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Using Green Chemistry and Engineering Principles to Design, Assess, and Retrofit Chemical Processes for Sustainability

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Outline

- Sustainability: Conceptual
- Process Design
- Sustainable Process Screening: WAR Algorithm
- Sustainable Process Assessment: GREENSCOPE
- Sustainable Process Retrofit: SustainPro
- Sustainable Process Design: Bringing it Together

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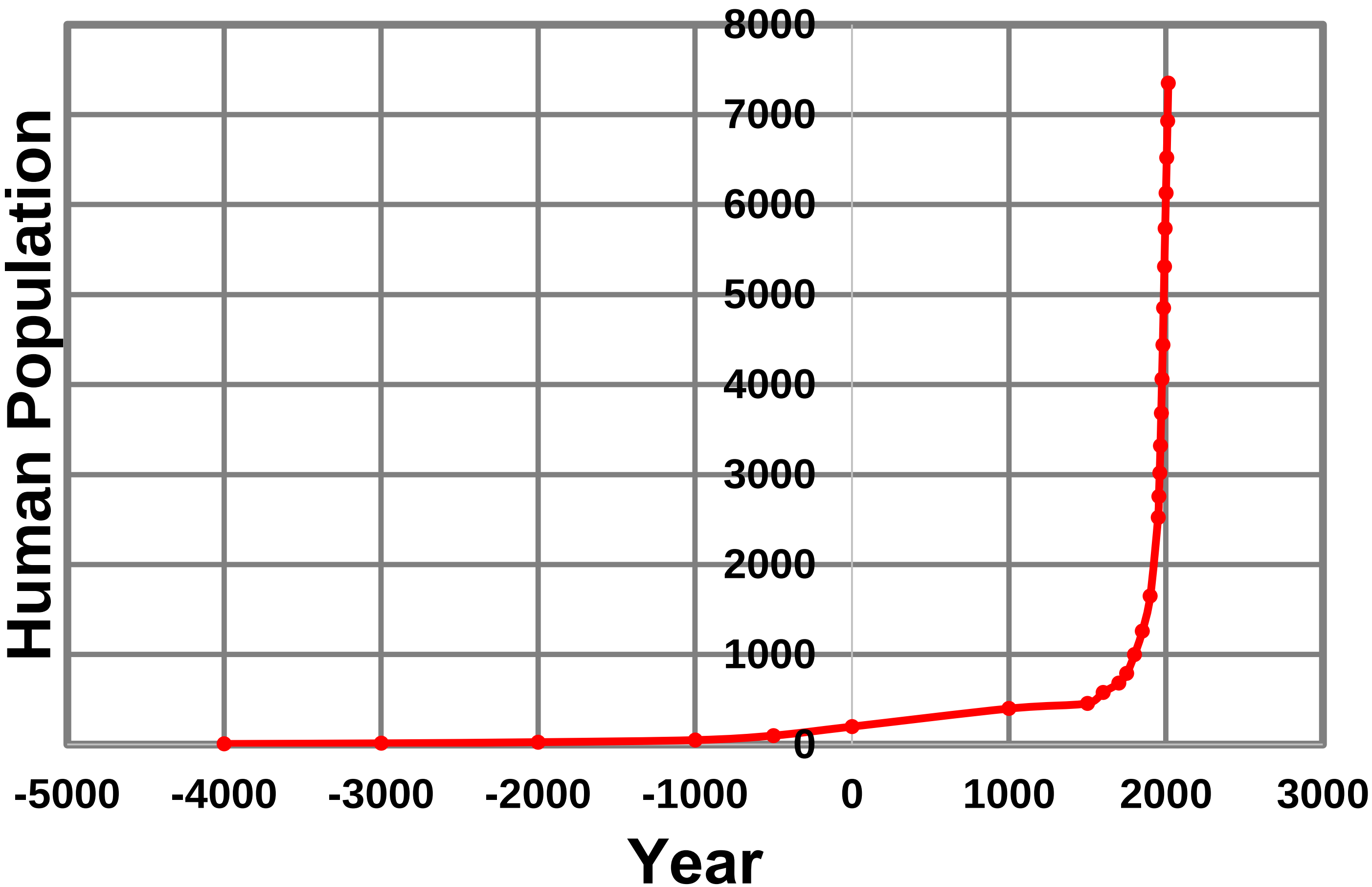
Sustainability: Conceptual

Historical World Population

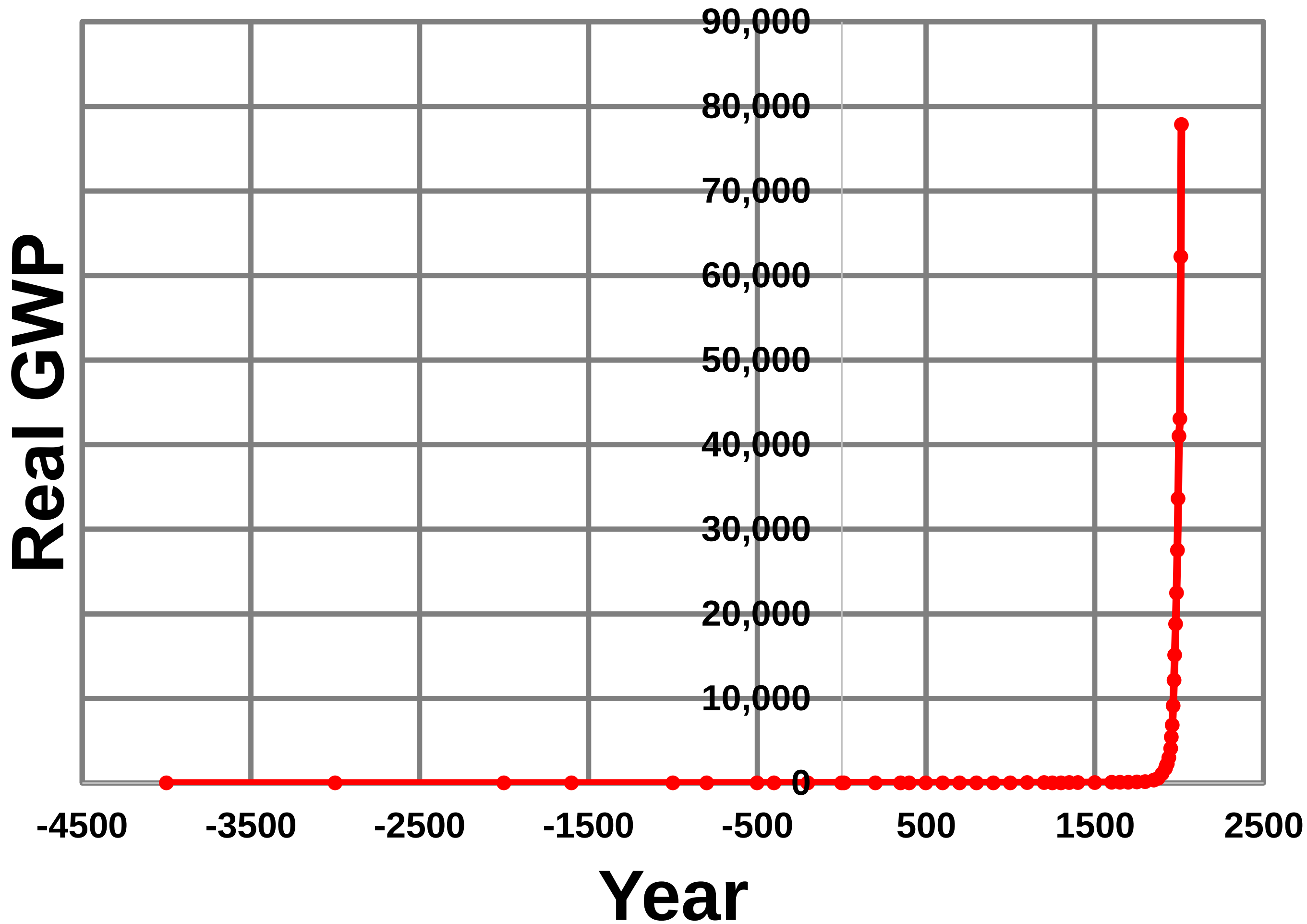
(https://en.wikipedia.org/wiki/World_population)



