Direct heating of chemical catalysts for hydrogen and fertilizer production using Microreactors

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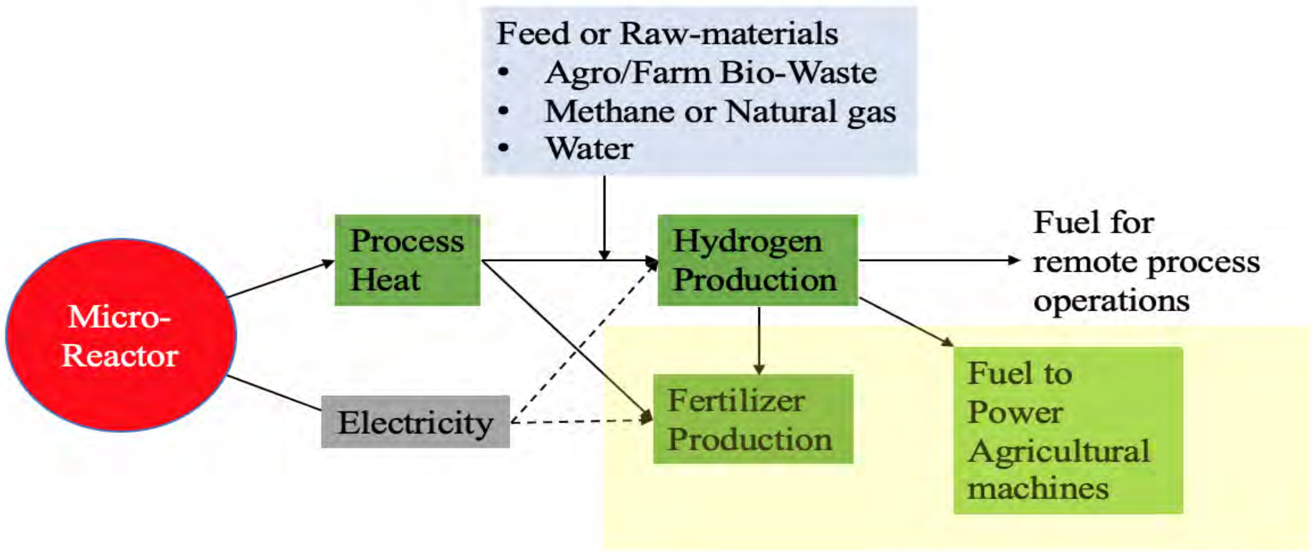
MRP Microreactor Program

Project Objectives

1) Design MPBHX and compare other IHX alternatives for microreactor integration.
2) Exergy and techno-economic feasibility of microreactor integration for hydrogen production and ammonia/fertilizer production.
3) Investigate feasibility of microreactors for achieving sustainable agriculture.

- Moving ceramic particles have high volumetric heat density.
- Store heat for later use.
- Catalyst carriers to sustain thermochemical reactions



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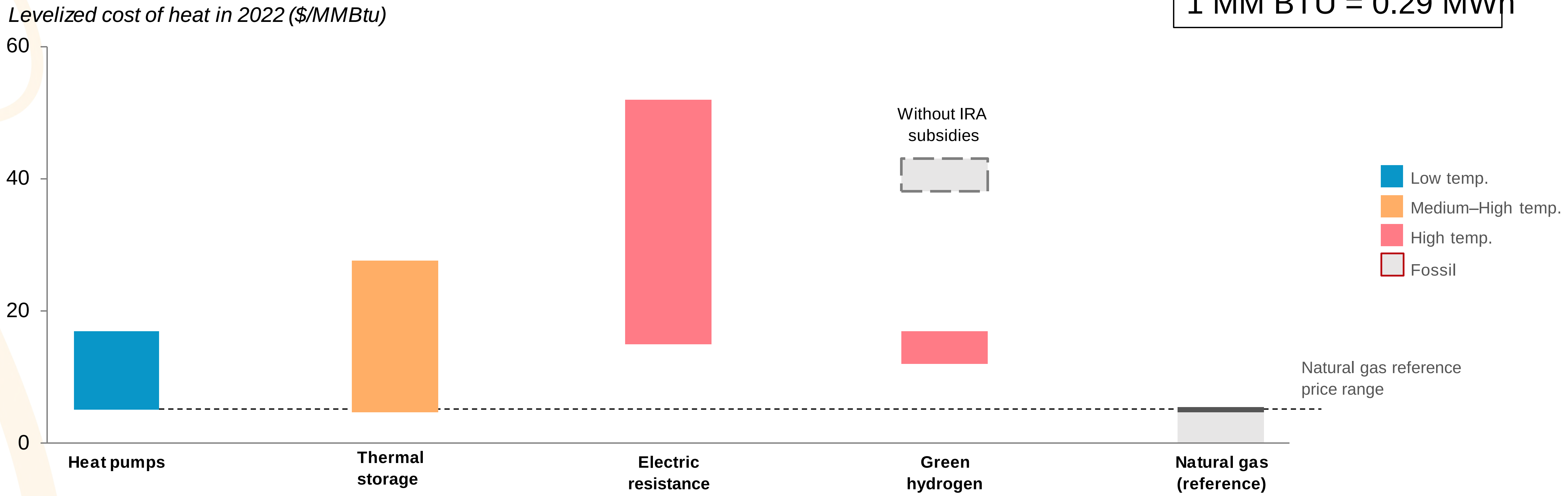
Review

Prioritized technologies offer competitive levelized cost of heat

Levelized cost of heat (LCOH) delivery across renewable thermal technologies[1]

1 MM BTU = 0.29 MWh



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Technologies must be strategically deployed as alternative to natural gas for industrial process heat

	Supply temp (ºC)	Nuclear LWRs	Nuclear Micro-Rx	Nuclear Advanced	Thermal storage	Electric	Green Hydrogen	RNG	Natural gas (Reference)
		300	650	900	1,500	1,800	2100	1950	1,950
Food	<130ºC	✓	✓	✓	✓	✓	✓	✓	✓
Refineries	<480ºC	✓	✓	✓	✓	✓	✓	✓	✓
Chemicals	<815ºC			✓	✓	✓	✓	✓	✓
Paper	<200ºC	✓	✓	✓	✓	✓	✓	✓	✓
Cement	600-1,500ºC				✓	✓	✓	✓	✓
Iron & Steel	1,600-2,000ºC					✓	✓	✓	✓

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Hydrogen generation – Thermochemical processes

	Process	Temperature	Efficiency	Fully mature
Steam Methane Reforming	SMR	850-900°C	51-85%	Yes
Partial Oxidation	POX	950°C	60-75%	Yes
Auto Thermal Reformer	ATR	575°C	60-75%	No
Coal Gasification	Coal Gasification	800°C	70%	Yes
Biomass Gasification	Biomass	750°C	35-50%	Yes
Aqueous Reforming	Aqueous Reforming	220-270°C	35-55%	No
Sulphur Iodine	SI	800°C	33-57%	No
Hybrid Sulphur	HyS	850°C	31-49%	No
UT-3	UT-3	750°C	13-45%	No
Copper Chloride Cycle	Cu-Cl	530°C	31-49%	No

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Some Microreactor designs with operating parameter details

Reactor	Design	Power	Max. process heat temperature	Operating Pressure	Coolant	Power Conversion System
Westinghouse eVinci	Heat Pipe	0.2-5 MW_e	600°C	<1atm	Na	Brayton Cycle
NuScale NPM	LWR	10-50 MW_e, 40-160MW_{th}	N/A	12.7 MPa	Water	Rankine Cycle
USNC MMR	HTGR	5 MW_e, 15 MW_{th}	565°C	3MPa(1°), 0.5MPa(2°)	He(1°), molten salt(2°)	Rankine Cycle[99]
HolosGen Holos Quad	HTGR	10-13MW_e	620°C	70bar(1°)/ 35bar(2°)	He, sCO_2	Brayton Cycle/ Organic Rankine Cycle
LeadCold SEALER	Lead-cooled	3-10 MW_e	417°C	N/A	Pb	Rankine Cycle
Urenco U-Battery	HTGR	10 MW_{th}, 4MW_e	710°C	N/A	He,N	Brayton Cycle
ARC Nuclear Generator	MSR	12 MW_e	700°C	N/A	Fluoride salt	N/A

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Integration Pathways

Process	Reactor	Primary, Secondary HTF	Heat Exchanger	Material
ATR 575°C	eVinci	Liquid metal, Molten Salt	All designs	Hastelloy
Coal Gasification 800°C	HTGRs	Helium, Molten Salts	Plate and Fin, PCHE	Alloy617, Hastelloy
Biomass 750°C	HTGRs	Helium, Molten salts	Plate and Fin	Alloy617, Hastelloy-N
Aqueous Reforming 220-270°C	All designs	Steam/Water	Shell and Tube, Plate and Frame	S/S
SI 800°C	HTGRs	Helium, Molten Salts	Plate and Fin, PCHE	Alloy617, Hastelloy-N
HyS 850°C	HTGRs	Helium, Molten Salts	PCHE	Alloy617, Hastelloy
UT-3 760°C	HTGRs	Helium, Molten Salts	Plate and Fin, PCHE	Alloy617, Hastelloy
Cu-Cl 530°C	USNC, eVinci	Molten salt, Helium, Liquid metals	All Types(TRL>6)	Alloy617, Hastelloy

Only ATR and Cu-Cl process are feasible with proposed microreactor designs.

