GREENSCOPE: A Tool for Chemical Process Sustainability Assessment and Design

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What is GREENSCOPE?

- Foundations
- Quantification of Sustainability for Chemical Processes
- Methodology
  - Taxonomy
  - Data Needs
- Application
- Tool
  - Excel®
  - Java
- Global Sustainability Assessment
- Conclusions

Motivation

The finite availability and accelerated depletion of ecological goods and services: The role of the chemical Industry

- ✓ Fundamental business sector for the global economy and society's quality of life
- ✓ 5% of the U.S. nominal gross domestic product
- ✓ directly employs ≅ 800,000 people nationwide
- ✓ 11% of all U.S. patents /yr
- ✓ 96% of all final goods are directly influenced

- Exposure of workers to toxic and carcinogenic substances
- Water pollution, air emissions and solid waste
- Product use impacts: e.g., agrochemicals, fossil fuels
- Disposal impacts: e.g., flame retardant substances, paint pigments
- 6% of the total U.S. energy consumption

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Sustainability for Chemical Processes

- Guidelines to achieve quality of life improvements
  - without affecting the availability of ecological goods & services
  - for new and existing manufacturing processes
- Address and assess environmental, social, and economic aspects that may be affected by industry
  - identify which system components are affected
  - localize process and product aspects which generate them
  - redesign relevant processes and products
  - demonstrate system improvements
- Minimize or eliminate the environmental impacts and maximizing the social/economic benefits

Quantitative Sustainability Assessment

Green objectives
- Green Chem. principles
- Green Eng. principles

→

GREENSCOPE
- Sustainability indicators
- Dimensionless scale

→

Sustainability indicator results
- Trends
- Clear visualization

→

Potential sustainable process

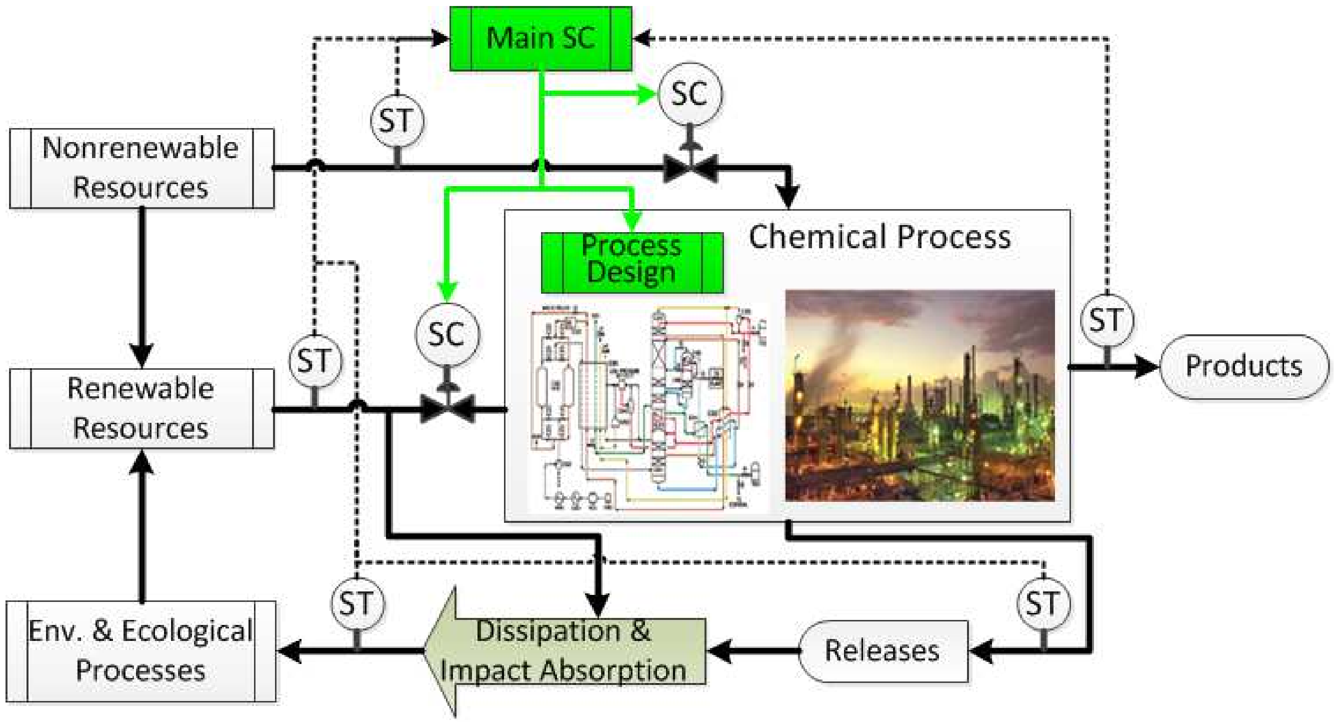
Qualitative Approaches
Apply all of them?
Levels of implementation?
A "win-win" situation?
Multiobjective function

Quantitative Approaches
Is this a sustainable process?
How sustainable is it?
Realistic limitations
Scale for measuring sustainability

Sustainability Criteria
Process areas for improvements
Identification of key factors (SA)
Multi-criteria decision making
Optimal tradeoff

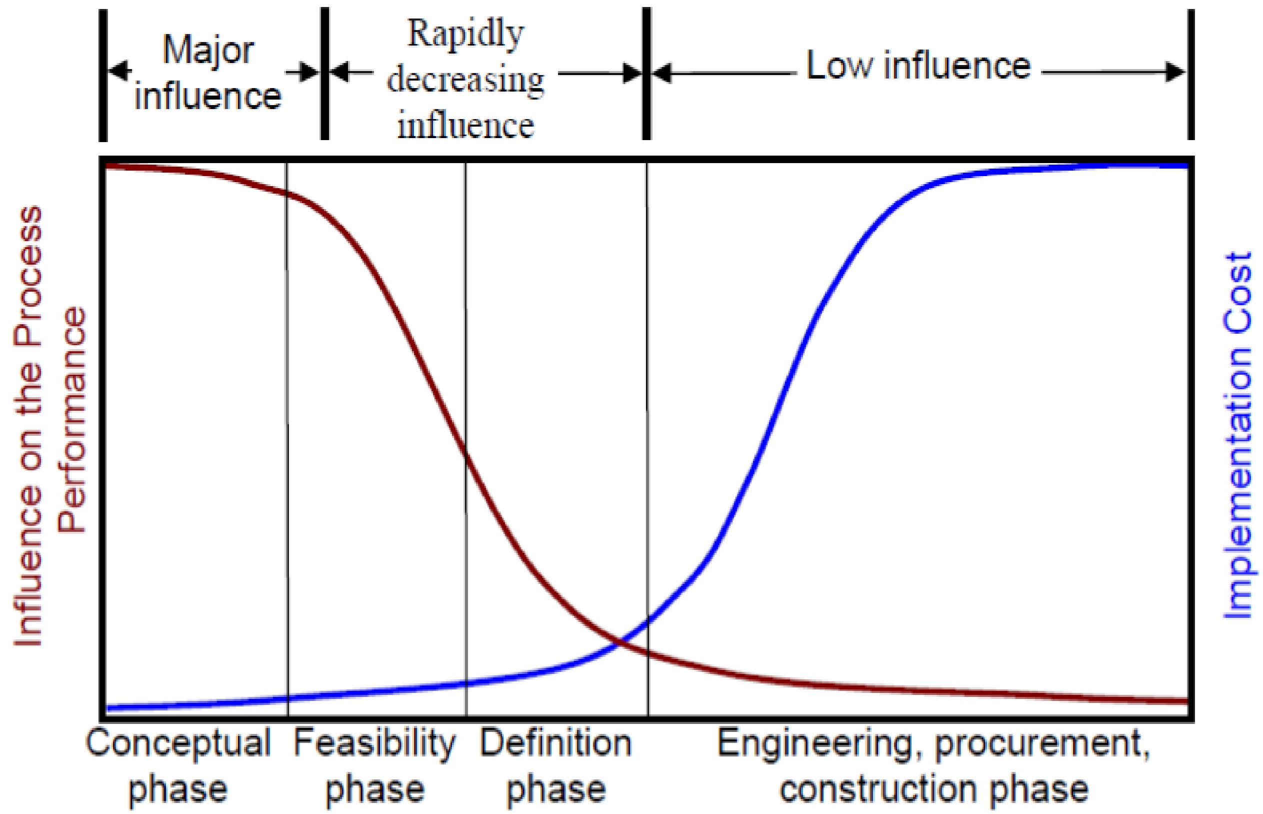
- From qualitative to quantitative
- Improvements achieved in one area may simultaneously affect other areas negatively
- A more sustainable process is the result of an optimal tradeoff

Sustainable Process Design Procedure



- Support decision-makers to determine whether a process is becoming more or less sustainable
  - Are we doing relatively good / bad?
- What benchmarks to use?
- How close are we to achieving absolute targets?

