Development of a Techno-Economic Analysis Framework for a Solar Thermochemical Fuel Production Process

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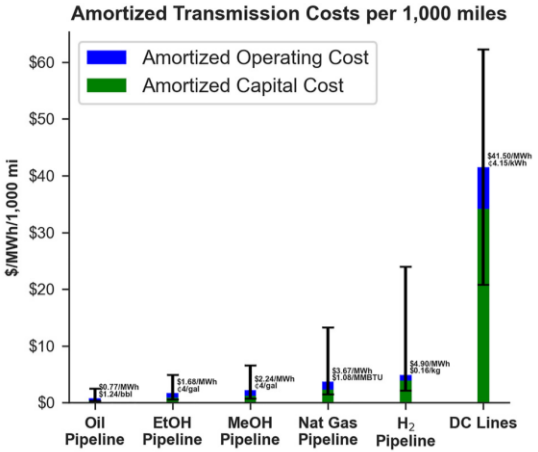
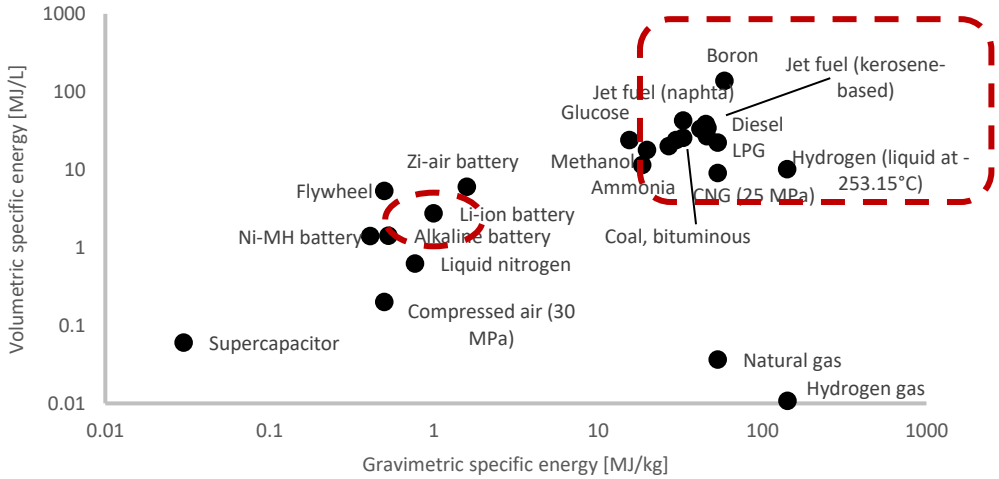
Background and Motivation (1)

- Liquid hydrocarbon fuels are critical and will remain part of the energy mix:
  - High specific energy (gravimetric/volumetric)
  - Ease of transport and storage, existing infrastructure (~800 Billion USD [2])
  - “Electrify everything” vs grid expansion and rising demand (data-centers)





[1] D. DeSantis, B. D. James, C. Houchins, G. Saur, and M. Lyubovsky, “Cost of long-distance energy transmission by different carriers,” *iScience*, vol. 24, no. 12, p. 103495, Dec. 2021, doi: 10.1016/j.isci.2021.103495.

[2] https://www.precedenceresearch.com/oil-and-gas-infrastructure-market

Background and Motivation (2)

- Syngas (H_2:CO mixture) is a chemical precursor that can be converted into fuels/chemicals via a variety of gas-to-liquid (GTL) technologies
- Today, syngas is produced via steam methane reforming (SMR) or coal gasification and is used in H_2 production (as an intermediate) or iron reduction
- CO_2 and H_2 can be converted to syngas via the *Reverse Water-Gas Shift (RWGS)* reaction:

$$CO_2 + H_2 \rightarrow CO + H_2O$$

- Catalytic RWGS currently considered as a pathway to synthetic fuels (e-fuels / Power-to-X). The following challenges/limitations exist:
  - Low CO_2 conversion -> **high energy/CAPEX** for downstream separation
  - High temperatures and excess H_2 are needed to improve conversion -> **higher CAPEX/OPEX**, challenges in tailoring syngas composition

<u>Our proposition: chemical looping RWGS process</u>

Chemical Regenerator Effect

Chemical regenerator design: using an oxygen carrier that can have continuous chemical potential while sequentially flowing reducing/oxidizing agent from opposite direction (analogy to thermal regenerator):

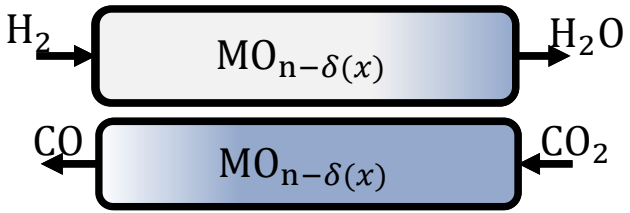
$$H_2 + \frac{1}{\Delta\delta} MO_{x-\delta_{ox}} \rightarrow \frac{1}{\Delta\delta} MO_{x-\delta_{red}} + H_2O$$

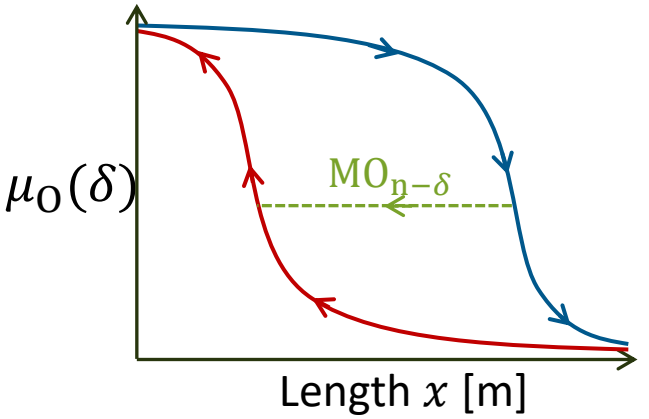
$$CO_2 + \frac{1}{\Delta\delta} MO_{x-\delta_{red}} \rightarrow \frac{1}{\Delta\delta} MO_{x-\delta_{ox}} + CO$$

With $\Delta\delta = \delta_{red} - \delta_{ox}$

This concept experimentally obtained **90% CO_2 conversion** at 800°C without excess H_2 when using CeO_2 (compared to ~55% when using CeO_2 catalytically at the same conditions)

