREET Encompass?

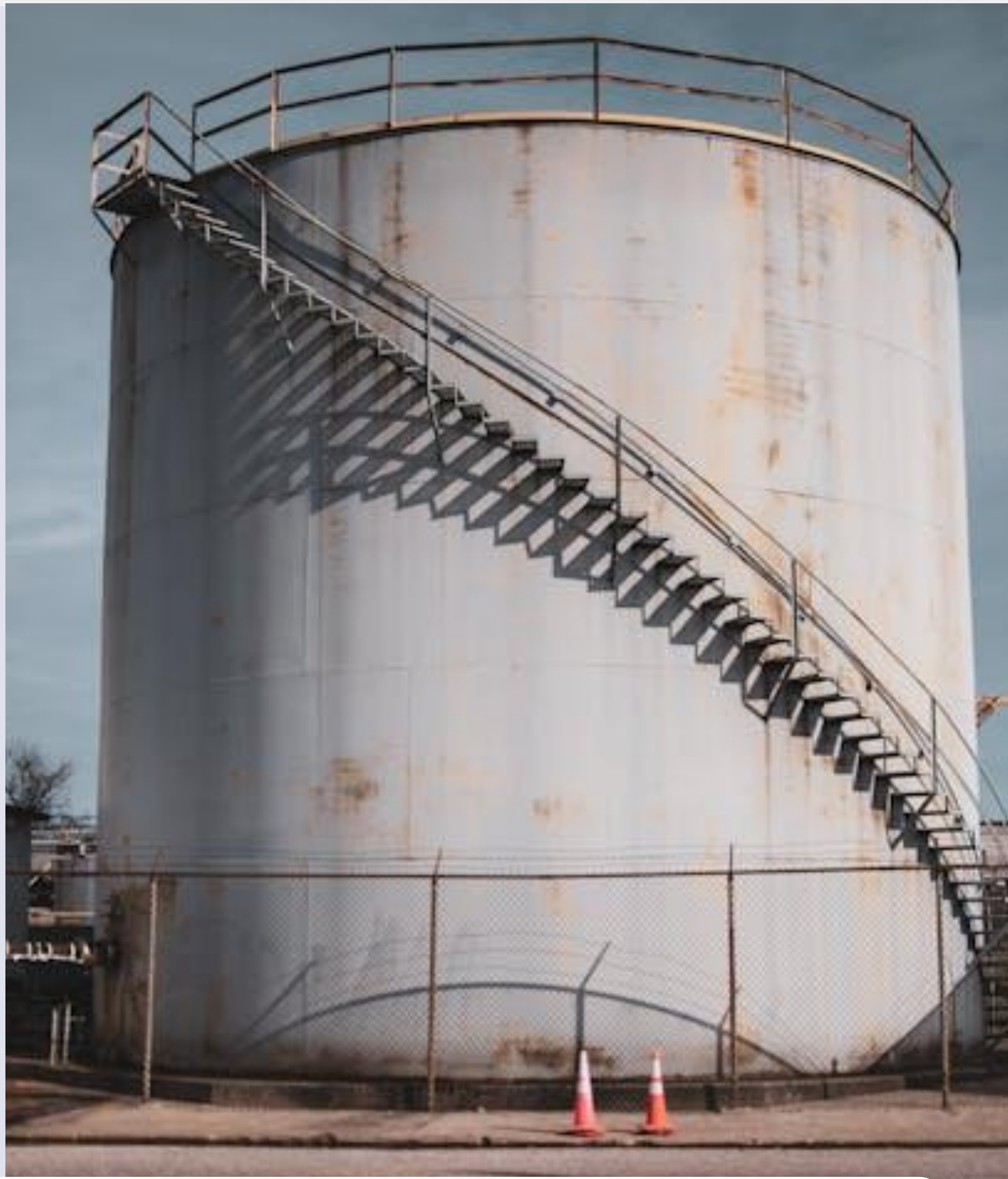
R&D GREET covers many groups of energy systems

- Petroleum
- Electric Systems
- Natural Gas
- Renewable Energy/Fuels
- Hydrogen
- Electro-fuels
- And More

R&D GREET in the hydrogen economy

Gaseous hydrogen
Liquid hydrogen
With carbon capture and sequestration (CCS), if applicable

Natural Gas
Biomass
Coal
Petroleum Coke
Coke Oven Gas
Electrolysis with Electricity
Nuclear Energy
and More



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Available hydrogen production pathways in R&D GREET

Electrolysis

- Low-temperature electrolysis: proton exchange membrane (PEM)
  - U.S. Mix, Regional Mix, Wind, Solar PV, Hydroelectric, and Nuclear LWR
- High-temperature electrolysis: solid oxide electrolyzer cell (SOEC)
  - Nuclear LWR

Natural Gas Reforming

- Steam methane reforming (SMR)
  - Natural Gas and Renewable Natural Gas
  - CCS available
- Autothermal reforming
  - Natural Gas and Renewable Natural Gas
  - CCS available

Gasification

- Biomass
  - Poplar, Willow, Switchgrass, Corn Stover, Forest Residue, and Miscanthus
- Coal
  - CCS available
- Pet coke
  - CCS available
- Coke oven gas

Co-product

- Chlor-alkali
- Steam cracker

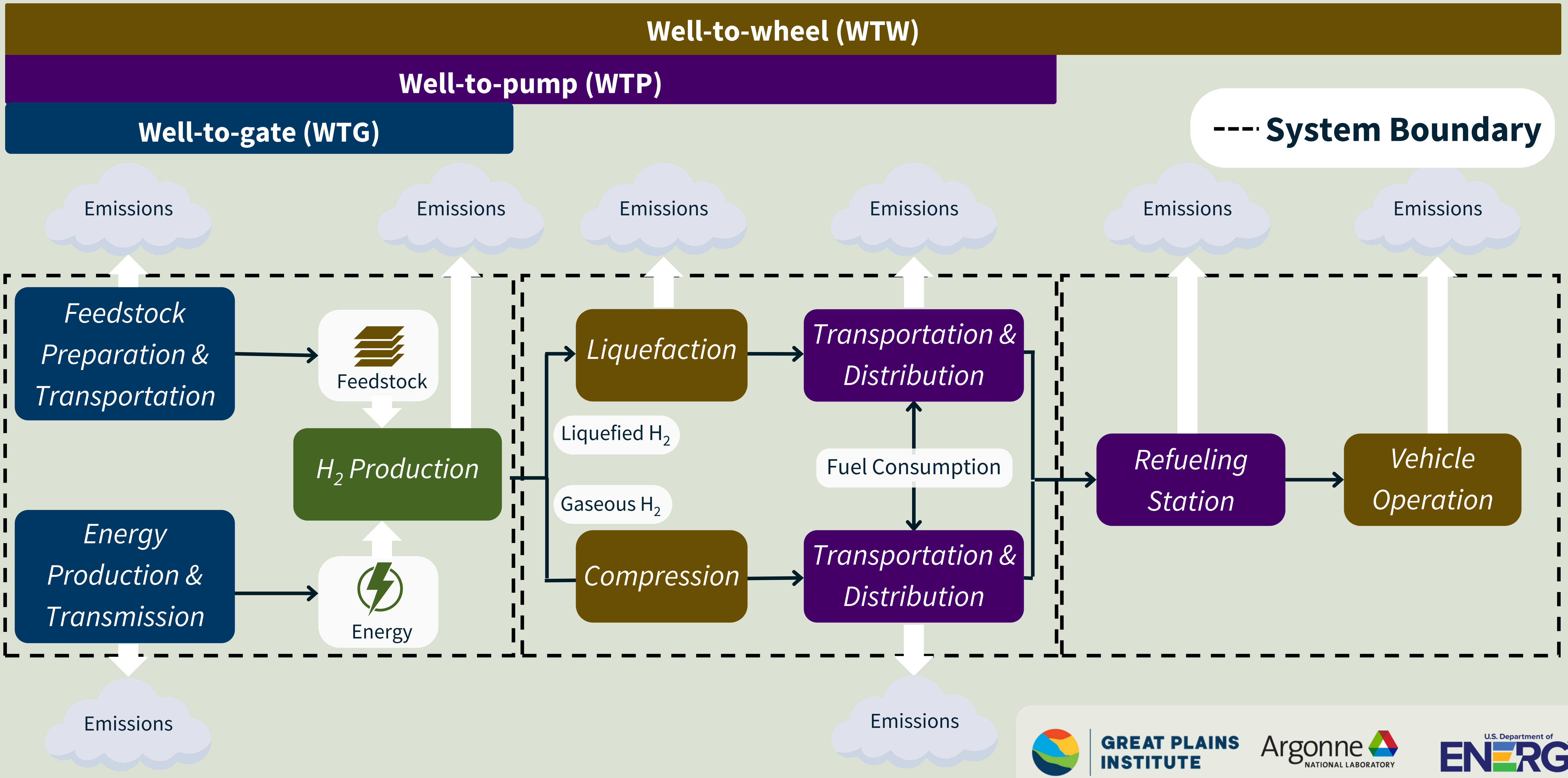
Biological

- Fermentation

and More

LCA of Hydrogen in R&D GREET

System boundaries of hydrogen production in R&D GREET



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System boundary of hydrogen production in R&D GREET

Hydrogen is used in many pathways in R&D GREET as both a fuel and a feedstock

Carbon Intensity

The carbon intensity of H_2 at each stage (WTG, WTP, and WTW) can be easily determined

