



Sustainable Design of Decarbonization Strategies via Process Integration

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The Grand Challenge: Sustainability



Complex Interactions



Systems-Based Paradigm Shifts & Enabling Design Concepts, Frameworks & Tools



KEY QUESTIONS

- **How to create decarbonization strategies using multi-scale process integration?**
- **Can we identify performance benchmarks (targets) ahead of detailed design?**
- **How to use these targets in decision making?**
- **How to handles appropriate level of details at all scales?**



OUTLINE

➔ Overview of Sustainable Design Through Multiscale Process Integration

- Application Examples:
 - Incorporation of renewables in energy integration and energy-water nexus
 - CO₂ monetization and reduction of carbon footprint for energy carriers and chemicals
- Use of Targets to Incorporate Sustainability in Decision Making
- Multi-scale Integration and Industrial Symbiosis
- Contemporary Challenges and Future Directions

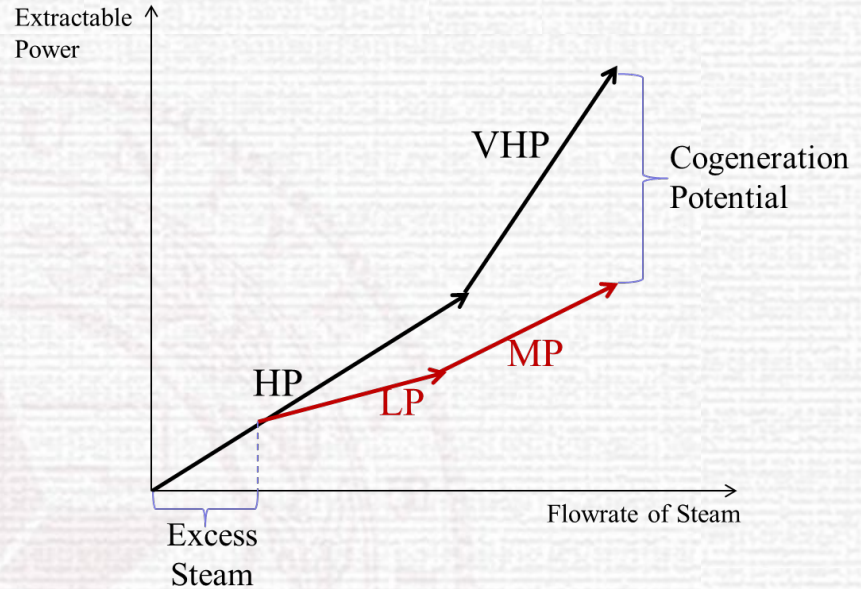
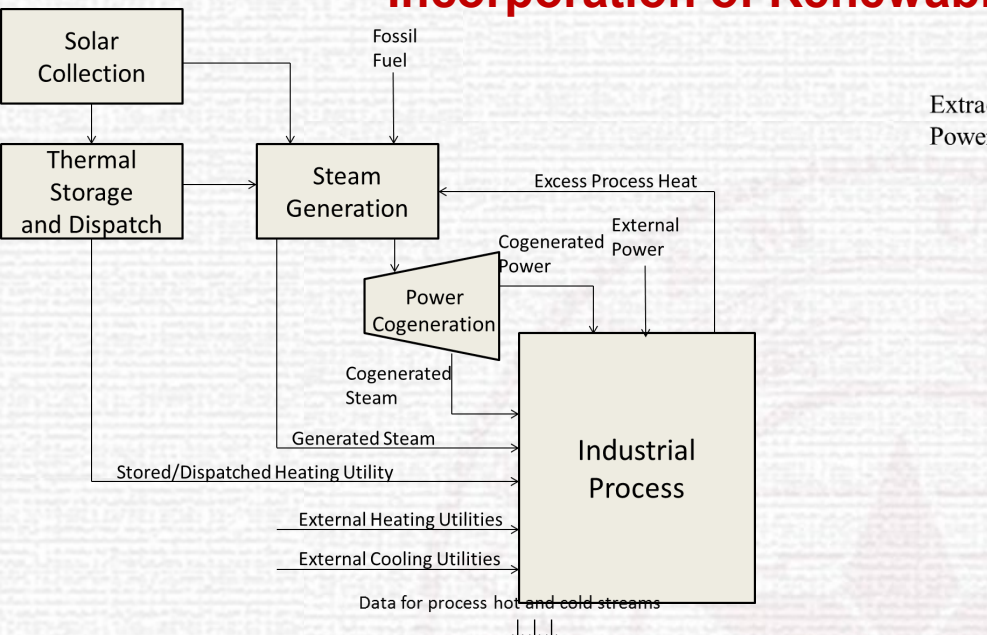




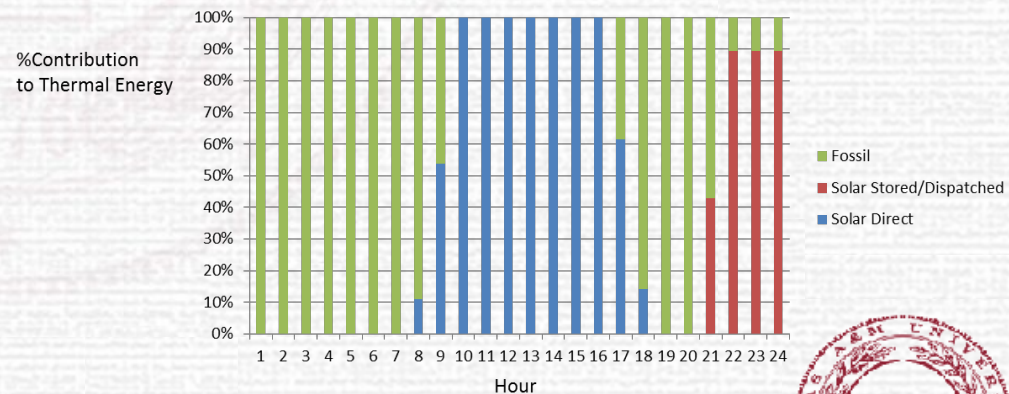
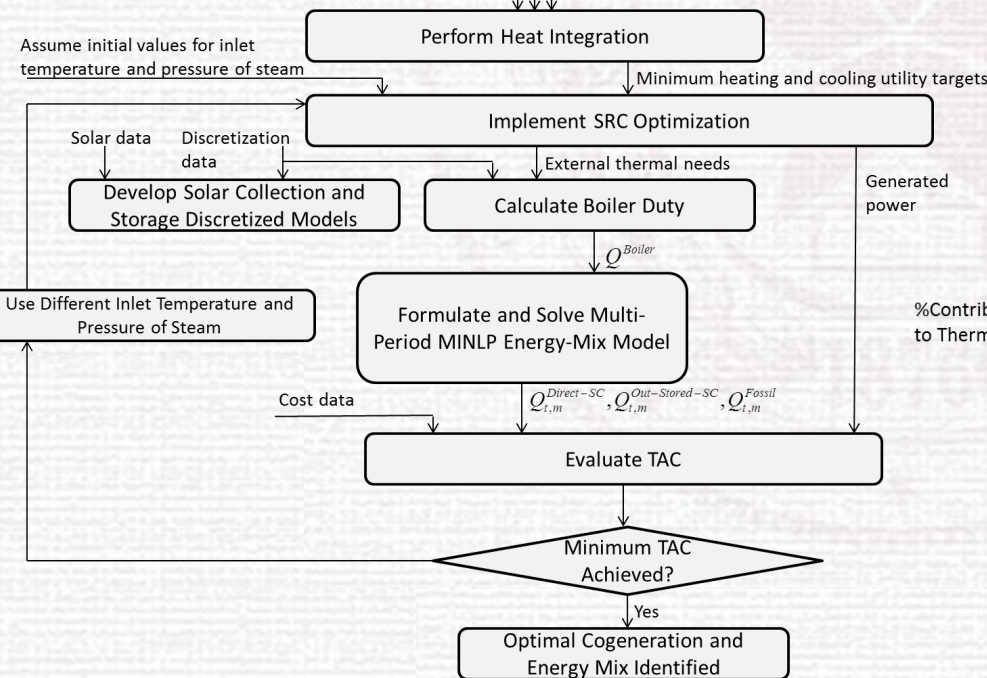
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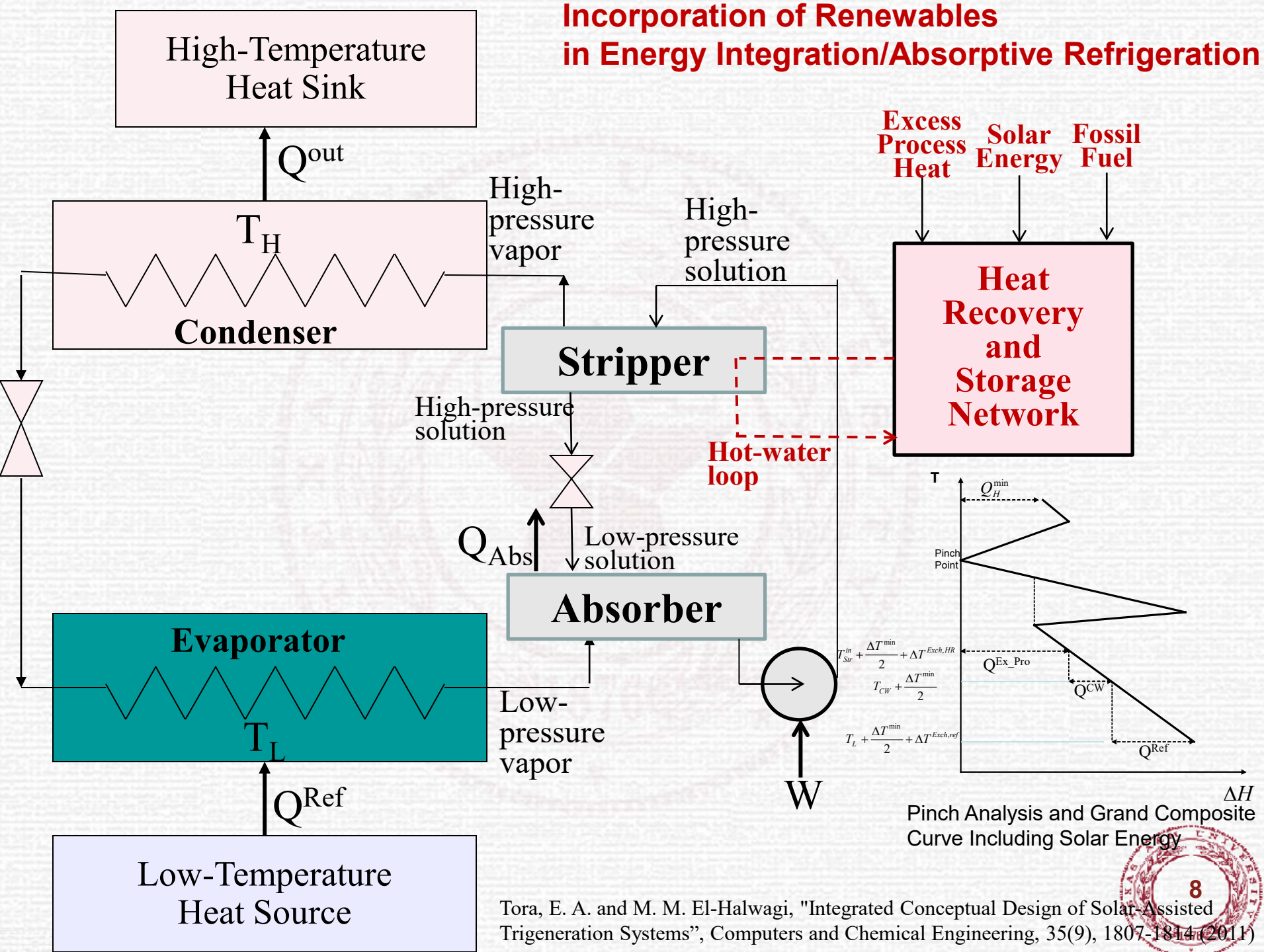
Incorporation of Renewables in Energy Integration/Cogeneration