Countercurrent regenerative reactor

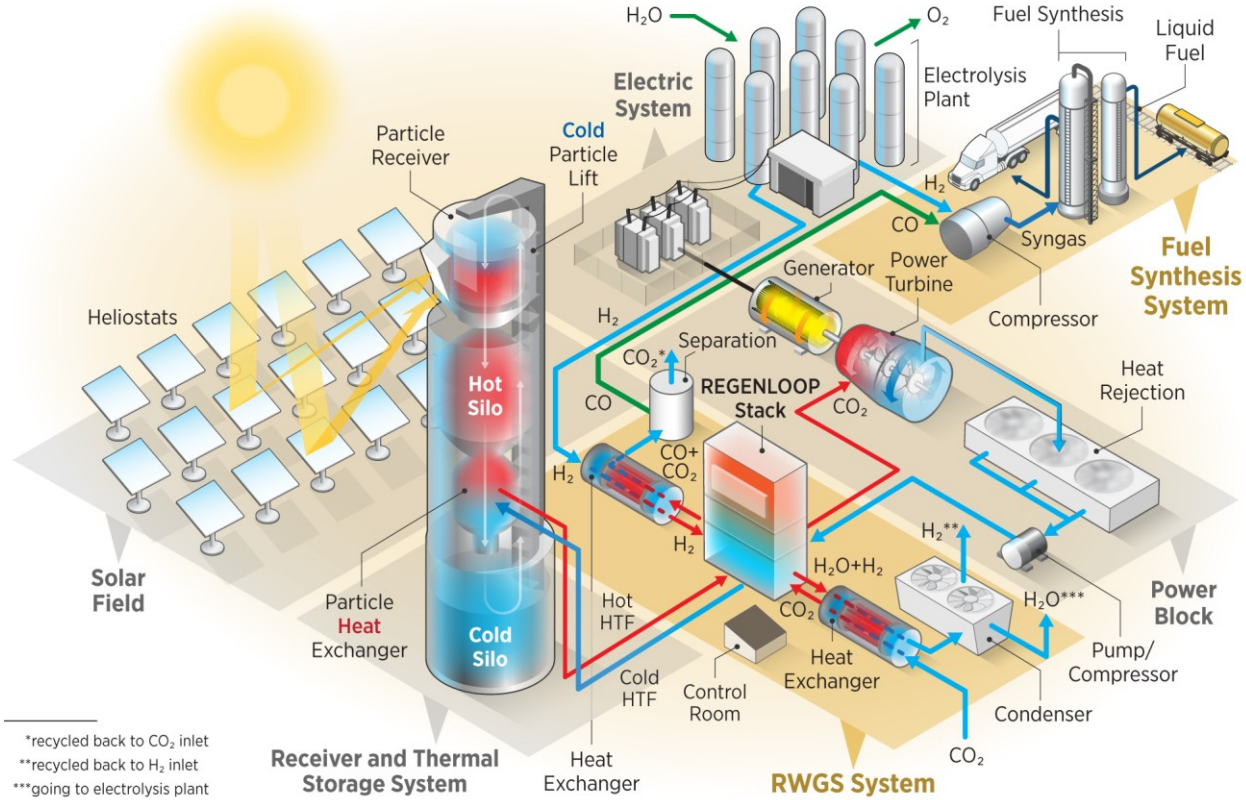




[3] B. Bulfin, M. Zuber, O. Gräub, A. Steinfeld, Intensification of the reverse water–gas shift process using a countercurrent chemical looping regenerative reactor, Chem. Eng. J. 461 (2023). https://doi.org/10.1016/j.cej.2023.141896.

Project Overview

- RWGS system with high energy and CO_2 conversion efficiencies
- CST-compatible reactor for Gen3 CST temperature range (600 - 800°C)
- Simple, scalable, and cost-effective design
- Development and demonstration of the RWGS: increasing TRL and de-risking
- Evaluate pathway to commercialization