Hydrogen Phase

R&D GREET includes modeling for both liquid and gaseous hydrogen

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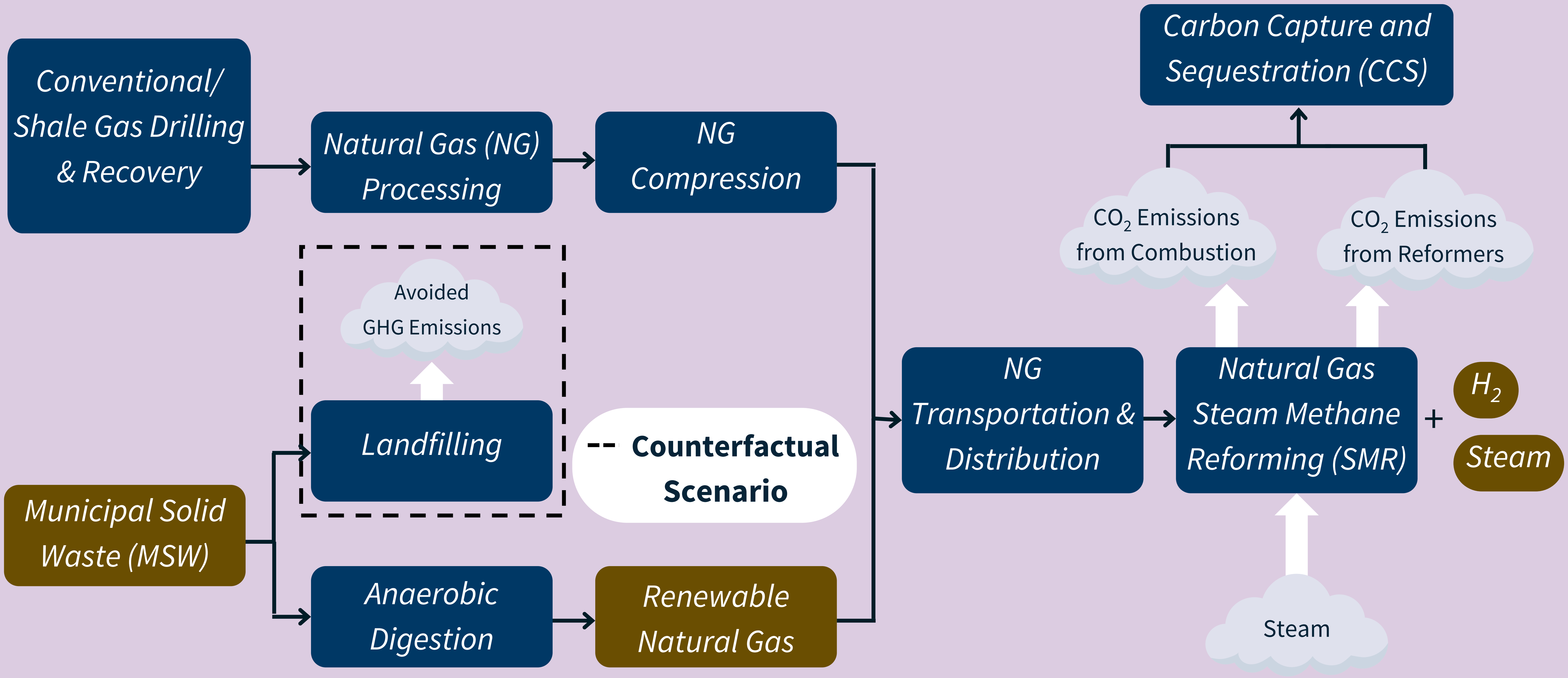
WTG life cycle of hydrogen: *NG & RNG reforming w/ and w/o CCS*



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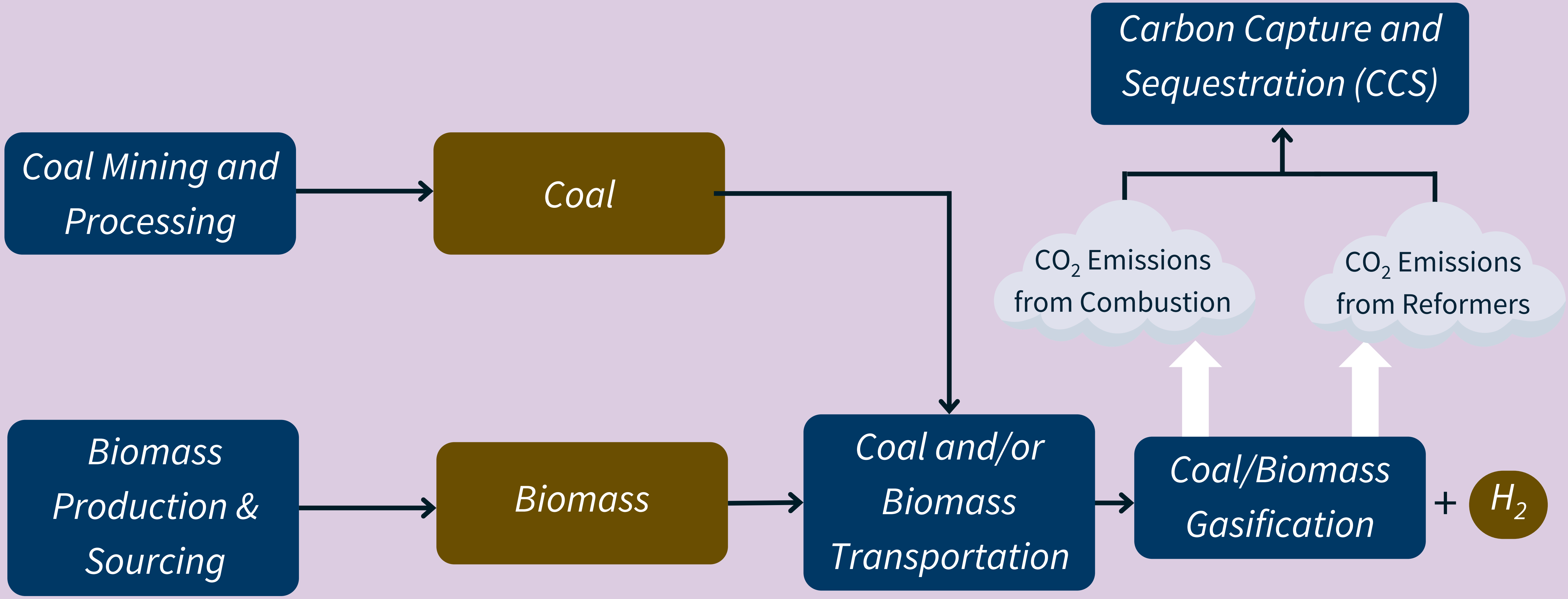
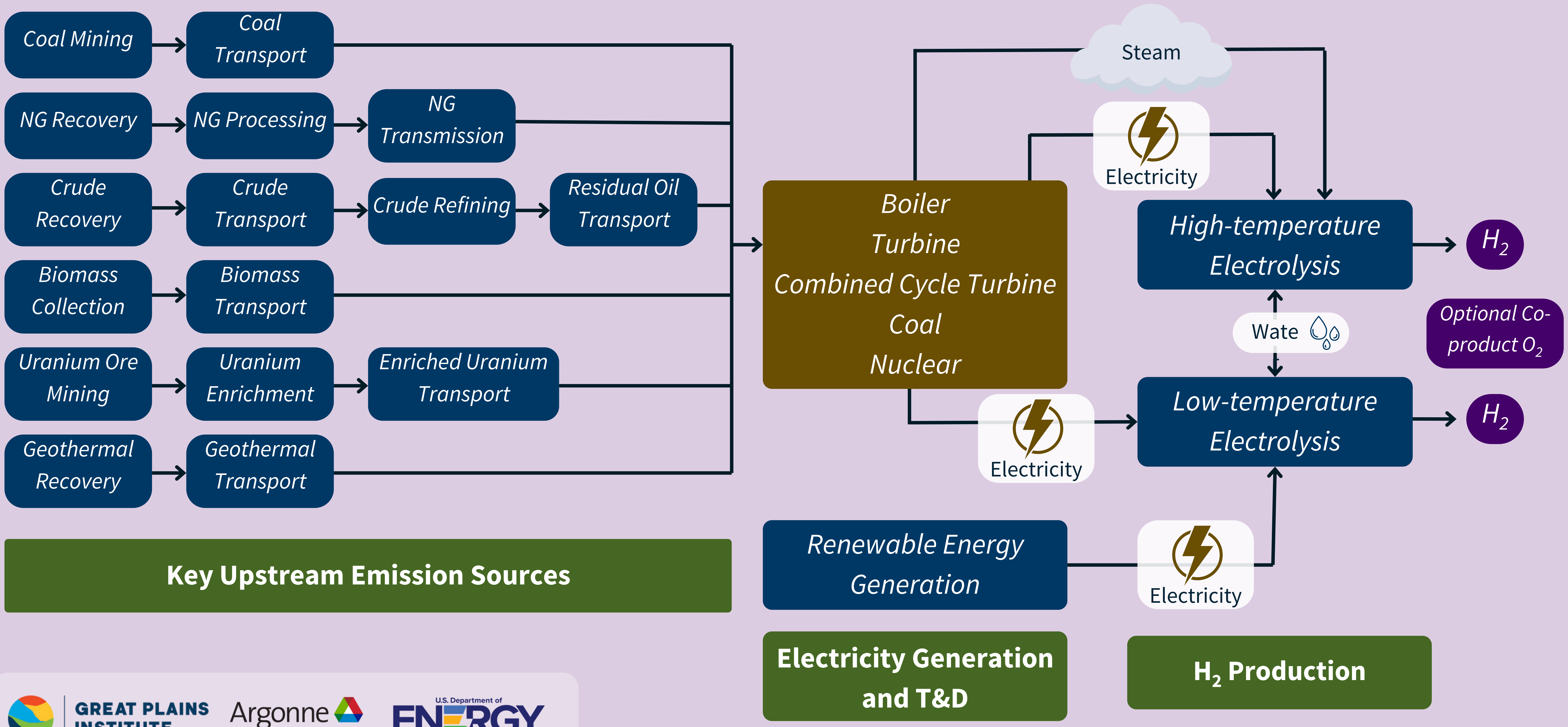
WTG life cycle of hydrogen: *gasification w/ and w/o CCS*



Types of Biomass

Willow
Poplar
Switchgrass
Corn Stover
Forest Residue
Miscanthus

WTG life cycle of hydrogen: *water electrolysis*



Natural Gas Reforming, Gasification, and Electrolysis

Fuel Phase

Natural gas reforming

Step 1

Apply high-temperature steam to natural gas (which contains methane) in the presence of a catalyst

Step 2

The carbon monoxide and the steam react over a catalyst in a water-gas shift reactor to produce more hydrogen