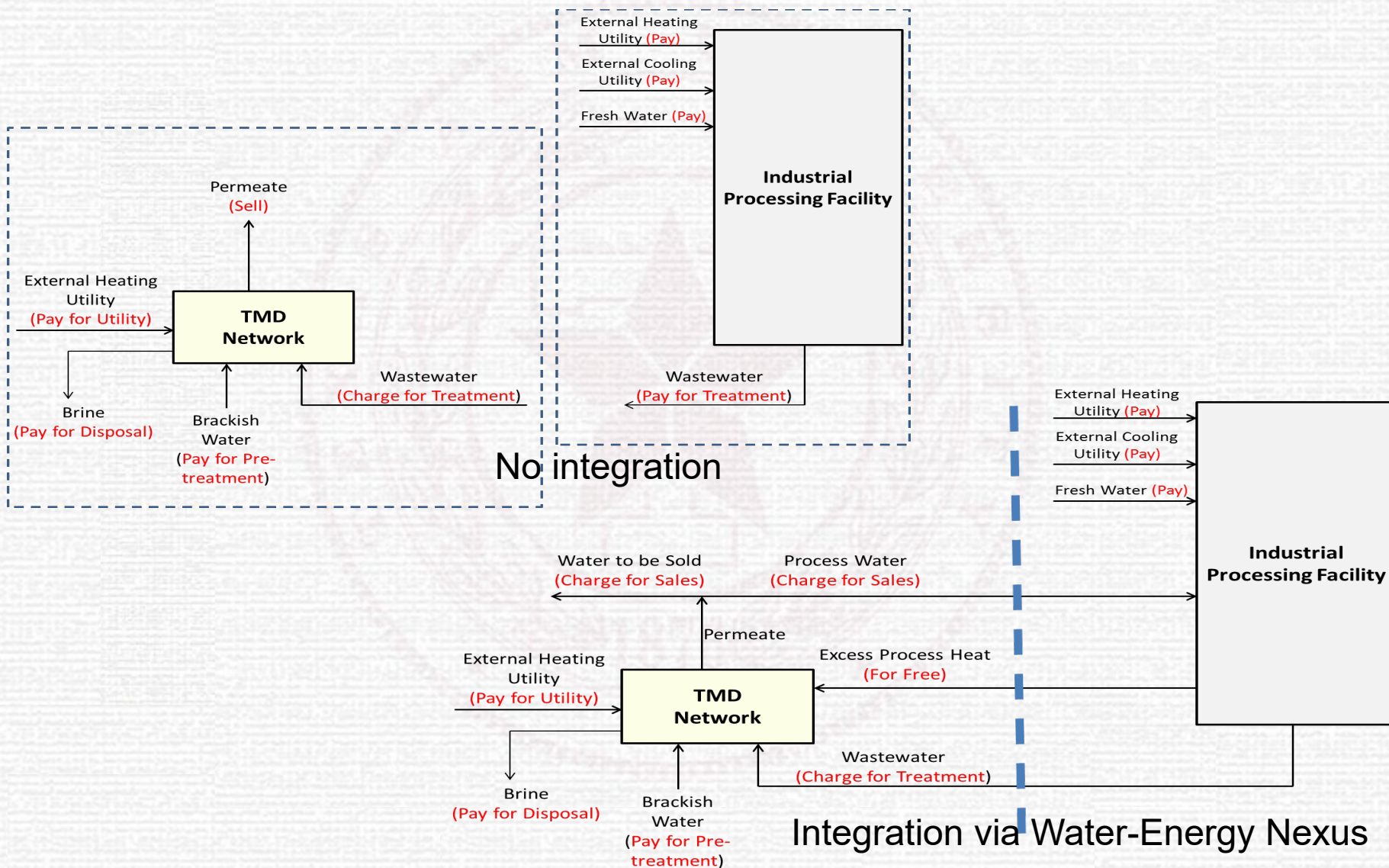
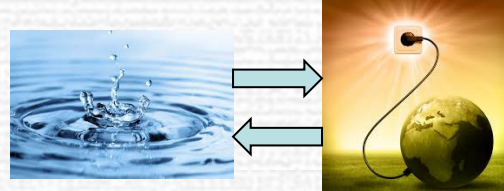
El-Halwagi, M. M., D. Harell, and H. D. Spriggs, "Targeting Cogeneration and Waste Utilization through Process Integration", *Applied Energy*, 86(6), pp. 880-887 (2009)



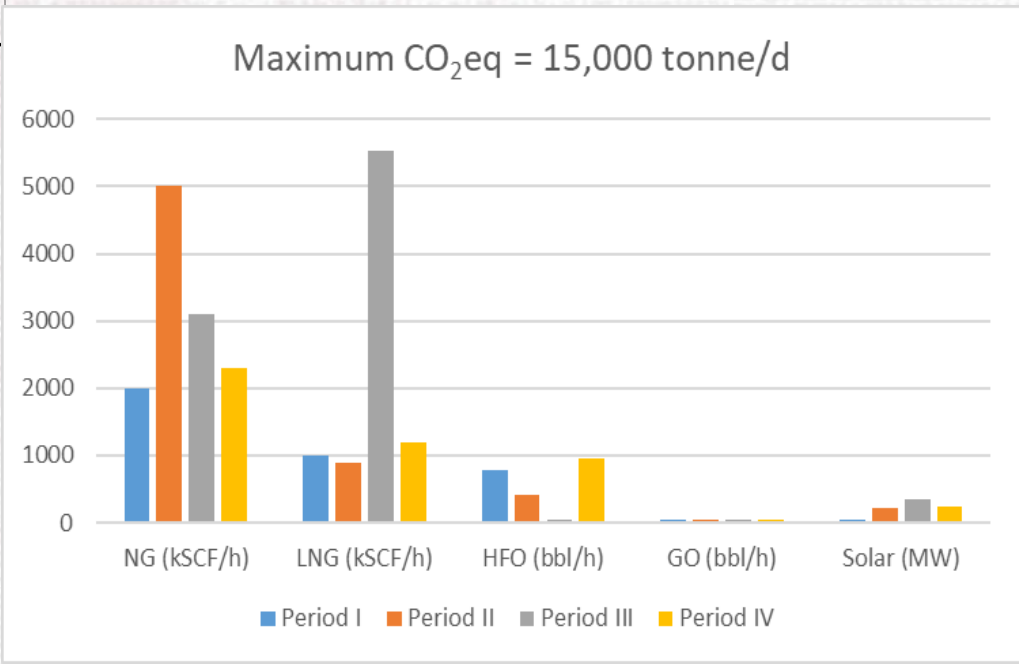
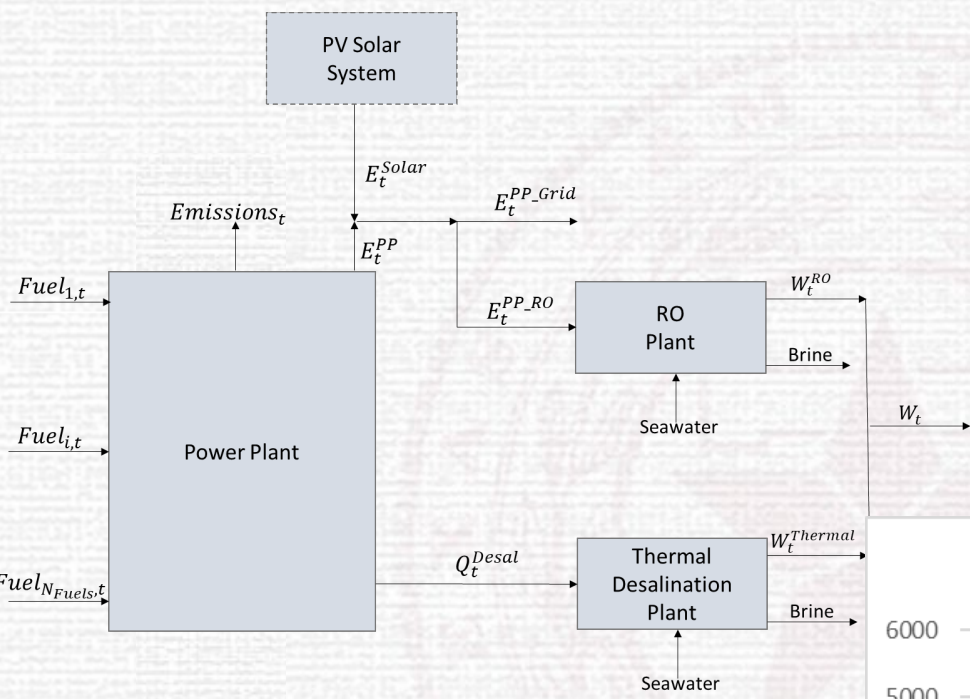
Incorporation of Renewables in Energy Integration/Absorptive Refrigeration



Water-Energy Nexus

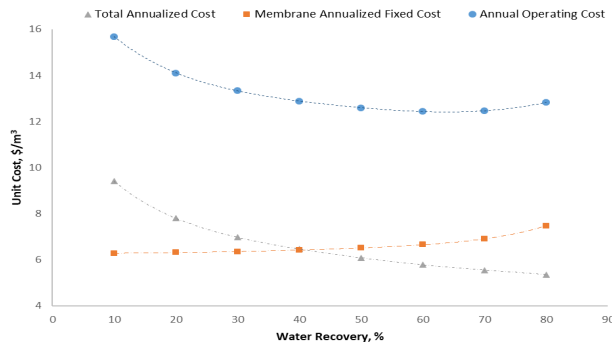
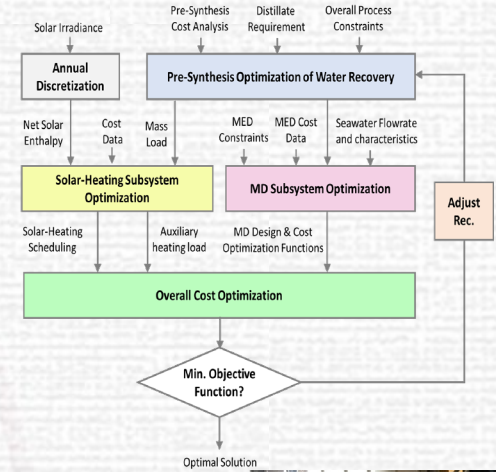
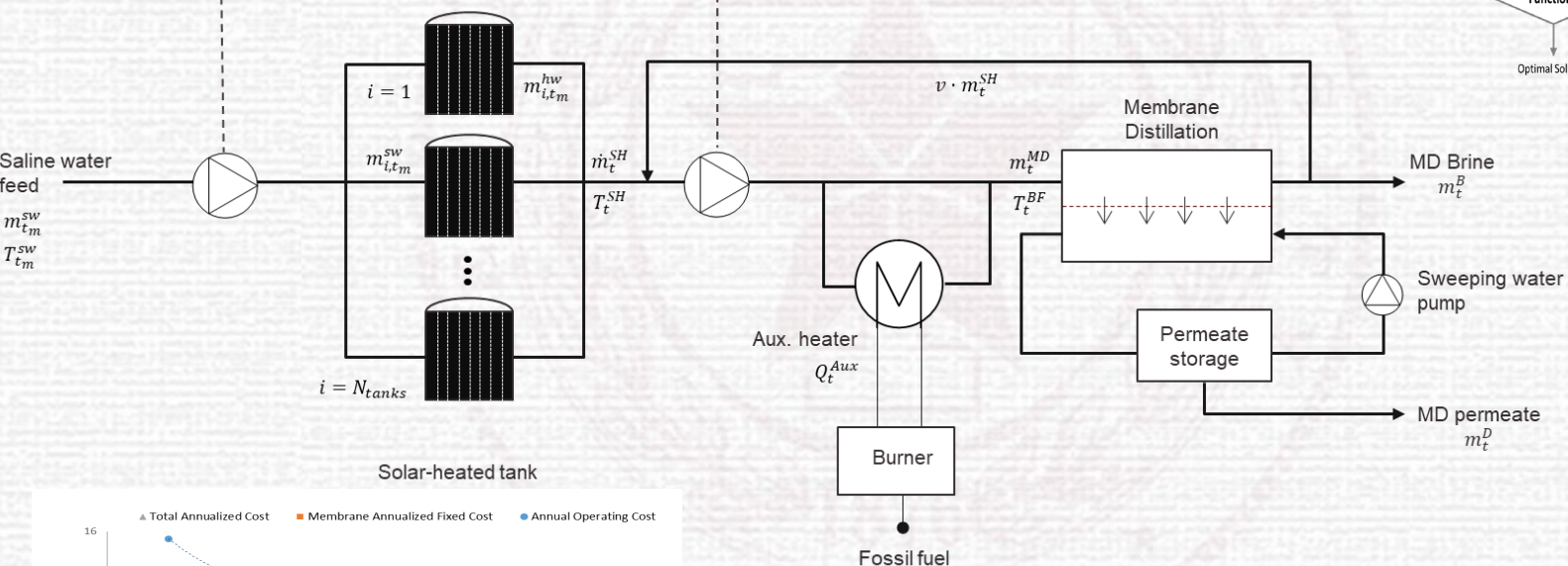
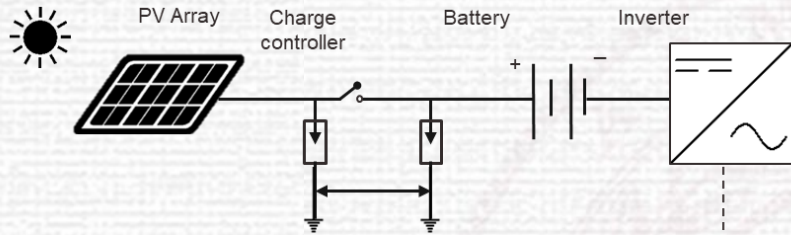


Incorporation of Solar Energy in Water-Energy Nexus



Al-Fadhli, F.M., N. Alhajeri, H. Ettouney, D. Sengupta, M. Holtzapple, and M. M. El-Halwagi, "Simultaneous optimization of power generation and desalination systems: a general approach with applications to Kuwait", Clean Techn Environ Policy (2022). <https://doi.org/10.1007/s10098-022-02303-3>