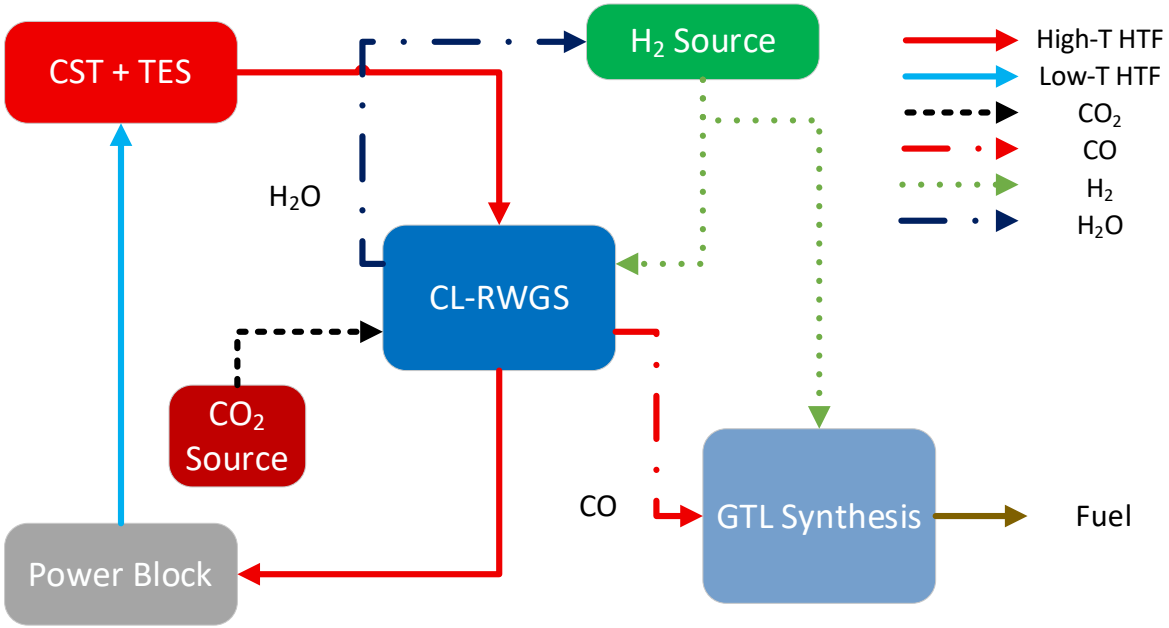


Credit: Alfred Hicks @ NREL

CST: concentrating solar thermal

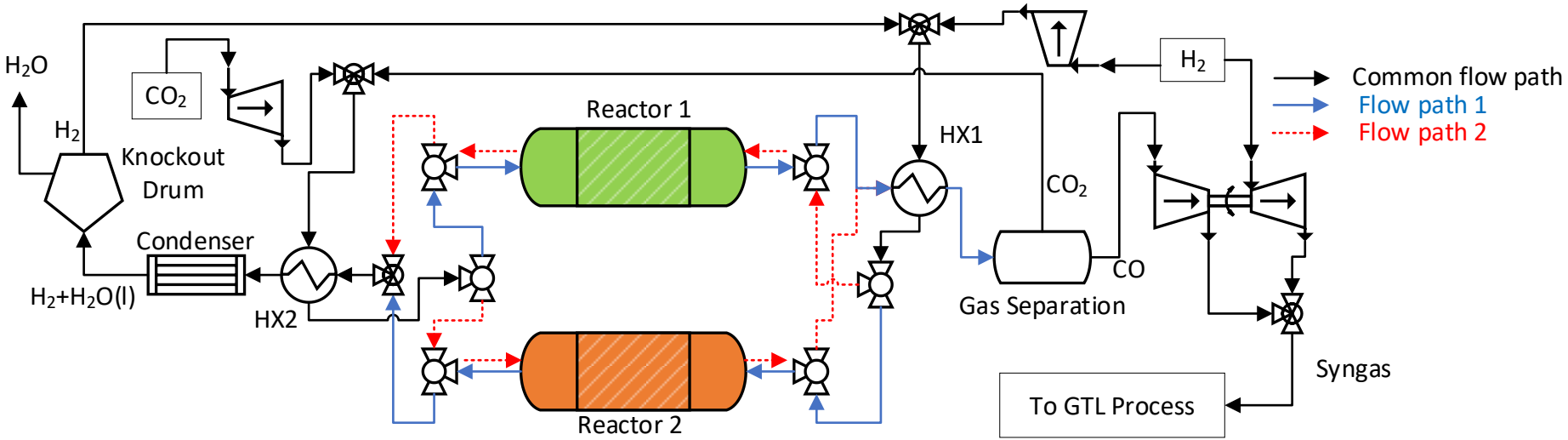
General System Design

- CST+TES for high capacity factor
- Bottoming power cycle
- Flexible syngas composition (H_2:CO)
- High CO_2 conversion: lower downstream separation
- Avoiding unwanted methanation reaction



CL-RWGS Process Integration

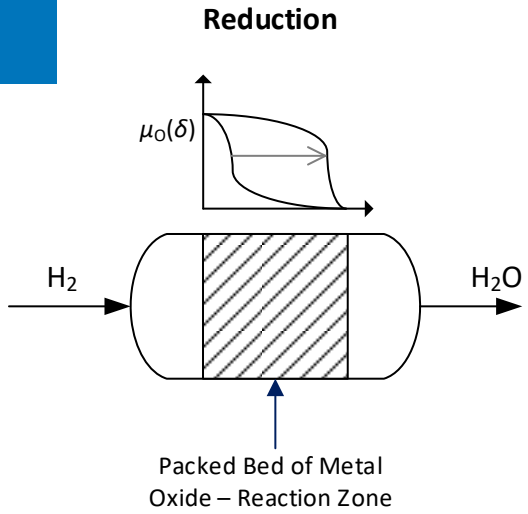
Downstream GTL process requires high-pressure steady-state steady-flow syngas:



- Gas separation is minimal; might be **fully omitted** based on CO_2 conversion and GTL requirements
- REGENLOOP reactors (CL-RWGS reactors): shell-and-tube heat exchange reactor type
- Sensible gas-gas heat recovery between feed and effluent of each reactor
- Recycling unconverted H_2 stream

Reactor Reduced Order Modeling

- Reduced order modeling developed by UCC and NREL
- Discretized batch equilibrium model for thermodynamic limits
- Using pre-calculated chemical potential curves
- Very rapid solution (avoid heavy numerical solutions)
- Validated against previous 1D model
- Allows for exploration of a large parameter space – useful for the TEA activities



For more details on the reactor ROMs:

[4] R. Ghotkar, R. Klostermeyer, J. Martinek, B. Bulfin, A. Lidor, "Modeling of a Countercurrent Regenerative Chemical Looping Reactor For the Reverse Water Gas Shift Reaction", *American Society of Mechanical Engineers Digital Collection* (in press).

[5] B. Bulfin, R. Ghotkar, A. Lidor, "Thermodynamic Modeling of Countercurrent Chemical Looping Reverse Water Gas Shift Process for Redox Material Screening", *Chemical Engineering Journal* (under review).

General Modeling Approach

Four subsystems

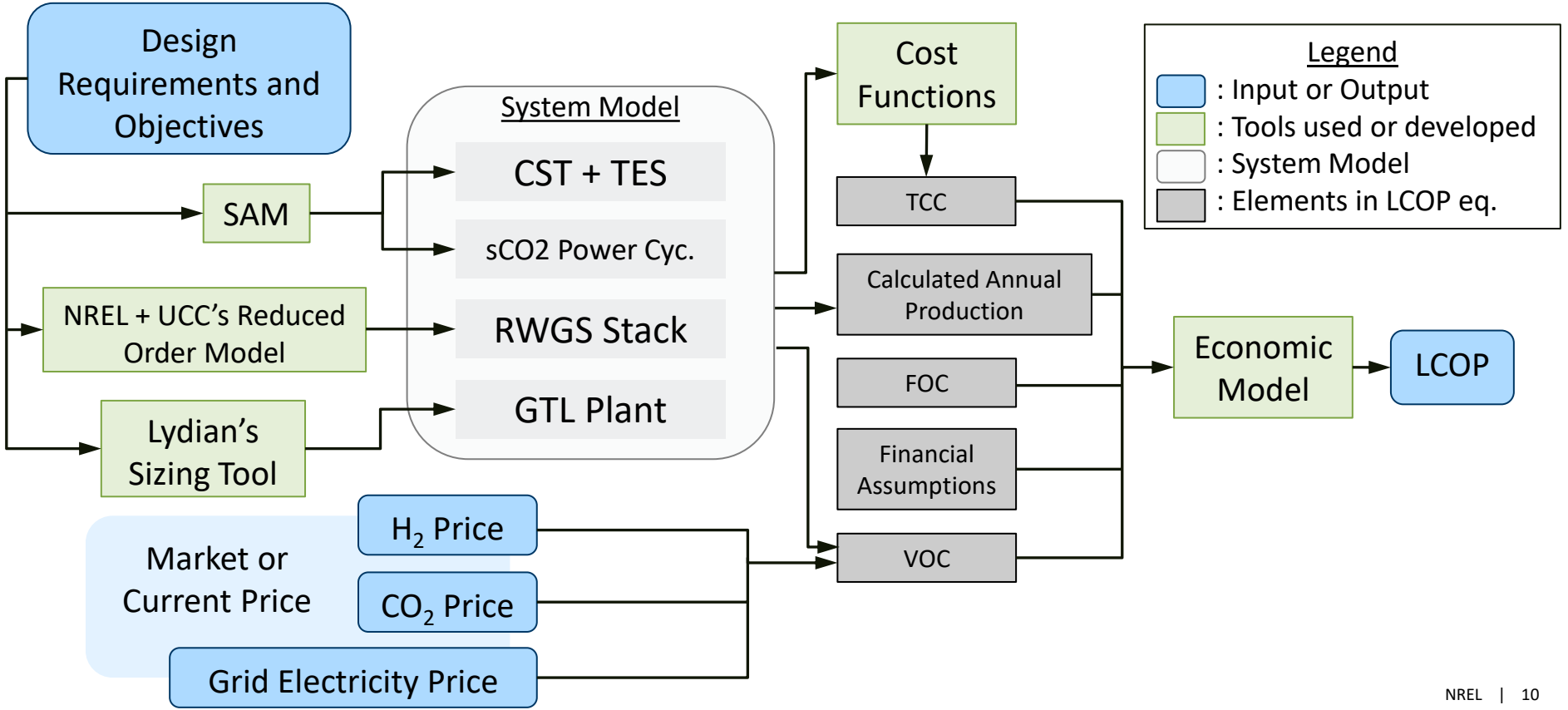
- CST+TES – energy input **(NREL's SAM [6])**
- Chemical looping RWGS (REGENLOOP) – syngas production **(NREL/UCC ROM)**
- Power Block (bottoming CST heat after CL-RWGS) **(NREL's SAM [6])**
- Gas-to-liquid (GTL) – getting to final product **(Lydian's proprietary model)**

