Green Chemistry in Process Engineering

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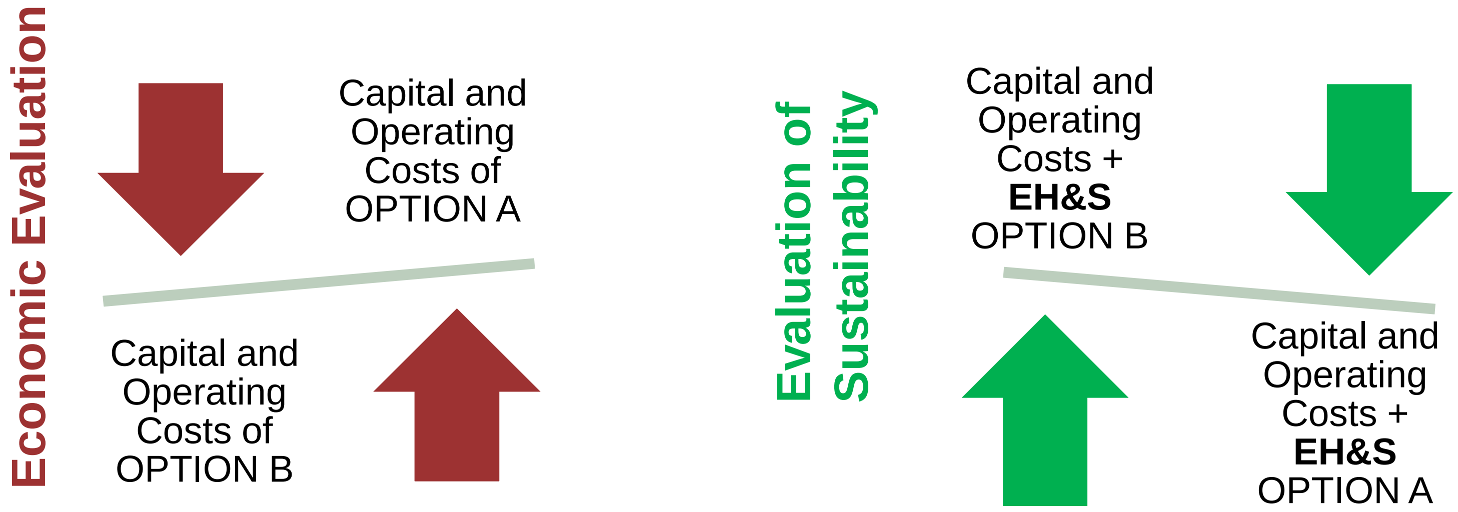
PROCESS SYNTHESIS AND SUSTAINABLE DEVELOPMENT

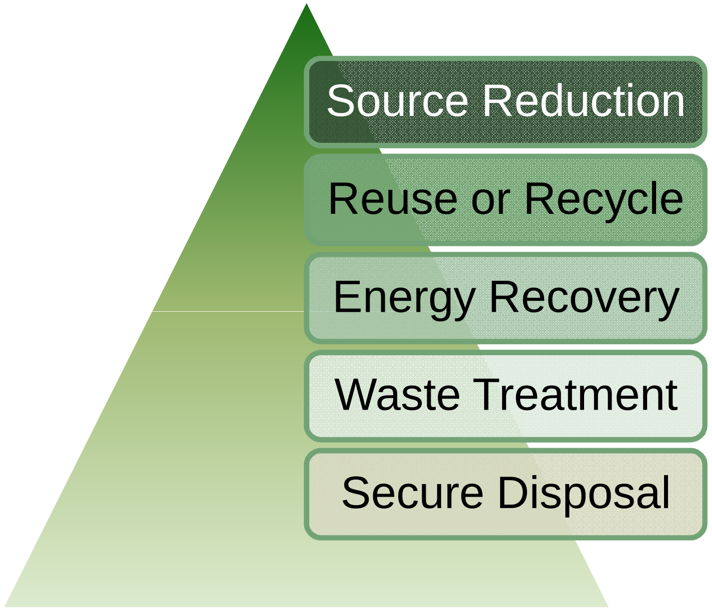
- Process synthesis is a systematic approach to the selection among potentially profitable process alternatives.

- **Process design aims for Sustainable Development**, the concept that development should meet the needs of the present without sacrificing the ability of the future to meet its needs.

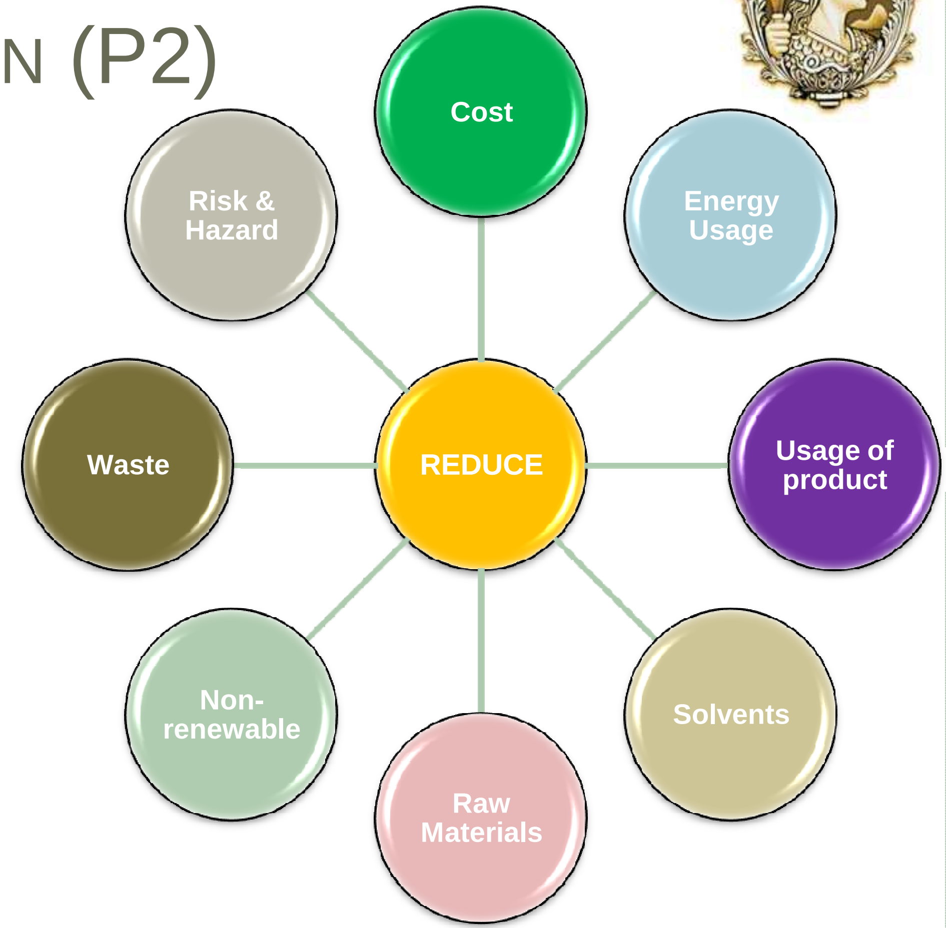
- **Process evaluation for process synthesis decision making:**



POLLUTION PREVENTION (P2)



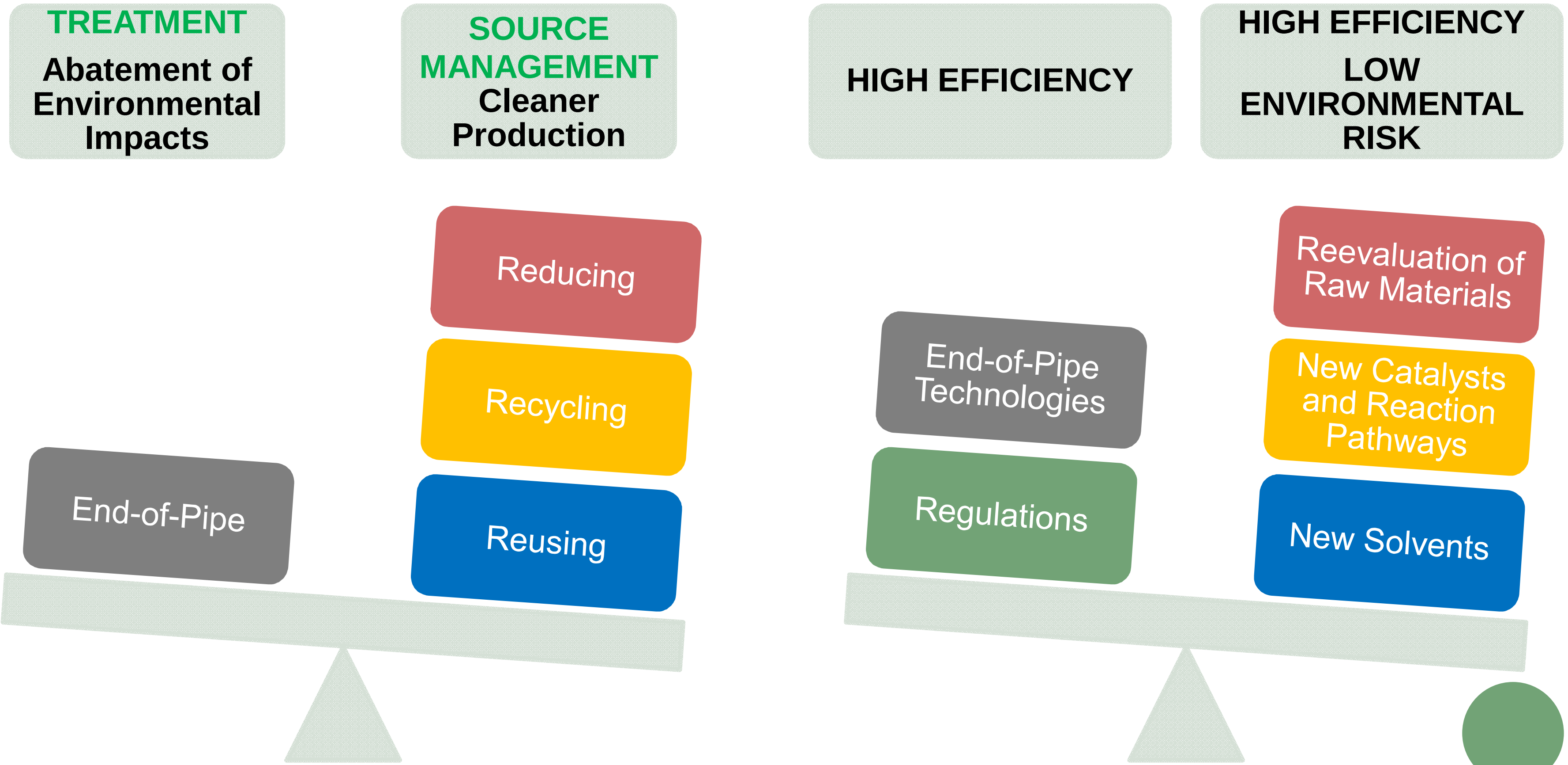
P2 Hierarchy



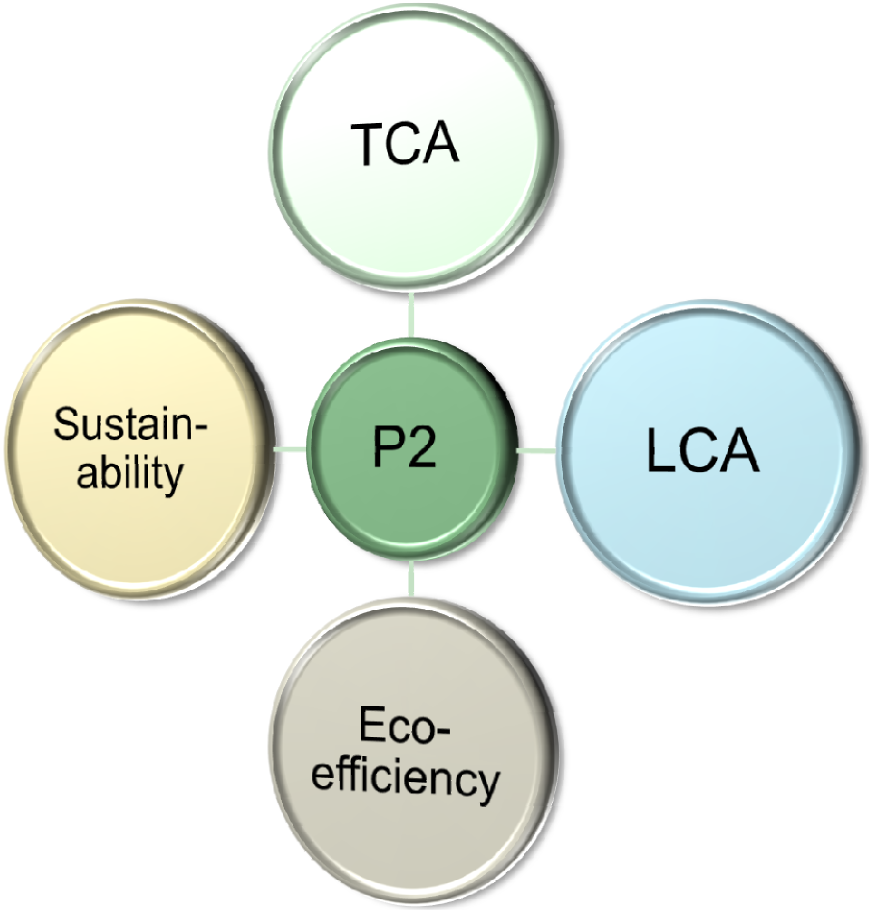
Reduction leads to sustainable development

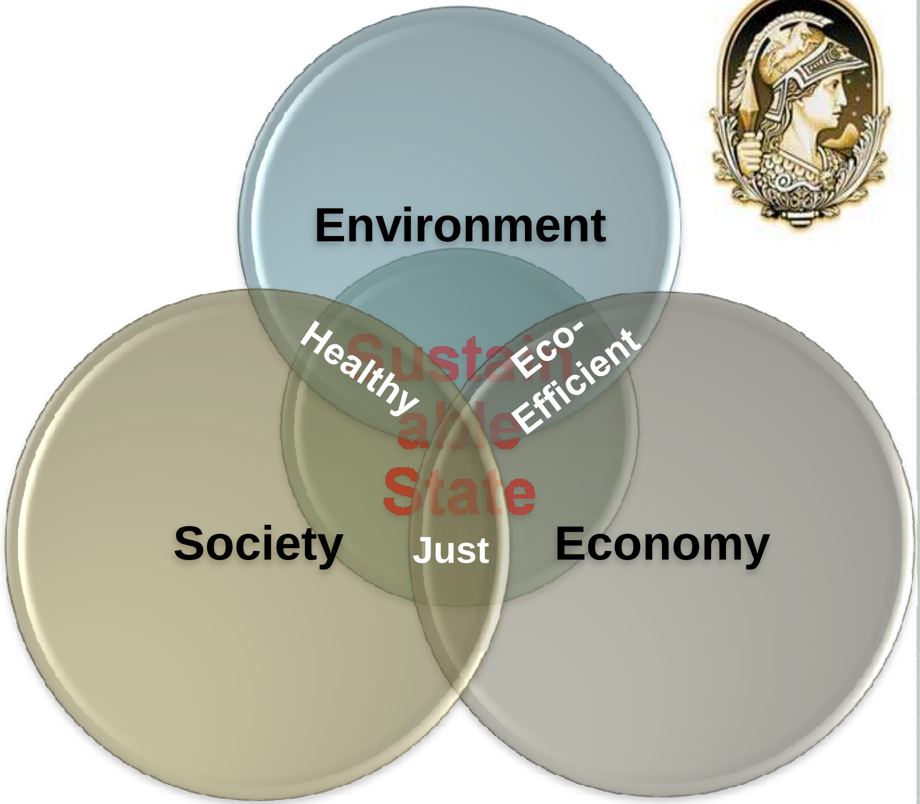
Green Chemistry and Engineering, Mukesh Doble & Anil Kumar Kruthiventi, Academic Press, 2007

