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Engineering



Fossil Energy in the H₂ Economy – A Carbon-Water-Energy Adaptive Evaluation Platform

Project number: DE-FE0032084

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U.S. Department of Energy
National Energy Technology Laboratory
Resource Sustainability Project Review Meeting
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 - Dashboard implementation status
 - Final considerations and future plans

Project Team

Current, past members and **collaborators** along the project



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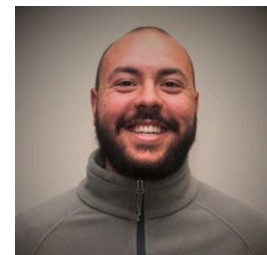
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Project objectives

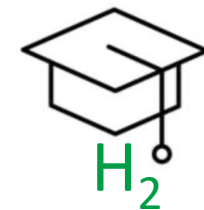
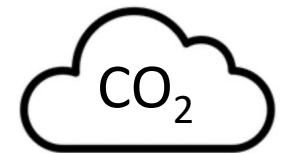
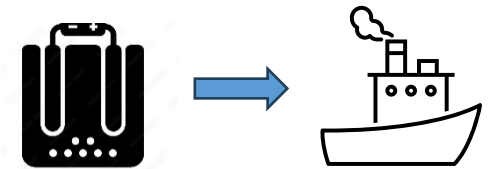
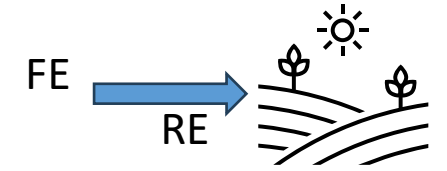


Major Goals and Objectives:

- Support the efficient, environmentally sound integration of fossil fuels into the H₂ economy as a complement - and not a competitor - to more renewable energy resources penetration;
- Review and assess fossil-focused hydrogen production and utilization within the hydrogen economy;

Specific Objectives:

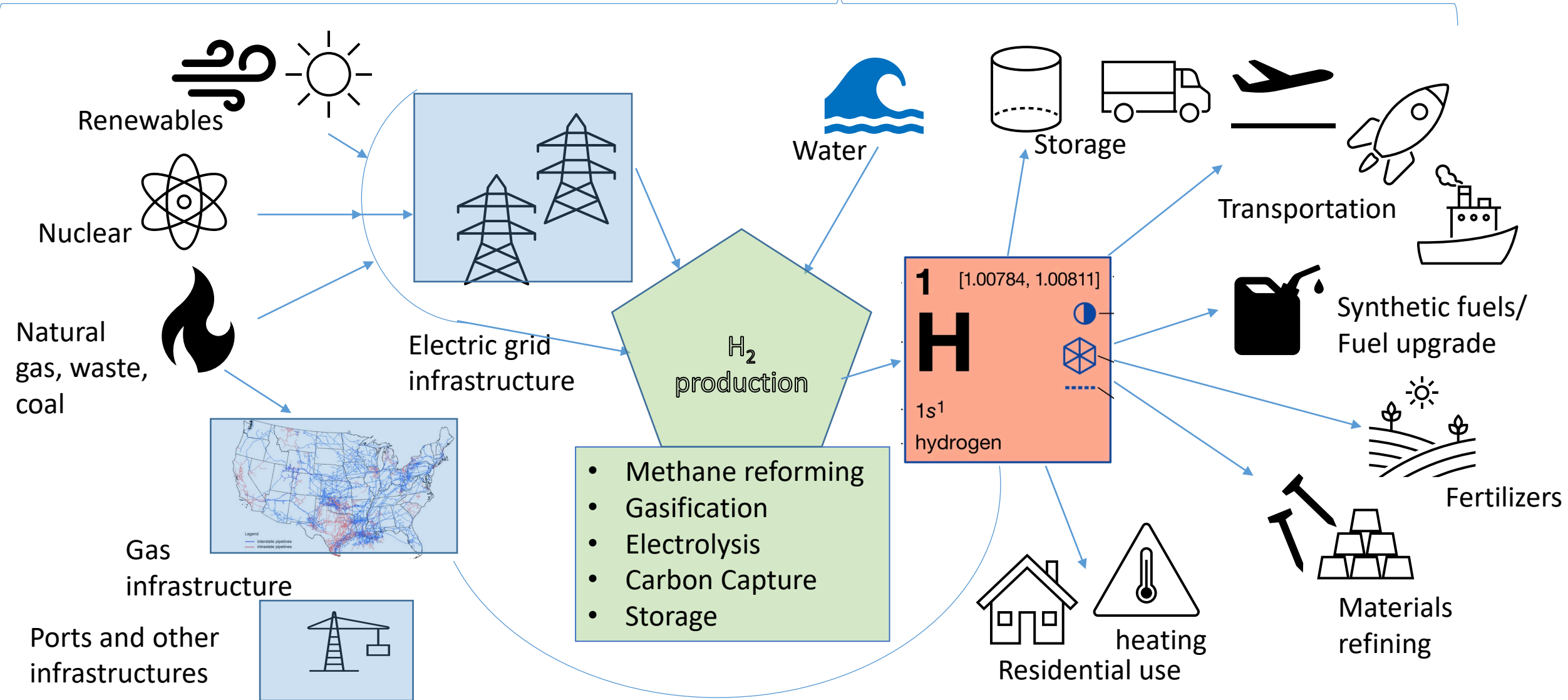
- Quantify the water intensity (water-energy nexus);
- Quantify the carbon footprint of the different fossil fuel hydrogen technologies (generation, transport, storage, and use) and identify existing and novel approaches to mitigate carbon footprint;
- Educate and prepare the next generation minority engineers on relevant aspects of the H₂ economy.



Fossil Energy in the Hydrogen Economy -A Carbon-Water-Energy Nexus Adaptive Evaluation Platform

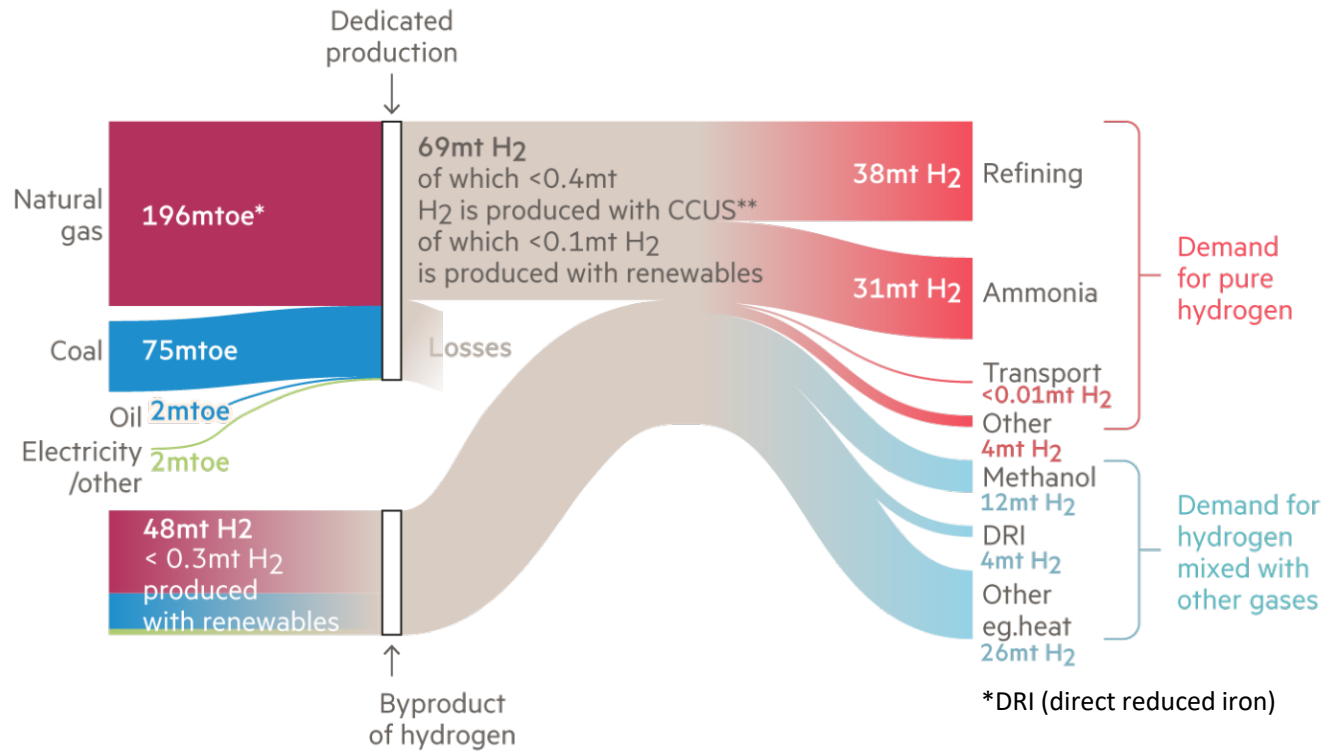


CO₂, GWP, Energy, Water

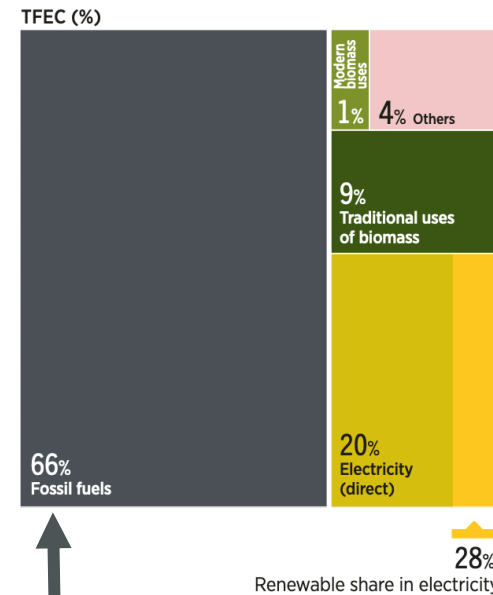
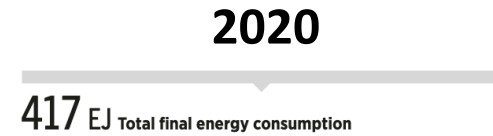


Hydrogen today and into the future

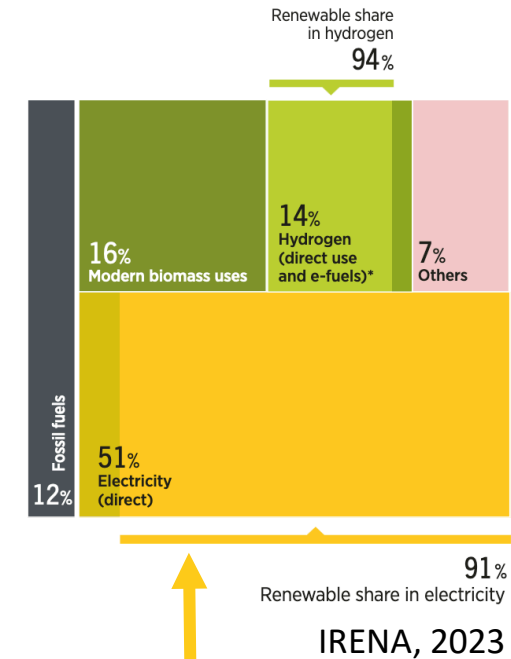
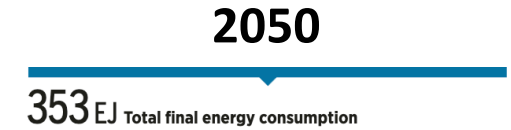
Hydrogen value chains



* mtoe=million tonnes of oil equivalent
 ** CCUS=carbon capture, utilisation and storage
 Source: International Energy Agency
 © FT

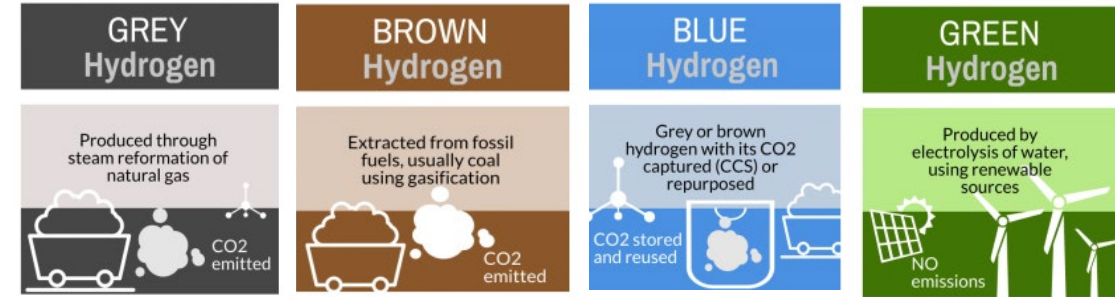
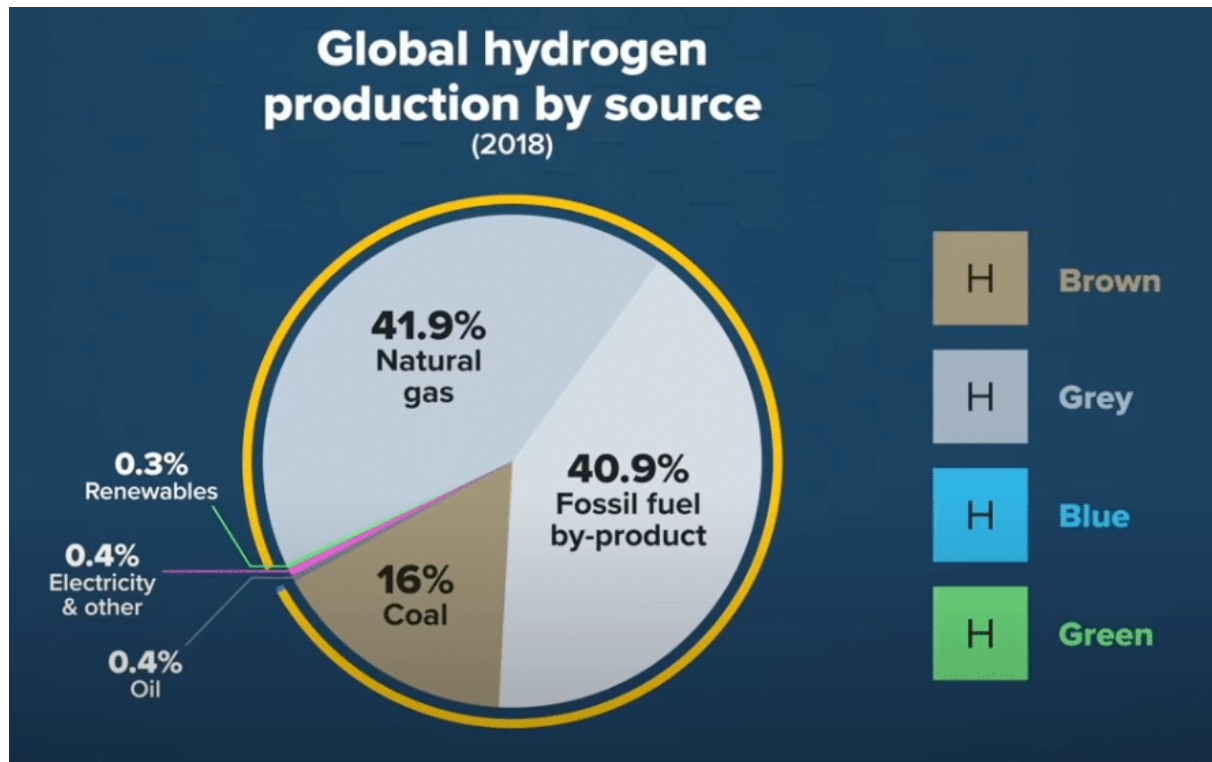


High fossil fuel reliance



Increase in renewables

Hydrogen today



COLOUR	DESCRIPTION: FEEDSTOCK
Grey	Grey: natural gas reforming without CCUS
Brown	Brown: brown coal (lignite) as feedstock
Blue	Blue: natural gas reforming with CCUS
Green	Green: electrolysis powered through renewable electricity
Pink	Pink: electrolysis powered through nuclear energy
Turquoise	Turquoise: methane pyrolysis
Yellow	Yellow: electrolysis powered through electricity from solar
Orange	Orange: electrolysis powered through electricity from wind

Use as fuel...