Methane CH_4 + **Water** H_2O + **Heat** → **Hydrogen** $3H_2$ + **Carbon Monoxide** CO

Carbon Monoxide CO + **Water** H_2O → **Hydrogen** H_2 + **Carbon Dioxide** CO_2 + **Heat**

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- Hydrogen Production: Natural Gas Reforming | Department of Energy

Gasification

Gasification includes a variety of reactions including the following

Pyrolysis
High temperatures break down chemical bonds and produce a char

Combustion
Products of pyrolysis react with oxygen to form CO_2 and CO

Gasification
Remaining char reacts with CO_2 and steam to produce CO and H_2

Water-gas-shift and Methanation
Additional reversible gas phase reactions

Coal →
Oxygen →
Steam →

Gasification with Oxygen

$$C + 1/2O_2 \longleftrightarrow CO$$

Combustion with Oxygen

$$C + O_2 \longleftrightarrow CO_2$$

Gasification with Carbon Dioxide

$$C + CO_2 \longleftrightarrow 2CO$$

Gasification with Steam

$$C + H_2O \longleftrightarrow CO + H_2$$

Gasification with Hydrogen

$$C + 2H_2 \longleftrightarrow CH_4$$

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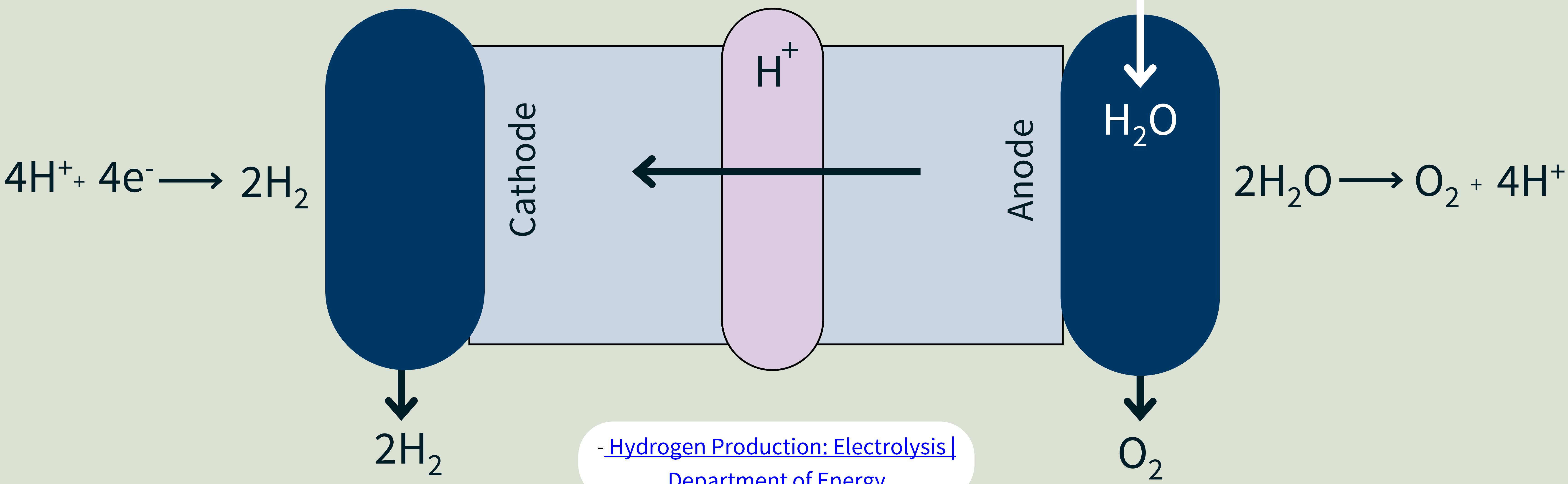
- 5.1.2. Reactions & Transformations | Department of Energy

Electrolysis

Electrolysis: splitting water in an electrolyzer

Electrolyzers have a cathode and an anode separated by an electrolyte



- Hydrogen Production: Electrolysis | Department of Energy

PEM electrolyzers

PEM: polymer electrolyte membrane

Electrolyte

A solid specialty plastic material

Anode

Water reacts to form oxygen and protons (H^+)

Movement

H^+ move across the PEM to the cathode while electrons move along the external circuit

Cathode

H^+ combine with electrons to form hydrogen gas

Solid oxide electrolyzers

Electrolyte
A solid ceramic material

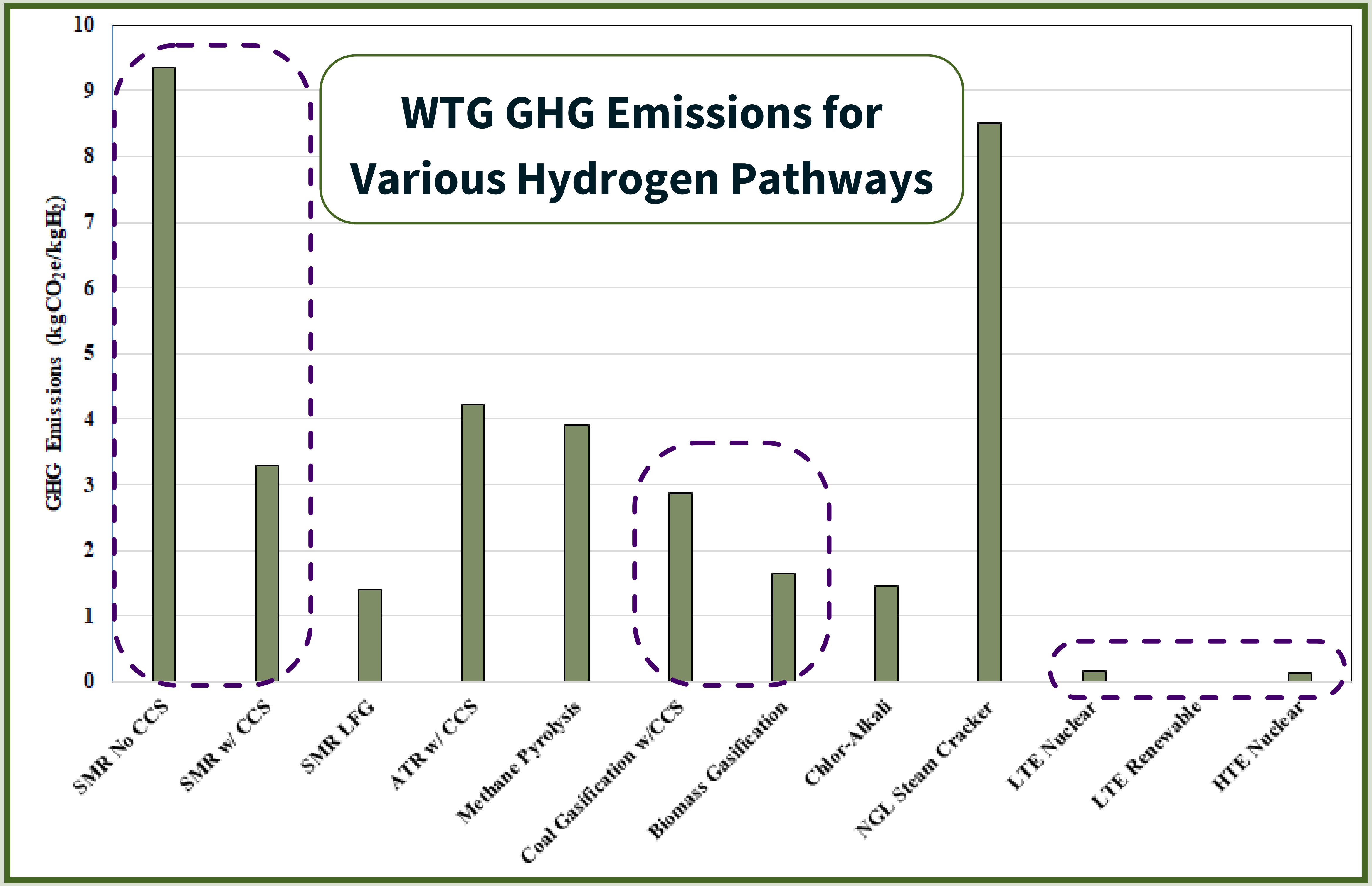
Cathode
Steam combines with the electrons from the external circuit and creates hydrogen gas and negatively charged oxygen ions

Movement
Oxygen ions pass through the electrolyte

Anode
Oxygen ions react to form oxygen gas

Well-to-Gate (WTG) GHG Emissions

Well-to-gate (WTG) GHG emissions in R&D GREET



SMR No CCS assumes a credit for co-produced steam

SMR w/ CCS does not assume a credit for co-produced steam

Biomass = Willow

Renewable = Solar or Wind power

Note: this figure was generated for illustrative purposes. As R&D GREET is updated, the values could change

[- R&D GREET 2023]