NEW PARADIGMES



P2 FOR A SUSTAINABLE STATE

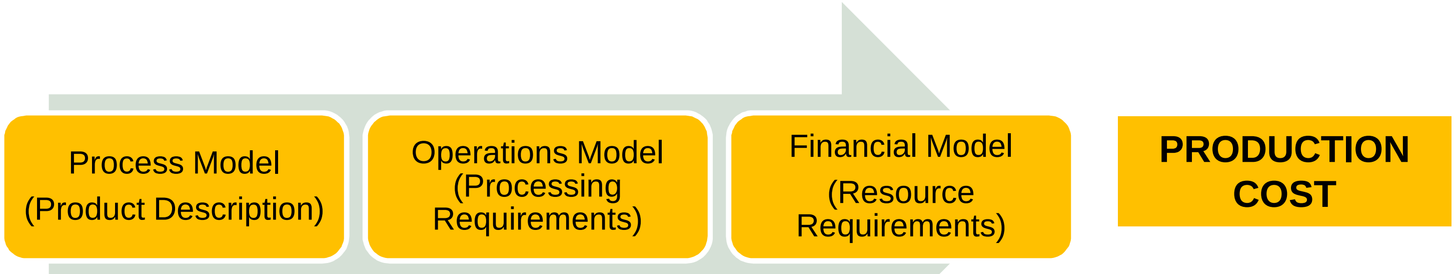




Combining economic, environmental and sustainability costs with new methodology for the **best process configuration.**

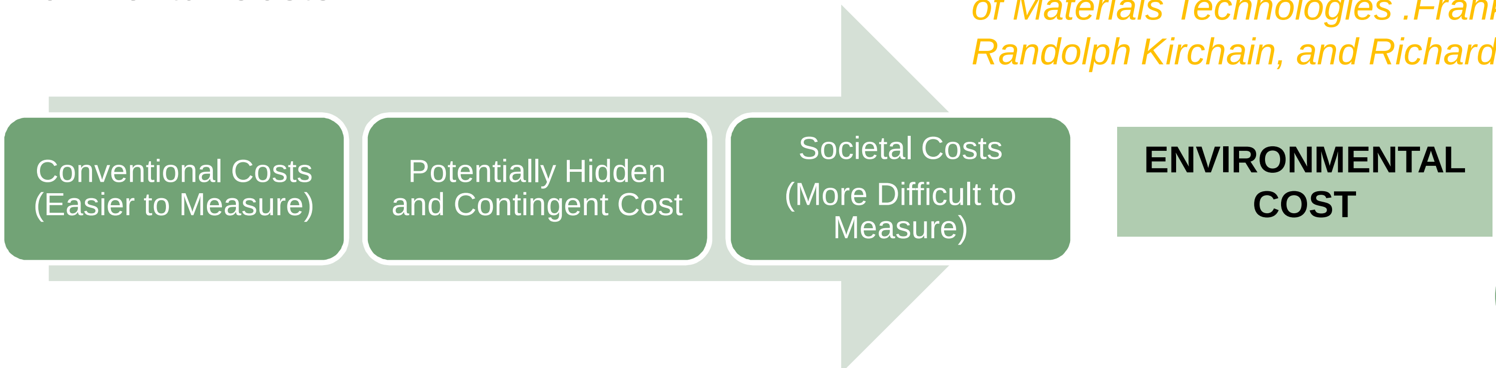
BEST PROCESS CONFIGURATION (DESIGN)

- Production cost is a central performance metric for engineering analysis, throughout the product development cycle.
- The key to good design lies in the conceptual framework that the designer employs to relate a design's properties to the design goals.



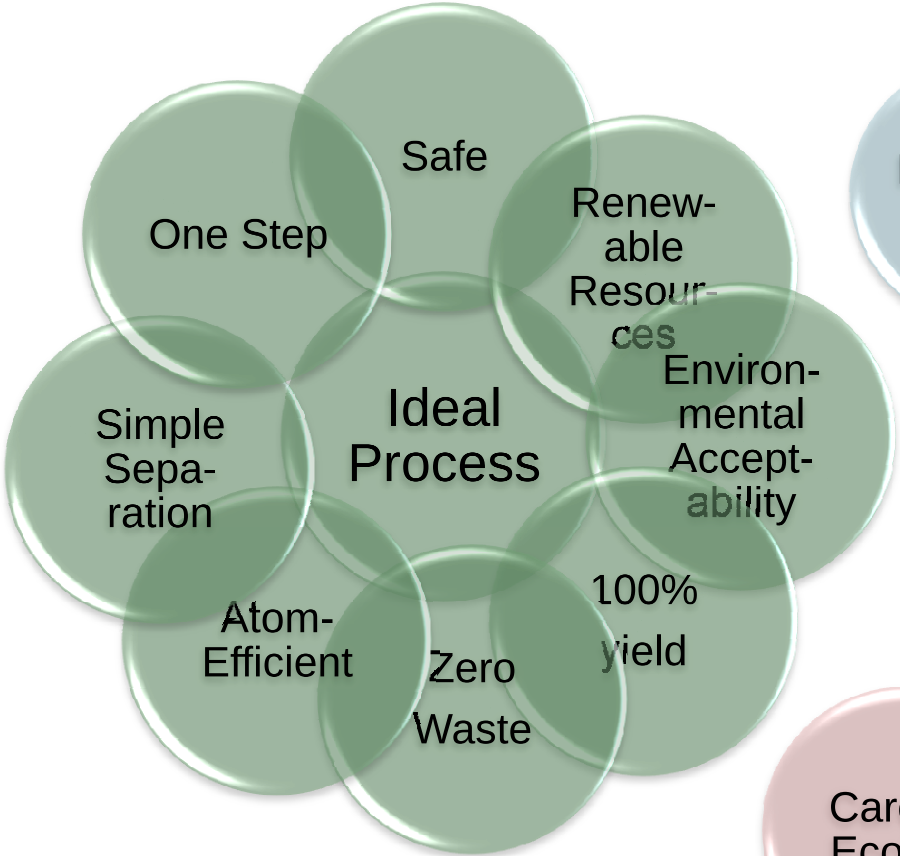
Process Cost Modeling: Strategic Engineering and Economic Evaluation of Materials Technologies .Frank Field, Randolph Kirchain, and Richard Roth

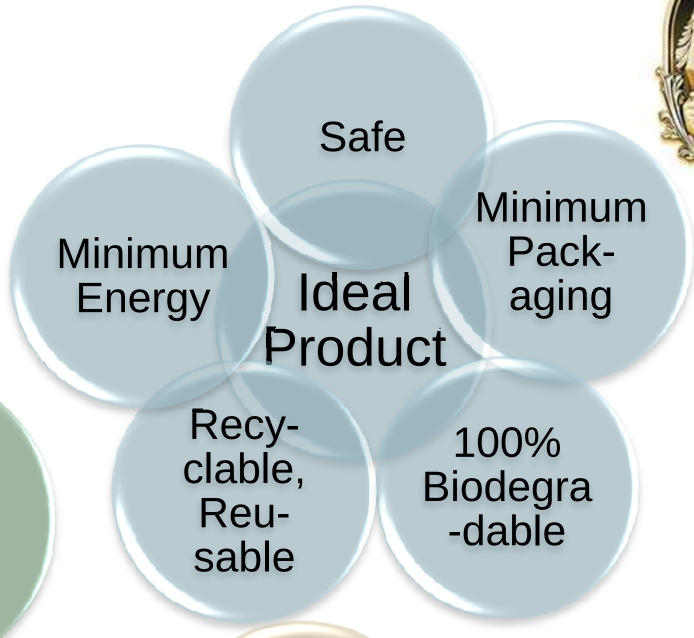
- Envionmental Costs



An Introduction to Environmental Accounting as a Business Management Tool: Key Concepts and Terms. EPA 742-R-95-001

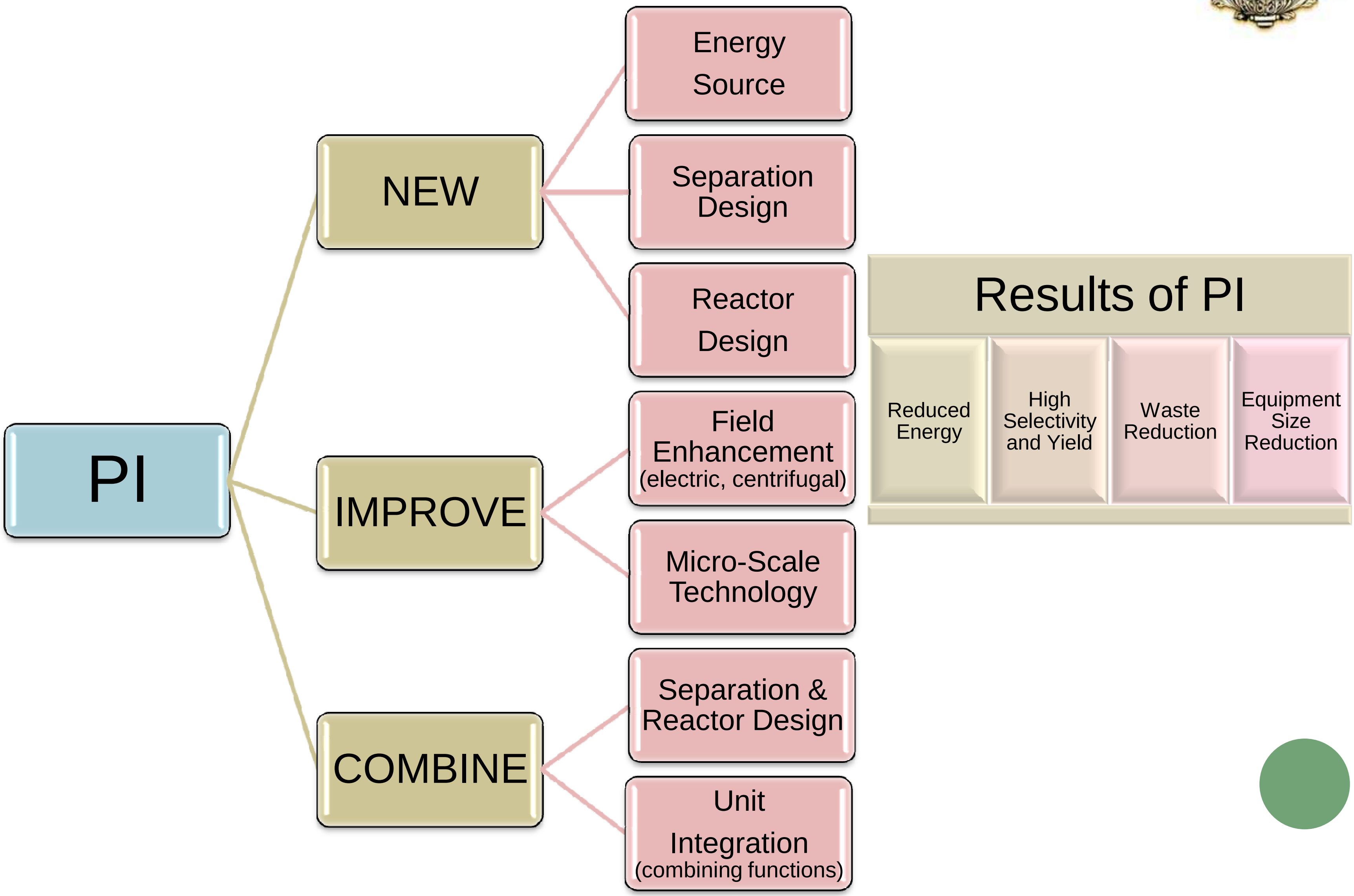
IDEAL PROCESS, PRODUCT AND USER





Green Chemistry and Engineering, Mukesh Doble & Anil Kumar Kruthiventi, Academic Press, 2007

PROCESS INTENSIFICATION (PI)



TRENDS IN PROCESS DESIGN

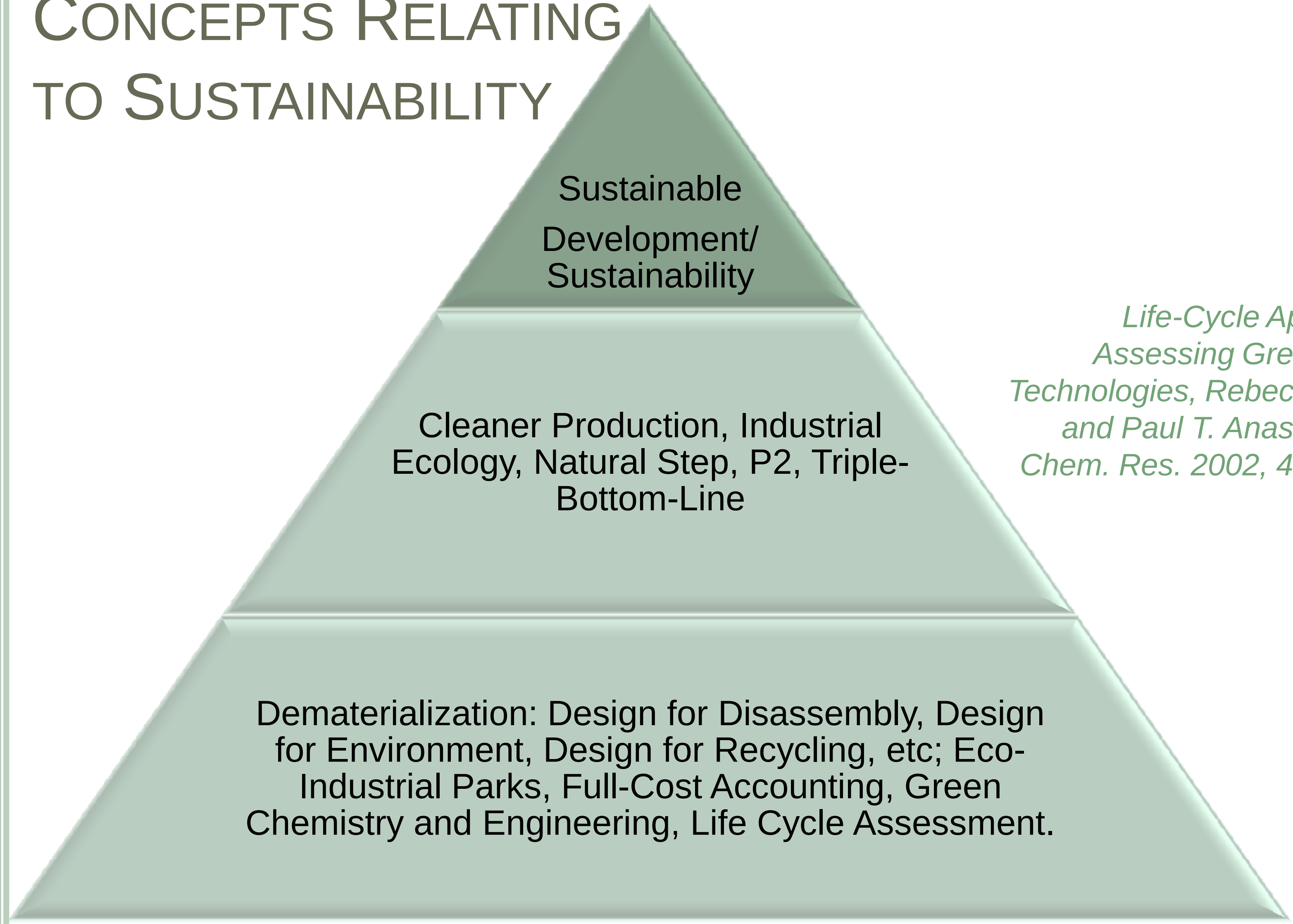
ECO-EFFICIENCY: minimizing waste, pollution and natural resource depletion (concept of P2).