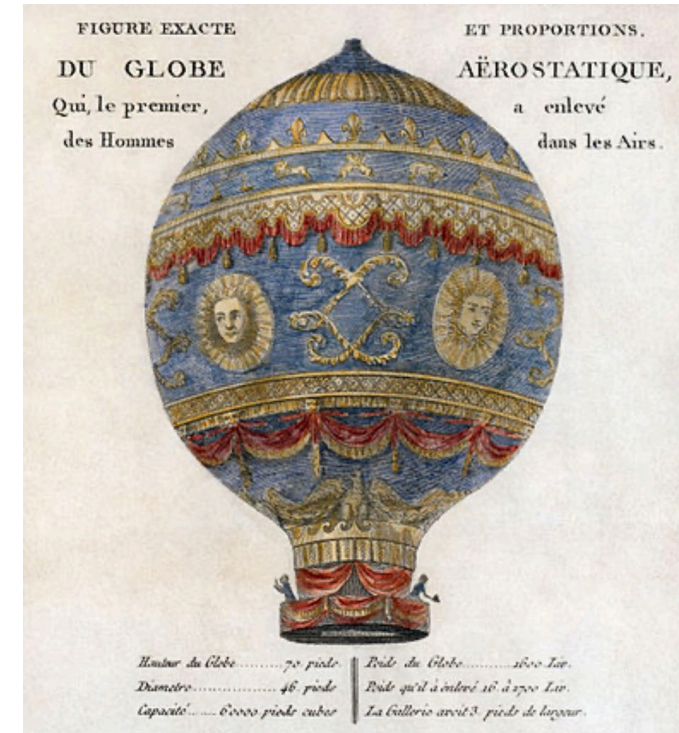
Uses

- → Direct combustion
 - Turbines
- → Fuel cells
- In modern aircraft its deployment requires significant changes to the airplane/propulsion system to accommodate fuel storage and address associated thermal management challenges.

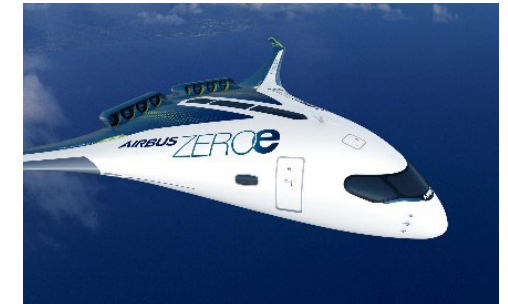
Global warming potential (GWP) values relative to CO₂

Industrial designation or common name	Chemical formula	GWP values for 100-year time horizon		
		Second Assessment Report (SAR)	Fourth Assessment Report (AR4)	Fifth Assessment Report (AR5)
Carbon dioxide	CO ₂	1	1	1
Methane	CH ₄	21	25	28
Nitrous oxide	N ₂ O	310	298	265

Montgolfier brothers, 1783

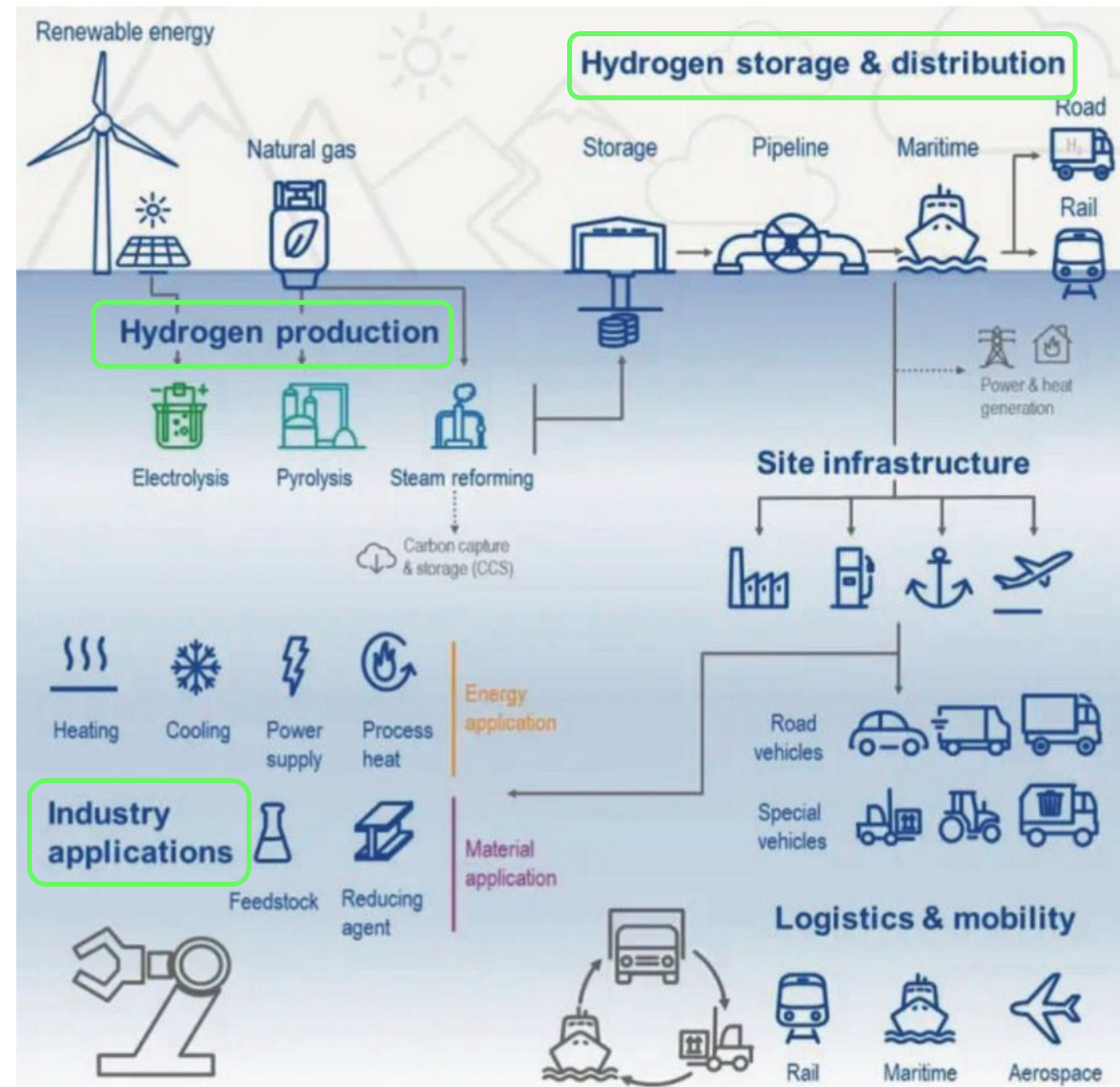


Airbus, 2023



Hydrogen value chain fields, interconnection and roles

- 1) Production
- 2) Storage
- 3) Distribution (storage)
- 4) End-user consumption



Source: Garcia-Navarro et al. (2023)

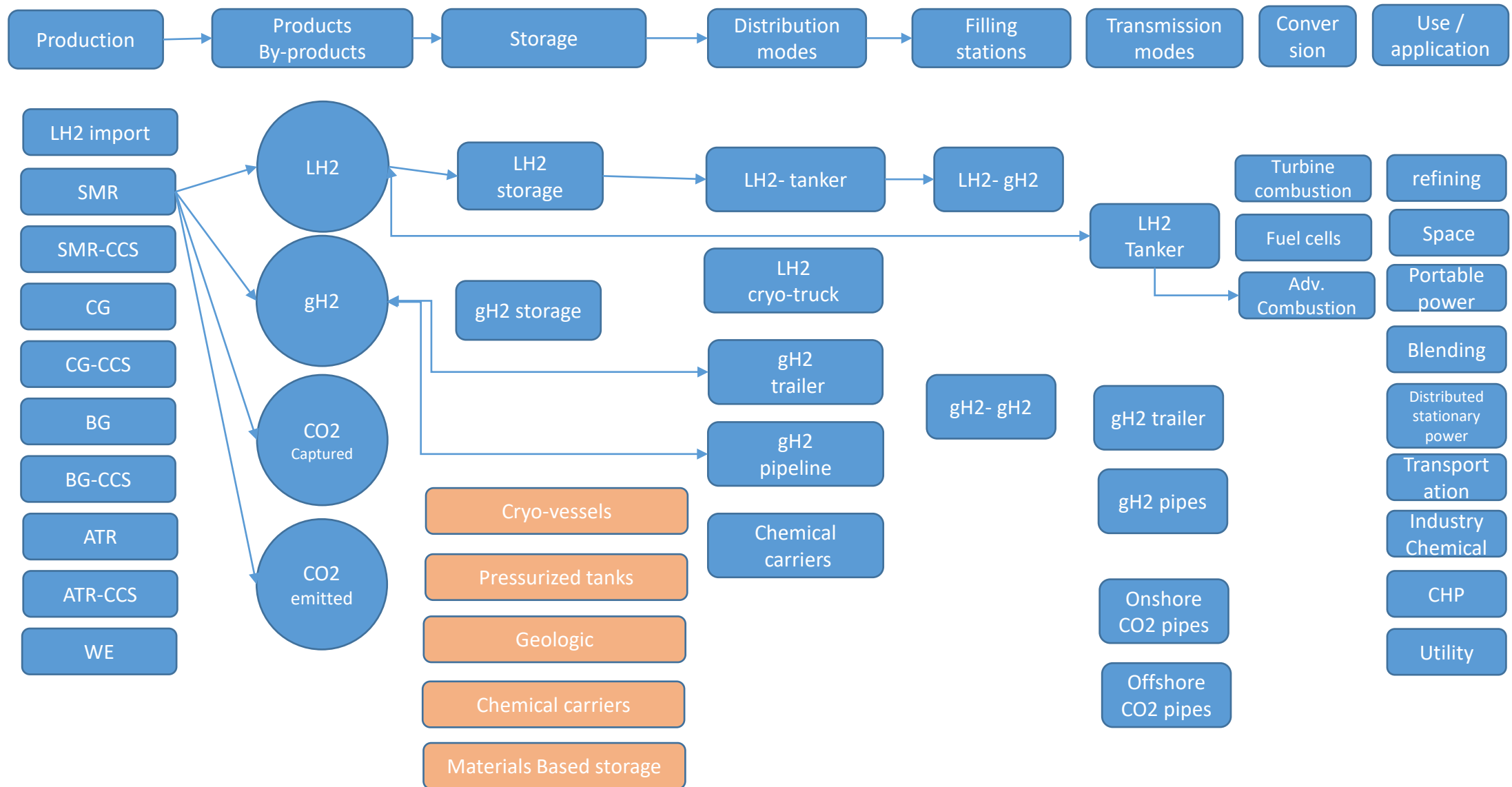
RESOURCES:

Fuel

Energy

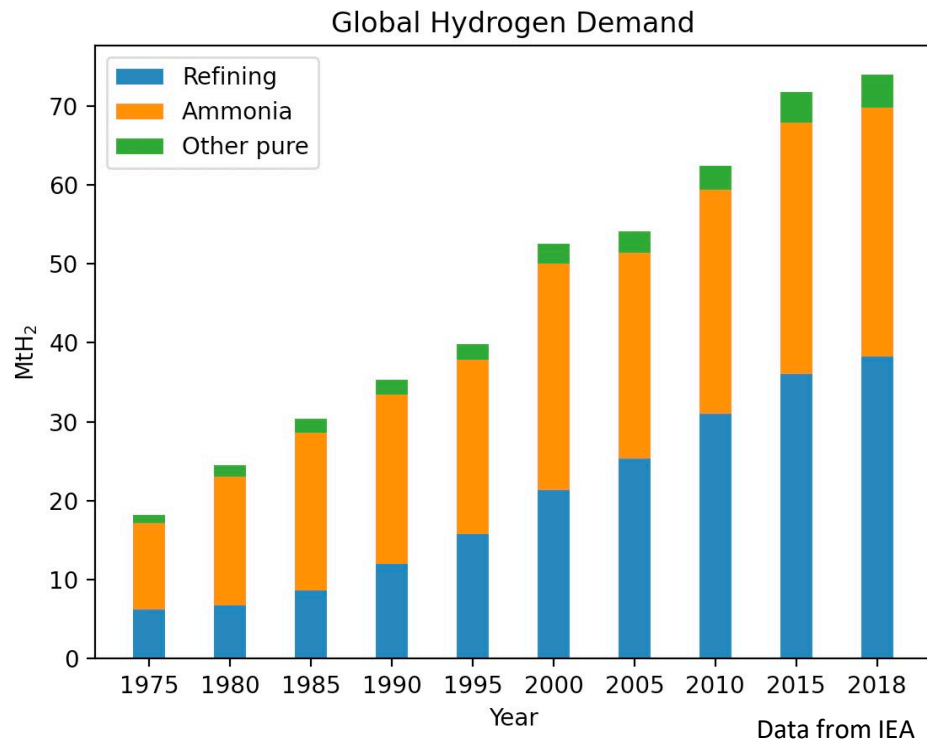
Water

Hydrogen supply chain superstructure



Big Picture Questions

- *What role should fossil fuels play in the development of the hydrogen economy?*
- *Can Fossil Energy (FE) complement the introduction of renewable forms of hydrogen production?*