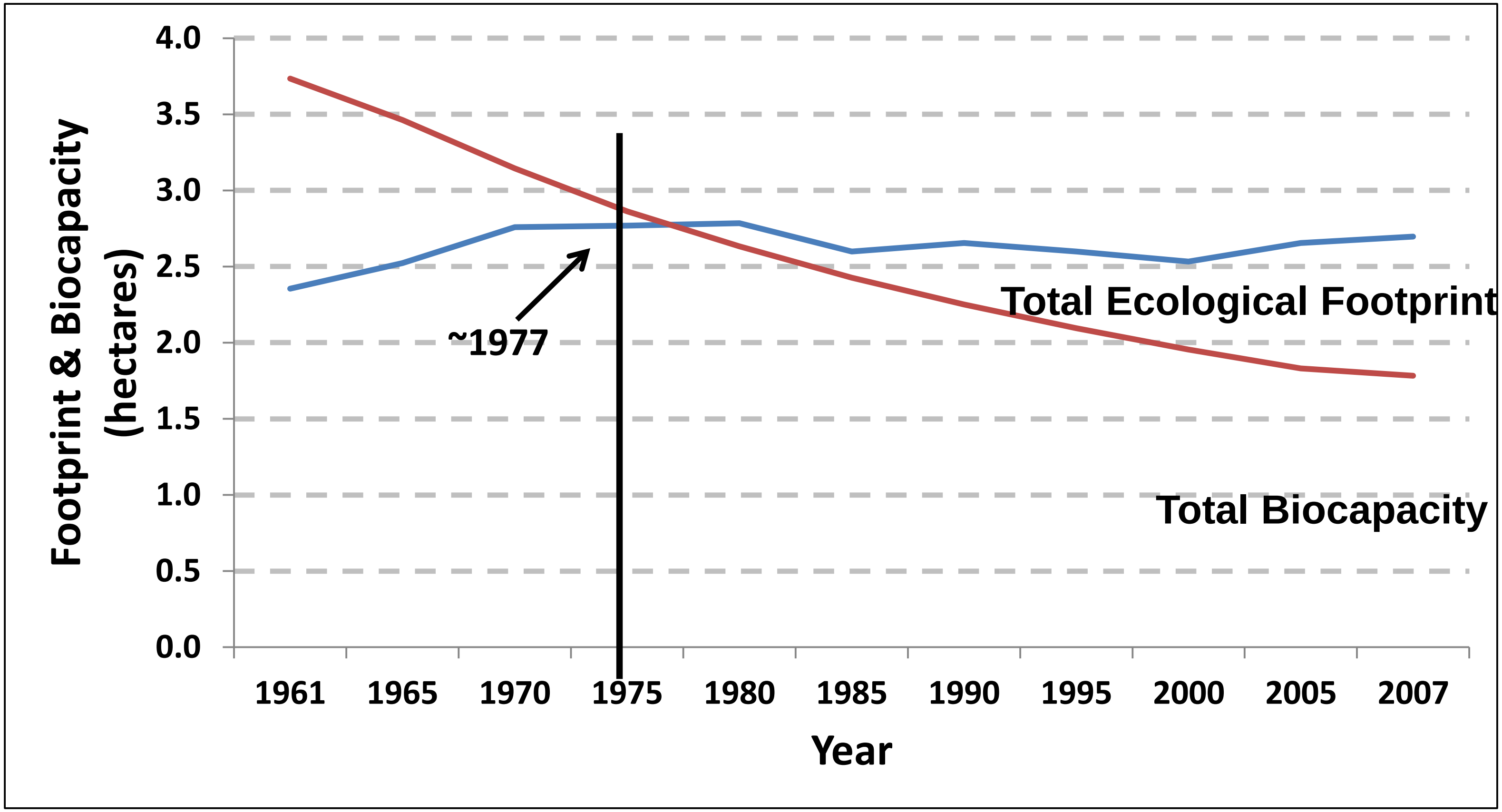
Real Gross World Product

(https://en.wikipedia.org/wiki/Gross_world_product)

($US billions, 1990 intl $US)



World Ecological Footprint & World Biocapacity



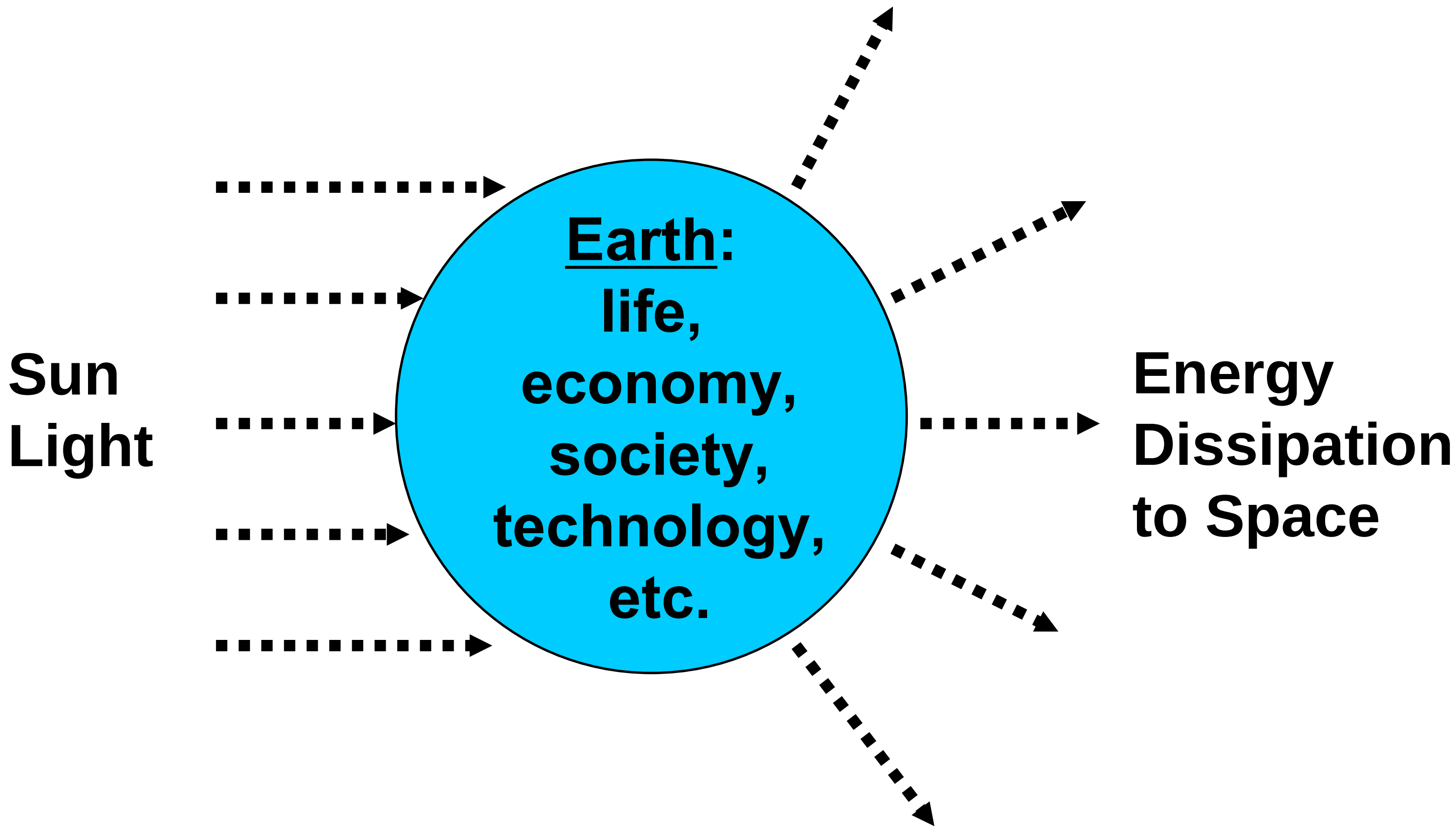
Source: National Footprint Accounts 2010 edition

www.footprintnetwork.org

Courtesy of M. Hopton, U.S. EPA

How does the biophysical world work?