Optimal Design and Scheduling of a Solar-Assisted Domestic Desalination System



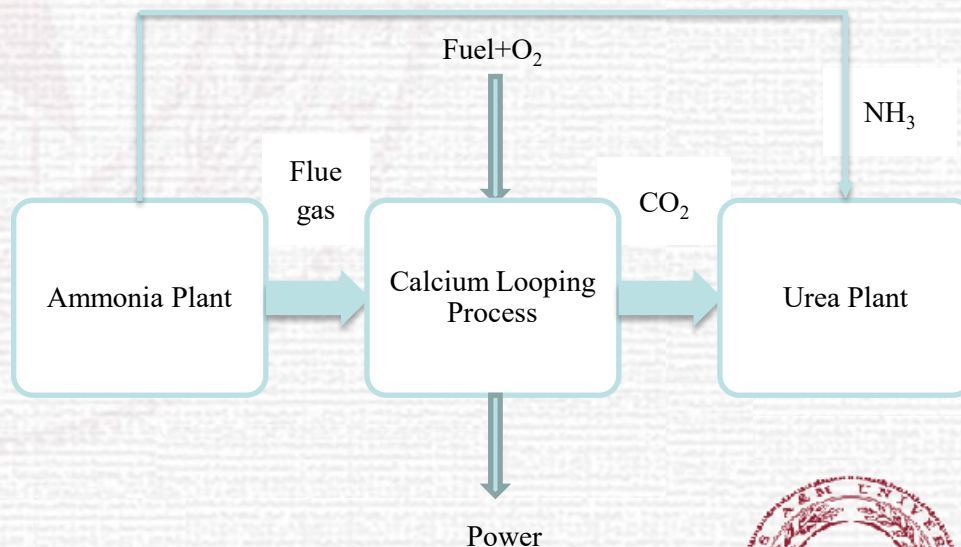
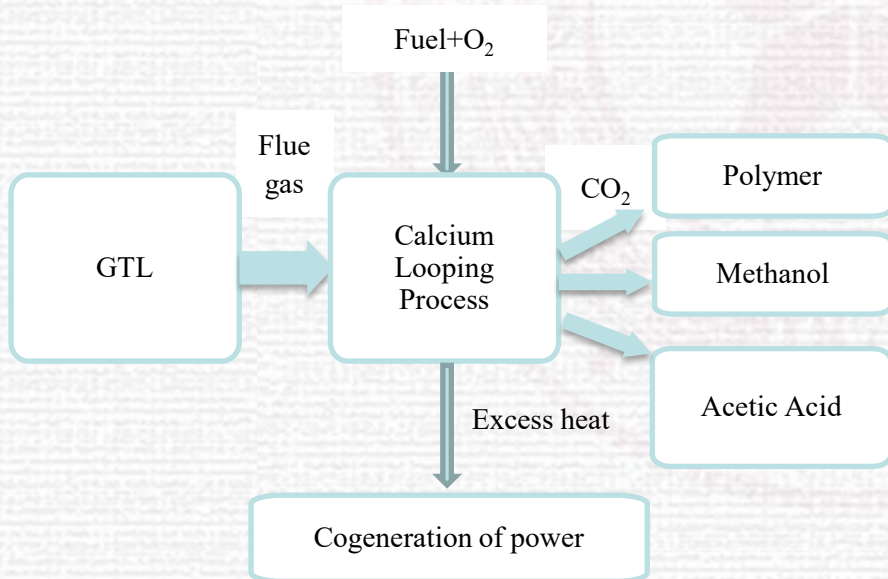
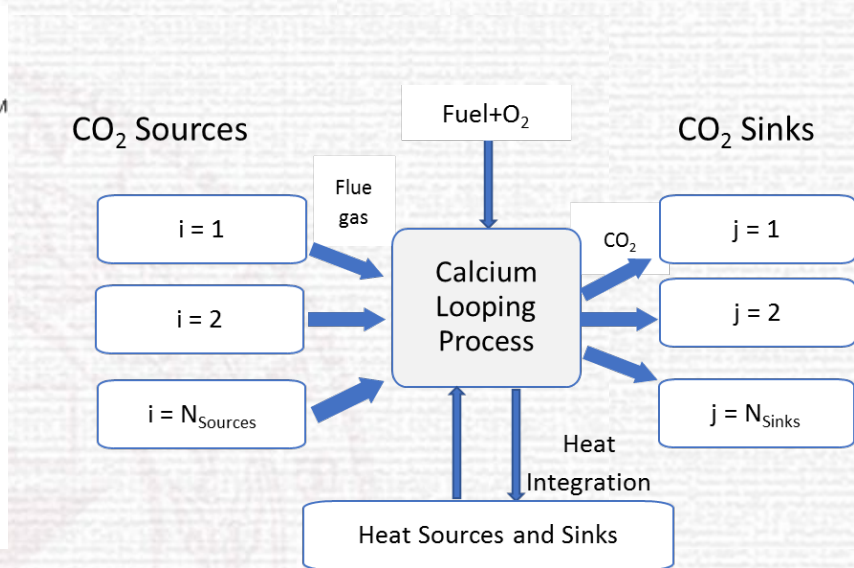
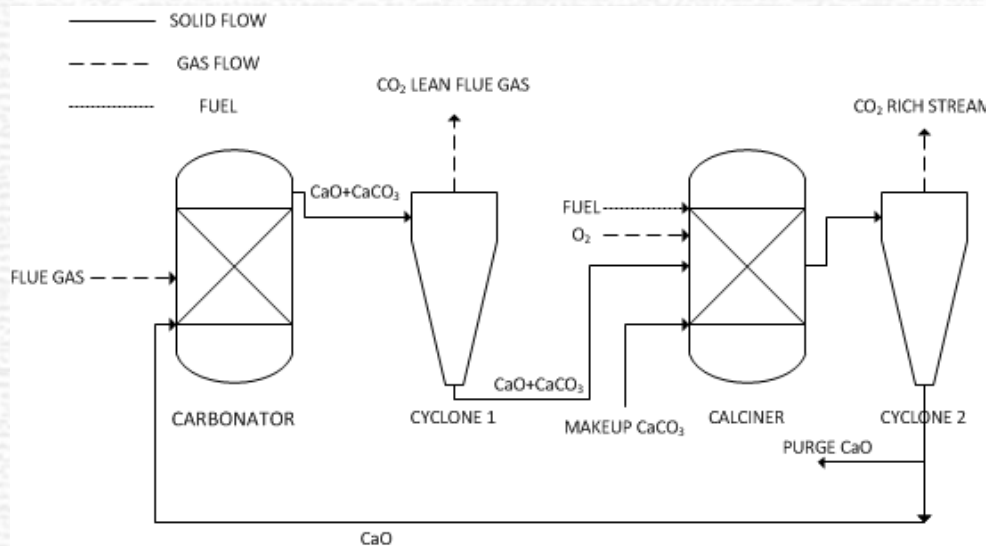
Baaqeel, H., A. Alghamdi, F. Abdelhady, and M. M. El-Halwagi, "Optimal Design and Scheduling of Solar-Assisted Domestic Desalination Systems", *Comp. Chem. Eng.* 132, p.106605 (2020) <https://doi.org/10.1016/j.compchemeng.2019.106605>



OUTLINE

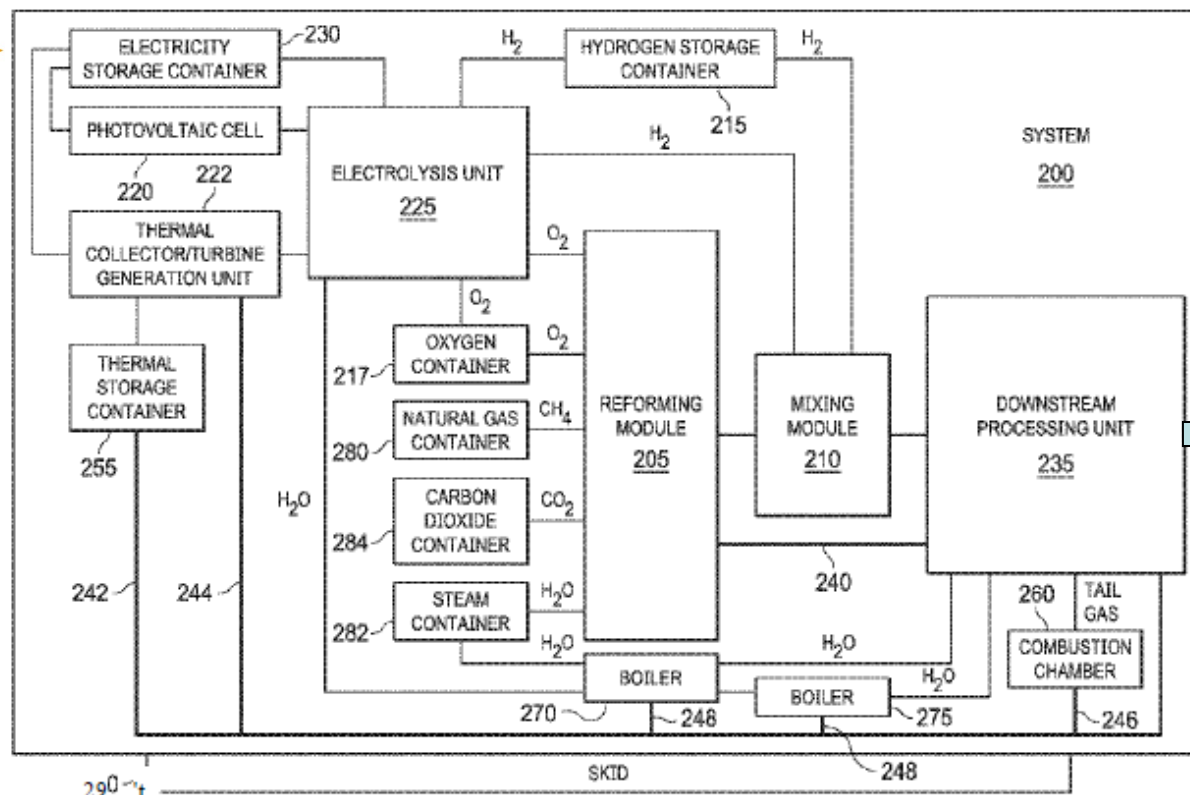
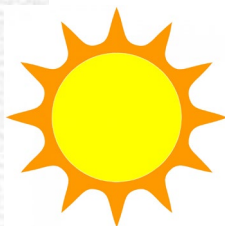
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CO₂ Monetization via Mass/Energy Integration with Calcium Looping



Use of Mass and Energy Integration to Create Novel Configurations for Energy Carriers and Chemicals

(54) Title: AN INTEGRATED AND TUNABLE SYSTEM FOR THE PRODUCTION OF SYNGAS AND CHEMICALS LAR-ASSISTED ELECTROLYSIS AND COMBINED REFORMING



Energy Carriers/
Chemical Supply Chains

Inventors: EL-HALWAGI, Mahmoud M.; 3369 TAMU, College Station, Texas 77843-3369 (US). CAMPBELL, Juliet E.; 3369 TAMU, College Station, Texas 77843-3369 (US).

(12) INTERNATIONAL APPLICATION PUBLISHED UNDER THE PATENT COOPERATION TREATY (PCT)

(19) World Intellectual Property Organization

International Bureau

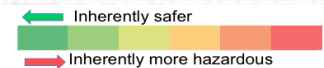
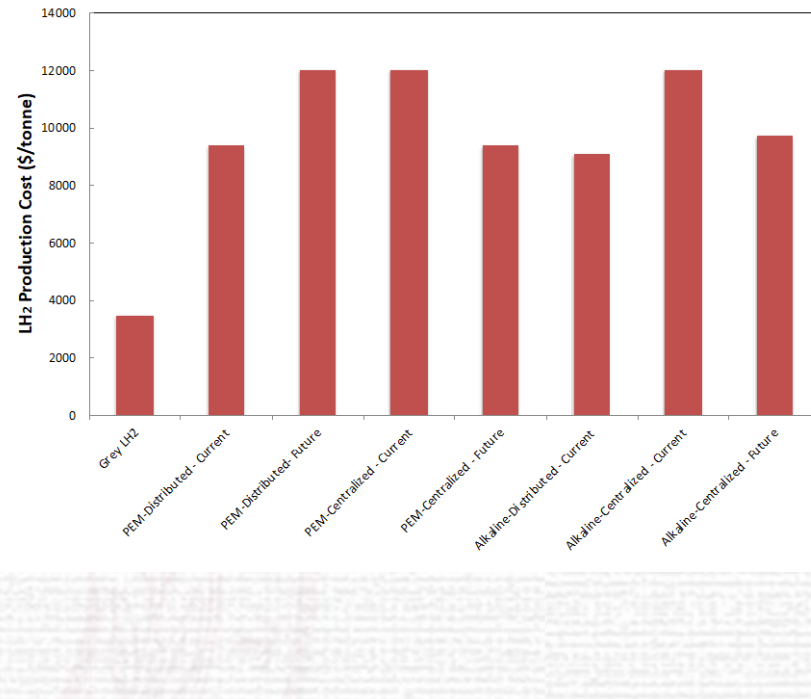
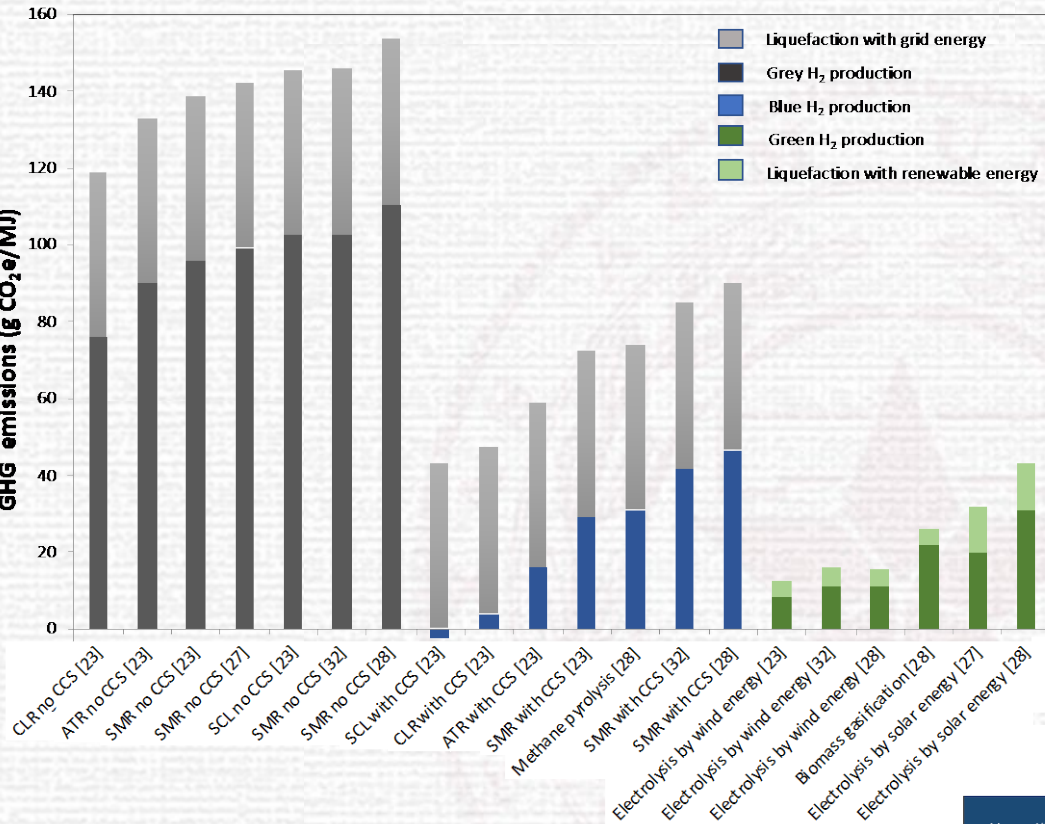
(43) International Publication Date
01 August 2019 (01.08.2019)



