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Sustainability in the Context of Process Engineering

Debalina Sengupta, PhD

**Associate Director, TEES Gas and Fuels Research Center
Lecturer, Artie McFerrin Department of Chemical Engineering**

**Environmental Engineering Symposium, AIChE Dallas Section
October 27th, 2017**



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Associate Director at the TEES Gas and Fuels Research Center

And

Lecturer at Artie McFerrin Department of Chemical Engineering, TAMU

Past Positions:

Post Doctoral Research Associate at the Artie McFerrin Department of Chemical Engineering, Texas A&M University, College Station, TX (May 2014 - December 2015)

ORISE Post Doctoral Fellow at the National Risk Management Research Laboratory, **US Environmental Protection Agency, Cincinnati, OH** (November 2010 - April 2014)

Doctorate (Chemical Engineering) : Louisiana State University (2005-2010)

Bachelor (Chemical Engineering) : Jadavpur University, India (1999-2003)

American Institute of Chemical Engineers

2nd Vice Chair, Environmental Division, AIChE 2017

Programming Chair, Environmental Division, AIChE 2015-2017

Director, Environmental Division, AIChE 2011-2014

Director, Fuels and Petrochemical Division, AIChE 2016-2019



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The GFRC is a Texas A&M Engineering Experiment Station (TEES) center that has been created to provide **research, educational, and outreach services** in the area of **gas and fuels**.

These activities and services support the **substantial growth of shale and natural gas exploration, production, processing, and monetization**, especially in the **United States and in Qatar**.

There is a **critical need** to support this growing industry and to offer novel approaches to its **sustainable development**. The GFRC aims to serve as a global leader in this area.



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UNIVERSITY *at* QATAR

Rainwater Harvesting?

Riding a bike?

Wind?

Solar?

Renewable Fuels?

Recycling?

Electric/Hybrid Cars?

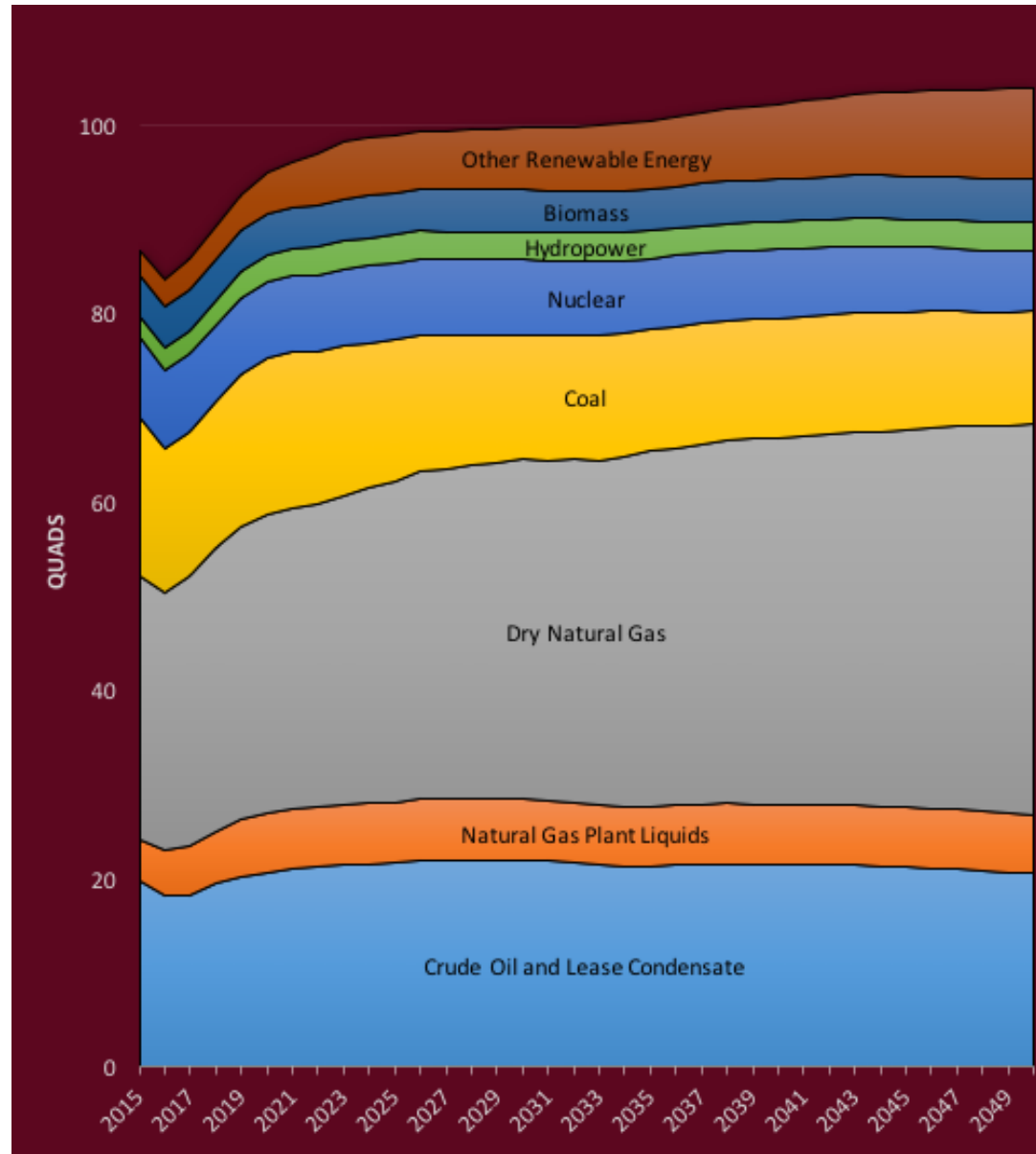


Total Energy Production, EIA, AEO 2017

Natural Gas, Coal and Crude are going to continue as primary energy sources.

Natural Gas is the "new" resource that the United States has, but not enough use other than LNG and electricity.

Natural gas liquids responsible for new boom in industrial development in the Gulf Coast.

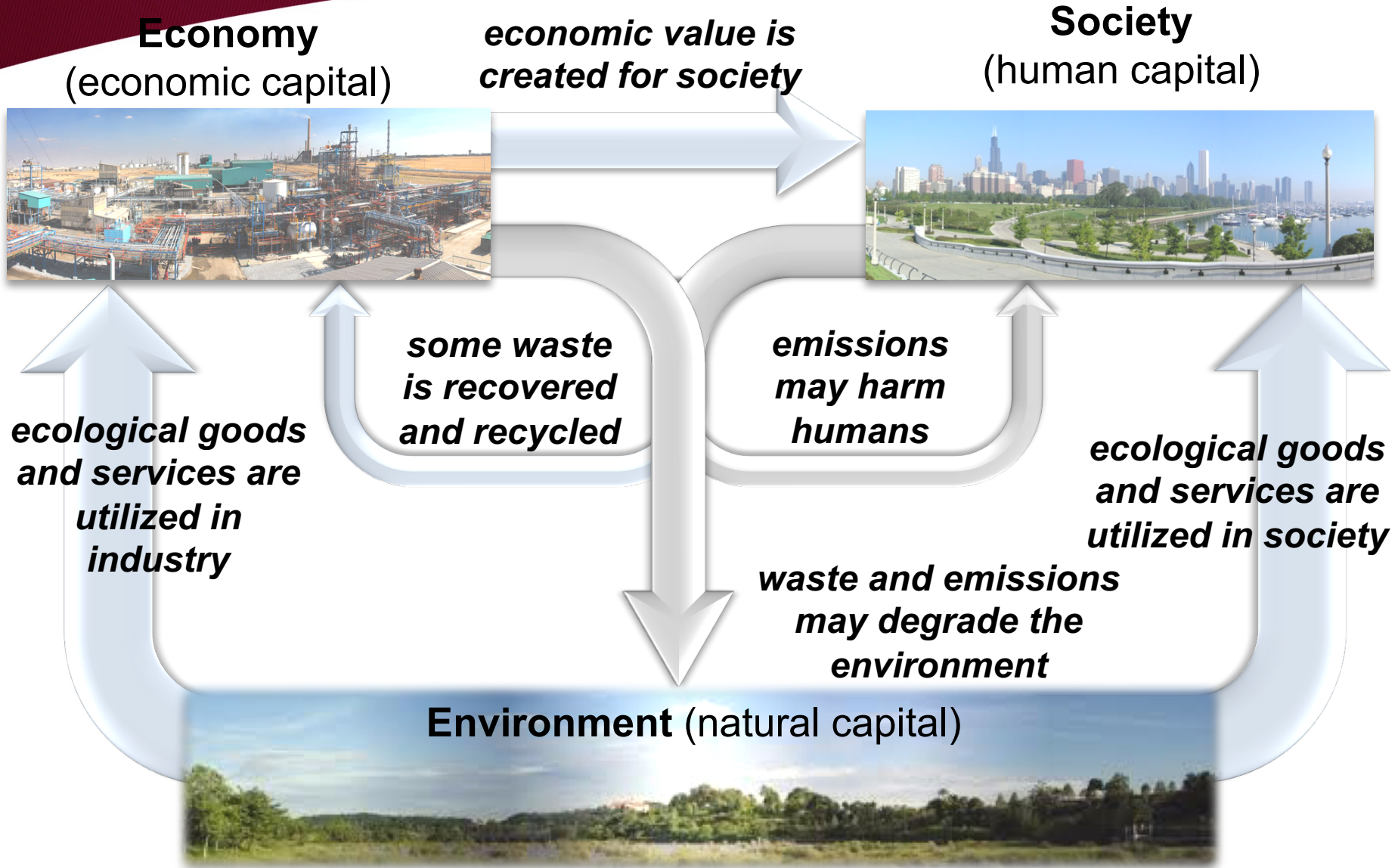


“Sustainable development is development that meets the needs of the present without compromising the ability of future generations to meet their own needs.” – Brundtland Report, United Nations World Commission on Environment and Development (WCED), 1987

There are numerous approaches to apply sustainable development by world organizations, countries and industries.



Systems View of Sustainability



Type I: Global Systems (e.g. global CO₂ budgeting)

Type II: Systems bounded by geographical boundaries, such as National Systems (energy system, material flow) and Regional Systems (e.g. watersheds, Brownfields)

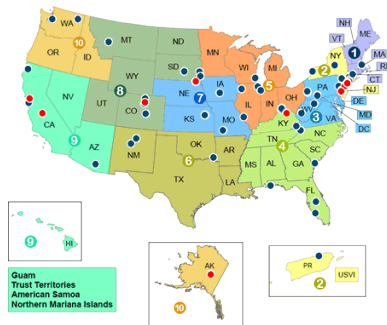
Type III: Business Systems (e.g. business networks, waste exchange networks)

Type IV: Sustainable technologies (e.g. green materials, sustainable products)

*I: Global Scale
(e.g. global CO₂ budgeting)*



*II. National Scale (e.g. energy)
and Regional Scale (e.g.
watersheds, epa regions)*



*III: Business or Institutional
Scale (e.g. eco-industrial
park)*



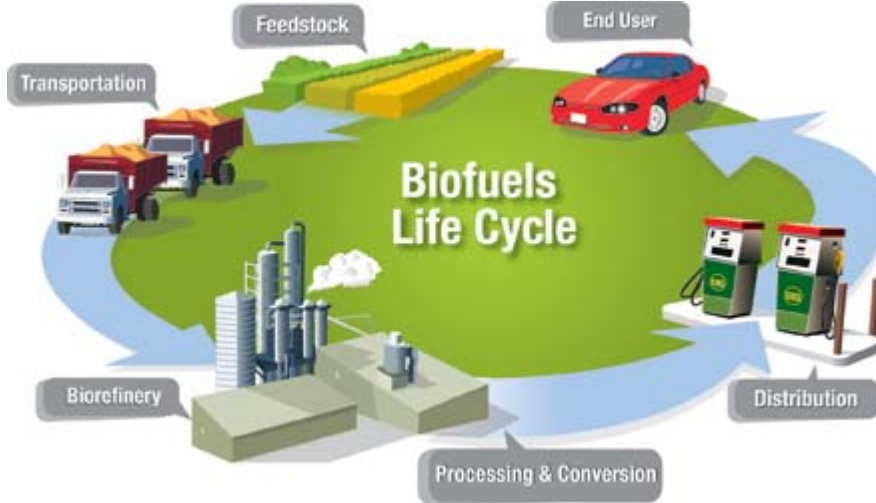
*IV: Sustainable
Technologies Scale
(e.g. sustainable products)*



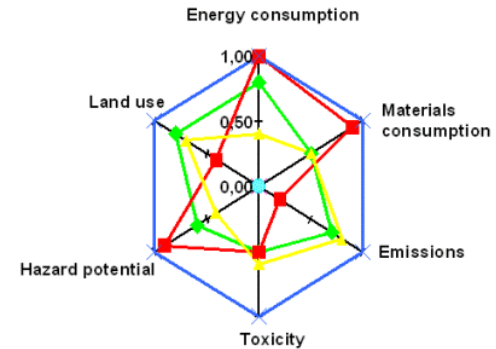
- How does the vision for the world organizations translate into what we do as process engineers?
- How do we link the information needs at the global scales to what is in our control?
- What methods exist in the academic community, and how does it differ from business perspectives?