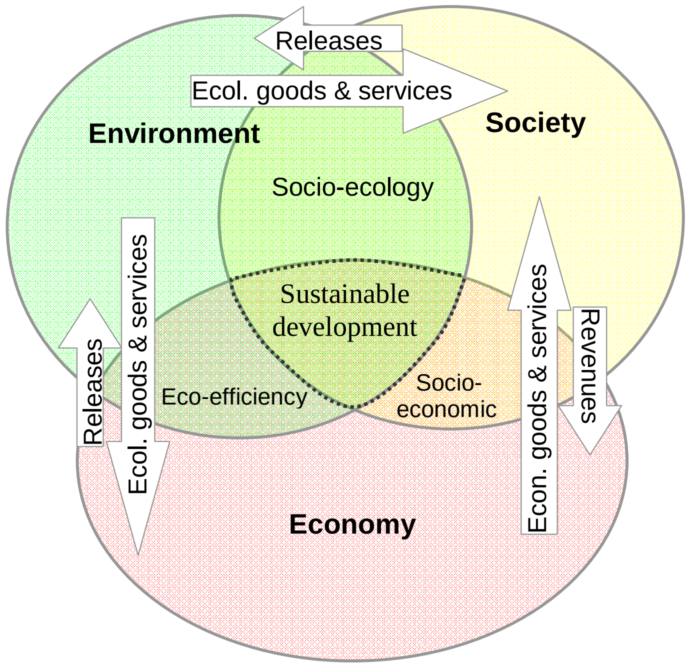
Sustainability & Process Design



Specific process changes to improve sustainability at early design stages will have greater potential influence on the sustainability of the process during operation

Taxonomy of Chemical Process Indicators

- Triple dimensions of Sustainable Development
  - –Environment, Society, Economy
  - –Corporate level indicators
  - –Assessment at corporate level



- Four areas of sustainable chemical processes
  - –Environmental, Efficiency, Economics, Energy (4E's)
  - –Process design level
  - –Taxonomy of chemical process indicators for use in process design

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The GREENSCOPE Tool



- Clear, practical, and user-friendly approach
- Monitor and predict sustainability at any stage of process design
- Currently developed into a spreadsheet tool, capable of calculating 139+ different metrics
- User can choose which indicators / metrics to calculate
- User can redefine absolute limits to fit circumstances

GREENSCOPE Sustainability Framework

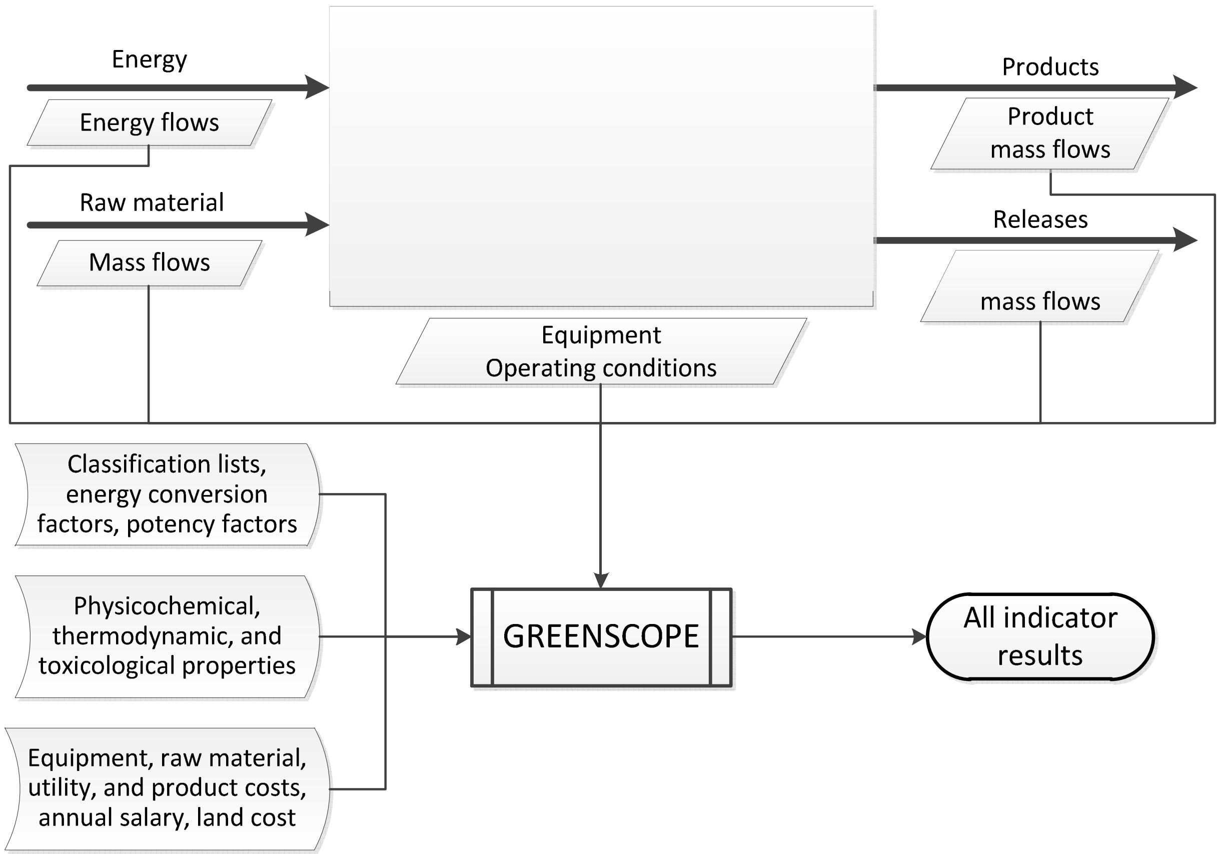
- Identification and selection of two reference states for each sustainability indicator:
  - Best target: 100% of sustainability
  - Worst-case: 0% of sustainability

- 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

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

GREENSCOPE: Systematic Evaluation Procedure



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Environmental Indicators

- 66 indicators
- Specifications of process input material
- Health & Safety hazards: operating conditions and operation failures
- Impact of components utilized in the system and releases
- 100% sustainability, best target, is no releases of pollutants and no hazardous material use or generation
- 0% sustainability, worst cases, all inputs are classified as hazardous, and/or all generated waste for each potential *EHS* hazard is released out of the process

Environmental Indicators: Example

Safety hazard, fire explosion

$$\text{SH}_{\text{fire/explosion}} = \frac{\text{Probable energy potential for reaction with O}_2}{\text{Mass of product}}$$

$$\text{SH}_{\text{fire/explosion}} = \frac{\left(-\Delta H_{c,i} \times 10^{4\times IndVal_i - 4}\right) \dot{m}_i}{\dot{m}_{\text{product}}}$$

If ΔT_{flash} is known

$$IndVal_i = \begin{cases} -0.005\Delta T_{\text{flash},i} + 1.0 & \text{if} \quad 0 < \Delta T_{\text{flash}} < 200 \\ 1 & \text{if} \quad \Delta T_{\text{flash}} \le 0 \\ 0 & \text{if} \quad \Delta T_{\text{flash}} \ge 200 \end{cases}$$

Elseif R_{code} is known

$$IndVal_i = \begin{cases} 1 & \text{if} \quad \text{R}_{\text{code}} = 12,15,17,18 \\ 0.875 & \text{if} \quad \text{R}_{\text{code}} = 11,30 \\ 0.75 & \text{if} \quad \text{R}_{\text{code}} = 10 \\ 0 & \text{if} \quad \text{R}_{\text{code}} = \text{other} \end{cases}$$

Elseif $\text{NFPA} - \text{f}$ is known

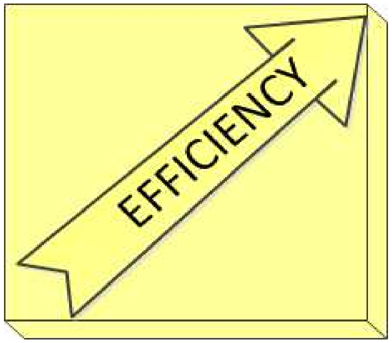
$$IndVal_i = \begin{cases} 1 & \text{if} \quad \text{NFPA-flamm=4} \\ 0.833 & \text{if} \quad \text{NFPA-flamm=3} \\ 0.667 & \text{if} \quad \text{NFPA-flamm=2} \\ 0.5 & \text{if} \quad \text{NFPA-flamm=1} \\ 0 & \text{if} \quad \text{NFPA-flamm=0} \end{cases}$$

end

Sustainability value	
Best, 100%	Worst, 0%
0 kJ/kg	All combustion enthalpy of each process substance is released

ΔH_c: combustion enthalpy, kJ/kg
ΔT_{flash}: temperature difference between the standard flash point and process temperature, ℃
R_{code}: Risk phrases of European community
NFPA-f: flammability hazard class according to the U.S. National Fire Protection Agency (NFPA)

Efficiency Indicators



- 26 indicators
- Amount of materials and inputs required to generate the desired product (reaction) or complete a specific process task (e.g., separation)
- Mass transfer operations have implicit influence in the amount of energy demand, equipment size, costs, raw materials, releases, etc.
- Efficiency indicators connect material input/output with the product or intermediate generated in the process or operating unit

Efficiency Indicators: Example

Actual atom economy

$$AAE = AE \times \varepsilon$$

$$AE_i = \frac{\left[(\text{Molecular weight}) \times (\text{stoichiometric coefficient})\right]_i}{\sum_{\text{reagents}} \left[(\text{Molecular weight}) \times (\text{stoichiometric coefficient})\right]_{\text{reagent}}}$$

$$\varepsilon = \frac{\text{Mass of product}}{\text{Theoretical mass of product}}$$

$$AAE = \frac{(\beta \times \text{MW})_{\text{product}} \times m^{\bullet}_{\text{product}}}{\sum_{i=1}^{I} (\alpha \times \text{MW})_{\text{reagent, } i} \times \frac{m^{\bullet\text{in}}_{\text{limit. reagent}}}{\text{MW}_{\text{limit. reagent}}} \times \frac{\beta_{\text{product}}}{\alpha_{\text{limit. reagent}}} \times \text{MW}_{\text{product}}}$$

Sustainability value	
Best,	Worst,
100%	0%
1	0

$m^{\bullet}_{\text{product}}$: mass flow of product *I* , kg/h
$m^{\bullet\text{in}}_{\text{limit. reagent}}$: input mass flow rate of the limiting reagent, kg/h
MW_i: molecular weight of the component *i*, kg/kmol
α_i: stoichiometric coefficient of the reagent *i*
β_{product}: stoichiometric coefficient of the desired product

Value mass intensity

$$MI_{\text{v}} = \frac{\text{Total mass input}}{\text{Sales revenue or value added}}$$

$$MI_{\text{v}} = \frac{\sum_{i=1}^{I} m^{\bullet\text{in}}_{m,i}}{S_m}$$

$$S_m = \sum_{i=1}^{I} m^{\bullet}_{m,\text{ product } i} \times C_{m,\text{product } i}$$

Sustainability value	
Best,	Worst,
100%	0%
1	40

$m^{\bullet\text{in}}_{m,i}$: input mass flow rate of the limiting reagent, kg/h
annual mass flow of substance *i* in year *m*, kg/yr
S_m: total income from all sales in year *m*, \$
$C_{m,i}$: cost of material *i* in year *m*, \$/kg
$m^{\bullet}_{\text{m, product, } i}$: : annual mass flow of product *i* in year *m*, kg/yr