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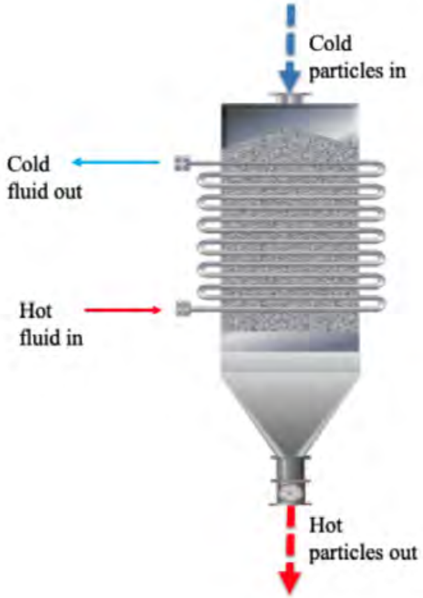
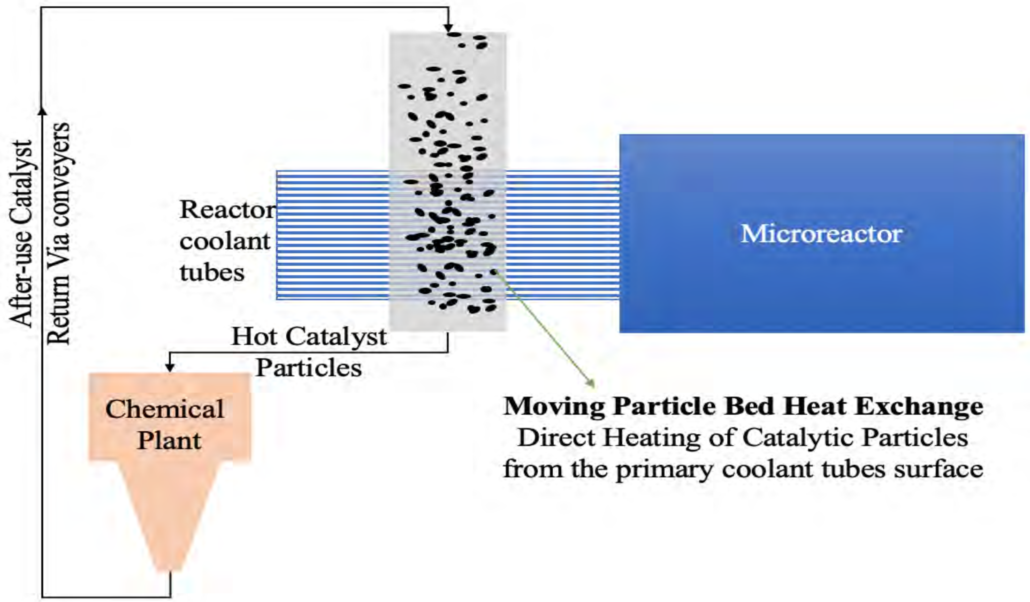
Design of Novel MPBHX

Moving Packed Bed Heat Exchanger (Design and Evaluation)

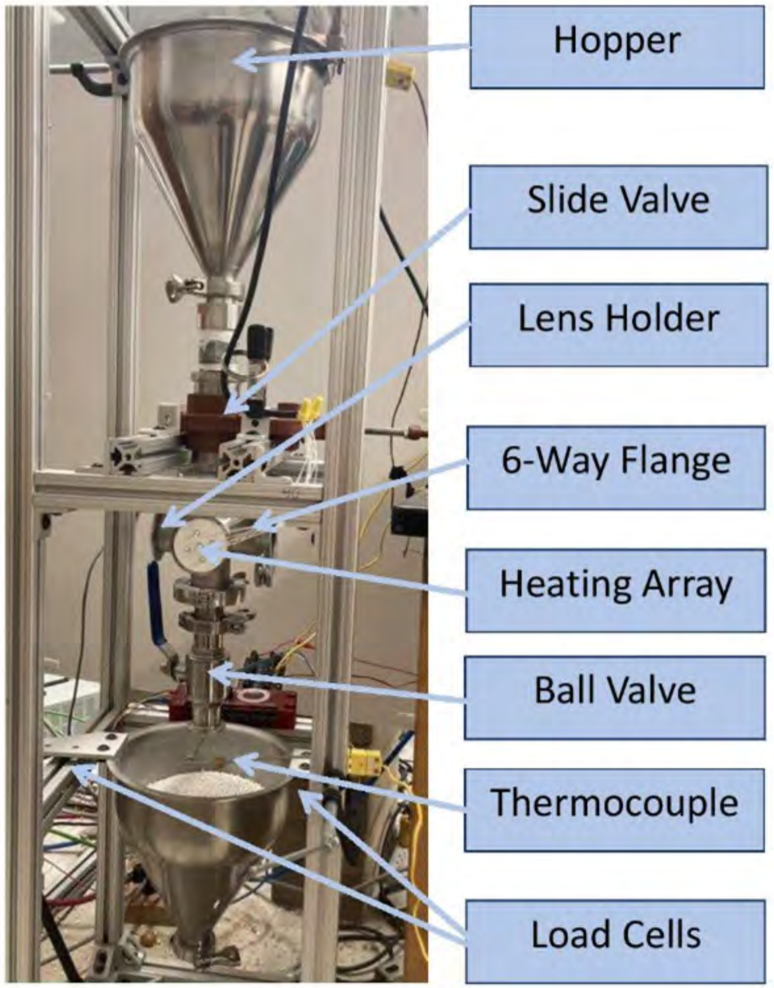


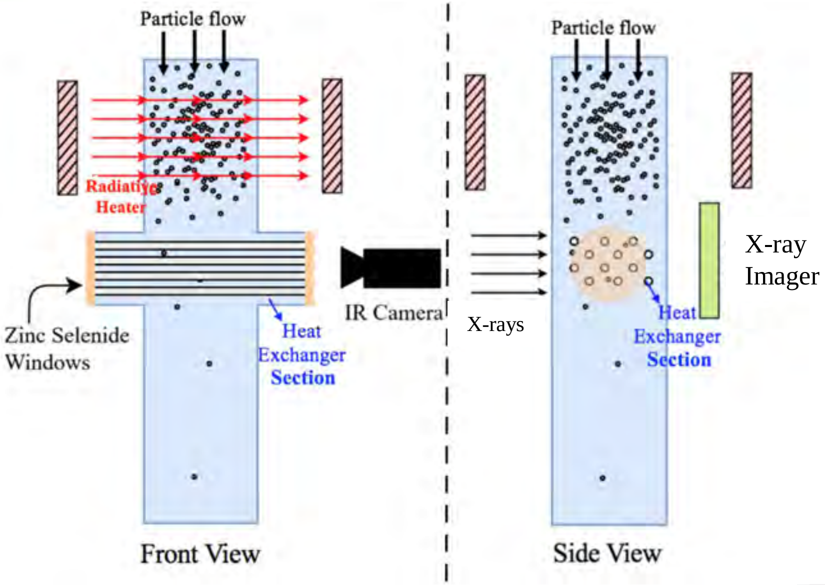
- Gaseous coolants-High Pressure drop- High parasitic Losses.
- Not too many liquid coolants compatible;
- Molten salt – security risk
- Ceramic granular flow – simple design
- Compare options

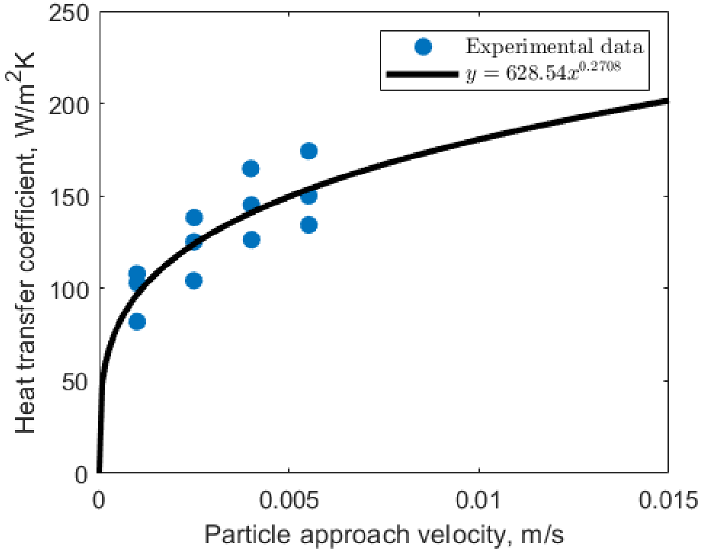


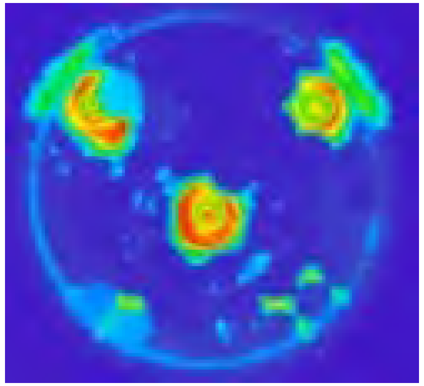
	FOM_ht	FOM_pumping
Air	0.07	40,000
Helium	0.12	25,000
Molten-Salt (Chloride)	0.55	15
Packed bed	0.31	12.5

Moving Packed Bed Heat Exchanger (Design and Evaluation)

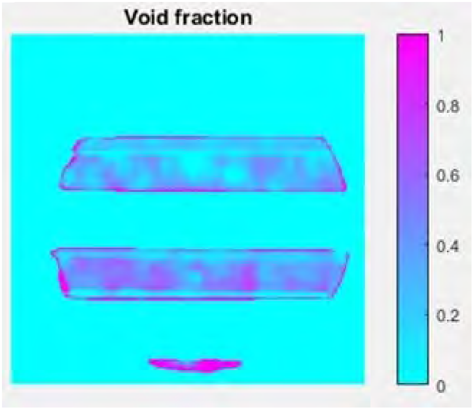








Infra-Red image showing azimuthal Asymmetry in heat transfer wake zone of granular flow



X-ray images showing higher Void in the wake zone below the Heater tubes

[A] K. J. ALBRECHT and C. K. HO,
Journal of Solar Energy Engineering,141, 3, 031006 (2019).