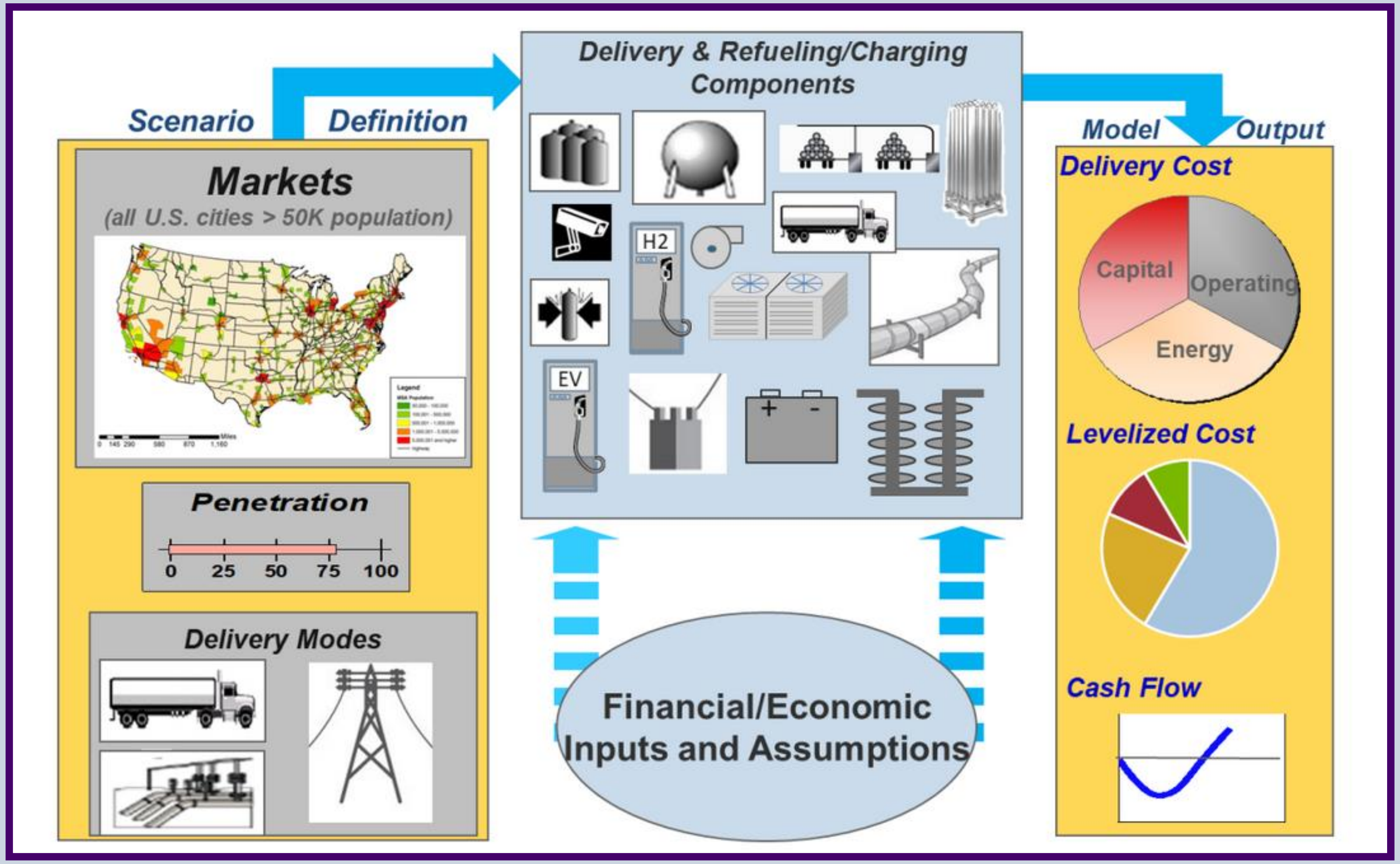
Hydrogen Packaging, T&D, and Fueling

Transportation and Distribution

Hydrogen packaging in R&D GREET

R&D GREET accounts for energy and emissions associated with hydrogen packaging

R&D GREET is consistent with Argonne's hydrogen delivery method (HDSAM)



[- Hydrogen Delivery Scenario Analysis Model (HDSAM) | Argonne National Laboratory]

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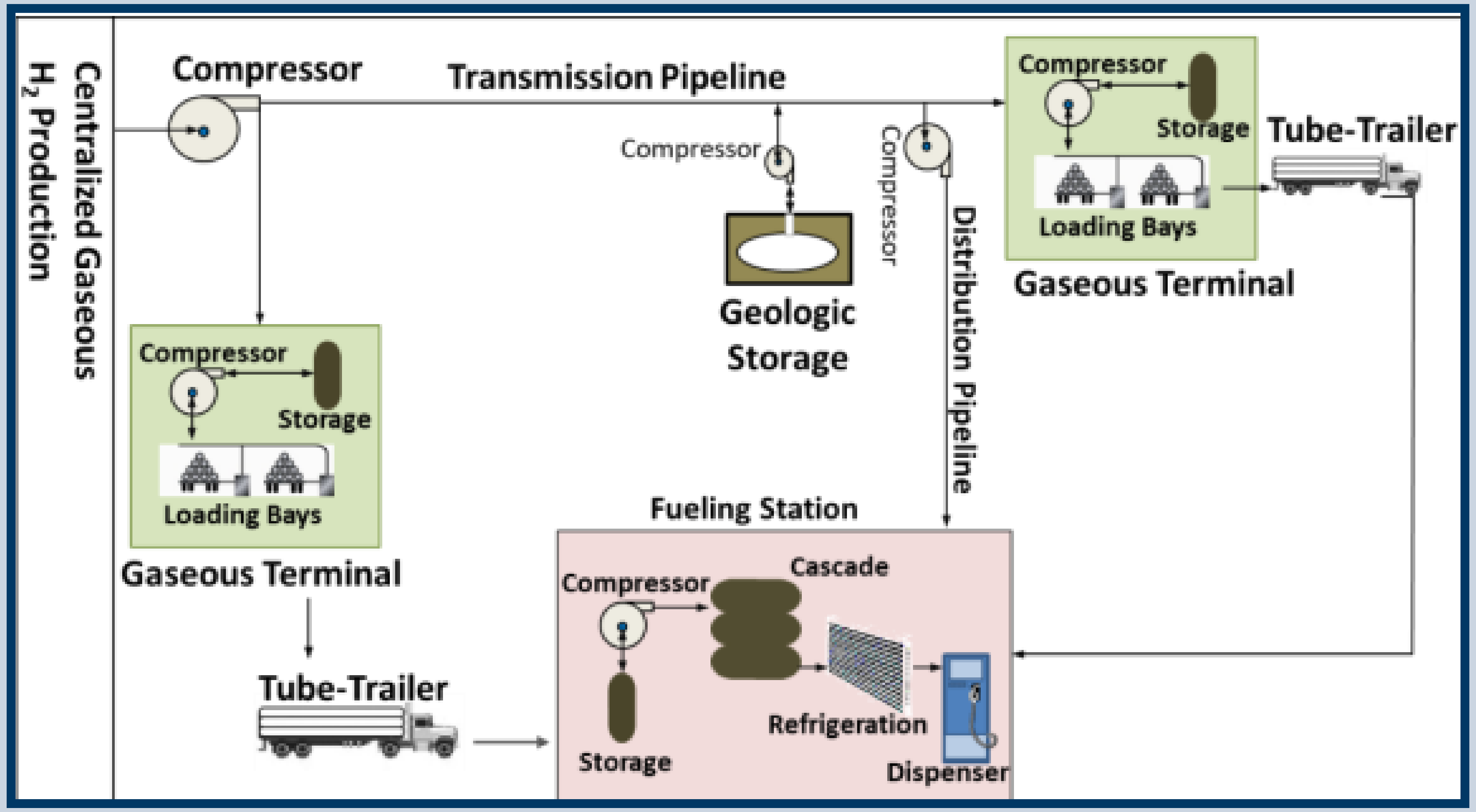
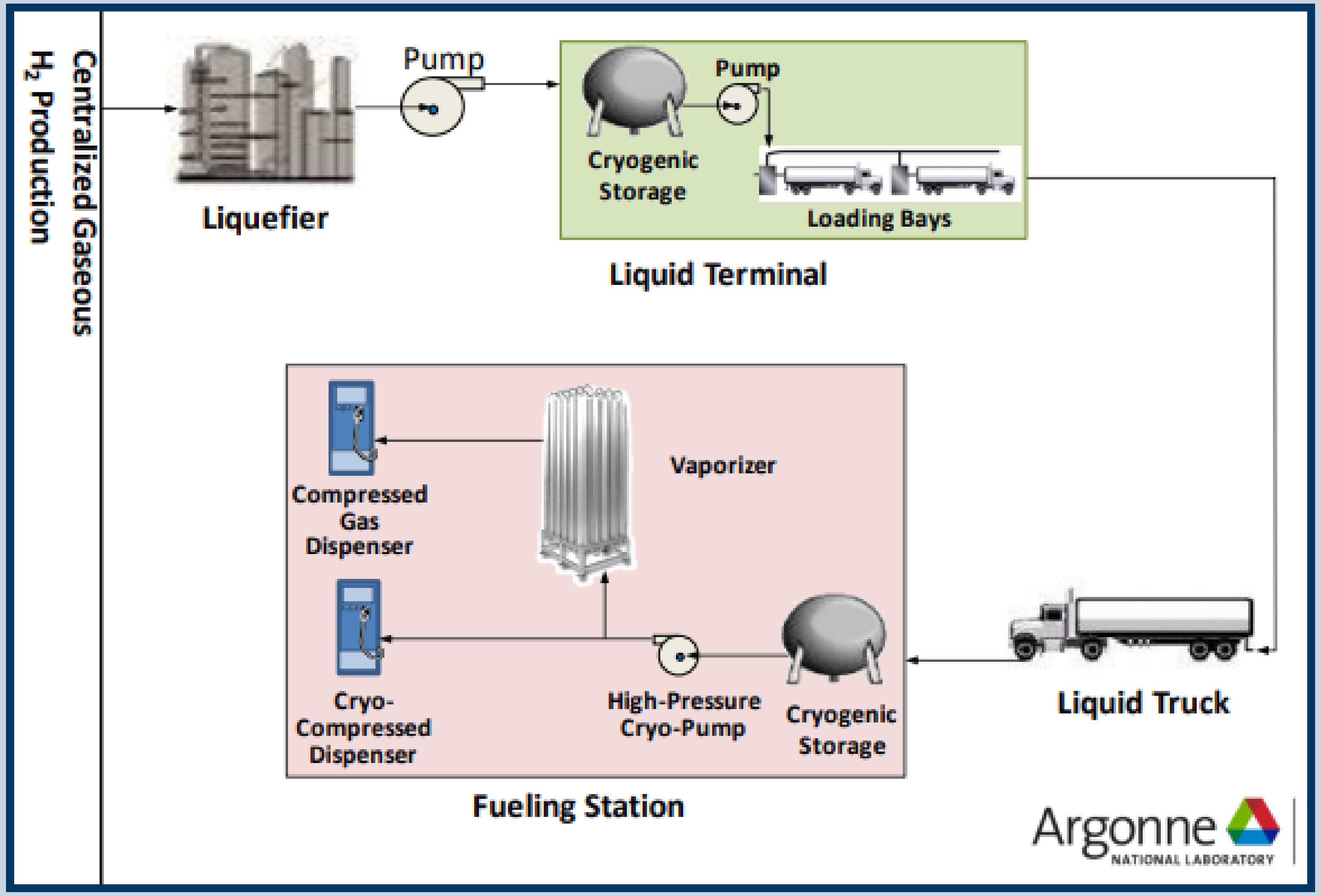
Hydrogen T&D and fueling in R&D GREET

