Evaluating Indicators and Life Cycle Inventories for Processes in Early Stages of Technical Readiness

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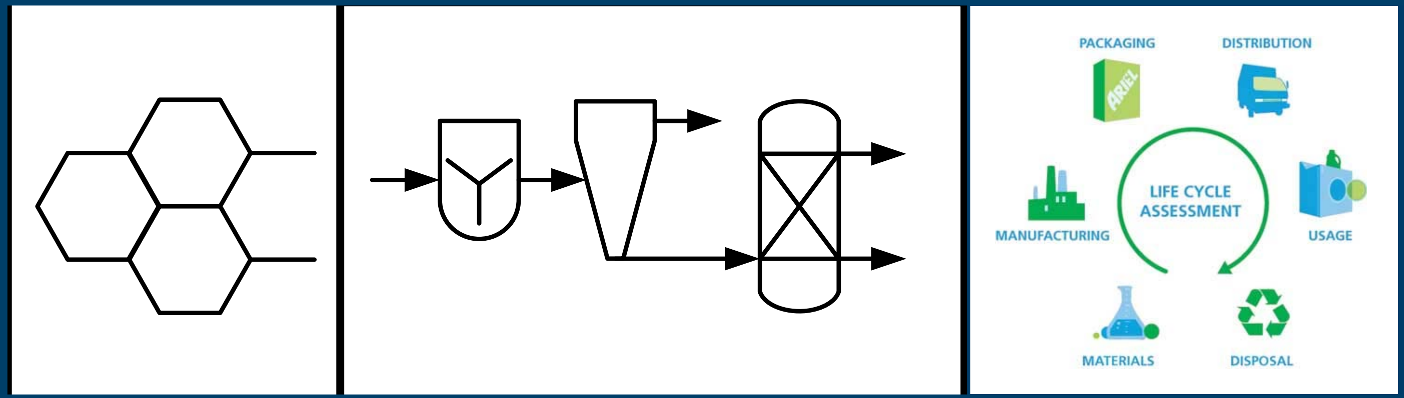

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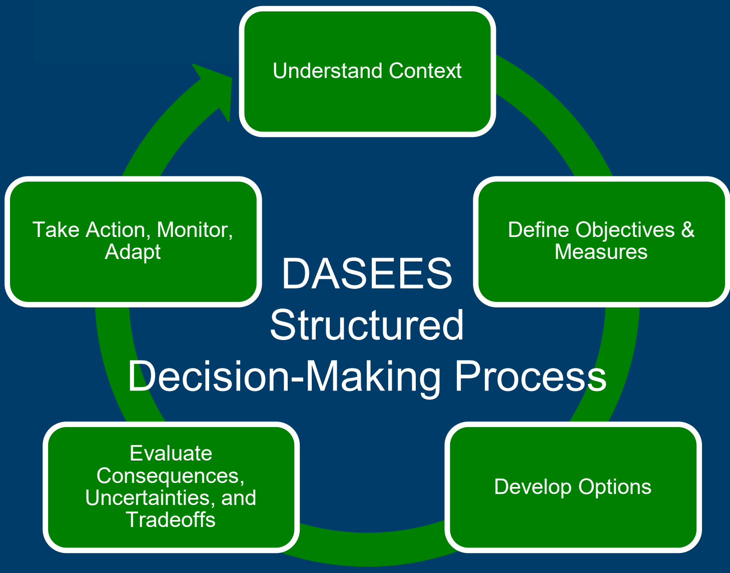
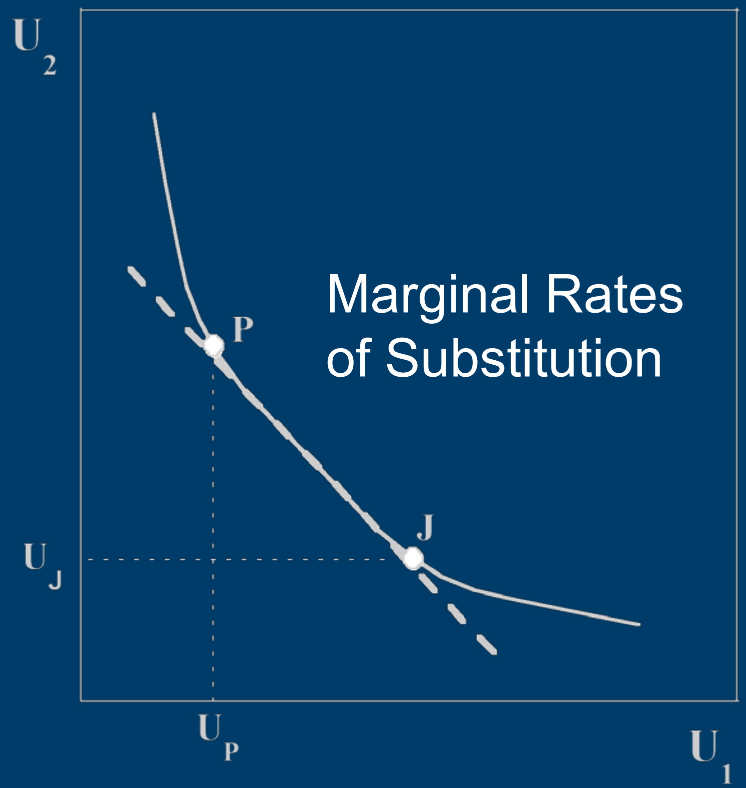
Motivation: Decision Making