- Sustainability is about **systems**
- Sustainability is always **relative**, never absolute
- Sustainability functions (economic, environmental, and societal) of systems are described by a **parsimonious set of indicators**
- **Scale of the system** determines the **nature of the set of indicators** and the sustainability analysis
- Indicators are **not pure** (in Brundtland sense); they are often two or three dimensional

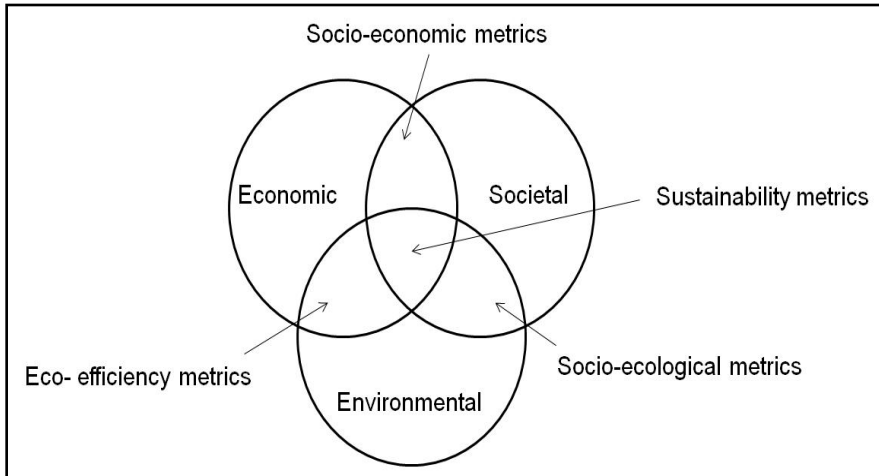
Life Cycle Assessment (LCA)



Eco-Efficiency Analysis



Sustainability Indicators: Metrics and Indices



Footprints (ecological, water, nitrogen, phosphorus etc.)

Industrial Ecology, Eco-Industrial Parks

Carbon Dioxide Sequestration
(geological sequestration, bio-sequestration, chemical sequestration)

Total Cost Assessment Methodology (TCA)
(Economic Costs, Environmental Costs, Societal Costs)

Sustainable Supply Chains

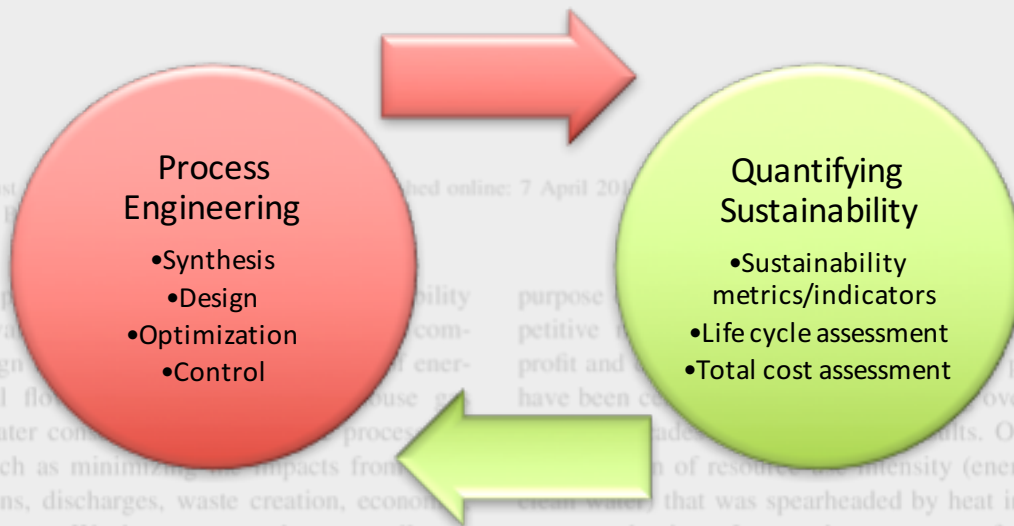
Sustainability in the context of process engineering

Rajib Mukherjee¹ · Debalina Sengupta² · Subhas K. Sikdar³

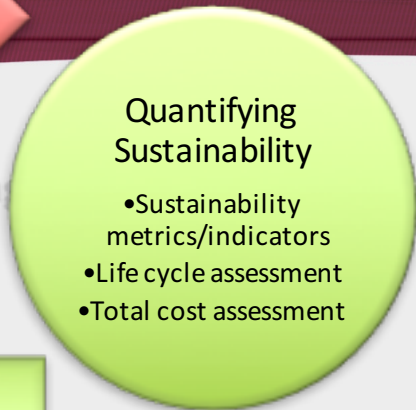
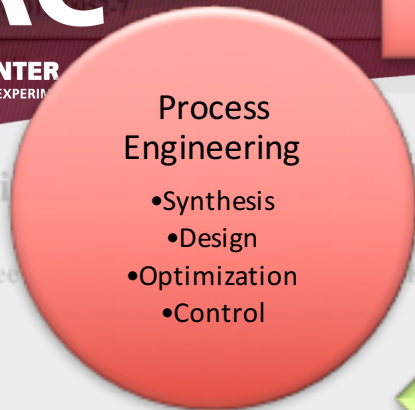
Received: 26 August 2014 / Accepted: 12 February 2015 / Published online: 7 April 2015
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Abstract Complexity in process engineering is increasing due to the use of various available technologies such as computer-aided design (CAD), process simulation, energy and material flow analysis, etc. This complexity demands more, such as minimizing the impacts from harmful emissions, discharges, waste creation, economic and societal impacts. We have proposed an overall sustainability footprint, which in theory represents impacts of a process on all three domains of sustainability. This perspective article provides a critical analysis of attaining sustainability by minimizing this sustainability footprint using impact data as indicators. We also propose the use of the integration of the sustainability footprint in the computer-aided process design itself, rather than checking the impacts after the data have been collected on actual process options designed ahead of the analyses.

purpose of this article is to provide a comprehensive overview of the current state of the art in the field of sustainability in process engineering. In a competitive market, companies are constantly seeking for ways to reduce their environmental footprint and improve their bottom line. This has led to parallel efforts in process engineering and sustainability. Over the last two decades, there has been a significant amount of research in this area. One of these is the concept of sustainability footprint, which is a measure of the total environmental impact of a process. This footprint is calculated based on the resource intensity (energy, materials, clean water) that was spearheaded by heat integration and waste reduction. Later, the concept of resource use minimization was extended to mass exchange networking, and to various process and cost optimization techniques. The other effort came from the concerns for the environment and was focused on quantifying process wastes into environmental impacts, particularly of toxic materials generated, emitted, or released from processes. With life-cycle assessment (LCA) techniques taking hold among process designers, process engineering started to combine the knowledge generated by researchers who were focused on devising measures for exposures of toxic compounds to the environment. This research has merged into an integrated design for safer processes that are efficient and cost-effective. We could call this com-

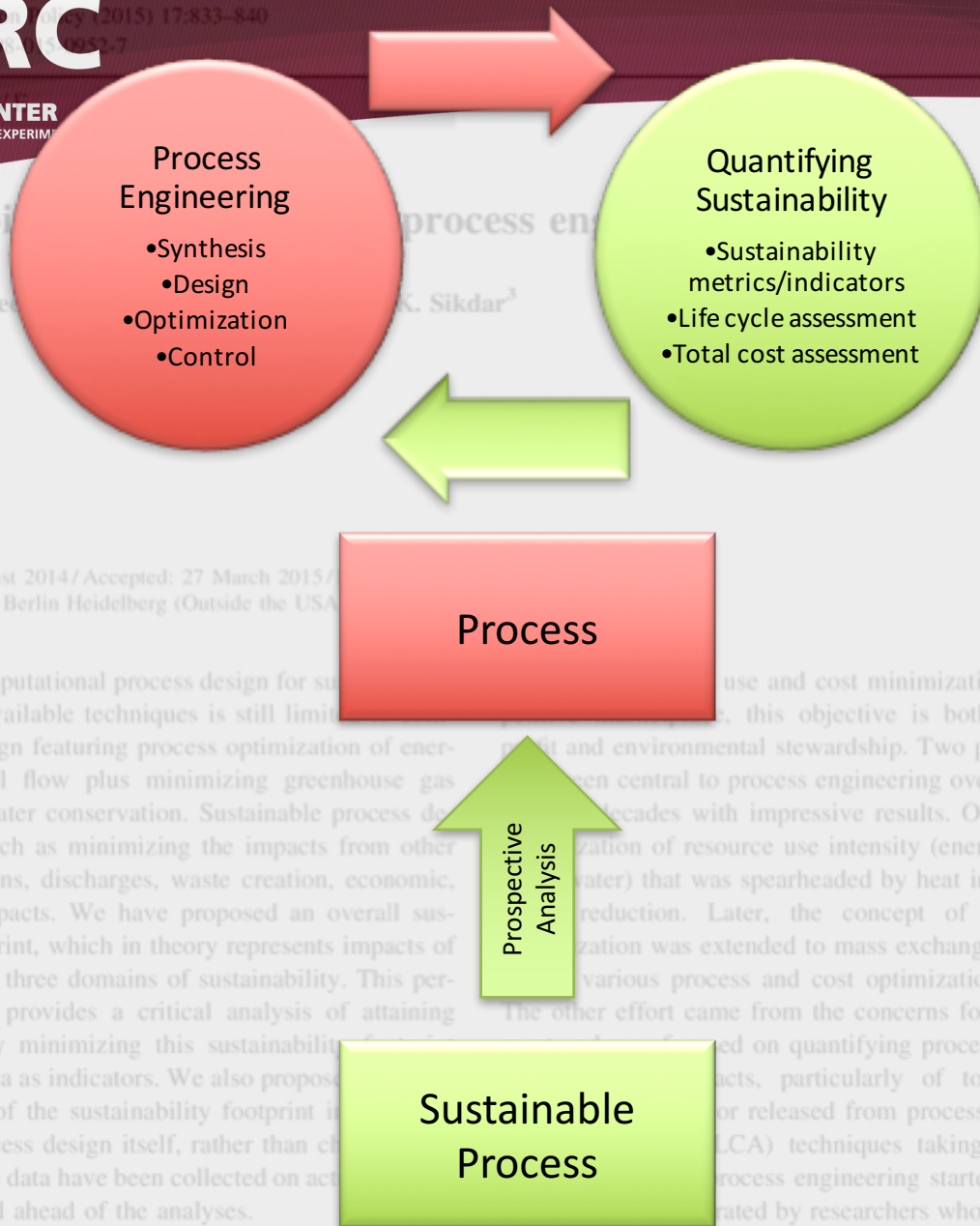


Motivation



Sustainability Assessment Methods

Motivation



Process Engineering

- Synthesis
- Design
- Optimization
- Control

Quantifying Sustainability

- Sustainability metrics/indicators
- Life cycle assessment
- Total cost assessment