(Mostly Closed to Mass & Open to Energy)



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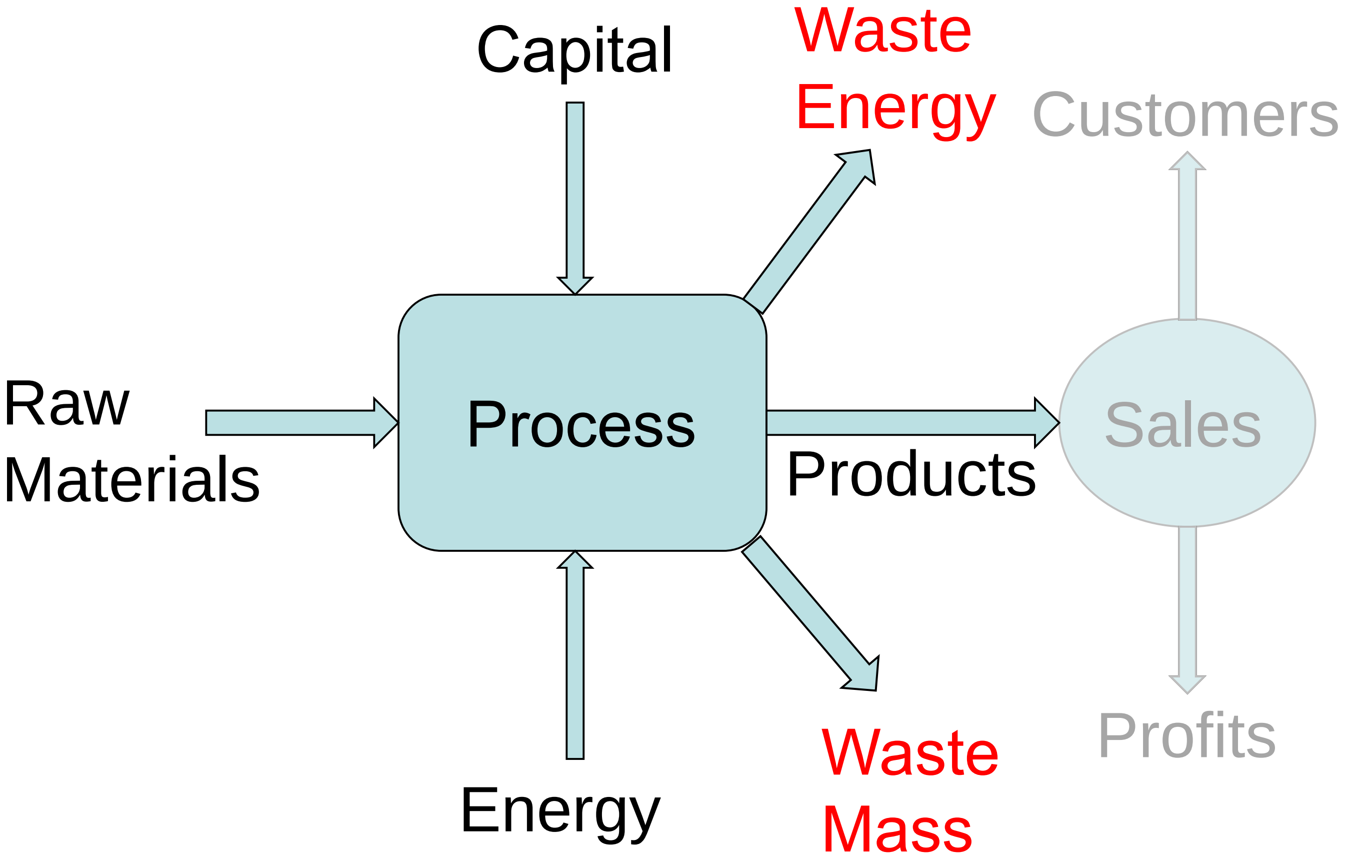
Process Design

Processes/Industrial Manufacturing



Sustainable Processes

IT HAS TO BE SYSTEMATIC SO THAT GOOD OPTIONS DONOT GET OVERLOOKED!

1. There is a hierarchical scheme for sustainable process design:
   a. WAR Algorithm for initial screening and analysis of new and existing designs.
   b. GREENSCOPE for detailed process analysis.
2. For established process designs, SustainPro provides an effective algorithm for retrofitting to make processes more sustainable.

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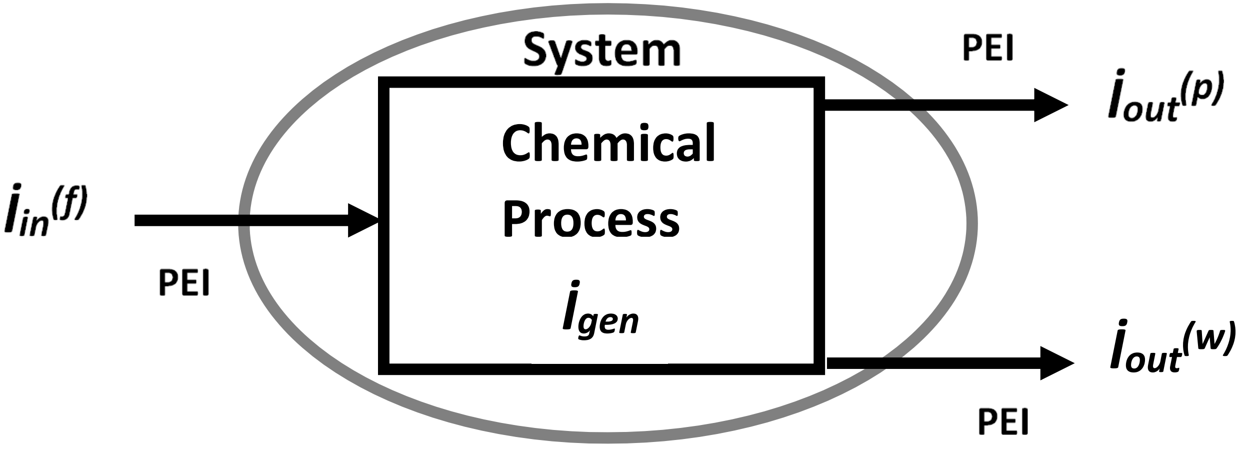
Sustainable Process Design: WAR Algorithm

Potential Environmental Impact (*I or PEI*)



$$\dot{I}_k^{(i)} = \frac{dI_k^{(i)}}{dt} = \frac{dM_k^{(i)}}{dt} \sum_l x_{kl} \psi_l$$

$$\psi_l = \sum_m \alpha_m \psi_{lm}$$

Potential Environmental Impact Balances

General Expression:

$$\frac{dI^{System}}{dt} = \sum_{k=f} \frac{dI_k^{(f)}}{dt} - \sum_{k=p} \frac{dI_k^{(p)}}{dt} - \sum_{k=w} \frac{dI_k^{(w)}}{dt} + \frac{dI_{gen}}{dt}$$

Steady State:

$$\frac{dI_{gen}}{dt} = \sum_{k=p} \frac{dI_k^{(p)}}{dt} + \sum_{k=w} \frac{dI_k^{(w)}}{dt} - \sum_{k=f} \frac{dI_k^{(f)}}{dt}$$

Design Criteria

Either Consume PEI or Minimize PEI Generation:

$$\frac{dI_{gen}}{dt} \leq 0$$

Minimize the Output of PEI:

$$\left[\sum_{k=p} \frac{dI_k^{(p)}}{dt} + \sum_{k=w} \frac{dI_k^{(w)}}{dt} \right] \geq 0$$

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Sustainable Process Design: GREENSCOPE