R&D GREET includes gaseous and liquid delivery pathways



Gaseous Hydrogen Pathway

R&D GREET default: tube trailer



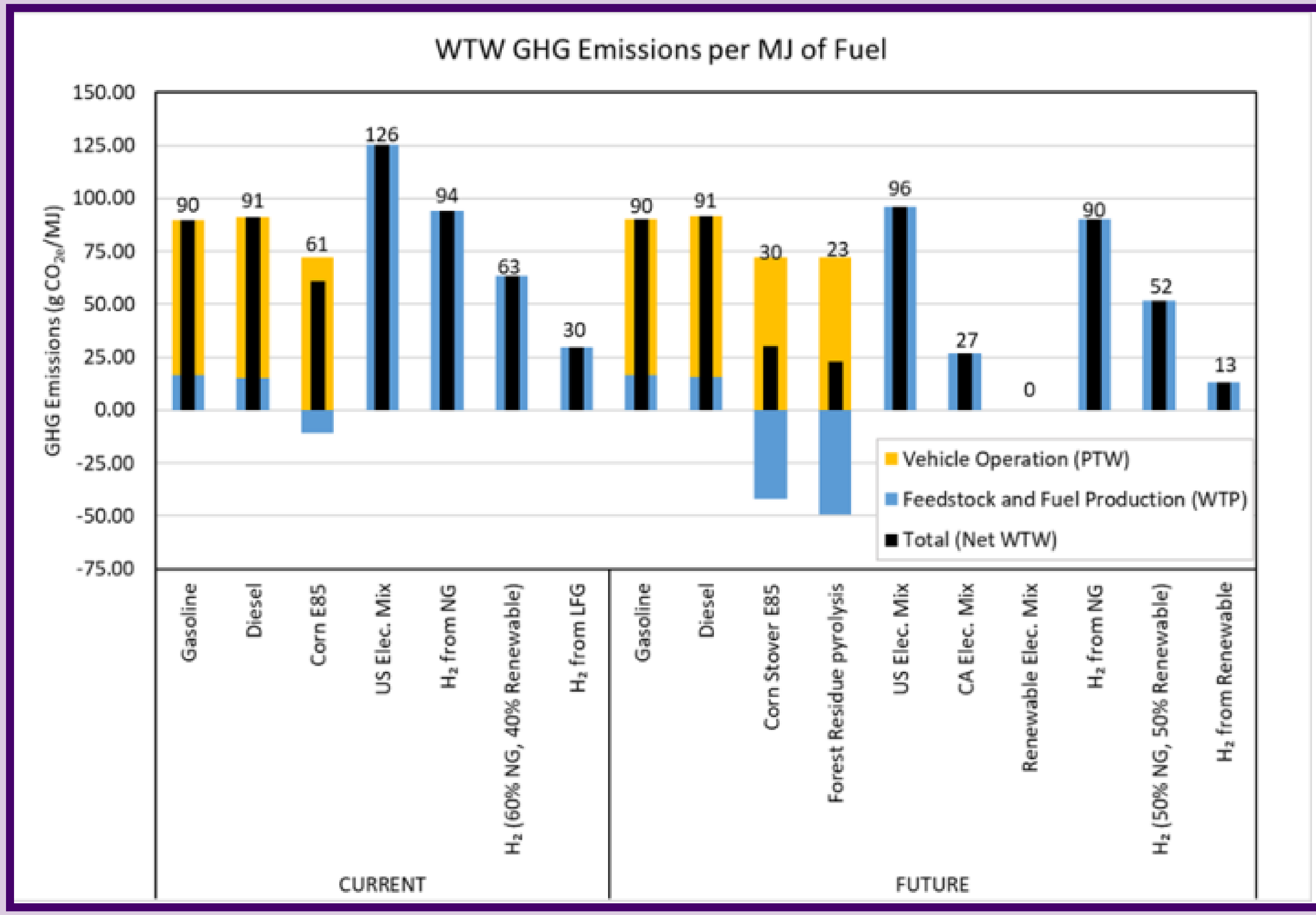
Liquid Hydrogen Pathway

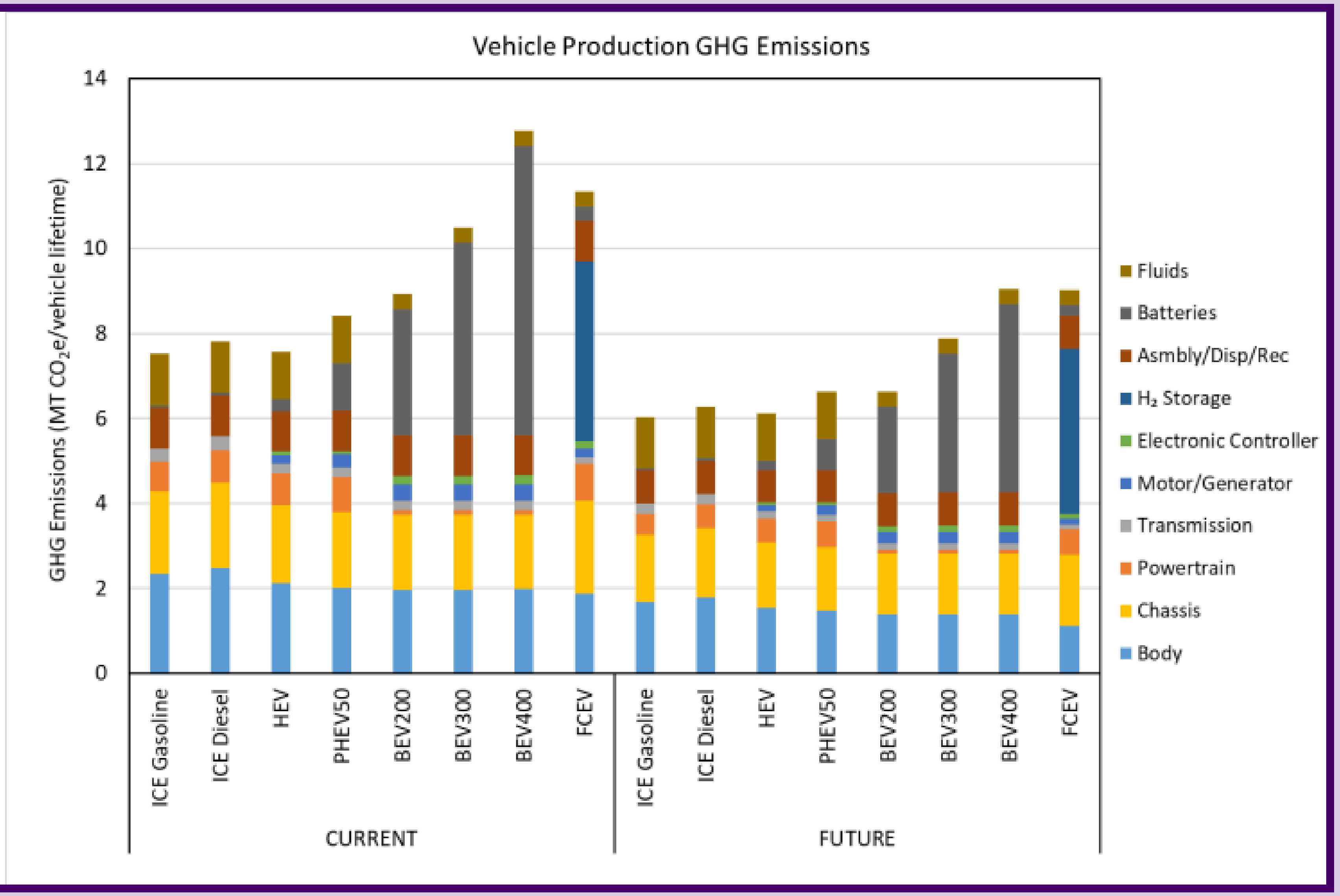
[- Hydrogen Delivery Scenario Analysis Model (HDSAM) | Argonne National Laboratory]

Well-to-Wheel (WTW) GHG Emissions

Well-to-wheel (WTW) GHG emissions in R&D GREET

R&D GREET evaluates WTW and vehicle manufacturing GHG emissions, including hydrogen pathways and fuel cell vehicles (FCVs)