Process

Sustainable Process

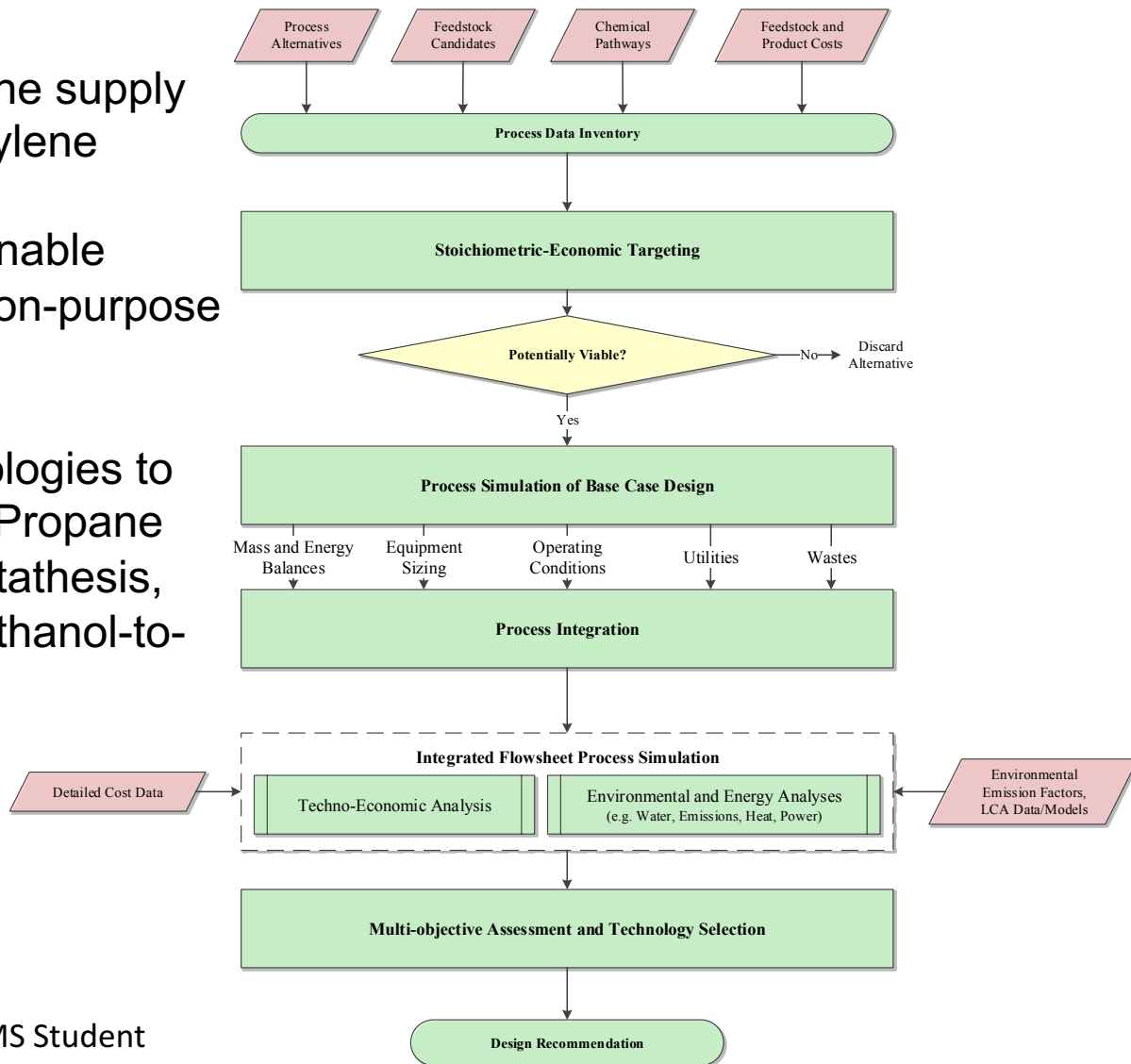
Prospective Analysis

Motivation

- Process Integration
 - **Single Process - PDH Process**
 - **Multiple Processes - Eco-Industrial Park**
- Life Cycle Assessment – Inventory Analysis
 - Sustainable Supply Chain Design of Biofuels
 - Sustainable Supply Chain Design of Consumer Products
 - Sustainability Metrics
 - Development of the Sustainability Footprint method

REMEMBER! SCALE OF PROCESS IMPORTANT FOR SUSTAINABILITY ANALYSIS!

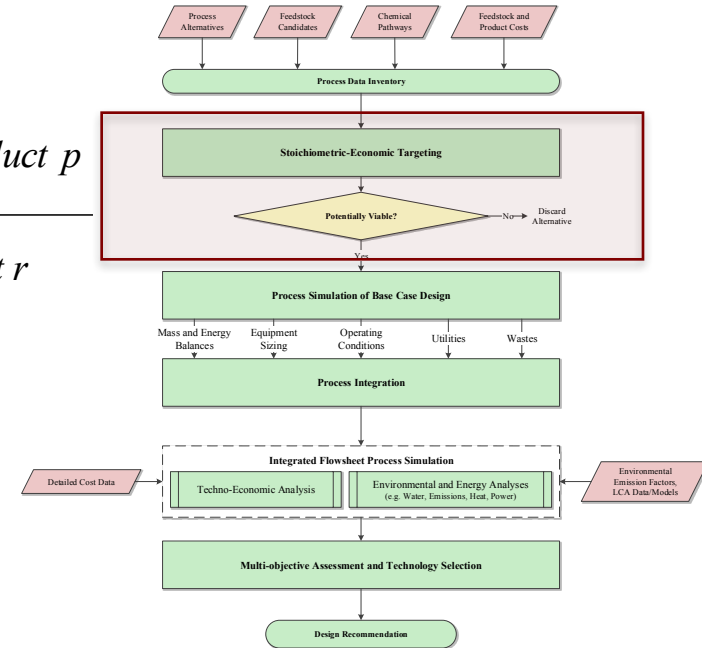
- Increasing spread between the supply and demand curves for propylene
- Aim is to investigate a sustainable process design approach to on-purpose propylene production
- Following established technologies to directly produce propylene : Propane Dehydrogenation (PDH), Metathesis, Methanol-to-Olefins and Methanol-to-Propylene (MTO/MTP)



Acknowledgement: **Mr. Ashwin Agarwal**, MS Student

$$MISR = \frac{\sum_{p=1}^{N_{products}} \text{Annual production rate of product } p \times \text{Purchase price of product } p}{\sum_{r=1}^{N_{reactants}} \text{Annual feed rate of reactant } r \times \text{Purchase price of reactant } r}$$

On-Purpose Propylene Process	MISR
Propane Dehydrogenation	2.07
Olefin Metathesis	0.95
Methanol to Olefins	0.98

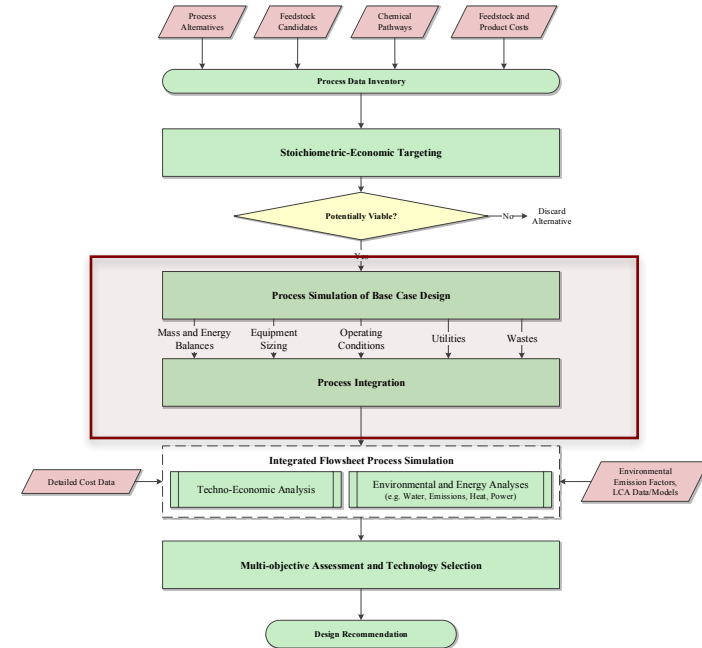
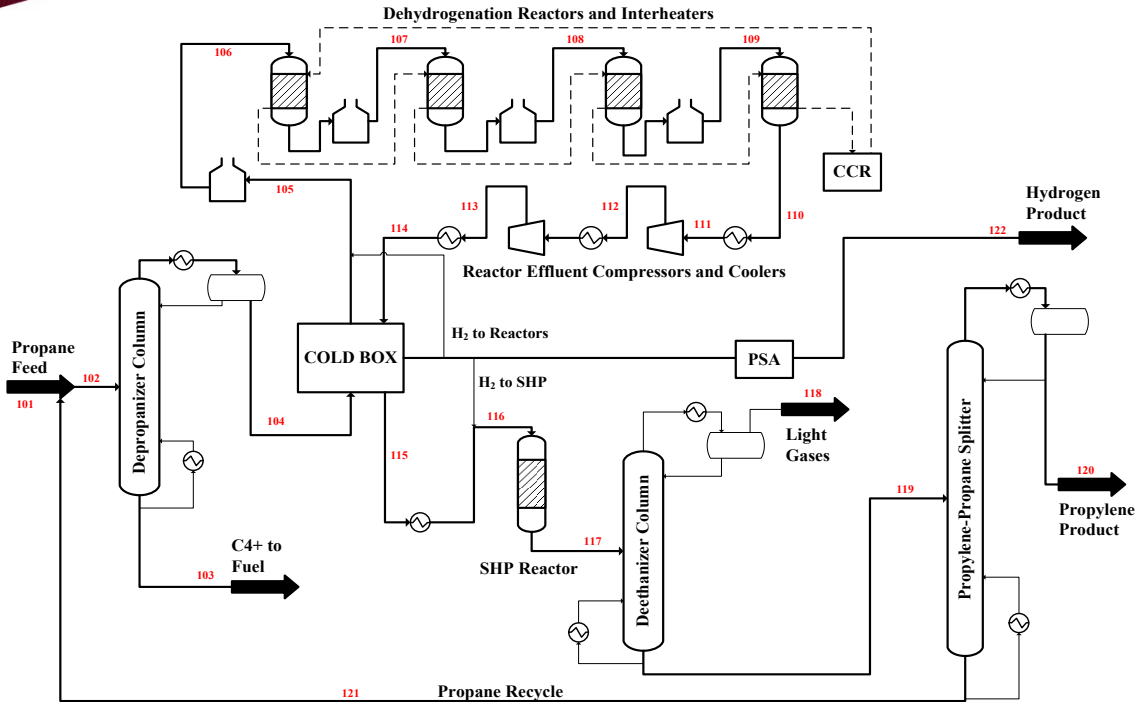