INDUSTRIAL ECOLOGY: designing and operating industrial systems, where wastes or byproducts from one facility provide feedstock for other facilities.

DESIGN FOR ENVIRONMENT: The systematic consideration during design of issues associated with environmental safety and health over the entire product life cycle

Hierarchy of Concepts Relating to Sustainability

CONCEPTUAL



PRACTICAL

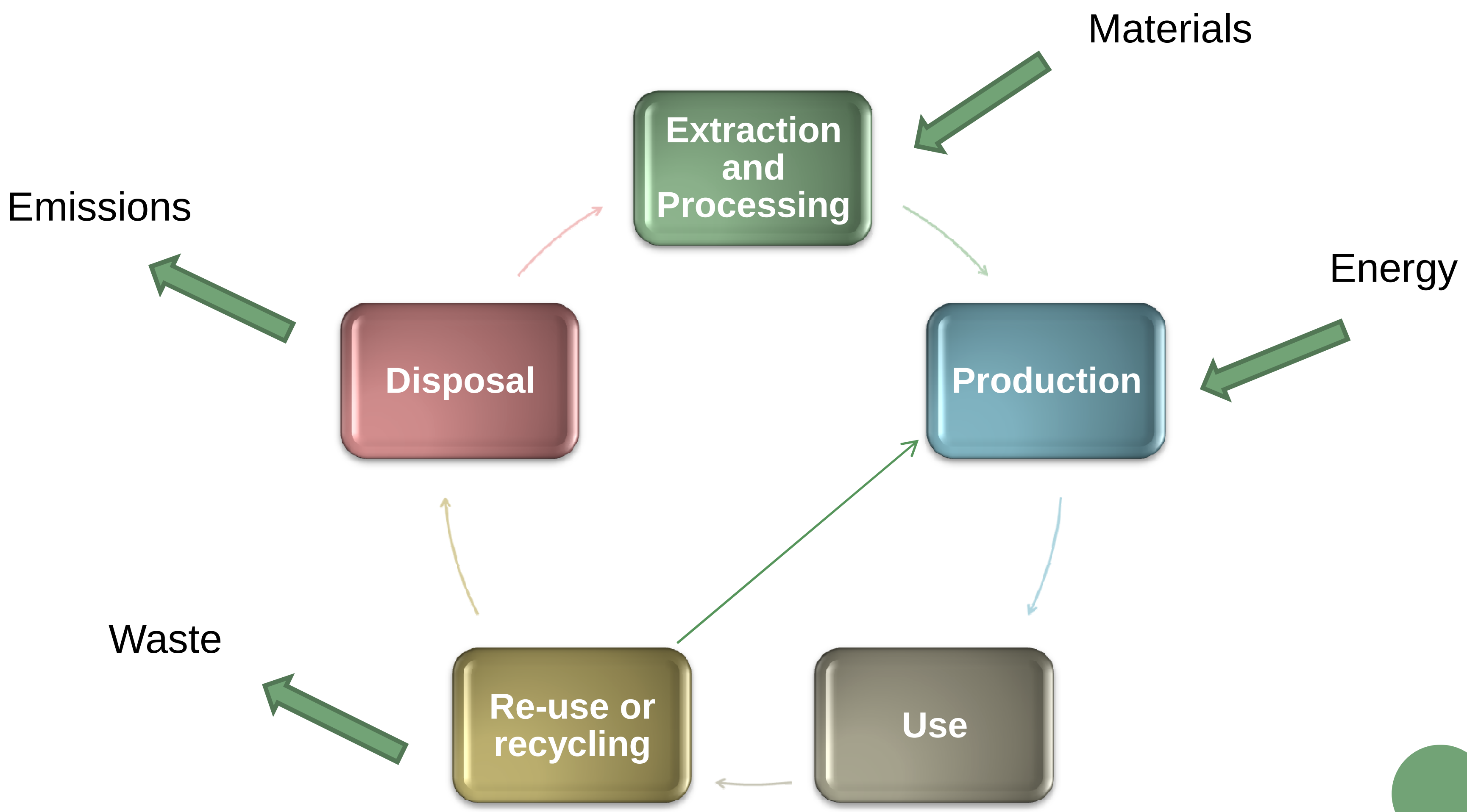
Life-Cycle Approaches for Assessing Green Chemistry Technologies, Rebecca L. Lankey, and Paul T. Anastas, Ind. Eng. Chem. Res. 2002, 41, 4498-4502

LCA FOR ASSESSING GREEN CHEMISTRY

- **Define the boundaries of the study** - within your sphere of influence, so that the changes indicated can be made.
- **Metrics should be specific and detailed** enough to provide useful information but **simple** enough to address the environmental issues within a useful time frame.
- **Desired metrics for LCA include:** (1) amounts of inputs, (2) emissions; (3) relative toxicities of materials; (4) process or product costs; (5) use of recycled material (waste or byproduct used as an input); and percentage of waste produced.
- Assessing the life-cycle impacts of a product or process and assigning metrics for the comparison of two options allow to **identify where environmental vulnerabilities occur over the life cycle.**

Life-Cycle Approaches for Assessing Green Chemistry Technologies, Rebecca L. Lankey, and Paul T. Anastas, Ind. Eng. Chem. Res. 2002, 41, 4498-4502

LCA Applied to Processes



12 Principles of Green Chemistry

1. Prevention
2. Atom economy
3. Less hazardous chemical synthesis
4. Design safer chemicals
5. Safety solvents and auxiliaries
6. Design for energy efficiency
7. Use renewable feedstocks
8. Reduce derivatives
9. Catalysis
10. Design for degradation
11. Real-time analysis for pollution prevention
12. Inherently safer chemistry for accident prevention

EPA Green Chemistry Mission: "To promote innovative chemical technologies that reduce or eliminate the use or generation of hazardous substances in the design, manufacture and use of chemical substances"

a. Green Chemistry is the application of P2 principles to the chemistry discipline;
b. Emphasis of Green Chemistry tends to be on synthesis routes and solvent selection, ignoring the role of equipment engineering

12 Principles of Green Engineering

1. All material and energy inputs and outputs are as inherently non-hazardous as possible
2. Prevention Instead of Treatment
3. Design for Separation and Purification
4. Maximize efficiencies *(Le Chatelier's Principle)*
5. Output-Pulled Versus Input Pushed
6. Conserve Complexity
7. Durability Rather than Immortality
8. Meet Need, Minimize Excess
9. Minimize Material Diversity
10. Integrate Material and Energy Flows
11. Design for Commercial "Afterlife"
12. Renewable Rather than Depleting

Anastas, P.T., and Zimmerman, J.B., "Design through the Twelve Principles, Principles of Green Engineering", Env. Sci. and Tech., 37, 5, 95 -101, 2003.

Process Alternatives Under GC and GE Perspectives

- Increase the integration of process chemistry into the generation of design alternatives.
- Predict by-products and emissions.
- Recognize opportunities to match waste streams with feed streams.
- Link process and environmental models (environmental databanks and process simulators).
- Detail used in process models should match the accuracy needed to make decisions.
- Allocate environmental impacts to specific processes and products in plants.
- Develop environmental impact indexes.
- Define preferences needed to weight multi-objective optimization.
- Sensitivity analysis and identification of the features that drive environmental impact.

J. A. Cano-Ruiz and G. J. McRae, ENVIRONMENTALLY CONSCIOUS CHEMICAL PROCESS DESIGN, *Annu. Rev. Energy Environ. 1998. 23:499–536*

Environmental Impact Assessment Based on Risks

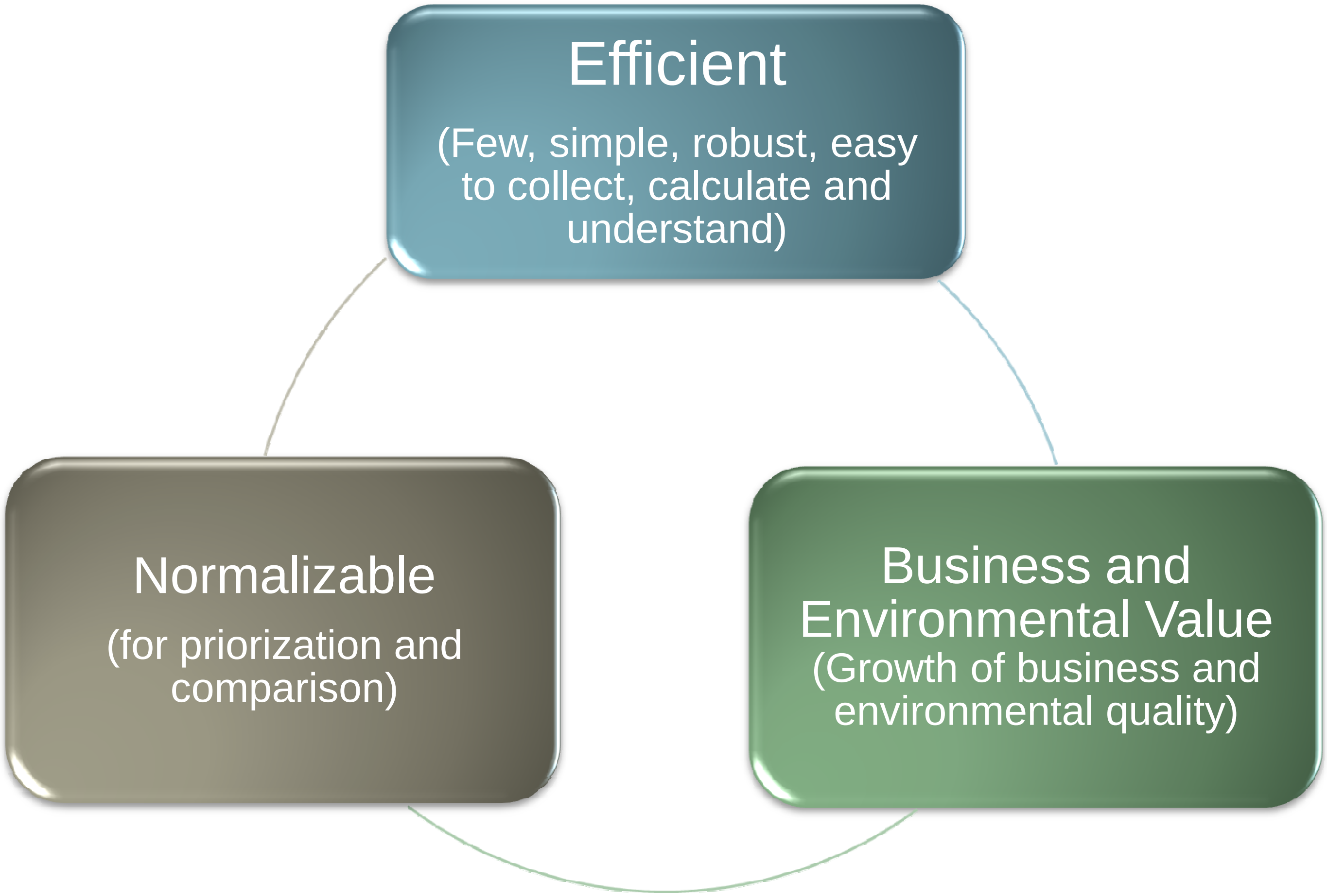
- **Risk** is a combination of the probability that an adverse event will occur and the consequences of the adverse event. Process designer should identify, evaluate, select and implement actions to reduce risk to **human health and to ecosystems**.

  Risk = f(hazard, exposure)

- **Hazard** is the potential for a substance or situation to cause harm or to create adverse impacts on persons or the environment. The magnitude of the hazard reflects the potential adverse consequences.

- **Exposure** denotes the magnitude and the length of time the organism is in contact with an environmental contaminant.

Qualities of Successful Metrics



Metrics of Environmental Risks for Flowsheet Evaluation

Abiotic Indexes

- Global Warming
- Stratospheric ozone depletion
- Acid deposition
- Smog formation

Health-Related Indexes

- Inhalation toxicity
- Ingestion toxicity
- Inhalation carcinogenicity
- Ingestion carcinogenicity

Ecotoxicity Indexes

- Fish aquatic toxicity

Sustainability Metrics

Environmental

- Greenhouse Gases, Ozone Depletion, Acidification, Eutrophication
- Incidents (Frequency, Severity, Worst-case Scenario)
- Waste (mass /output),
- Toxic Dispersion (Airborne toxics, Carcinogens, VOC, Particulates, Acid gases, aquatic toxicity, etc)

Material Intensity

- Percent yield
- Water Consumption (Volume of fresh water/Output)
- Material Efficiency (unit consumptions)
- Percent Atomic Efficiency

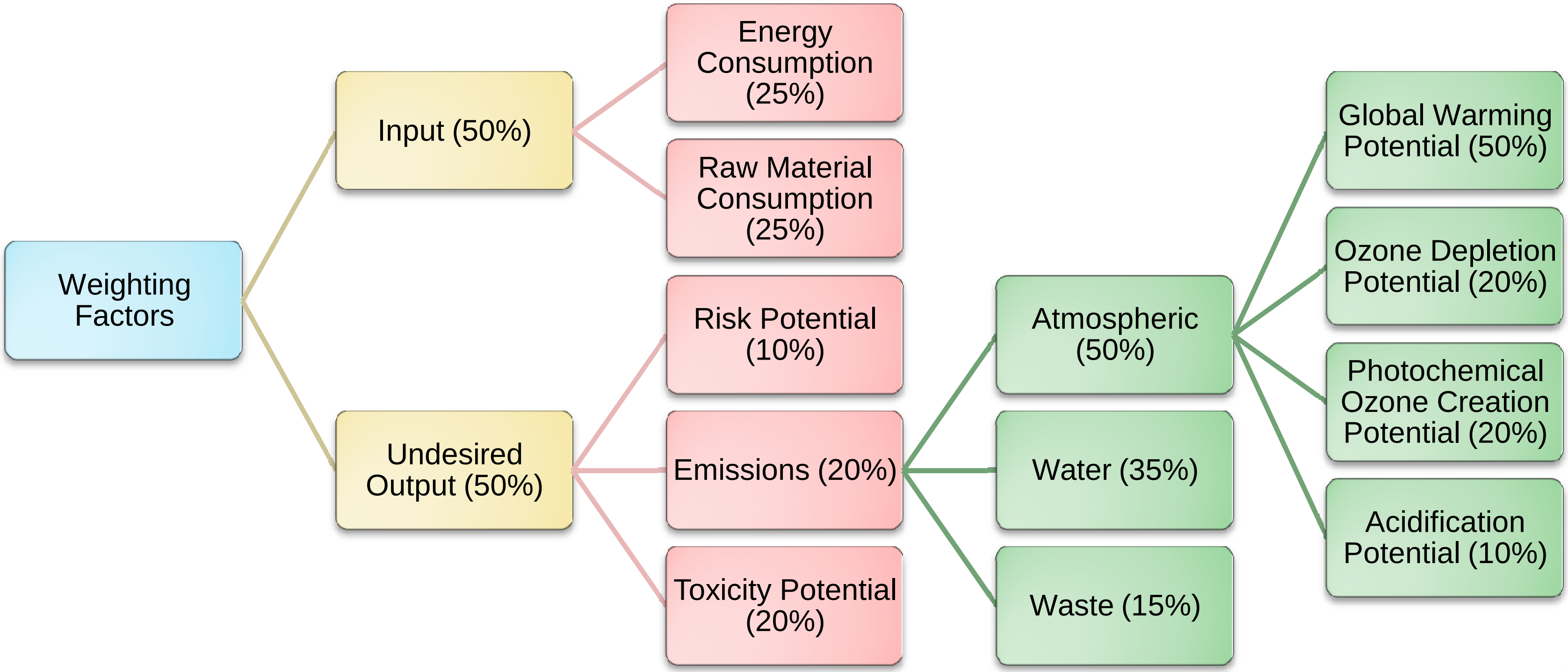
Societal

- Forestation (Total C offset, monetized eutrophication reductions,etc)
- Ecological footprint (ha/output)
- Ratio of Highest/Lowest Salary
- Employee Turnover, age of death of employees, etc

Energy Intensity

- "Emergy" (embodied energy ratio)
- BTU/pound
- Minimum practical energy use
- Total Energy Used (Energy used/output)

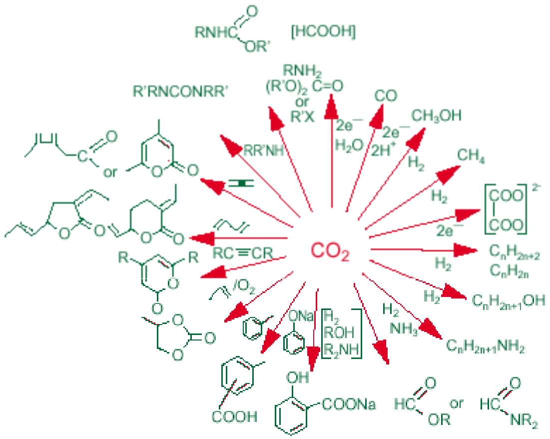
SUSTAINABILITY METRICS – WEIGHTING FACTORS

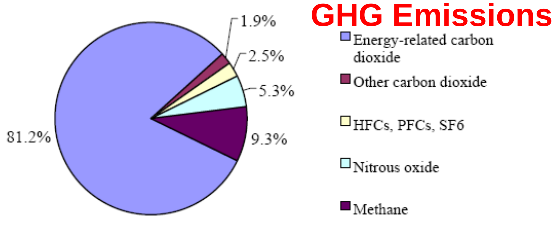


CASE STUDY
CHEMICAL SEQUESTRATION OF CO_2

CO_2 SEQUESTRATION

- Carbon dioxide use as a raw material (production of urea, methanol, DMC, plastics, etc).