Economic Indicators

- 33 indicators
- A sustainable economic outcome must be achieved for any new process technology or modification proposed for the commercial scale
- Based in profitability criteria for projects (process, operating unit), may or may not account for the time value of money
- Indicators supported in cost criteria:
  - –Processing costs: capital cost, manufacturing cost
  - –Process input costs: raw material cost, utility costs
  - –Process output costs: waste treatment costs

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Economic Indicators: Example

Net present value

$NPV =$ The total of the present value of all cash flows minus the present value of all capital investments

$$NPV = \sum_{m=1}^{n} \mathrm{PWF}_{cf,m} \left[(S_m - COM_m - d_m)(1-\Phi) + \mathrm{rec}_m + d_m \right] - \sum_{m=-b}^{n} \mathrm{PWF}_{v,m} TCI_m$$

$$S_m = \sum_{i=1}^{I} \dot{m}_{m,\text{ product } i} \times C_{m,\text{product } i}$$

$$COM_m = 0.280 FCI_{L,m} + 2.73 C_{OL,m} + 1.23 \left(C_{UT,m} + C_{WT,m} + C_{RM,m} \right)$$

$$d_m = 0.1 FCI_L$$

$$\mathrm{rec}_m = \begin{cases} C_{\text{Land}} + WC + FCI_L - \sum_{m=1}^{n} d_m & \text{if } m = n \\ 0 & \text{if } m \neq n \end{cases}$$

$$TCI_m = \mathrm{C}_{\text{Land},m} + FCI_{L,m} + WC_m$$

$$FCI_L = C_{TM} = 1.18 \sum_{i=1}^{u} C_{BM,i}$$

$$C_{BM,i} = C^{o}_{p,i} F_{BM,i}$$

$$C_{OL} = 4.5 N_{OL} \times (\text{annual salary})$$

$$N_{OL} = \left(6.29 + 31.7 P^2 + 0.23 N_{np} \right)^{0.5}$$

$$N_{np} = \sum \text{Equipment}$$

Sustainability value	
Best, 100%	Worst, 0%
NPV @ discount rate (r_d)= 0%	*NPV* @ r_d= minimum acceptable rate of return (*MARR*)=40% for very high risk projects

n: life of the plant or equipment, yr
$\mathrm{PWF}_{cf,m}$: the selected present worth factor
S_m: total income from all sales in year m, \$
COM_m: cost of manufacture without depreciation, \$
FCI_L : Fixed capital investment without including the land value
d_m: depreciation charge. Here, it is assumed as 10% of the FCI_L evaluated in year m, however it can be estimated by different methods
Φ: fixed income tax rate given by the IRS
rec_m: salvage-value recovered from the working capital, land value, and the sale of physical assets evaluated at the end of the plant life. Often this salvage value is neglected, \$

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Energy Indicators

- 14 indicators
- Different thermodynamic assessments for obtaining an energetic sustainability score
  - Energy (caloric); exergy (available); emergy (embodied)
- Zero energy consumption per unit of product is the best target (more products per unit of consumed energy)
- Most of the worst cases do not have a predefined value
  - They depend on the particular process or process equipment
  - The designer has to choose which value is unacceptable
  - Some worst cases can be assigned by taking the lowest scores found through comparing several sustainability corporate reports

Energy Indicators: Example

Exergy intensity

$$R_{Ex} = \frac{\text{Net exergy used}}{\text{Mass of product}}$$

$$R_{Ex} = \frac{\text{Ex}^{\bullet\,\text{in}} - \text{Ex}^{\bullet}_{\text{lost}}}{m^{\bullet}_{\text{product}}}$$

$$\text{Ex}^{\bullet\,\text{in}} = \left[\text{Ex}^{\bullet}(\text{physical}) + \text{Ex}^{\bullet}(\text{chemical})\right]_{\text{input flows}} + \text{Ex}^{\bullet}(\text{work}) + \text{Ex}^{\bullet}(\text{heat})$$

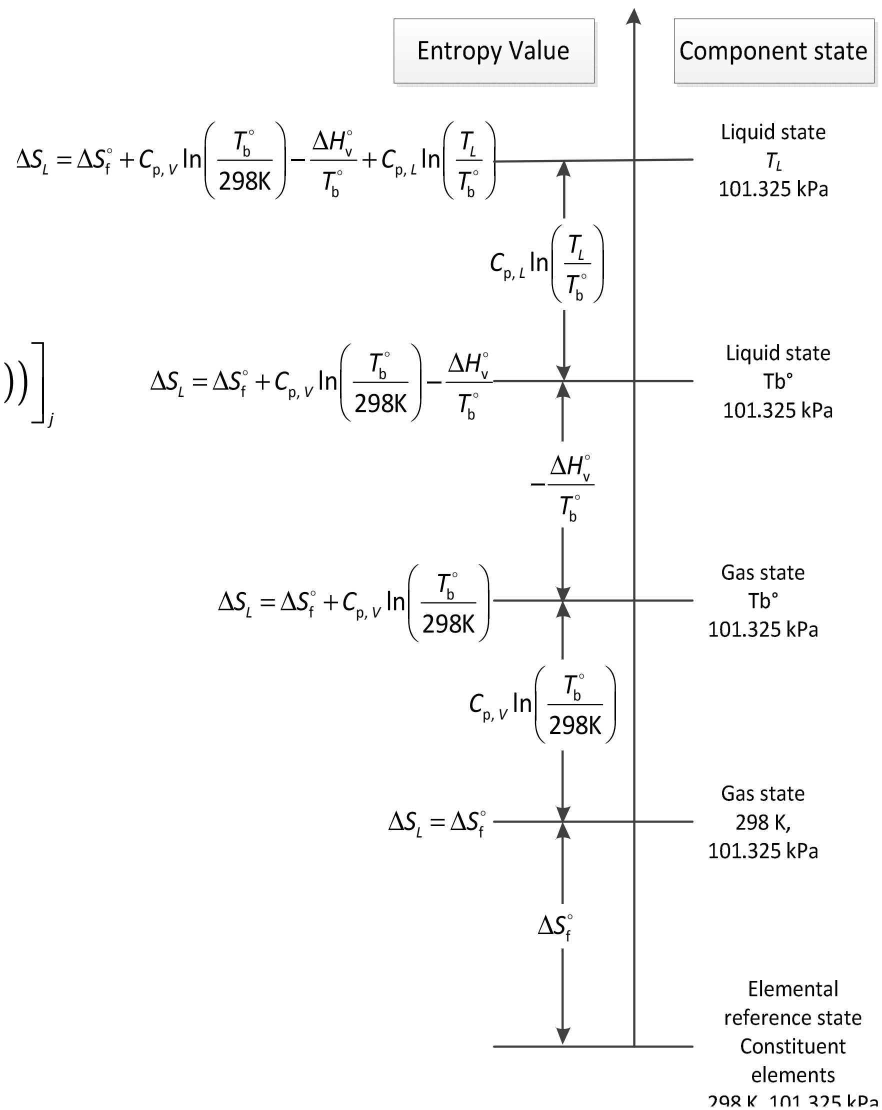
$$\text{Ex}^{\bullet\,\text{in}} = \sum_{j=1}^{J} m_j^{\bullet\text{in}} \left(\Delta H - T_0 \Delta S\right)_j + \sum_{j=1}^{J}\left[\sum_{i=1}^{c} n_i^{\bullet} \sum_{i=1}^{c}\left(x_i \text{Ex}_i^{\circ\text{ch}} + RT_0 x_i \ln(x_i)\right)\right]_j + \sum_{k=1}^{K'} W_k^{\bullet} + \sum_{k=1}^{K} Q_k^{\bullet}\left(1 - T_0 / T_{*,k}\right)$$

$$\text{Ex}^{\bullet}_{\text{lost}} = T_0 S^{\bullet}_{\text{generated}}$$

$$S^{\bullet}_{\text{generated}} = \sum_{j=1}^{J} m_j^{\bullet\text{in}} \times \Delta S_j - \sum_{j=1}^{J'} m_j^{\bullet\text{out}} \times \Delta S_j - \sum_{k=1}^{K} \frac{Q_k^{\bullet}}{T_0}$$

$$\Delta S_{L,j} = \sum_{i=1}^{c} x_{i,j} \Delta S_{L,ij} + \Delta S_{L,j\ \text{mix}} \qquad \Delta S_{V,j} = \sum_{i=1}^{c} y_{i,j} \Delta S_{V,ij} + \Delta S_{V,j\ \text{mix}}$$

Sustainability value	
Best, 100%	Worst, 0%
0	Max Ex_{total}/kg product



Indicators and Data Needs

- To generate a sustainability assessment a model must have available data
- Data is not the final goal, but it is mandatory to get there
- *M & E* flows , operating conditions and equipment specifications; substance properties: physicochemical, thermodynamic, and toxicity; manufacturing and capital costs
- Data-source alternatives can be used to fulfill potential data gaps
  - Simulators
  - Physiochemical
  - Toxicological
  - QSAR models
  - Databases
  - Classification lists