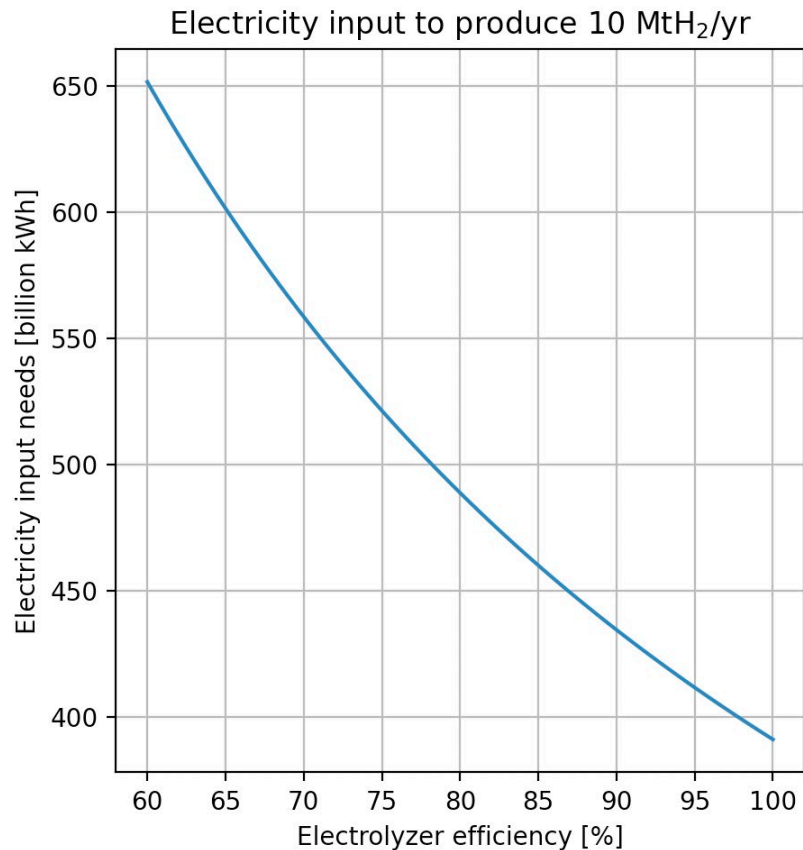


Mt = 10⁹ kg = billion kg

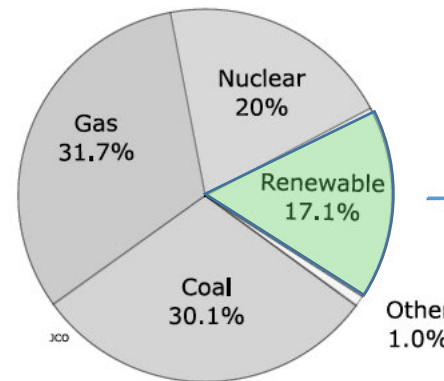
- US ~ 10 MtH₂.
- Worldwide, approximately 96% of H₂ is generated from fossil fuels, particularly from steam methane reforming (SMR) of natural gas but also from coal gasification.
- Could we, today, generate all H₂ via electrolysis from renewables?

Context

- $10 \text{ MtH}_2 = 10 \times 10^9 \text{ kg H}_2$ (10 billion kg); (Others use MMT).
- Ideal electrolysis electricity requirement (HHV) $141.9 \text{ MJ/kg} = 39.4 \text{ kWh/kg}$



- US electricity generation in 2020 ~ 4009 billion kWh (utility scale) + 41.7 billion small scale. [EIA]

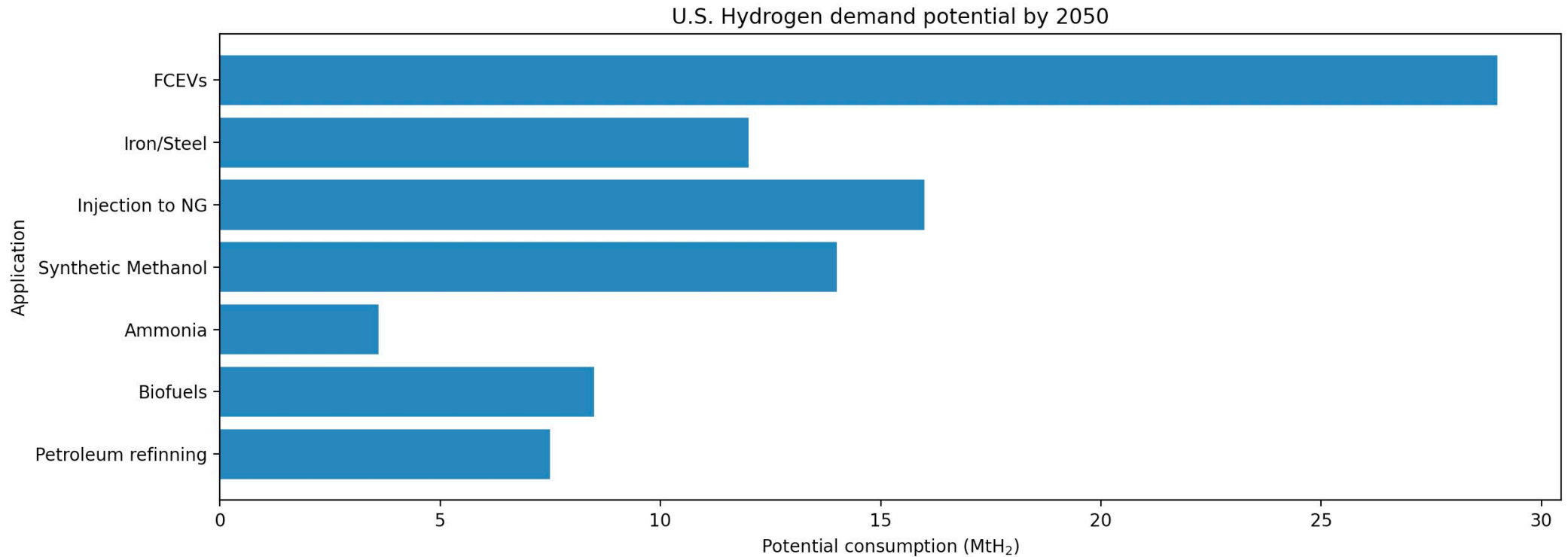


~**693 billion kWh** (from renewables) (17.1%).

Da Rosa, Ordonez, 2021

How much H₂ will we need?

U.S. Current use: 10 Mth₂



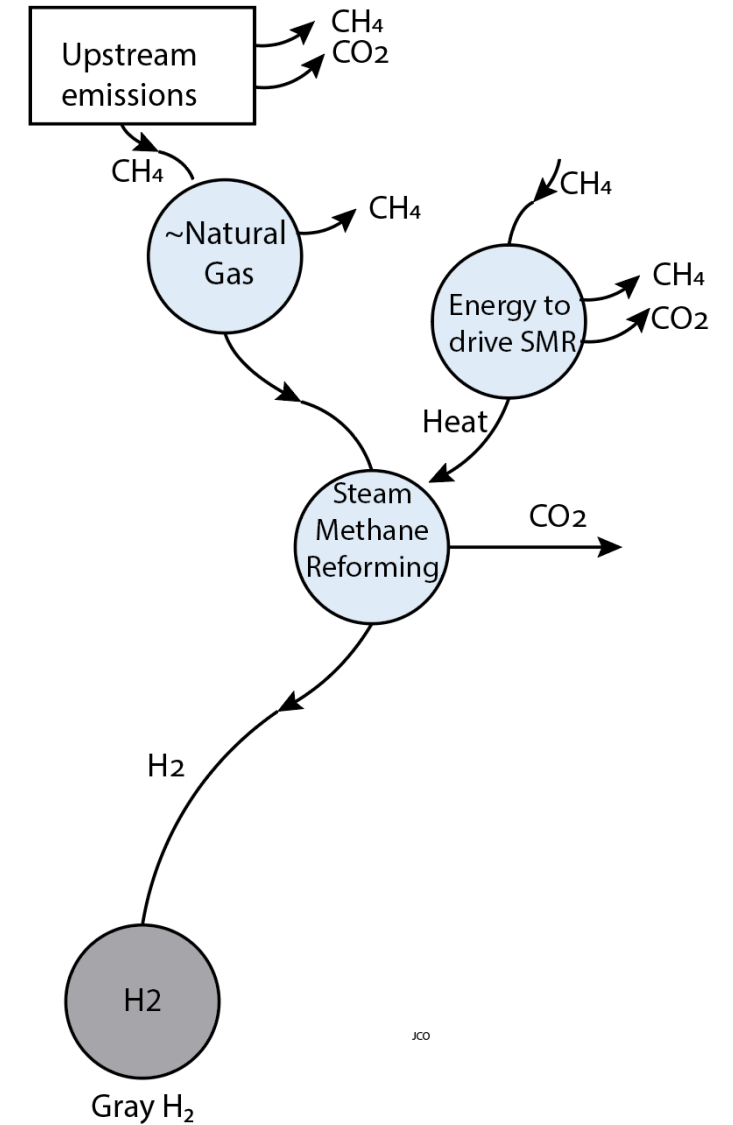
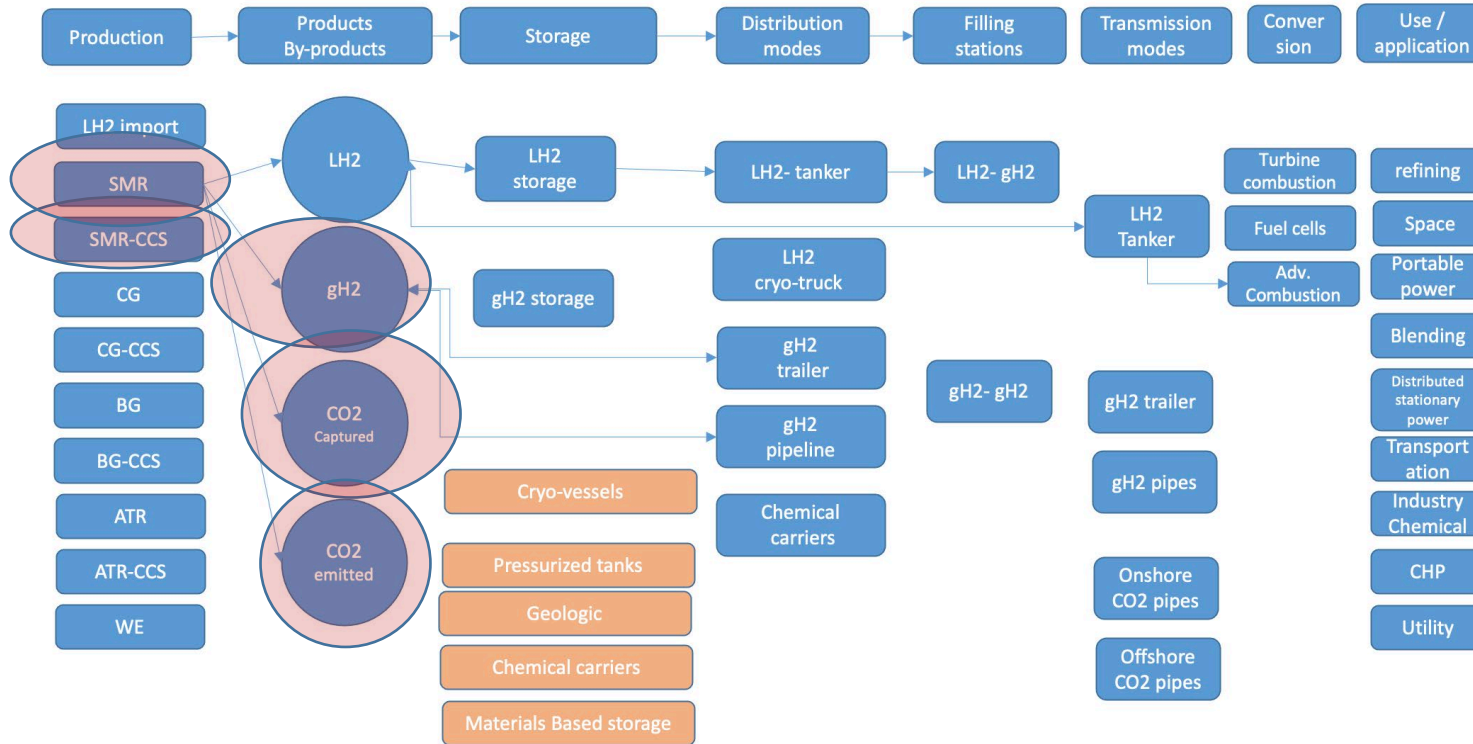
Future: ~85 Mth₂

Plot from data from ANL, 2020 (Warning, categories may not be additive)