DOE - U.S. DEPARTMENT OF ENERGY, OFFICE OF SCIENCE OFFICE OF FOSSIL ENERGY. ***Carbon Sequestration Research and Development,*** *(www.ornl.gov/carbon_sequestration/), Dec. 1999*

- Processes should overcome challenges of economics, performance, and associated environmental impacts;

- Most commercial plants capturing CO_2 from power plant flue gas use is based on chemical absorption with monoethanolamine (MEA) solvent (\$41/t CO_2).

Waste Reduction Algorithm (WAR)

- WAR was selected to calculate the EI of DMC production in each route.
- It characterizes sustainability with an index that measures **Potential Environmental Impacts (PEI)**, meaning **it works with hazards rather than risks**.
- Although the algorithm defines seven hazard categories, only three of them were taken into consideration in the present work: human toxicity potential by ingestion (HTPI), human toxicity potential by inhalation or dermal exposure (HTPE), and aquatic toxicity potential (ATP).
- The scores for these categories measured using easily obtainable data (LD_{50}, TLV_{50} e LC_{50}).
- Terrestrial toxicity potential is also measured using LD_{50} being, therefore, proportional to HTPI.
- Global warming potential (GWP) of both routes would be negative, since both routes sequestrate CO_2 (and produce no carbon-equivalent substances).
- Additionally, none of the chemicals involved appear in Ozone Depletion Potential (ODP) or Acidification Potential (AP).
- The only chemical which has Photochemical Oxidation Potential (PCOP) in both routes is methanol. But methanol consumption of the routes can be directly compared.

WAR (...)

$$\frac{\partial I_t}{\partial t} = \hat{I}_{in} - \hat{I}_{out} + \hat{I}_{gen}$$

$$\hat{I}_{in} = \sum_{i}^{Categories} \alpha_i \sum_{j}^{Streams} M_{j,in} \sum_{k}^{Components} x_{kj}\psi_{ki}$$

$$\hat{I}_{out} = \sum_{i}^{Categories} \alpha_i \sum_{j}^{Streams} M_{j,out} \sum_{k}^{Components} x_{kj}\psi_{ki}$$

$$\psi_{ki} = \frac{score_{ki}}{< score_k >_i}$$

$$score_{k,HTPI} = \frac{1}{LD_{50,k}}$$

$$score_{k,HTPE} = \frac{1}{TLV_{50,k}}$$

$$score_{k,ATP} = \frac{1}{LC_{50,k}}$$

The scores for the remaining categories are available in the literature (tables).

The values used in the WAR GUI software are from Heijungs et. al. (1992).

Heijungs, R. et al; Life Cycle Assessment; United Nations Environment Program - UNEP, Paris, France (1996)

Human Health and Environmental Impact Indexes

Dimensionless Risk Index	Eqn. #	Equation	Parameter / Software Source(s)
Ingestion Route Toxicity Potential	1	$INGTP_i = \dfrac{C_{i,a}/RfD_i}{C_{Toluene,a}/RfD_{Toluene}}$	$C_{i,a}$ & $C_{Toluene,a}$ – Mackay Model, 1992-4; **RfD** $_i$ **& RfD** $_{Toluene}$ – EPA 1994, 1997
Inhalation Route Toxicity Potential	2	$INHTP_i = \dfrac{C_{i,a}/RfC_i}{C_{Toluene,a}/RfC_{Toluene}}$	$C_{i,a}$ & $C_{Toluene,a}$ – Mackay Model, 1992-4; **RfC** $_i$ **& RfC** $_{Toluene}$ – EPA 1994, 1997
Ingestion Route Carcinogenicity Potential	3	$INGCP_i = \dfrac{C_{i,w} \times (SF_i)_{ING}}{C_{Benzene,w} \times (SF_{Benzene})_{ING}}$	$C_{i,w}$ & $C_{Benzene,w}$ – Mackay Model, 1992-4; ***SF*-** EPA 1994, 1997
Inhalation Route Carcinogenicity Potential	4	$INHCP_i = \dfrac{C_{i,a} \times (SF_i)_{INH}}{C_{Benzene,a} \times (SF_{Benzene})_{INH}}$	$C_{i,w}$ & $C_{Benzene,w}$ – Mackay Model, 1992-4; ***SF*-** EPA 1994, 1997
Fish Toxicity Potential	5	$FTP_i = \dfrac{C_{i,w} \times LC_{50f,PCP}}{C_{PCP,w} \times LC_{50f,i}}$	$C_{i,w}$ & $C_{PCP,w}$ – Mackay Model, 1992-4; LC_{50f} - Verschueren, 1996; Davis, 1994

C_i is the concentration if species "i".
RfD is the reference dose; LD50 may be substituted for RfD.
RfC is the reference concentration, LC50 may be substituted for RfC, and Hazard Value (HV, Davis 1994) may be substituted for SF (slope factor).

HUMAN HEALTH AND ENVIRONMENTAL IMPACT INDEXES

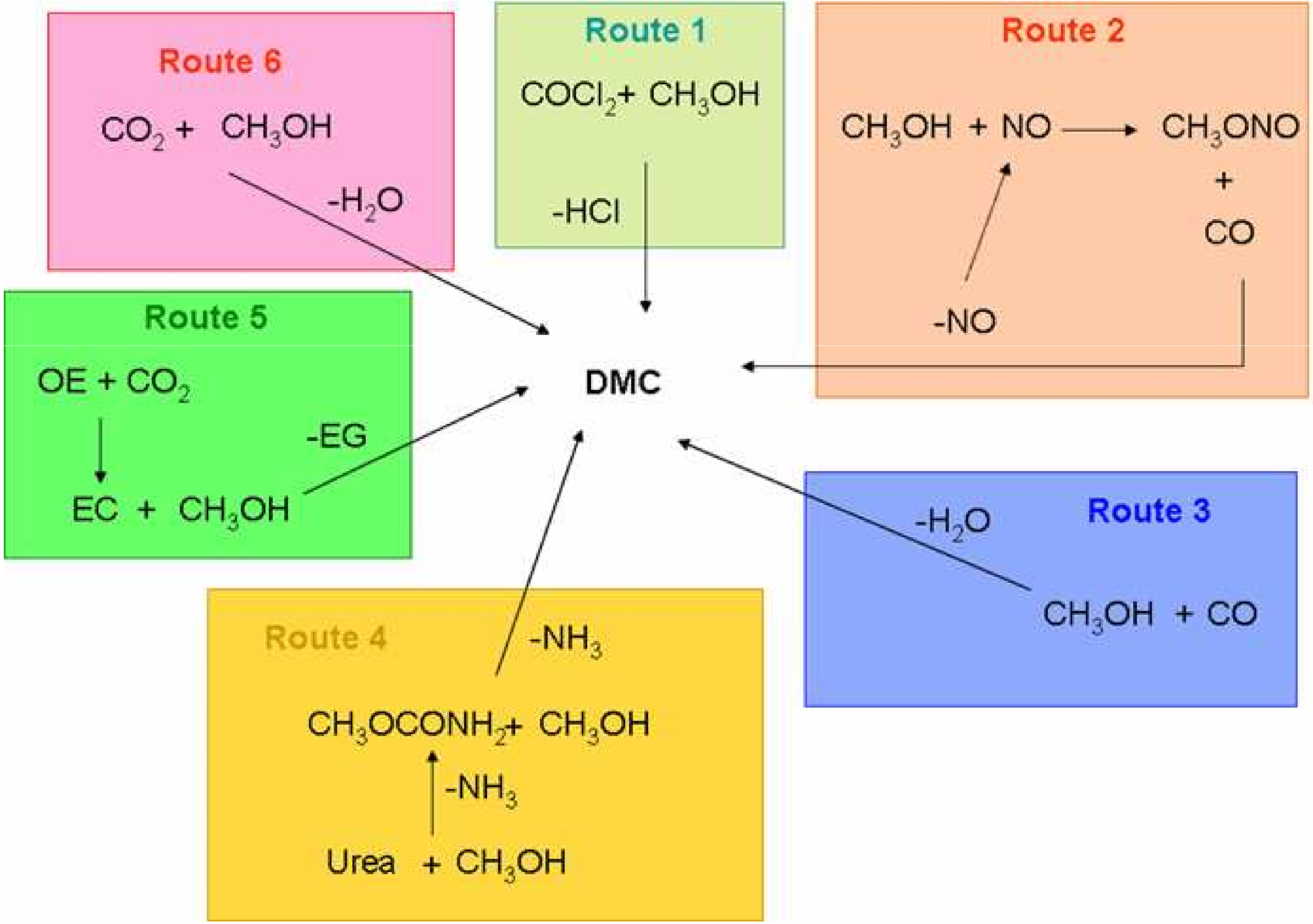
Dimensionless Risk Index	Eqn. #	Equation	Parameter / Software Source(s)
Global Warming	6	GWP_i	***GWP-*** Fisher, 1990a; WMO, 1992a; IPCC, 1991, 1996
	6a	$GWP_i = N_C \times \frac{MW_{CO_2}}{MW_i}$	N_C –
Ozone Depletion	7	ODP_i	***ODP-*** Fisher, 1990b; WMO, 1990a; WMO 1992b
Smog Formation	8	$SFP_i = \frac{MIR_i}{MIR_{ROG}}$	***MIR-*** Carter, 1994; Heijungs, 1992
Acid Rain	9	ARP_i	***ARP-*** Heijungs, 1992; Goedkoop, 1995

GWP is global warming potential.
ODP is the ozone depletion potential.
MIR is the maximum incremental reactivity for forming ozone in the lower atmosphere.
ARP is the acid rain potential.

DMC Production

- DMC market is broadening and it is moving to the category of chemical commodity: DMC can be used, for example, as alkylation agent, gas or diesel additive and as a monomer in polycarbonate synthesis
- Exploratory Analysis of six routes for DMC production (three of which have sequestration potential), briefly described as:
  - **ROUTE 1**: production of DMC and co-production of HCl from methanol and phosgene
  - **ROUTE 2**: production of methyl nitrite from methanol and NO, followed by production of DMC from methyl nitrite and CO, recovering NO
  - **ROUTE 3**: production of DMC and water from CO and methanol
  - **ROUTE 4**: production of DMC and NH_3 from urea and methanol (urea production involves CO_2 sequestration)
  - **ROUTE 5**: production of DMC and ethylene glycol from ethylene oxide and CO_2
  - **ROUTE 6**: production of DMC and water from CO_2 and methanol
- ROUTES 4, 5 and 6 show CO_2 sequestration potential

ROUTES FOR DMC PRODUCTION



Simple Sustainability Metrics

Environmental

Toxicity Index

$$TX_j = \sum_{i=1}^{n} tx_{ji}$$

$$TXI_j = \frac{TX_j}{TX_4}$$

Ecoefficiency

ec = economical indicator ; *en* = environmental indicator

$$\varepsilon = \frac{ec}{en}$$

Profit Potential

$$PP_j = \sum_{i=1}^{n} \nu_{ji} P_{ji}$$

$$PI_j = \frac{PP_j}{PP_4}$$

WAR Algorithm

(HTPI, HTPE, TTP, ATP, GWP, ODP, PCOP, AP)

Material Intensity

Material index

p = products mass flow (kg/h); *rm* = raw material mass flow (kg/h);

$$M = \frac{p}{rm}$$

Energy Intensity

Energy Index

e = energy consumption (KJ/h), *p* = products mass flow (kg/h)

$$E = \frac{e}{p}$$

Profit Potential for Ranking Routes

Chemical	Route 1	Route 2	Route 3	Route 4	Route 5	Route 6
Stoichiometric coefficients (gate-to-gate domain) ν_{ji}						
Hydrochloric acid	2					
Water		1	1			1
Ammonium				1		
Ethylene carbonate					0	
Dimethyl carbonate	1	1	1	1	1	1
Carbon dioxide					-1	-1
Ethylene glycol					1	
Phosgene	-1					
Methanol	-2	-2	-2	-3	-2	-2
Methyl carbamate				0		
Carbon monoxide		-1	-1			
Methyl nitrite		0				
Ethylene oxide					-1	
Nitric oxide		1				
Oxygen		- 1/2	- 1/2			
Urea				-1		
Cradle-to-gate domain						
Carbon	●	●	●	●	●	●
Sodium chloride	●					
Chlorine	●					
Carbon dioxide				●		
Ethane					●	
Ethylene					●	
Hydrogen	●	●	●	●	●	●
Methane	●	●	●	●	●	●
Carbon monoxide	●	●	●	●	●	●
Nitrogen				●		
Oxygen		●	●		●	

The symbol (●) was used in the cradle-to-gate domain to indicate the presence of the chemical in the route.