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Cost Benefit Analysis

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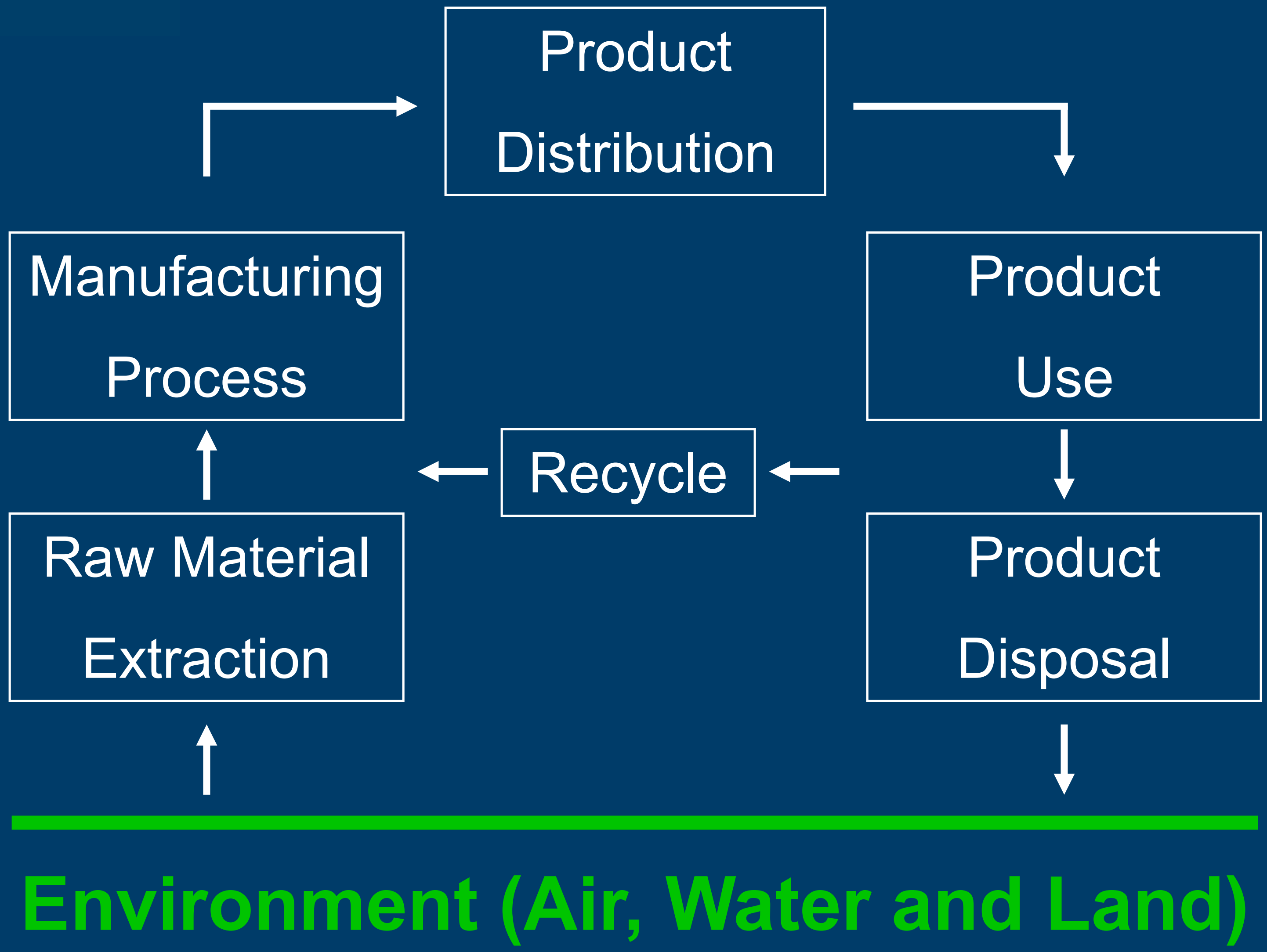
Numerical Methods

- Pareto fronts
- Optimization with constraints
- Heuristics

Motivation: Life Cycle Assessment



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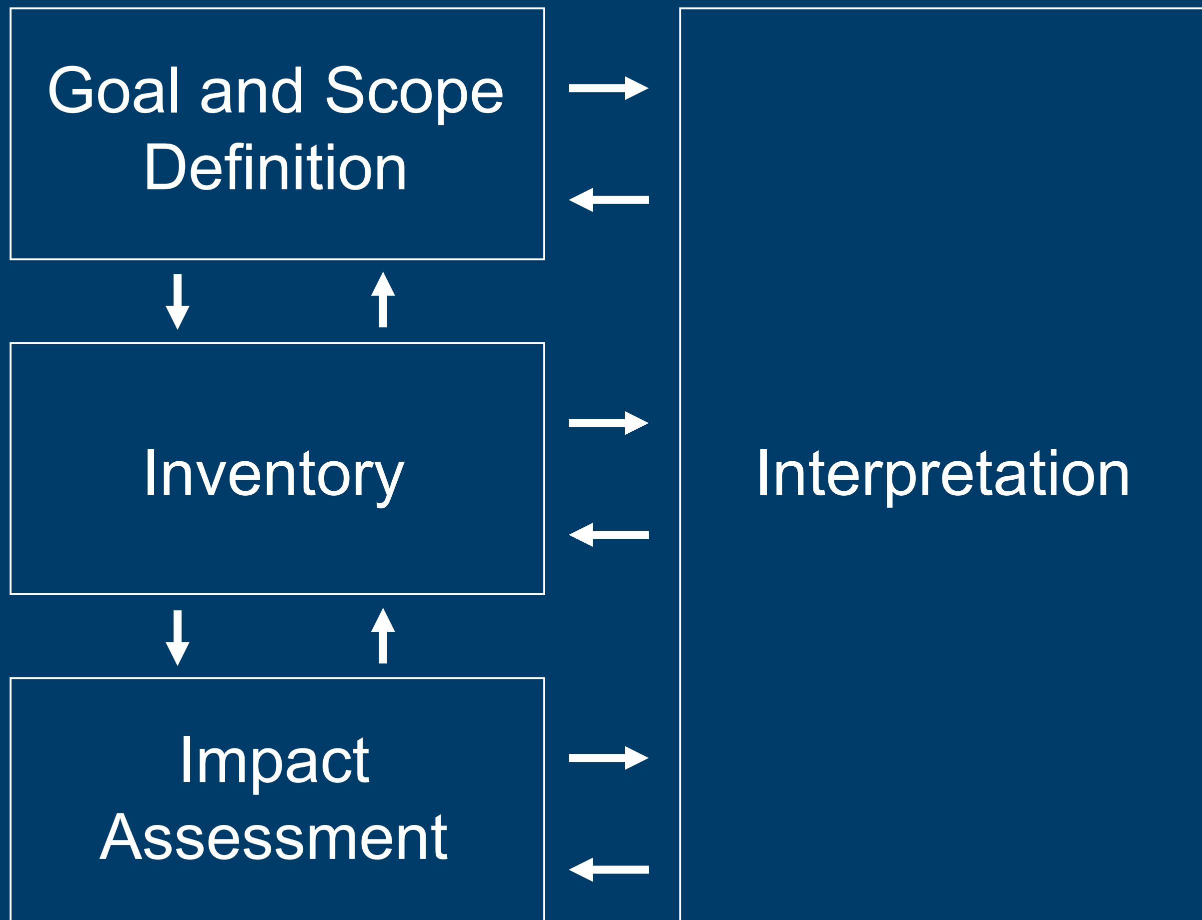
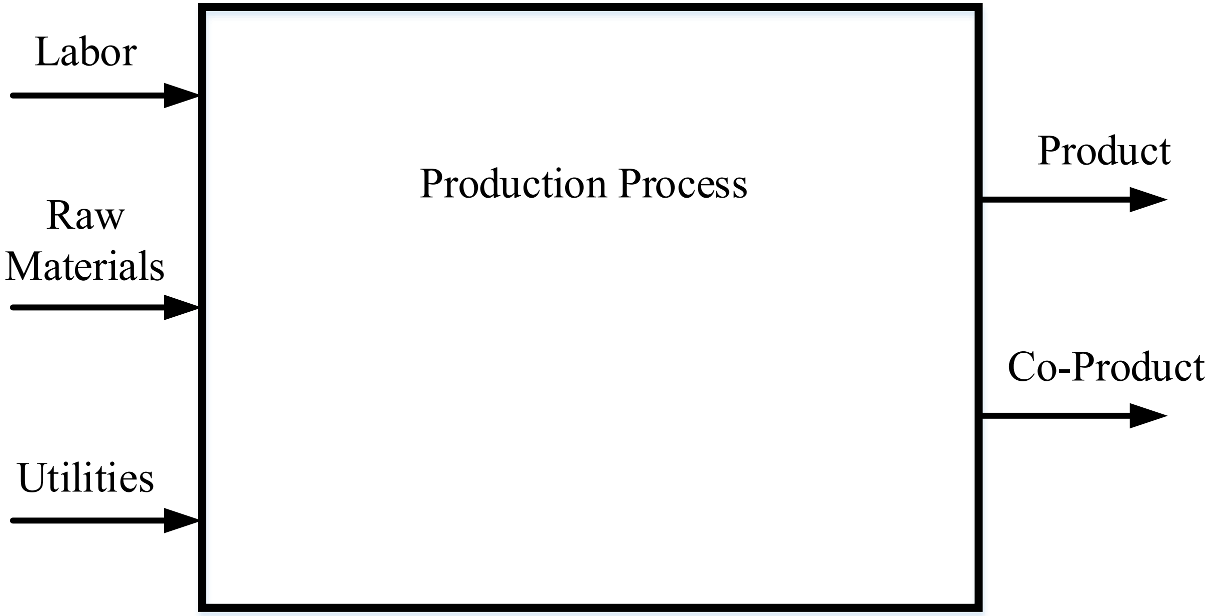
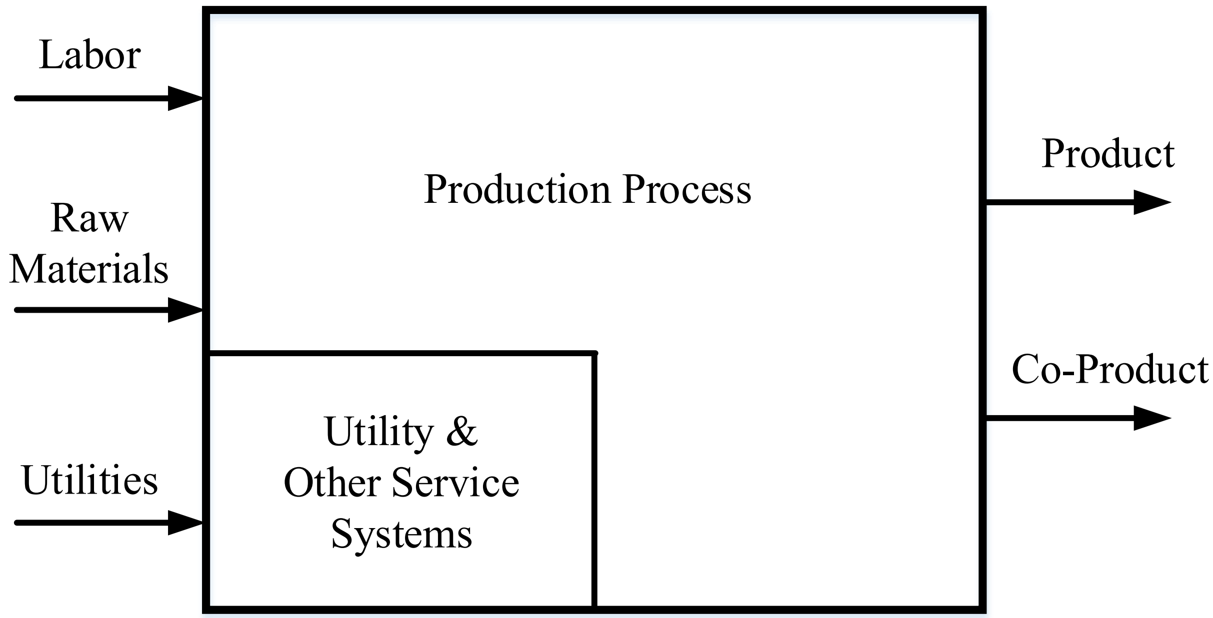
Life Cycle Assessment