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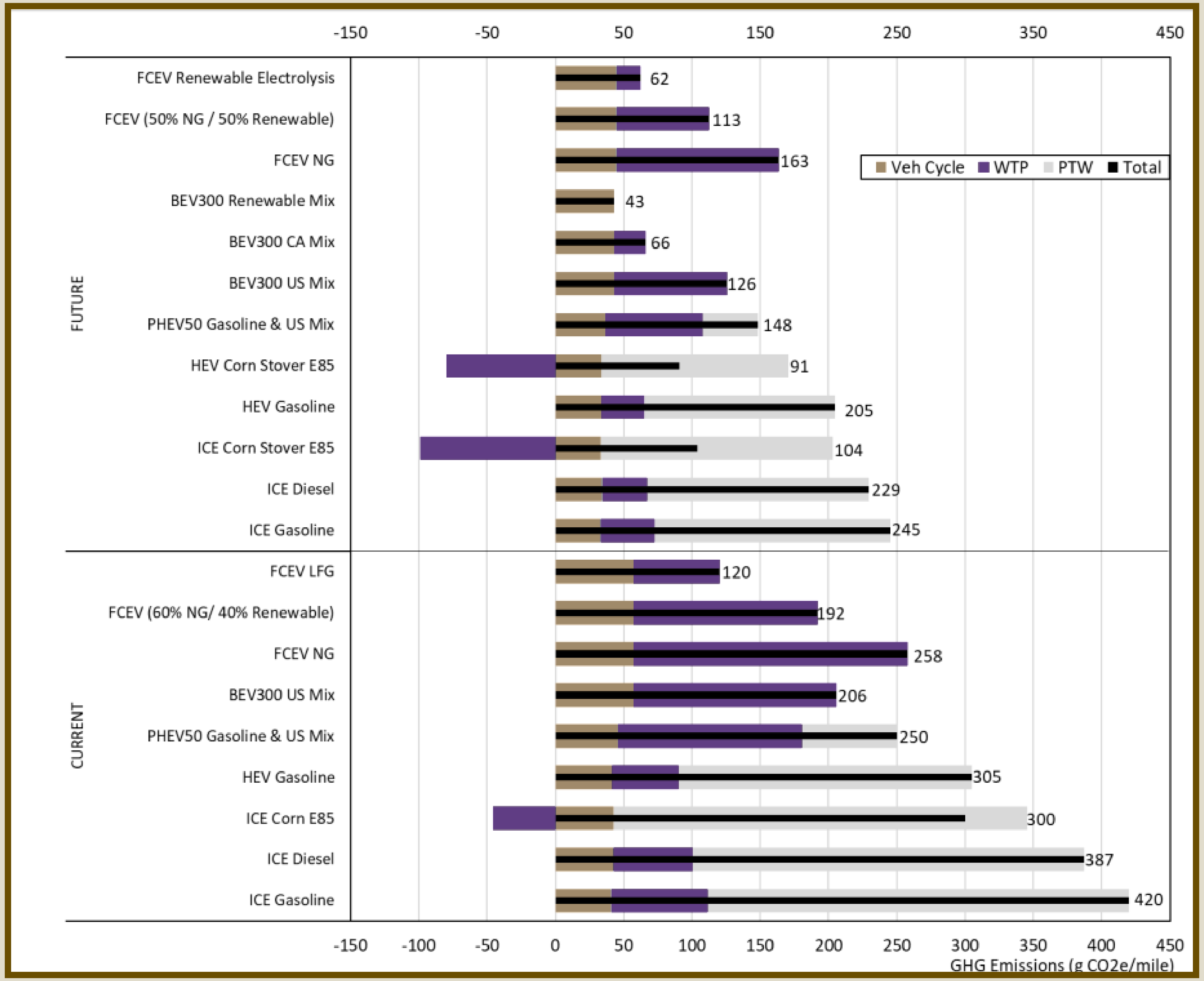
- Elgowainy et al., 2021, Department of Energy EERE Record

Cradle-to-grave (C2G) GHG emissions in R&D GREET

R&D GREET combines WTW and vehicle cycle GHG emissions into cradle-to-grave (C2G) emissions for alternative fuels and vehicle systems



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- Elgowainy et al., 2021, Department of Energy EERE Record

Hydrogen as a feedstock

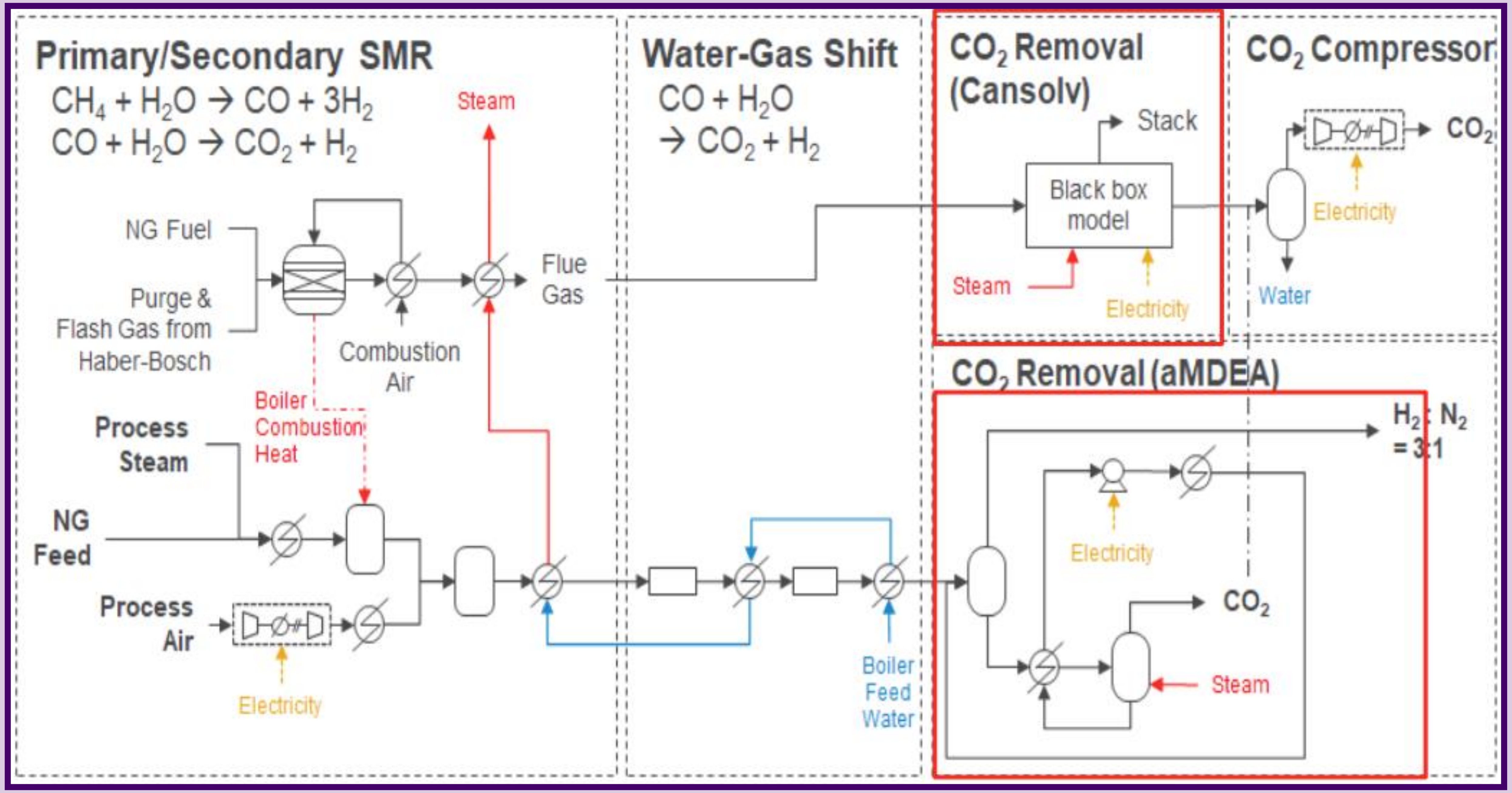
Hydrogen is used as a feedstock in several other pathways in R&D GREET

Renewable ammonia
E-fuels
Methanol
Green steel production
and more

Ammonia, FT-Fuels, and Methanol Production

Ammonia production in R&D GREET

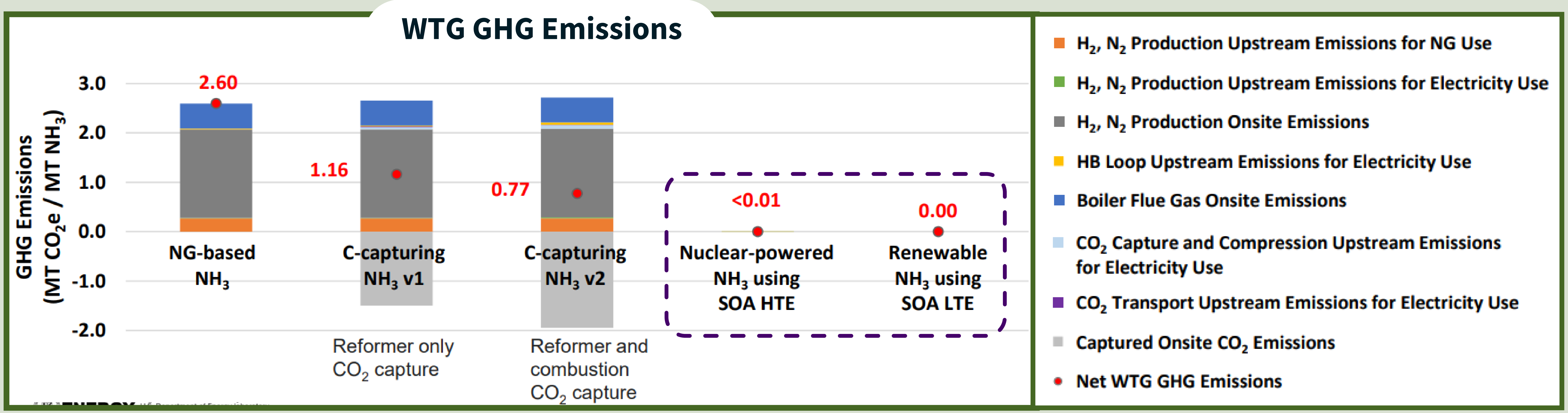
Ammonia production Aspen process modeling