(10) International Publication Number

WO 2019/147786 A1

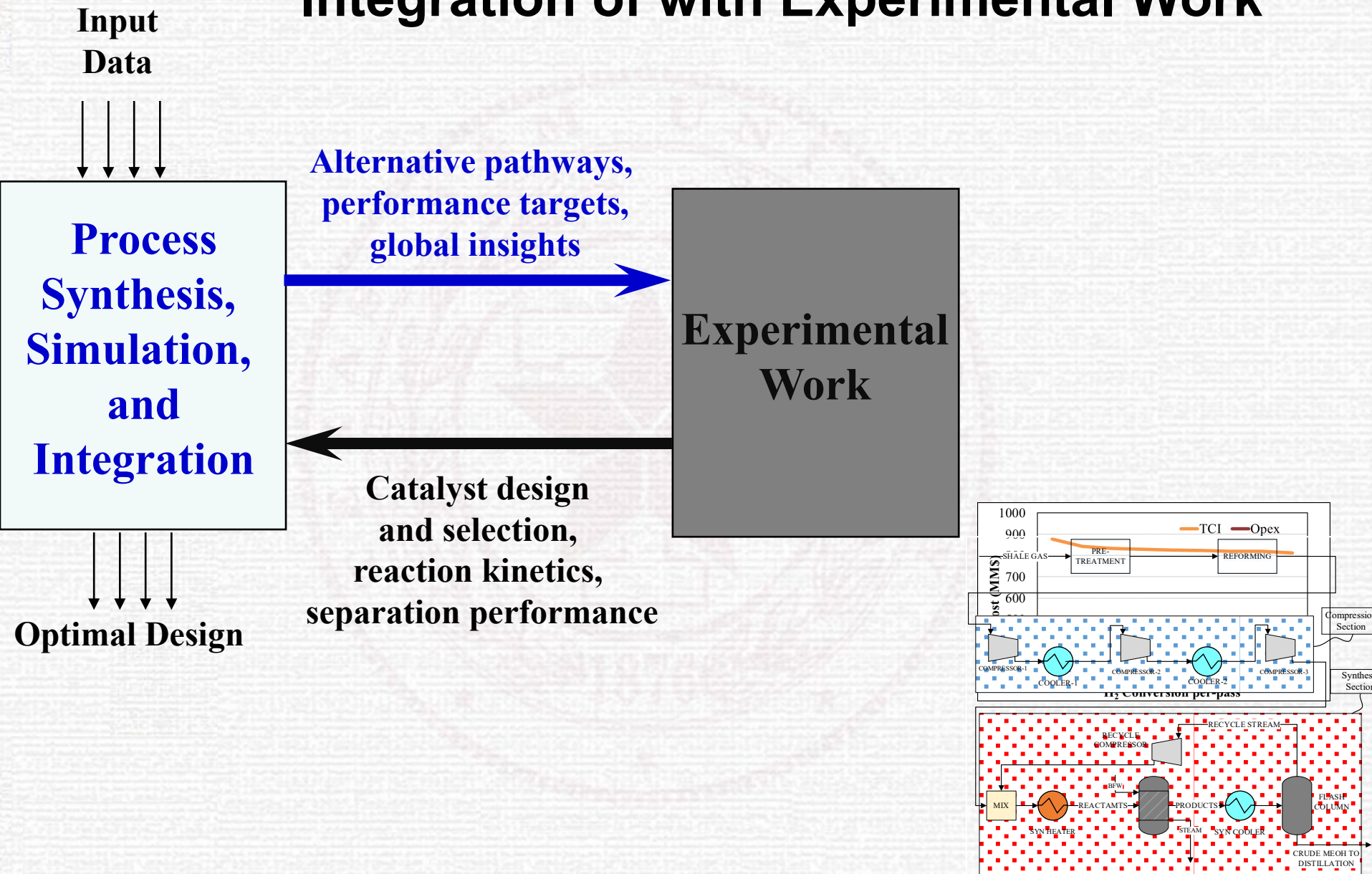
Benchmarking Production of Green Hydrogen



Hazard/Safety Category	Fuels							
	LH ₂	HFO/MGO	Biodiesel	LPG	LNG	MeOH	EtOH	Ammonia
Criterion 1: Flammability limits- vapor-air mixtures will ignite and burn over a well-specified range fo compositions.								
A wider range increases the limits in which a fire or explosion could commence.								
Lower heating value [MJ/kg]	120	42.7	37.4	46	50	19.9	26.7	18.6
Flammable limit range	71.0	9.7	-	7.5	9.7	29.3	15.7	13.0
Criterion 2: the potential of self-ignition								
In presence of oxygen all materials heated above their ignition temperature will burn								
Auto ignition point [C°]	520	250	220	470	540	464	363	650.9
Boiling point [C°]	-252.9	175.0	315.0	-42	-161.5	64.7	78.0	-33.3
Flash point [C°]	-259.2	61	100	-104	-175	12	17	-64.2
Criterion 3: Cloud formation and Flame propagation								
-'vapor density' or 'diffusion coefficient' would be related to buoyancy (e.g., LH ₂ evaporates for a short period due to its high buoyancy)								
Vapor Density air=1	0.10	5	0.88	0.56	0.55	1.10	1.60	0.80

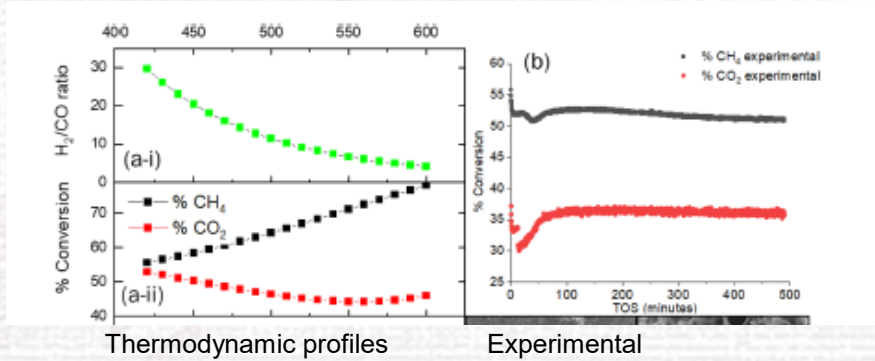
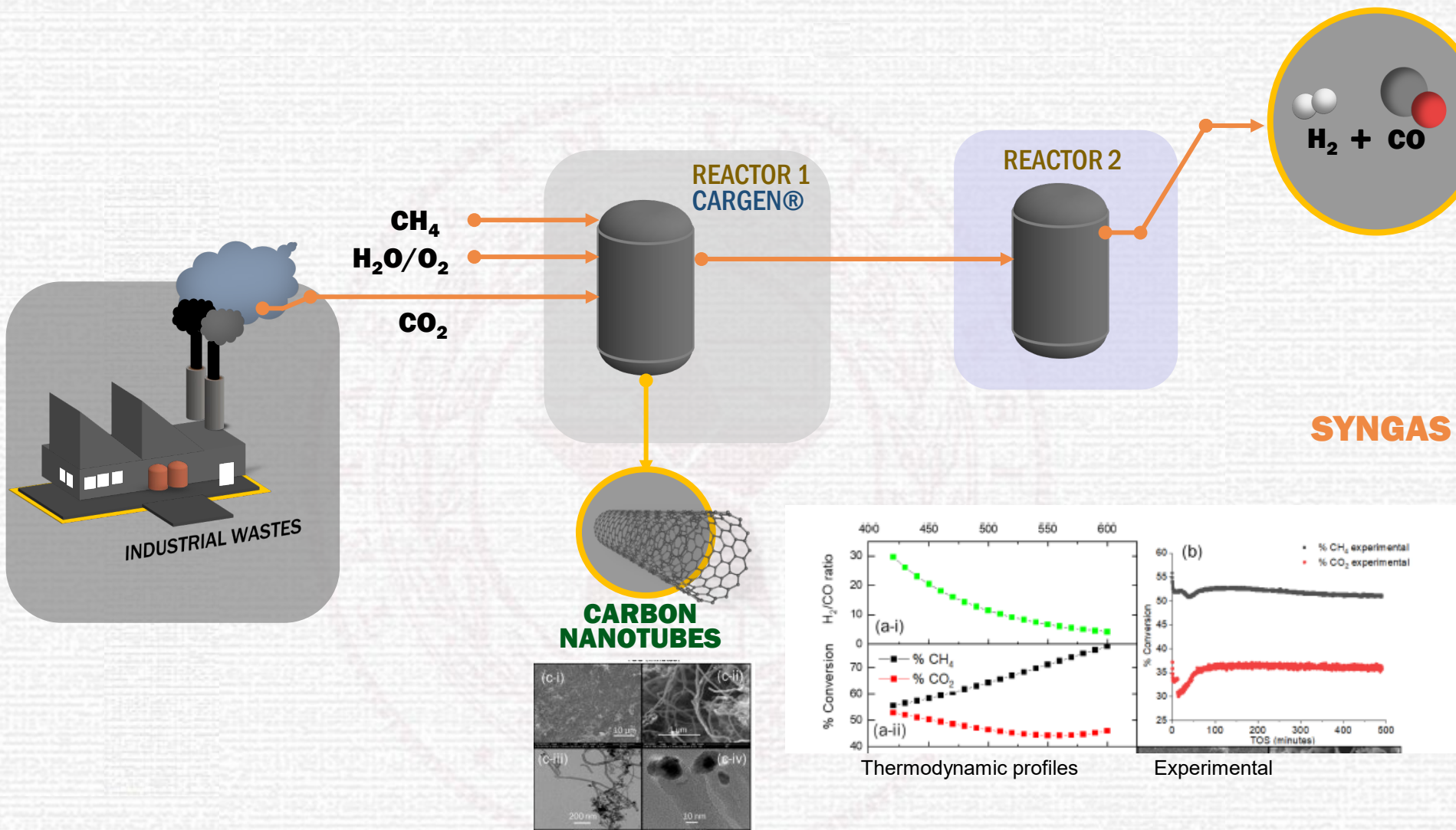
Atilhan, S., S. Park, M. M. El-Halwagi, M. Atilhan, M. Moore, and R. B. Nielsen, "Green Hydrogen as an Alternative Fuel for the Shipping Industry", Current Opinion in Chemical Engineering, Vol. 31, 100668 (2021)

Integration of with Experimental Work





Monetizing CO₂ into Carbon Nanotubes and Syngas (CARGEN[®])



Chaliwalla, M. S., N. O. Elbashir, D. Sengupta, and M. M. El-Halwagi, "System and Method for Carbon and Syngas Production", Patent Pub. No.: US 2020/0109050 A1, Apr. 9, 2020
 Chaliwalla, M. S., H. Choudhury, D. Wang, M. El-Halwagi, E. Weitz, and N. Elbashir, "A novel CO₂ utilization technology for the synergistic co-production of multi-walled carbon nanotubes and syngas", Scientific Reports 11(1), 1-8 (2021)



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INCORPORATING SUSTAINABILITY AND TARGETING IN PROFITABILITY CALCULATIONS

- Process improvement projects are typically driven/assessed by profitability criteria (e.g., return on investment, payback period, net present value)
- Sustainability goals are well aligned with process integration activities (natural-resource conservation, process-efficiency enhancement, pollution prevention, etc.)
- Targeting approaches can set goals for sustainability
- Sustainability considerations are best included in the early stages of decision making

How to use a consistent platform for including sustainability in development and assessment of process integration and improvement projects?