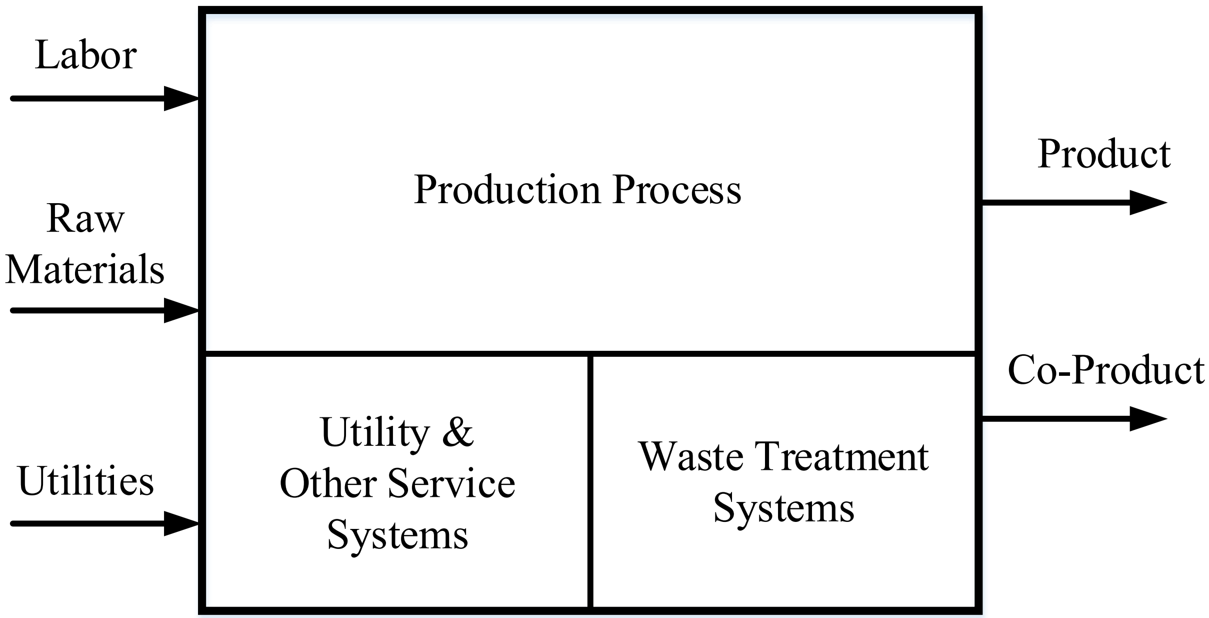
Process Model



Process Model



Process Model



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