Operational mode:

1. Steady-state GTL
2. Quasi-steady-state REGENLOOP subsystems (i.e., constant syngas->fuel production at stable conditions)
3. Solar intermittency is absorbed/buffered by the CST+TES

[6] Blair et al., *NREL Tech. Rep.* **2014**, NREL/TP-6A20-61019.

TEA Framework



Quantifying the LCOP

Generalized levelized cost of product (LCOP) using a simple fixed-charge rate (FCR) method [7,8]:

$$\mathrm{LCOP} = \frac{(\mathrm{FCR} * \mathrm{TCC} + \mathrm{FOC})}{\mathrm{AP}} + \mathrm{VOC}$$

LCOP : Levelized cost of product [$/gal]
TCC : Total capital cost [$]
FOC : Fixed operating cost [$/yr]
AP : Annual production [gal /yr]
VOC : Variable operating cost, normalized with production [$/gal]

TCC to calculate levelized cost of product (syncrude):

$$\mathrm{TCC} = C_{\mathrm{CST}} + C_{\mathrm{sCO_2}} + C_{\mathrm{RWGS}} + C_{\mathrm{GTL}}$$

CST : Concentrating solar thermal
sCO2 : sCO2 power cycle
RWGS: Reverse water-gas shift stack
GTL : Gas-to-liquid plant

FOC and VOC :

$$\mathrm{FOC} = C_{\mathrm{labor}} + C_{\mathrm{land}} + C_{\mathrm{insur}} + C_{\mathrm{maint}}$$

$$\mathrm{VOC} = C_{\mathrm{H_2}} + C_{\mathrm{CO_2}} + C_{\mathrm{electricity}}$$

[7] Hughes et al., *NETL Tech. Rep.*, DOE/NETL—2023/3870.
[8] Martin et al., *Environ. Sci. Technol.* **2024**, 58, 13737-13747.

Feasibility Study of the System Design

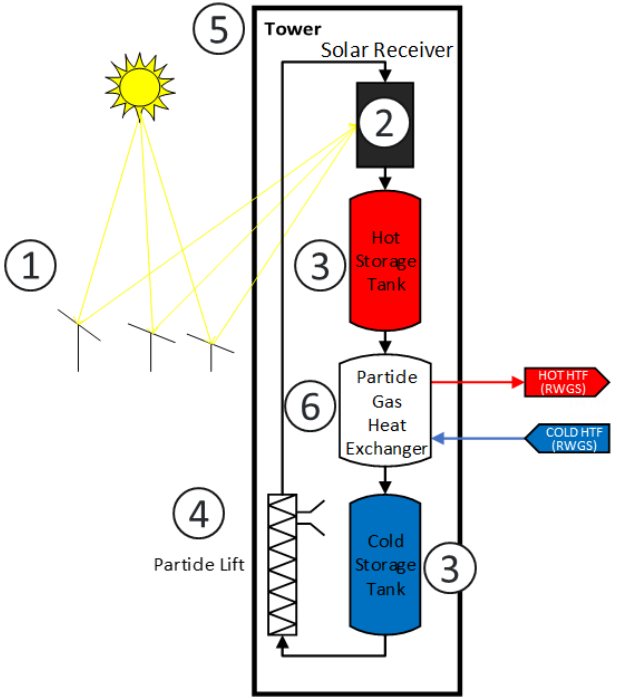
Subsystem Design: CST (1)

Sized with target of 150 MW_{th} solar power input and the following:

- Nominal DNI = 950 W/m^2
- Full storage duration = 10 - 14 hr
- HTF (bauxite particle) hot temp = ≥ 900°C
- Solar Multiple = ~3

Size and calculate cost of the following component:

1. Heliostat Field
2. Receiver
3. Hot and Cold Storage
4. Particle Lift
5. Solar Tower
6. Particle-Gas HX



Schematic of the CST and TES subsystem along with 6 main components

Subsystem Design: CST (2)

Optimization for field, receiver, and tower sizing is conducted for a *3 falling particle curtain receiver* design:

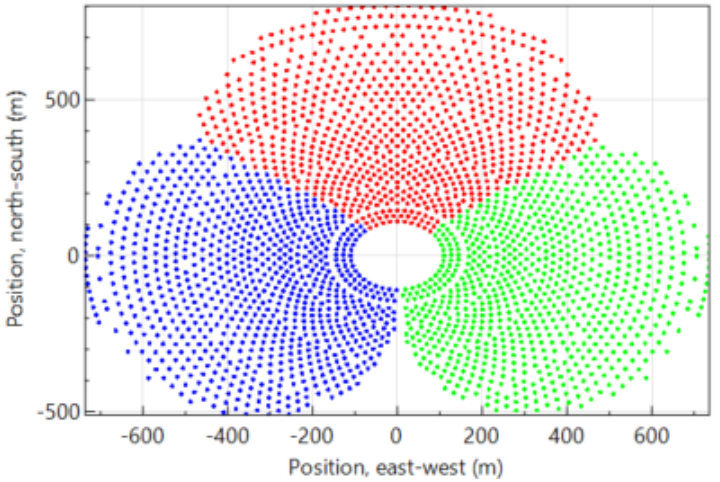
- 7.5 x 7.5 m receiver height x width.
- 147 m tower height.
- 2,441 heliostat count.