Progress and current status of the project

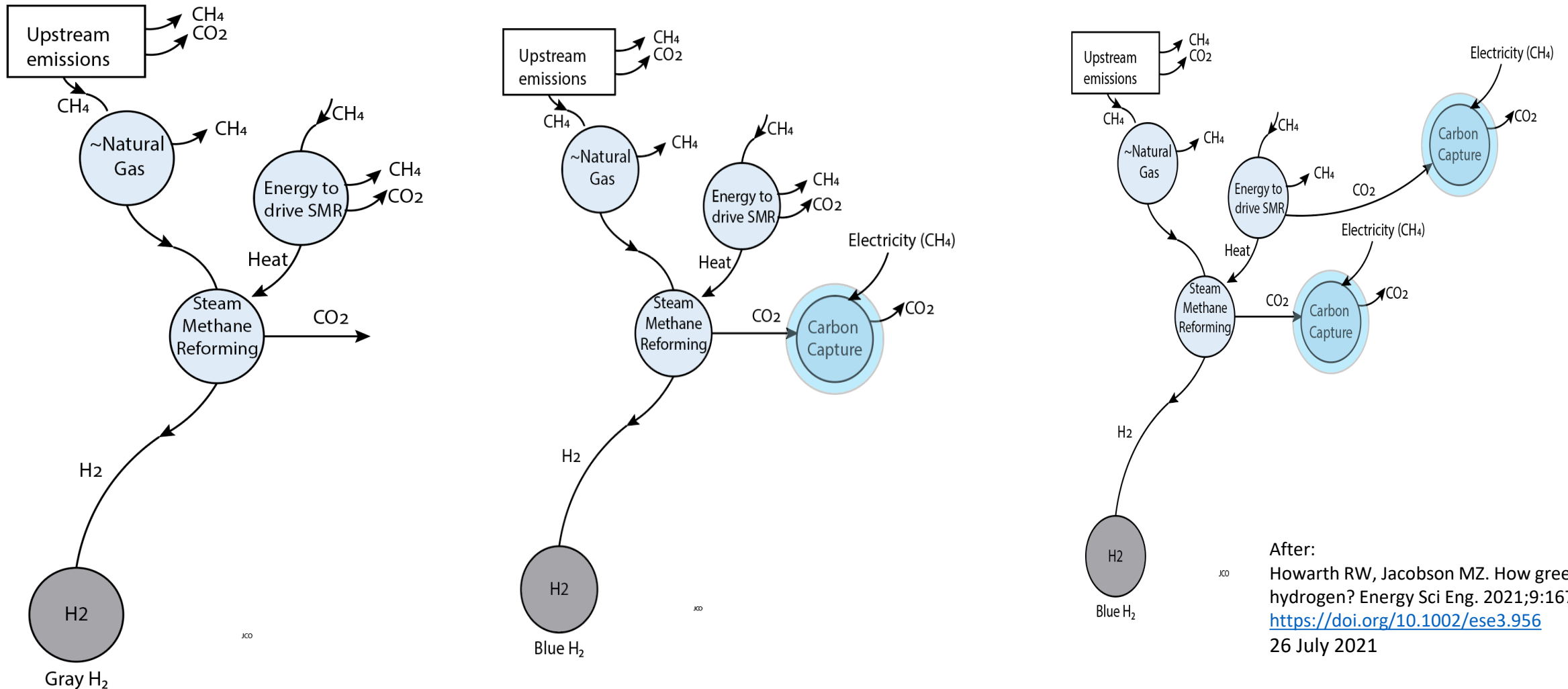
1. CO_{2e} emissions
2. Water use considerations – Explicit and Implicit
3. Levelized Cost of Hydrogen and dynamic maps representation
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5. Final considerations and future plans

1. CO2 footprint



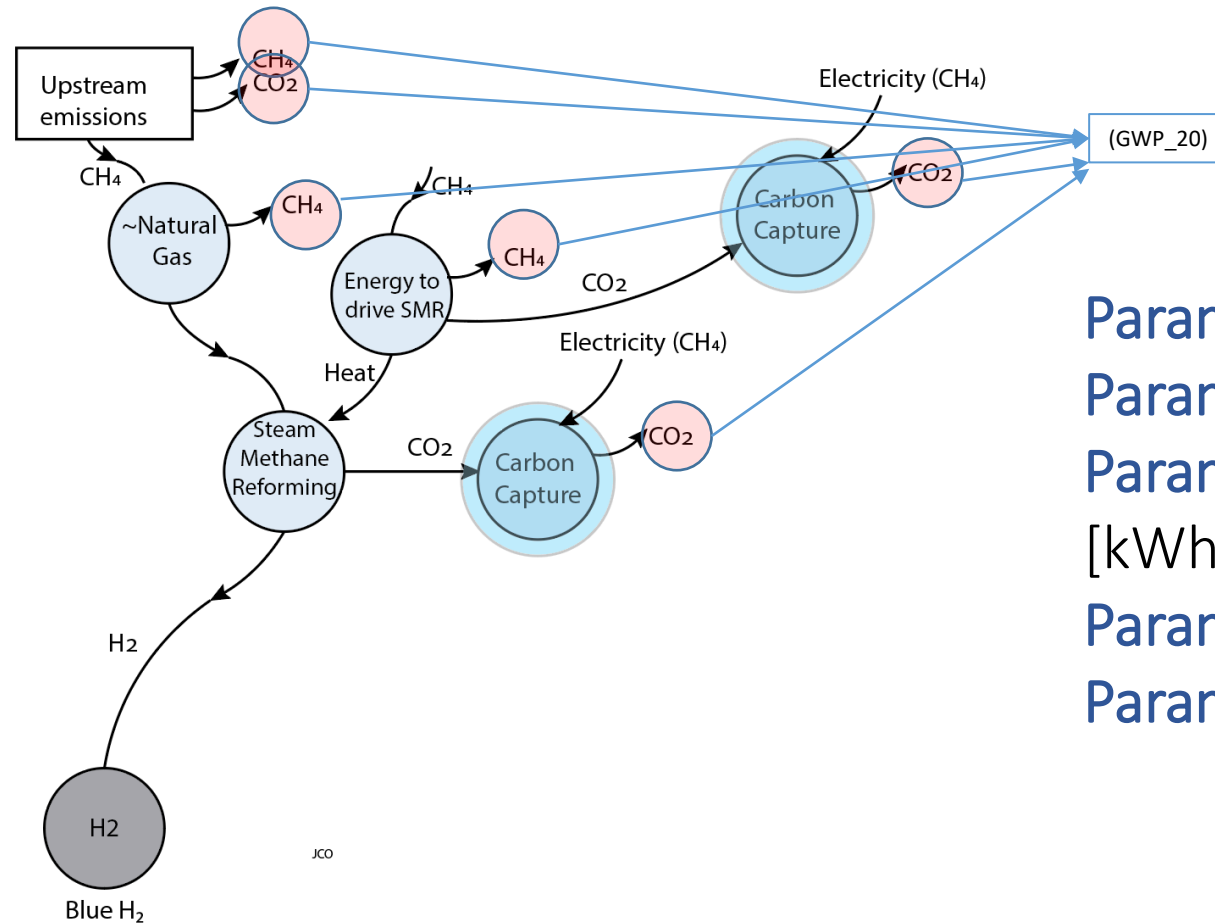
JCO

Three different levels of carbon capture



After:
 Howarth RW, Jacobson MZ. How green is blue hydrogen? *Energy Sci Eng.* 2021;9:1676– 1687.
<https://doi.org/10.1002/ese3.956>
 26 July 2021

Blue H₂- carbon capture in heat production to drive SMR

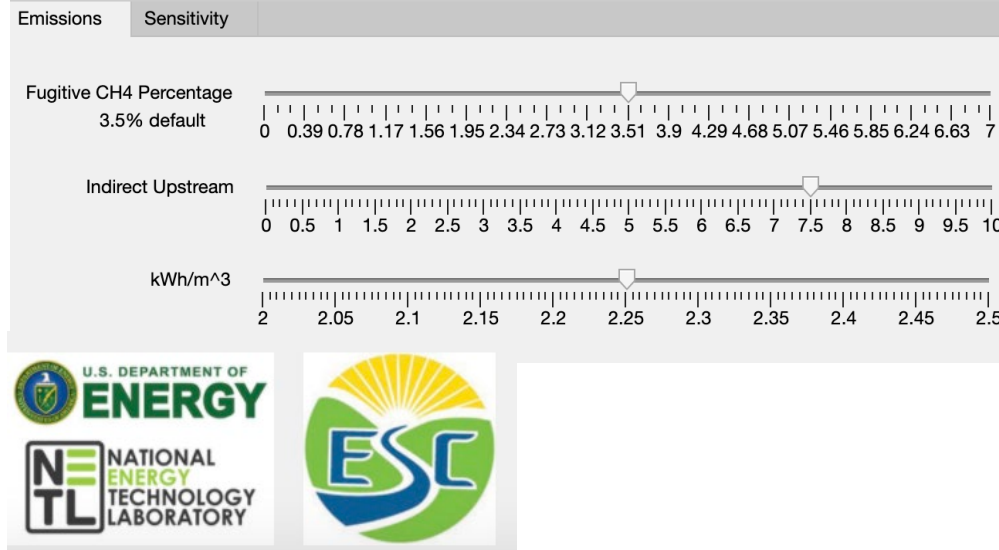


- Parameter 1:** CH₄ leakage (fugitive CH₄).
- Parameter 2:** Indirect upstream emissions.
- Parameter 3:** Energy consumption in SMR [kWh/m³]
- Parameter 4:** CO₂ capture efficiency in SMR.
- Parameter 5:** CO₂ capture in flue

After:
 Howarth RW, Jacobson MZ. How green is blue hydrogen? Energy Sci Eng. 2021;9:1676– 1687.
<https://doi.org/10.1002/ese3.956>
 26 July 2021

MATLAB (and Python)

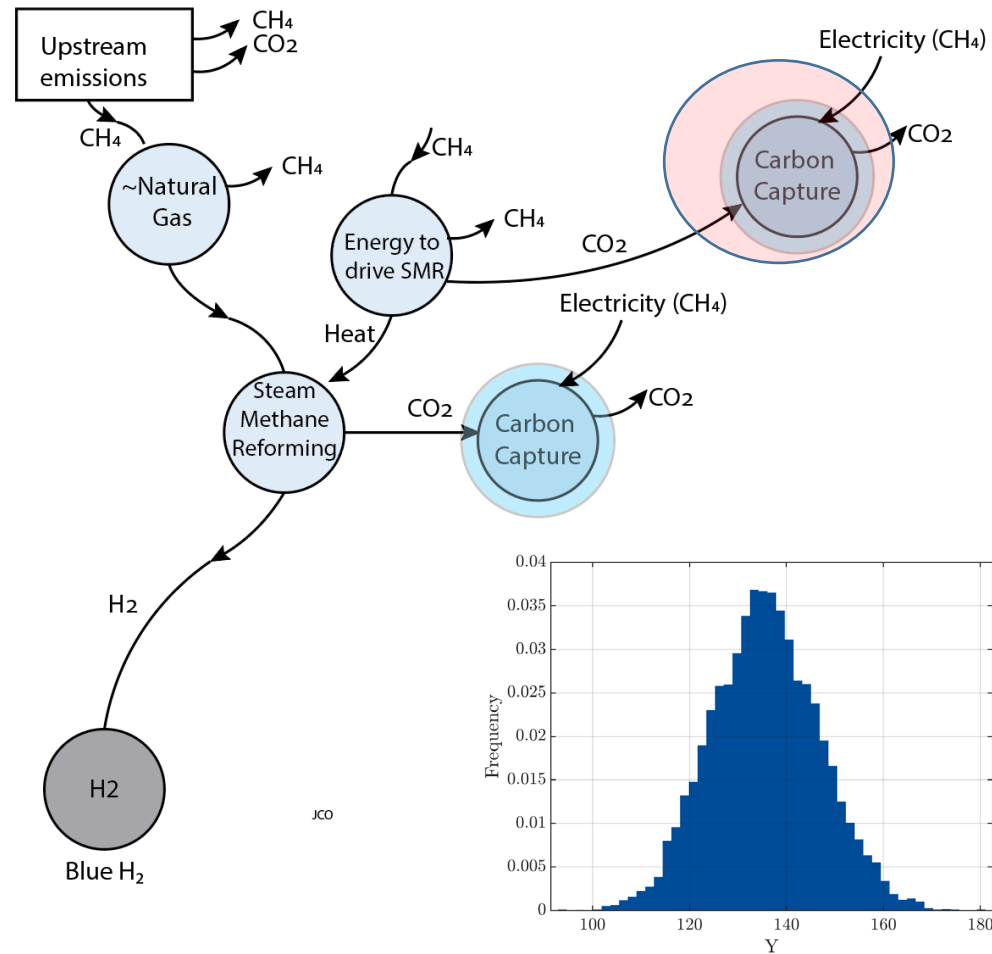
An application that allows the user to set (using sliders) the primary emission parameters for SMR under three cases of CC has been developed in MATLAB



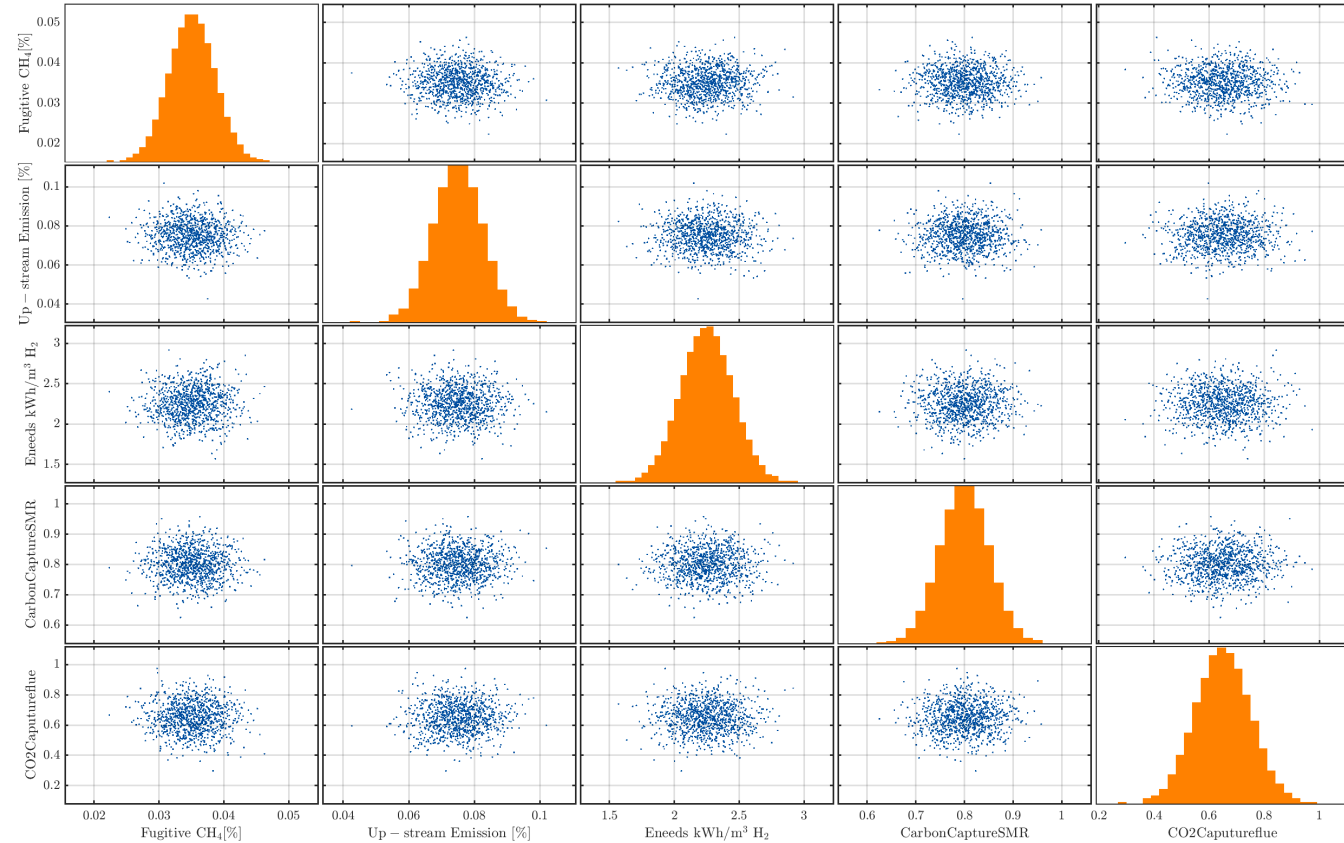
Next:
Enable
exploration of
uncertainty in
these
parameters