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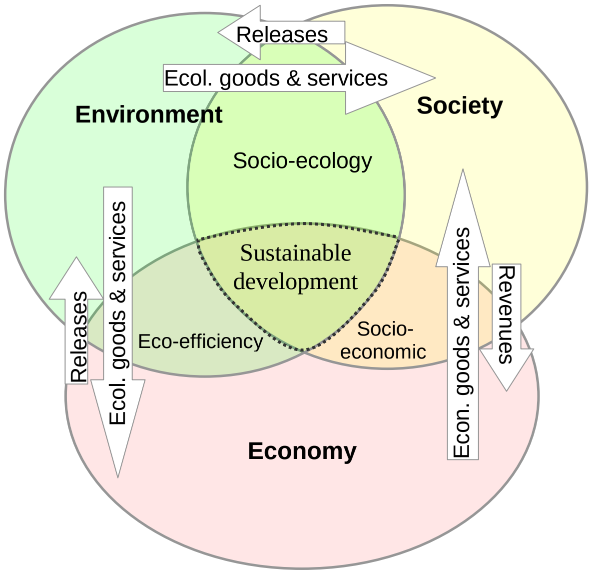
Chemical Process Indicators

- Triple dimensions of sustainable development
  - –Environment, Society, Economy
  - –Corporate level indicators
  - –Assessment at corporate level



- Four areas for promoting & informing sustainability
- Environmental, Efficiency, Economics, Energy (4E's)
- Decision-making at process design level
- Taxonomy of chemical process indicators for use in process design

GREENSCOPE Indicators

Environmental (66)	Efficiency (26)	Economic (33)	Energy (14)
•Specifications of process input material (e.g., hazardous) •Operating conditions and process operation failures (health and safety hazards) •Impact of components utilized in the system •Potential impact of releases •100% sust., best target, no pollutants release, & no hazardous material use or generation	•Quantities of inputs required/product or a specific process task (e.g., separation) •Mass transfer operations, energy demand, equipment size, costs, raw materials, releases •Connect input/output with product, intermediate or operation unit •The reference states are defined as mass fractions $0 \leq x \leq 1$	•A sustainable economic outcome must be achieved •Based on profitability criteria for projects (process, operating unit), may or may not account for the time value of money •Some cost criteria Indicators: capital & manufacturing costs; Input costs: raw material cost; Output costs: waste treatment cost	•Different thermodynamic properties used to obtain energetic sustainability scores •Energy (caloric); exergy (available); emergy (embodied) •Zero energy consumption per unit of product trend can be best target •Most of the worst cases depend on the particular process or process equipment

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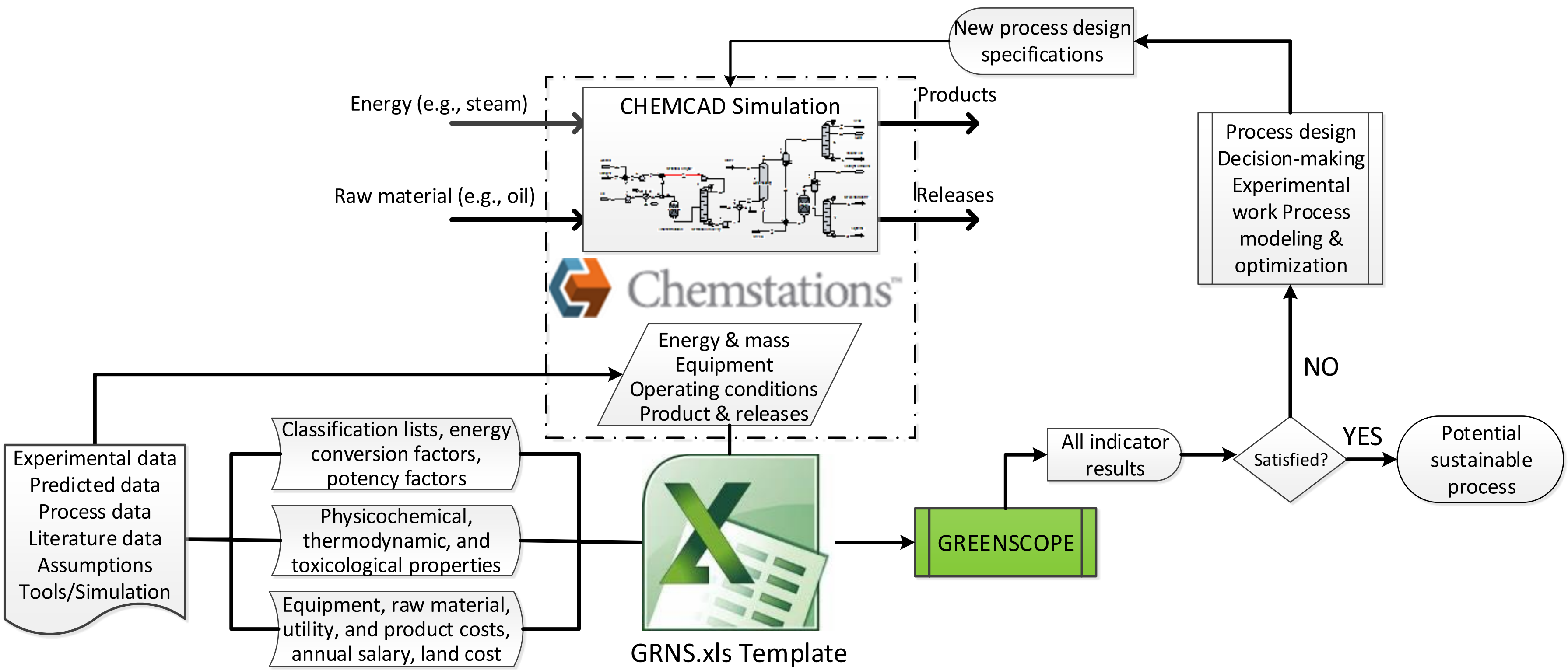
GREENSCOPE Sustainability Framework

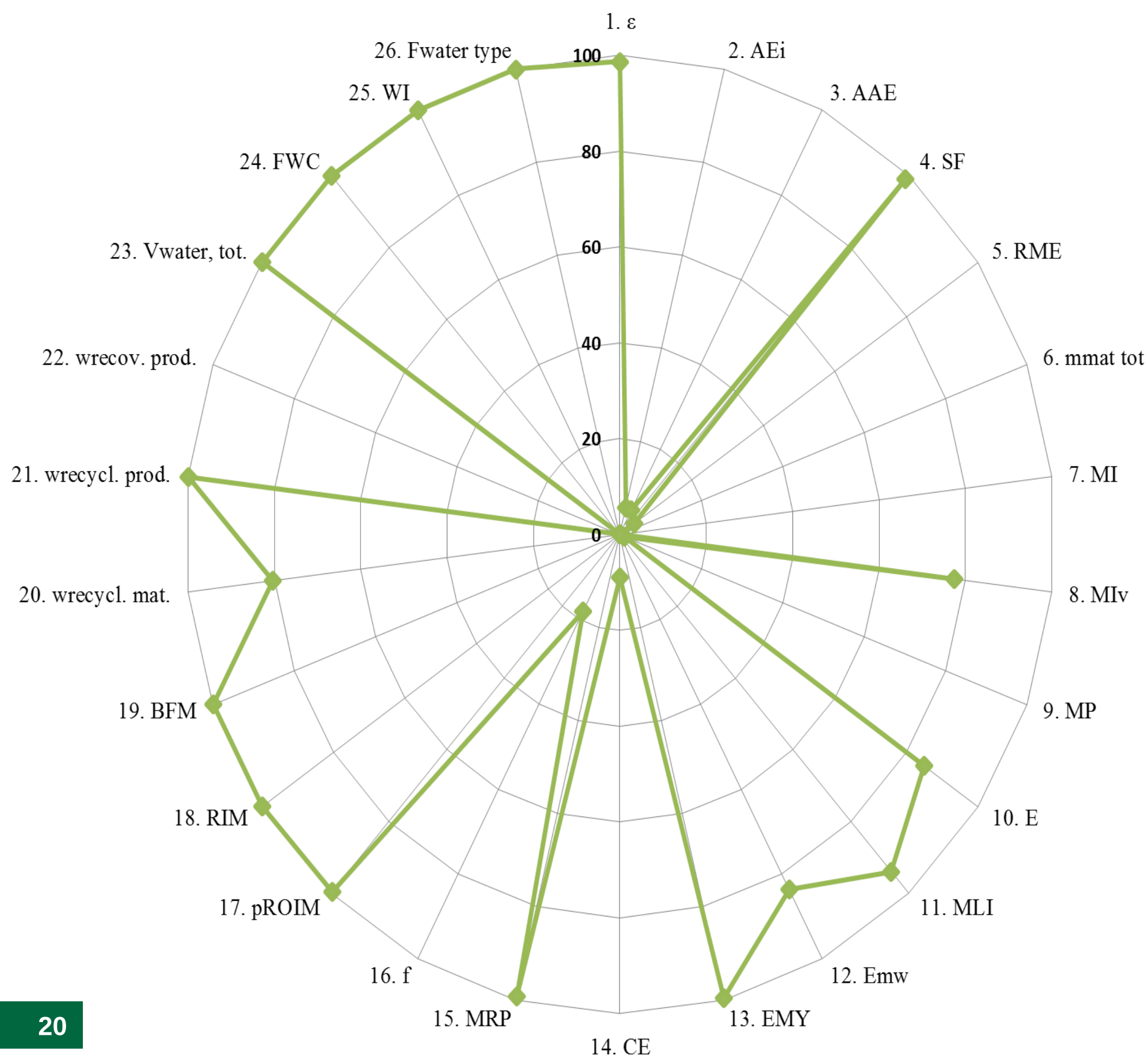
- Identification and selection of two reference states for each sustainability indicator:
- Best target: 100% of sustainability
- Worst-case: 0% of sustainability
- Two scenarios for normalizing the indicators on a realistic measurement scale
- Dimensionless scale for evaluating current process or tracking modifications/designs of new (part of a) process