1 mm alumina particles

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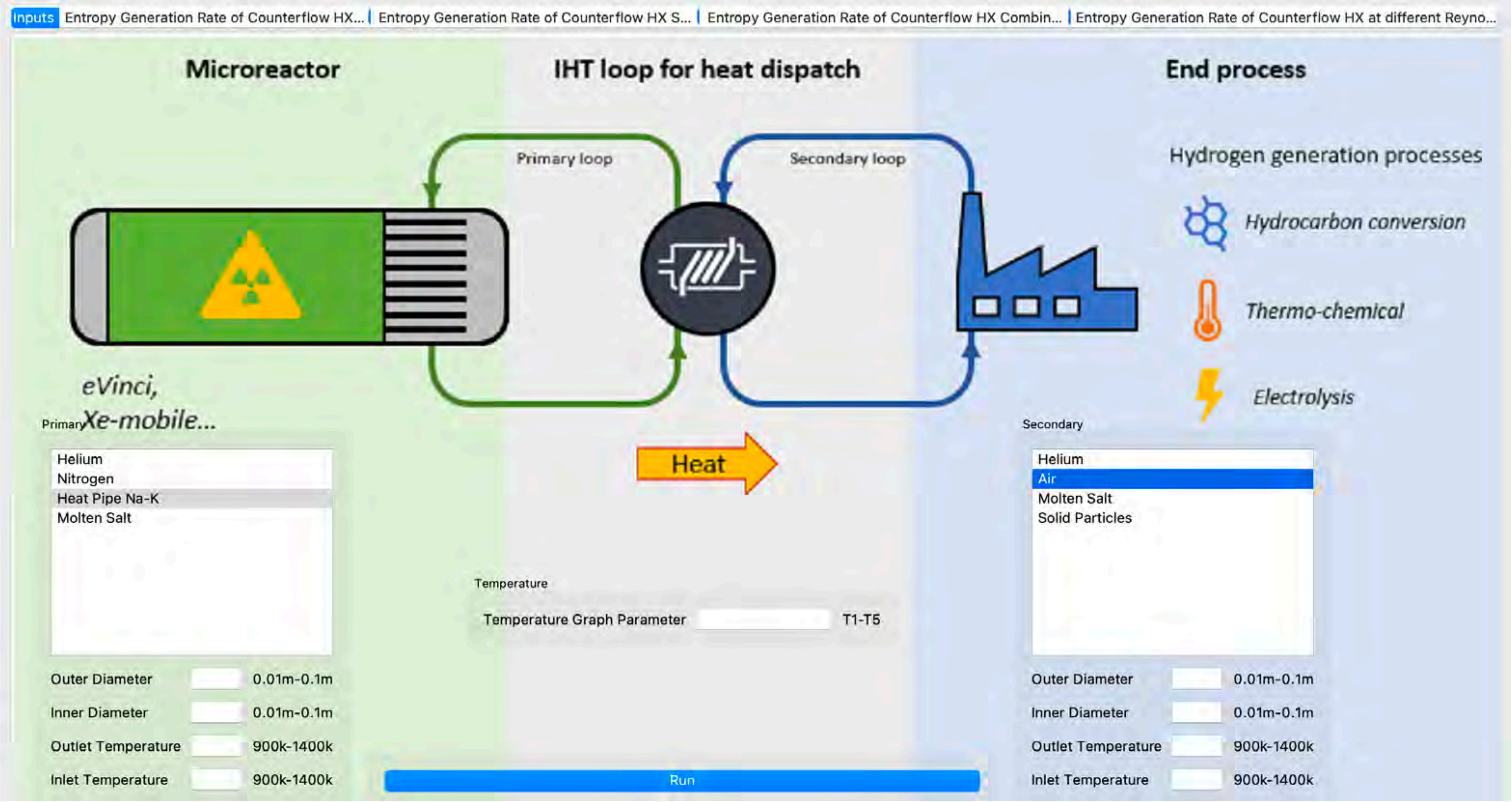
Technoeconomic Feasibility

Exergy based integration assessment tool



H. BINDRA, P. BUENO, and J. F. MORRIS, *Applied thermal engineering*, 64, 1-2, 201–208 (2014).
A. BEJAN, G. TSATSARONIS, and M. J. MORAN, *Thermal design and optimization*, John Wiley & Sons (1995).

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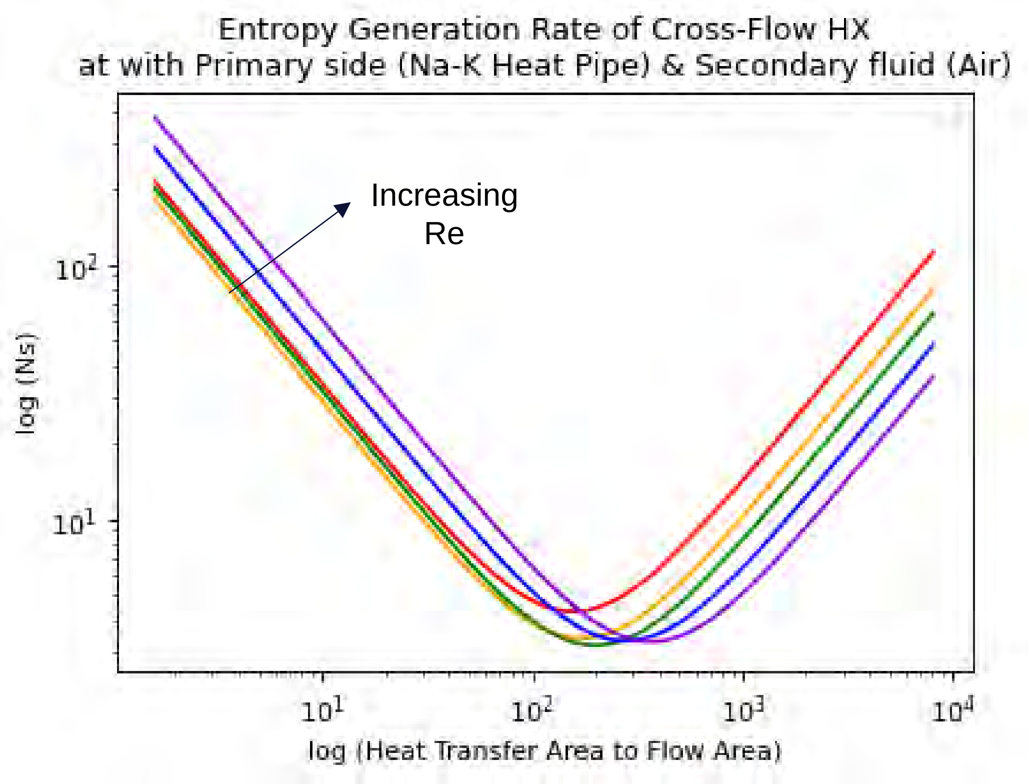
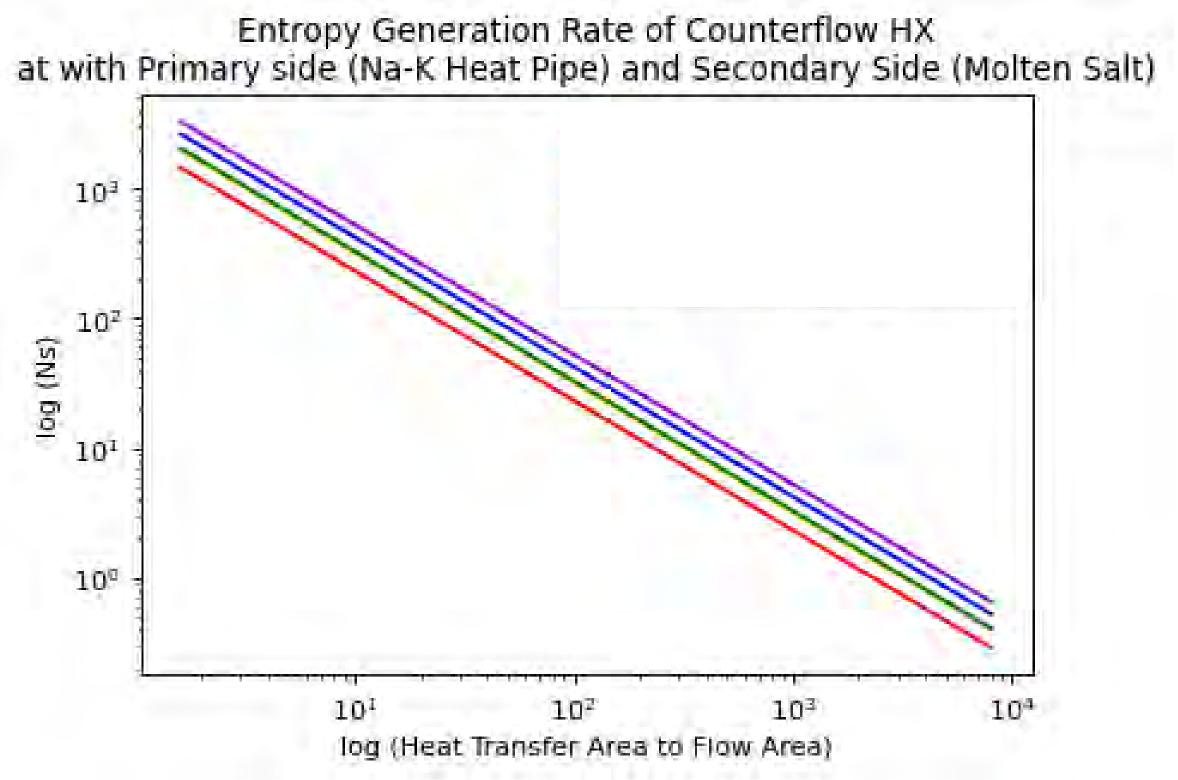
Entropy generation number- Assessment parameter