Solar field sized with solar resource and weather data in Dagget, CA:

- 1.5 km (east-west) and 1.3 km (north-south).
- 413 acres total land area.

Optimization summary for the CST components using SAM[6].

Optimized Variable	Value	Unit
Receiver height x width	7.5 x 7.5	m
Receiver azimuth	[108, 0, -108]	°
Tower height	147	m
Heliostat count	2441	-



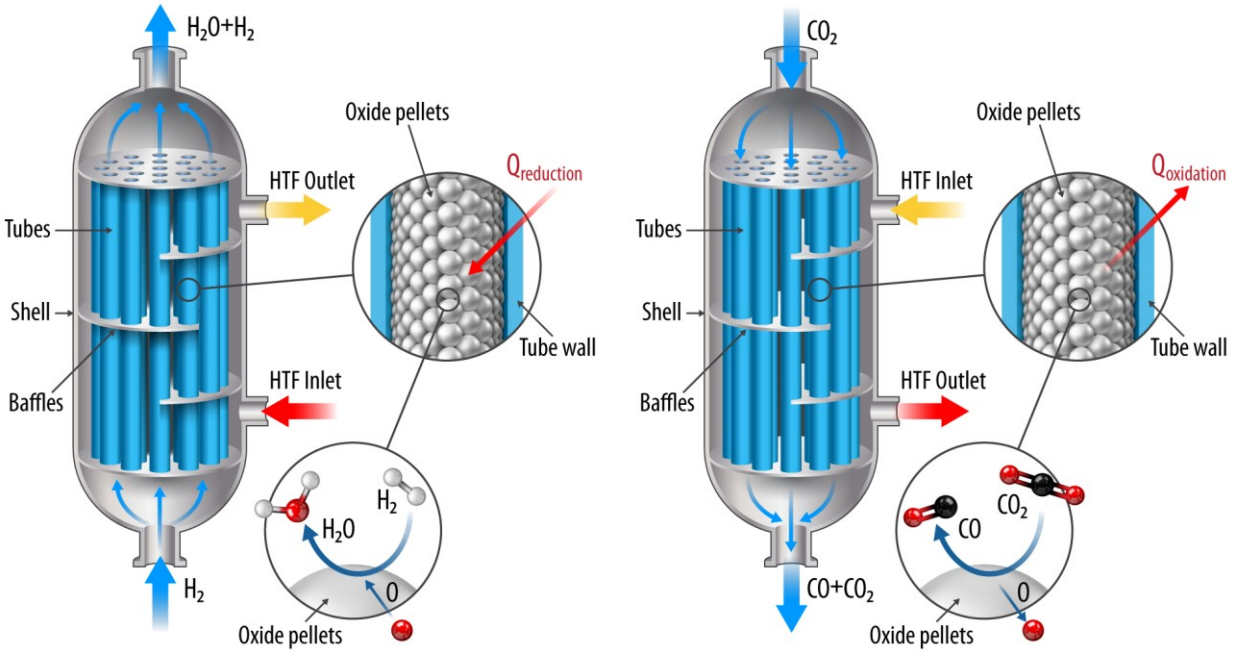
Heliostat field layout result from SAM

[6] Blair et al., *NREL Tech. Rep.* **2014**, NREL/TP-6A20-61019.

Subsystem design: RWGS Reactor

RWGS reactor is designed as a shell and tube heat exchanger - reactor with consideration:

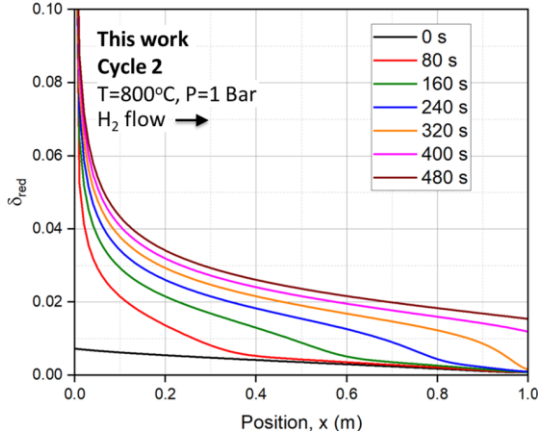
- Cost model developed with raw material and fabrication estimation.
- Tube is Nickel alloy stainless steel with coated inner wall.
- Shell is low alloy steel with inner refractory lining.

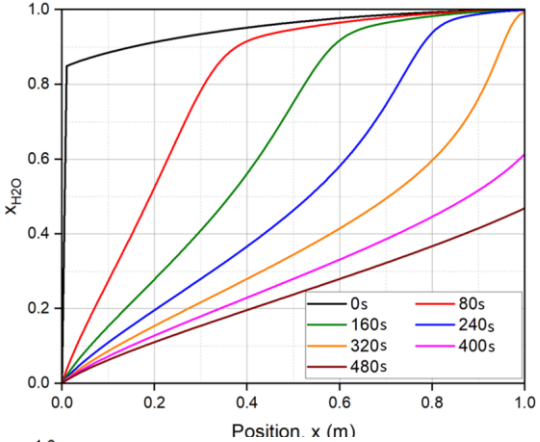


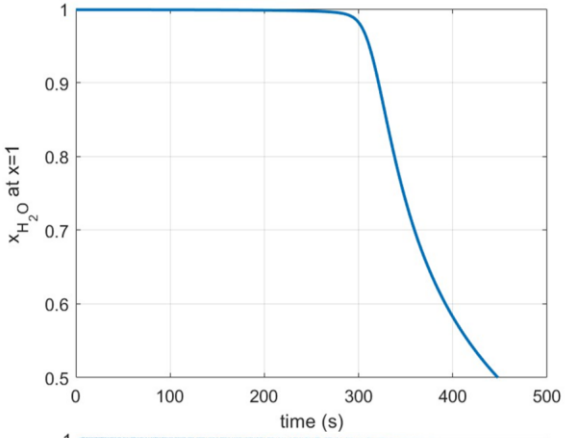
Reactor design as shell and baffled tube. The tube bank contains packed bed of oxide pellets (credits: Al Hicks @ NREL).