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

Sustainability Assessment & Design: GREENSCOPE Tool

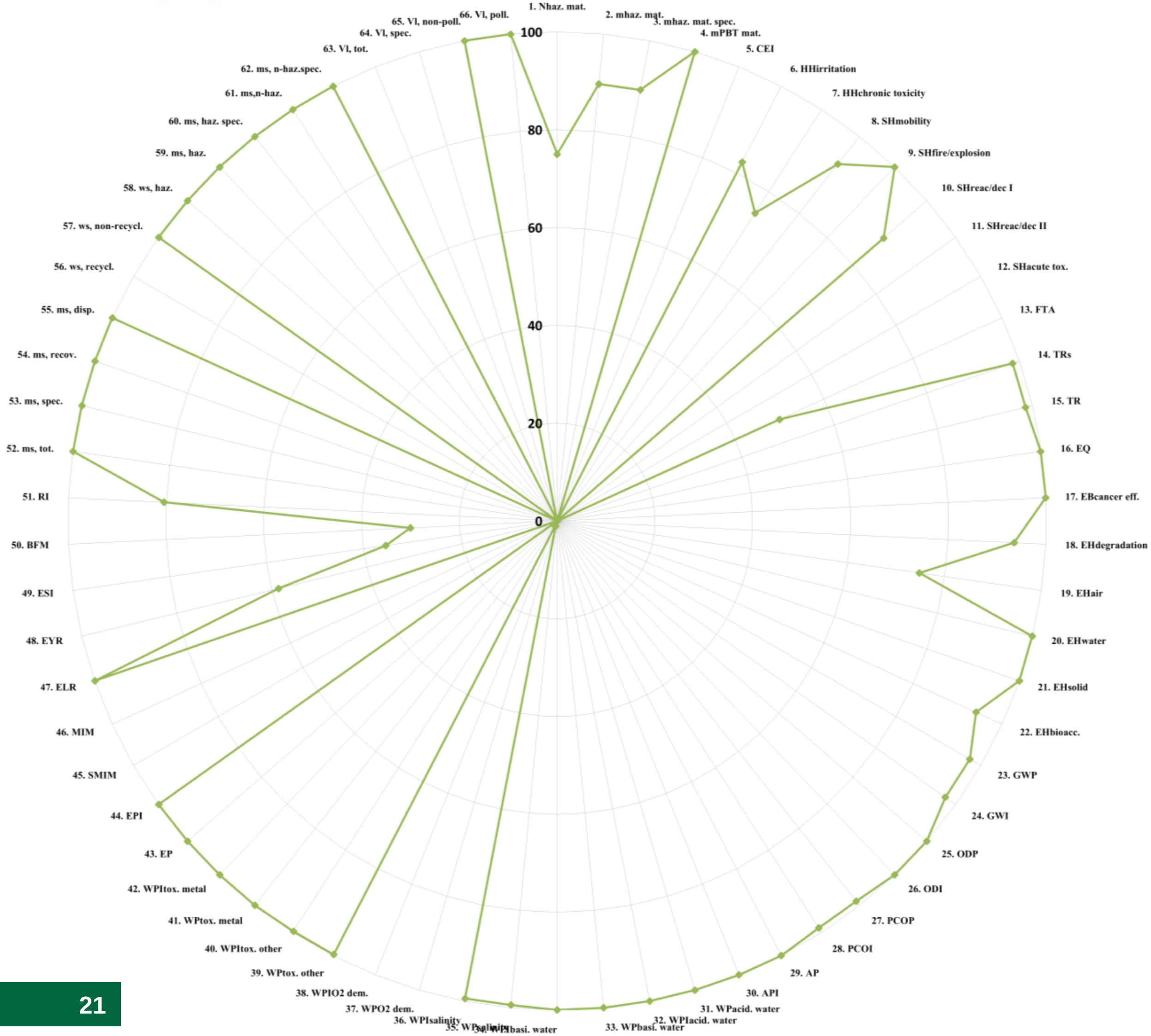


Efficiency Indicator Results



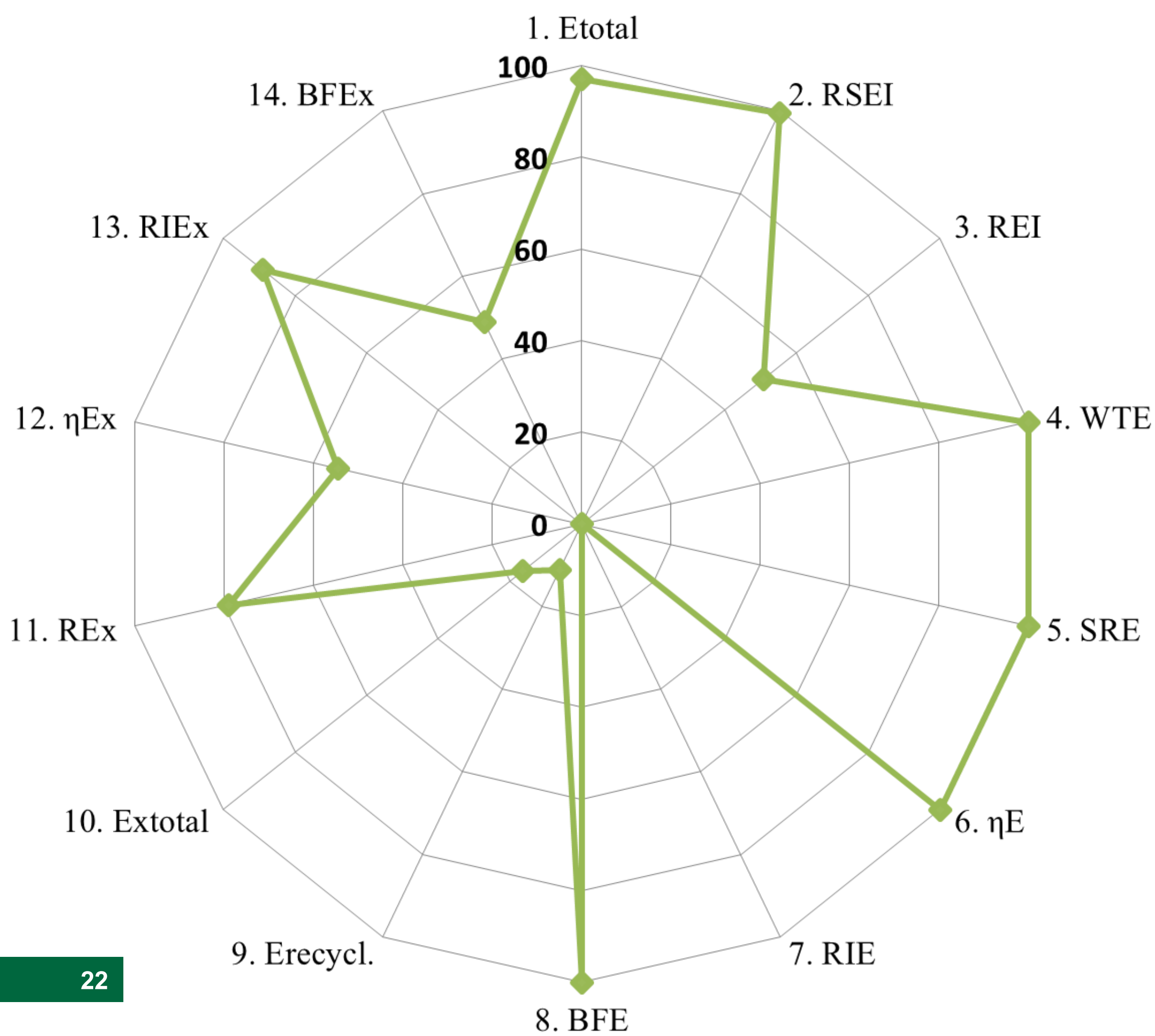
Indicator	Description	Sust. (%)
2. AE_i	Atom economy	5.8
7. MI_v	Value mass intensity	0
15. MRP	Material recovery parameter	0
17. $pROI_M$	Physical return on investment	99.4
23. $V_{water, tot.}$	Total water consumption	100