$$N_s = \frac{S_{gen}}{mC_p}$$

Molten Salt is more appropriate choice based on exergy analysis

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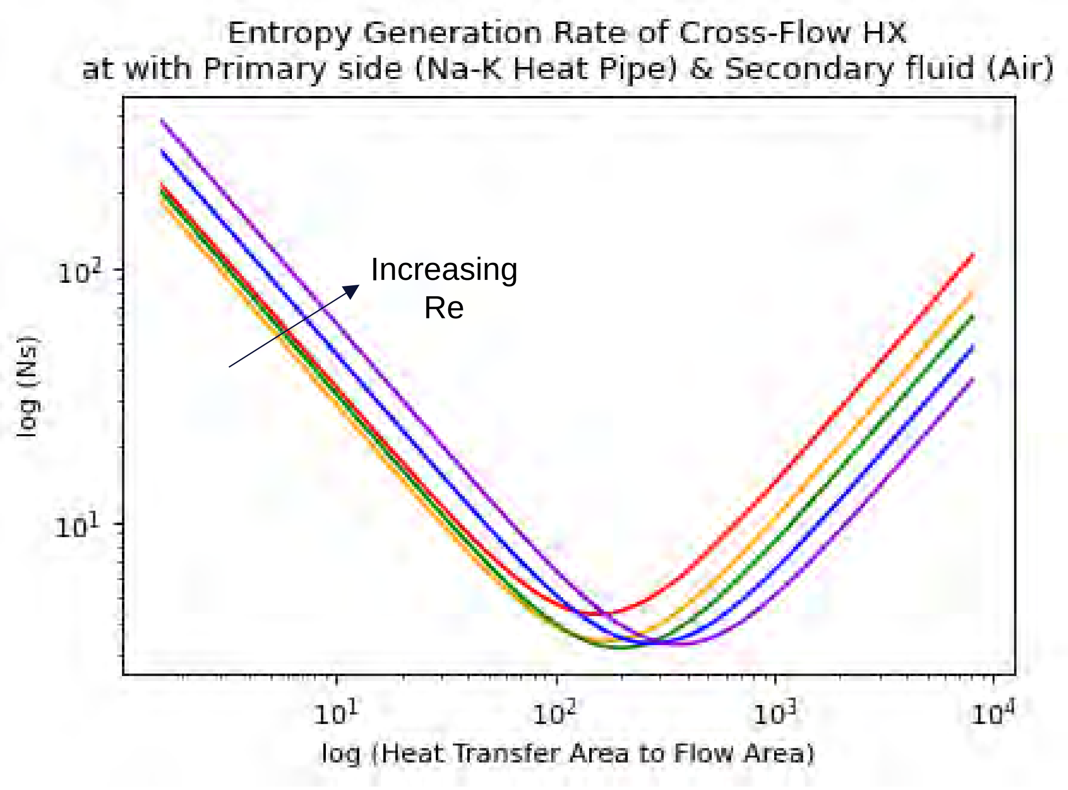
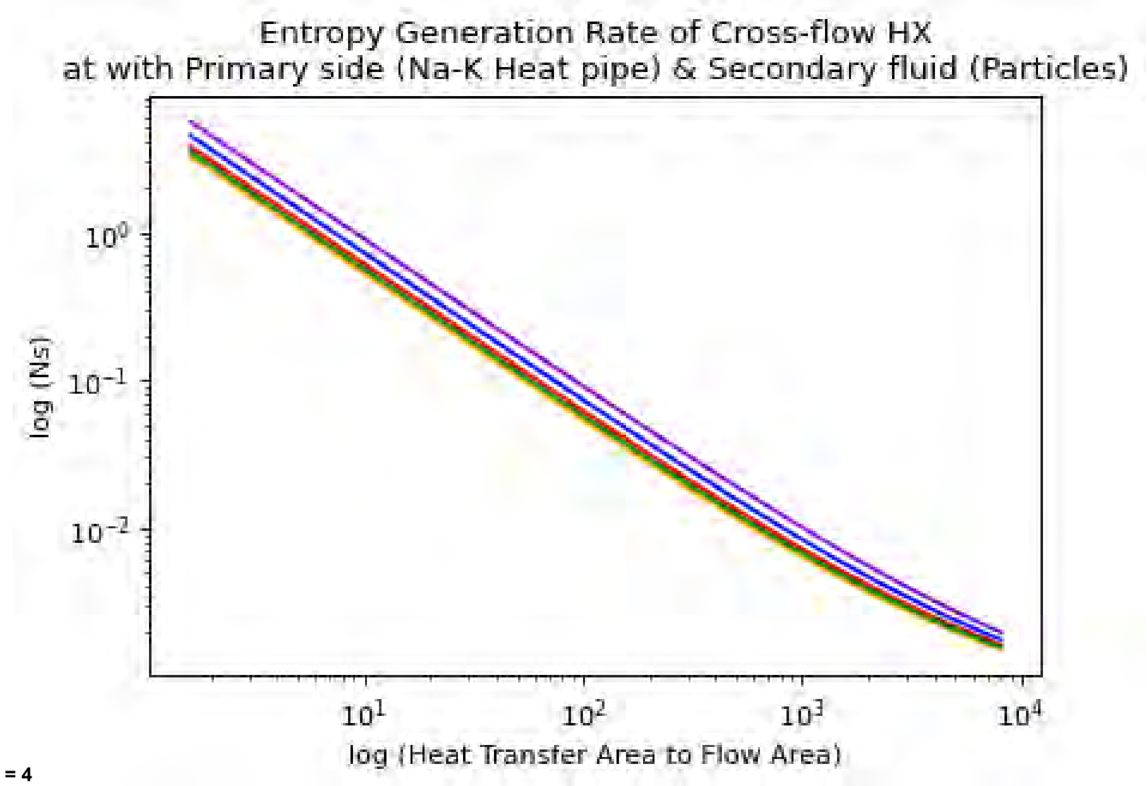
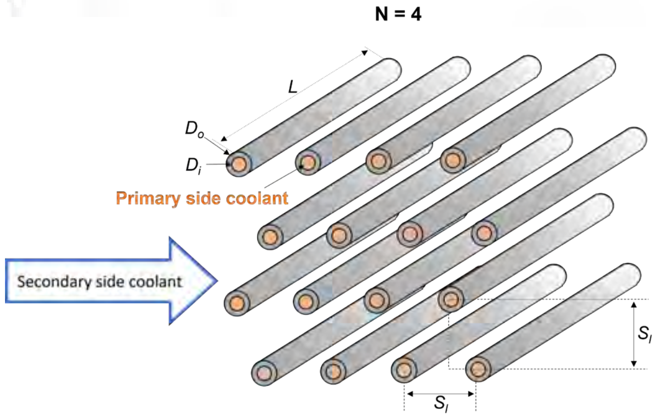
Entropy generation number- Assessment parameter