Reactor Modeling: Sample Results

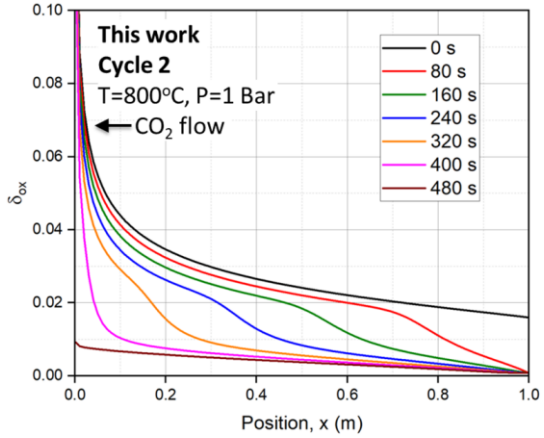
Reduction

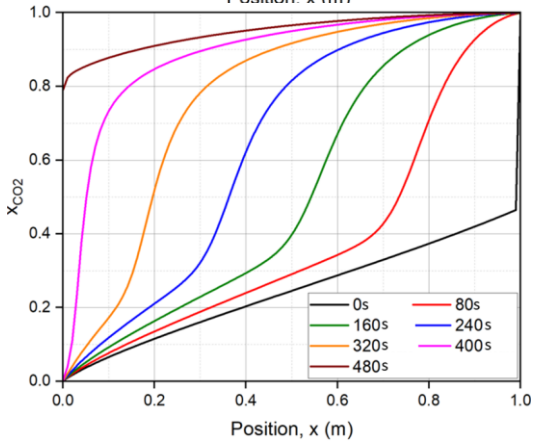


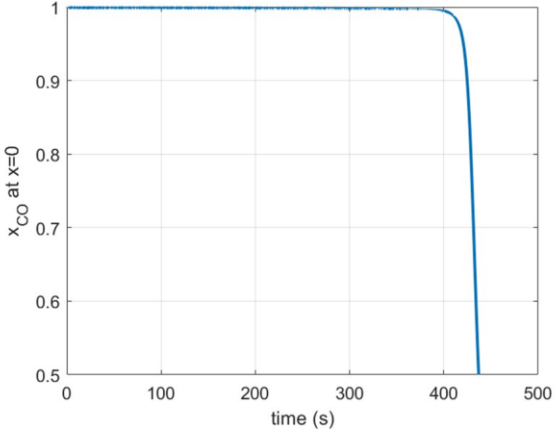




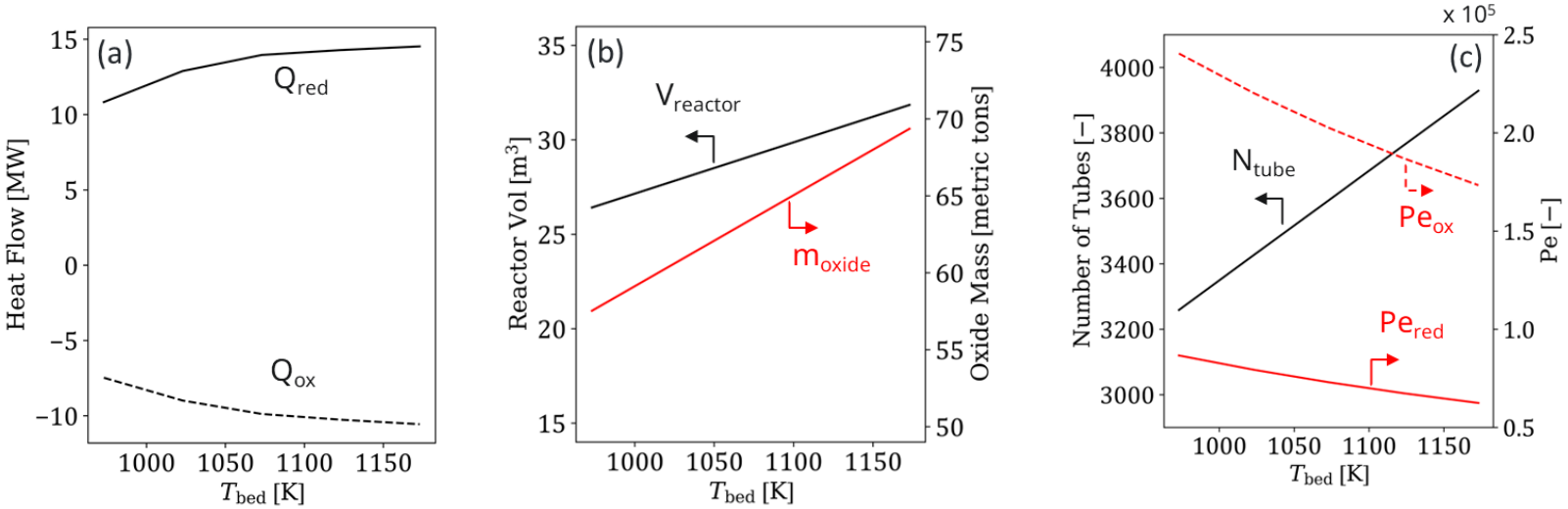
Oxidation







Subsystem design: RWGS Reactor

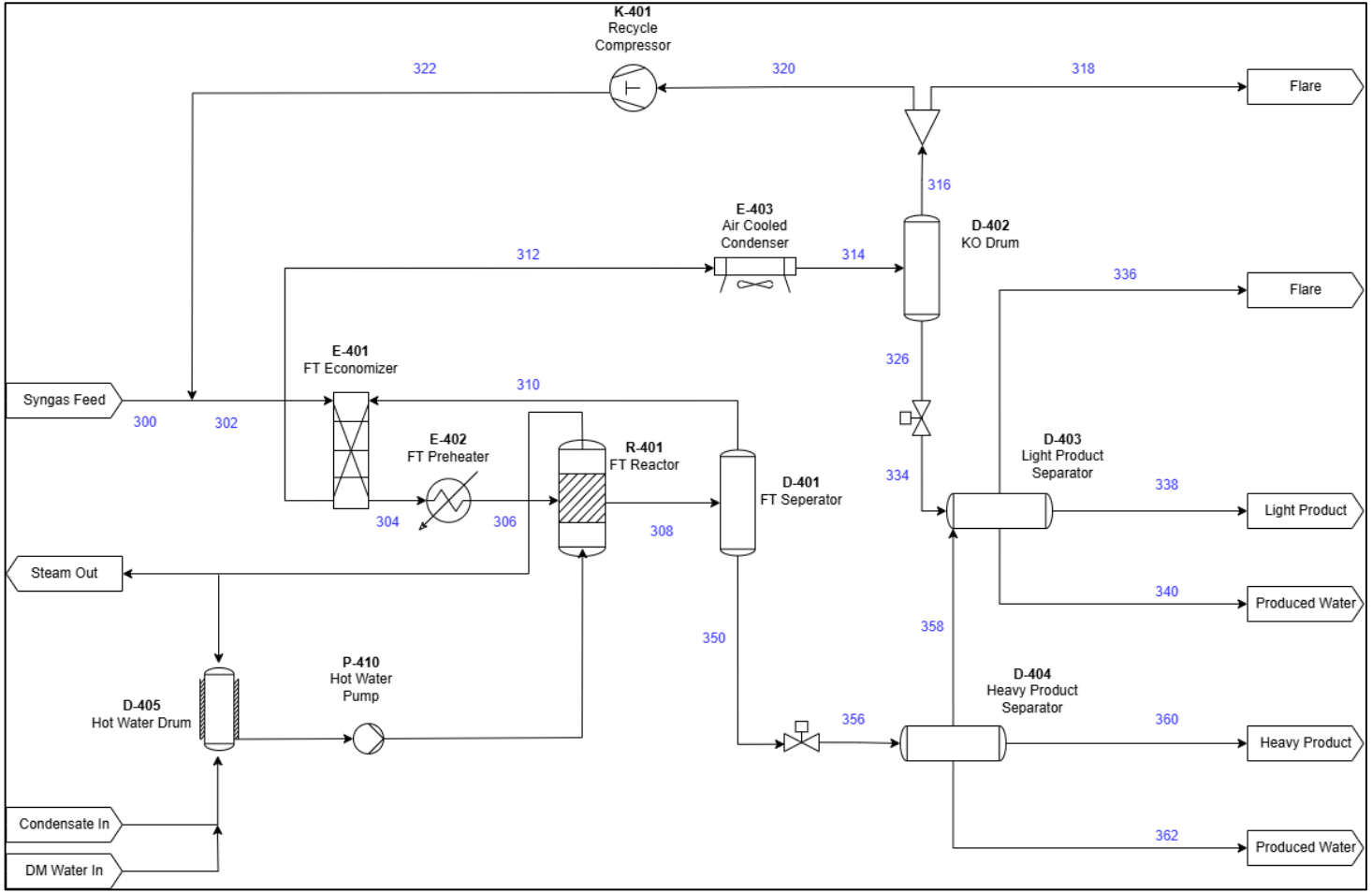


- Sized to meet the downstream GtL requirements of n_{H2}/n_{CO} = 2.05 and syngas flow = 1260 kmol/h → H_2 flow = 847 kmol/h and CO flow = 413 kmol/h.
- At 95% CO_2 conversion, inlet CO_2 flow required is ~435 kmol/h.
- Sizing results are shown for Heat Duty, Volume, Oxide Mass, Tube count for 0.10 m 4 m tube and $Ce_{0.85}Zr_{0.15}O_2$.

GTL Model Process Design

- Multipass FT reactor with recycling loop
- Co-based lower alpha (0.87) FT catalyst
- PFD, HMB, Aspen Plus models
- AACE Class V cost estimates (Aspen Capital Cost Estimator and internal quotes)

*PFD: Process Flow Diagram
HMB: Heat and Mass Balance



Subsystem design: GTL Plant

Gas-to-Liquids (GtL) Model: **System Performance Summary**

Summary of Outputs:

- Syncrude output of 950 Bbl/d
- Total CO conversion of 95%
- Syngas → Liquid Product LHV Efficiency : 46%
- Total System Efficiency : 87%

Future Technology Considerations:

- Flare Gas Waste Heat Recovery
- Flare Gas reforming / Chemical looping
- FT Process recycle
- Steam utilization / LT Steam power generation

Model Summary	Value	Units
Syngas Inlet Flow (MW = 10.5)	13279	kg/h
Syncrude Yield	950	Bbl/d
Product Split & Mass Balance		
Light Prod. (Mol Wt. = 125)	3356 (733)	kg/h (Bbl/d)
Heavy Prod. (Mol. Wt. = 196)	973 (217)	kg/h (Bbl/d)
Purge / Flare (Mol Wt. = 23)	1836	kg/h