Chemical	*P* (US$/mol)
Hydrochloric acid	0.00342
Ammonium	0.00496
Carbon credits	0.00084
Dimethyl carbonate	0.10810
Ethylene glycol	0.06238
Phosgene	0.16571
Methanol	0.01047
Carbon monoxide	0.00140
Ethylene oxide	0.05487
Nitric oxide	0.00150
Oxygen	0.00477
Urea	0.02019

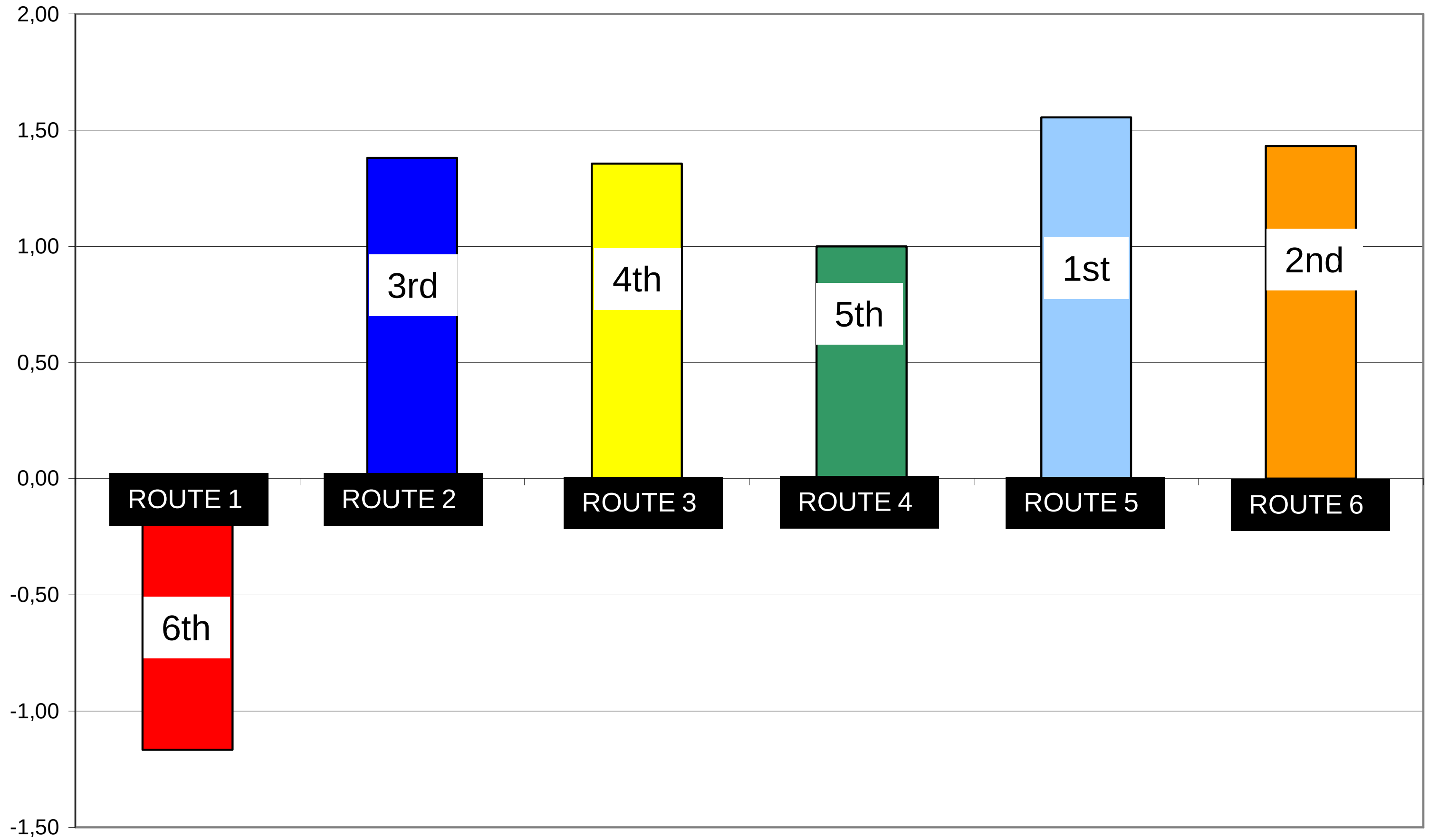
Profit Potential

ν_{ji} = stoichiometric coefficient of chemical i on route j; P_{ji} = price in US$/mol of chemical i on route j

$$PP_j = \sum_{i=1}^{n} \nu_{ji} P_{ji} \qquad PI_j = \frac{PP_j}{PP_4}$$

ANATAS, P. T. e ALLEN, D. Green Chemistry. In: ALLEN, D. T. Green Engineering: Environmentally Conscious Design of Chemical Processes. Prentice Hall PTR: New Jersey, 2002. pp 177-196.

RESULT OF EXPLORATORY ANALYSIS

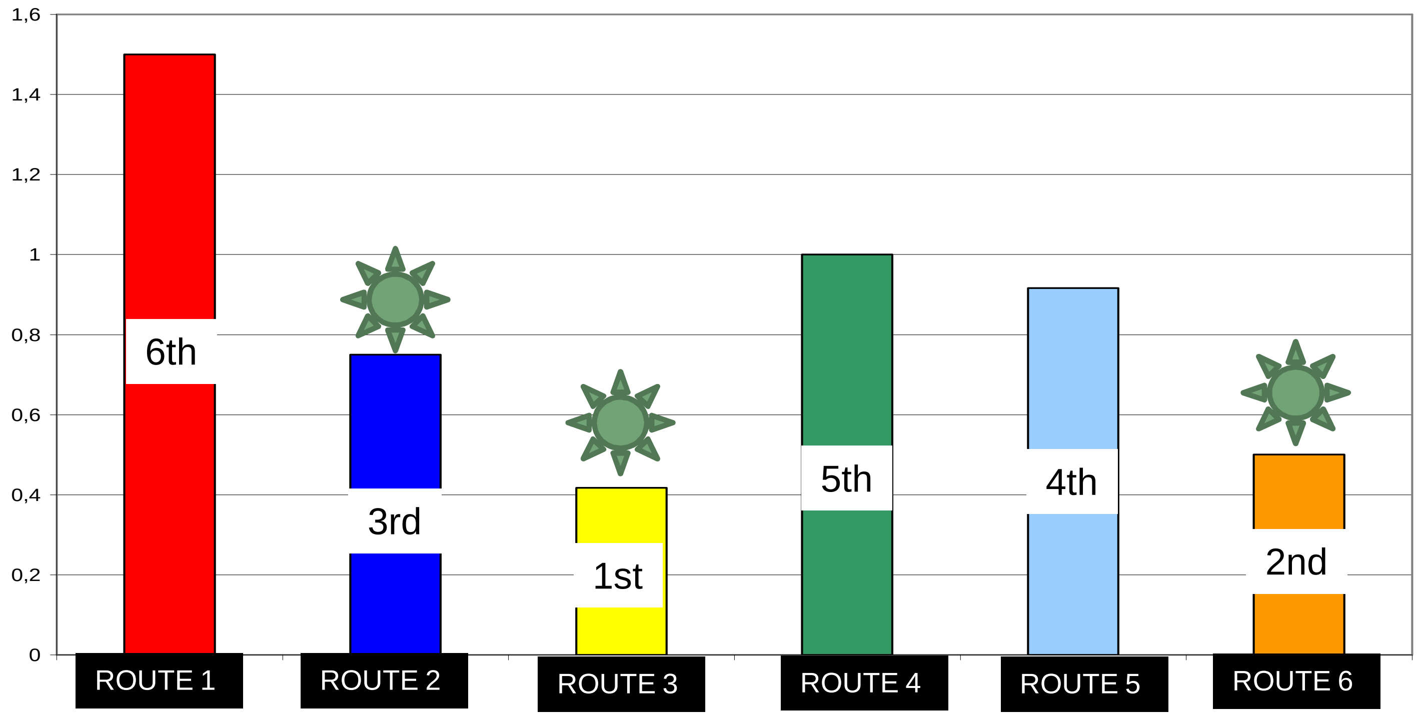


TOXICITY RANKING

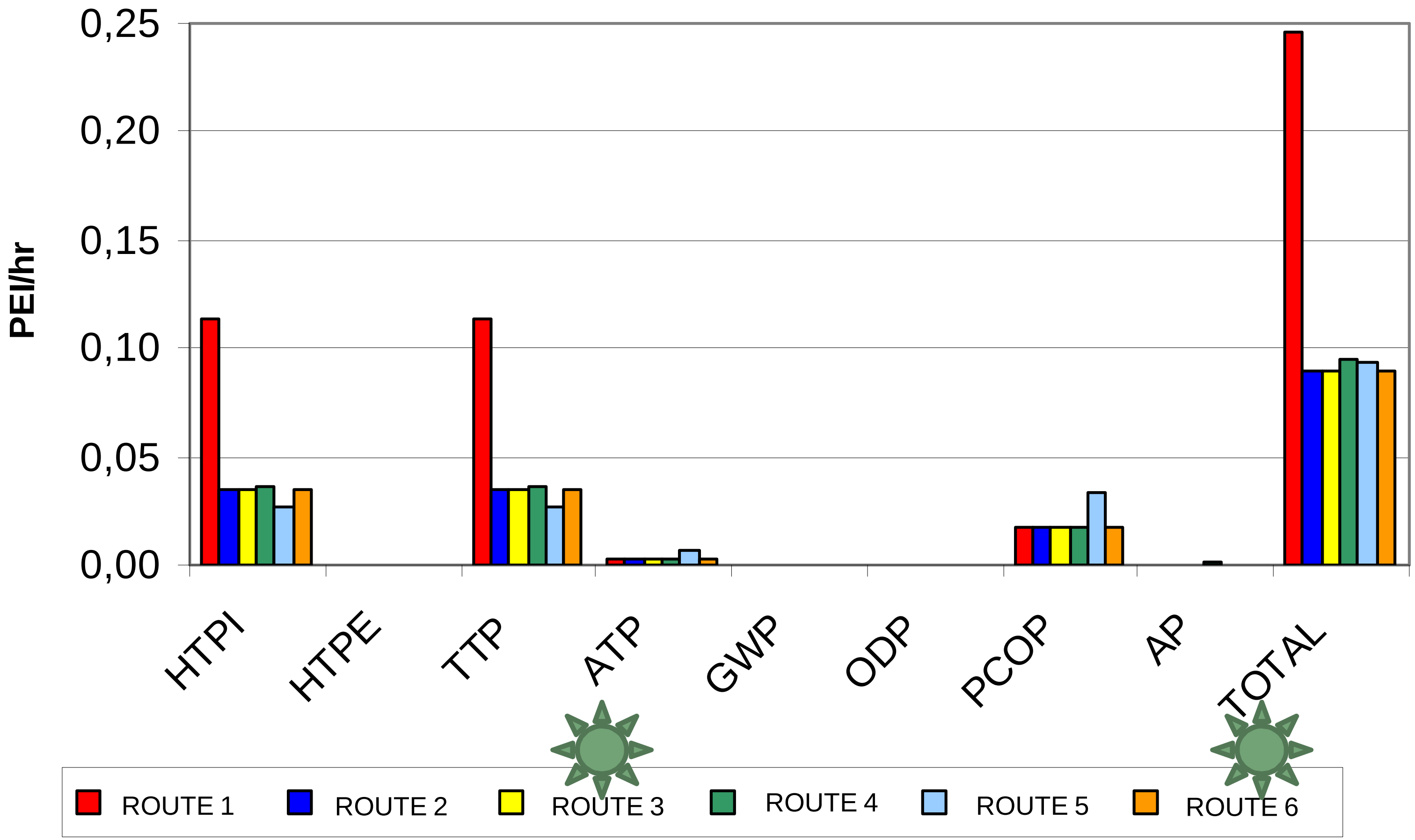
- The toxicity index of each route was calculated, using ROUTE 4 as basis

$$TX_j = \sum_{i=1}^{n} tx_{ji} \qquad TXI_j = \frac{TX_j}{TX_4}$$

where: TX_j = toxicity of route j; tx_{ji} = toxicity of chemical i on route j; TXI_j = toxicity index of route j.



WAR RANKING



The toxicity index results are in general agreement with the WAR (PEI) results

Overall Ranking

- Total score = sum of economical ranking position + the average of environmental ranking positions (toxicity and PEI criteria). The lower the score, the greener the route.

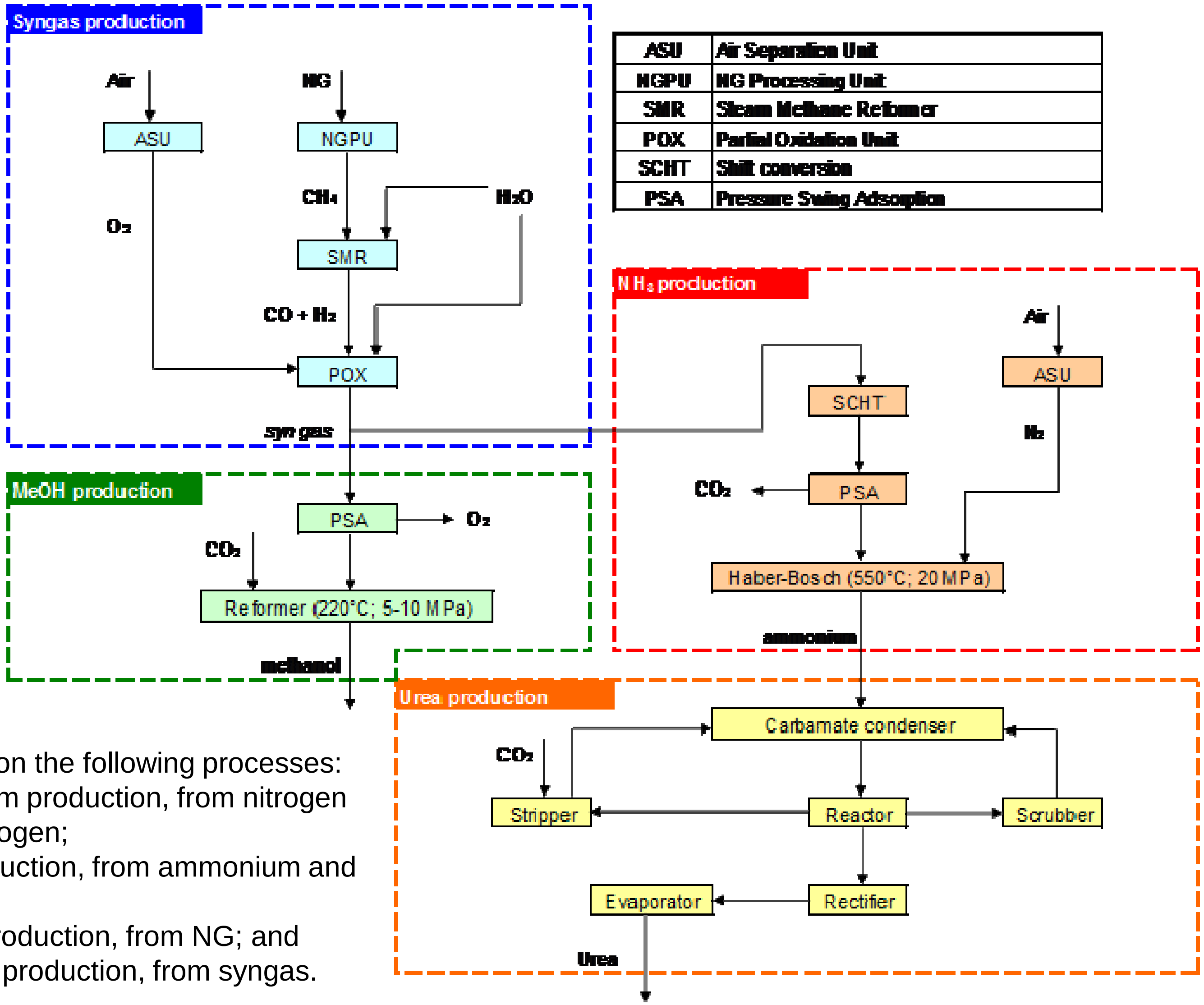
Route	Economical ranking	Environmental ranking		Total score
		Toxicity	PEI	
1	6	6	6	12
2	3	3	1	5
3	4	1	1	5
4	5	5	4	9.5
5	1	4	4	5
6	2	2	1	3.5