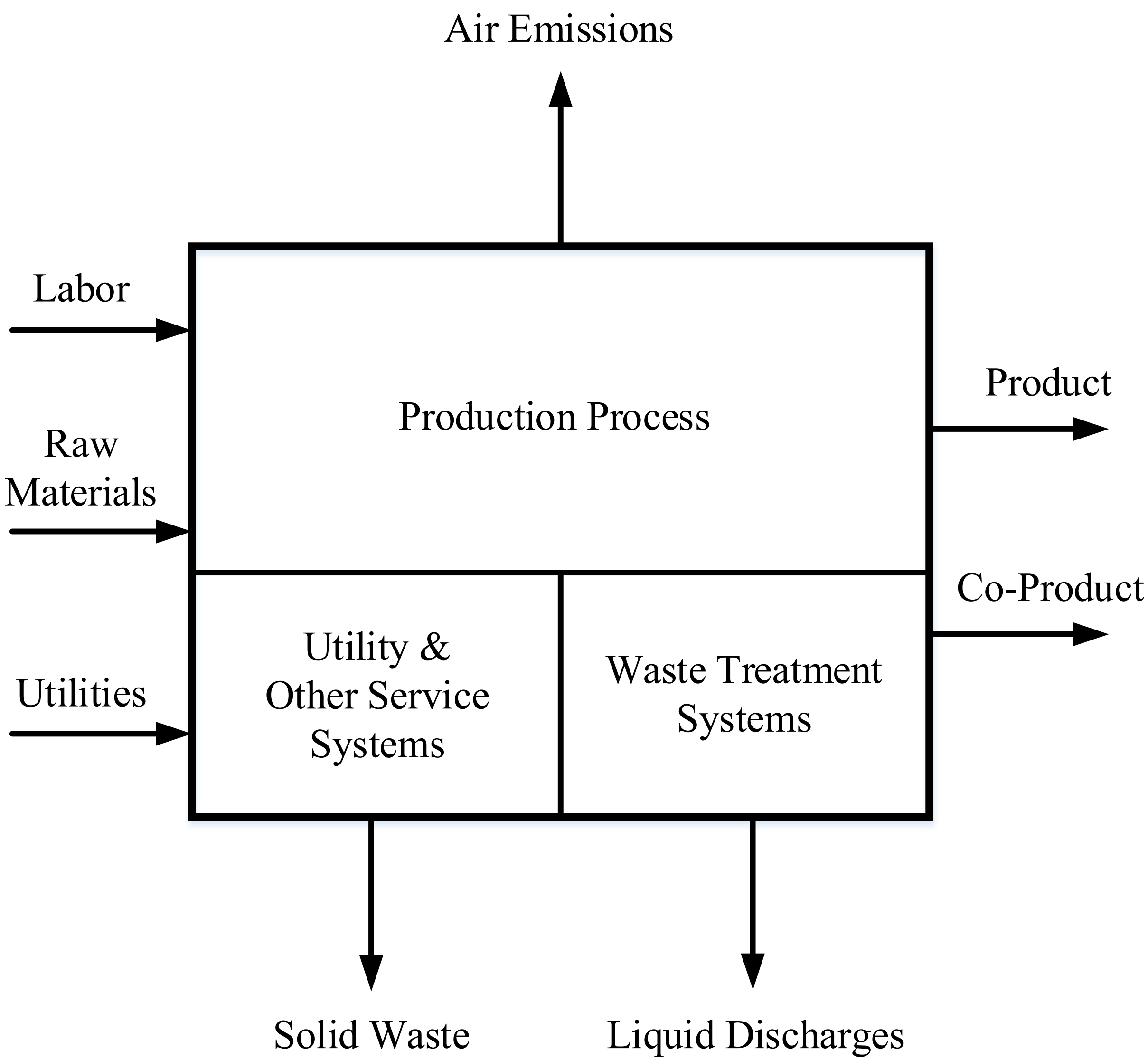
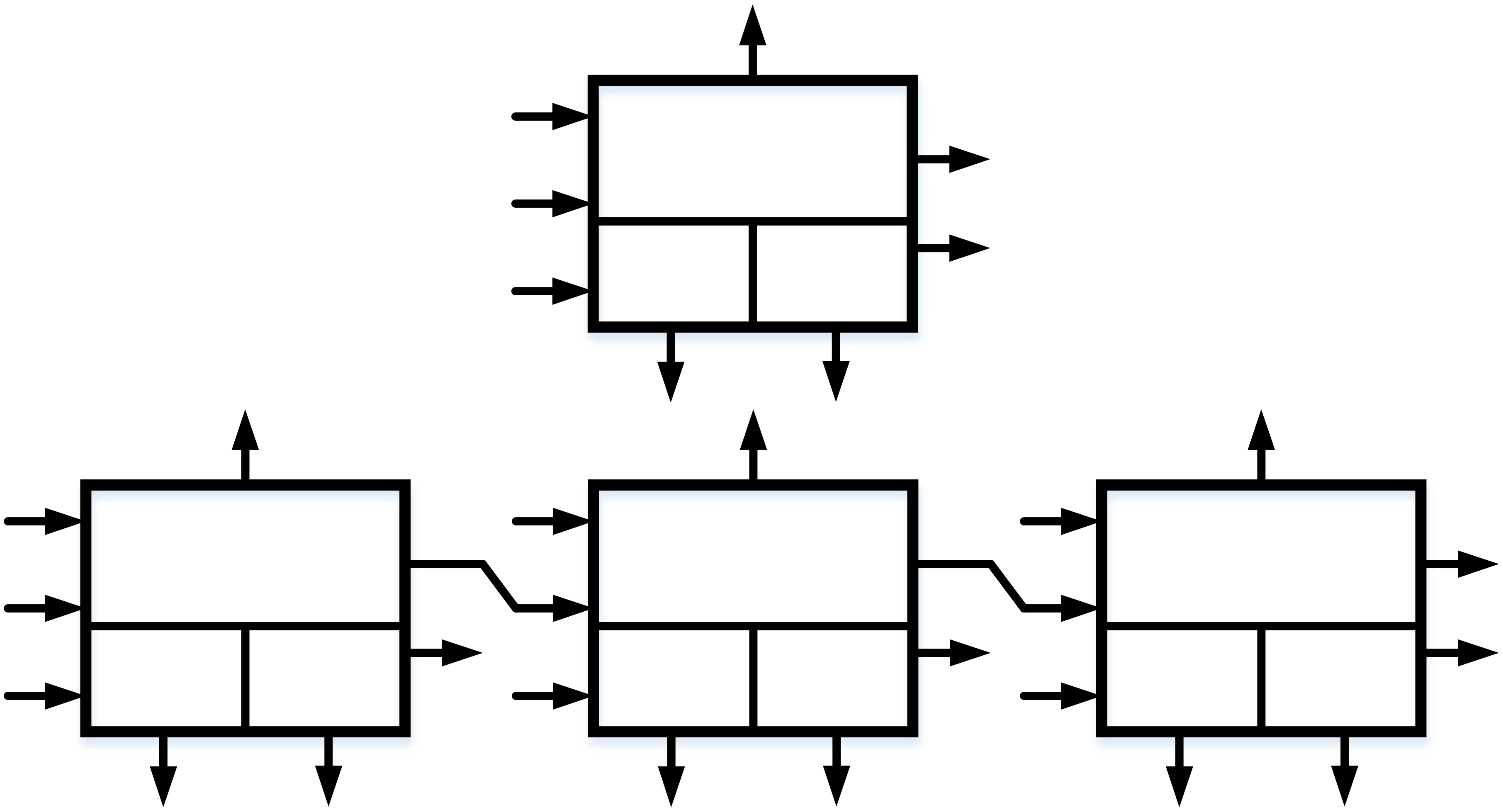
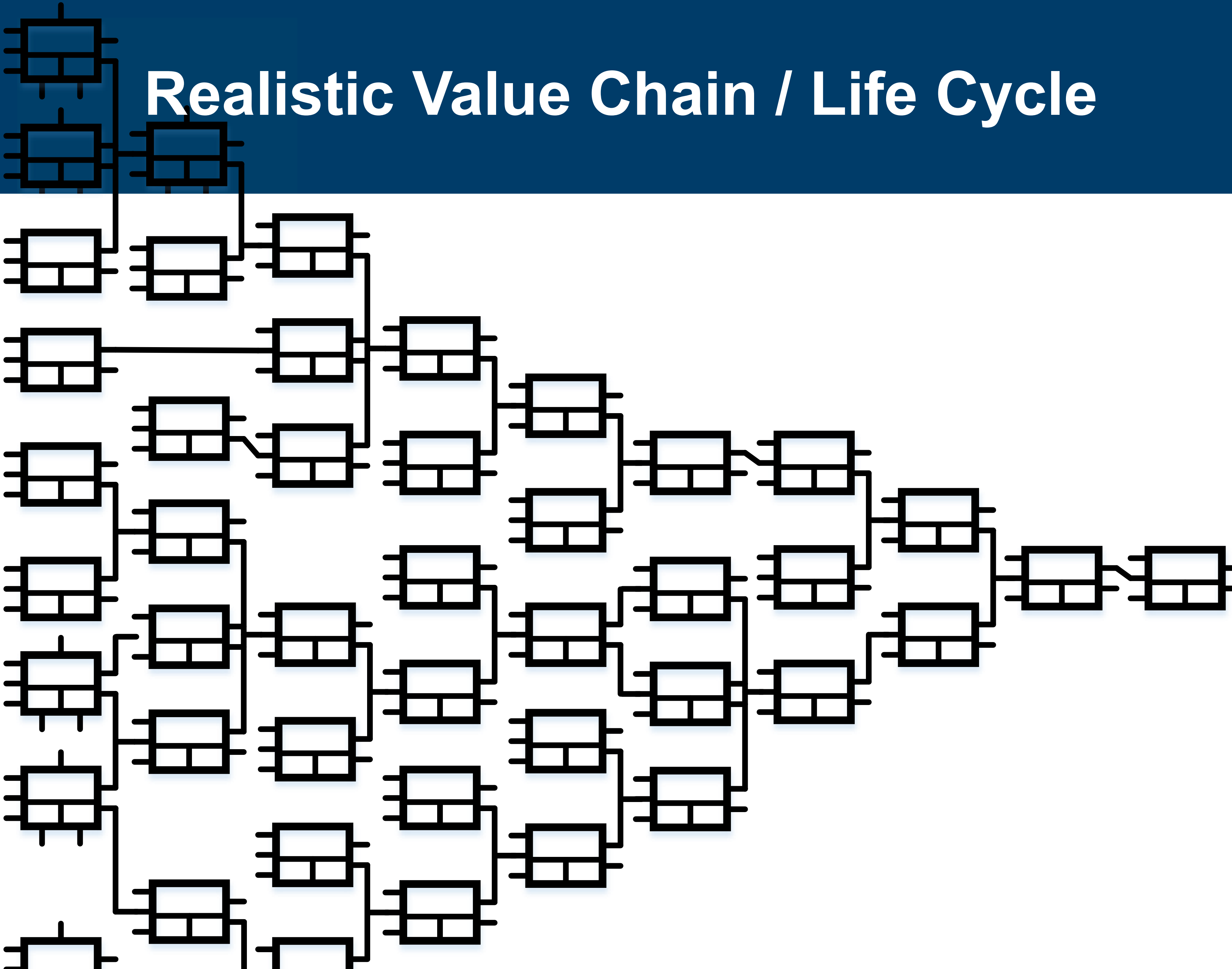