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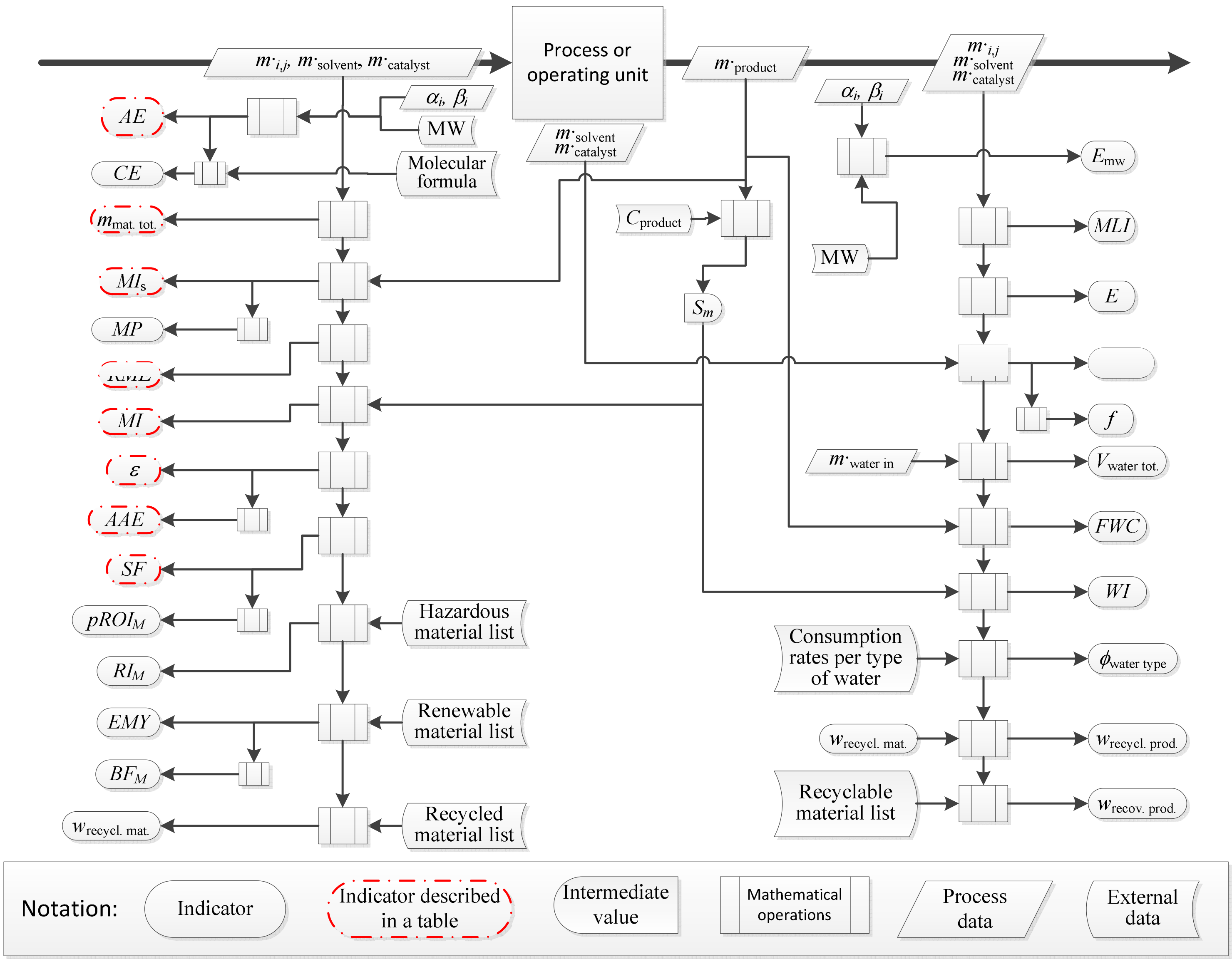
Indicators and Data Needs: Efficiency



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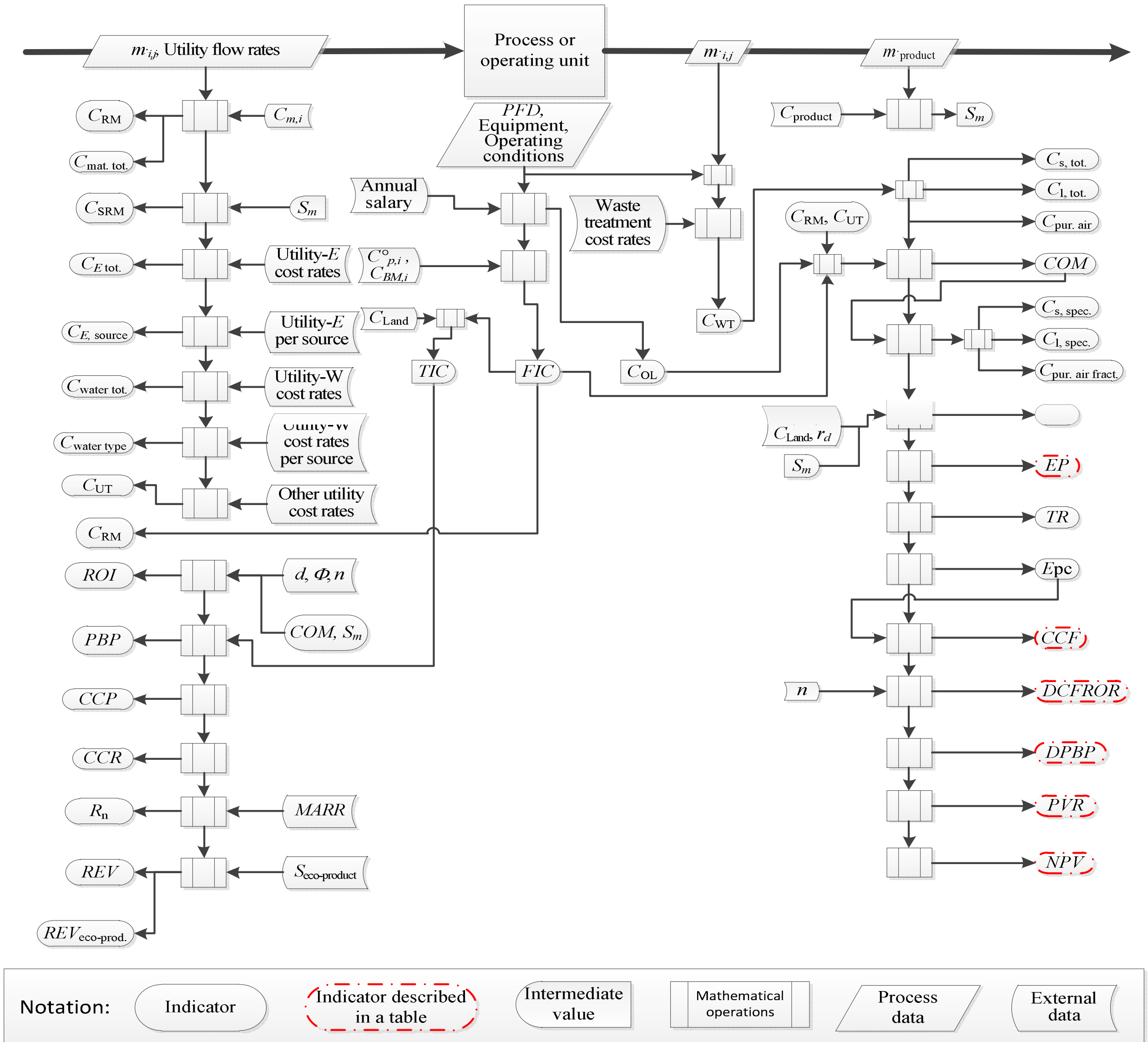
Indicators and Data Needs: Economic



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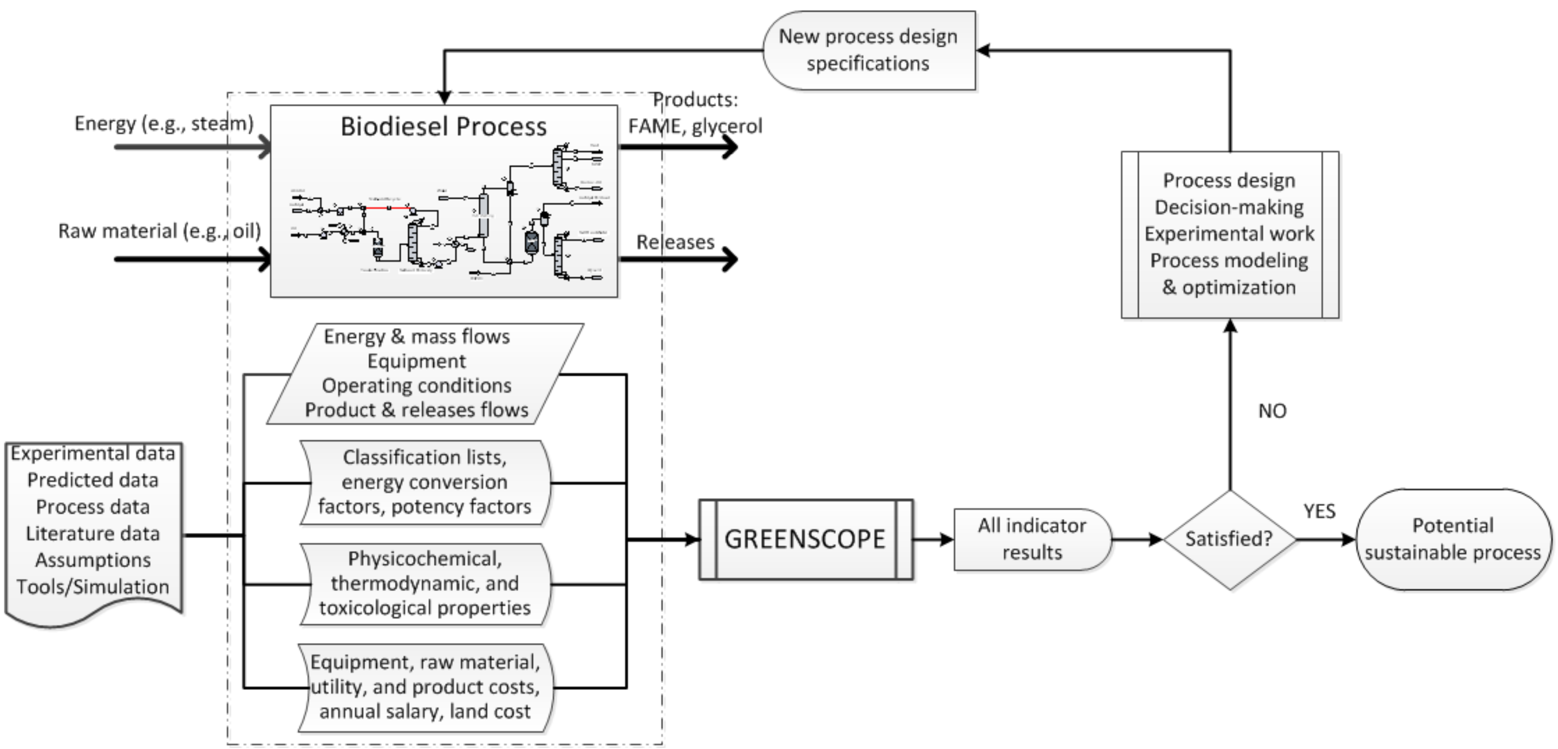
Data Sources