- ROUTE 6 might be the greener route, but ROUTE 5 has a better profit potential and its total score is close to ROUTE 6's
- ROUTE 6 is eliminated as there's no indication that it is feasible in industrial scale
- ROUTES 2 and 3 have the same total score as ROUTE 5, but only intermediate profit potential.
- For CO_2 sequestration, ROUTES 2 and 3 must be abandoned.
- **ROUTES 4 and 5 should be further investigated, as they combine intermediate total score, sequestration potential, and industrial feasibility.**

LIFE CYCLE ASSESSMENT

- DMC production via ROUTES 4 and 5 were conceived in two domains: **cradle-to-gate** (raw material production processes) and **gate-to-gate** (DMC production processes).
- Domain **gate-to-gate is the actual industrial venture in focus**, which receives raw materials produced in cradle-to-gate domain processes.
- Processes of **cradle-to-gate domain are herein seen as auxiliary**, and were addressed exclusively to allow LCA. In this sense, there are other possible processes that were not taken into consideration and could equally be used.
- For the gate-to-gate domain analysis, DMC production processes were **simulated and optimized using HYSYS** (Aspentech).
- To assess the **environmental impact of the considered routes, the WAR algorithm,** which requires streams' information, was implemented in the simulation environment.
- **The cradle-to-gate domain was analyzed exclusively based on the WAR algorithm** using information estimated from stoichiometric data available in literature

ROUTE 4 (DMC FROM UREA) – CRADLE-TO-GATE

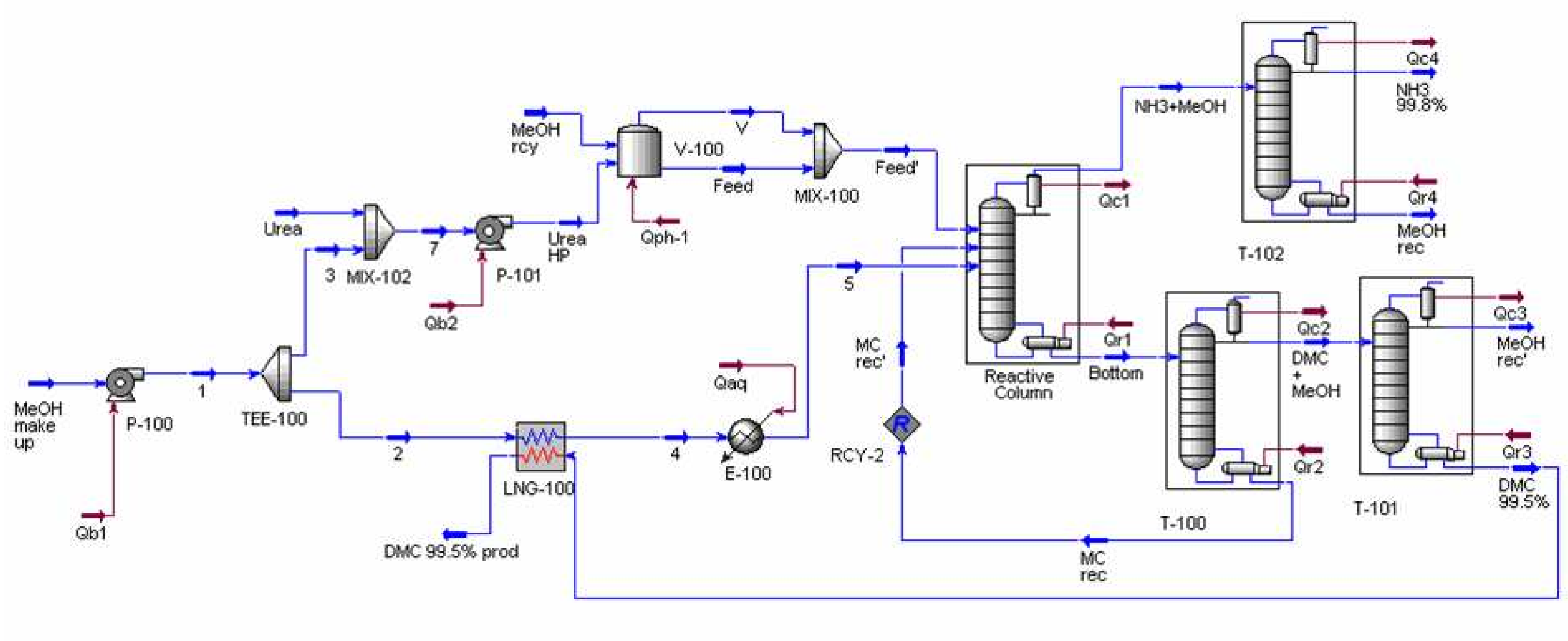


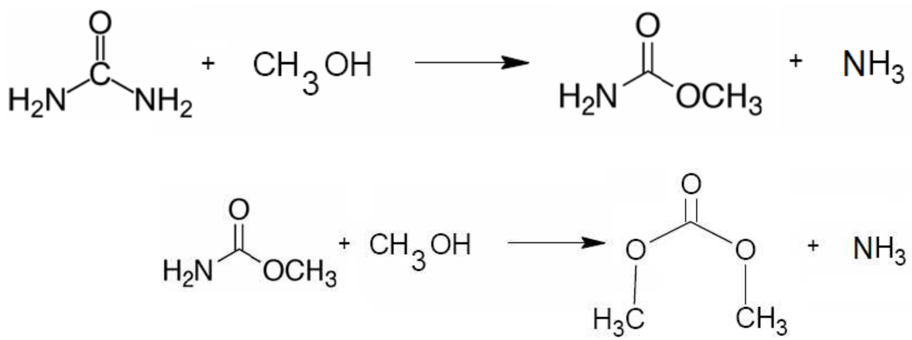
ASU	Air Separation Unit
NGPU	NG Processing Unit
SMR	Steam Methane Reformer
POX	Partial Oxidation Unit
SCHT	Shift conversion
PSA	Pressure Swing Adsorption

Consists on the following processes:

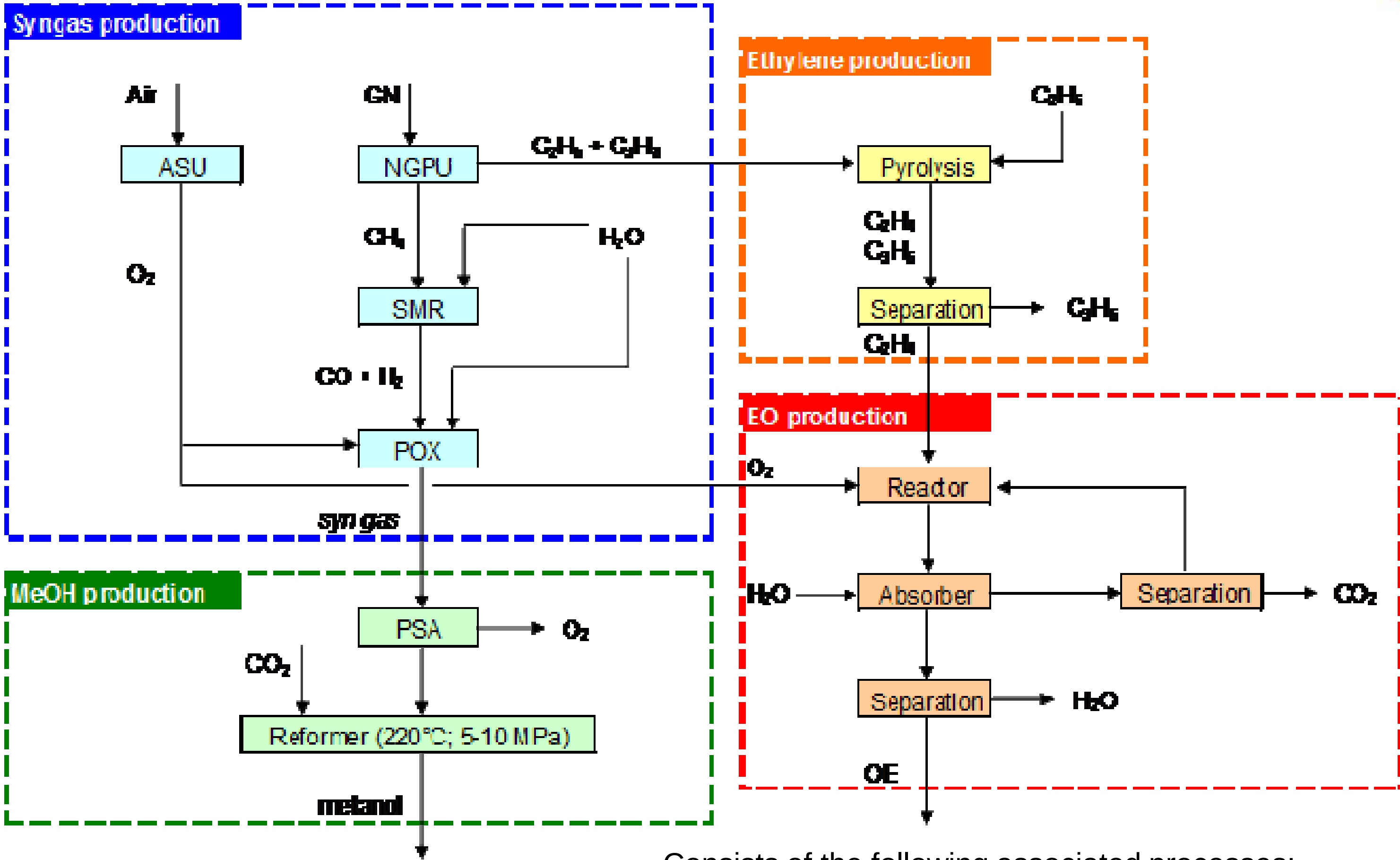
- ammonium production, from nitrogen and hydrogen;
- urea production, from ammonium and CO_2;
- syngas production, from NG; and
- methanol production, from syngas.

Route 4 (DMC from Urea) – Gate-to-Gate





Route 5 (DMC from EO) – Cradle-to-Gate

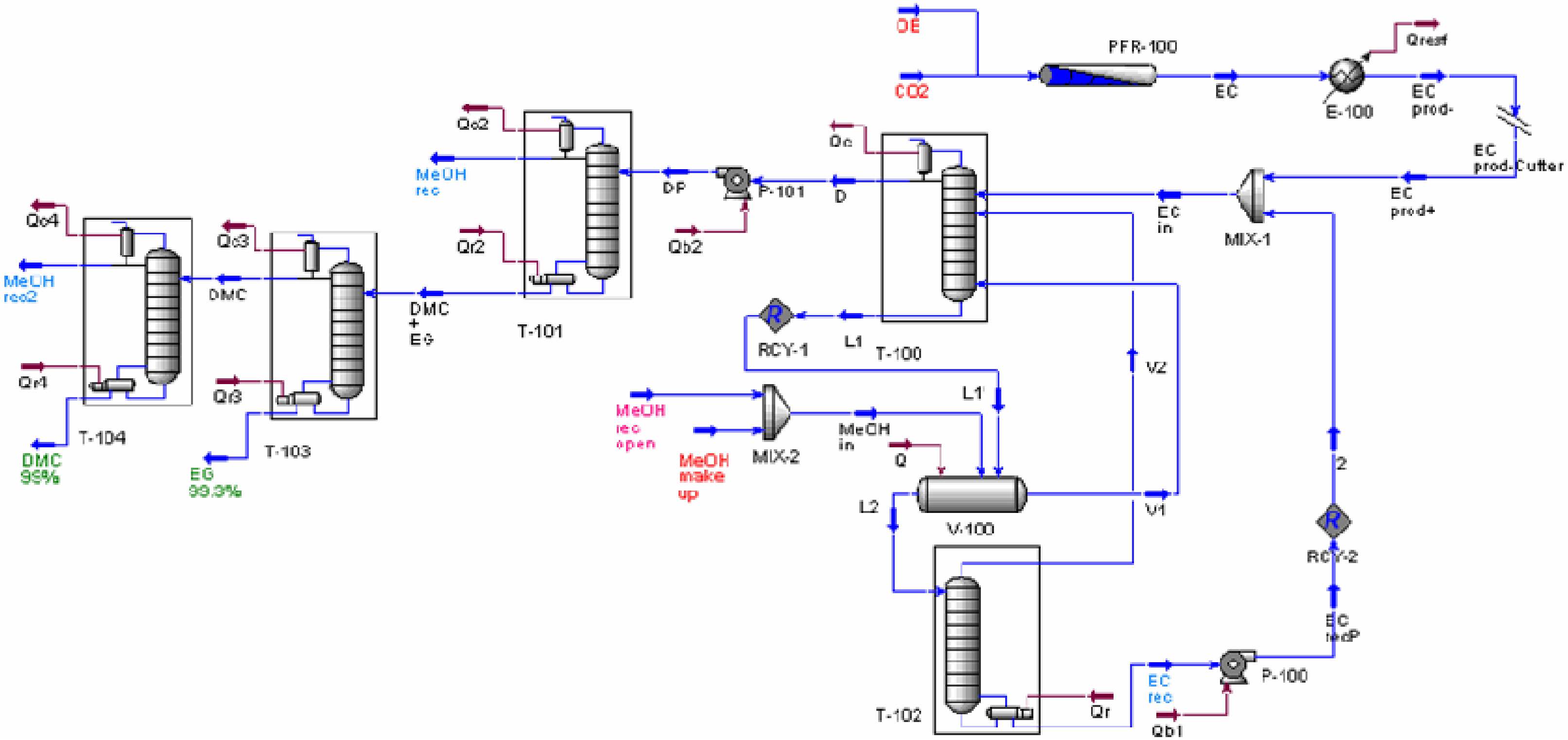


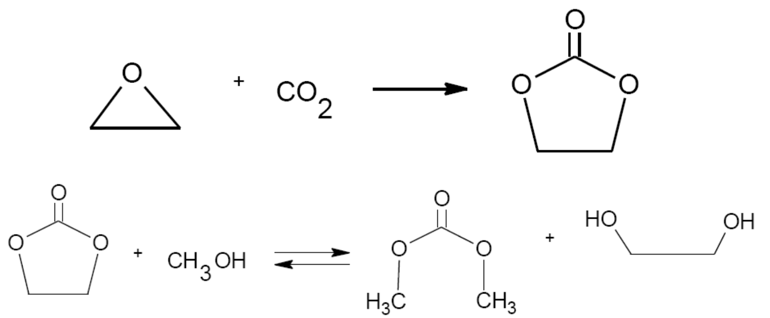
ASU	Air Separation Unit
NGPU	NG Processing Unit
SMR	Steam Methane Reformer
POX	Partial Oxidation Unit
PSA	Pressure Swing Adsorption

Consists of the following associated processes:

- Ethylene production from ethane (obtained from natural gas – NG – and oil);
- EO production from ethylene and oxygen; and
- Syngas production (steam methane reform – SMR); methanol production from syngas

Route 5 (DMC from EO) – Gate-to-Gate





Environmental + Economic Factors

- Objective Function for searching Optimal Design must incorporate **environmental and economic factors** together.
- The economic assessment uses **economic indexes** that include Total Revenue, Capital Costs and Operational Costs.
- The environmental indexes used to **quantify environmental impact** (global warming, ozone depletion, acid rain, smog formation, human-ingestion-route toxicity, human-inhalation-route toxicity, human-ingestion-route-carcinogenicity toxicity, human-inhalation-route carcinogenicity toxicity and ecotoxicity). An environmental process composite index is found (**EI**) .
- A Sustainability Function (**S**)

$$S = \omega_P P - \omega_{EI} EI$$

Economic Objective

$$P(\$/yr) = 0.48 Incomes - 0.54 ISBL - 0.68 Outcomes$$

$Price_{DMC}$(US$/kg)*$Production_{DMC}$(kg/yr)
+ $Price_{EG}$(US$/kg)*$Production_{EG}$(kg/yr)
+ $Price_{MeOH}$(US$/kg)*$Recovery_{MeOH}$(kg/yr)