	Blue H2 (with flue gas capture);
SMR process	
CH4 consumed (g CH4/MJ)	14.0350
CO2 produced (g CO2/MJ)	38.5087
Fugitive CH4 emissions (g CH4/MJ)	38.5087
Fugitive CH4 emissions (g CO2eq/MJ)	42.2454
Direct CO2 emissions (g CO2/MJ)	5.7763
CO2 capture rate	0.8500
Energy to drive SMR	
CH4 consumed (g CH4/MJ)	11.5724
CO2 produced (g CO2/MJ)	31.7520
Fugitive CH4 emissions (g CH4/MJ)	0.4050
Fugitive CH4 emissions (g CO2eq/MJ)	34.8330
Direct CO2 emissions (g CO2/MJ)	11.1132
CO2 capture rate	0.6500
Energy to power carbon capture	
CH4 consumed (g CH4/MJ)	5.9160
CO2 produced (g CO2/MJ)	16.2322
Fugitive CH4 emissions (g CH4/MJ)	0.2071
Fugitive CH4 emissions (g CO2eq/MJ)	17.8073
Direct CO2 emissions (g CO2/MJ)	16.2322
Indirect upstream CO2 emissions (g CO...	6.4870
Total CH4 consumed (g CH4/MJ)	31.5235
Total CO2 emitted (g CO2/MJ)	39.6087
Total fugitive CH4 emissions (g CO2eq/...	94.8856
Total emissions (g CO2eq/MJ)	134.4944

Distribution of CO₂eq estimates for the given input

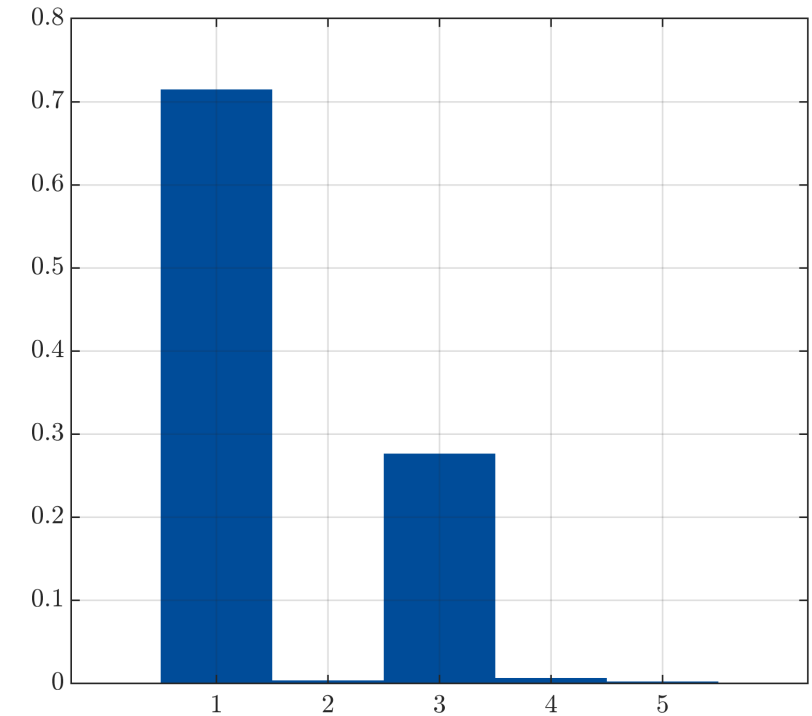
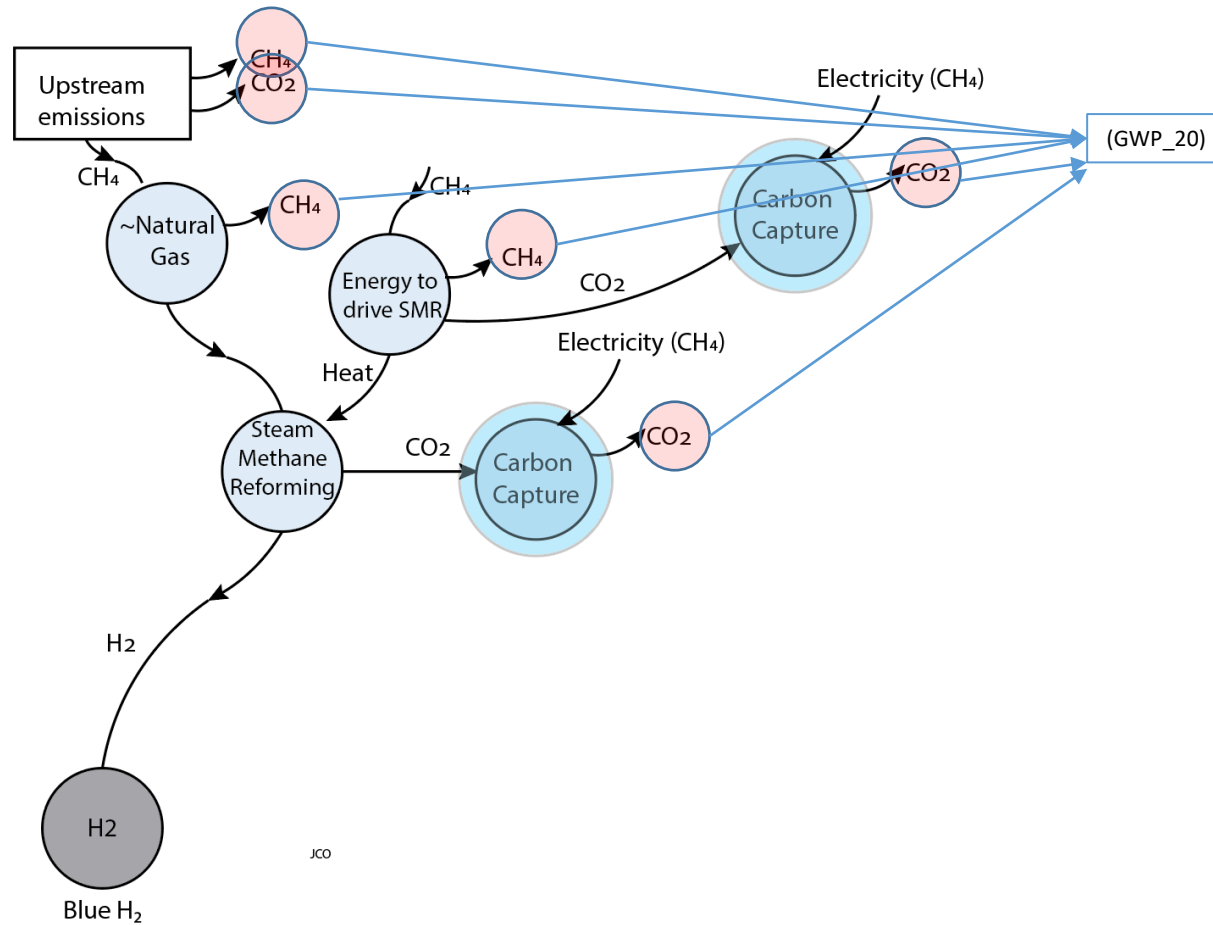


Total emissions (g CO₂eq/MJ)



Sampling using gaussians around base case estimate; 10⁵ samples (Sobol). Implemented in MATLAB via UQLab.

Blue H2- carbon capture in heat production to drive SMR



- Parameter 1:** CH₄ leakage (fugitive CH₄).
- Parameter 2:** Indirect upstream emissions.
- Parameter 3:** Energy consumption in SMR [kWh/m³]
- Parameter 4:** CO₂ capture efficiency in SMR.
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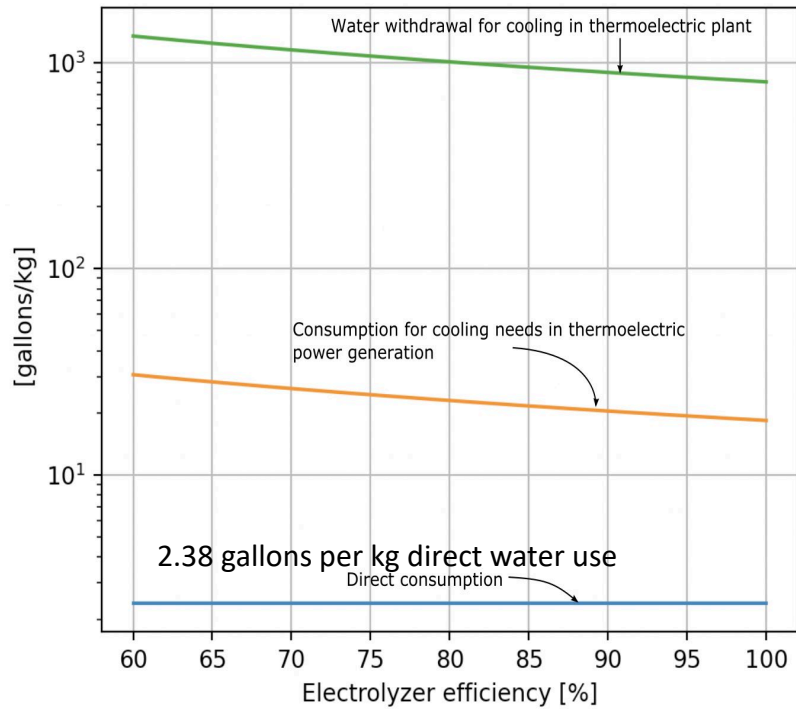
Explicit and implicit water considerations for H₂

This effort seeks to quantify water usage in H₂ production.

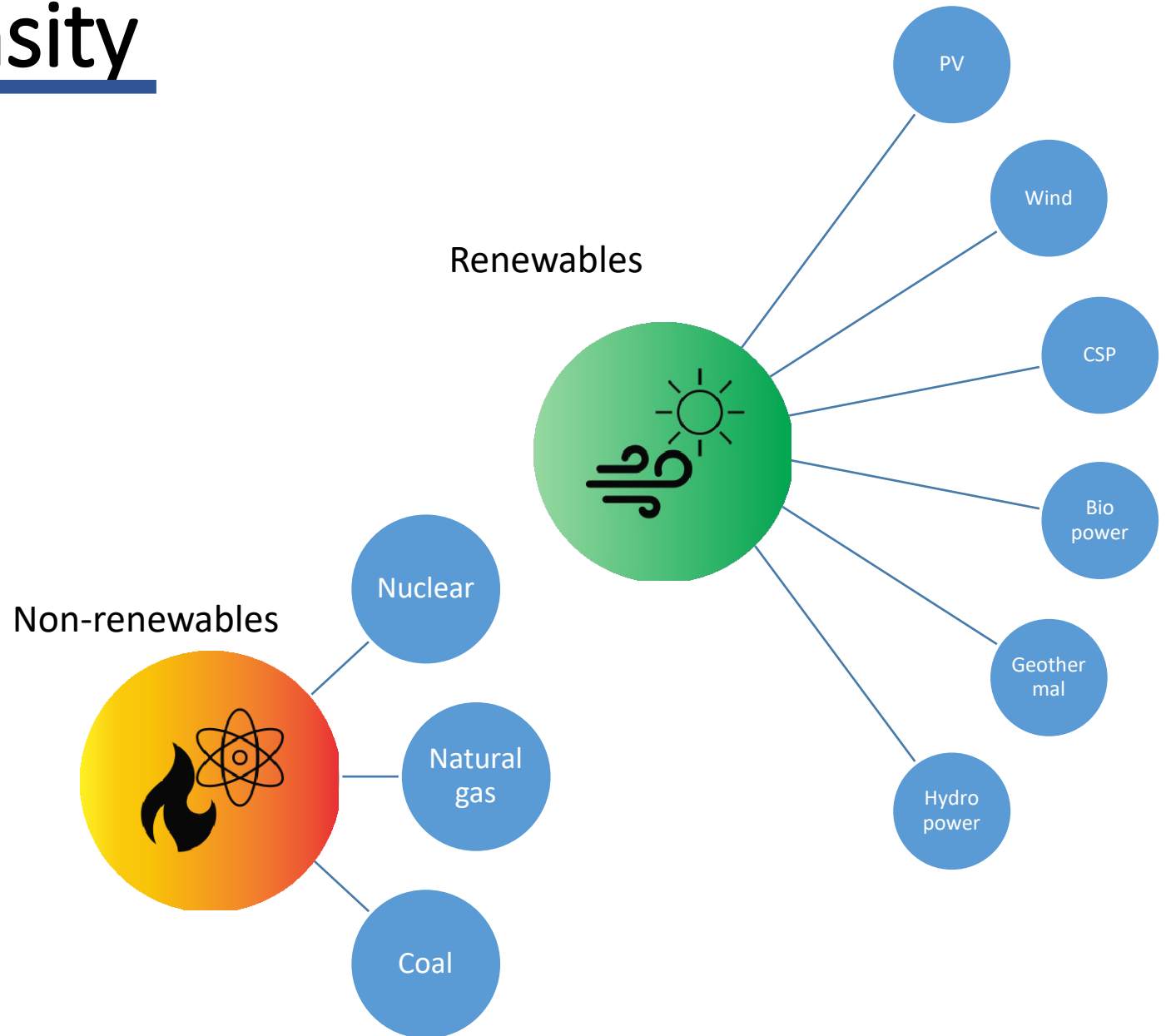
- Explicit (those dictated by the stoichiometry).
- Implicit opportunities for water savings primarily associated with meeting the energy needs.

Water – Energy Nexus

Explicit Water Intensity

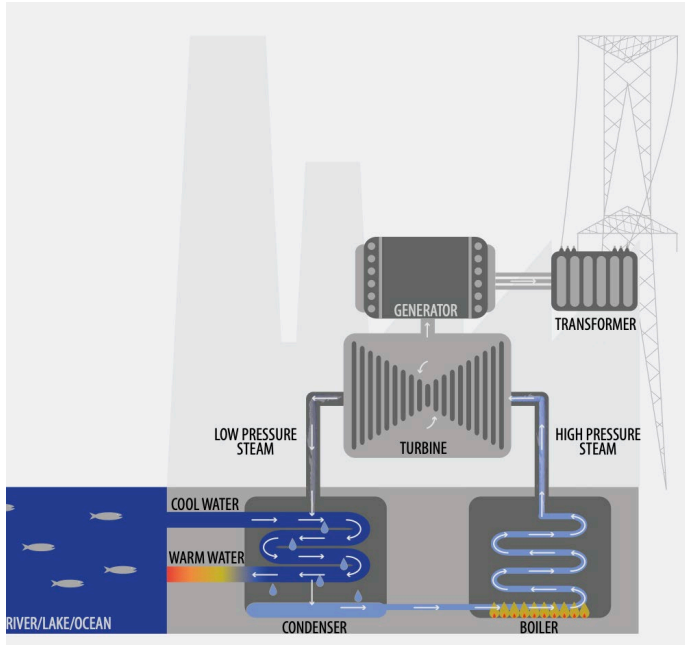


We have explored the disaggregation of this average [water withdrawal is around 20.6 gallons per kWh ^[1, 2, 3] and the average water consumption for cooling is about 0.47 gallons kWh⁻¹ ^{[1].}] leveraging mostly NREL studies of water consumption for different modes of electricity generation ^[4].