Environmental Indicator Results



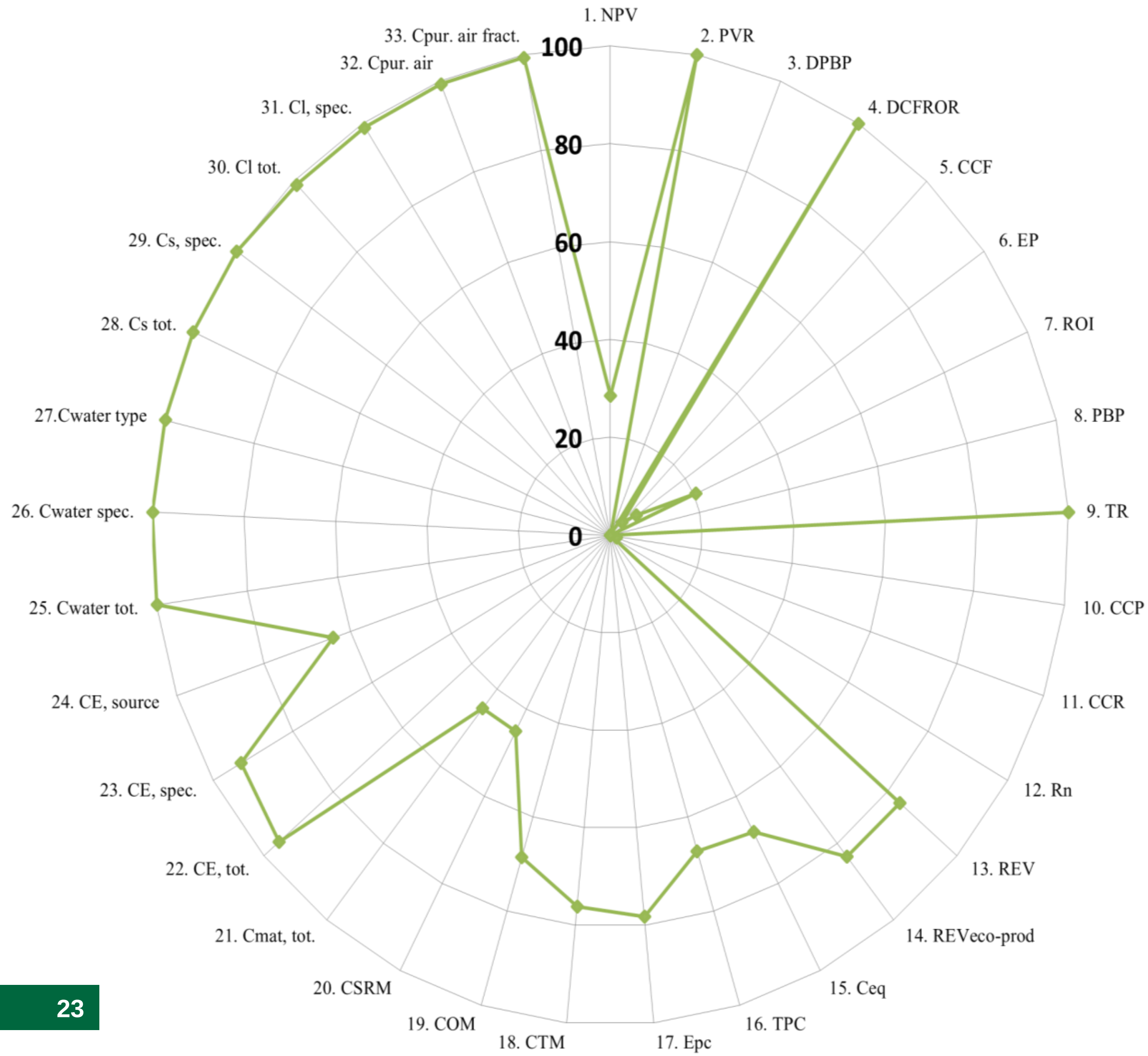
Indicator	Description	Sust. (%)
1. $N_{haz.\ mat.}$	Number of hazardous materials input	75
6. $HH_{irritation}$	Health hazard, irritation factor	68.5
10. $SH_{reac/dec\ I}$	Safety hazard, reaction / decomposition I	88.3
22. $EH_{bioacc.}$	Environmental hazard, bioaccumulation (the food chain or in soil)	89.3
43. EP	Eutrophication potential	100

Energy Indicator Results



Indicator	Description	Sust. (%)
2. R_{SEI}	Specific energy intensity	98.9
6. η_E	Resource-energy efficiency	77.0
8. BF_E	Breeding-energy factor	100.0
10. Ex_{total}	Exergy consumption	0.0
14. BF_{Ex}	Breeding-exergy factor	36.1

Economic Indicator Results



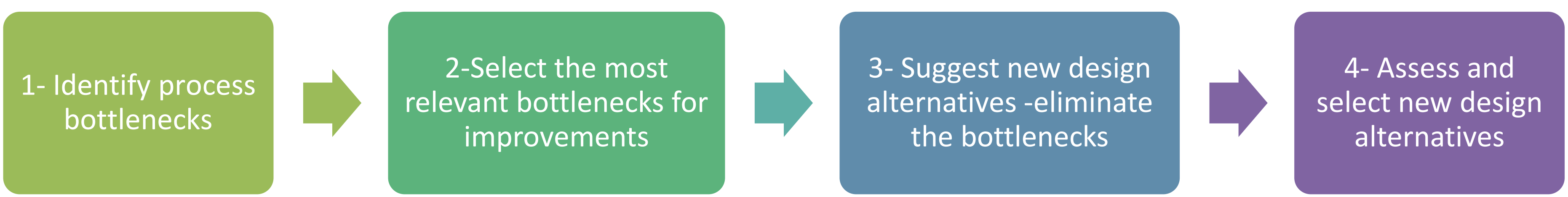
Indicator	Description	Sust. (%)
1. NPV	Net present value	45.9
8. PBP	Payback Period	92.0
19. COM	Manufacturing cost	68.0
23. $C_{E,\ spec.}$	Specific energy costs	63.1
33. $C_{pur.\ air\ fract.}$	Fractional costs of purifying air	0.0