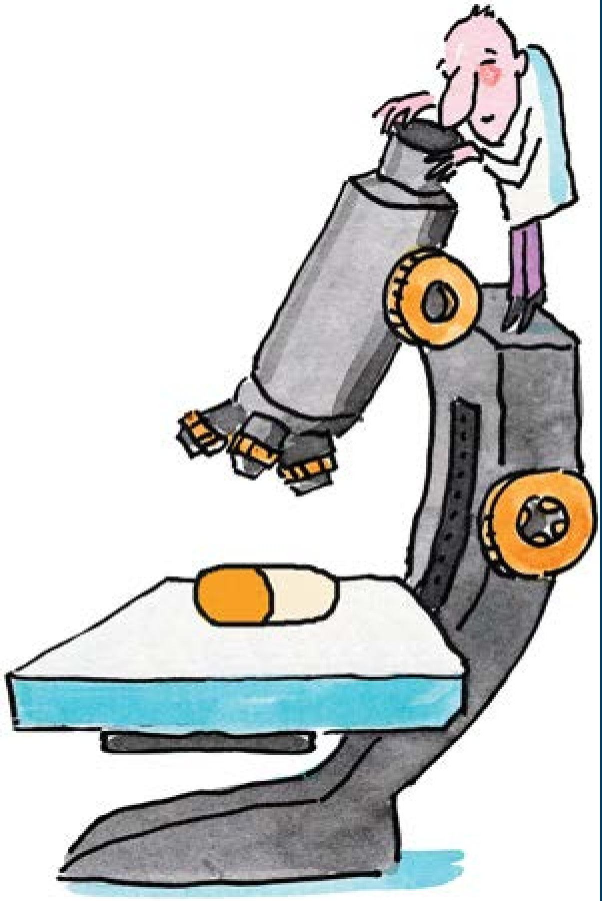
Process Model in the Value Chain



Realistic Value Chain / Life Cycle



GREENSCOPE Tool



Gauging Reaction Effectiveness for ENvironmental Sustainability of Chemistries with a multi-Objective Process Evaluator

GREENSCOPE Tool

- Spreadsheet and online software tool, capable of calculating ~140 different indicators.
- User can choose which indicators to calculate.
- User can redefine absolute limits to fit circumstances.