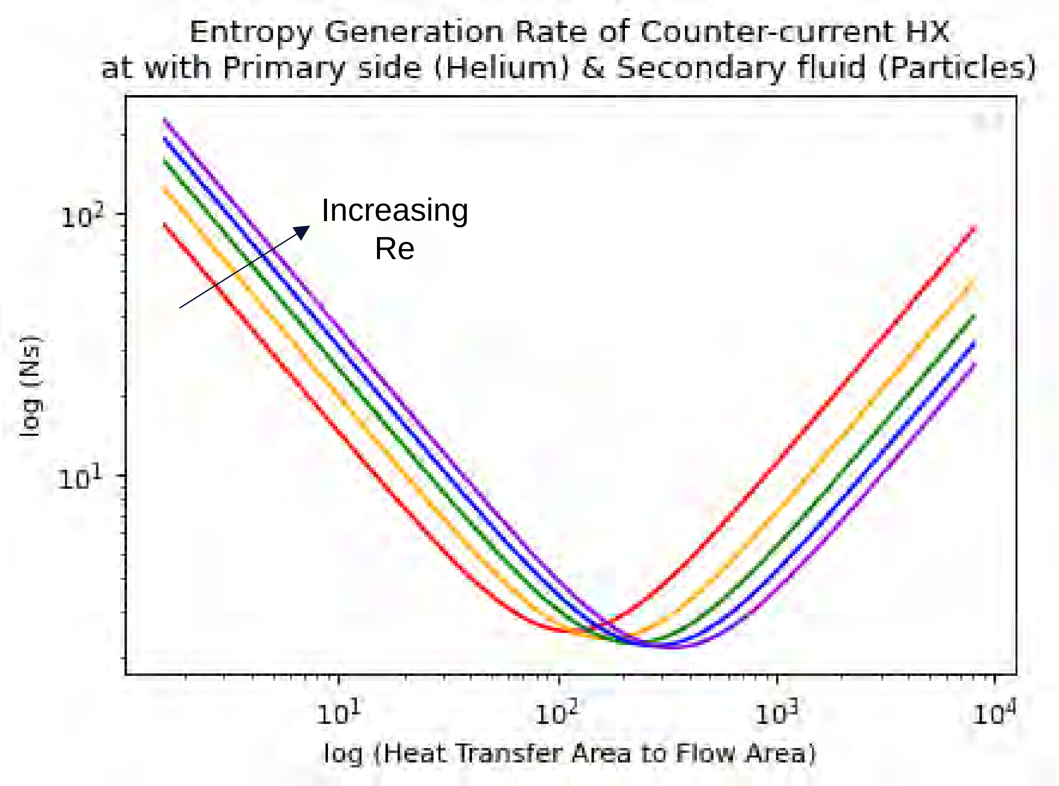


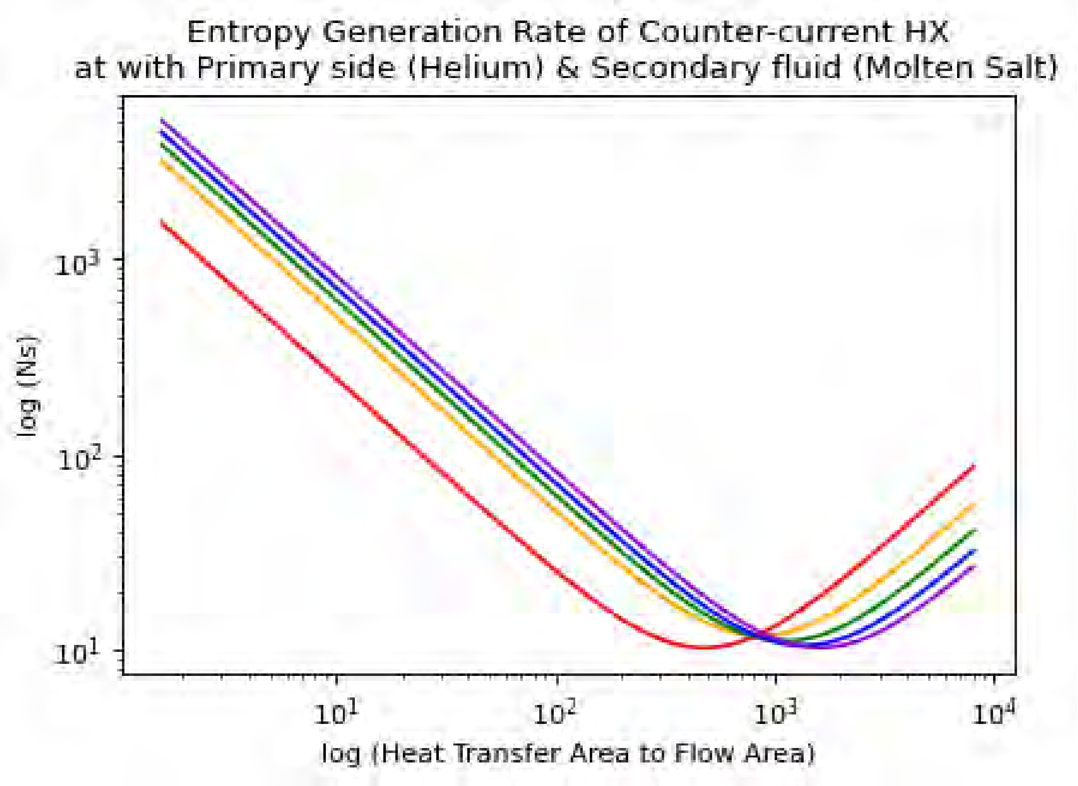


$$N_s = \frac{S_{gen}}{mC_p}$$



Entropy generation number- Assessment parameter





$$N_s = \frac{S_{gen}}{mC_p}$$

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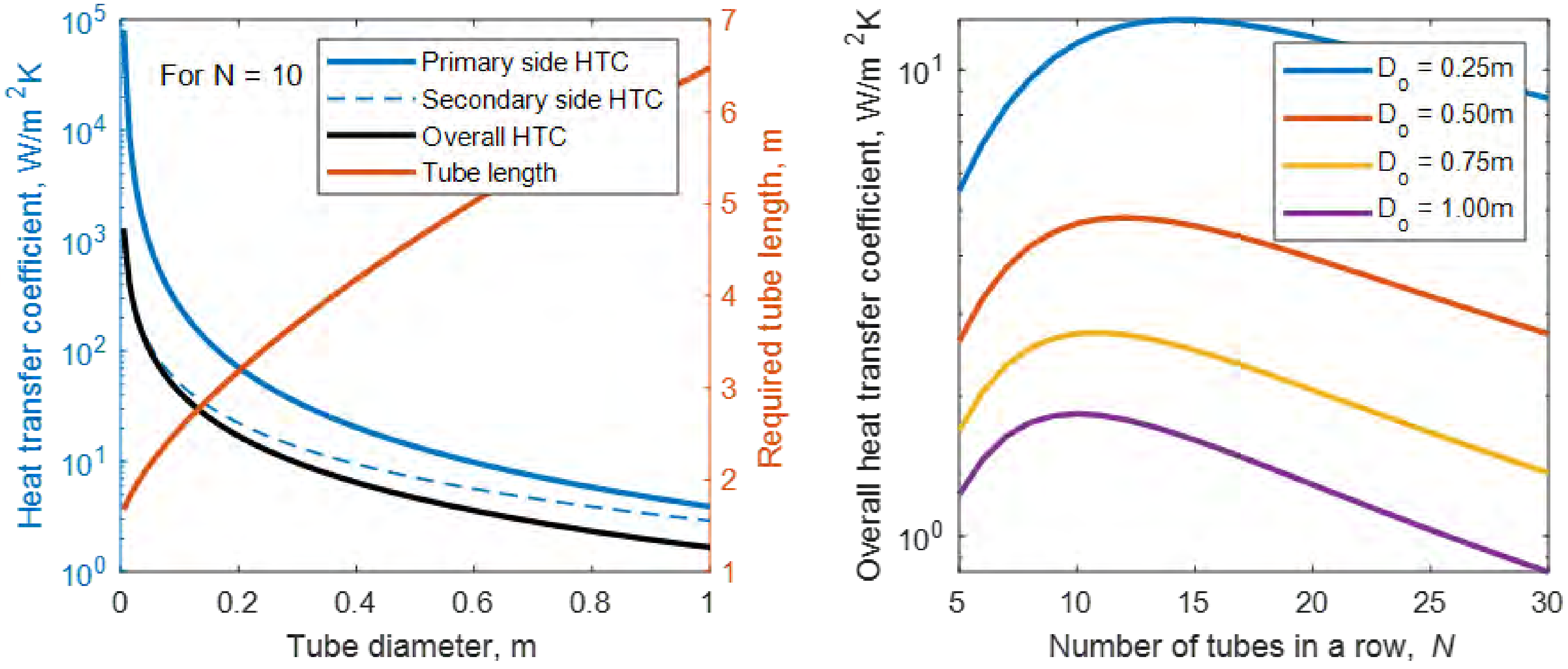
Variation of the overall heat transfer coefficient with geometric parameters



He-He cross-flow heat exchanger

- Larger tube diameter → decreased h
- Requires more surface area to meet thermal requirements