- Lee et al., 2022, Green Chemistry

Ammonia production in R&D GREET

Ammonia GHG emissions depend strongly on the source of hydrogen



- Lee et al., 2022, Green Chemistry

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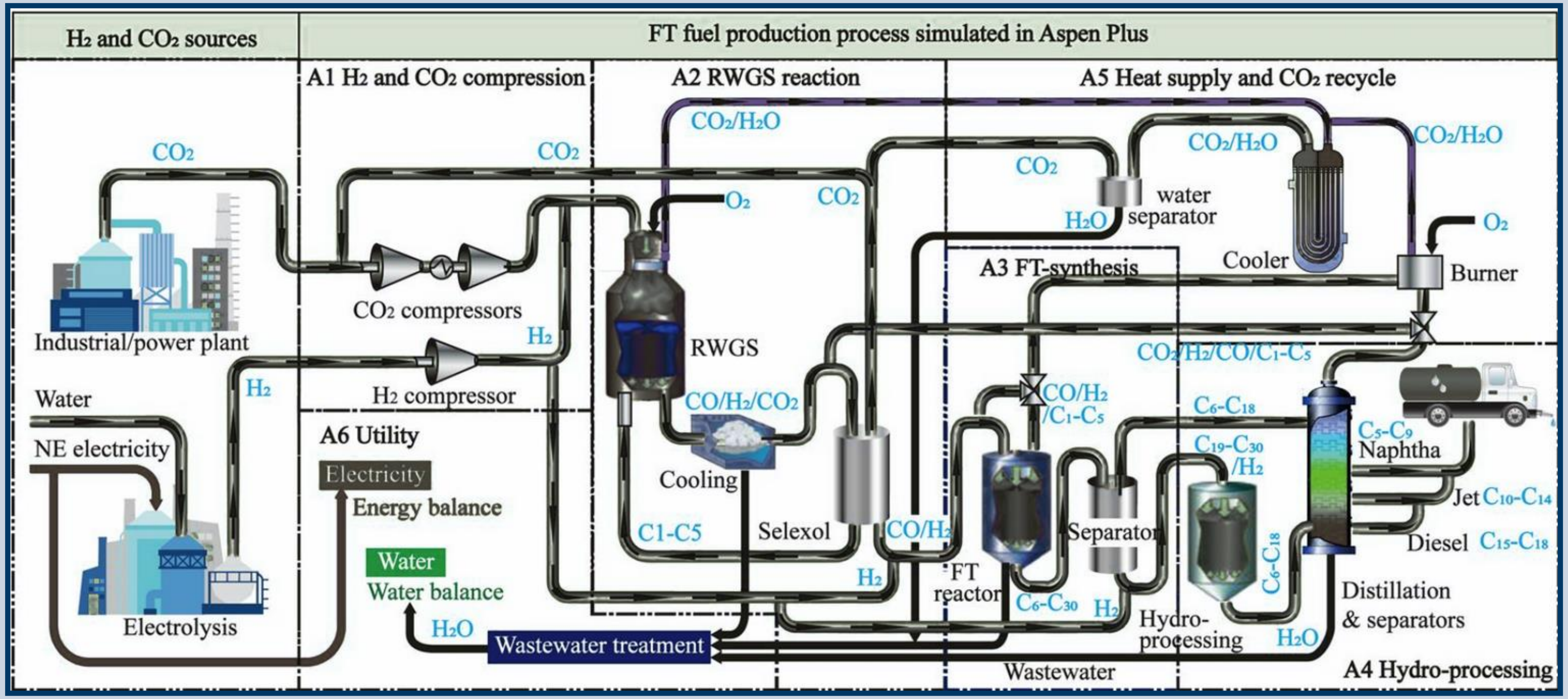
Fischer-tropsch fuels in R&D GREET

Carbon Dioxide CO_2 + **Hydrogen** H_2 → **Syngas** → **FT Fuels**

FT fuels can be synthesized by using **carbon dioxide** and **hydrogen** via a water-gas shift reaction (RWGS) and FT reaction



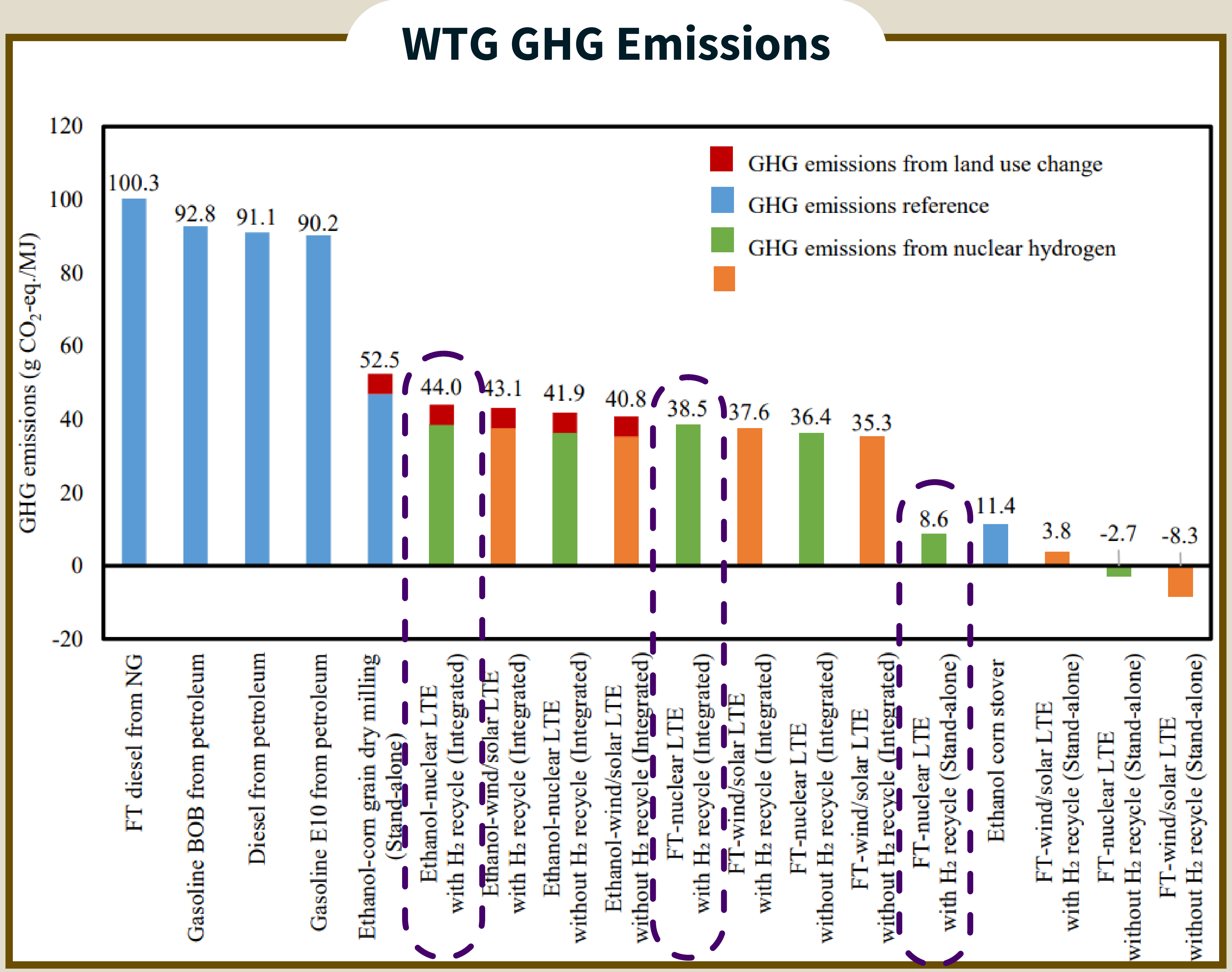
[- Zang et al., 2022, Argonne National Laboratory]

Fischer-tropsch fuels in R&D GREET

Fischer-tropsch GHG emissions depend strongly on the source of hydrogen

Standalone system has a system boundary only around the FT process

Not considering corn ethanol production as the CO_2 source



- Zang et al., 2022, Argonne National Laboratory

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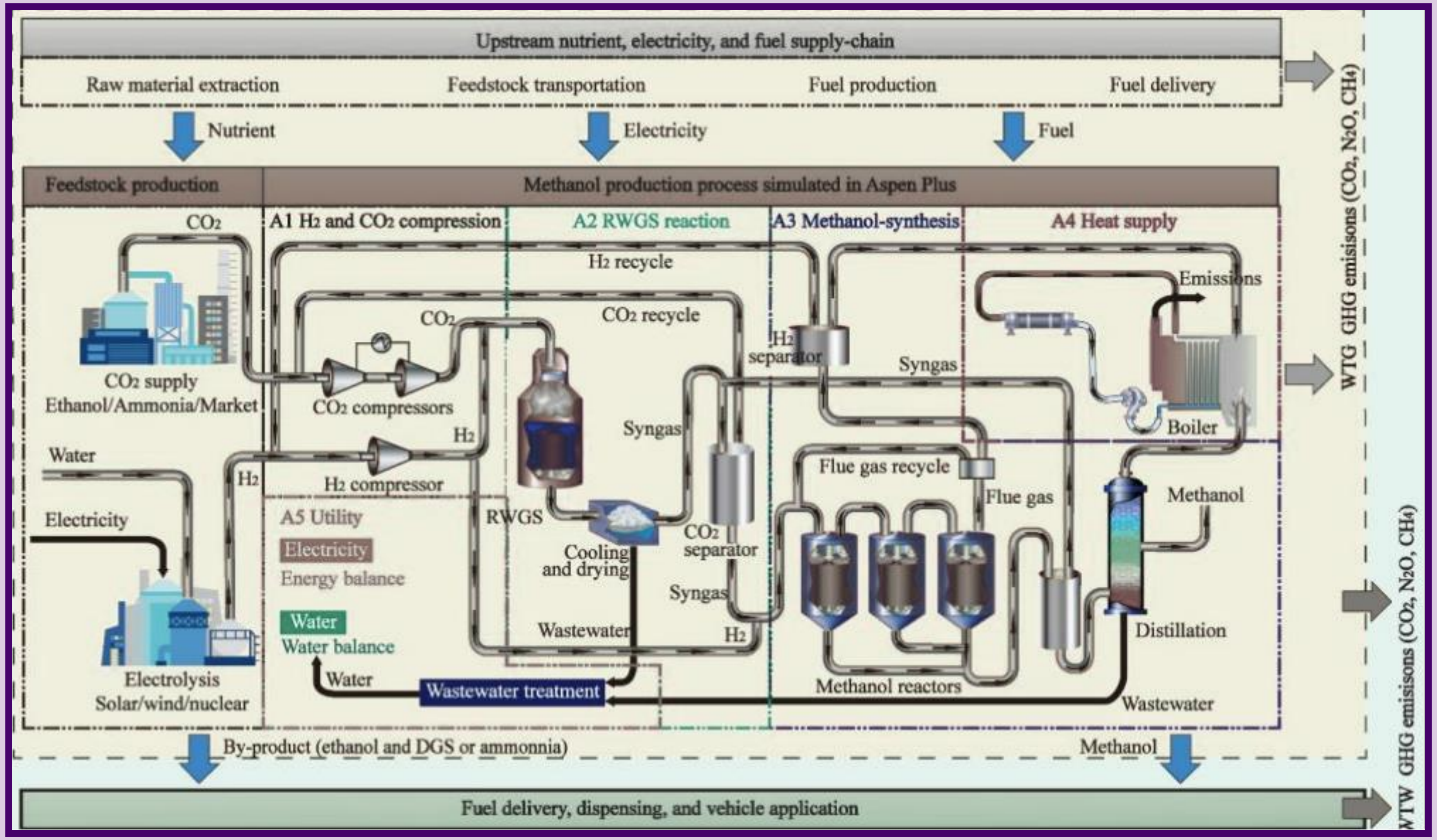
Methanol in R&D GREET