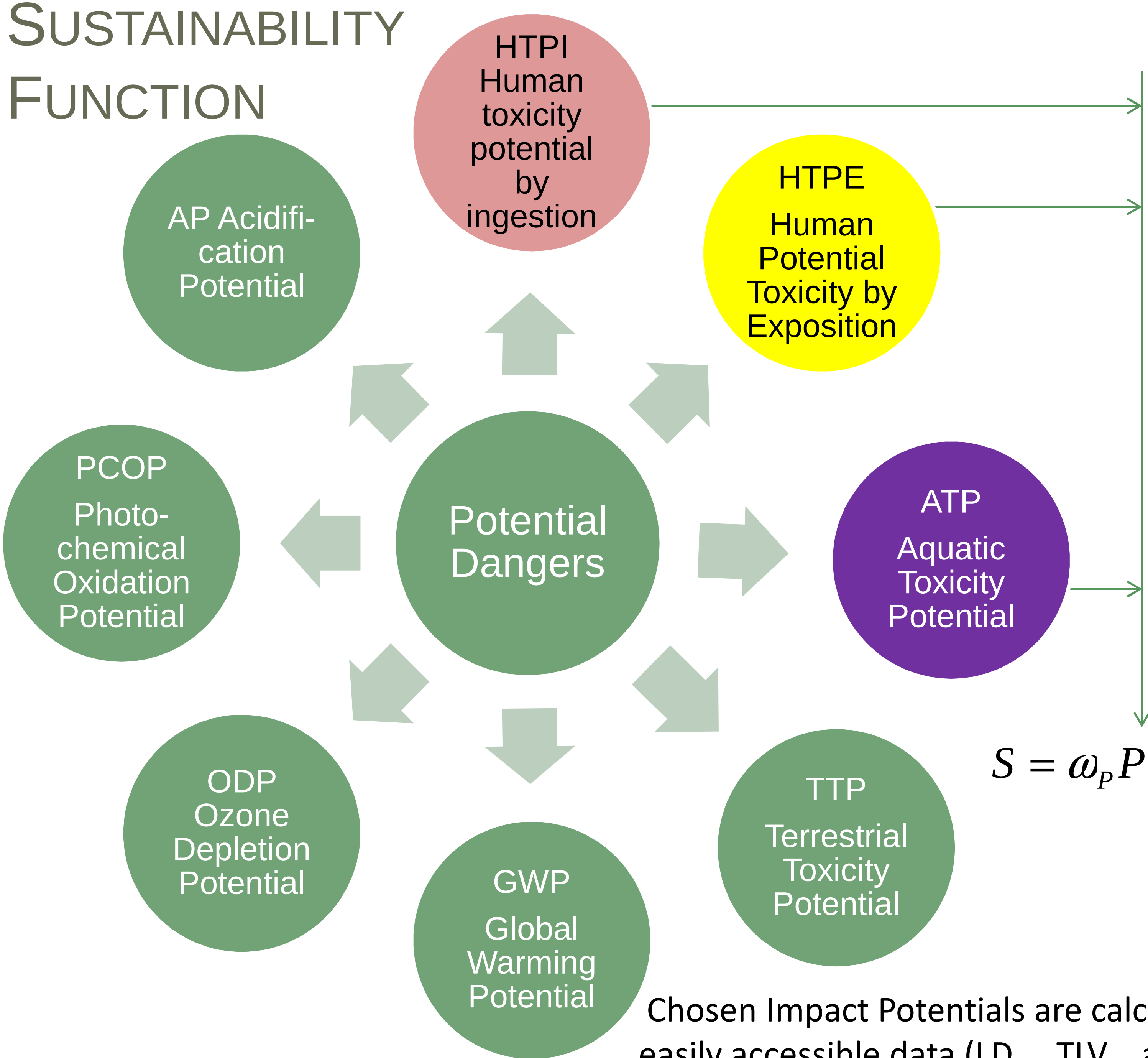
Heat exchangers, columns, vessels, reactors and pumps

$Price_{EO}$(US$/kg)*$Production_{EO}$(kg/yr)
+ $Price_{MeOH}$(US$/kg)*$Feed_{MeOH}$(kg/yr)
+ $Price_{Water}$(US$/kg)*$Consumption_{Water}$(kg/yr)
+ $Cost_{Vapour}$(US$/kg)*$Consumption_{Vapour}$(kg/yr)
+ $Cost_{EE}$(US$/kg)*$Consumption_{EE}$(kg/yr)

ISBL

Cost of Equipments (US$)	
Heat Exchanger	$$C = \frac{(M\ \&\ S)}{280} 101{,}3 A^{0,65} (2{,}29 + F_c)$$ F_c=0,85 A = surface of heat exchange; em ft²
Vessesl, colums and reactors	$$C = \frac{(M\ \&\ S)}{280} 101{,}9 D^{1,066} H^{0,802} (2{,}18 + F_c)$$ F_c=1,00 H = height; ft² D = diameter; ft²
Internals of distillation columns	$$C = \frac{(M\ \&\ S)}{280} 4{,}7 D^{1,55} H \cdot F_c$$ F_c=1,00 H = height; ft² D = diameter; ft²
Pumps	30.000,00* *estimated cost

SUSTAINABILITY FUNCTION



$$S = \omega_P P - \omega_{EI} EI$$

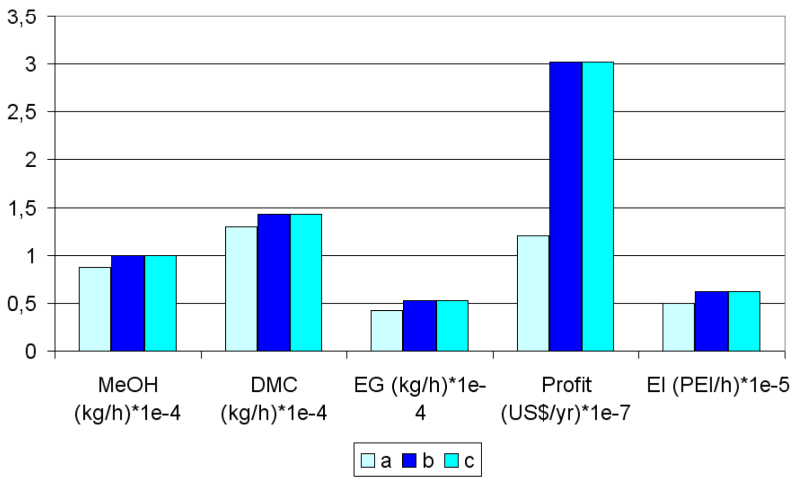
Chosen Impact Potentials are calculated from easily accessible data (LD_{50}, TLV_{50} and LC_{50}).

PROCESS OPTIMIZATION – GATE-TO-GATE

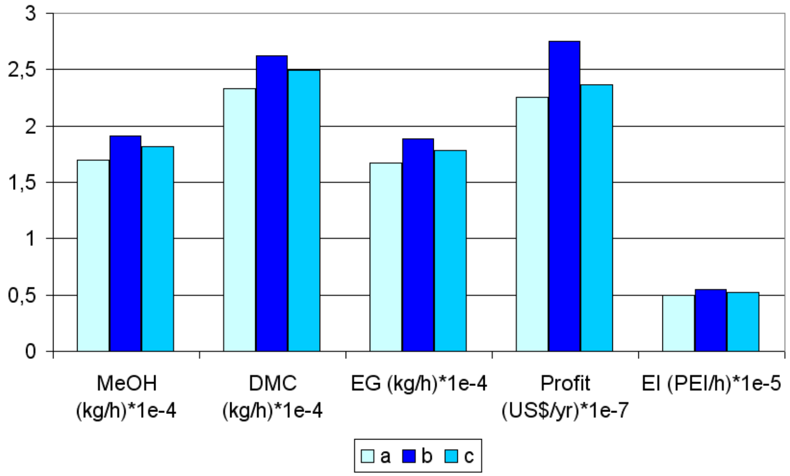
Problem Formulations

- sustainability maximization constrained by maximum EI of 50.000 PEI/h;
- sustainability maximization with ω_I=0 (i.e., profit maximization);
- sustainability unconstrained maximization.