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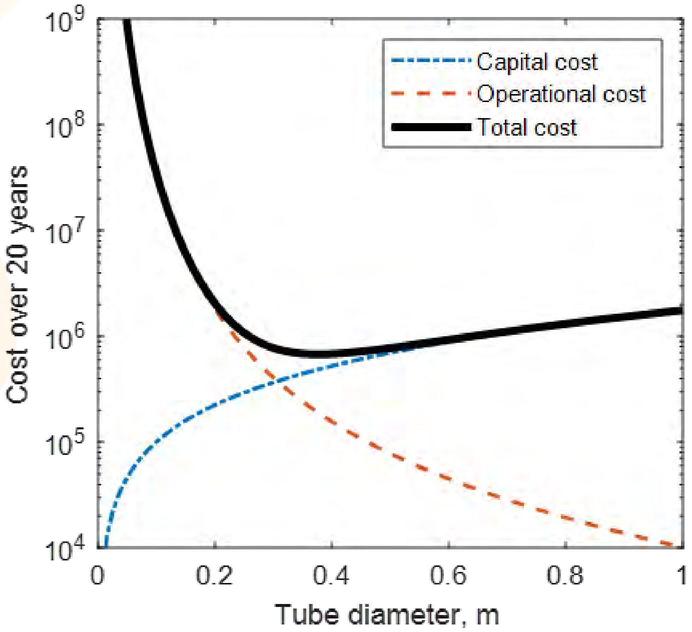
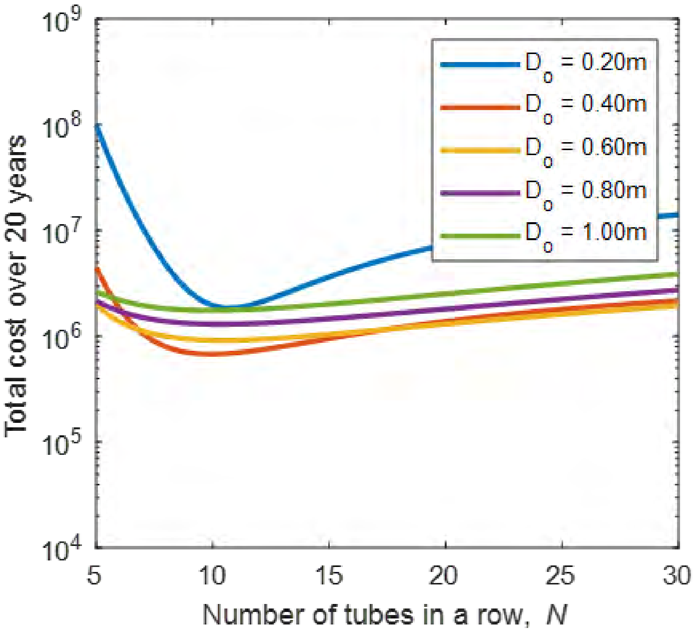
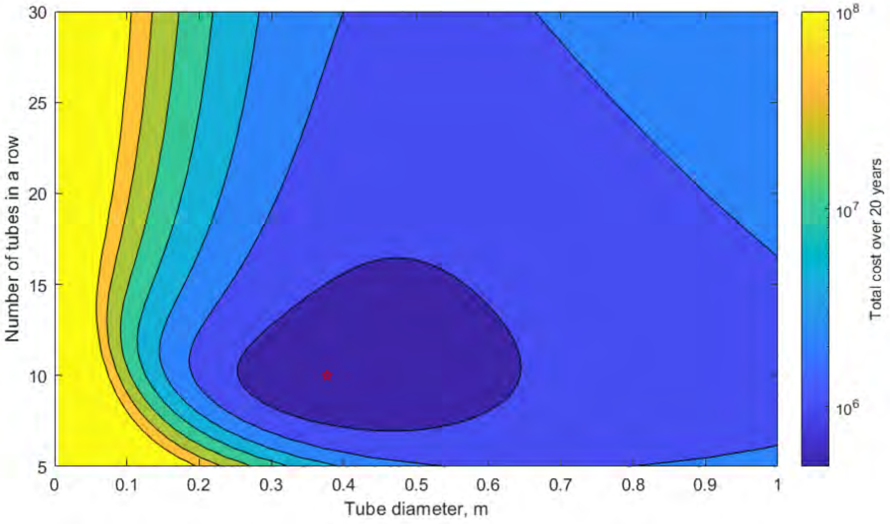
Variation of the total cost (in USD) of the heat exchanger with geometric parameters





- Larger tube diameter increases material cost.
- Larger diameter reduces pressure drop, lowering pump work and operational cost.



Case: He-He cross-flow heat exchanger

Total lifetime Cost, $		Primary		
		He	Molten Salt	Alumina Particles
Secondary	He	6.7E4+5	4.33E+5	3.22E+5
	Molten Salt	6.14E+5	5.80E+4	5.62E+4
	Liquid Metal	3.87E+5	3.49E+4	2.78E+4

Heat duty = 10 MWth

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Ammonia production- Economics

Microreactor Program

Haber-Bosch process is an industrial method for producing ammonia

$$N_2 + 3H_2 \rightarrow 2NH_3$$

Reactants

Nitrogen and Hydrogen

Conditions

Temperature: 400-550 °C

Pressure: 250-350 bar

Energy Intensive Process

27.4 -31.8 GJ/t_{NH_3}

Industrial Ammonia Production

Scale: 1000-1500 t/d

Technology: Microreactors for H_2

Haber Bosch Process

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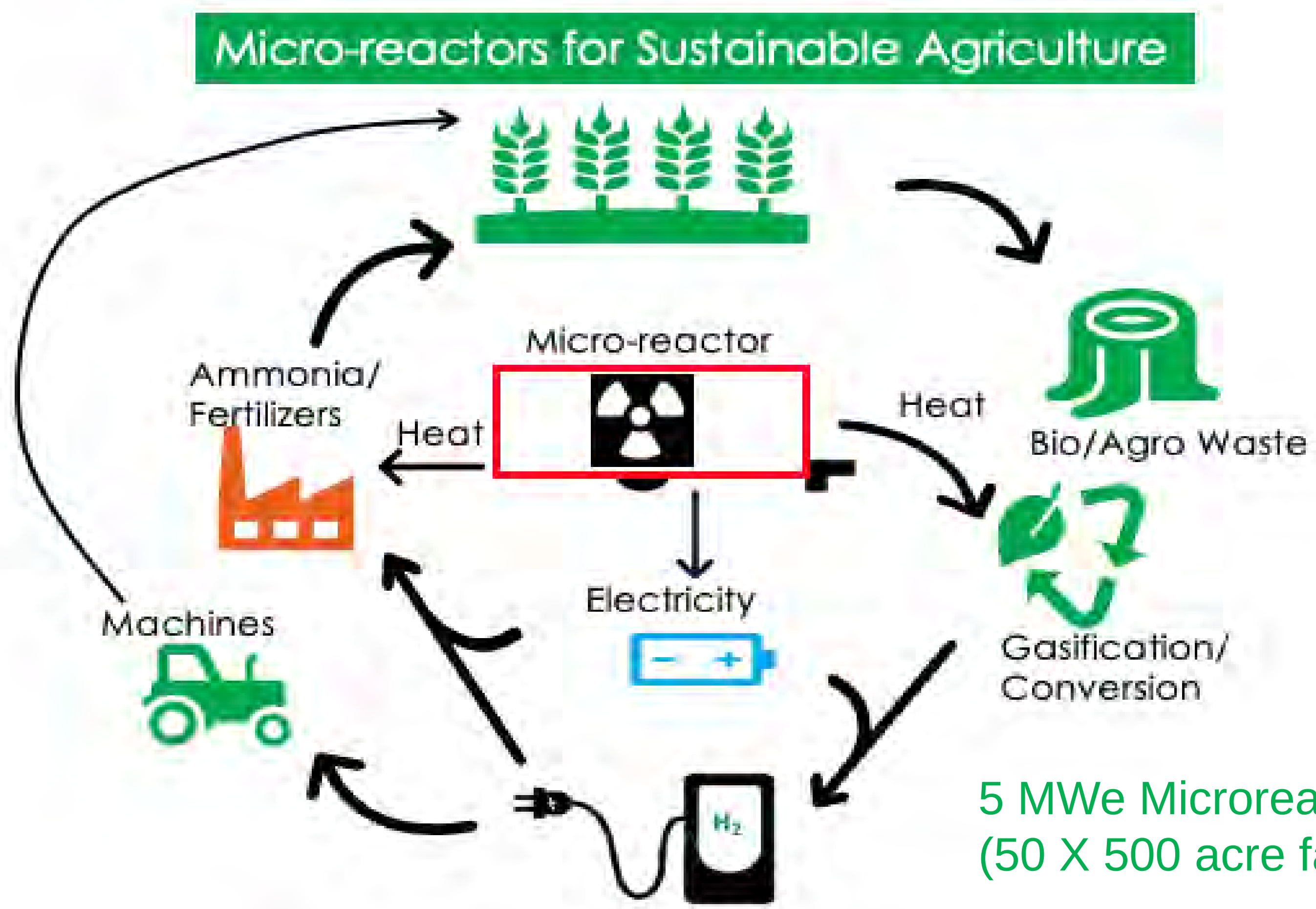
Carbon Neutral farm



Produces

1 acre – 170 Bushel (Corn)
1.5 Ton (Residue Corn Stover)
180 kg H_2 gas (Gasification yield)

Needs

1 acre – 150 lbs (Ammonia) ~ 30 kg H_2
48 kWh to produce 1 kg H_2
4320 kWh Total energy

5 MWe Microreactor
(50 X 500 acre farms)

[D] David, W. I. F. "Ammonia: zero-carbon fertiliser, fuel and energy store." Policy Briefing, The Royal Society (2020).
[E] Carpenter, Daniel L., et al. Industrial & Engineering Chemistry Research 49.4 (2010): 1859-1871.
[F] Technologies for hydrogen production