Water	7113	kg/h
Energy Input / Output		
Cooling Duty Req'd	4500	kW
Air Cooler Power	86	kW
Steam Duty Produced (225 °C)	18000	kW
System Performance		
Liquid Product LHV Efficiency	46%	-
Total LHV Efficiency	87%	-

Cost Estimation and TEA Results

Summary of Cost Functions and Estimation

No	Sub-System	Cost Model Source	Total Capital Cost (TCC)
1	Concentrating Solar Thermal (CST) and Thermal Energy Storage (TES) at 150 MW_{th} field	SAM [6], DOE Sunshot 2030 [10], Ma et al. [11,12].	$ 261.3 M
2	sCO2 Power Cycle at 10 Mw_e output	SAM [6], Weiland et al. [13].	$ 50.8 M
3	Chemical Looping – Reverse Water Gas Shift at 33 x 10^6 kmol syngas/year yield.	NREL's developed model complemented with commercial pricing of auxiliary equipments.	$ 114.2 M
4	Gas to Liquid Plant at 1.04 x 10^6 Bbl syncrude/year yield.	Lydian's proprietary data.	$ 33.6 M

* TCC includes both direct and indirect cost for the investment of each subsystem.

[12] Ma et al., *NREL Tech. Rep.* **2023**, NREL/TP--5700-84728.
[13] Weiland et al., in *Proc. ASME Turbo Expo* **GT2019** (2019): 90493.

[12] Ma et al., *NREL Tech. Rep.* **2023**, NREL/TP--5700-84728.
[13] Weiland et al., in *Proc. ASME Turbo Expo* **GT2019** (2019): 90493.

LCOP Estimation (1)

Feed Price of H_2 and CO_2

H_2 price is varied between $ 2 – 10 per kg of H_2:

- Considering high uncertainty in current green H_2 process.
- Also looking at sensitivity of LCOP to grey - green H_2.

CO_2 price is varied between $ 50 – 200 per metric tons of CO_2:

- Depends on sources DAC, CCUS, Biogenic, etc.
- Price per kg compared to H_2 is low, hence low sensitivity to CO_2 price expected.