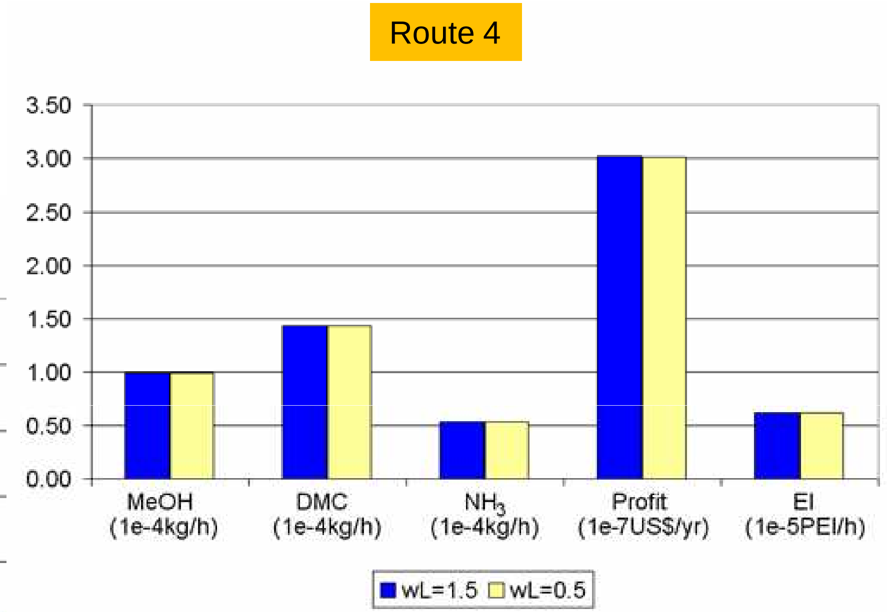
Route 4

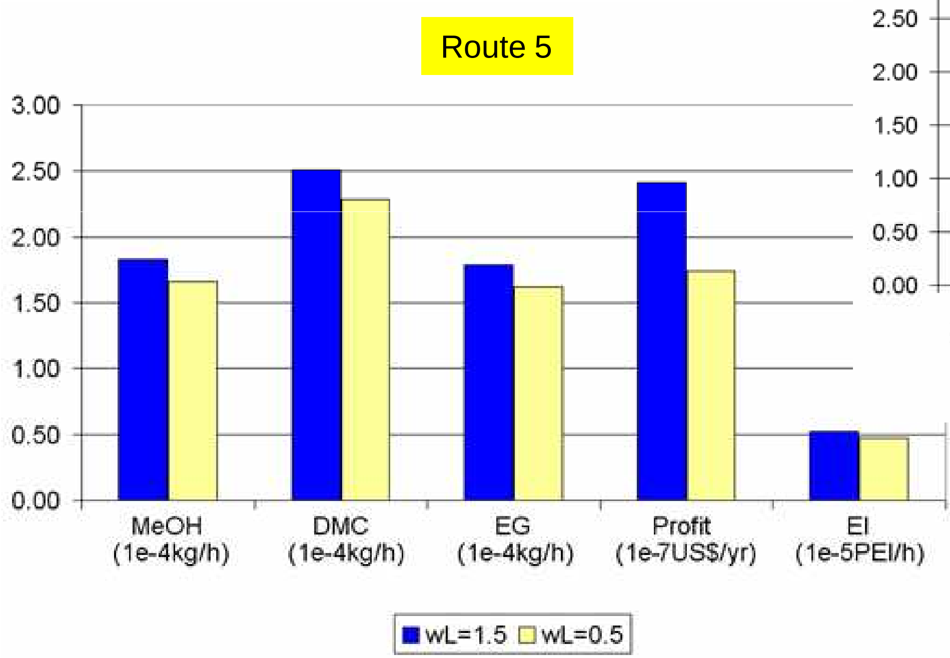


Route 5



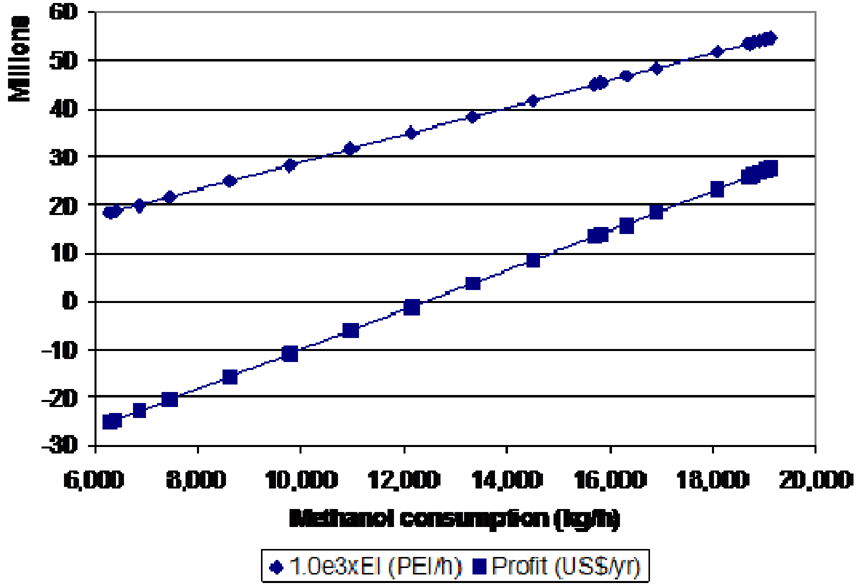
OPTIMIZATION OF SUSTAINABILITY

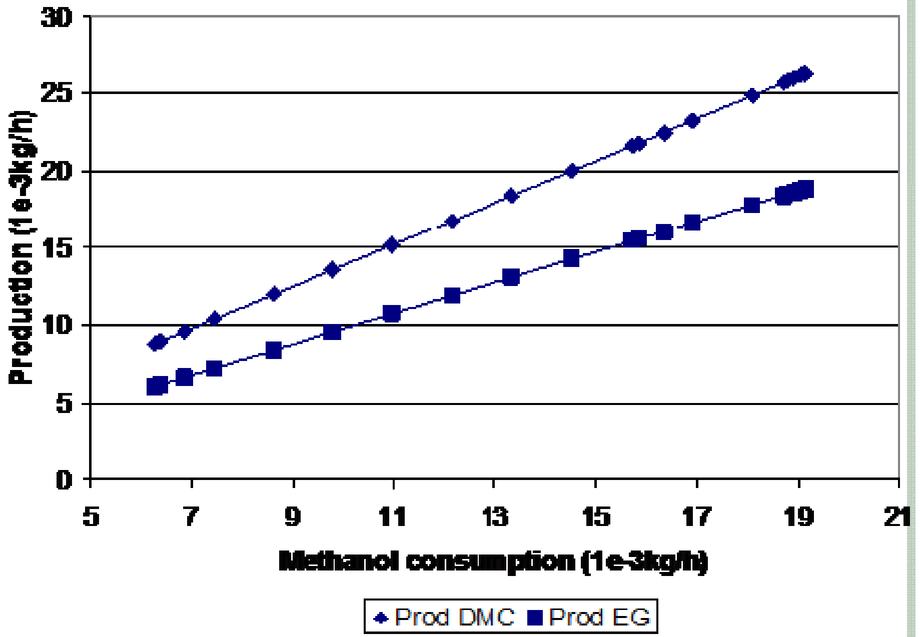


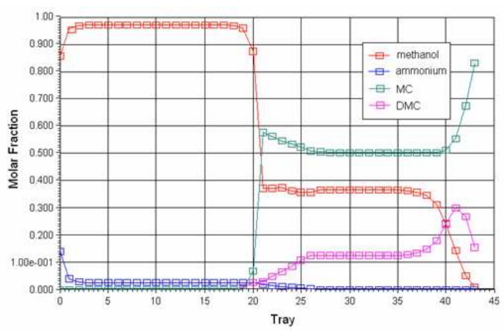


ω_P=1.5 and ω_{EP}=0.5

ROUTE 4 – GATE-TO-GATE

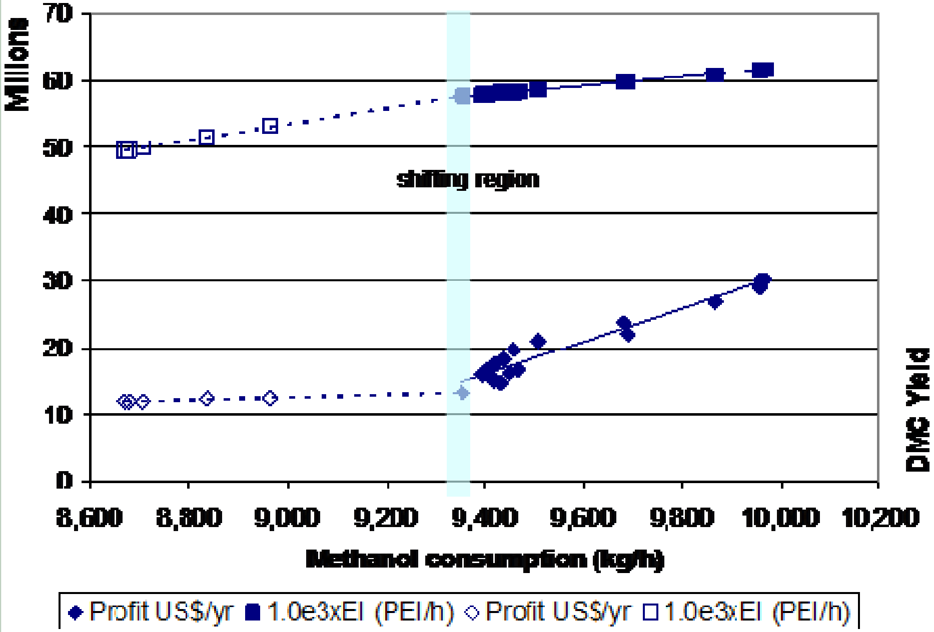


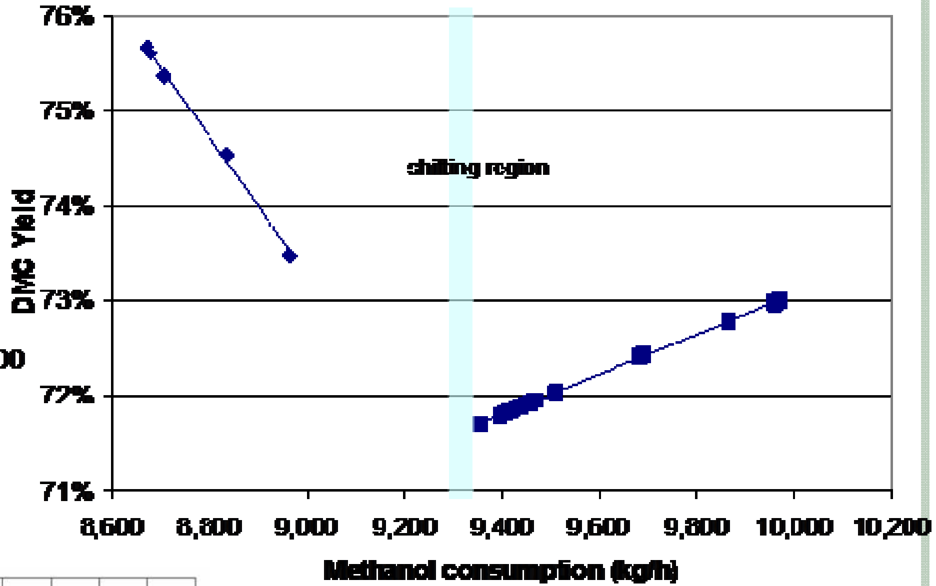


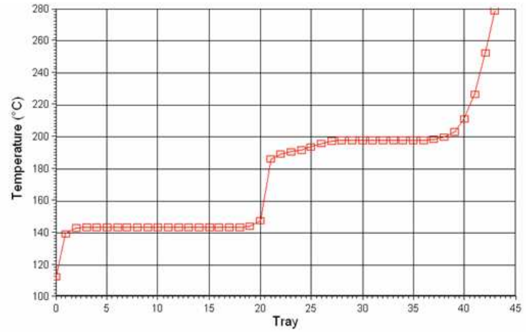


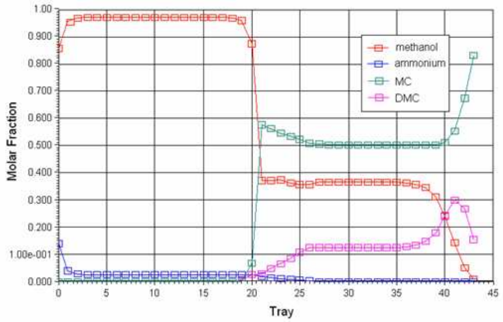
DMC from Urea

ROUTE 5 – GATE-TO-GATE







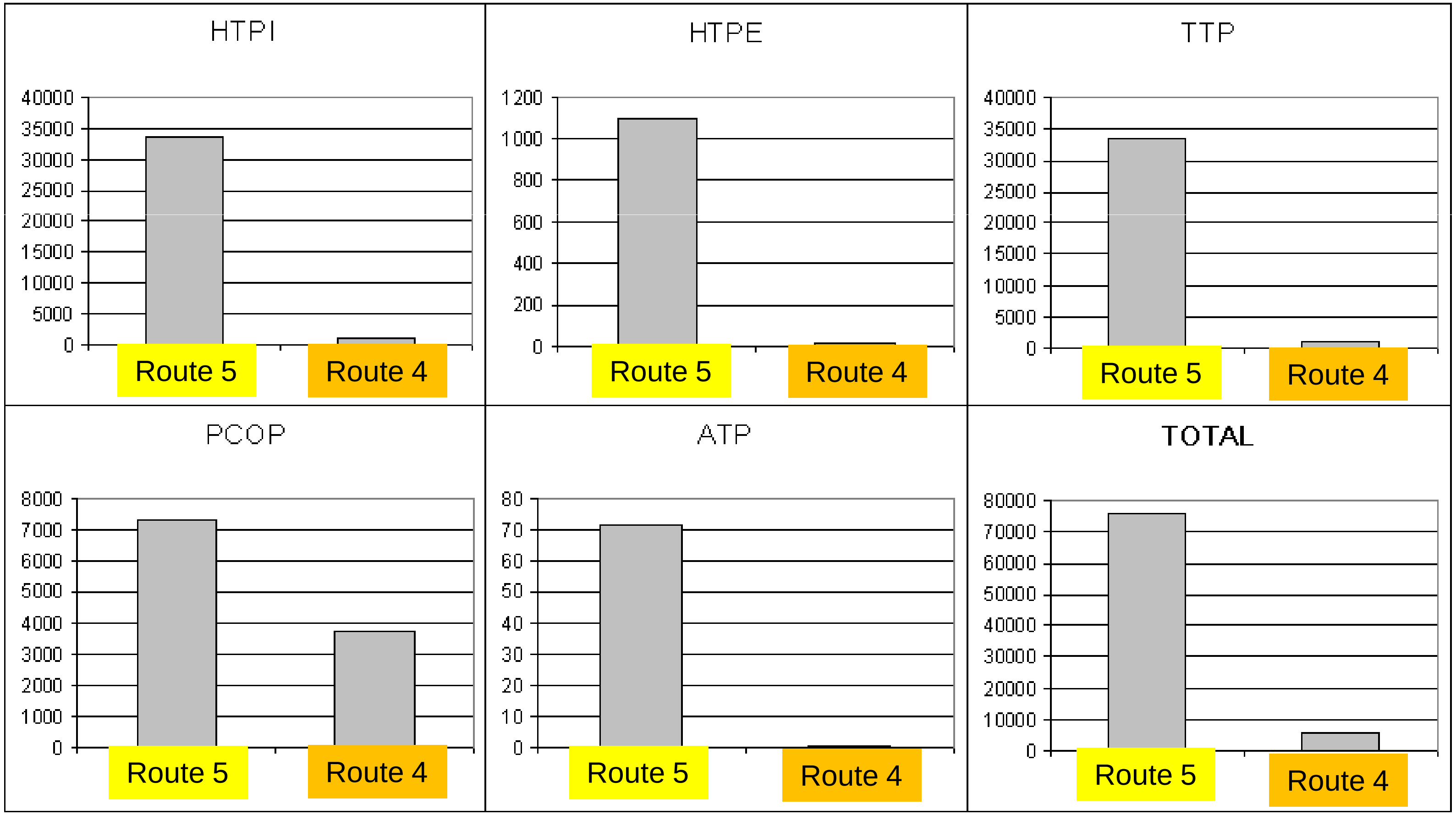


DMC from EO

Reactive Column – Concentration Profile

CRADLE-TO-GATE DOMAIN

Problem Formulation: WAR Algorithm



Route 4 x Route 5

	ROUTE 5	ROUTE 4
EI cradle-to gate	75,600	5,740
EI gate-to gate	50,000	50,000
Profit (M$)	27.26	14.5
ω_P	1	
ω_{EI}	100	
Sustainability (M)	14.7	8.9

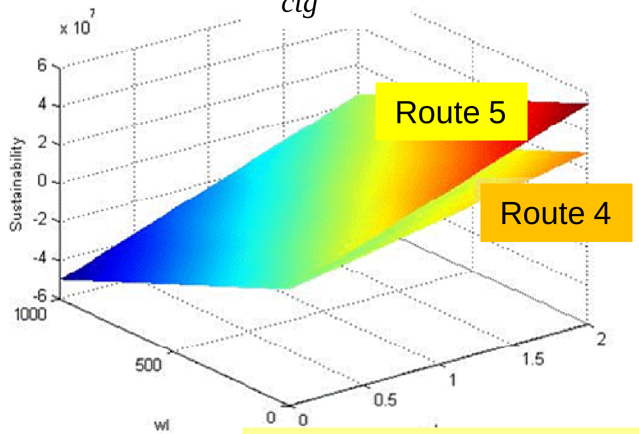
Sensitivity	ROUTE 5		ROUTE A	
	ω_P=1.5	ω_P=0.5	ω_P=1.5	ω_P=0.5
EI	0.66%	-8.48%	0.006%	0.003%
Profit	2.18%	-26.30%	0.013%	-0.031%

$$\sigma = \frac{f(\omega_P = 1)}{f(\omega_P = k) - f(\omega_P = 1)}$$

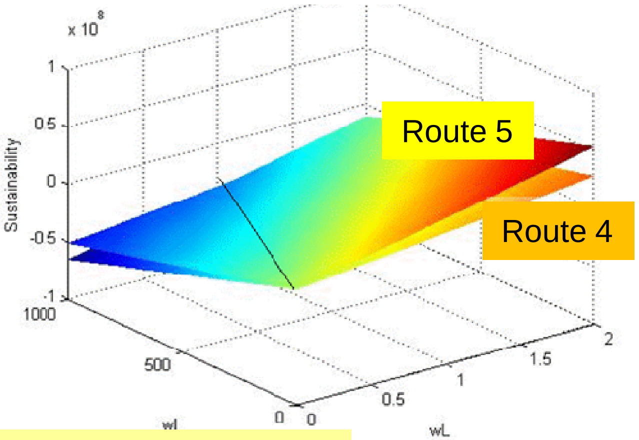
Function	Importance grade		
	Low	Normal	High
EI	$0 \le \omega_{EI} < 500$	$500 \le \omega_{EI} < 1000$	$\omega_{EI} \ge 1000$
P	$0 \le \omega_P < 0.75$	$0.75 \le \omega_P < 1.25$	$\omega_P \ge 1.25$

Route 4 x Route 5

$\omega_{ctg} = 0$

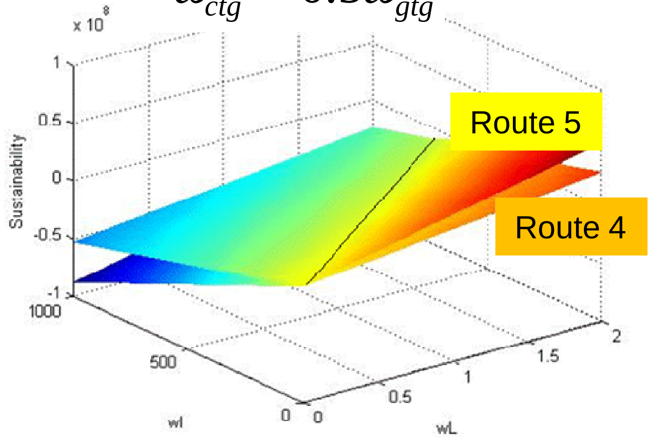


$\omega_{ctg} = 0.2\omega_{gtg}$



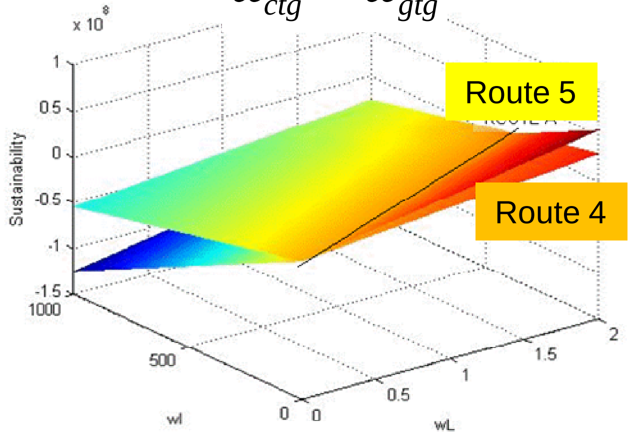
$$S_i = \omega_P P_i - \omega_{EI} EI_i - \omega_{ctg} EI_{i,ctg}$$

$\omega_{ctg} = 0.5\omega_{gtg}$



(c)

$\omega_{ctg} = \omega_{gtg}$



(d)

Route 4 x Route 5

CO_2 Mass Balance in Cradle-to-Gate Domain

Route	CO_2 mass flow (kg/h)		
	Inlet	Outlet	Sequestration
5	16,161	4,165	11,996
4	8,468	1,952	6,517

Additional Sustainability Metrics

Metric	**EI_{max}=50,000**	
	ROUTE 5	**ROUTE 4**
M (kg/kg)	1.30	0.97
E (kJ/kg)	225,114	104,128
ec (US$/h)	22.198	9,136
en (PEI_{out}/h)	50,000	50,000
ε (US$/$PEI_{out}$)	0.44	0.18

CONCLUDING REMARKS

- P2 was introduced as the basis for **GC** and **GE**
- Sustainability Metrics were presented for screening Process Alternatives
- A CASE STUDY was used to illustrate the Selection of the best ROUTE among process alternatives.
- An Exploratory Metric was first used to reduce the candidate processes.
- For the 2 most promising alternatives (ROUTES 4 and 5), process simulation and optimization in HYSYS was employed for SUSTAINABILITY ANALYSIS.
- CRADLE-TO-GATE and GATE-TO-GATE domains for each routes were defined.
- A sensitivity analysis was used to stress the impact of the “degree of relevance” attributed to a given metric and/or domain.
- Sustainability metrics show that ROUTE 5 has better Ecoefficiency and Material index. In contrast, ROUTE 4 has better Energy index. The EI of cradle-to-gate domain (global impact) of ROUTE 5 is around 12
- The simultaneous consideration of the two domains reveals that the choice of the better route depends on the aspects that are being prioritized. In general, profit and local impact should be given priority. If this rule is applied, then ROUTE 5 is the most sustainable.