SUSTAINABILITY WEIGHTED RETURN ON INVESTMENT METRIC “SWROIM”

- consider a set of process integration project alternatives: $p = 1, 2, \dots, N_{Projects}$.
- For the p^{th} project, a new term called the *Annual Sustainability Profit “ASP”* is defined as follows

$$ASP_p = AEP_p \left[1 + \sum_{i=1}^{N_{Indicators}} w_i \left(\frac{Indicator_{p,i}}{Indicator_i^{Target}} \right) \right]$$

Annual Economic Profit

Index for sustainability indicators

weighing factor: a ratio representing the relative importance of the i^{th} sustainability indicator compared to the annual net economic profit

Value of the i^{th} sustainability indicator for the p^{th} project: may be positive, 0, or negative

Target value of the i^{th} sustainability indicator (obtained from process integration benchmarking or taken as the largest value from all projects, or set by the company as a goal): always positive indicating improvement

$$SWROIM_p = \frac{ASP_p}{TCI_p}$$



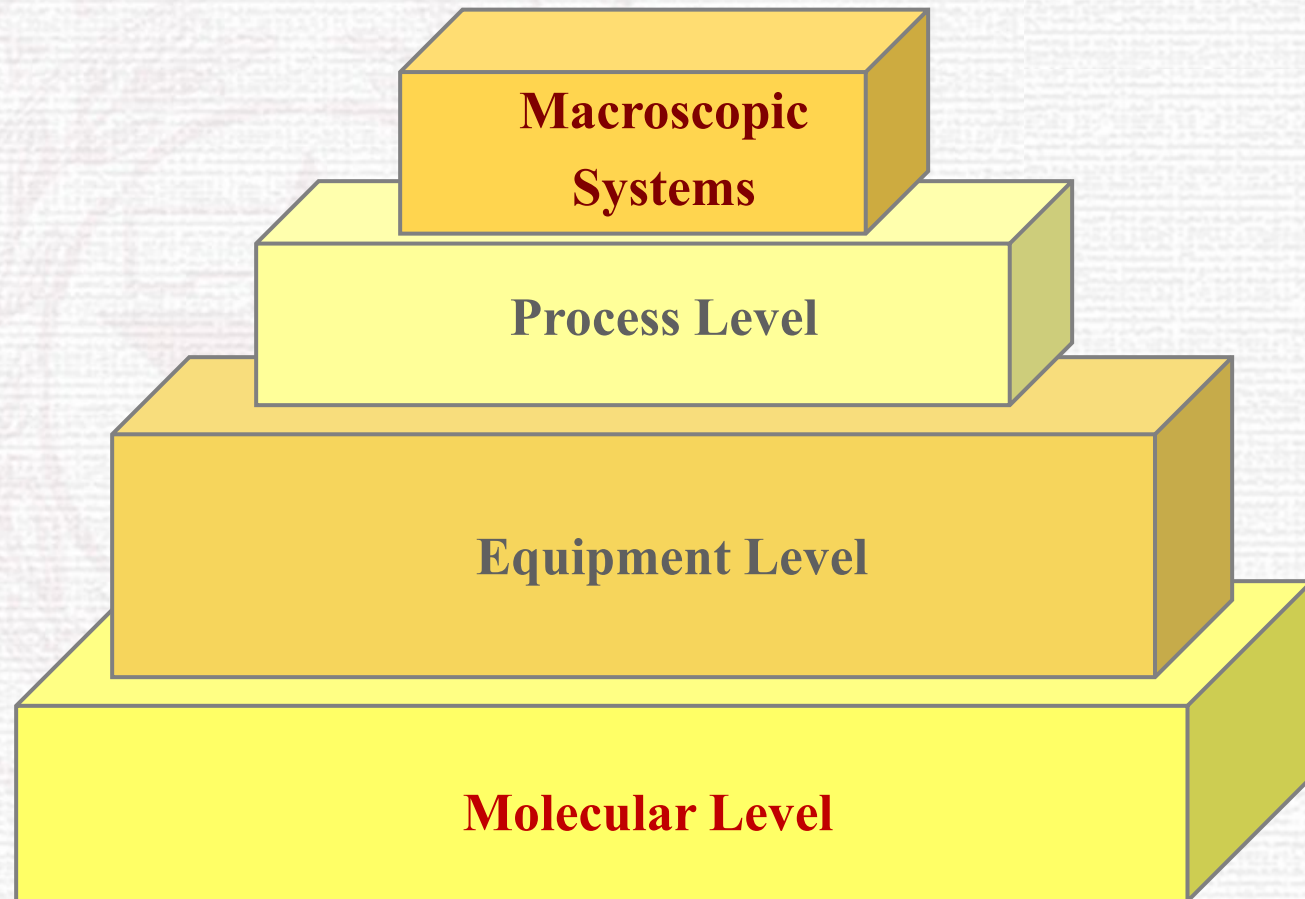
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THE MULTI-SCALE NATURE PROCESS INTEGRATION

Example:

- Eco-Industrial Parks



What is an EIP?

An EIP may be defined as “a community of manufacturing and service businesses located together on a common property. Members seek enhanced environmental, economic, and social performance through collaboration in managing environmental and resource issues”

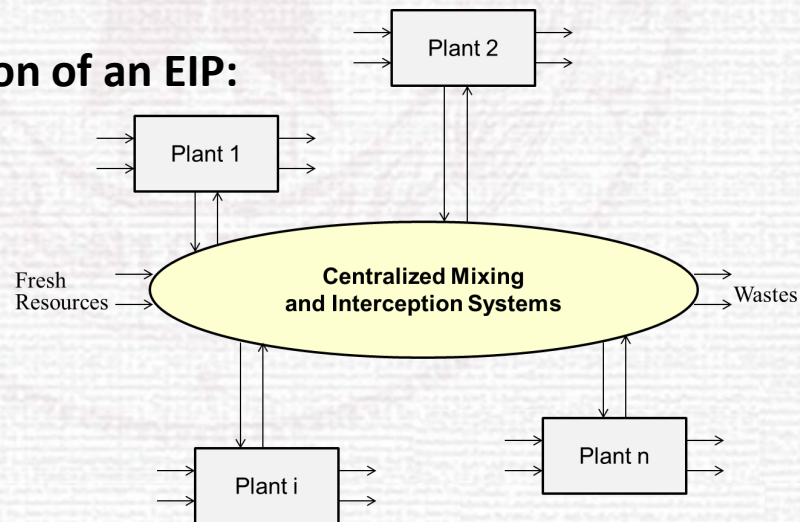
(Source: Lowe E. A, “Eco-Industrial Park Handbook for Asian Developing Countries”, A Report to Asian Development Bank. Indigo Development, Santa Rosa, California (2001)).

Key Characteristic of a Successful EIP:

Synergism to promote industrial symbiosis is essential for the creation of an EIP and “a key condition for an EIP to successfully attract industrial participants is that it should demonstrate that the sum of the benefits achieved by working as collective is greater than working as a stand-alone facility”

(Source: Lovelady, E. M. and M. M. El-Halwagi, “Design and Integration of Eco-Industrial Parks”, Environmental Progress and Sustainable Energy, 28(2), pp. 265-272 (2009))

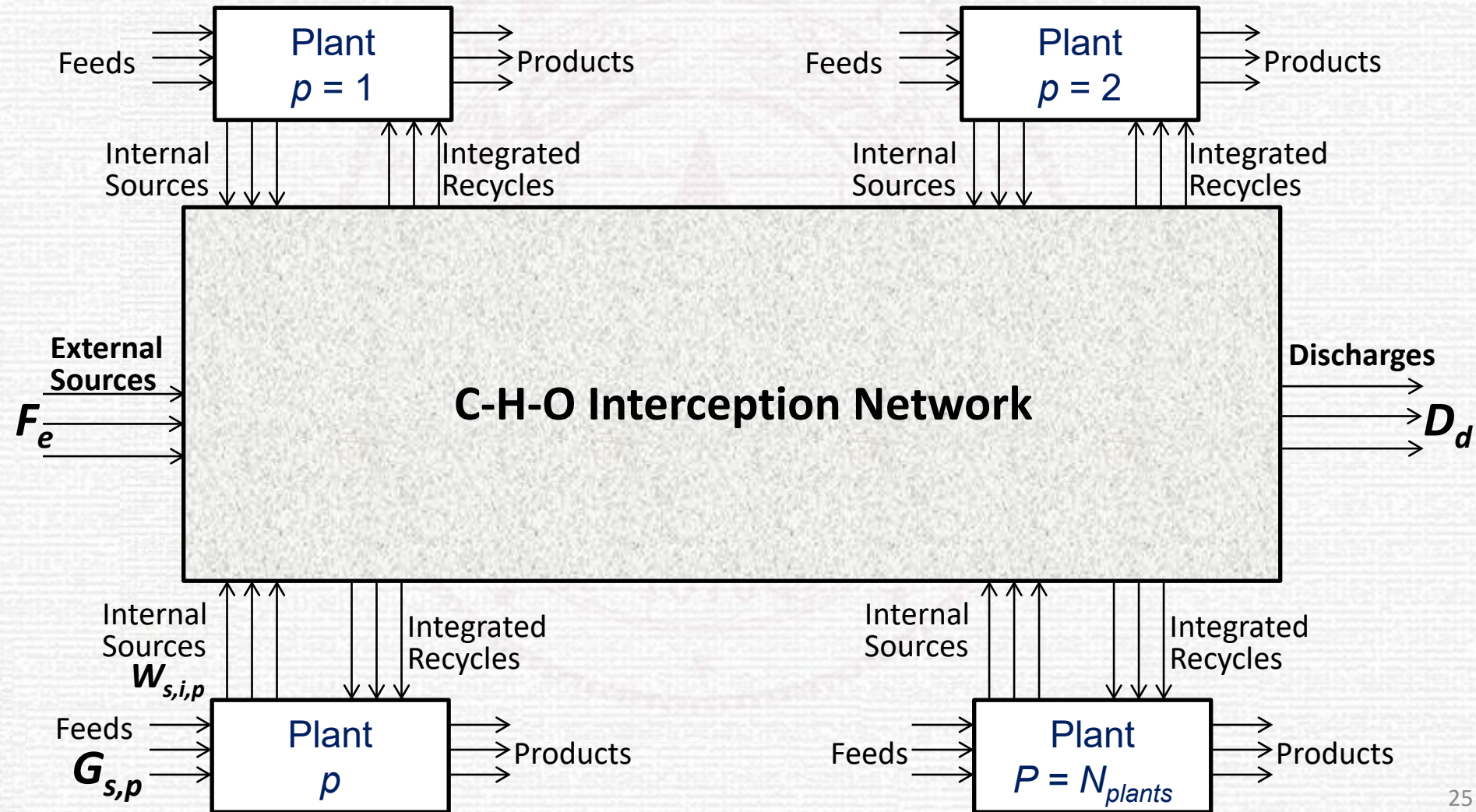
Mass Integration Representation of an EIP:



Source: Spriggs, H. D., E. A. Lowe, J. Watz, M. M. El-Halwagi, and E. M. Lovelady, “Design and Development of Eco-Industrial Parks”, paper #109a, AIChE Spring Meeting, New Orleans, April, (2004)

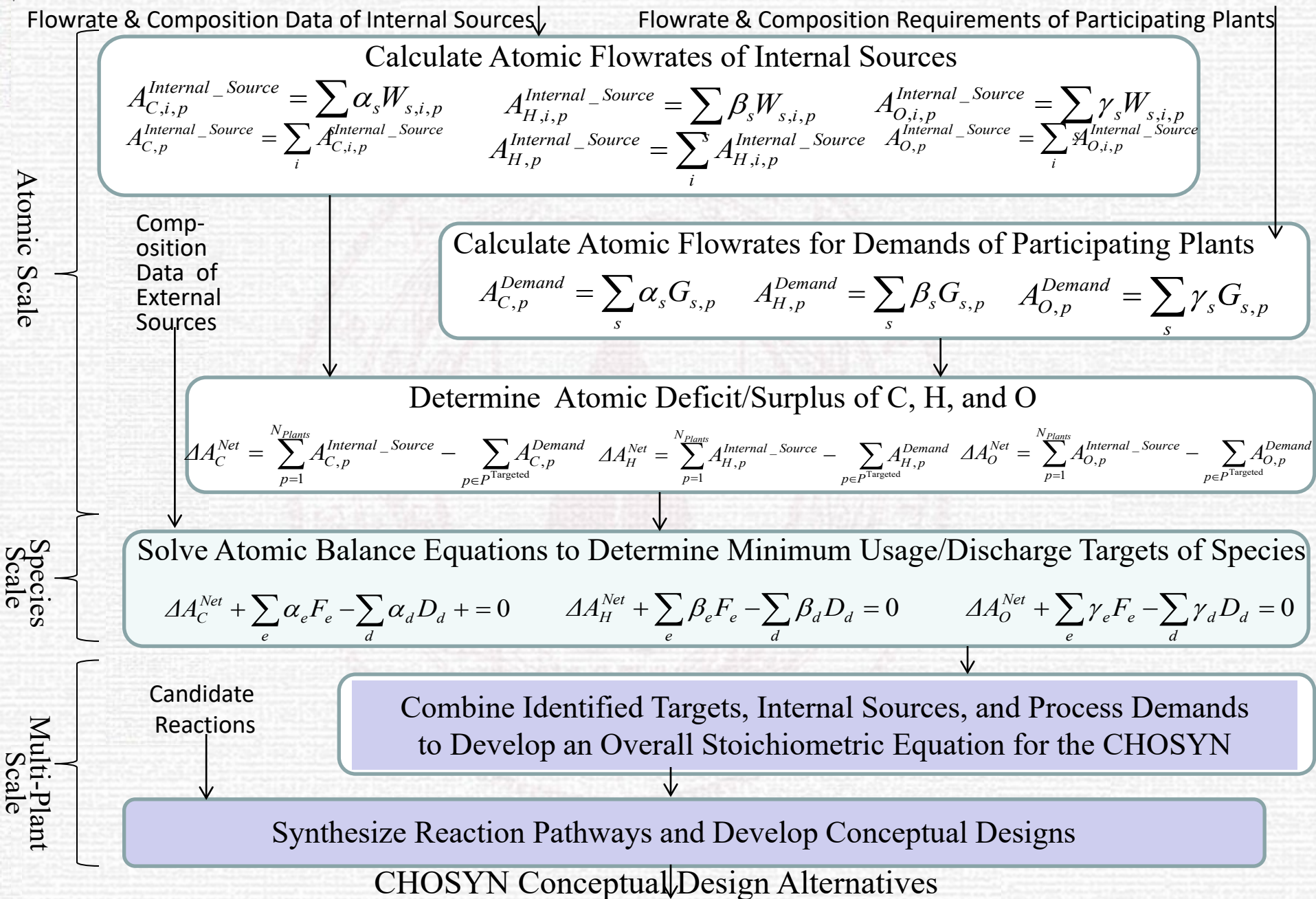
CARBON-HYDROGEN-OXYGEN SYBIOSIS NETWORK (CHOSYN)