Process Retrofit: SustainPro

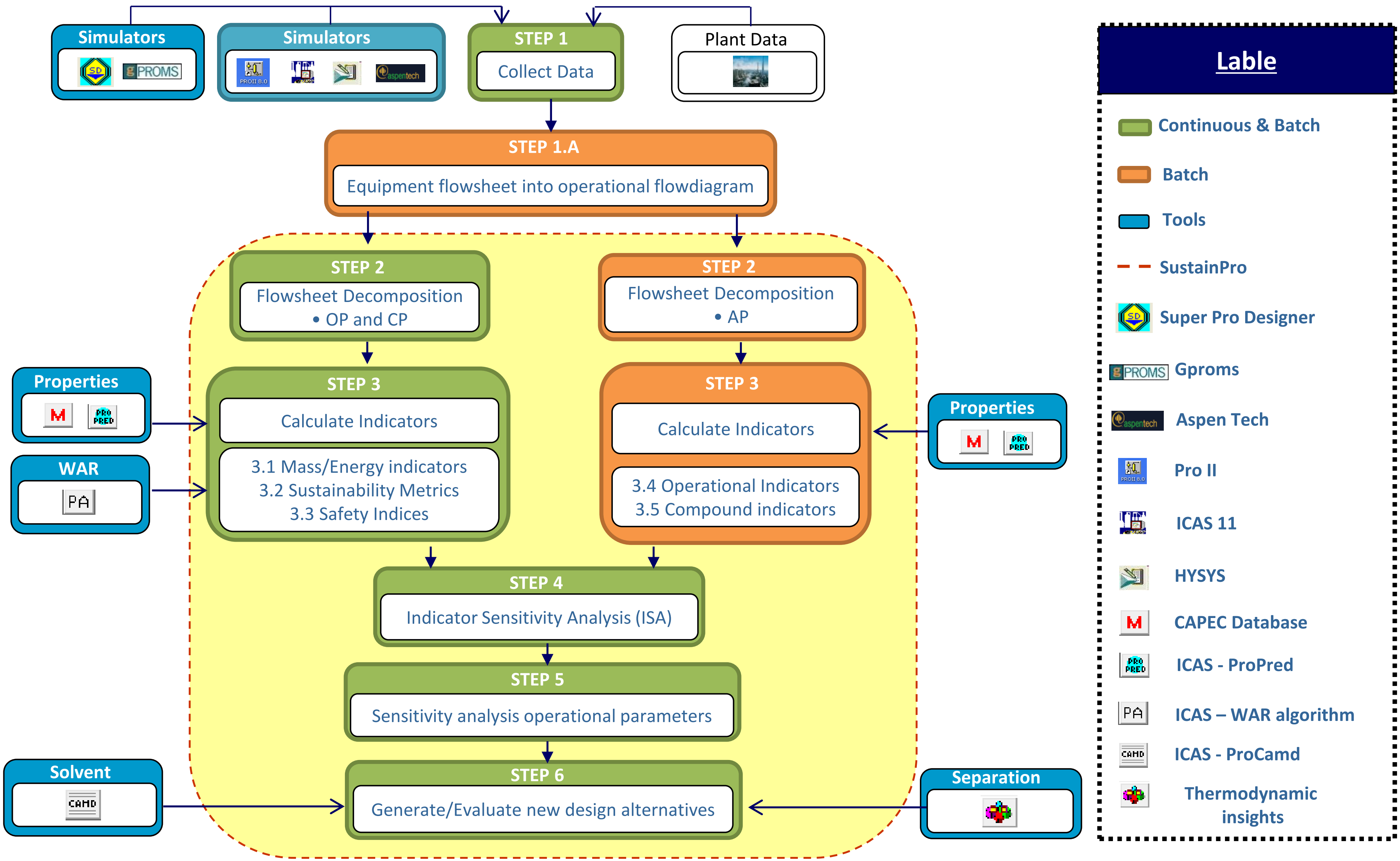
Process Retrofit

Retrofit design has been defined by Guinand (2001) as follows: “Process retrofitting is the redesign of an operating chemical process to find new configuration and operating parameters that will adapt the plant to changing conditions to maintain its optimal performance.”

Retrofit Generic Methodology



SustainPro- Retrofit Tool



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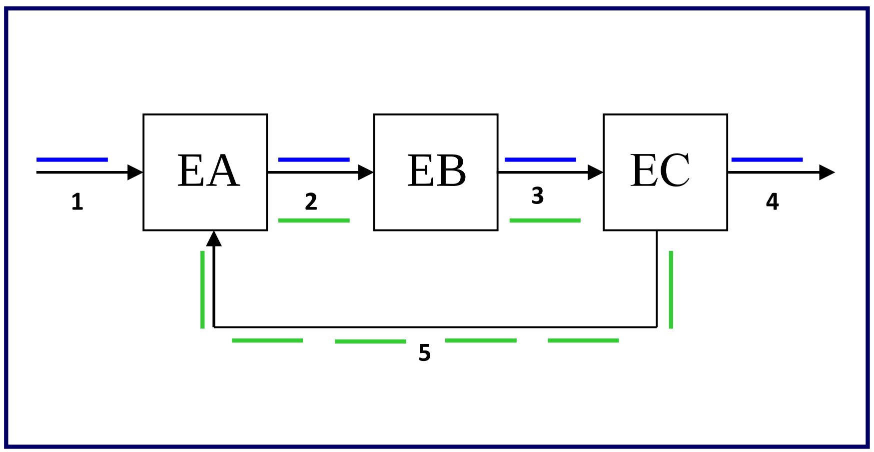
SustainPro- Retrofit Tool.