Carbon Dioxide CO_2 + **Hydrogen** H_2 → **Syngas** → **Methanol**

Methanol can be synthesized by using **carbon dioxide** and **hydrogen** via a RWGS and methanol reaction

- Zang et al., 2021, Environmental Science & Technology



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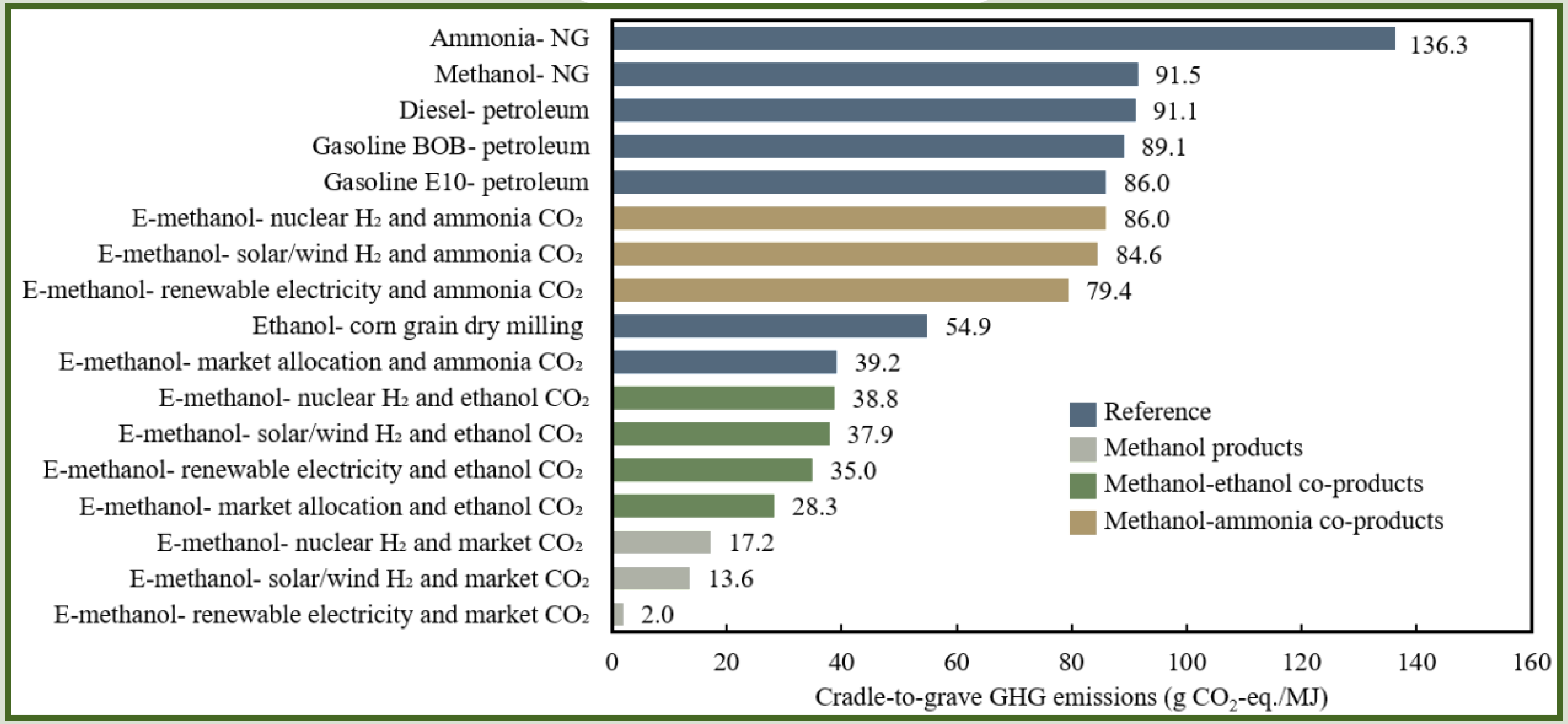
Methanol in R&D GREET

Methanol GHG emissions depend strongly on the source of hydrogen

C2G GHG Emissions



- Zang et al., 2021, Environmental Science & Technology

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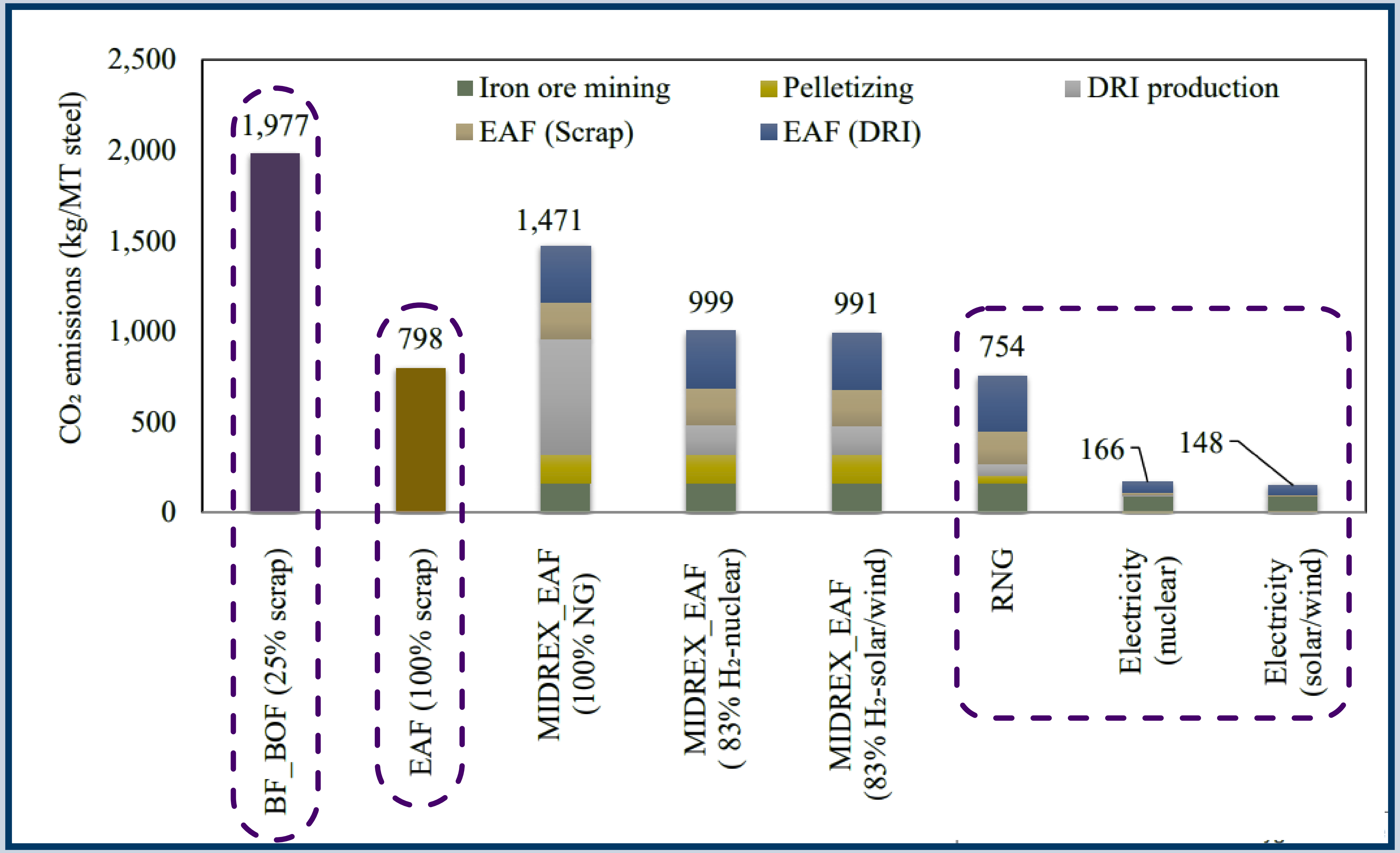
Steel decarbonization in R&D GREET

R&D GREET evaluates steel decarbonization technology options



BF-BOF=blast furnace-basic oxygen furnace
EAF=electric arc furnace
DRI=direct reduction of iron
RNG=renewable natural gas
WTG=well-to-gate

- R&D GREET 2023

Note: this figure was generated for illustrative purposes. As R&D GREET is updated, the values could change

R&D GREET capabilities for LCA of hydrogen

Feedstock Types

PEM electrolysis, solid oxide electrolysis, SMR, auto thermal reforming, methane pyrolysis, biomass gasification, and coal gasification

Refining Products

Hydrogen fuel, ammonia, e-fuels, ethanol, direct reduced iron (DRI), steel, methanol, SAF, rare earth oxides, LPG, propane, butane, asphalt, propylene, diesel, residual oil, gasoline, PLA, HDPE, algae oil, nickel refining, and monocrystalline silicon

Energy and Environmental Metrics

Energy intensities of total, fossil (petroleum, gas, coal), water use intensities, GHG emission intensities (total and CO_2, CH_4, and N_2O separately), air pollutants' emissions intensities of VOC, CO, NO_x, $PM_{2.5}$, PM_{10}, SO_x, BC, and OC

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Hydrogen tabs in R&D GREET 1

Primary
Hydrogen

Some Secondary
Ag_Inputs
Petroleum
EtOH
MeOH
E-fuels
Algae
PUP Conversion
Plastics

Inputs
Results
Fuel_Prod_TS
Fuel_Specs
Electricity
Car_TS
Vehicles
Tractor WTW
Rail PTW
EF
T&D
T&D Flowcharts

Hydrogen tabs in R&D GREET 2

Primary

Silicon

Rare Earth

Steel

Nickel

Some Secondary

TEC_Results

MHDV_TEC_Results

Questions?

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Visit https://greet.anl.gov/

Contributors

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