“A cluster of multiple plants with shared centralized facilities to enable the exchange, conversion, separation, treatment, splitting, mixing, and allocation of streams containing C-H-O compounds”





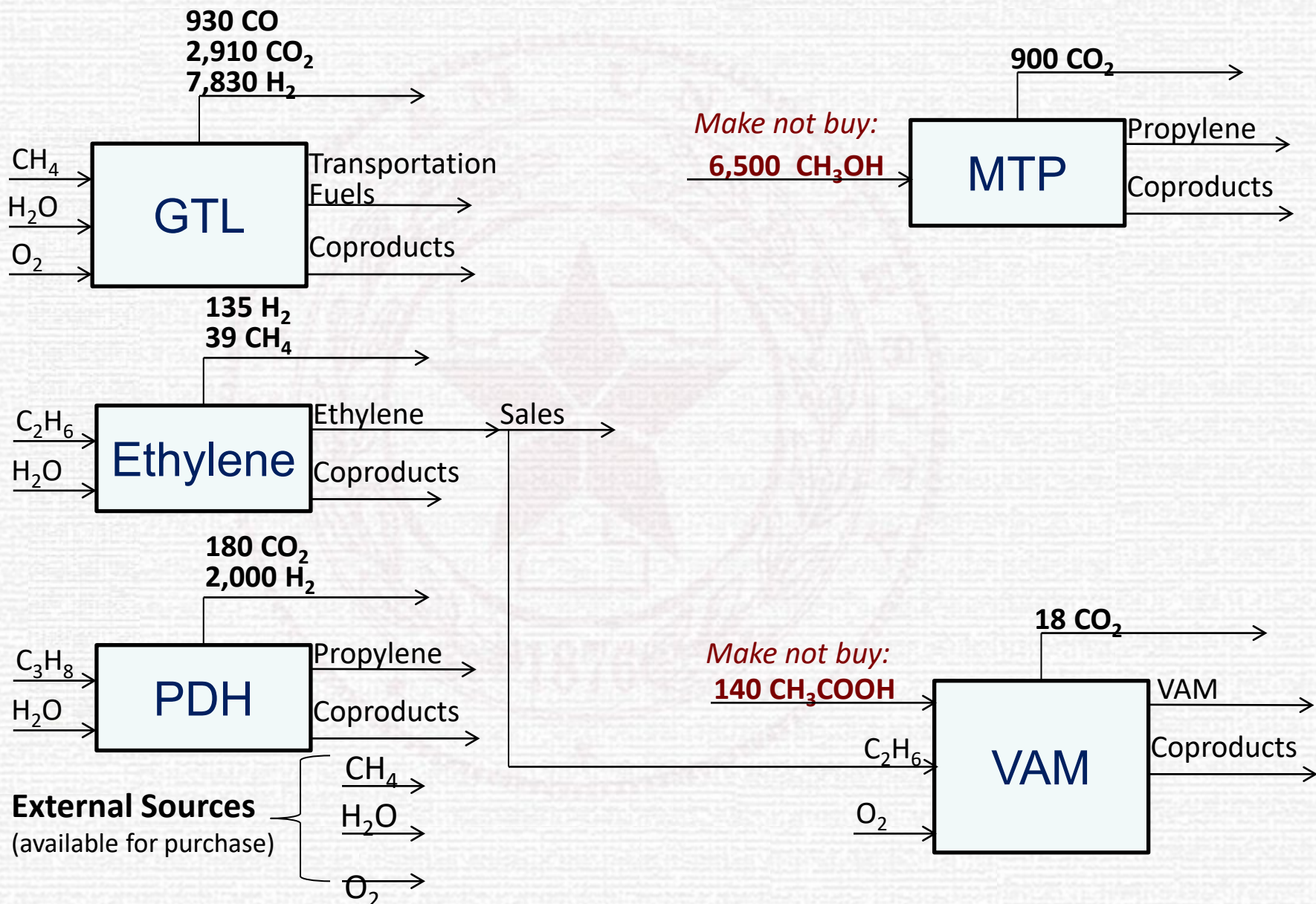
SUMMARY OF CHOSYN MULTI-SCALE TARGETING APPROACH



EXAMPLE

1. How to Best Integrate Discharges and Feedstocks?

2. How to Establish Targets (Atomic, Chemical Species, and Multi-Plant)for Integration Opportunities?



Key Targeting Results for the CHOSYN Case Study

Atomic Targeting

$$\Delta A_C^{Net} = -1,803 \text{ kmol C/h (target for deficit in carbon)}$$

$$\Delta A_H^{Net} = -6,474 \text{ kmol H/h (target for deficit in hydrogen)}$$

$$\Delta A_O^{Net} = 2,166 \text{ kmol O/h (target for surplus oxygen)}$$

Molecular Targeting

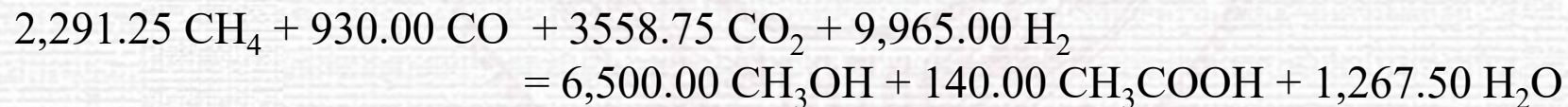
$$F_{CH_4} = 2,252.25 \text{ (external)}$$

$$F_{H_2O} = -1,267.50 \text{ (-ive } \rightarrow \text{ net discharge)}$$

$$D_{CO_2} = -449.25 \text{ (-ive } \rightarrow \text{ net discharge)}$$

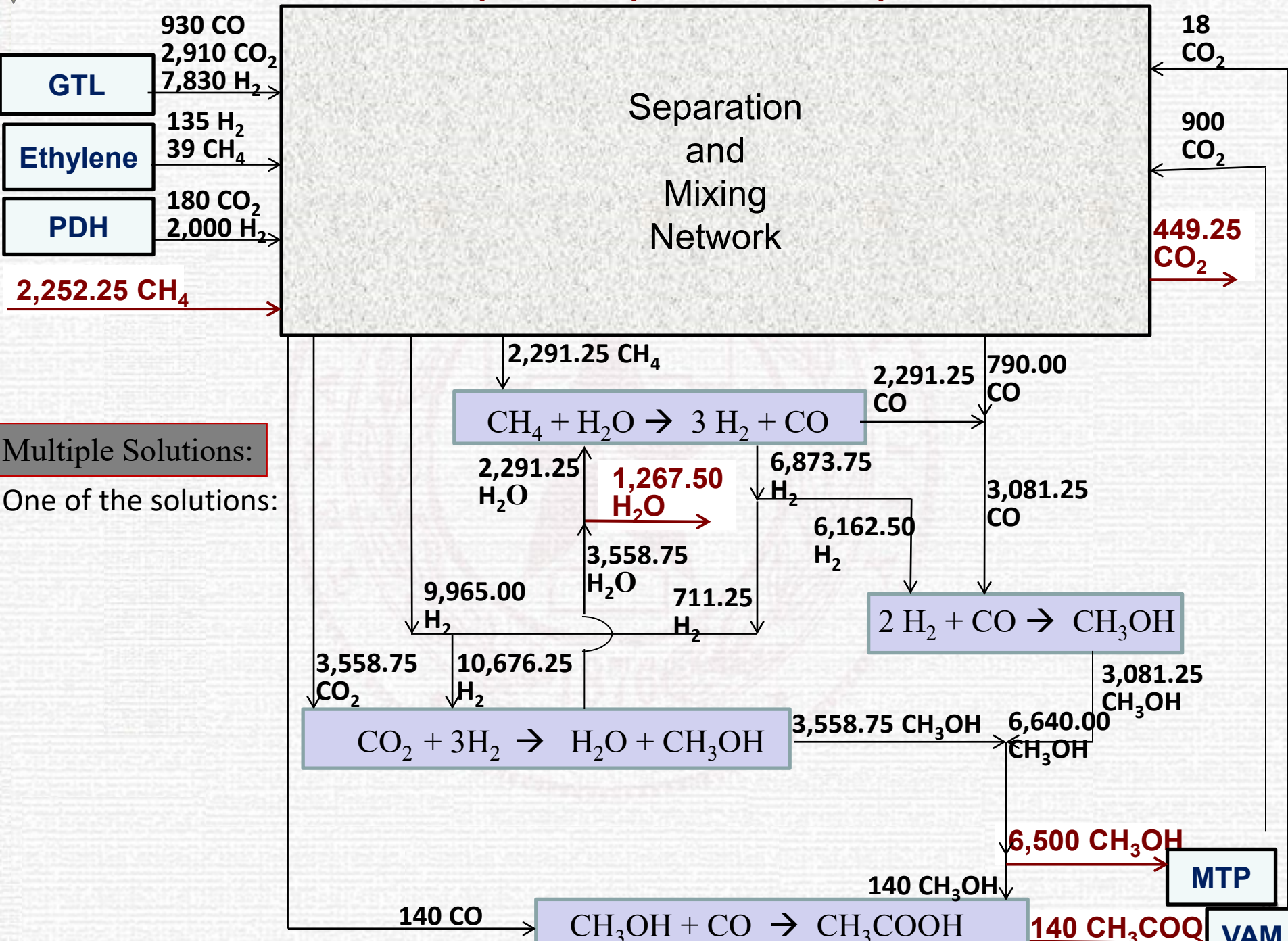
Chemical Species Targets for Minimum
External Resource Usage and Discharge
How to achieve?

Overall stoichiometric equation for the internal streams & external (fresh + discharges) :