Sustainability Framework

Identification and selection of two reference states for each sustainability indicator:

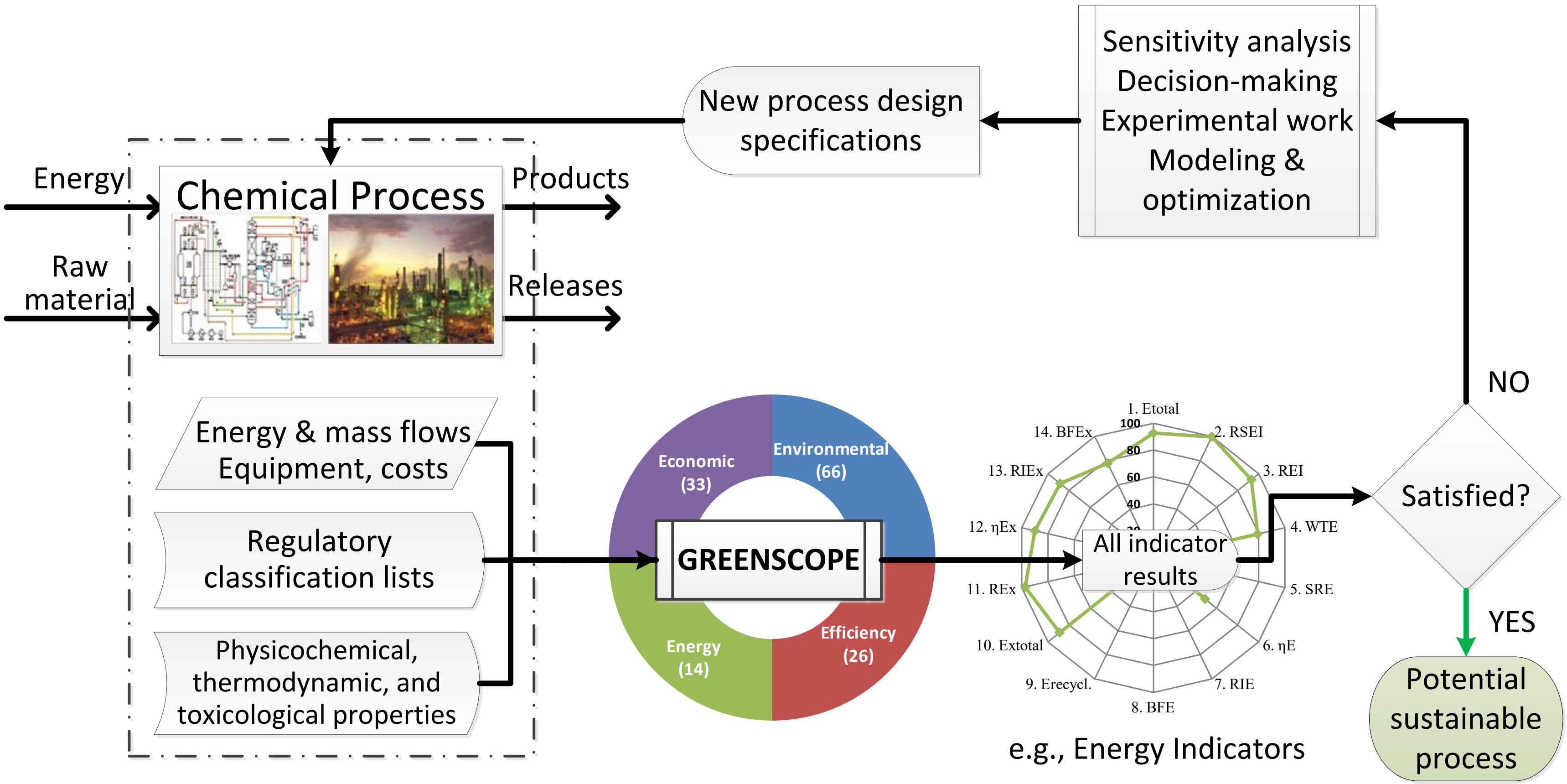
- Best target: 100% of sustainability
- Worst-case: 0% of sustainability

Two scenarios for normalizing the indicators on a realistic measurement scale

Dimensionless scale for evaluating a current process or tracking modifications/designs of a new (part of a) process

$$\text{Percent Score} = \%G_i = \frac{(\text{Actual-Worst})}{(\text{Best-Worst})} \times 100\%$$

Using GREENSCOPE



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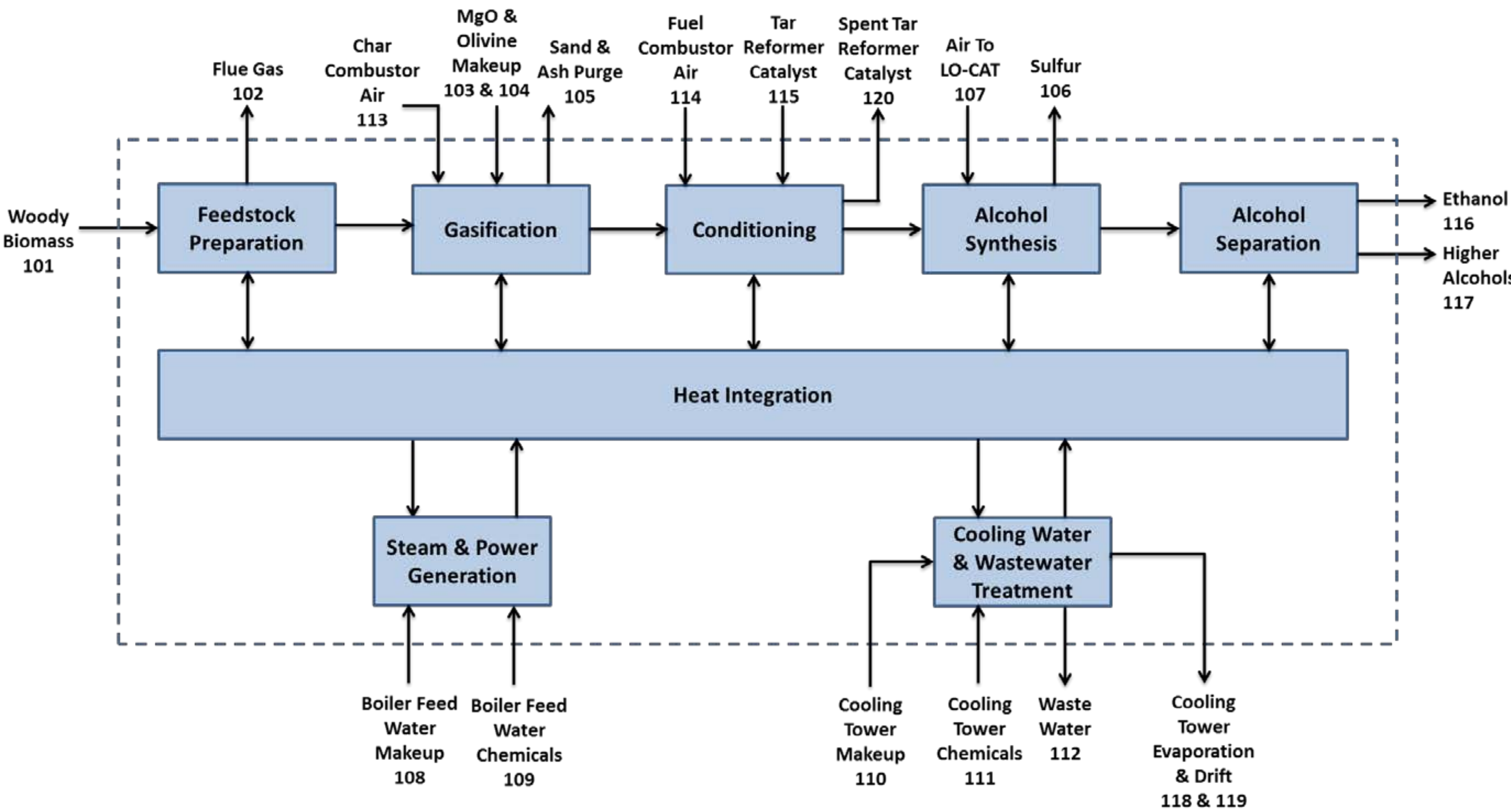
Early Stage Processes