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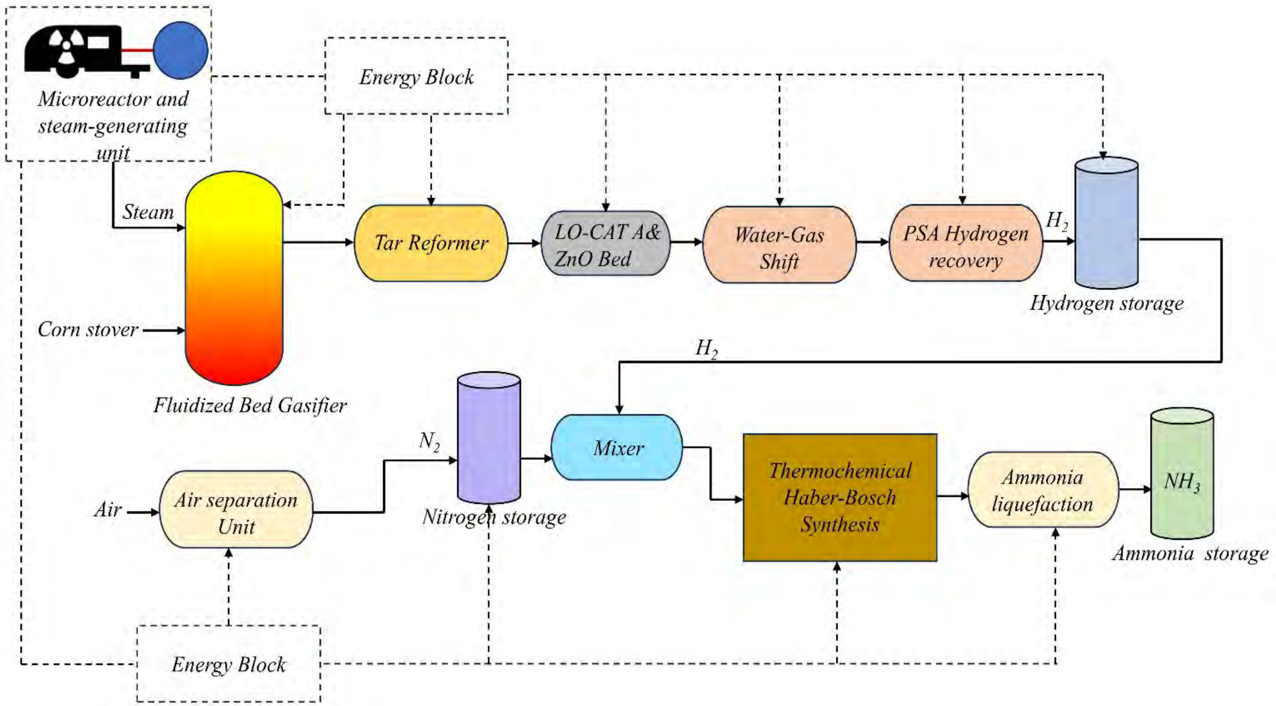
Nuclear-Integrated Biomass -to-Ammonia Production



Plant annual ammonia production: 340 tonnes (which is equivalent to the annual ammonia requirement for 10 × 500-acre farms)

Plant annual working hours: 7488

Biomass requirement: Corn stover = 1158 tonnes
Wheat straw = 1107 tonnes
Wood chips = 830 tonnes

Energy requirement: Corn stover = 3409 MWh
Wheat Straw = 3212 MWh
Wood Chips = 3331 MWh

Gasifier: Fluidized bed
Gasification temperature: 650 °C
Gasification yield is referenced from the literature [Carpenter, 2010]
Tar reformer CO and H_2 conversion efficiency: 90%
PSA H_2 recovery rate: 85%
H-B overall conversion efficiency: 97%

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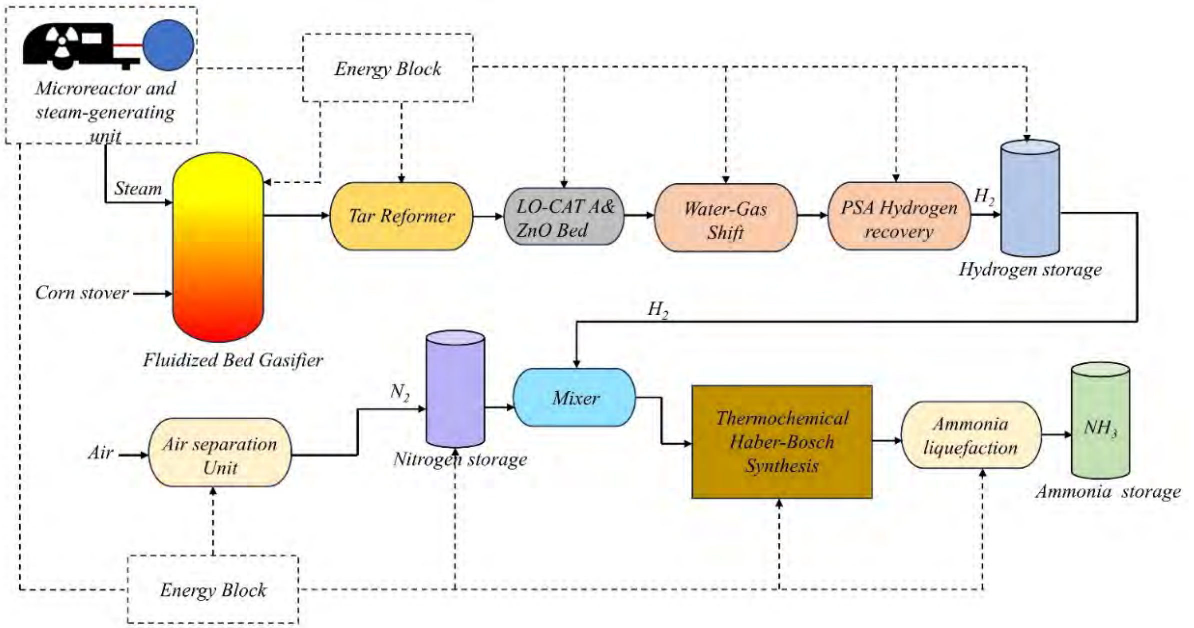
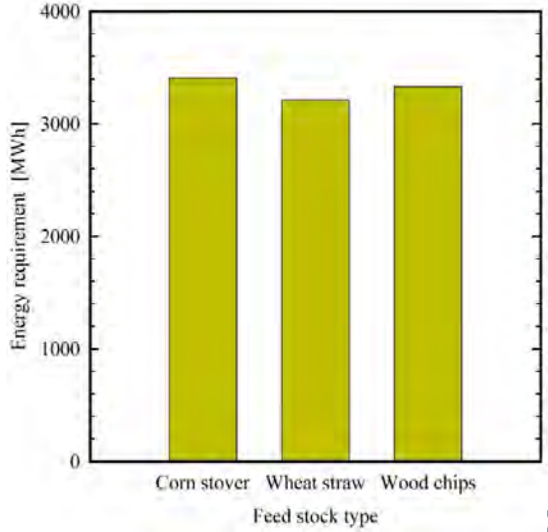
Nuclear-integrated biomass-to-ammonia production



Process	Energy Requirement, MWh		
	Corn stower	Wheat Straw	Wood Chips
Gasification	2766	2570	2689
PSA for H_2	32	32	32
Nitrogen separation from air	364	364	364
Ammonia synthesis (H-B)	247	247	247



The energy requirement is for the equivalent ammonia production to meet the demand of 50 × 500-acre farms (340 t/y) ~ 5 MW

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Process Description

- Biomass gasification: Converts agricultural residues to syngas (H_2, CO, etc.).
- Syngas cleaning and conditioning: Removes impurities.
- Air separation: Supplies nitrogen for ammonia synthesis.
- Ammonia synthesis (Haber-Bosch): Converts H_2 and N_2 to NH_3 using nuclear microreactor energy.

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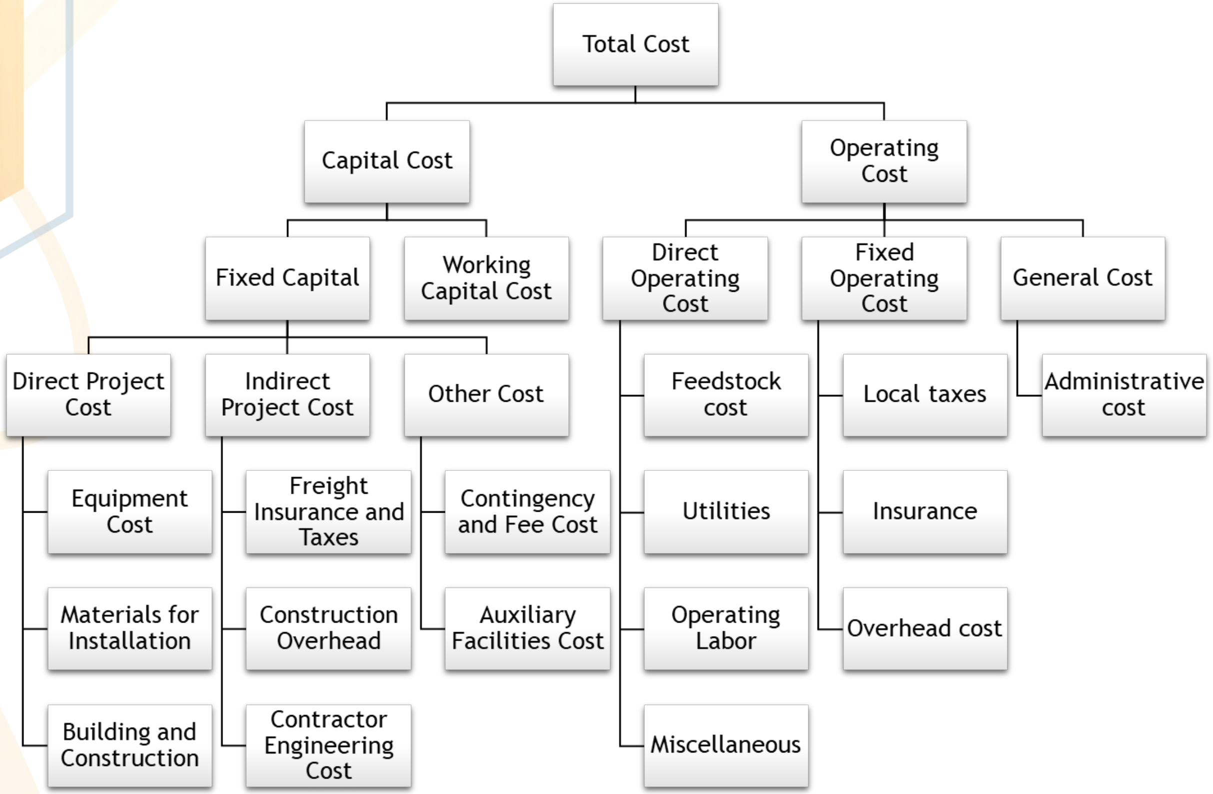
Economic Parameters