Data source	Property or type of provided data
DOT, TOXNET, ACToR	Hazardous material list
TRI program	TRI PBT chemical list
TOXNET/HSDB	ERPG-2, ERPG-3, MW, ΔH_c, ρ, pH, K_{OW}, P_v, T_{flash}, NFPA-r, NFPA-f, IDLH, EC_{50}, LC_{50}, LD_{50}, TWA
NIST Chemistry WebBook	MW, ΔH_r, $C_p(T)$, ΔH_f, ΔH_c, ΔH_v,, T_{flash}, $P_v(T)$, U, ΔG_r,
AIHA	ERPG-2, ERPG-3
ACToR	MW, IDLH, LC_{50}, LD_{50}, ρ, K_{OW}, P_v, MAK-CH, TWA, hazard, acute toxicity, chronic toxicity, carcinogenicity, reproductive toxicity, neurotoxicity, immunotoxicity, dermal toxicity, respiratory toxicity, nephrotoxity, endocrine effects, ecotoxicity
ACToR/ICSC	MW, EU_{class}, R_{code}, NFPA, MAK-CH, T_{flash}, , μ, EC_{class}, TWA
IRIS	MW, P_v, K_{OW}, RfD, toxicity kinetics, pharmacokinetic modeling, hazard identification, mode-of-action and dose-response, cancer factors, and cancer descriptors

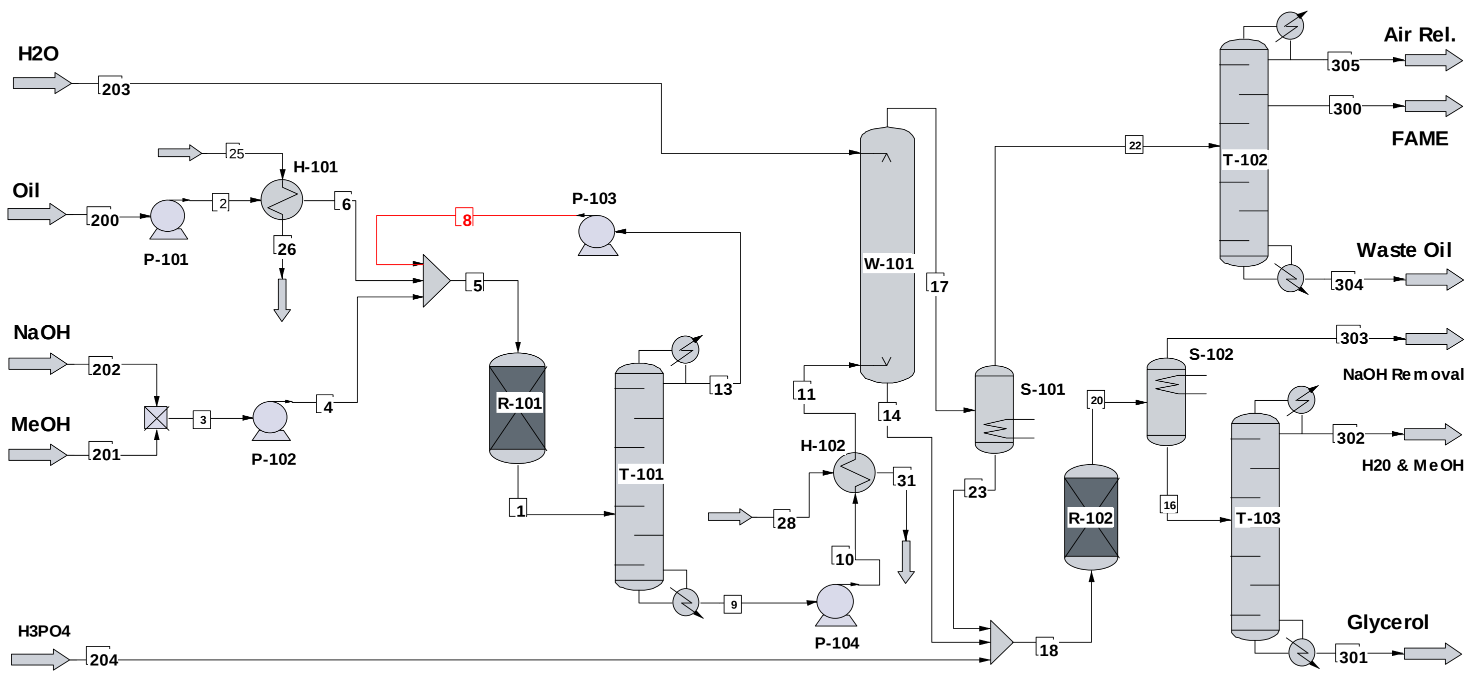
Sustainability Assessment: Biodiesel Case Study

- External data: ERPG, IDLH, T_b, T_m, LC_{50}, etc.
- Process data: $\dot{m}_{i,\,in}$, $\dot{m}_{i,\,out}$, C_{RM}, C_{UT}, $C_{equipment}$, etc.
- Definition of best & worst case scenarios



Biodiesel: Process Description

- Soybean oil
- 95% Oil conversion
- 1 Ton FAME/h
- 99.60% Purity
- 0.1 Ton Glycerol/h
- Utilities: steam, electricity, cooling water
- Solid, liquid, & air releases



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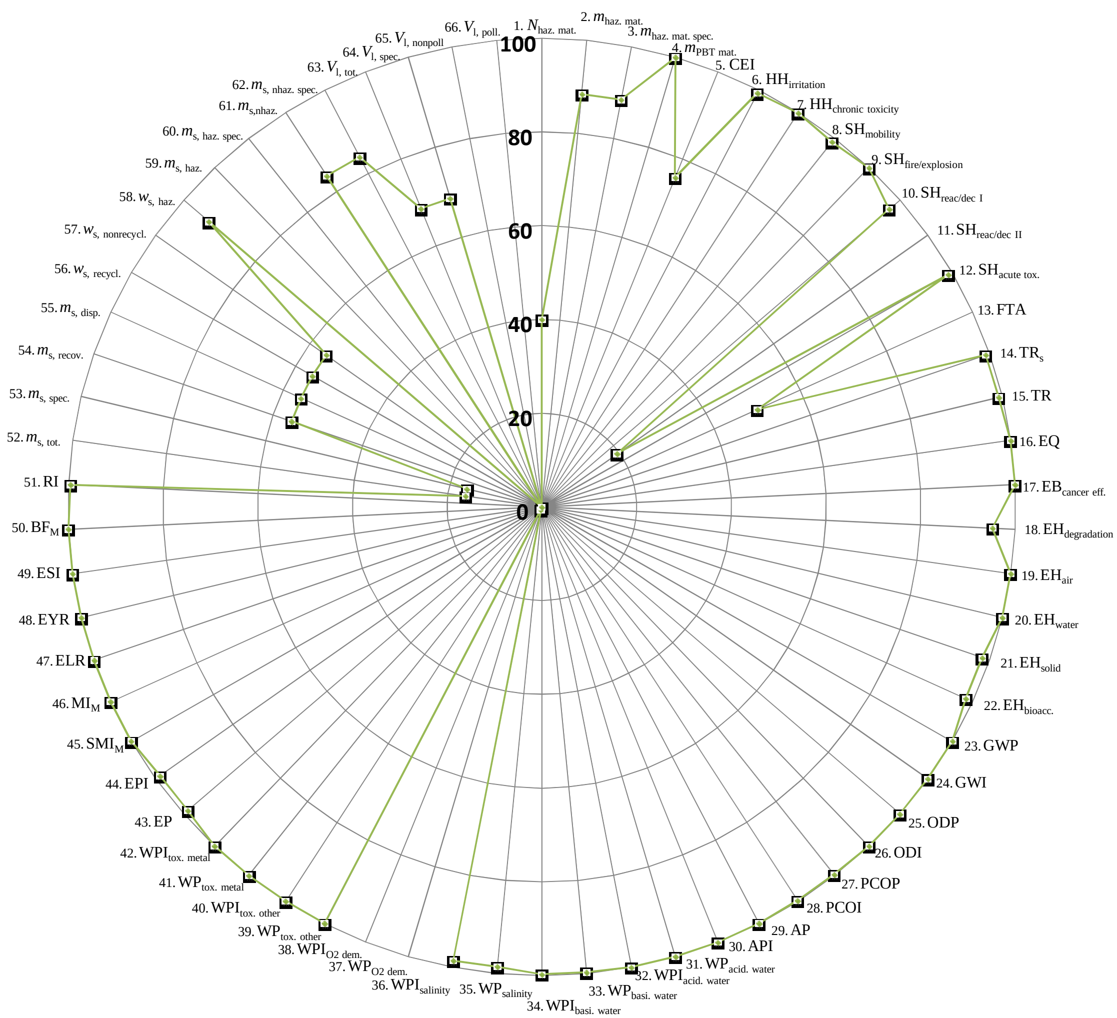
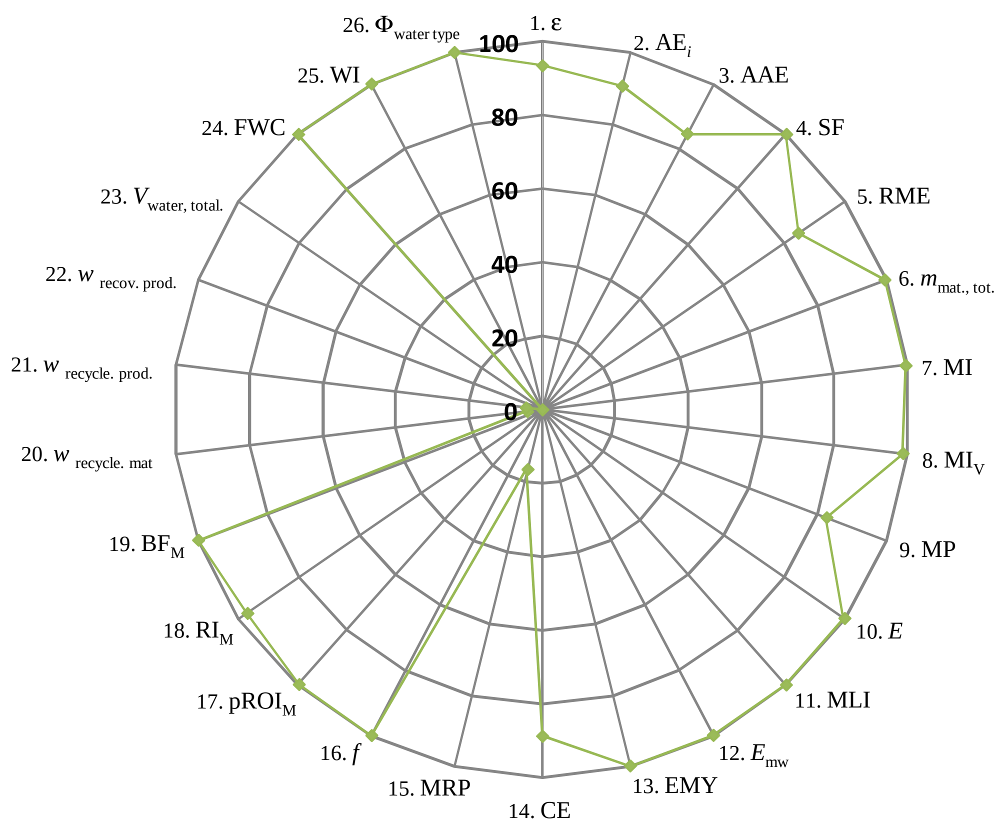
Environmental Indicator Results