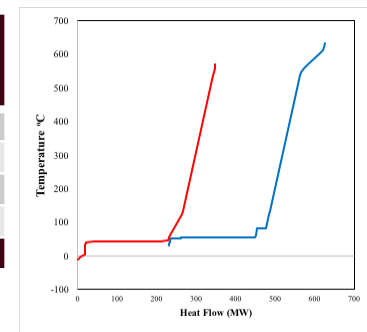
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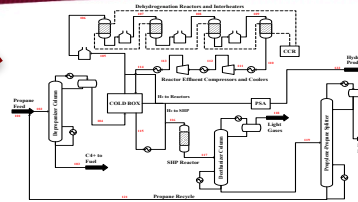
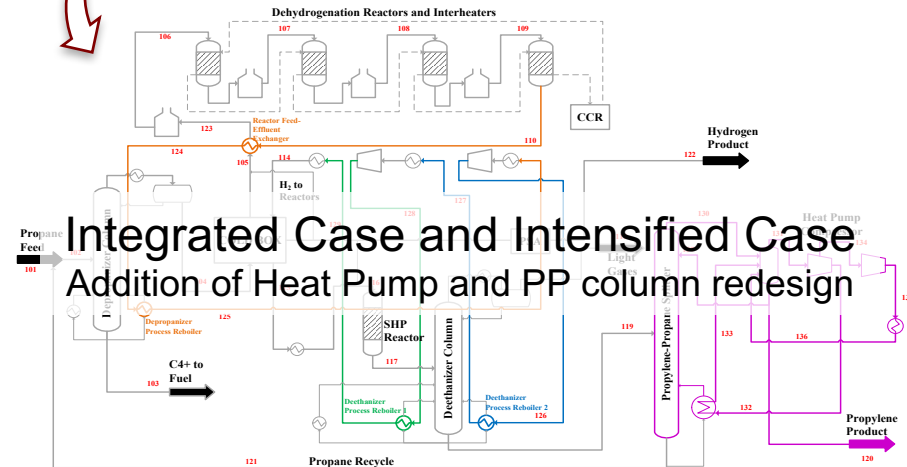
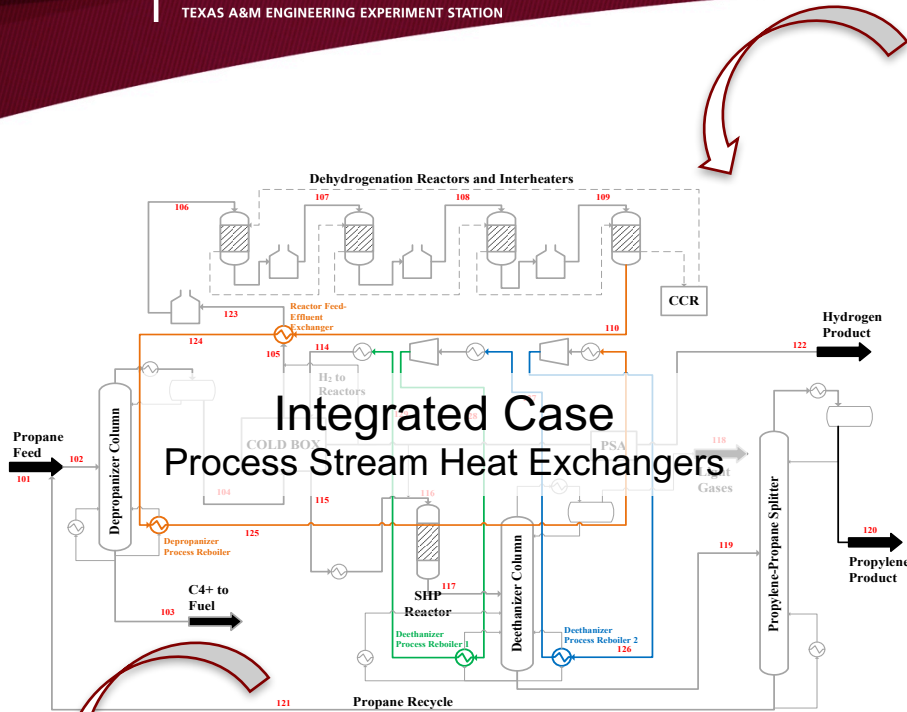
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On-purpose Propylene Production

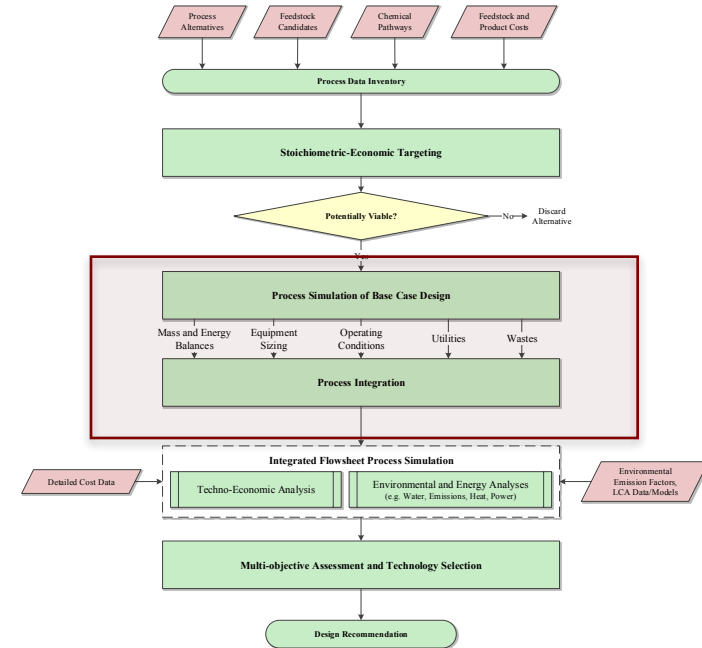


Utility Type	Unit Cost	Duty (MW)	Cost (MM\$/yr)	% of Total Utility	Major Consumer in Process
Cooling Water	\$0.023/m ³	358	8.4	10.7%	PP Splitter Condenser and Reactor Effluent Coolers (83%)
LP Steam	\$10.7/kg	237.4	35.5	45%	PP Splitter Reboiler (80%)
Natural Gas	\$10.1/MW-hr	159.3	15.7	19.9%	Fired Heaters (100%)
Electricity	\$0.065/KW-hr	35.6	19.2	24.4%	Reactor Effluent Compressors (95%)
Total Utility		790.3	78.8	100%	



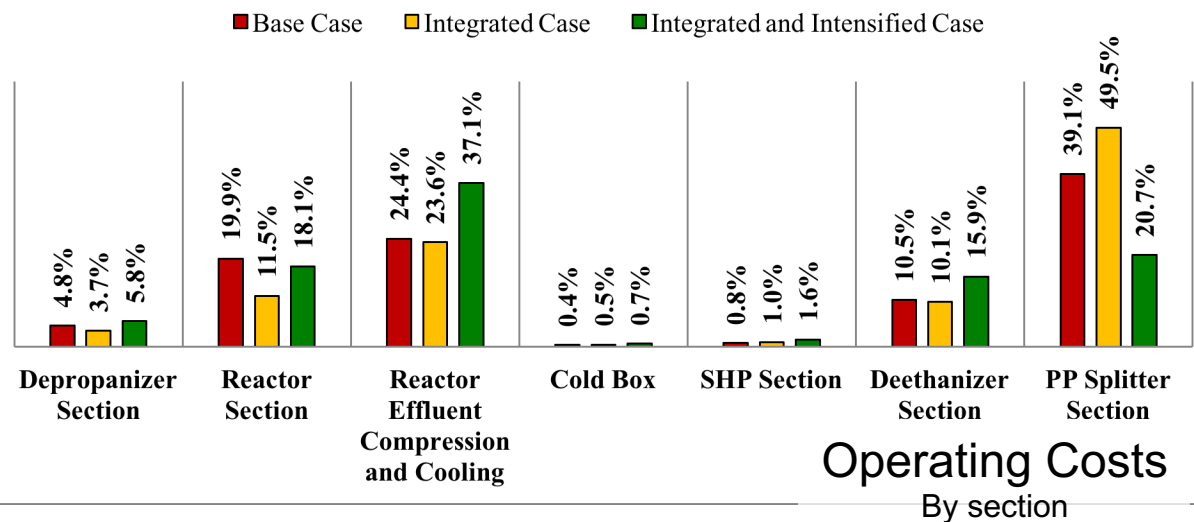
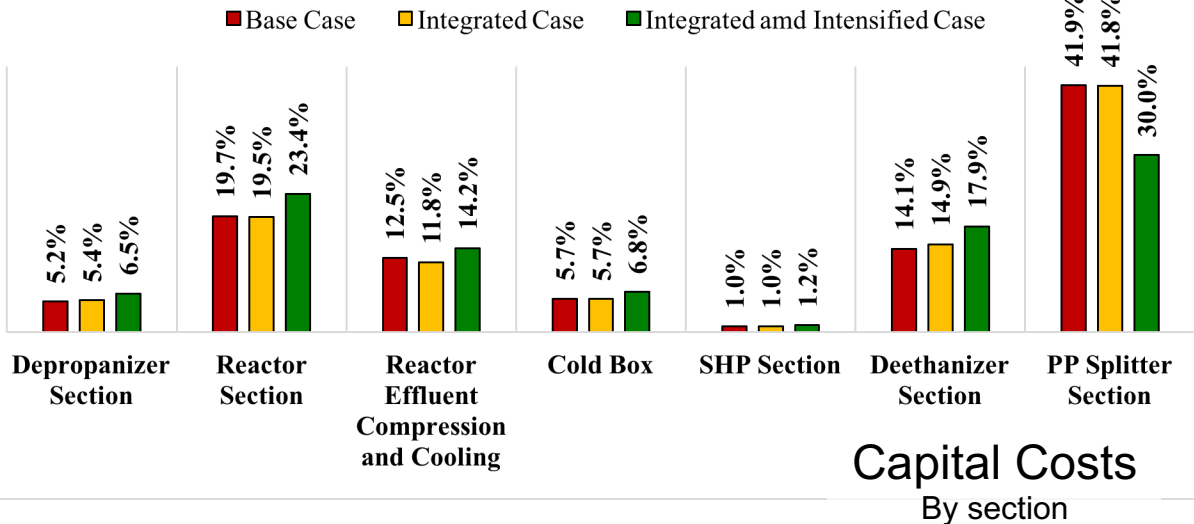


Base Case
Completely unintegrated design
(no information available, other than stoichiometry)

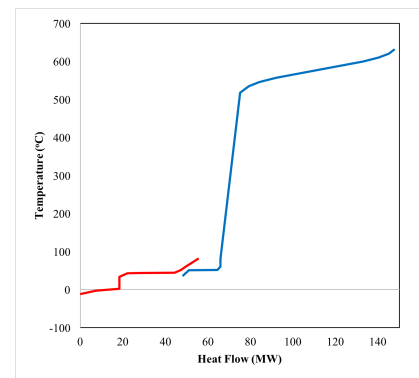
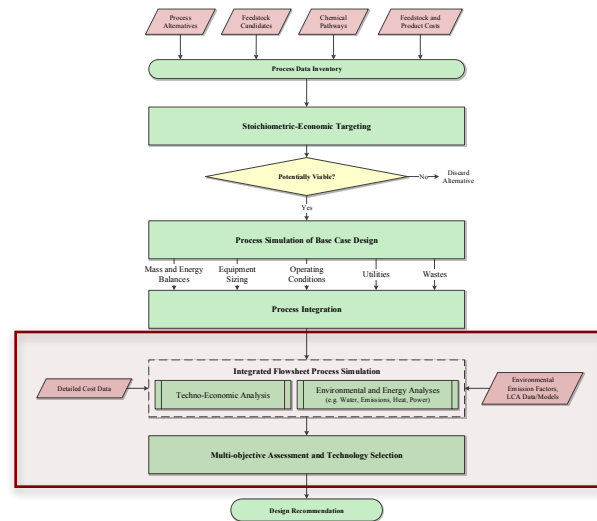


**Integrated Case and Intensified Case +
WHR + OGR**

Waste heat recovery from fired heaters
Off gas recovery as fuel



Economic Criteria	Base Case	Integrated Case	Integrated and Intensified Case
Simple Pay-back (yrs)	5.82	5.34	4.06
Return on Investment (15yrs)	15%	17%	25%
NPV (15 yrs) [\$MM]	240.7	314.6	489.5
IRR (15 yrs)	14%	16%	22%





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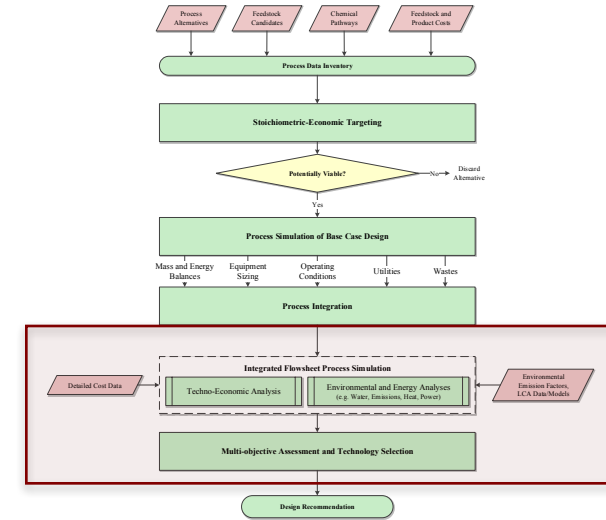
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On-purpose Propylene Production