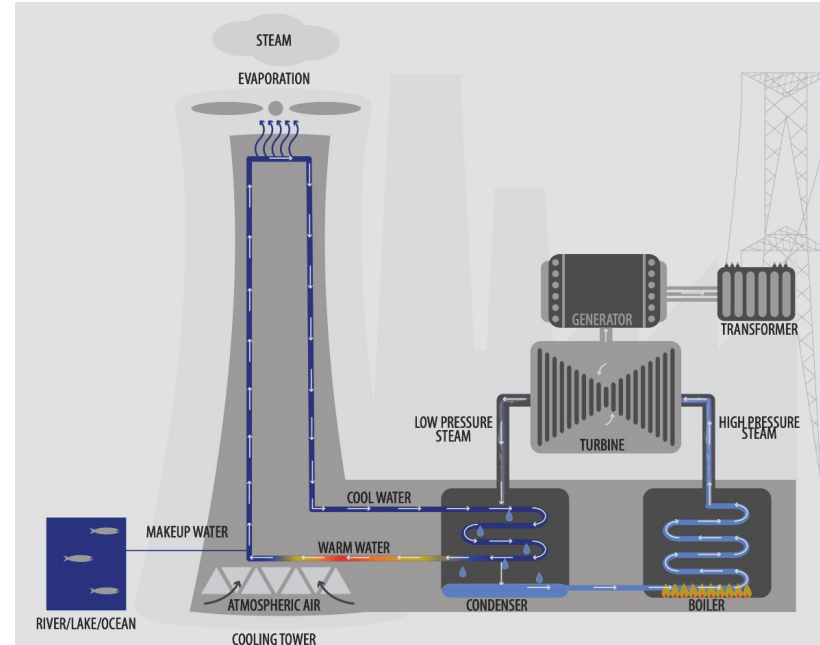


Cooling Technologies

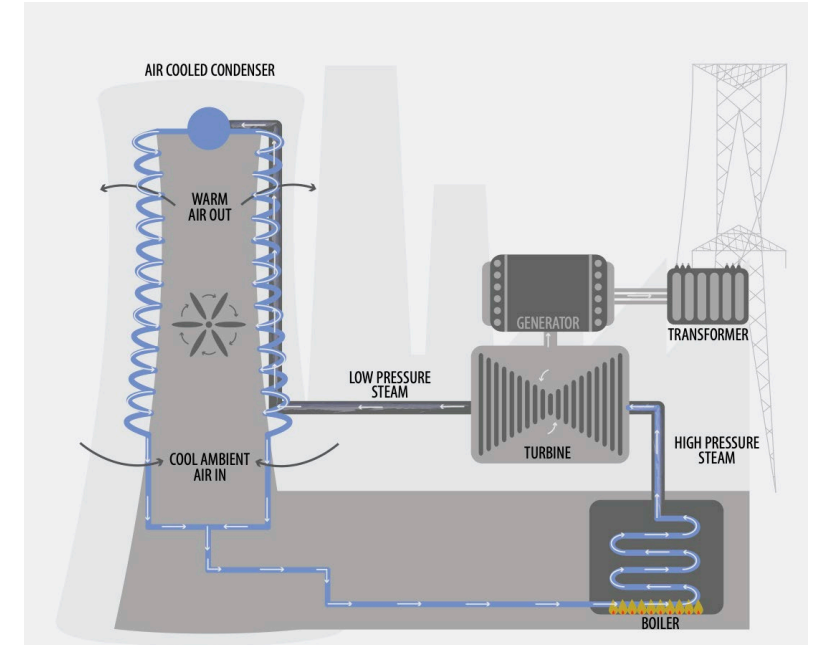
<https://www.nrdc.org/sites/default/files/power-plant-cooling-IB.pdf>



Once-Through



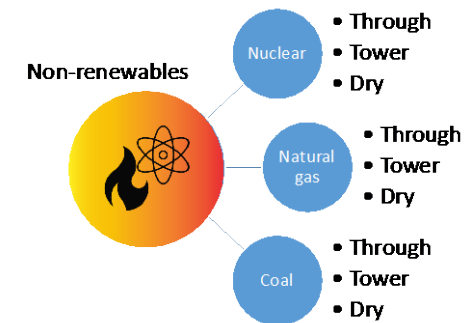
Tower



Dry

- The water footprint is divided between water **consumption** and water **withdrawal**.
- Water usage is, in most cases, tied to the cooling technology employed in the energy conversion system.

Many alternatives



Cooling Technologies

Renewables

Fuel Type	Cooling	Technology
PV	N/A	Utility Scale PV
Wind	N/A	Wind Turbine
CSP	Tower	Trough
		Power Tower
		Fresnel
	Dry	Trough
		Power Tower
	Hybrid	Trough
		Power Tower
	N/A	Stirling
Biopower	Tower	Steam
		Biogas
	Once-through	Steam
		Pond
Dry	Biogas	
Geothermal ¹	Tower	Dry Steam
		Flash (freshwater)
		Flash (geothermal fluid)
		Binary
	Dry	EGS
		Flash
		Binary
		EGS
	Hybrid	Binary
		EGS
Hydropower	N/A	Aggregated in-stream and reservoir

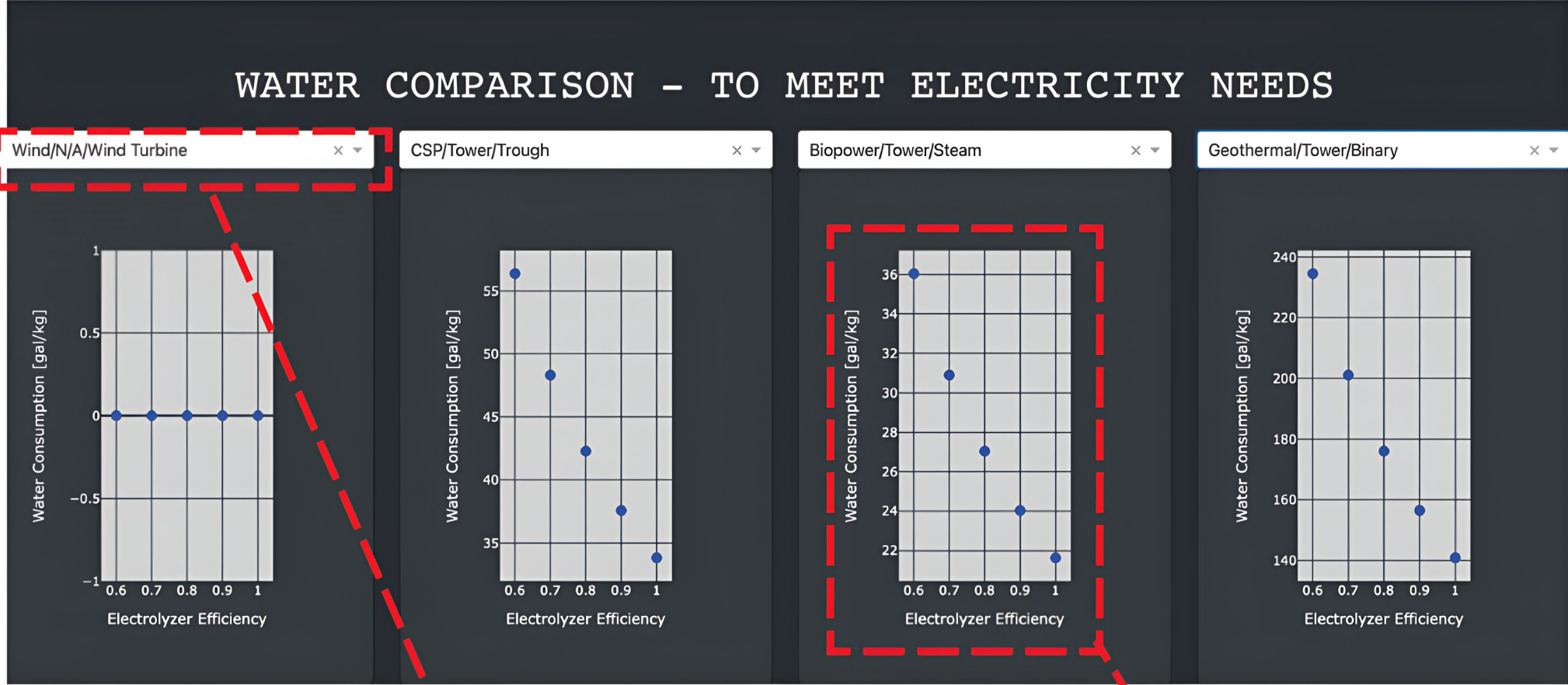
¹Most geothermal facilities can use geothermal fluids or freshwater for cooling.

Non-renewables

Fuel Type	Cooling	Technology
Nuclear	Tower	Generic
	Once-through	Generic
	Pond	Generic
Natural Gas	Tower	Combined Cycle
		Steam
		Combined Cycle with CCS
	Once-through	Combined Cycle
		Steam
	Pond	Combined Cycle
	Dry Inlet	Combined Cycle
Coal	Tower	Steam
		Generic
		Subcritical
		Supercritical
		IGCC
		Subcritical with CCS
	Once-through	Supercritical with CCS
		IGCC with CCS
		Generic
		Subcritical
Pond	Supercritical	
	Generic	
	Subcritical	
		Supercritical

Source:
 NREL/TP-6A20-50900 March 2011
 A Review of Operational Water Consumption and Withdrawal Factors
 for Electricity Generating Technologies
 Jordan Macknick, Robin Newmark, Garvin Heath, and KC Hallett

Water Consumption Comparisons



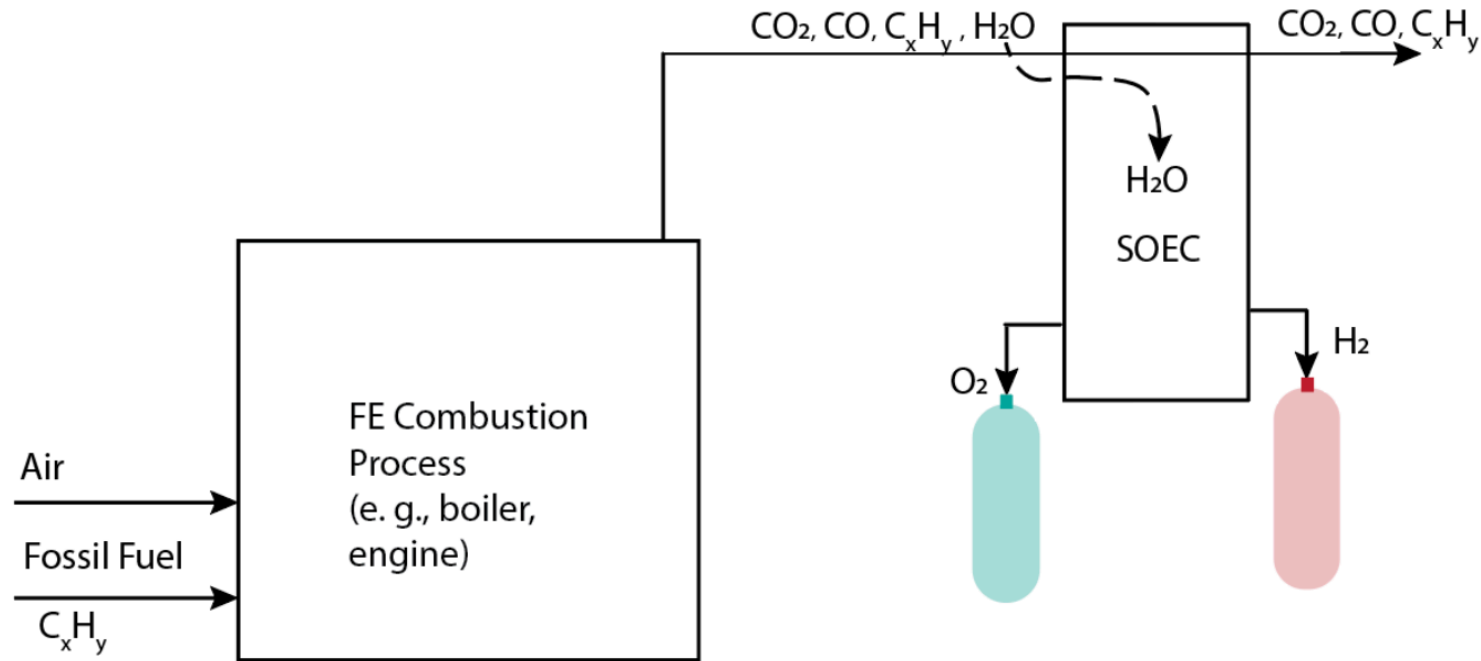
Drop down menu to specify user selected technology

Specific water consumptions for different needs according to electrolyzer efficiencies.

Dashboard Utility screenshot – A water requirements comparison tool.

Implicit Water Savings

- We have started exploring approaches to combine combustion processes and SOEC systems.
- We are interested in efficient ways to obtain flue gas composition (and water molar fraction in particular).

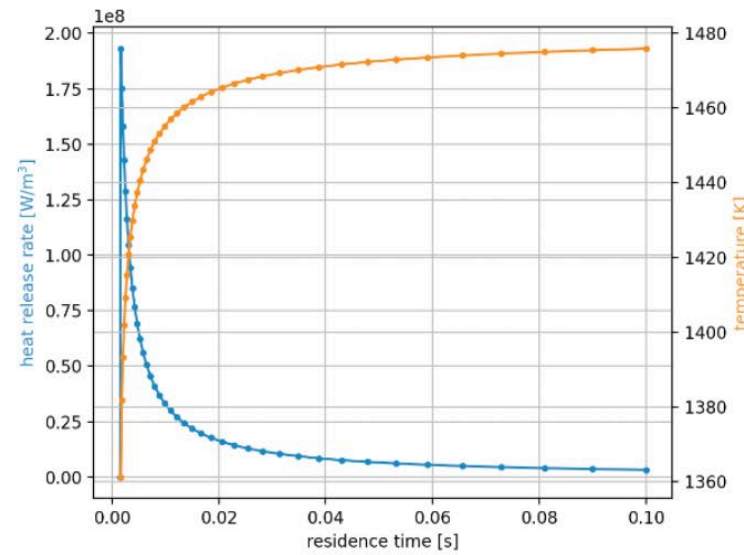


Schematic representation of potential use of flue gas water content in SOEC electrolysis.