Next, Reaction Pathway Synthesis

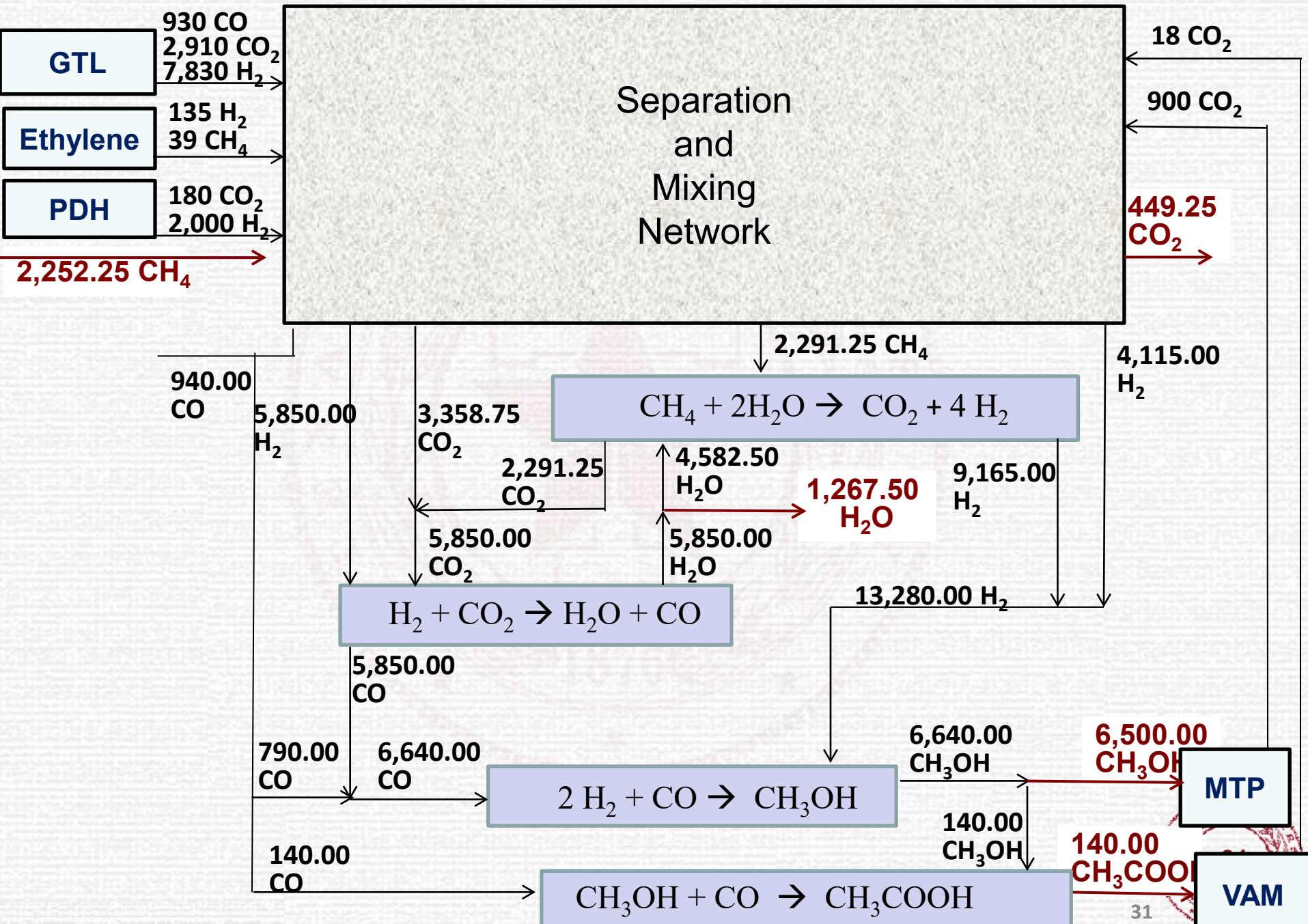
Examples of Implementation: Option 1



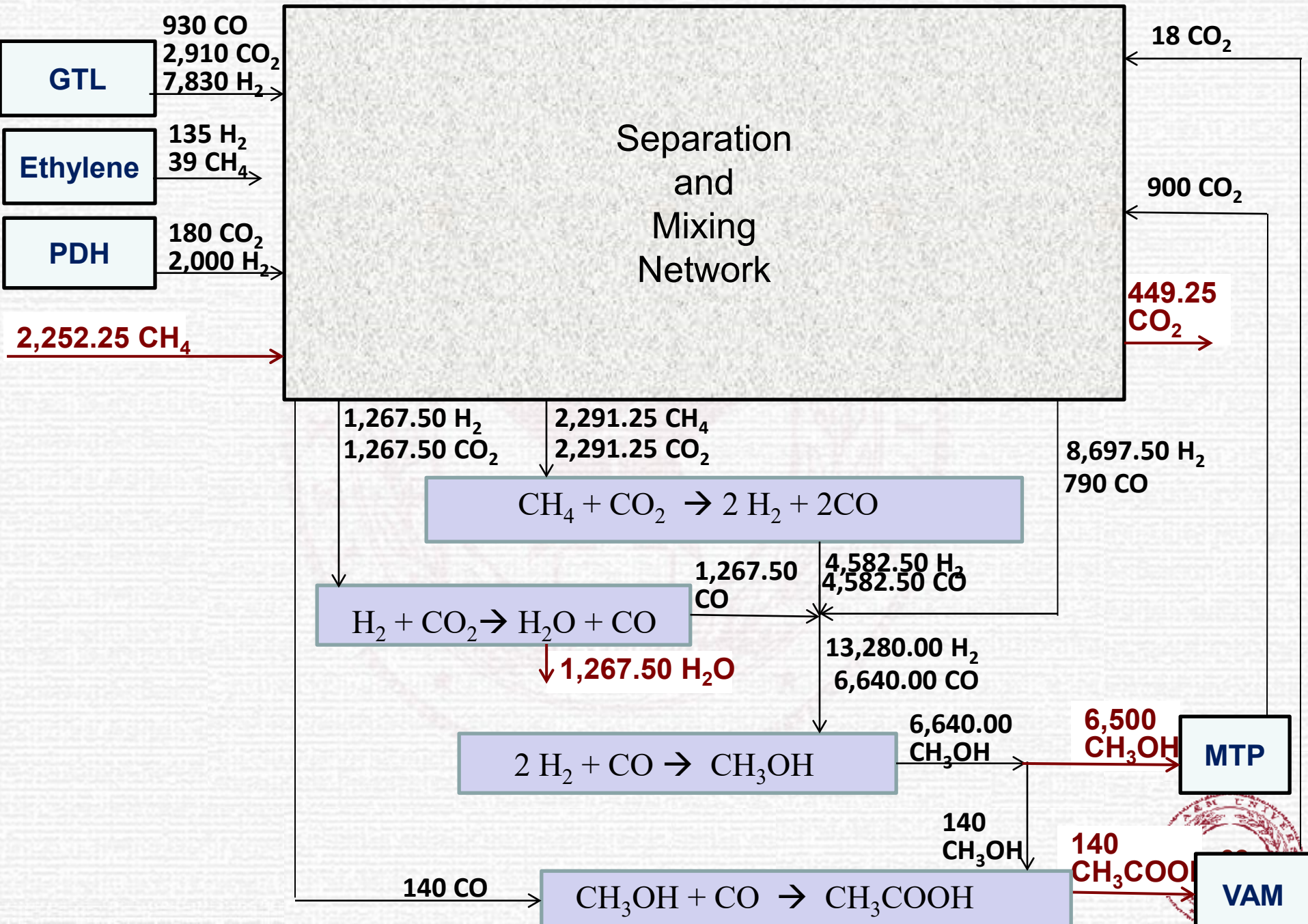
Multiple Solutions:

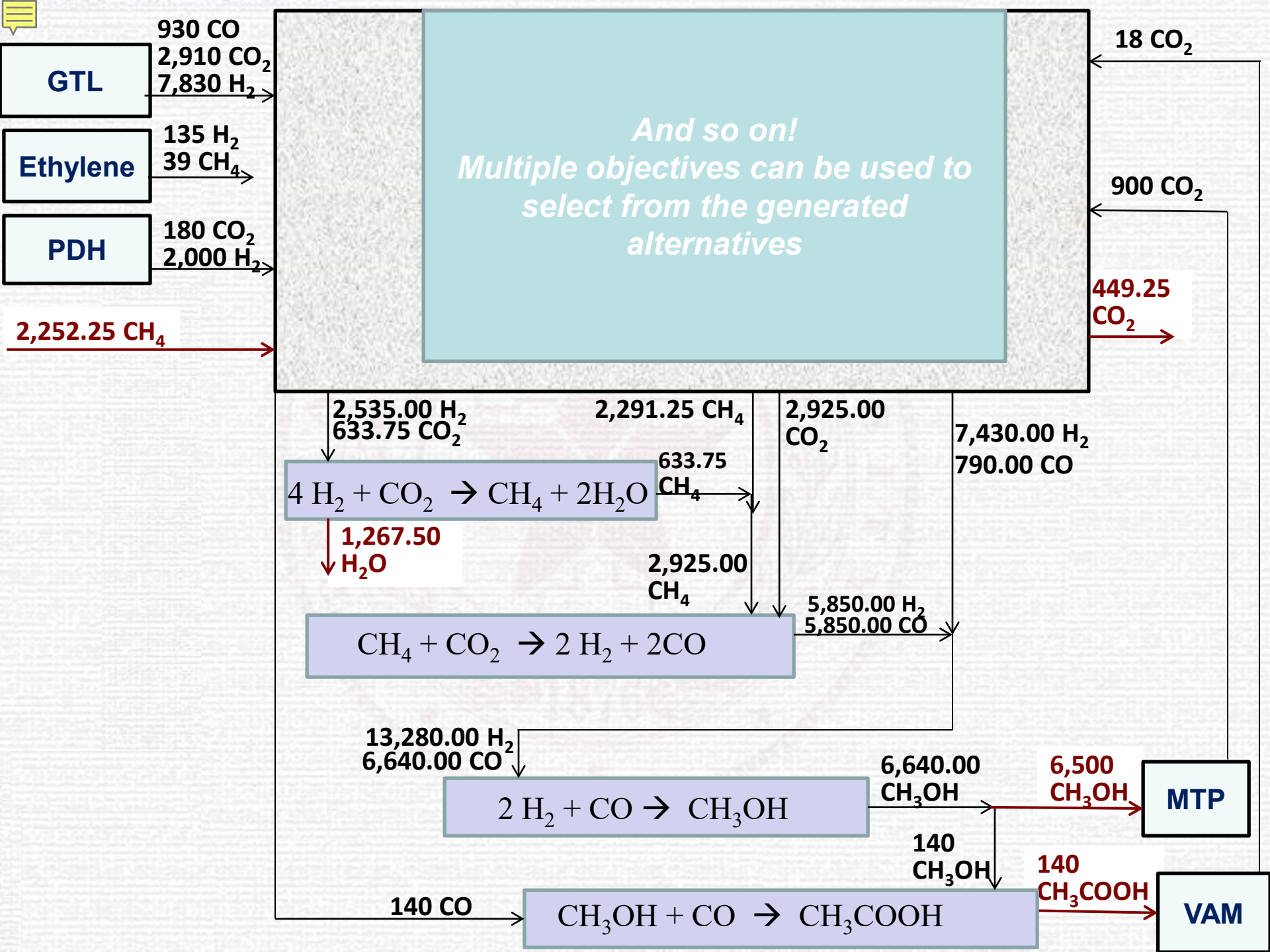
One of the solutions:

Examples of Implementation: Option 2



Examples of Implementation: Option 3





Sample Categories of CHOSYN Synthesis

AICHE

Synthesis of C-H-O Symbiosis Networks


Mohamed M. B. Noureldin and Mahmoud M. El-Halwagi
Ferrin Dept. of Chemical Engineering, Texas A&M University, College Station, TX 77843

DOI 10.1002/aic.14714

Process Integration and Optimization for Sustainability (2019) 3:199–212
<https://doi.org/10.1007/s41660-018-0065-y>

ORIGINAL RESEARCH PAPER

A Disjunctive Programming Approach for Optimizing Carbon, Hydrogen, and Oxygen Symbiosis Networks

Maricruz Juárez-García¹ · José María Ponce-Ortega¹  · Mahmoud M. El-Halwagi^{2,3}



Contents lists available at ScienceDirect

Chemical Engineering Science

journal homepage: www.elsevier.com/locate/ces

CO₂ footprint reduction via the optimal design of Carbon-Hydrogen-Oxygen SYmbiosis Networks (CHOSYNs)

Marc Panu^a, Kevin Topolski^a, Sarah Abrash^a, Mahmoud M. El-Halwagi^{a,b,*}

Smart and Sustainable Manufacturing Systems

Rajib Mukherjee¹ and Mahmoud M. El-Halwagi^{1,2}

DOI: 10.1520/SSMS20180022

Reliability of C-H-O Symbiosis Networks under Source Streams Uncertainty

Process Integr Optim Sustain (2017) 1:3–13
DOI 10.1007/s41660-016-0001-y

ORIGINAL RESEARCH PAPER

A Shortcut Approach to the Multi-scale Atomic Targeting and Design of C–H–O Symbiosis Networks

Mahmoud M. El-Halwagi¹



Contents lists available at ScienceDirect

Computers and Chemical Engineering

journal homepage: www.elsevier.com/locate/compchemeng

An anchor-tenant approach to the synthesis of carbon-hydrogen-oxygen symbiosis networks[☆]

Kevin Topolski^a, Mohamed M.B. Noureldin^b, Fadwa T. Eljack^c, Mahmoud M. El-Halwagi

Chemical Engineering & Processing: Process Intensification 141 (2019) 107535



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journal homepage: www.elsevier.com/locate/cep



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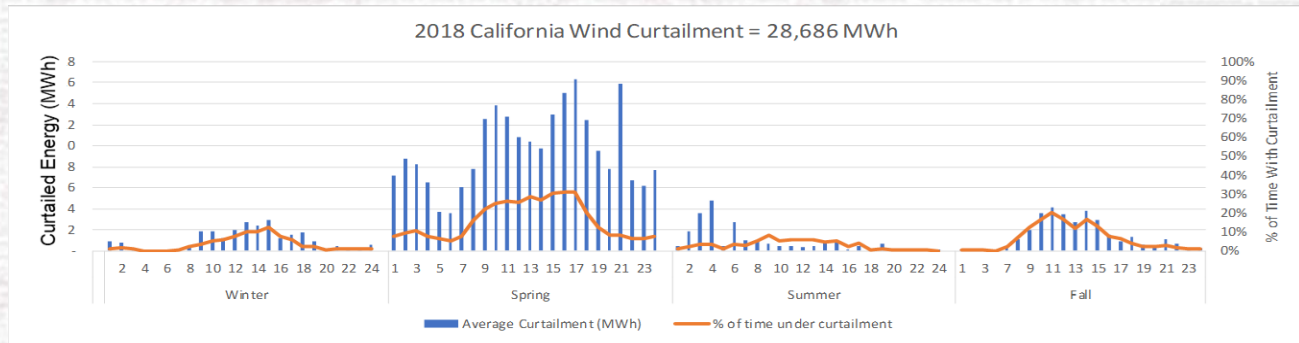
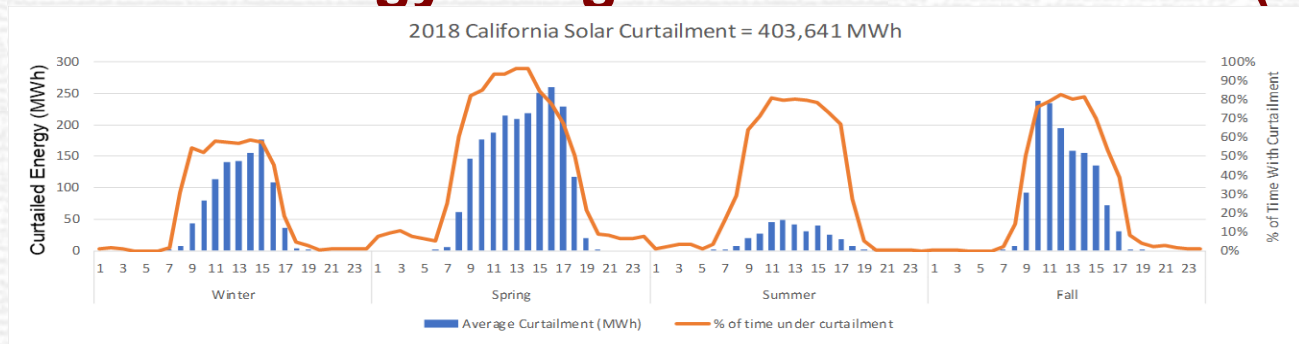
pubs.acs.org/IECR