Pollutant	Emission Factor (lb/10 ⁶ scf)	Emission Factor Rating
CO ₂	120,000	A
N ₂ O (Low NOx Burner)	0.64	E
SO ₂	0.6	A
TOC	11	B
Methane	2.3	B
VOC	5.5	C

Electricity Source	CO ₂ (lb/MWhr)	Methane (lb/GWhr)	N ₂ O (lb/GWhr)
ERCOT (Texas) Grid	1142.8	81.8	11.6
US Avg.	1122.9	110.9	16.0
SRMW (SERC Midwest)	1772.0	208.8	30.4



Pollutant	Base Case			Integrated Case			Integrated + Intensified Case		
	Base Case	Base Case + WHR	Base Case + WHR + OGR	Integrated Case	Integrated Case with WHR	Integrated case +WHR + OGR	Integrated + Intensified Case	Integrated + Intensified Case with WHR	Integrated + Intensified case with WHR+ OGR
	tons/yr			tons/yr			tons/yr		
CO ₂	1,013,054	911,646	748,282	820,723	776,074	612,710	531,606	480,676	317,312
Methane	21.94	20.00	20.00	18.25	17.40	17.40	15.99	15.01	15.01
SO ₂	3.57	3.07	3.07	2.61	2.39	2.39	0.85	0.60	0.60
TOC	65.50	56.20	56.20	47.87	43.77	43.77	15.63	10.96	10.96
VOC	32.75	28.10	28.10	23.93	21.89	21.89	7.81	5.48	5.48
N ₂ O	4.98	4.44	4.44	3.95	3.72	3.72	2.71	2.44	2.44
Total Emissions	1,013,182	911,758	748,394	820,819	776,164	612,800	531,649	480,711	317,347
Cost of CO₂ Emissions @\$25/ton \$MM/yr	25.33	22.79	18.71	20.52	19.40	15.32	13.29	12.02	7.93

OGR – Off Gas Recovery
WHR – Waste Heat Recovery

Sustainability Weighted Return on Investment (SWROI) metric which is an extension of the Return on Investment concept with the augmented sustainability metrics and process integration targeting approaches.

Considering a set a process alternatives: $p = 1, 2, 3, N_{\text{projects}}$. For the p^{th} project, a new term called the Annual Sustainability Profit (ASP) is given by:

$$ASP_p = AEP_p \left[1 + \sum_{i=1}^{N_{\text{indicators}}} w_i \left(\frac{\text{Indicator}_{p,i}}{\text{Indicator}_i^{\text{Target}}} \right) \right]$$

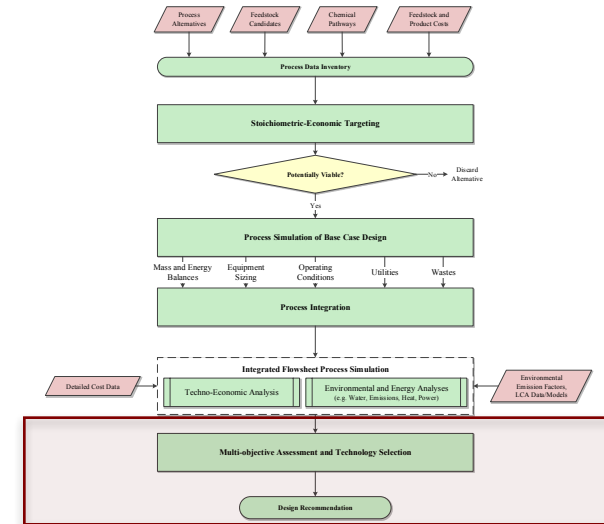
AEP_p is the Annual Economic Profit

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

$\text{Indicator}_{p,i}$: represents the value of the i^{th} sustainability indicator associated with the p^{th} project

$\text{Indicator}_i^{\text{Target}}$: target of the i^{th} sustainability indicator (benchmarking or taken as the largest value from all project)

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





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

AEP_p is the Annual Economic Profit

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

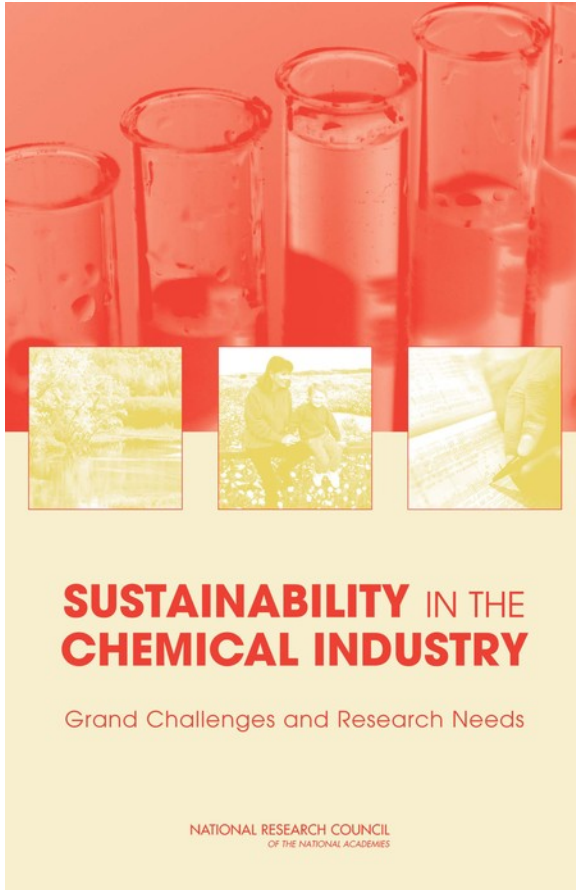
$Indicator_{p,i}$: represents the value of the i^{th} sustainability indicator associated with the p^{th} project

$Indicator_{i,Target}$: target of the i^{th} sustainability indicator (benchmarking or taken as the largest value from all project)

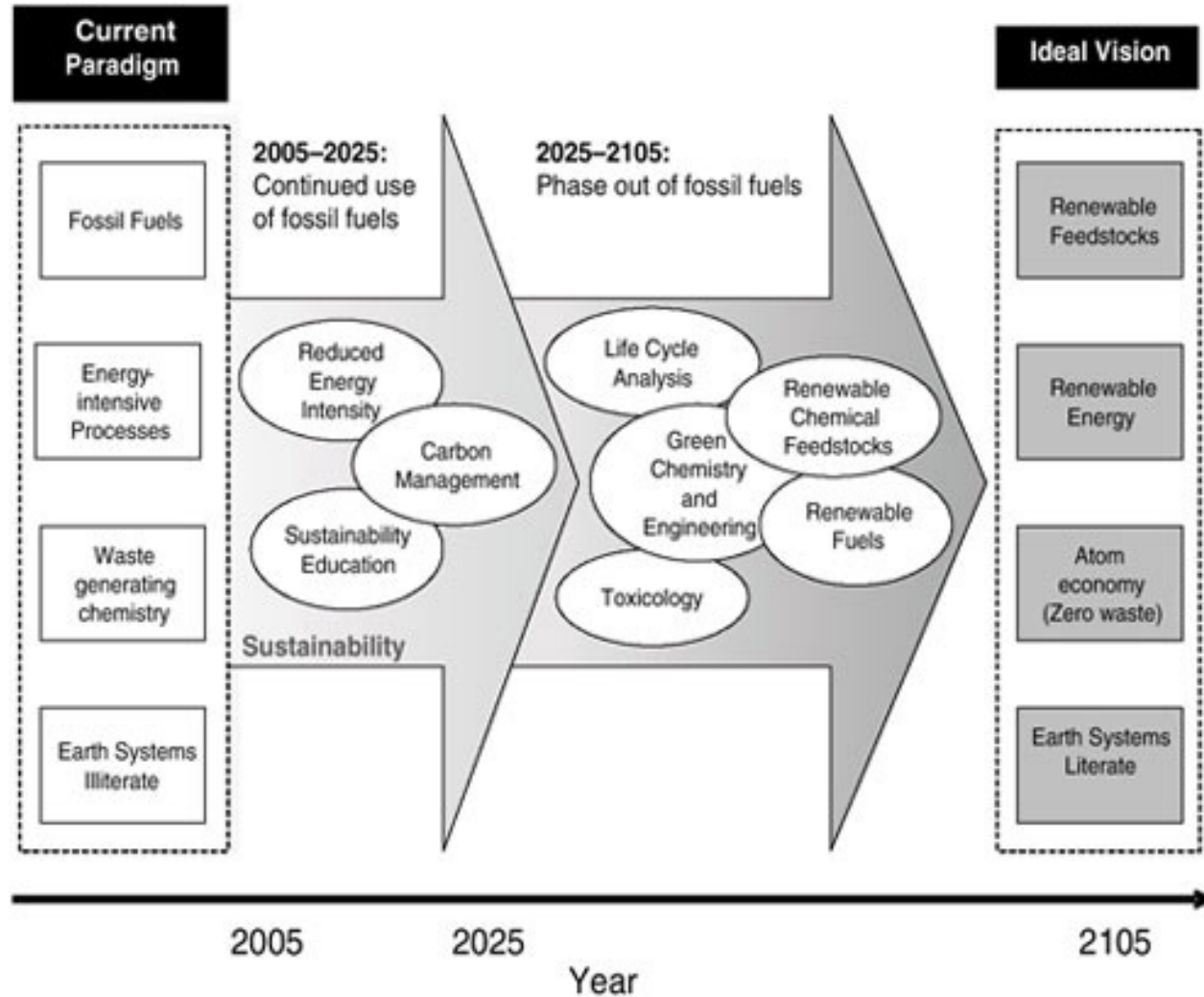
Description	10 yr. Avg. Taxable Income	Total Capital Investment	Water Reduction (Steam + CW)	Electrical Energy Savings (Power)	Fuel Savings (NG Firing in Fired Heaters)	CO ₂ emission Reductions	VOC Reduction	ROI (10 yrs)	SWROI
	MM\$/yr	MM\$	10 ⁶ kg/hr	MW	MW	10 ³ tons/yr	tons/yr		
Weight Factors			0.1	0.1	0.07	0.25	0.05		
Targets			45.08	36	159	1013	32.7		
Base Case + WHR	67	643	0	0	0	101.4	4.6	10.38%	10.71%
Base Case + WHR + OGR	67	643	0	0	0	264.8	4.6	10.38%	11.13%
Integrated Case	79	645	25.6	0	87	192.3	8.8	12.29%	14.21%
Integrated Case + WHR	79	645	25.6	0	87	237	10.9	12.29%	14.38%
Integrated Case + WHR + OGR	79	645	25.6	0	87	400.3	10.9	12.29%	14.88%
Integrated + Intensified Case	104	536	38.7	-14.5	87	481.4	24.9	19.45%	24.12%
Integrated + Intensified Case + WHR	104	536	38.7	-14.5	87	532.4	27.3	19.45%	24.43%
Integrated + Intensified Case + WHR + OGR	104	536	38.7	-14.5	87	695.7	27.3	19.45%	25.21%

Recap:

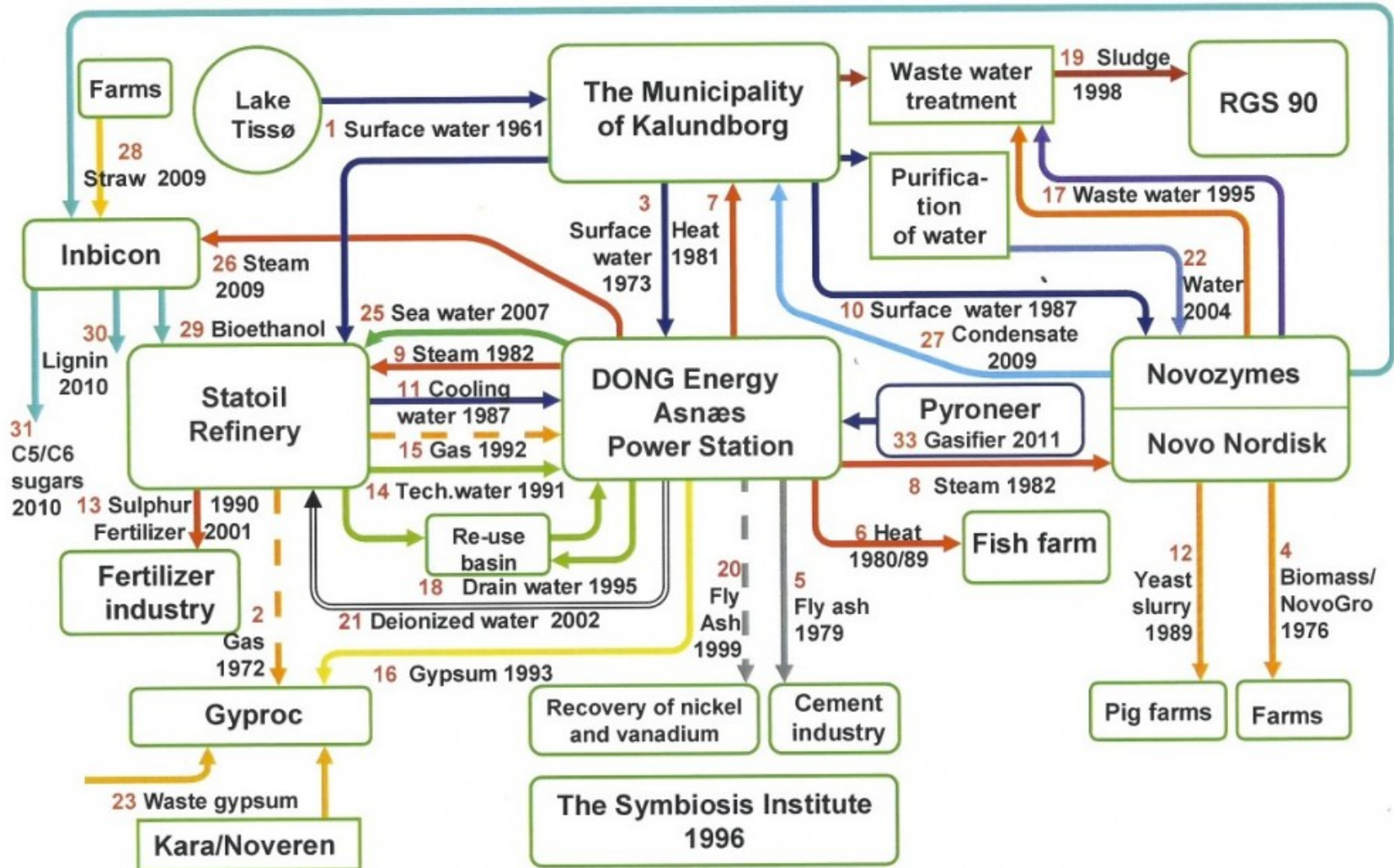
- Calculate your common economic metrics for your projects.
- Calculate your environmental (and possible social metrics) metrics.
- Use the ASP (Annual Sustainability Profit) and SWROI (Sustainability Weighted ROI) to make a decision about a project.
- If your ROI is reasonable, but you can show a much higher SWROI, project justification can be made.
- SWROI provides a reflection of how sustainable your project is from different competing choices.



Status: Final Book
Downloads: 1,890

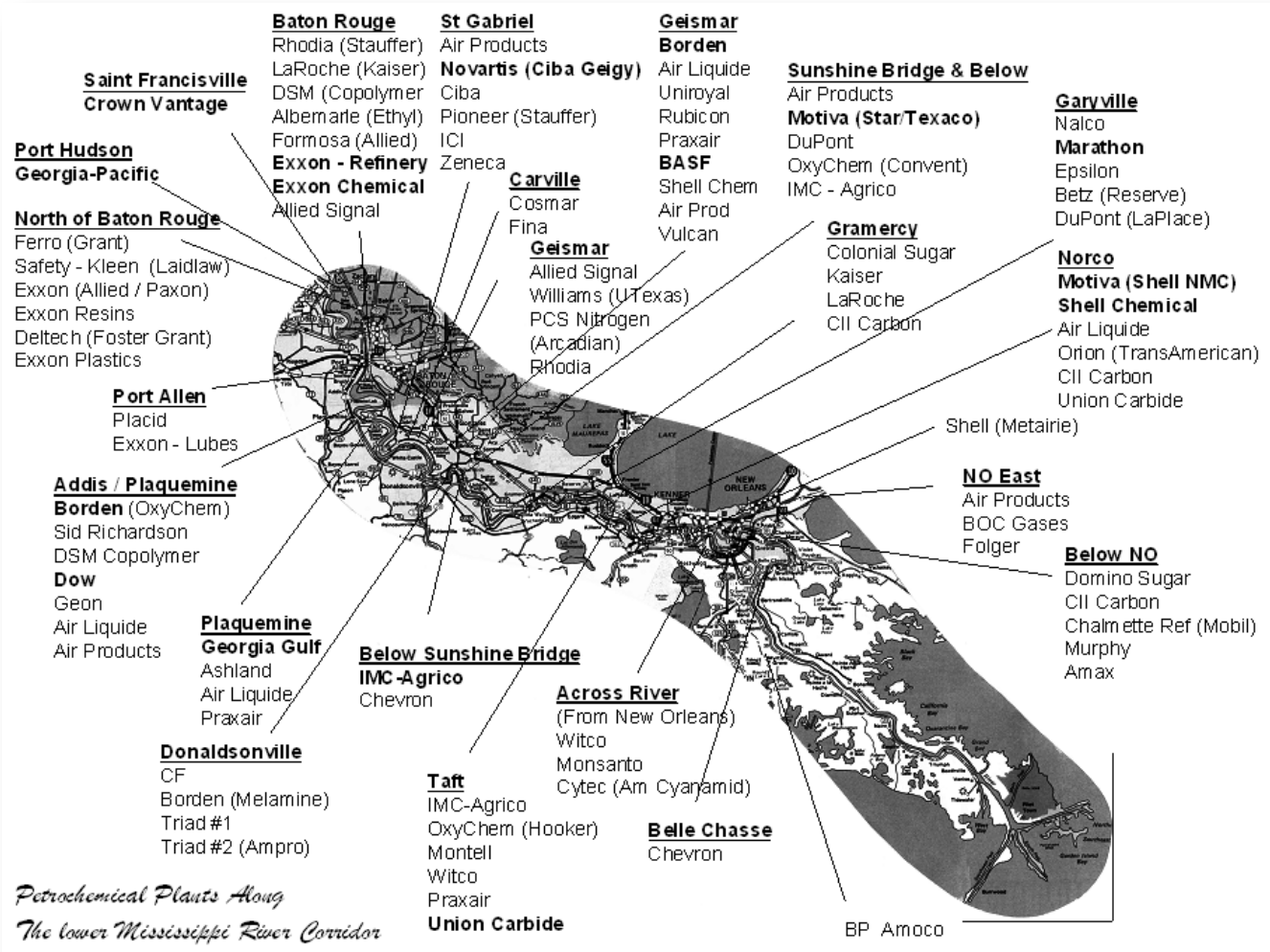


Kalundborg, Denmark

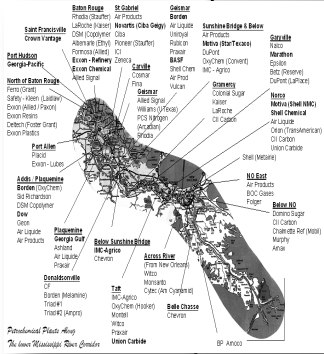
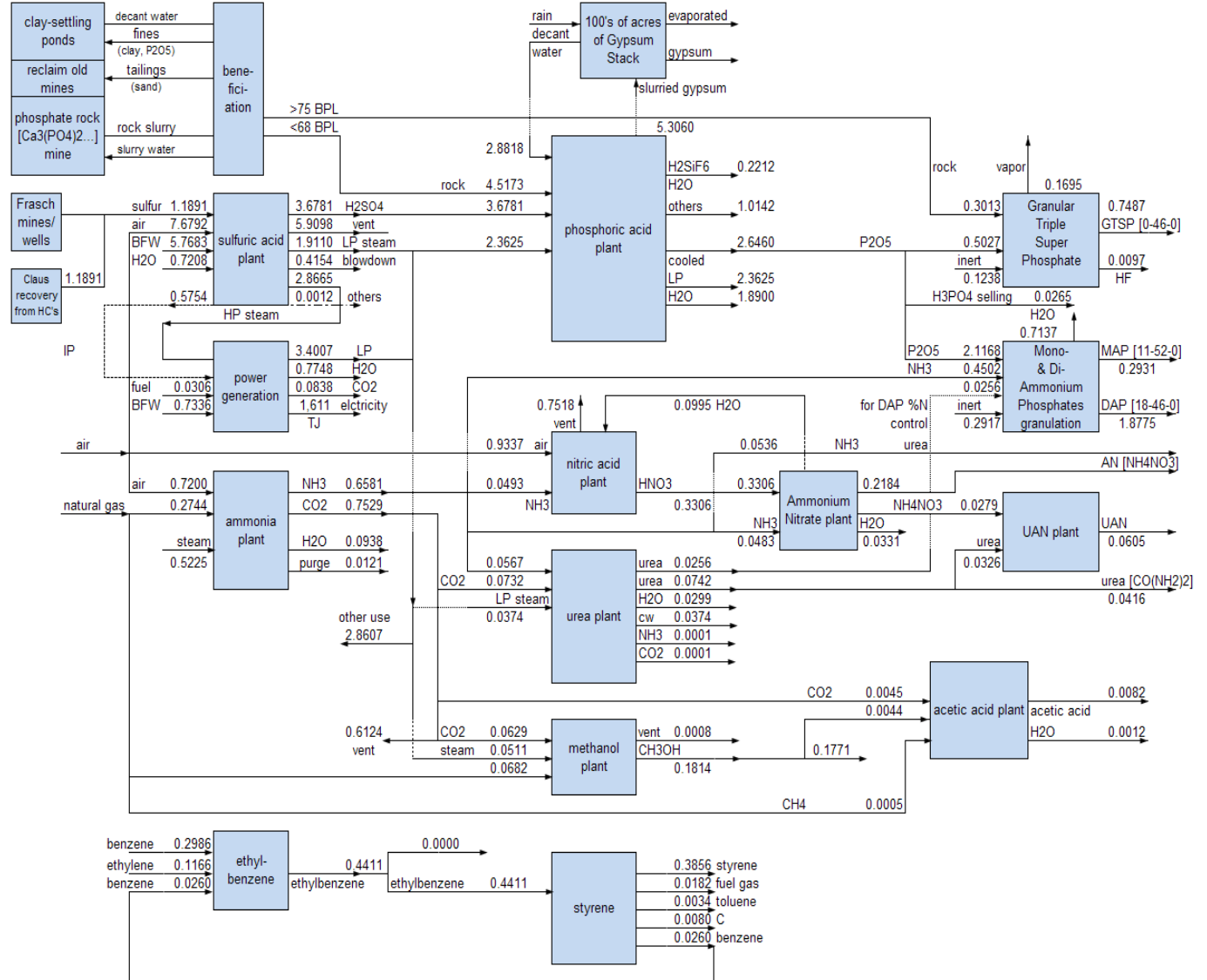


Petrochemical complex in the lower Mississippi River Corridor

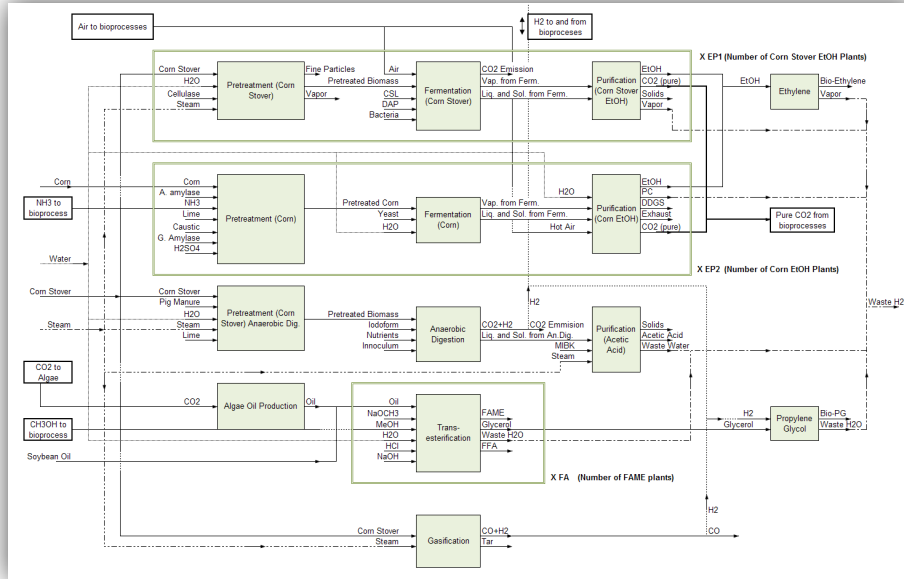
- Dow
- DuPont
- BASF
- Shell
- Exxon
- Monsanto
- Mosaic
- and others