Step 1- Data Collection

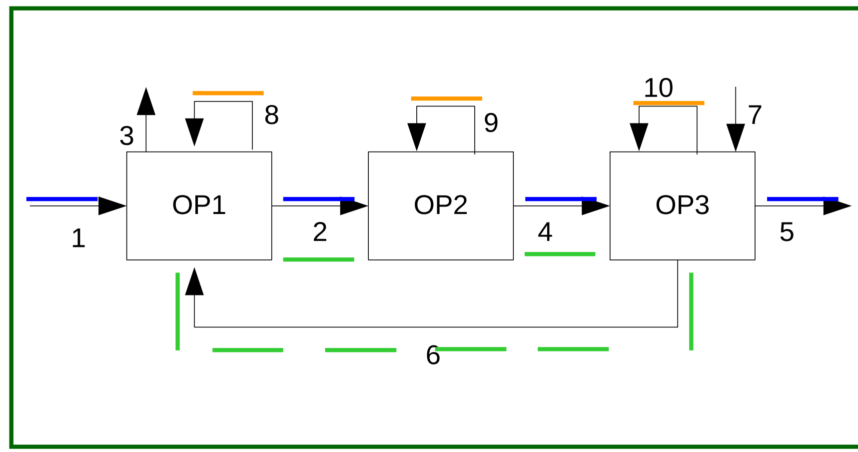
OR

Simulators

Step 2- Flowsheet Decomposition



Continuous Process



Batch Process

Closed-path Open-path Accumulation-path

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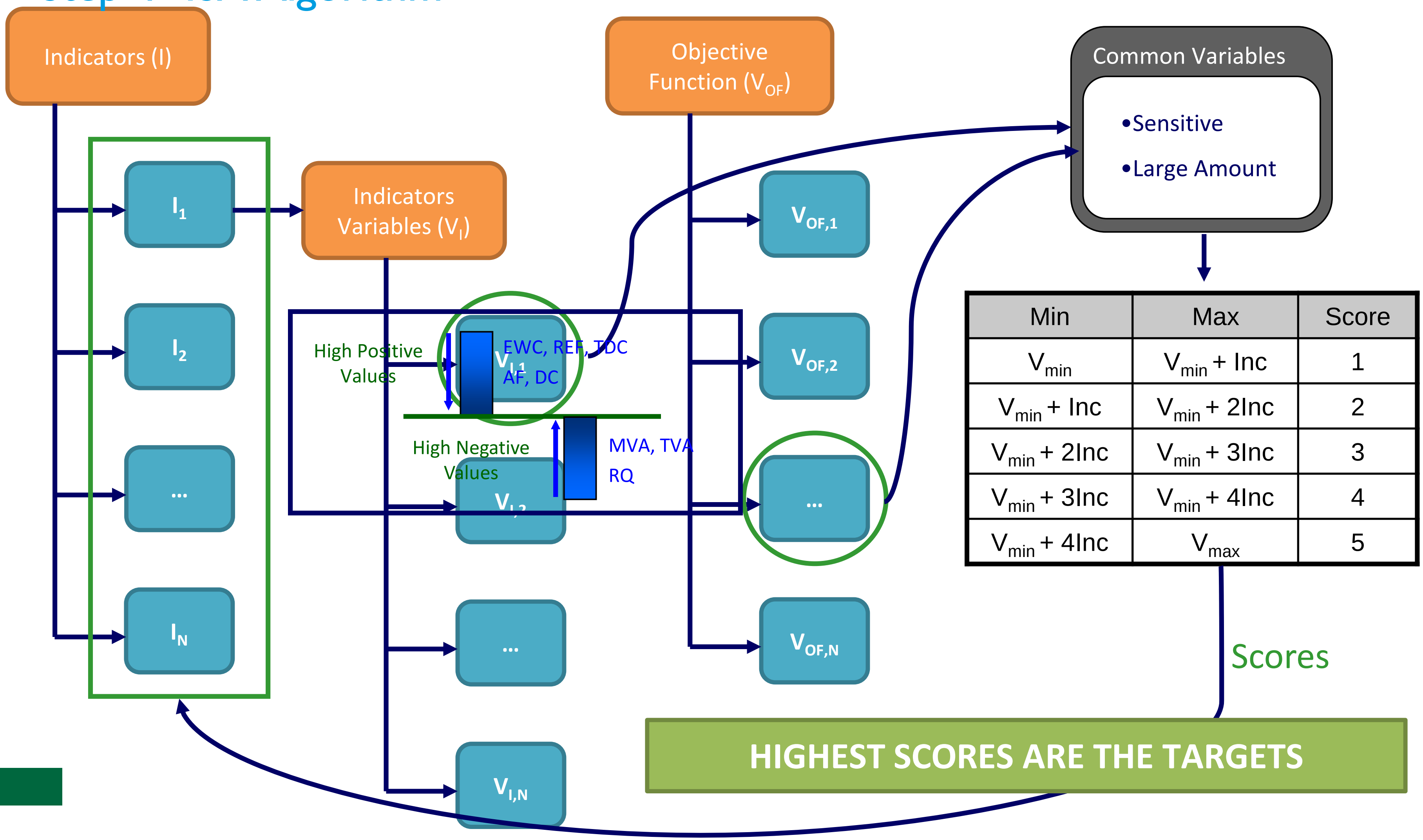
SustainPro- Retrofit Tool: Indicators

Step 3- Indicators Calculation

Indicator	Description	Definition
MVA	Material Value Added	$MVA = M_T*(P_{sale}-P_{cost})$
EWC	Energy & Waste Cost	$EWC = E\ P_E\ M_i\ \theta_i/(\Sigma_i\ M_i\ \theta_i)$
TVA	Total Value Added	$TVA = MVA - EWC$
RQ	Reaction Quality	$RQ = R_X\ \theta_R/\ (\Sigma_p\ M_p)$
AF	Accumulation Factor	$AF = M_{i\text{-cycle}}\ /(\Sigma_{k\text{-cycle}}\ M_{k\text{-cycle}})$
REF	Reusable Energy Factor	$REF = E_{used\text{-cycle}}/\ E_{exit\text{-cycle}}$
DC	Demand Cost	$DC = P_{utility}E_{open\text{-path}}$
TDC	Total Demand Cost	$TDC = \Sigma\ DC_k$

SustainPro- Retrofit Tool: Algorithm

Step 4- ISA Algorithm



Min	Max	Score
V_{min}	V_{min} + Inc	1
V_{min} + Inc	V_{min} + 2Inc	2
V_{min} + 2Inc	V_{min} + 3Inc	3
V_{min} + 3Inc	V_{min} + 4Inc	4
V_{min} + 4Inc	V_{max}	5

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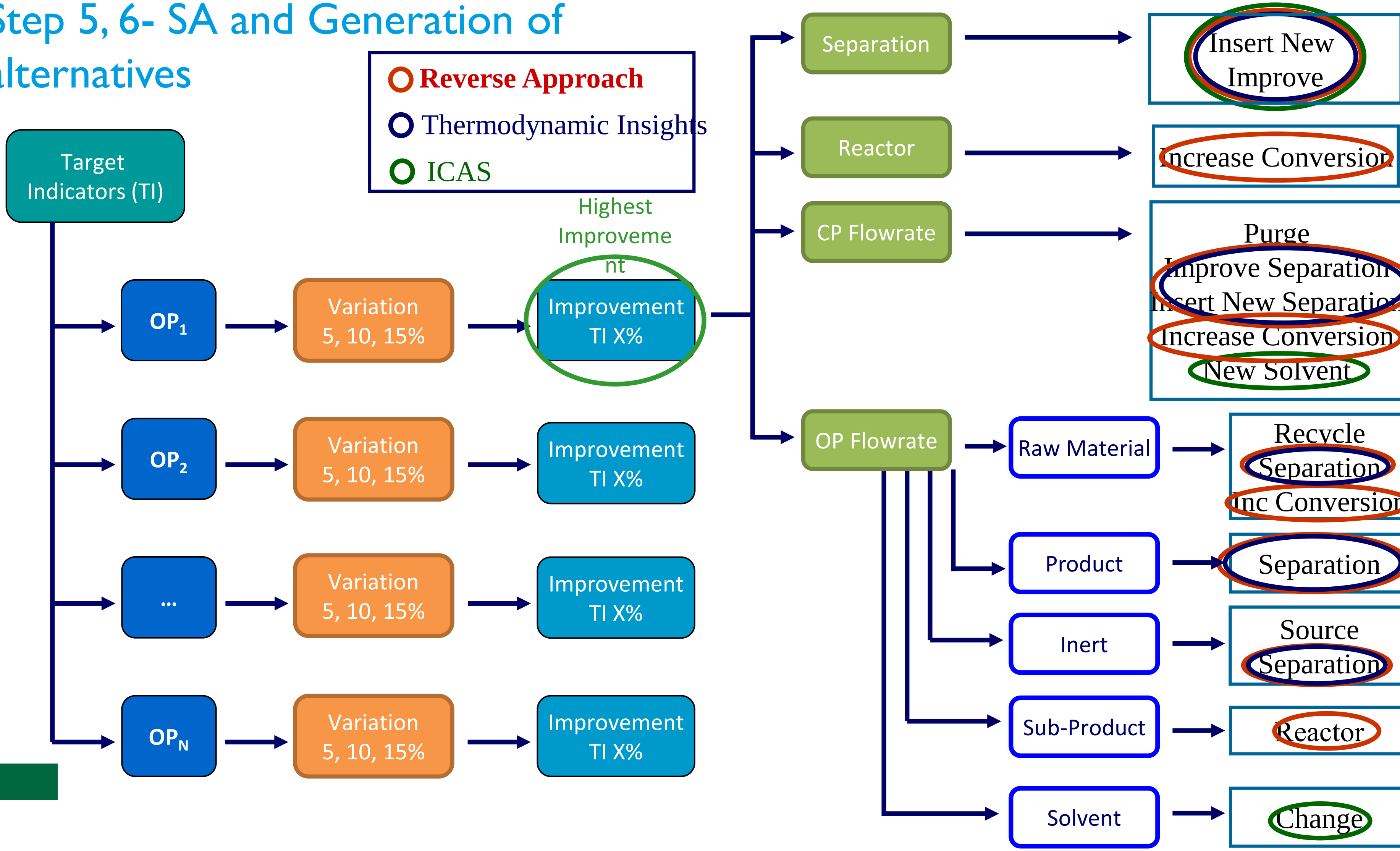
SustainPro- Retrofit Tool: Alternatives

Step 5, 6- SA and Generation of alternatives



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Sustainable Processes: Bringing It All Together

Some Final Thoughts

- **There is a hierarchical scheme for sustainable process design of new designs:**
  - **WAR Algorithm for initial screening analysis.**
  - **GREENSCOPE for detailed process analysis.**
- **For established process designs, SustainPro provides an effective algorithm for retrofitting to make processes more sustainable.**
- **However, these tools do not and can not substitute for the skill of the engineer. A fine hammer is wonderful in the hands of a skilled carpenter but useless in unskilled hands.**