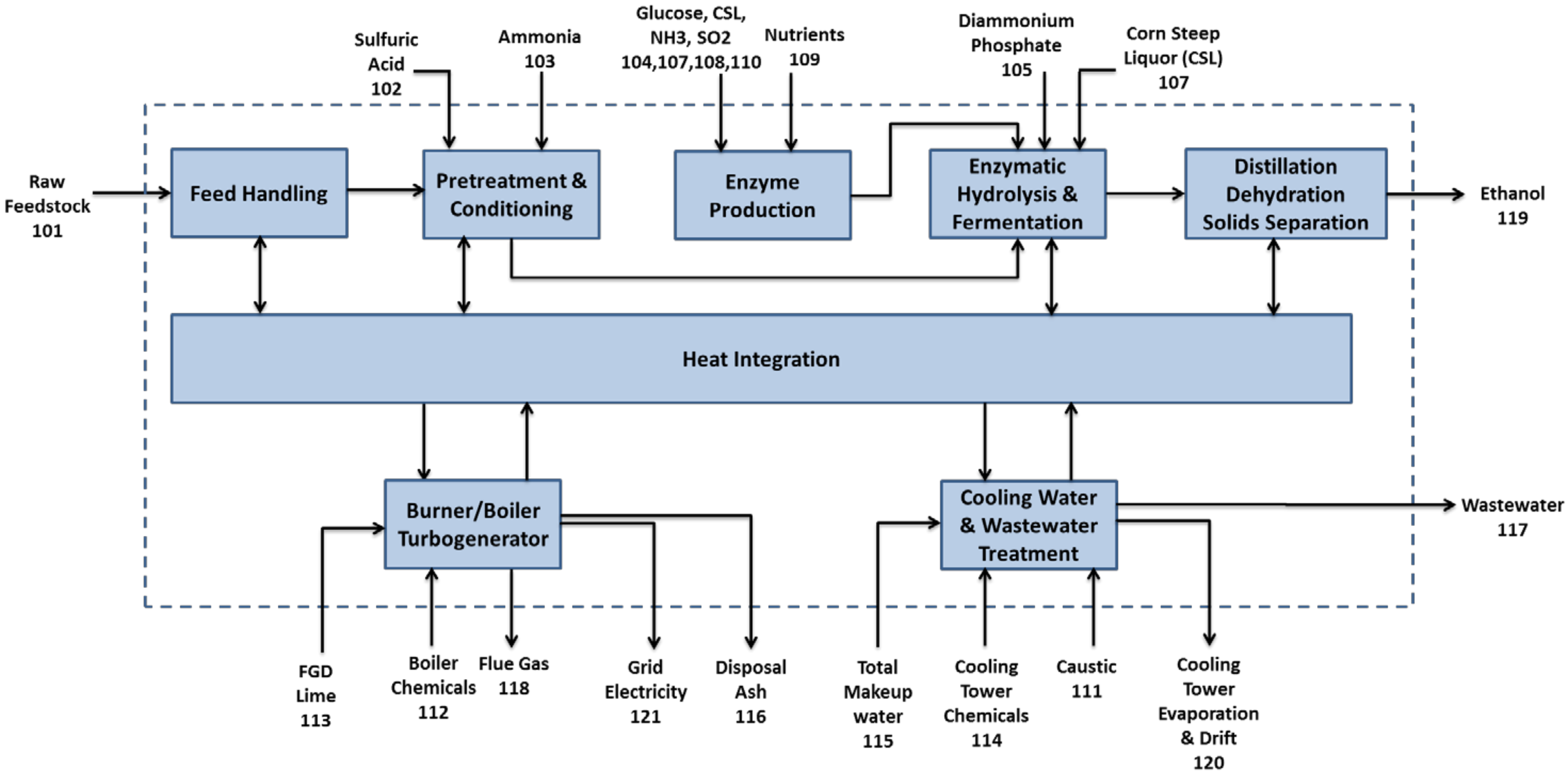
Two conversion pathways for producing cellulosic ethanol from biomass, via thermochemical and biochemical routes (NREL's 2011 design reports).

Thermochemical Conversion Pathway



Dutta A. et al, Process Design and Economics for Conversion of Lignocellulosic Biomass to Ethanol: Thermochemical... NREL, 2011 Report No. TP-5100-51400

Biochemical Conversion Pathway



Humbird D. et al, Process Design and Economics for Biochemical Conversion of Lignocellulosic Biomass to Ethanol... NREL, 2011 Report No. TP-5100-47764

Storage Emissions

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Working losses from filling and emptying liquid tanks

$$L_W = \frac{\dot{V}}{22.4}\left(\frac{273.15}{T}\right)\left(\frac{P_i^{sat}}{760}\right)(MW)K_N K_P$$

Breathing losses from daily fluctuations in temperature

$$L_B = 16.3 V_V \left(\frac{273.15}{T}\right)\left(\frac{P_i^{sat}}{760}\right)(MW)\left(\frac{T_R}{T}\right)$$

U.S. EPA (2016) *AP-42*, Ch. 7; Peress, J. (2001) *CEP*, Aug. 44-45

Process Vent Emissions

Non-condensable gases exiting vents (*F*) take evaporated liquids with them (*kA*),

$$S_i = \frac{P_i^b}{x_i \gamma_i P_i^{sat}} = \frac{k_i A}{k_i A + F}$$

S describes the approach to vapor-liquid equilibrium. The emissions are described by,

$$E_i = \frac{F x_i \gamma_i P_i^{sat}}{RT} S_i (MW_i)$$

U.S. EPA (1994) *Hdbk Control Techniques for Fugitive VOC Emissions...*; Hatfield, J.A. (2004) *Env. Prog.*, 23, 45

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Fugitive Emissions

Calculate fugitive emissions based on stream compositions and number of sources for each unit operation,

Equipment Type	Service	Emission Factor (kg/h/source)
Pumps	Light liquid	0.0199
	Heavy liquid	0.00862
Compressors	Gas	0.228
Valves	Gas	0.00597
	Light liquid	0.00403
	Heavy liquid	0.00023
Connectors (e.g., flanges)	All	0.00183
Open-ended lines	All	0.0017
Sampling connections	All	0.0150
Pressure relief valves	Gas	0.104