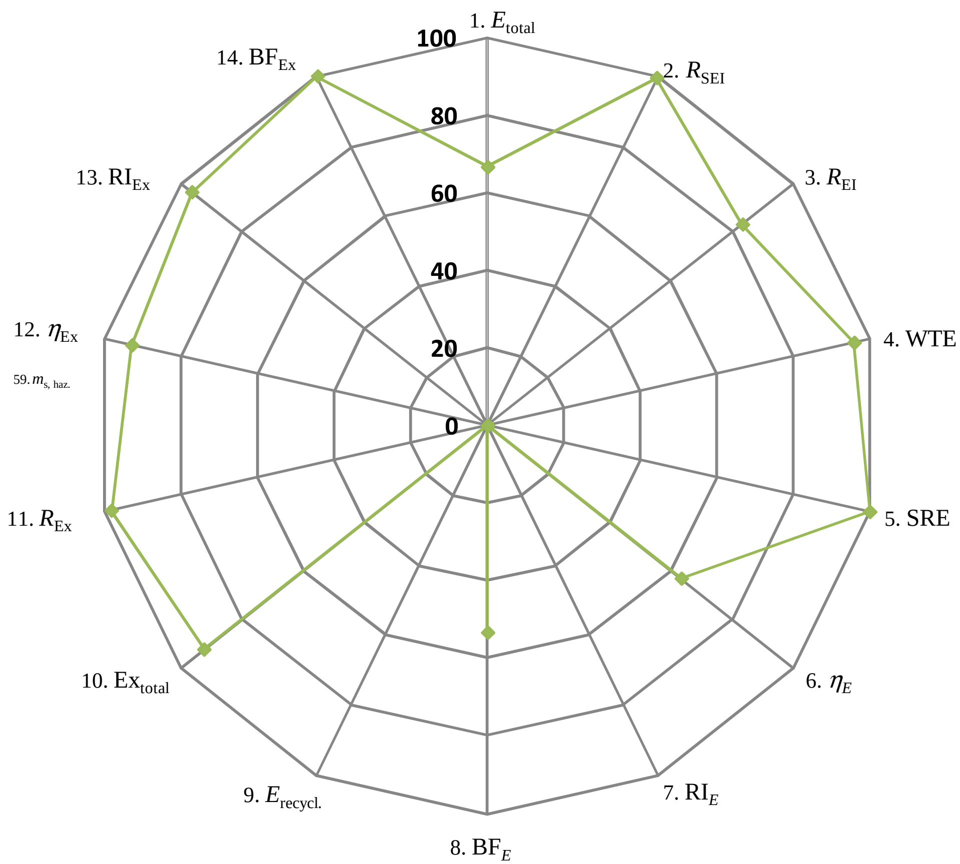
Indicator	Description	Sust. (%)
1. $N_{haz. mat.}$	Number of hazardous materials input	40.00
6. $HH_{irritation}$	Health hazard, irritation factor	99.31
10. $SH_{reac/dec I}$	Safety hazard, reaction / decomposition I	97.00
22. $EH_{bioacc.}$	Environmental hazard, bioaccumulation (the food chain or in soil)	98.34
27. PCOP	Photochemical oxidation (smog) potential	99.83
32. $WPI_{acid. water}$	Aquatic acidification intensity	99.88
38. $WPI_{O2 dem.}$	Aquatic oxygen demand intensity	0.60
43. EP	Eutrophication potential	98.89

Efficiency Indicator Results



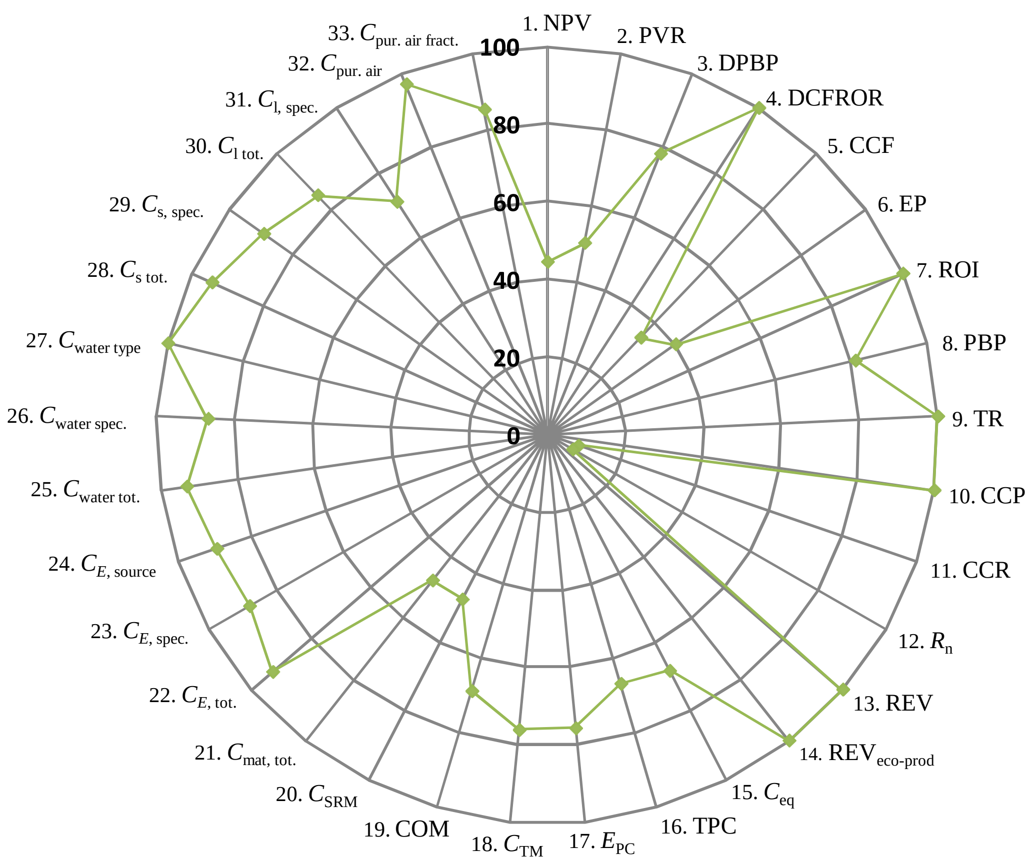
Indicator	Description	Sust. (%)
2. AE_i	Atom economy	90.60
7. MI_v	Value mass intensity	99.46
17. $pROI_M$	Physical return on investment	99.76
21. $w_{recycl. prod.}$	Mass fraction of product from recyclable materials	4.50
25. WI	Water intensity	100

Energy Indicator Results



Indicator	Description	Sust. (%)
2. R_{SEI}	Specific energy intensity	99.49
6. η_E	Resource-energy efficiency	63.26
8. BF_E	Breeding-energy factor	53.38
10. Ex_{total}	Exergy consumption	92.59
14. BF_{Ex}	Breeding-exergy factor	100.00

Economic Indicator Results



Indicator	Description	Sust. (%)
1. NPV	Net present value	44.52
8. PBP	Payback Period	81.10
19. COM	Manufacturing cost	68.70
23. $C_{E,\ spec.}$	Specific energy costs	88.07
33. $C_{pur.\ air\ fract.}$	Fractional costs of purifying air	85.26