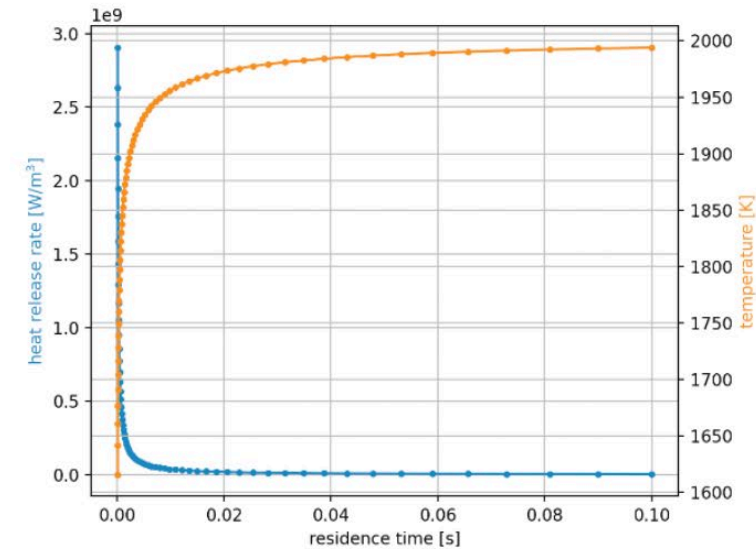
Implicit Water Savings



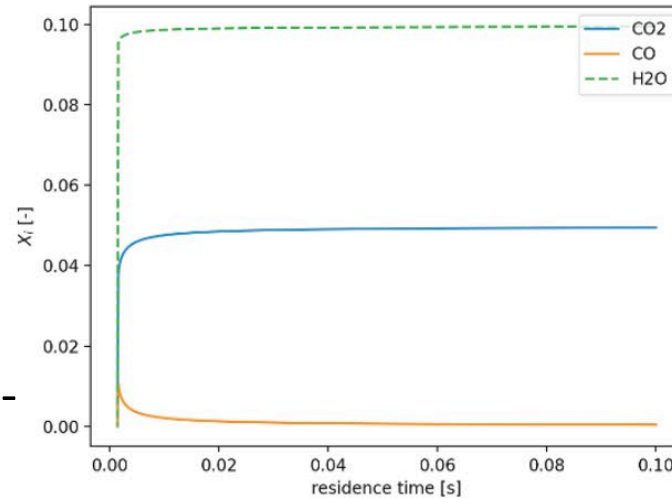
- Example: a steady-state combustor modeled as a well-stirred reactor (evaluation of the effect of residence time on heat release and temperature).
- CANTERA toolkit will be useful in future explorations of the combustion-SOEC.



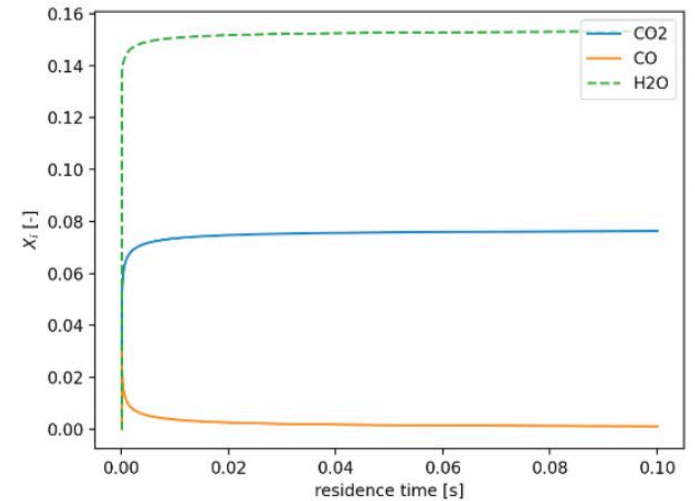
(a)



(b)



(c)



(d)

CANTERA results for a combustor burning natural gas with air. (a) Base case: equivalence ratio = 0.5. Output from combustor example: Heat release and Temperature. (b) Modified case: equivalence ratio = 0.5; (c) Added computation of Molar Fractions. Equivalence ratio = 0.5; (d) Added computation of Molar Fractions. Equivalence ratio = 0.8.

Source: Goodwin et al. (2023).

Levelized Cost of Hydrogen



Fundamental calculation used in the preliminary assessment of a H2 project.

Cost of Hydrogen and Electricity.

Considers the average net current cost of H2 generation over the lifetime of the plant.

Hydrogen plants:

- NG SMR with CCS
- NG SMR without CCS
- NG ATR with CCS

- Coal Gasification with CCS
- Coal Gasification without CCS
- Coal/Biomass Co-Gasification with CCS

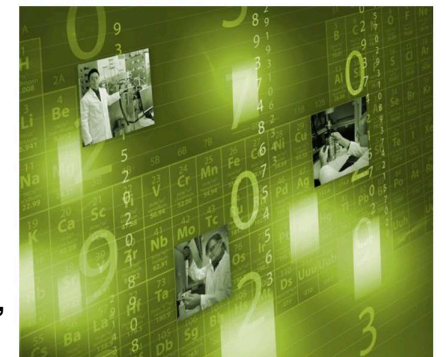
Sub-costs:

- Levelized Costs of Capital
- Levelized Fixed Operating Costs
- Levelized Variable Operating Costs
- Levelized Fuel Costs
- Levelized CO₂ Transportation and Storage Costs

Eric Lewis, Shannon, Matthew Jamieson, Megan S. Henriksen, H. Scott Matthews, John White, Liam Walsh, Jadon Grove, Travis Shultz, Timothy J. Skone, Robert Stevens (2022)



COMPARISON OF COMMERCIAL, STATE-OF-THE-ART, FOSSIL-BASED HYDROGEN PRODUCTION TECHNOLOGIES



April 12, 2022

DOE/NETL-2022/3241

Dynamic maps

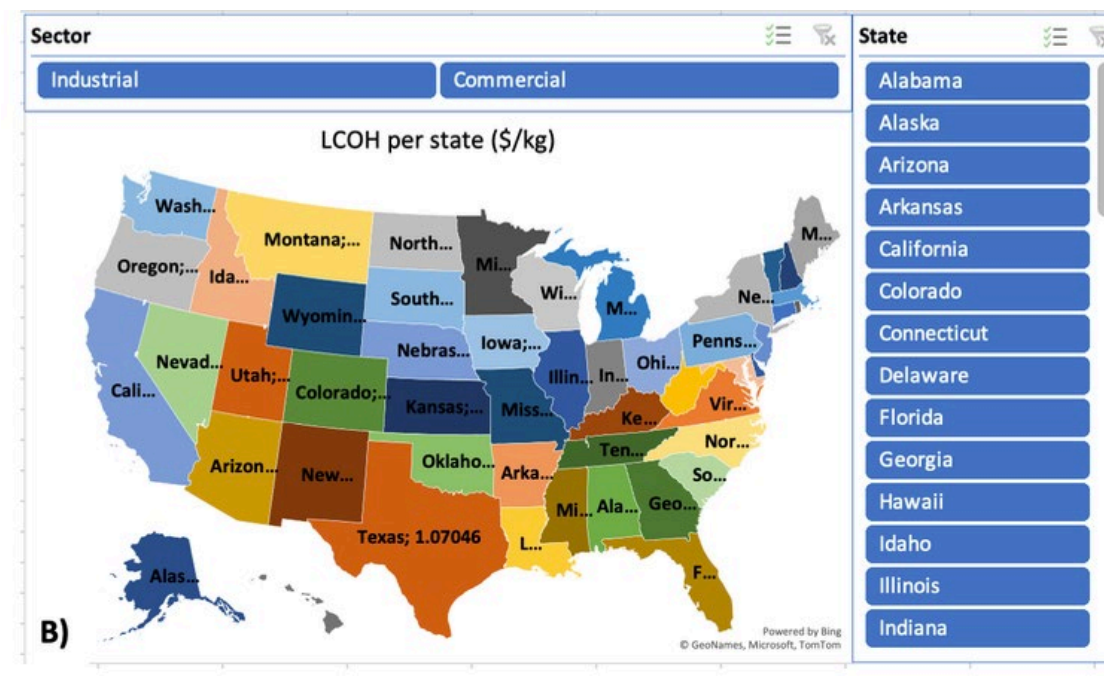
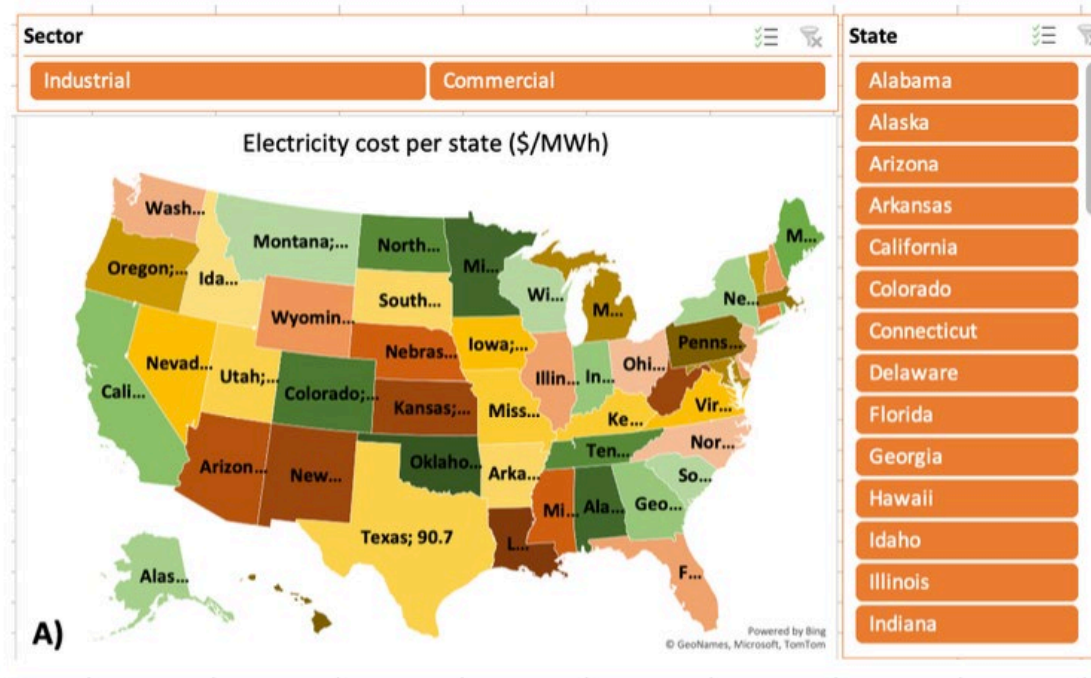
Development of dynamic maps to visualize and evaluate

- The maps are used to display quantifiable data supported in a dynamic and interactive solution.

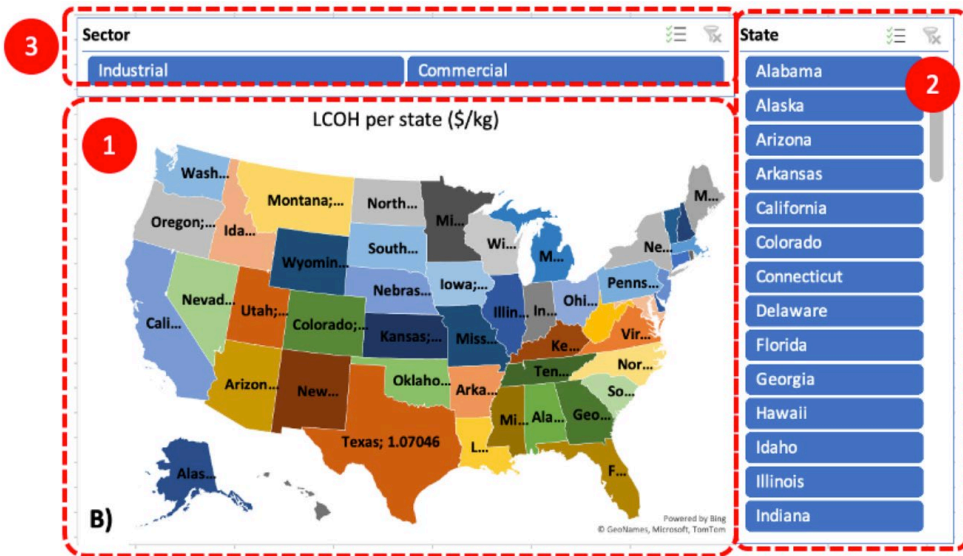
Electricity cost (\$/MWh)

Levelized cost of hydrogen (LCOH) (\$/kg)

in different regions of the U.S.



Dynamic maps

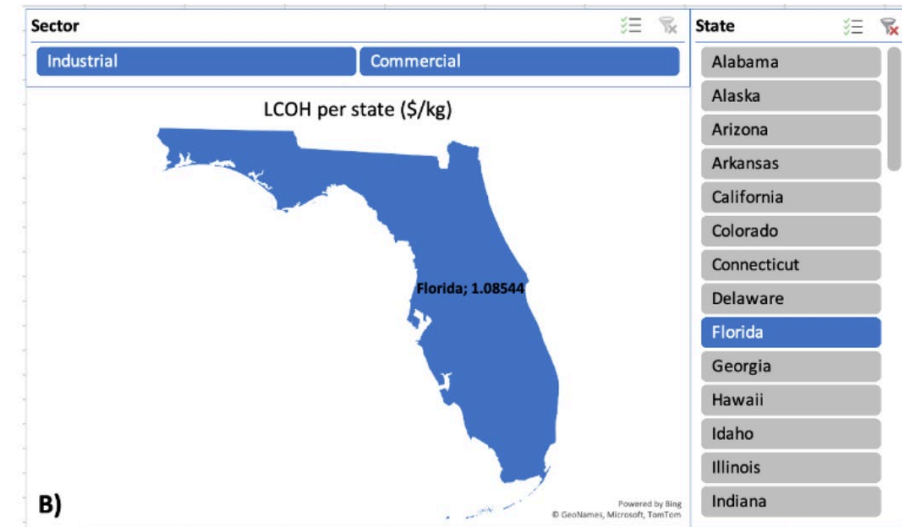


The user can Interact with the maps by:

- 1) LCOH Nationwide
- 2) Allows for state selection for closer look
- 3) Sectors: Industrial and Commercial

- LCOH for other technological routes will be considered for integration into the dashboard.