Categorization of total cost

Parameters and assumptions for the estimation of LCOA

Money value	US $ (Aug 2023)			
Plant lifespan	20 years			
Construction year	1 year			
Interest rate	8%			
Inflation rate	2%			
Operations and maintenance cost growth rate	0.65%			
Working hours	52 weeks in year, 6 days in a week, 8 hours per day for one shift			
No of operating labor	2 laborers per shift			
Efficiency of microreactor	36%			
Electricity cost	$0.21/kWh			
Feedstock cost	80$/tonne			
Operating labor cost	20 $/h			
Equipment cost estimation				
Equipment	Attribute	Designed capacity		
		Corn stover	Wheat straw	t wood
Gasifier, including gas cleaning and tar	Feedstock, t/d	3.71	3.55	2.66
WGS reactor	Producer gas entering the shift reactor, kg/h	180.39	178.95	175.57
PSA for hydrogen	kg/h (H_2)	8.26	8.26	8.26
PSA for nitrogen	kg/h (N_2)	38.51	38.51	38.51
H-B synthesis process	kg/h (NH_3)	45.43	45.43	45.43

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Results and Discussion

- LCOA Findings:
- - Corn stover: $5.13/kg (FOAK)
- - Wheat straw: $4.83/kg
- - Wood: $5.00/kg
- Sensitivity analysis:
- - Reactor cost dominates (88-90% of total capital cost).
- - Feedstock and labor costs have a modest impact.
- NOAK- using guidelines published by INL, the LOCA costs were found to be lower.

$$LCOA = \frac{\sum_{t=0}^{n_{life}} \frac{TCC_t + OPC_t}{(1+r)^t}}{\sum_{t=0}^{n_{life}} \frac{P_t}{(1+r)^t}}$$

TCC : capital cost
OPC: operating cost
P : annual ammonia production
r: discount rate

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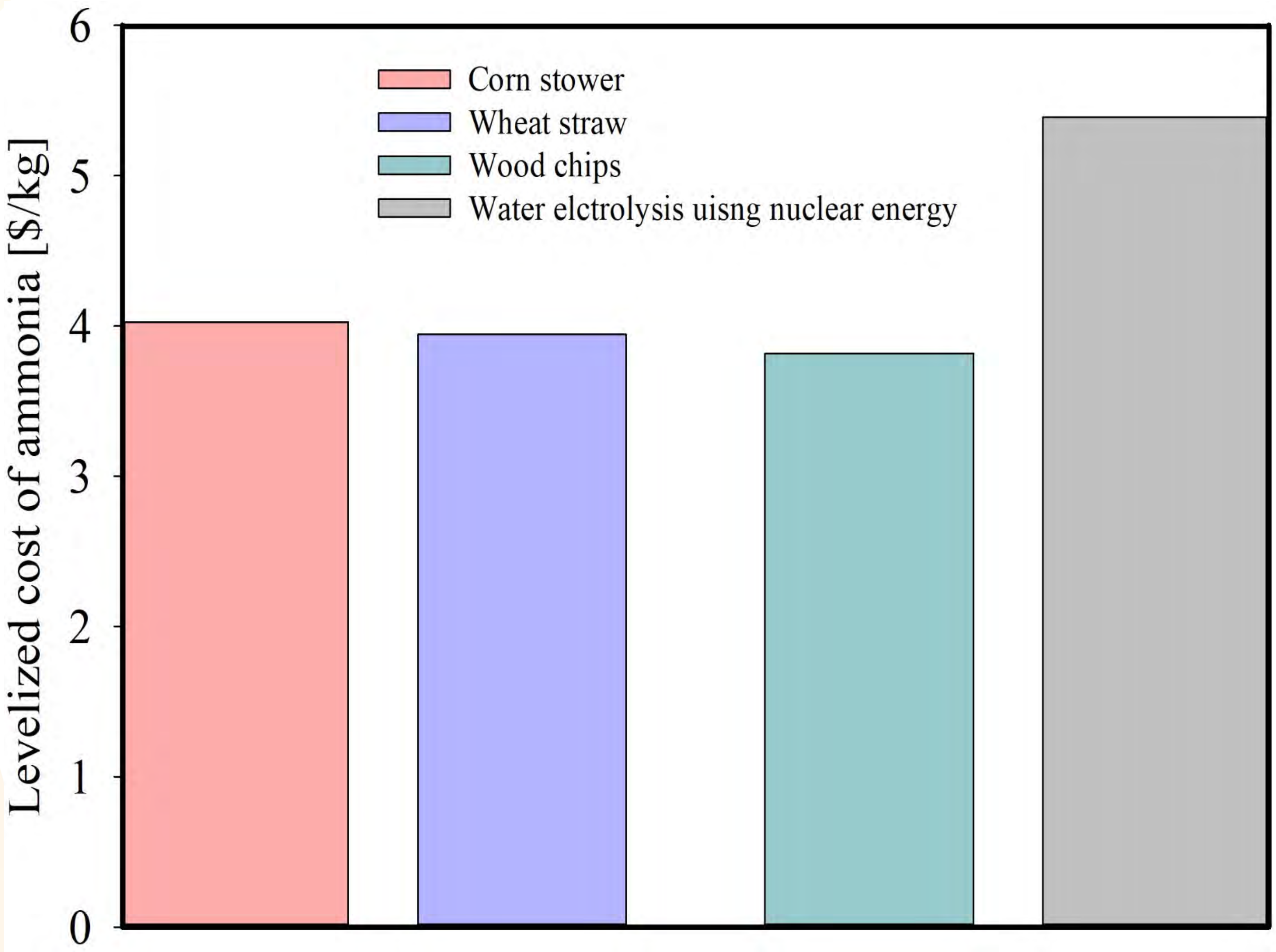
Estimated levelized cost of ammonia production



$$LCOA = \frac{\sum_{t=0}^{n_{life}} \frac{TCC_t + OPC_t}{(1+r)^t}}{\sum_{t=0}^{n_{life}} \frac{P_t}{(1+r)^t}}$$

TCC : capital cost
OPC: operating cost
P : annual ammonia production
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The cost of hydrogen production based on water electrolysis using nuclear energy is obtained using the IAEA HydCalc tool.

www.iaea.org/topics/non-electric-applications/nuclear-hydrogen-production

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Summary

- Industrial process heat is an important sector which needs carbon emission reductions.
- Ammonia production powered by nuclear microreactors can be a critical pathway to address these goals.
- Economic feasibility was conducted for ammonia production using nuclear microreactors.
- Ammonia production using electrolysis based nuclear hydrogen is significantly more expensive as compared to steam methane reforming based hydrogen.
- This cost can be reduced by adopting agro-feedstocks and thermochemical gasification process to produce hydrogen and then ammonia.
- Current LCOA higher than traditional methods but competitive with nuclear-powered electrolysis.
- Cost reduction possible with reactor standardization and improved learning rates.

MRP Microreactor Program

List of students

- Zayed Ahmed (Obtained PhD and now working as Research Engineer at Applied Cooling Technologies)
- Bailey Strine (Obtained MS and now working as Engineer at Black & Veatch)
- Ketan Ajay (Postdoctoral fellow, now Research Associate at McMaster University)
- Anshuman Chaube (Now PhD Student at Penn State)
- Jake Marr (Undergrad, Now MS student at Purdue)

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[1] Gupta, D., Kafle, A., & Nagaiah, T. C. (2023). Sustainable ammonia synthesis through electrochemical dinitrogen activation using an Ag 2 VO 2 PO 4 catalyst. *Faraday Discussions*.

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[8] Morgan, E. R., Manwell, J. F., & McGowan, J. G. (2017). Sustainable ammonia production from US offshore wind farms: a techno-economic review. *ACS Sustainable Chemistry & Engineering*, *5*(11), 9554-9567.

[9] Ghavam, S., Vahdati, M., Wilson, I. A., & Styring, P. (2021). Sustainable ammonia production processes. *Frontiers in Energy Research*, *9*, 34.

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