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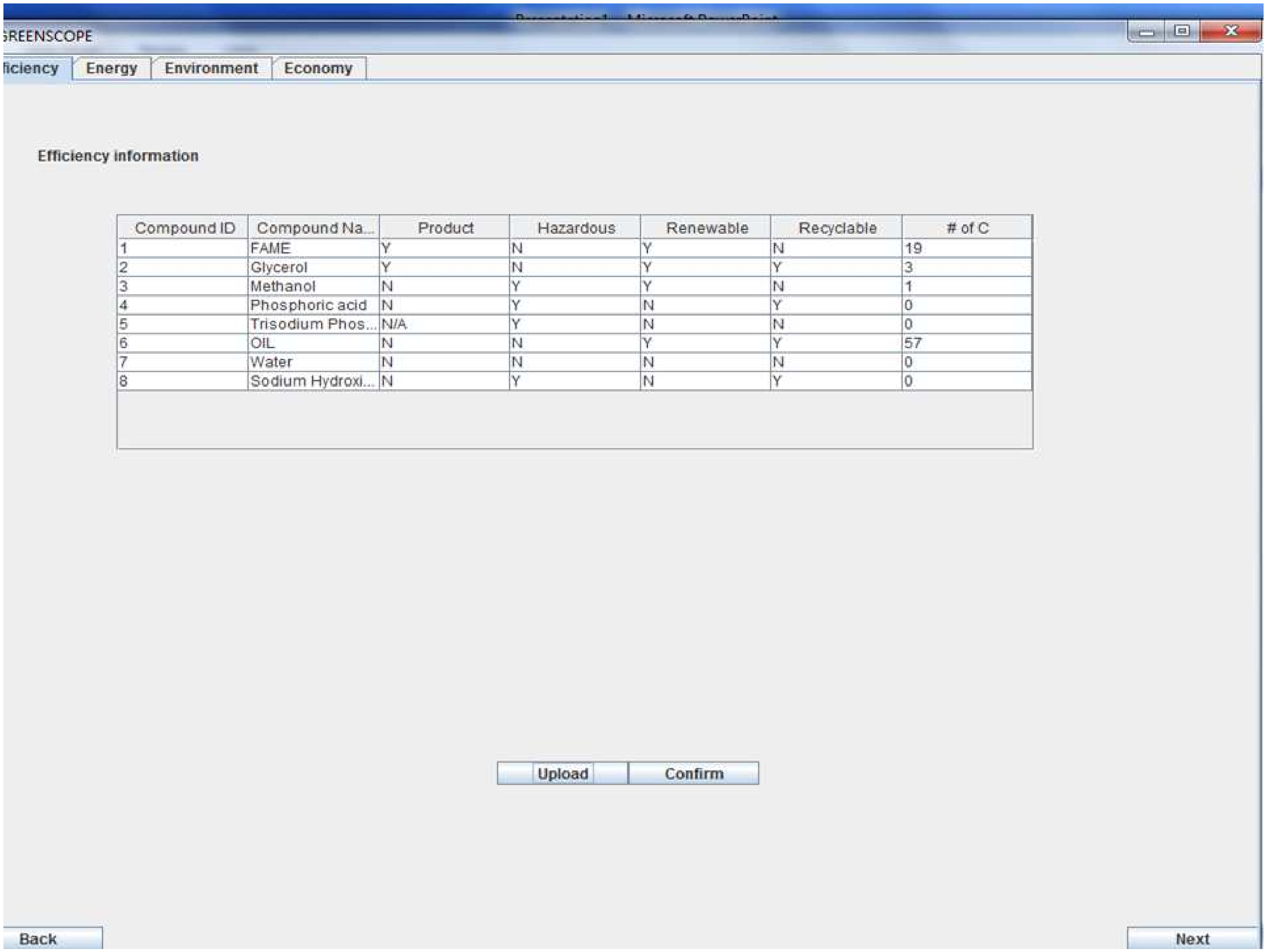
	Indicator	Symbol	Definition	Equation	Value	Input	unit	Range: Best case	Range: Worst case	Percent Sc
1	Total energy consumption	1. E total	Total energy consumed by the process or process unit as primary fuel equivalent	$E_{total}=(C_{fuel}E^{*})_{natural\ gas}+(C_{fuel}E^{*})_{fuel\ oil}+(C_{fuel}E^{*})_{steam}+\ldots+(C_{fuel}E^{*})_{electricity}$; $E^{*}_{k}=\begin{cases}Q^{*}_{k} & \text{heat requirements}\\ W^{*}_{k} & \text{power requirements}\end{cases}$; $\sum_{j=1}^{J} m_j^{*in}\times\Delta H_j+\sum_{k=1}^{K} Q^{*}_k+\sum_{k=1}^{K'} W^{*}_k-\sum_{j=1}^{J} m_j^{*out}\times\Delta H_j=0$	2970.331629	E^{*}: energy flow rate as a heat flow or power provided by utilities such as natural gas, fuel oil, steam, and electricity, MJ/h; C_{fuel}: conversion factor to fuel energy; Q_k^{*}: heat flow stream k, MJ/h; W_k^{*}: energy flow k for power needs, kWh/h; m_j^{*}in: total mass flow rate of the input stream j, kg/h; mj•out: total mass flow rate of the output stream j, kg/h; ΔH_j: mass enthalpy of the	MJ/h	2740.1	27401	**99.07**
2	Specific energy intensity	2. R_{SEI}	Total energy consumed by the process or process operating unit as primary fuel equivalent per unit mass of product	$R_{SEI}=\frac{(C_{fuel}E^{*})_{natural\ gas}+(C_{fuel}E^{*})_{fuel\ oil}+(C_{fuel}E^{*})_{steam}+\ldots+(C_{fuel}E^{*})_{electricity}}{m^{*}_{product}}$	2.714752602	E^{*}: energy flow rate as a heat flow or power provided by utilities such as natural gas, fuel oil, steam, and electricity, MJ/h; C_{fuel}: conversion factor to fuel energy; Q_k^{*}: heat flow stream k, MJ/h; W_k^{*}: energy flow k for power needs, kWh/h; m•product: total mass flow rate of the	MJ/kg	0	1949	**99.86**
3	Energy intensity	3. R_{EI}	Measurement of the net fuel-energy consumed to provide the heat and the power requirements for the process per unit of sales revenue or value addedd	$R_{EI}=\frac{(C_{fuel}E^{*})_{natural\ gas}+(C_{fuel}E^{*})_{fuel\ oil}+(C_{fuel}E^{*})_{steam}+\ldots+(C_{fuel}E^{*})_{electricity}}{S_{s}}$	1.6972	E^{*}: energy flow rate as a heat flow or power provided by utilities such as natural gas, fuel oil, steam, and electricity, MJ/h; C_{fuel}: conversion factor to fuel energy; Q_k^{*}: heat flow stream k, MJ/h; W_k^{*}: energy flow k for power needs,	MJ/$	0	37.3	**95.45**
4	Waste treatment energy	4. WTE	This is the net amount of energy required by the waste process unit per mass of product	$\mathrm{WTE}=\frac{\left[(C_{fuel}E^{*})_{natural\ gas}+(C_{fuel}E^{*})_{fuel\ oil}+(C_{fuel}E^{*})_{steam}+\ldots+(C_{fuel}E^{*})_{electricity}\right]_{waste\ section}}{m^{*}_{product}}$	0.040679198	E^{*}: energy flow rate as a heat flow or power provided by utilities such as natural gas, fuel oil, steam, and electricity, kJ/h; C_{fuel}: conversion factor to fuel energy; Q_k^{*}: heat flow stream k, kJ/h; W_k^{*}: energy flow k for power needs, kWh/h; m•product: total mass flow rate of the product stream, kg/h. All energy flows to the waste	MJ/kg	0	0.27147526	**85.02**
5	Solvent recovery energy	5. SRE	This is the net amount of energy required by the process to recover and reuse solvents per mass of product	$\mathrm{SRE}=\frac{\left[(C_{fuel}E^{*})_{natural\ gas}+(C_{fuel}E^{*})_{fuel\ oil}+(C_{fuel}E^{*})_{steam}+\ldots+(C_{fuel}E^{*})_{electricity}\right]_{solvent\ recovery\ section}}{m^{*}_{product}}$	0	E^{*}: energy flow rate as a heat flow or power provided by utilities such as natural gas, fuel oil, steam, and electricity, kJ/h; C_{fuel}: conversion factor to fuel energy; Q_k^{*}: heat flow stream k, kJ/h; W_k^{*}: energy flow k for power needs, kWh/h; m•product: total mass flow rate of the product stream, kg/h. All energy flows to the solven recovery	MJ/kg	0	0.27147526	**100**
6	Resource-energy efficiency	6. η_E	The ratio of the physical "value" of the products (YE) to the total resource use in the same energetic unit. YE is the quantity of the raw materials energy remains in the desired product	$\eta_E=\frac{m^{*}_{product}\times\Delta H_{product}}{\sum_{j=1}^{J} m_j^{*in}\times\Delta H_j}$	0.631606851	m_j^{*}in: total mass flow rate of the input stream j, kg/h; m•product: product flow rate, kg/h; ΔH_j: mass enthalpy of the stream j in the respective phase (L: liquid, V: vapor), kJ/kg	fraction	1	0	**63.16**
7	Renewability-energy index	7. RI_E	The ratio of the consumption of renewable energy to total energy consumption	$RI_E=\frac{(E_{total})_{renewable}}{E_{total}}$	0	E^{*}: energy flow rate as a heat flow or power provided by utilities such as natural gas, fuel oil, steam, and electricity, kJ/h; C_{fuel}: conversion factor to fuel energy; Q_k^{*}: heat flow stream k, kJ/h; W_k^{*}: energy flow k for power needs, kWh/h;	fraction	1	0	**0**
8	Breeding-energy factor	8. BF_E	The total energy output of the process divided by the non-renewable material input energy	$BF_E=\frac{m^{*}_{product}\times\Delta H_{product}}{\sum_{j=1}^{J} m^{*in}_{non\text{-}renewable,j}\times\Delta H_j}$	5.338203779	m_j^{*}in: total mass flow rate of the input stream j, kg/h; m•product: product flow rate, kg/h; ΔH_j: mass enthalpy of the stream j in the respective phase (L: liquid, V: vapor), kJ/kg; utility rates from non-renewable sources	scalar	10	0	**53.38**
9	Energy for recycling	9. $E_{recycl.}$	This is the net amount of energy required by the recycling operating units per mass of product	$E_{recycl.}=\left[\begin{matrix}(C_{fuel}E^{*})_{natural\ gas}+(C_{fuel}E^{*})_{fuel\ oil}+(C_{fuel}E^{*})_{steam}\\ +\ldots+(C_{fuel}E^{*})_{electricity}\end{matrix}\right]_{Recycling\ section}/m^{*}_{product}$	0.832567995	E^{*}: energy flow rate as a heat flow or power provided by utilities such as natural gas, fuel oil, steam, and electricity, kJ/h; C_{fuel}: conversion factor to fuel energy; Q_k^{*}: heat flow stream k, kJ/h; W_k^{*}: energy flow k for power needs, kWh/h.	MJ/kg	0	0.27147526	**0**
10	Exergy consumption	10. Ex_{total}	It describes quantitatively the amount of resources in exergy units in order to deliver a product	$\mathrm{Ex}_{total}=\mathrm{Ex}^{*in}-\mathrm{Ex}^{*}_{product}$; $\mathrm{Ex}^{*in}=[\mathrm{Ex}^{*}(\text{physical})+\mathrm{Ex}^{*}(\text{chemical})]_{input\ flows}+\mathrm{Ex}^{*}(\text{work})+\mathrm{Ex}^{*}(\text{heat})$; $\mathrm{Ex}^{*in}=\sum_{j=1}^{J} m_j^{*in}(\Delta H-T_0\Delta S)_j+\sum_{j=1}^{J}\left[\sum_{i=1}^{I} n_i^{*}\sum_{i=1}^{I}(x_i\mathrm{Ex}^{ch}_i+RT_0x_i\ln(x_i))\right]_j+\sum_{k=1}^{K'} W^{*}_k+\sum_{k=1}^{K} Q^{*}_k[1-T_0/T_{s,k}]$; $\mathrm{Ex}^{*}_{product}=m^{*}_{product}(\Delta H-T_0\Delta S)_{product}+n^{*}_{product}\mathrm{Ex}^{ch}_{product}$	2966.554424	Ex•in: total exergy flow input to the process or process unit, kJ/h; m•j: total mass flow rate of the stream j, kg/h; ΔH_j: mass enthalpy of the stream j, kJ/kg; T_0: temperature of reference, T_0=298 K; ΔS_j: mass entropy of the stream j, kJ/(kg K); n•i: molar flow rate of substance i, kmol/h; Ex$^{ch}_i$: standard chemical exergy of substance i, kJ/kmol; R: the gas constant, R = 8.314 kJ/(kmol K); x_i: molar fraction of specie i; W^{*}_k: energy flow k for power needs, kWh/h; Q^{*}_k: heat flow stream k, kJ/h; $T_{s,k}$: temperature at which a heat flow stream k is supplied, K; S•generated: generated entropy	MJ/h	▪	42962.6154	**93.1**