- More comprehensive overview of H2 economy.



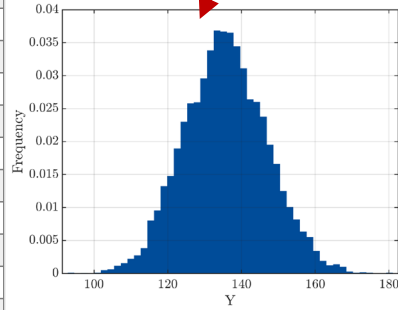
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Fugitive CH4 emissions (g CH4/MJ)	0.4050
Fugitive CH4 emissions (g CO2eq/MJ)	34.8330
Direct CO2 emissions (g CO2/MJ)	11.1132
CO2 capture rate	0.6500
Energy to power carbon capture	
CH4 consumed (g CH4/MJ)	5.9160
CO2 produced (g CO2/MJ)	16.2322
Fugitive CH4 emissions (g CH4/MJ)	0.2071
Fugitive CH4 emissions (g CO2eq/MJ)	17.8073
Direct CO2 emissions (g CO2/MJ)	16.2322
Indirect upstream CO2 emissions (g CO2/MJ)	6.4870
Total CH4 consumed (g CH4/MJ)	31.5235
Total CO2 emitted (g CO2/MJ)	39.6087
Total fugitive CH4 emissions (g CO2eq/MJ)	94.8856
Total emissions (g CO2eq/MJ)	134.4944

Emissions



Uncertainty



HYDROGEN ECONOMY

Effects of Hydrogen generation on the US electric resources.

Production Type

- Shell Gasif. w/o CCS
- SMR w/ CCS
- SMR w/o CCS

State: Kansas
Climate Zone: 4A

Fuel Cost: 0 to 10

Capacity Factor: 0 to 1

Impact of H2 Integration (e.g., buildings)

CO2 eq. Emissions

BUILDING TYPE: SINGLE FAMILY RESIDENTIAL

Annual Energy Cost

Emission	gray H2	blue H2 w/o flue gas capture	blue H2 with flue gas capture
SMR process		null	null
CH4 consumed	14.035	14.035	14.035
Co2 produced	38.50875	38.50875	38.50875
Fugitive CH4 emissions	0.491225000000000	38.50875	38.50875
Fugitive CH4 emissions	42.24535000000001	42.24535000000001	42.24535000000001
Direct CO2 emissions	38.50875	5.7763125	5.7763125
CO2 capture rate	0	0.85	0.85
Energy to drive SMR			
CH4 consumed	11.57241717791410	11.57241717791410	11.57241717791410
CO2 produced	31.751999999999999	31.751999999999999	31.751999999999999

Annual Electric Bill (\$) vs Percent of energy met by H2

Load: Daily Variance

Levelized Cost of Hydrogen



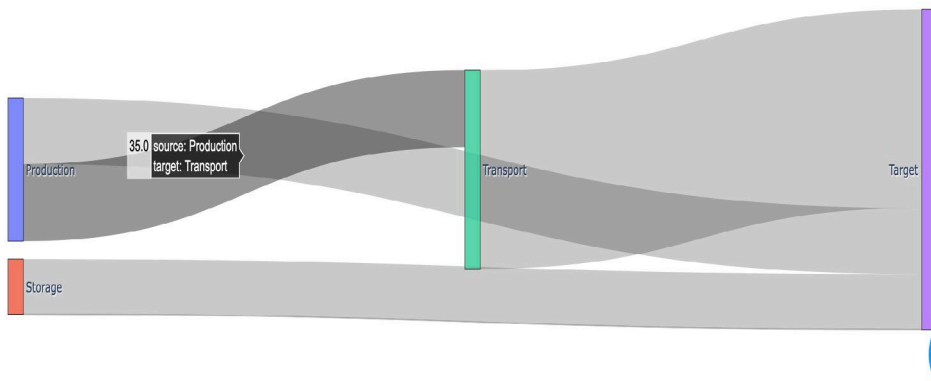
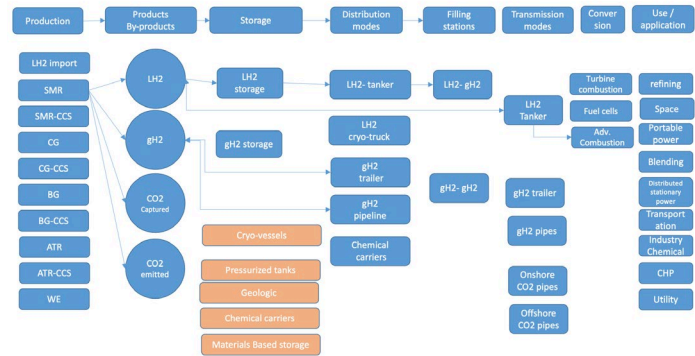
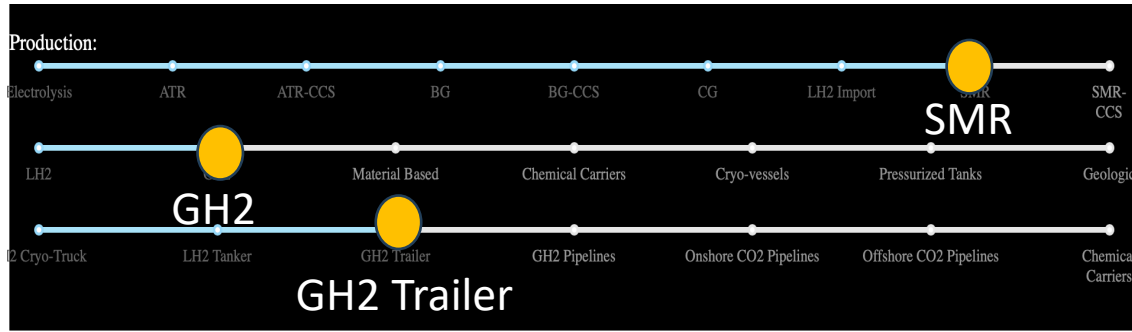
Sliders for key parameters

Geographically dependent building load variance and electricity cost

LCOH

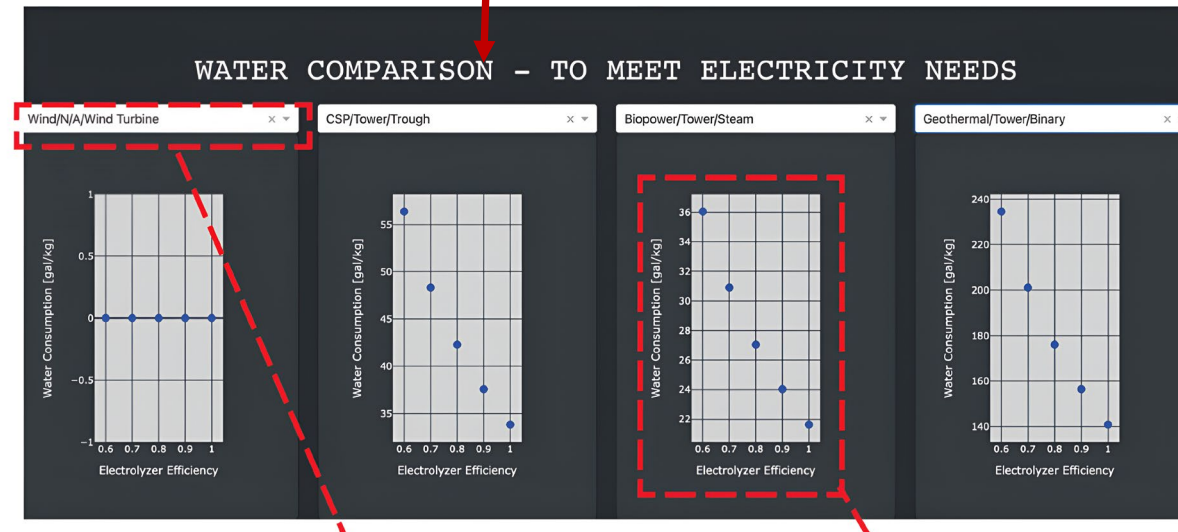


Comparison among H2 routes



Water Consumption Comparisons

Water comparisons among electricity sources for hydrogen electrolysis



Drop down menu to specify user selected technology

Specific water consumptions for different needs according to electrolyzer efficiencies.



Final Considerations

Future plans

In this project:

a. Finalize the H2Dash with information from the last reports:



1) LCOH and electricity costs for different end-use sectors (dynamic maps);



2) Use of water to produce electricity to generate H₂ via electrolysis.

b. Submission of collaborative publications:



1) Journal publication: manuscript being prepared reviewing the integration of fossil fuels and different technologies in the H₂ economy;



2) Conference: participation and publication of a paper summarizing the main results of the project.



Final Considerations

After this project:

We plan to explore as a next project:

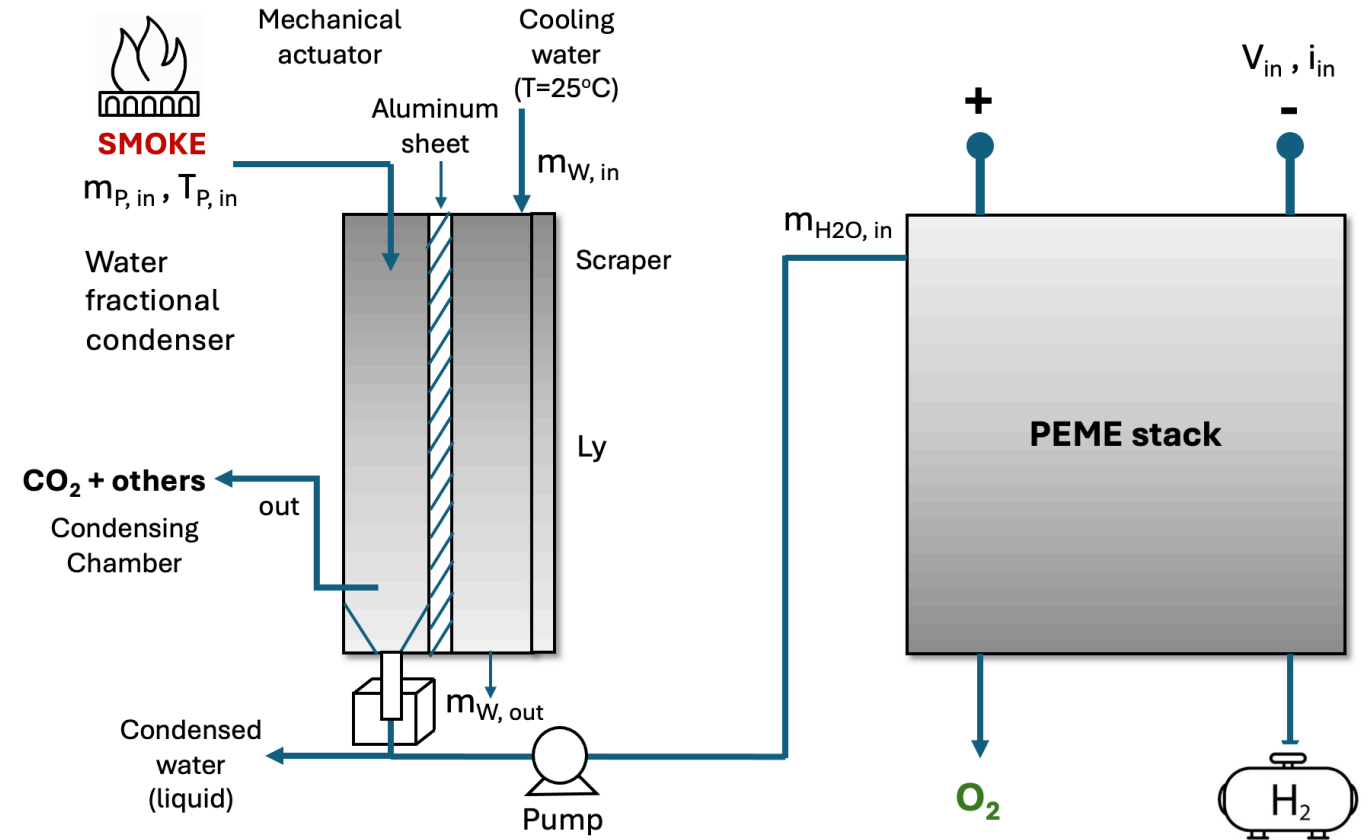
Fossil fuel emissions derived water for H₂ production

Using a Proton Exchange Membrane Electrolyzer Stack (FFEDW / PEME stack)

*Could be used as reverse/regenerative fuel cell (either as a Fuel Cell or [Water Electrolysis](#))

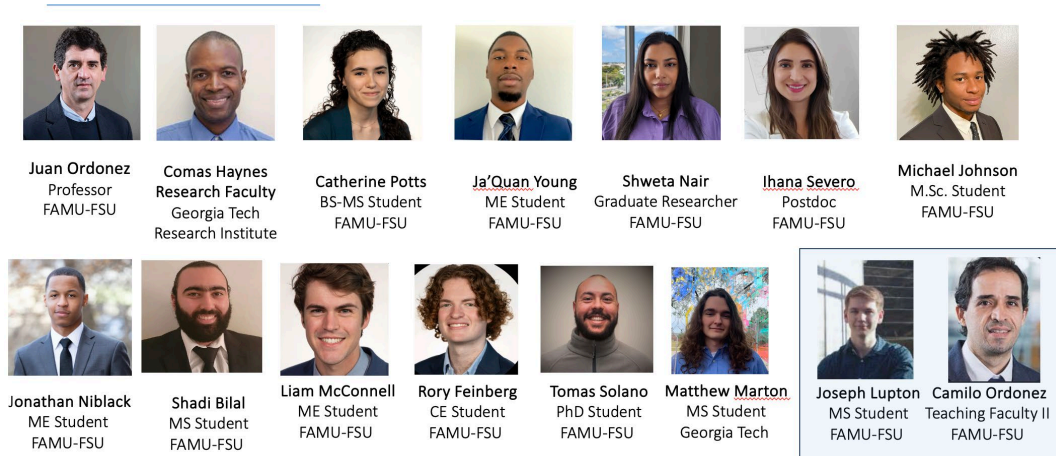
m_p – products of combustion:

$\text{CO}_2 + \text{H}_2\text{O} + \text{others (NO}_x, \text{SO}_x, \text{CO, dioxins, furans, particulates...)}$



Other achievements

- Workforce training



- Training and development of students in the use of new tools and water-CO2-Energy relevant processes,



- PI engaged with colleagues at UFPR (Brazil) on H₂ generation strategies for transportation;
- Co-PI involved in H2Hub activities.

Appendix

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Thank you!

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