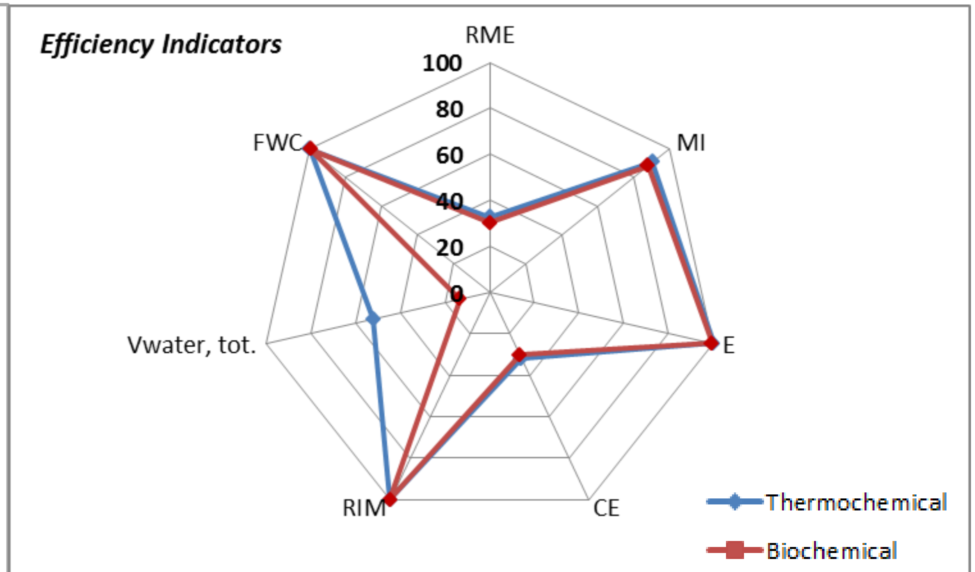
Synthetic Org. Chem. Mfg. Ind., U.S. EPA (1995) *Protocol for Equipment Leak Emission Estimates*

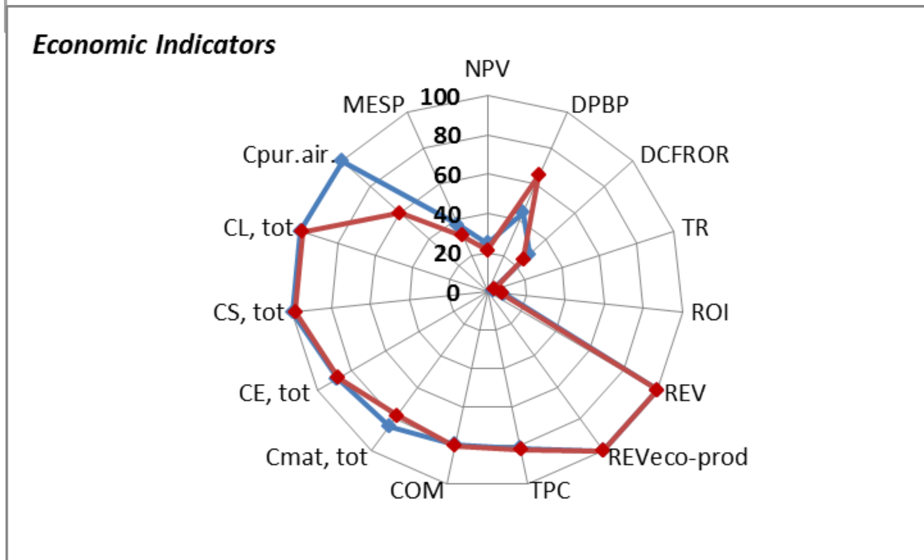
Life Cycle Gate-to-Gate Emissions

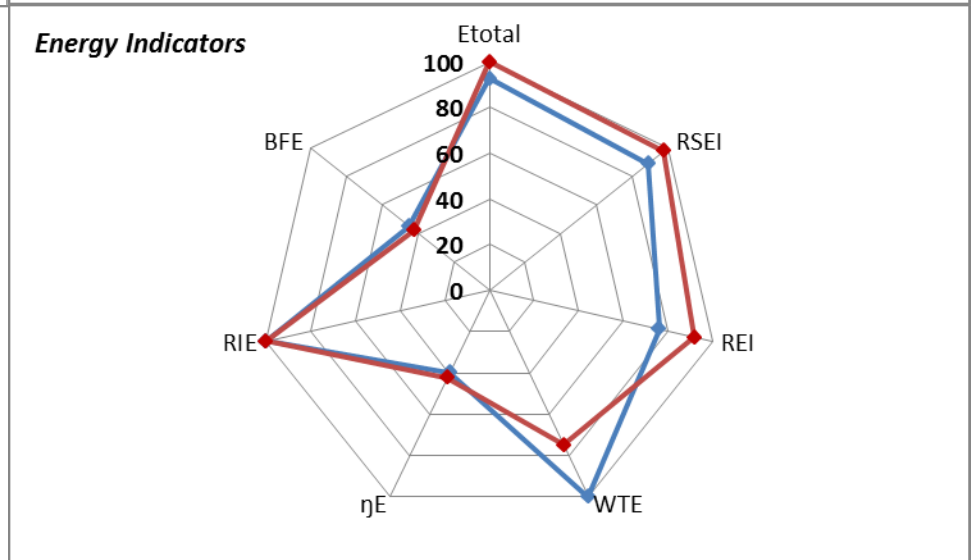
LCI Outputs	Thermochemical			Biochemical		
(kg/kg Alcohol Product)	Fugitive	Storage	Vents	Fugitive	Storage	Vents
Acetic Acid	4.40E-07			6.25E-07		
Ammonia	6.38E-06			7.36E-06		
Benzene	1.23E-07			0		
Carbon Dioxide	8.81E-06		4.16E+00	0		3.39E+00
Carbon Monoxide	1.86E-05			0		2.86E-03
Ethanol	8.99E-05	2.30E-05		1.05E-04	1.98E-05	
Ethylene	1.52E-06			0		
Furfurals	1.30E-06			1.76E-06		
Methane	4.00E-06			1.00E-06		
Methanol	1.74E-06			0		
NOx	0		1.23E-03	0		2.86E-03
SOx	1.89E-06		5.27E-04	2.20E-06		2.48E-03
Sulfuric Acid	1.68E-05			1.97E-05		

Incorporating Sustainability into Process Design Development Using GREENSCOPE Methodology

- (Efficiency) The total water consumption score for TC is much better than BC.
- (Energy) The waste treatment energy score for TC is better than BC.
- (Energy) The total energy use and energy intensity scores are better for BC than TC.
- (Economics) The cost of purifying air score is much better for TC than BC.
- (Economics) The Discounted Payback Period score is much better for BC than TC.
- (Economics) The cost of materials score is a bit better for TC than BC.







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Summary

Analyses provide indicators for processes and life cycle inventories on gate-to-gate basis

Indicators allow direct comparison of different kinds of processes, even at early stages of development

Life cycle inventories are improved over common methods with incorporation of fugitive, storage, and vent emissions