Stream&Compound Data / Equipment&Cost Inputs / Utility Data / Material Efficiency / Environment / **Energy** / Economics / Best&Worst-Economics / CEI / Potency Factors / Exergy

EPA United States Environmental Protection Agency

Stand Alone GREENSCOPE Software

- Currently in development
- Dr. Rajib Mukherjee (ORISE Post-Doc)
- JAVA Language
- Based on the Excel® version
- User can define
  - level of interaction
  - which indicators to calculate
  - best and worst case scenarios



Compound ID	Compound Na...	Product	Hazardous	Renewable	Recyclable	# of C
1	FAME	Y	N	Y	N	19
2	Glycerol	Y	N	Y	Y	3
3	Methanol	N	Y	Y	N	1
4	Phosphoric acid	N	Y	N	Y	0
5	Trisodium Phos...	N/A	Y	N	N	0
6	OIL	N	N	Y	Y	57
7	Water	N	N	N	N	0
8	Sodium Hydroxi...	N	Y	N	Y	0

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GREENSCOPE

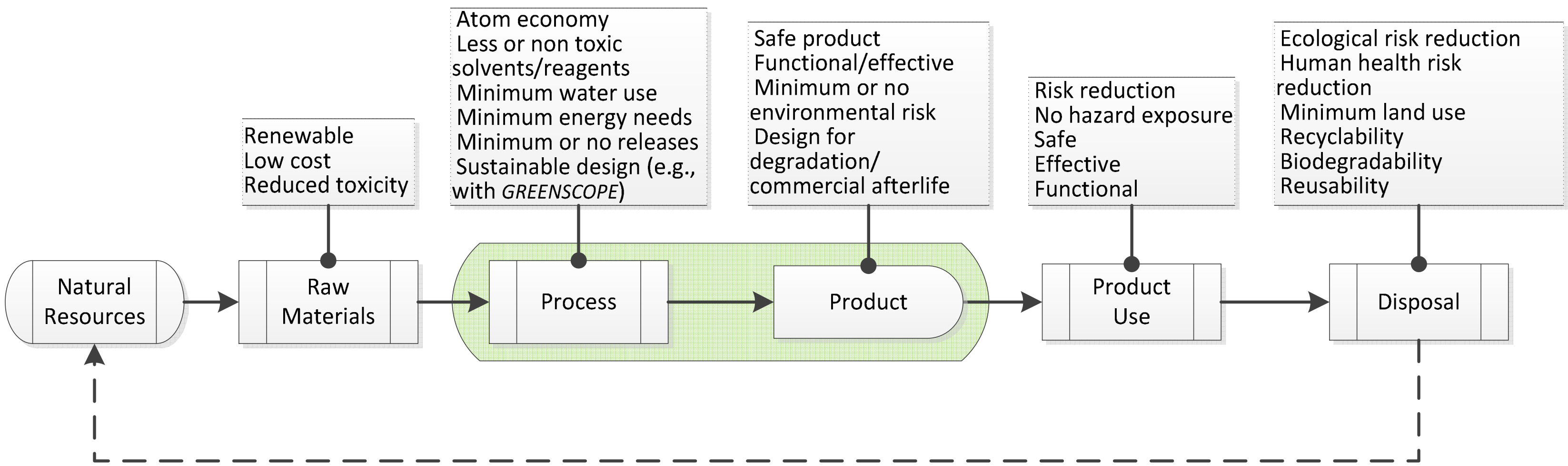
Calculate efficiency indicators, choose from the list :

- 1. Reaction Yield
- 2. Atom Economy
- 3. Actual Atom Economy
- 4. Stoichiometric Factor
- 5. Reaction Mass Efficiency
- 6. Total material consumption
- 7. Mass Intensity
- 8. Value mass intensity
- 9. Mass Productivity
- 10. Environmental Factor
- 11. Mass Loss Index
- 12. Environmental Factor based on molecular weight
- 13. Effective Mass Yield
- 14. Carbon Efficiency
- 15. Material Recovery Parameter
- 16. Solvent and Catalyst Environmental impact Parameter
- 17. Physical Return on Investment
- 18. Renewability-Material Index
- 19. Breeding-Material factor
- 20. Recycled material fraction
- 21. Mass fraction of products from recyclable materials
- 22. Mass fraction of products designed for disassembly, reuse or recycling
- 23. Total water consumption
- 24. Fractional water consumption
- 25. Water intensity
- 26. Volume fraction of water type

- Select All

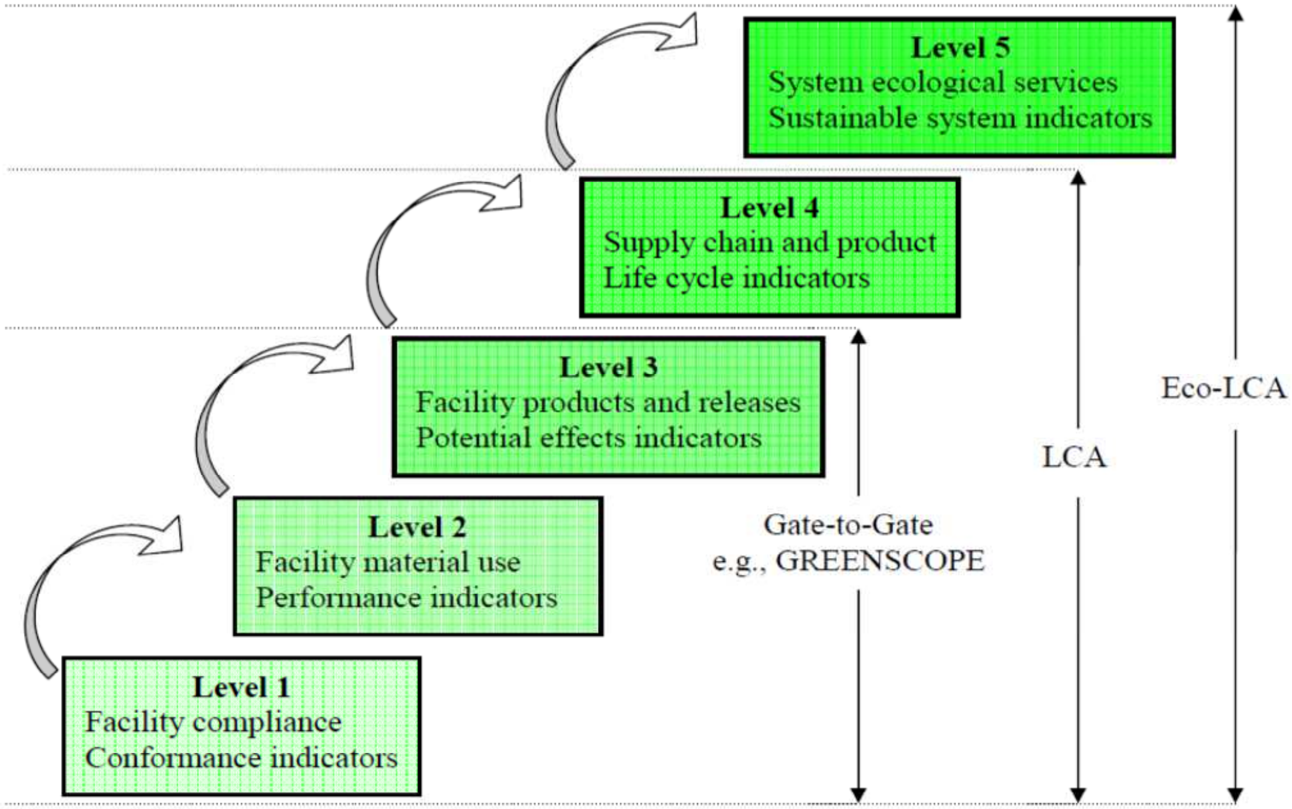
Commit

Global Sustainability Assessment



- Impact assessment beyond the process to decide which design alternative is more sustainable based on the life-cycle considerations
- Identifying stages contributing greater than any other stage to the global life-cycle impact within the product life cycle

Global Sustainability Assessment



A complete quantification of sustainability performance requires an extensive evaluation of the entire system beyond the manufacturing facility

Conclusions

- Performance indicators for designing sustainable chemical processes at any level:
  - Provides direction to the designer (0% and 100% sustainability)
  - Modifying existing processes as well as implementing new chemistries
  - Approximates manufacturing scale sustainability from a bench or pilot scale
- With GREENSCOPE, the results of sustainable chemical practices are quantified:
  - Modifications in the type and magnitude of goods and services
  - Preventing and minimizing all types of releases
  - Manufacturing the desired product without negatively affecting the economic profitability
- GREENSCOPE can be used as a reliable and robust tool for the development of chemical processes

Disclaimer

The views expressed in this presentation are those of the author and do not necessarily represent the views or policies of the U.S. Environmental Protection Agency.

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Thanks!

Questions?