Base Case of Plants in the Lower Mississippi River Corridor

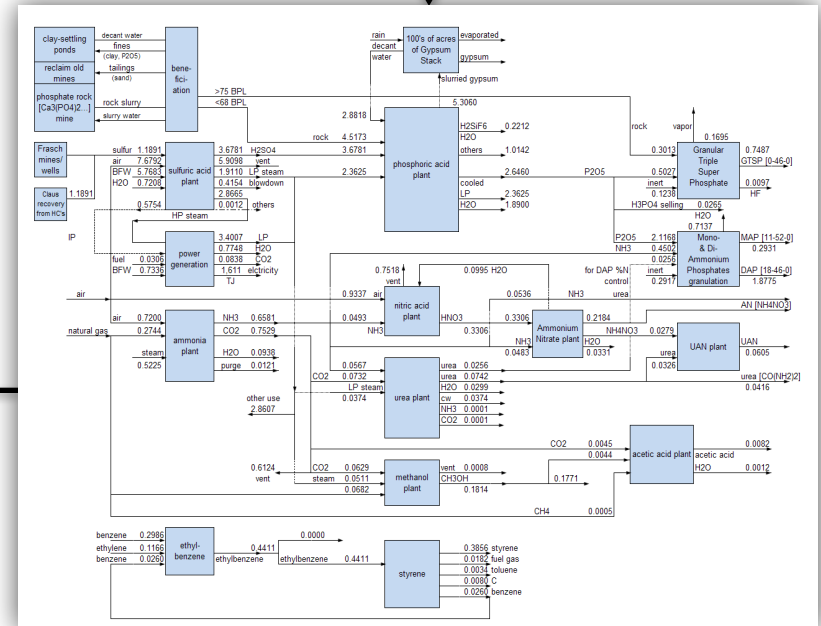


Integrated Chemical Production Complex



Biomass Complex

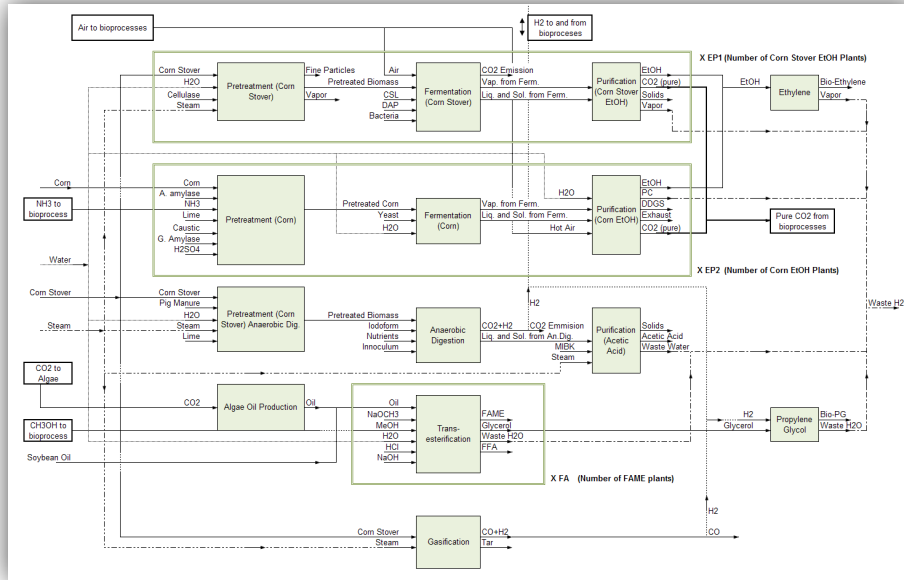
Hydrogen, CO₂



Base Case Complex

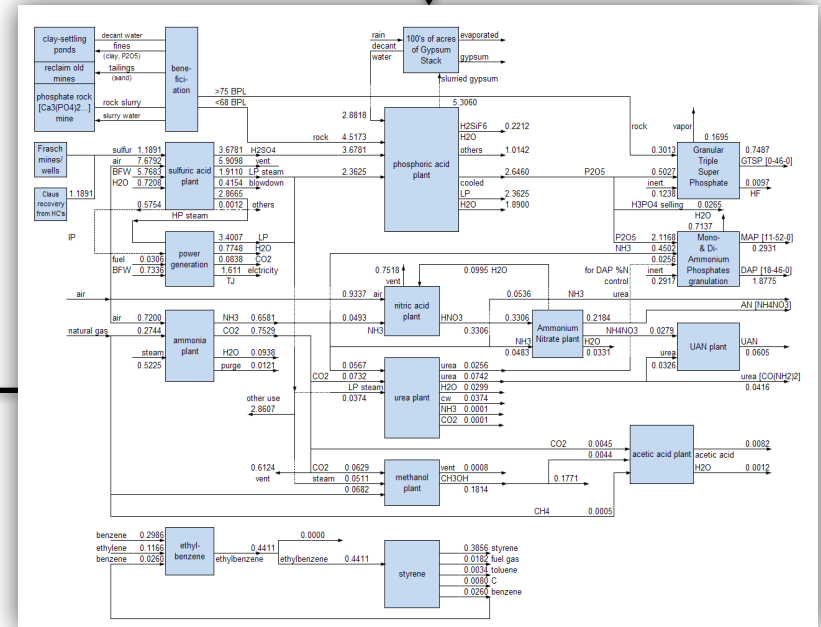
Air, Methanol, Ammonia

Integrated Chemical Production Complex



Biomass Complex

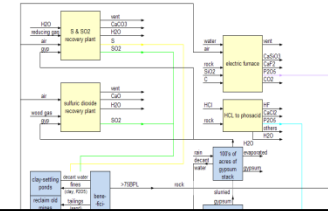
Hydrogen, CO₂



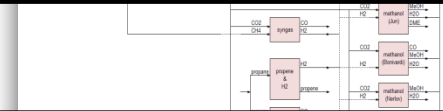
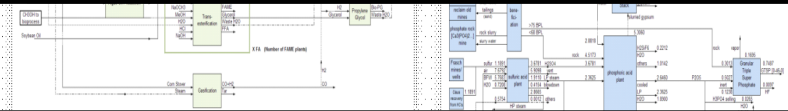
Air, Methanol, Ammonia

Base Case Complex

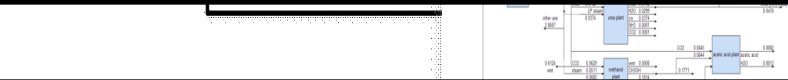
Superstructure



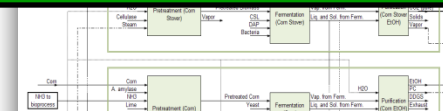
Profit



Environmental Costs



Sustainability (Credits – Costs)



Triple Bottom Line = Σ Profit - Σ Environmental Costs + Σ Sustainable (Credits – Costs)



Eco-Industrial Park

Plants in Base Case

(blue)

Ammonia
Nitric acid
Ammonium nitrate
Urea
UAN
Methanol
Granular triple super phosphate (GTSP)
MAP and DAP
Contact process for sulfuric acid
Wet process for phosphoric acid
Acetic acid – conventional method
Ethyl benzene
Styrene
Power generation

Plants Added to Form the Superstructure

Bioprocesses and CO₂ consumption by Algae (green)

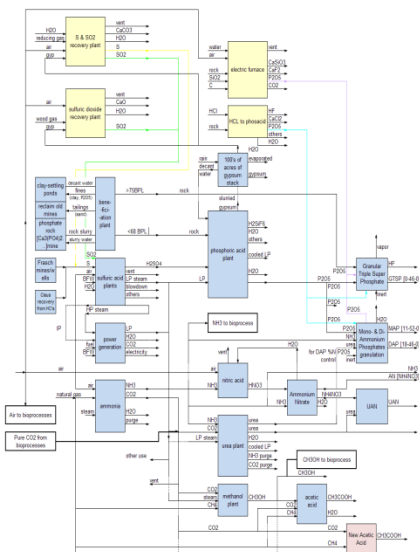
Fermentation ethanol (corn stover)
Fermentation ethanol (corn)
Anaerobic Digestion to acetic acid (corn stover)
Algae Oil Production
Transesterification to FAME and glycerol (soybean oil and algae)

CO₂ consumption for Chemicals (red)

Methanol – Bonivardi, et al., 1998
Methanol – Jun, et al., 1998
Methanol – Ushikoshi, et al., 1998
Methanol – Nerlov and Chorkendorff, 1999
Ethanol
Dimethyl ether
Formic acid
Acetic acid - new method
Styrene - new method
Methylamines
Graphite
Hydrogen/Synthesis gas
Propylene from CO₂
Propylene from propane dehydrogenation

Choice for phosphoric acid production and SO₂ recovery (yellow)

Electric furnace process for phosphoric acid
Haifa process for phosphoric acid
SO₂ recovery from gypsum waste
S and SO₂ recovery from gypsum waste