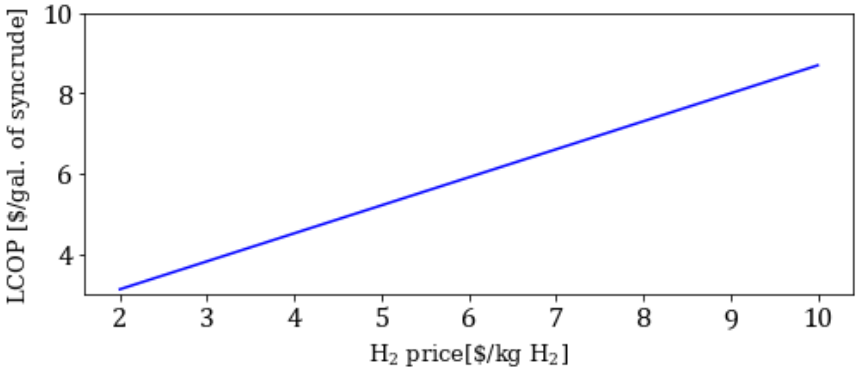
Financial Decisions

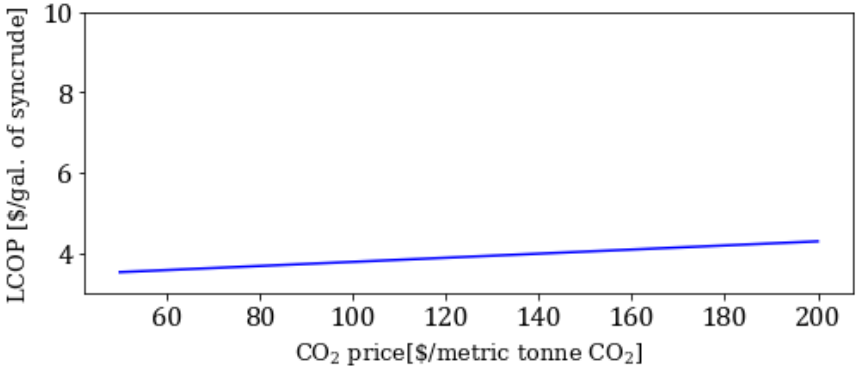
Assumptions and Analysis Period:

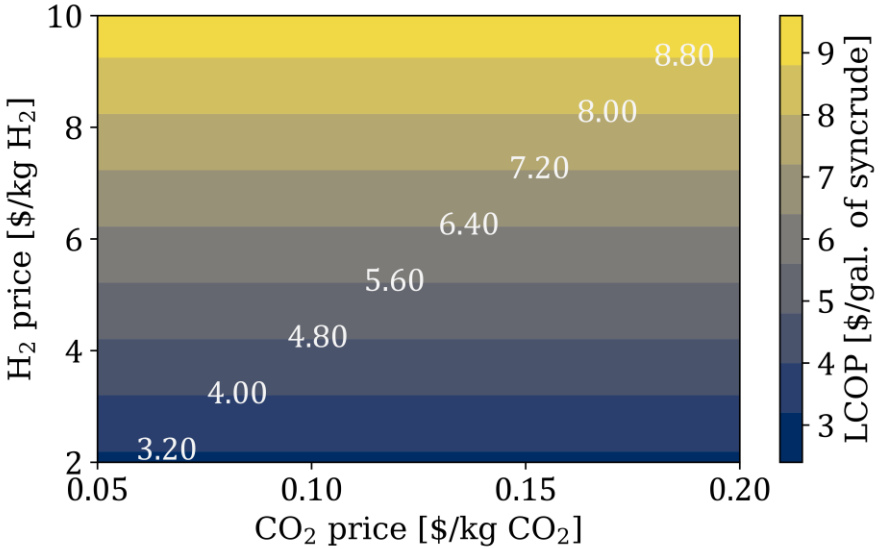
- Construction period = 3 years
- Analysis period = 30 years
- Inflation rate = 2% / year
- Internal rate of return = 1 %
- Nominal debt interest rate = 7% / year
- Effective tax rate = 15.7% / year

LCOP Estimation (2)

Sensitivity to Different Feed Price of H_2 and CO_2







LCOP Estimation (3)

Findings

LCOP is highly sensitive to TCC

- There is value in omitting expensive system (e.g., sCO2 PC and separation system) that is not justified by improvement in system performance or yield.
- Future iteration of system design needs to be optimized to maximize yield and minimize cost.

LCOP less sensitive to CO_2 price compared to H_2

due to significant difference in price per unit mass between CO_2 and H_2, but comparable usage.

LCOP is also highly sensitive to financial assumptions, but current analysis is not focusing in the most realistic financial assumptions yet.

Summary and Conclusions

1. Preliminary system design and techno-economic analysis framework developed
2. Levelized Cost of Product (syncrude), heavily dependent on TCC and H_2 price. Current estimates, without optimizing system design, still mostly yields price above target of $ 4/ gal. of jet fuel.
3. Future analysis will look at :
   - Designing optimum system to maximize yield an minimize cost.
   - Extending the system design to get to jet fuel instead of syncrude.
   - Looking at integration with other system: SOEC for H_2 production, fossil fuel energy as backup, and effective heat recovery.
   - Omitting separation (due to high X_{CO2}) and sCO_2 PC due to low oxidation enthalpy that is hard to justify investment.

The Project Team

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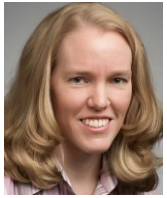

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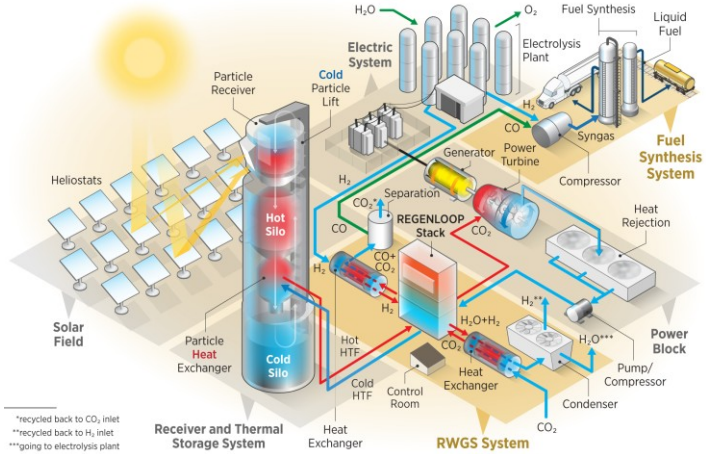

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Patent Pending

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