Integrating Mass and Energy through the Anchor-Tenant Approach for the Synthesis of Carbon-Hydrogen-Oxygen Symbiosis Networks

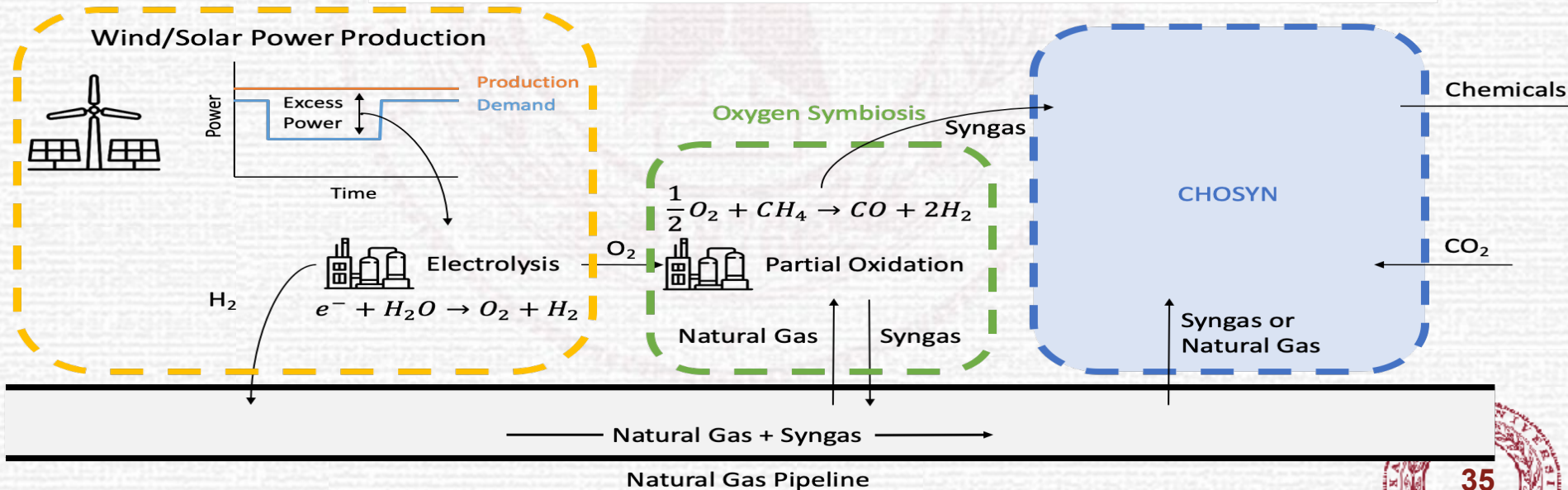
Kevin Topolski,[†] Luis Fernando Lira-Barragán,[‡] Marc Panu,[†] José María Ponce-Ortega,[‡] and Mahmoud M. El-Halwagi^{*,†,§,¶}

Curtailed Wind/Solar Energy Integration with CHOSYN (PtG)

“Curtailement of energy which is the activity of lowering the delivery of energy from a source (e.g., solar energy collector) to the electric grid. Curtailement may be driven by limited capacity of the grid, energy supply exceeding demand, and the desire to avoid unfavorable selling price of energy.”



Power to Gas





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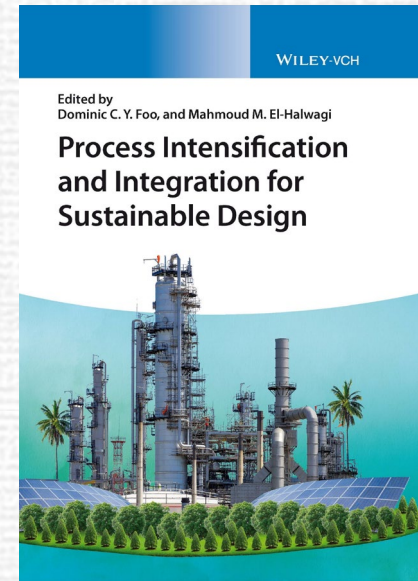
Contemporary Challenges and Future Directions

- **Process intensification and modular integration**
- **Scaleup of decarbonization technologies**
- **Integration of Renewable Energy and Creation of Global Chains of Energy Carriers**
- **Process Safety**
- **Disaster-Resilient Design**

Process Intensification

- Reduce plant size for a given throughput
- Increase throughput (raw materials or products) for a given size of plant
- Reduce number of processing steps
- Increase performance of the process (as a whole):
 - Higher profit
 - Lower cost (CAPEX/OPEX)
 - Higher mass intensity (e.g., process yield, use of material utilities per unit product, less waste per unit product)
 - Higher energy intensity

Enhanced Sustainability

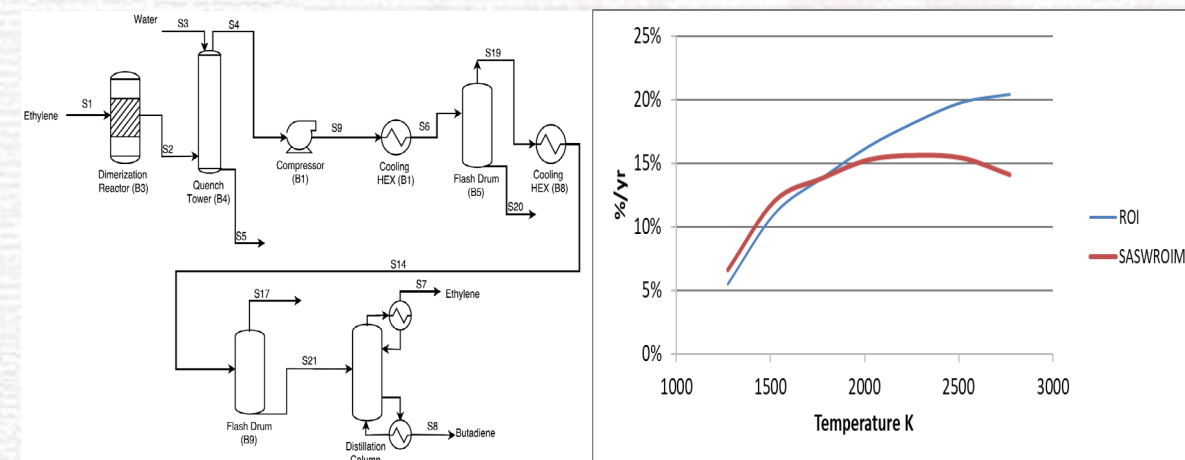


Process Safety: e.g., Sustainability and Safety Weighted Return on Investment Metric “SASWROIM”

- consider a set of process integration project alternatives: $p = 1, 2, \dots, N_{Projects}$.
- For the p^{th} project, a new term called the *Annual Sustainability and Safety Profit* “*ASSP*” is defined as follows

$$ASSP_p = AEP_p \left[1 + \sum_{i=1}^{N_{Indicators}} w_i \left(\frac{Indicator_{Base,i} - Indicator_{p,i}}{Indicator_{Base,i} - Indicator_{Target,i}} \right) \right]$$

$$SASWROIM_p = \frac{ASSP_p}{TCI_p}$$





Contents lists available at [ScienceDirect](https://www.sciencedirect.com)

Journal of Loss Prevention in the Process Industries

journal homepage: <http://www.elsevier.com/locate/jlp>

Incorporating inherent safety during the conceptual process design stage: A literature review

Sunhwa Park^{a,b}, Sheng Xu^b, William Rogers^{a,b}, Hans Pasman^a, Mahmoud M. El-Halwagi^{a,b,c,*}

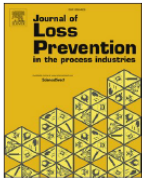
Journal of Loss Prevention in the Process Industries 67 (2020) 104261



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Mitigation of operational failures via an economic framework of reliability, availability, and maintainability (RAM) during conceptual design

Journal of Loss Prevention in the Process Industries 74 (2022) 104635

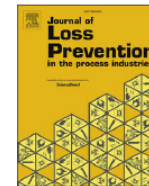
n^{a,d,1}, Mahmoud M. El-



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Integrating flare gas with cogeneration system: Hazard identification using process simulation

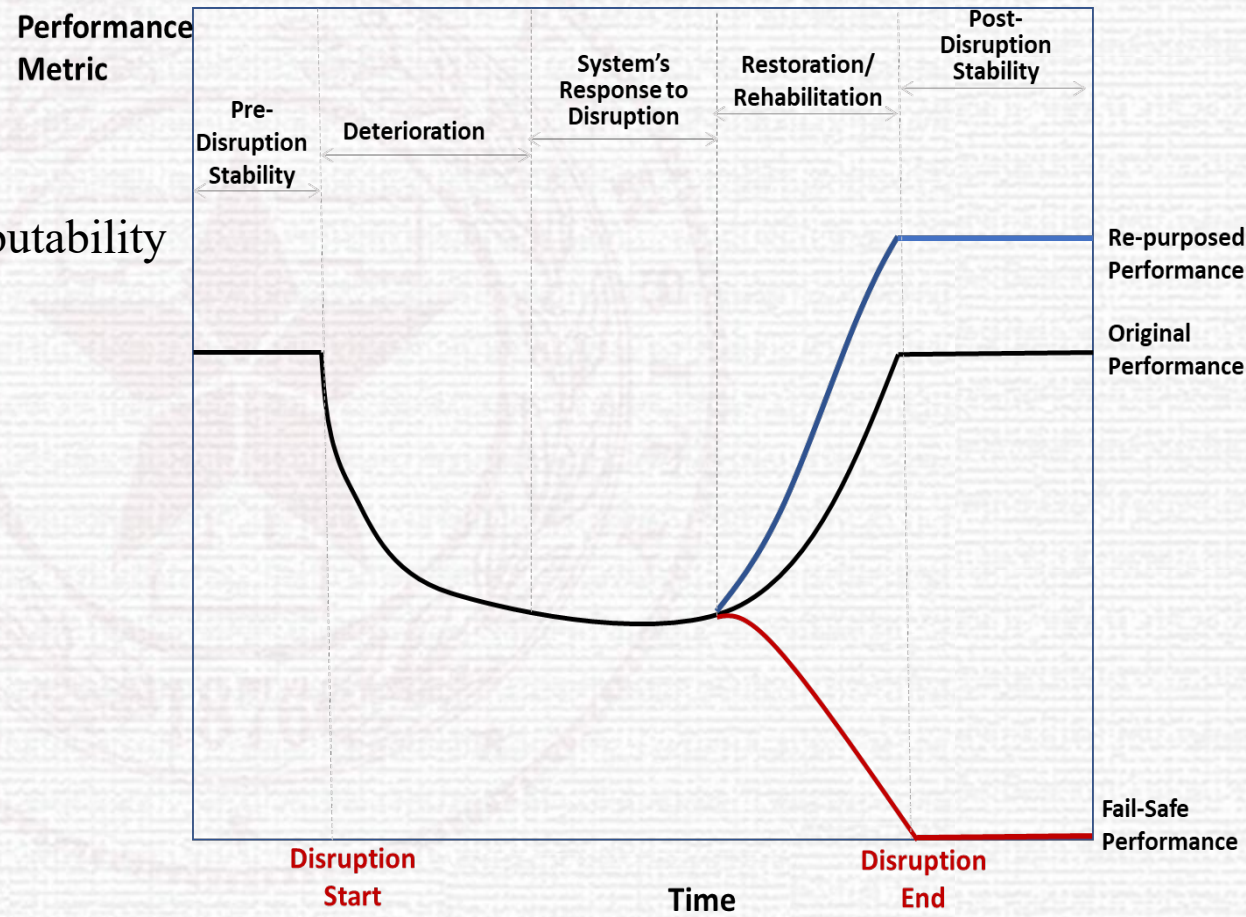
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Disaster-Resilient Design through Process Integration

12 principal strategies for creating disaster-resilient designs:

- (1) Fail-safe by design
- (2) Redundancy
- (3) Reconfigurability
- (4) Modularity/Mobility/Distributability
- (5) Repurposability,
- (6) Flexibility,
- (7) Controllability,
- (8) Reliability,
- (9) Recoverability/restorability,
- (10)Rapidly,
- (11)Robustness, and
- (12)Resourcefulness.



CONCLUDING THOUGHTS

- **Effective decarbonization requires a systems approach**
- **Multi-scale system integration provides a powerful framework at atomic, unit, process, and macroscopic scales with multiple objectives**
- **Paradigm shift of integrating energy and monetizing CO₂ and other GHG gases creates exciting opportunities**

Thank you!
Questions?