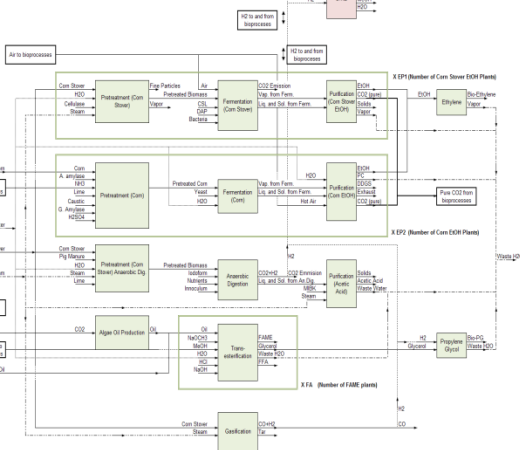


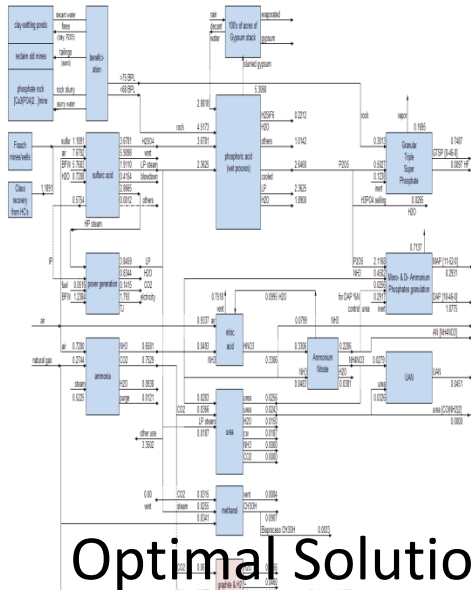
Continuous Variables: 969

Integer Variables: 25

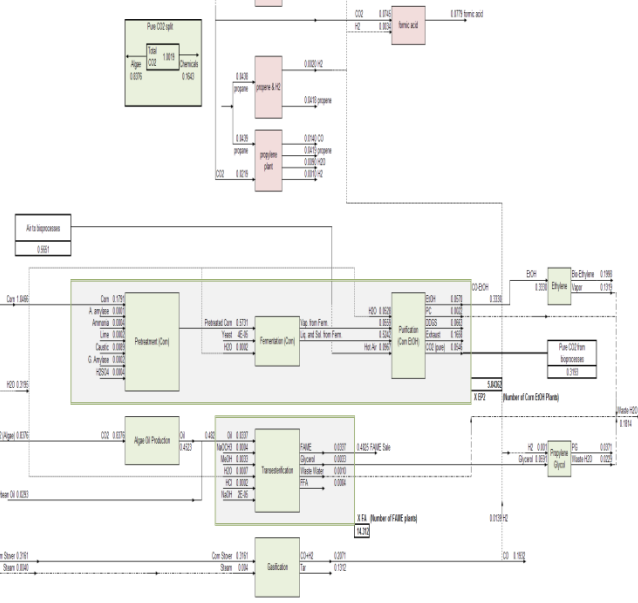
Equality Constraints: 978

Inequality Constraints: 91

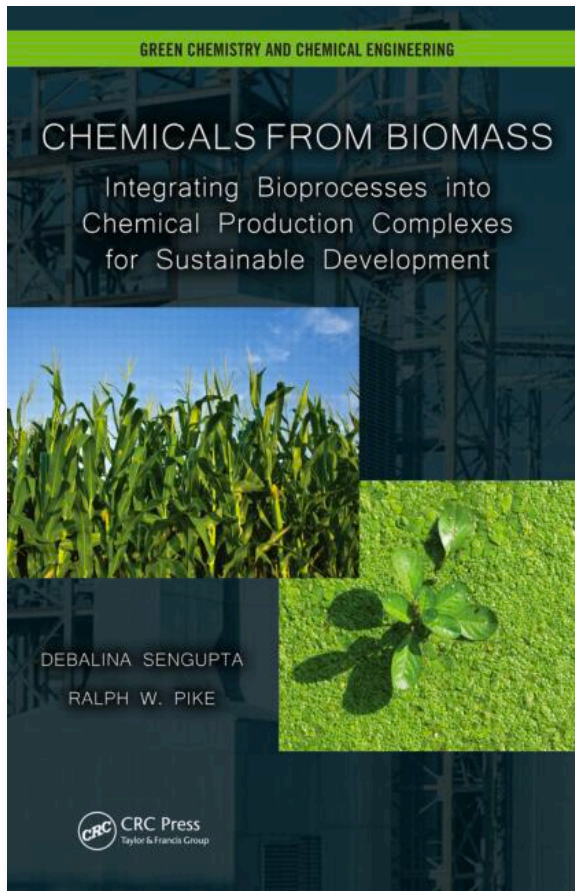




Optimal Solution



Existing Plants in the Optimal Structure	New Plants in the Optimal Structure
Ammonia Nitric acid Ammonium nitrate Urea UAN Methanol Granular triple super phosphate (GTSP) MAP and DAP Contact process for Sulfuric acid Wet process for phosphoric acid Power generation	Fermentation to ethanol (corn) Bio-ethylene from dehydration of bio-ethanol Transesterification to FAME and glycerol (soy oil and algae) Algae oil production Bio-propylene glycol from glycerol Gasification to syngas (corn stover) Formic acid Graphite Propylene from CO2 Propylene from propane dehydrogenation
Existing Plants Not in the Optimal Structure	New Plants Not in the Optimal Structure
Acetic acid Ethylbenzene Styrene	Fermentation to ethanol (corn stover) Anaerobic Digestion to acetic acid (corn stover) Methanol – Bonivardi, et al., 1998 Methanol – Jun, et al., 1998 Methanol – Ushikoshi, et al., 1998 Methanol – Nerlov and Chorkendorff, 1999 Methylamines (MMA and DMA) Ethanol Dimethyl ether Hydrogen/synthesis gas Acetic acid – new process Styrene - new method Electric furnace process for phosphoric acid Haifa process for phosphoric acid SO2 recovery from gypsum waste S and SO2 recovery from gypsum waste



Recap:

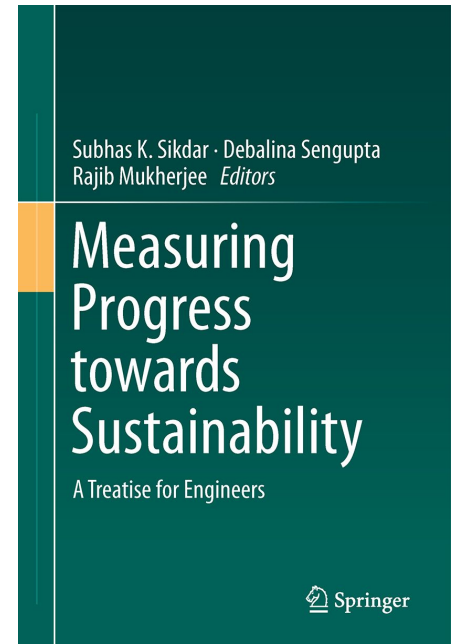
- Eco-industrial parks provide shared resources, outlets for byproducts, and utilities
- The Louisiana Case Study demonstrated that a biomass based chemical complex can be sustainable, provided there is an outlet for the CO_2
- A Triple Bottomline Profit allows the screening of potential processes for further evaluation
- Model reduction methods can be applied to high fidelity process models and used for optimization model
- An optimization based mathematical framework for a region allows for relatively simple analysis for potential process plants

Remember?



- Measuring Progress Towards Sustainability was written for Engineers, giving them a way to quantify sustainability for engineering decisions
- Key impact areas can be identified, and improved based on the Sustainability Footprint Method

"Measure what is measurable, and make measurable what is not so" - Galileo Galilei





GFRC

**GAS & FUELS
RESEARCH CENTER**

TEXAS A&M ENGINEERING EXPERIMENT STATION

We look forward to collaborating with talents and leaders in academia, industry, and government in a true partnership to achieve advancement and make a difference in the area of gas and fuels.

Questions, Comments:

debalinasengupta@tamu.edu

(225) 223 - 9046

Comparison of Base Case with Optimal Structure (Triple Bottomline)

	Base Case Million \$/year	Optimal Structure Million \$/year
Income from Sales	2,026	2,490
Economic Costs	697	516
Raw Material Costs	685	470
Utility Costs	12	46
Environmental Costs	457	313
Sustainable Credits(+)/Costs(-)	-18	-10
Triple Bottomline	854	1,650

Comparison of Base Case with Optimal Structure (Energy Requirement)

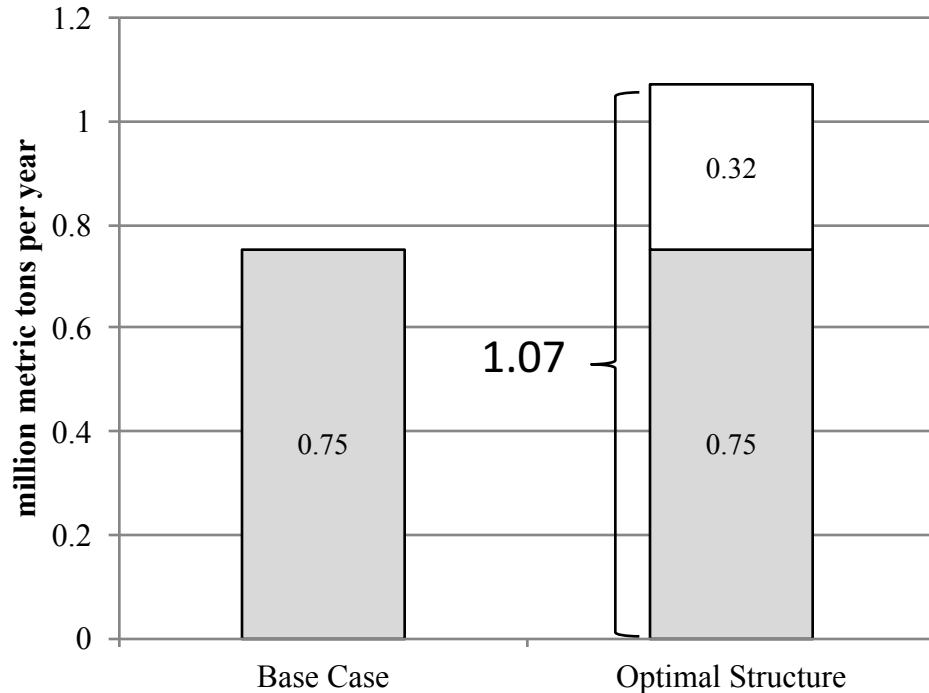
	Base Case (TJ/yr)	Optimal Structure (TJ/yr)
Ammonia	3,820	3,820
Methanol	2,165	1,083
Sulfuric acid	-14,642	-14,642
Wet process phosphoric acid	5,181	5,181
Corn Ethanol	na	4,158
Fatty Acid Methyl Esters	na	1,293
Others	4,374	5,512
Total Energy	898	6,405

Comparison of CO₂ use in Base Case and Optimal Structure

Base Case CO₂ Emission (million metric tons per year) : $0.75 - 0.14 = \mathbf{0.61}$

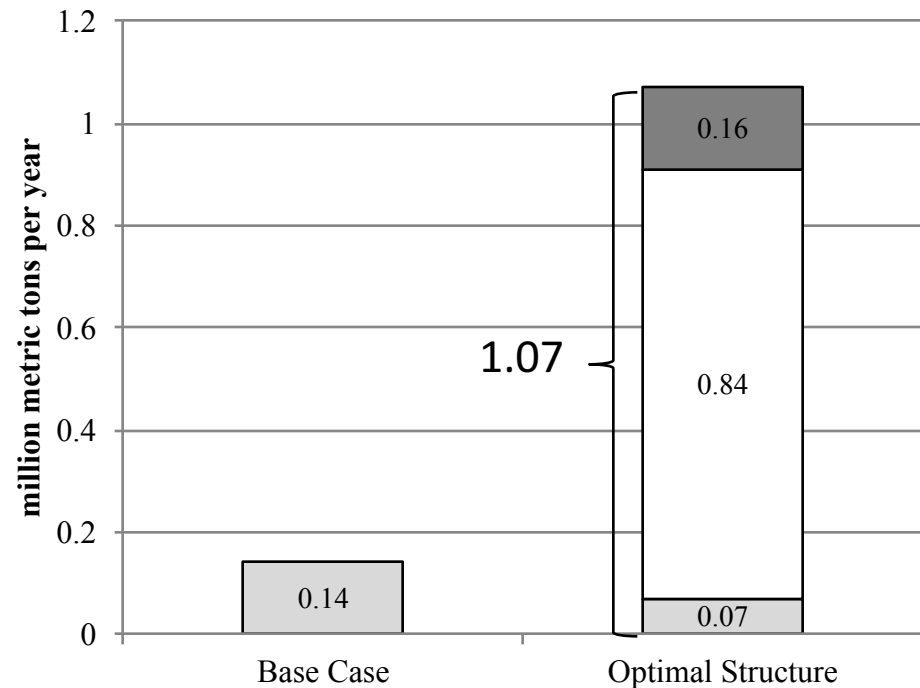
Optimal Structure CO₂ Emission (million metric tons per year) : $1.07 - 1.07 = \mathbf{0}$

Pure Carbon Dioxide Sources



- Pure CO₂ (ammonia plant)
- Pure CO₂ (bioprocesses)

Pure Carbon Dioxide Consumption



- Pure CO₂ (new CO₂ chemicals)
- Pure CO₂ (algae)
- Pure CO₂ (existing chemical plants)

Utility Type	Base Case Utility Cost (MM\$/yr)	Integrated Case Utility Cost (MM\$/yr)	Integrated and Intensified Case Utility Cost (MM\$/yr)
Cooling Water	8.4	3.6	1.2
LP steam	35.5	31.9	4.0
Natural Gas Firing	15.7	7.1	7.1
Electricity	19.2	19.2	27.1
Total Utility	78.8	61.8	39.4

Equipment Type	Base Case Capital Cost (\$MM, 2016)	Integrated and Intensified Case Capital Cost (\$MM, 2016)
Columns	90	71
Vessels	14	14
Reactors	46	46
Exchangers	100	54
Pumps	1	0.5
Compressors	34	54
Fired Heaters	19	11
Refrigeration Equipment	17	17
Total Installed Capital Cost	321	268
Outside Battery Limits(OSBL) 30% (as a percentage of Total Installed Cost)		
Detailed Engineering and Construction 30 % (as a percentage of Total Installed Cost + OSBL)		
Contingency 10% (as a percentage of Total Installed Cost + OSBL)		
Total Fixed Capital Investment	585	488

