Chemical Process Development for Sustainability

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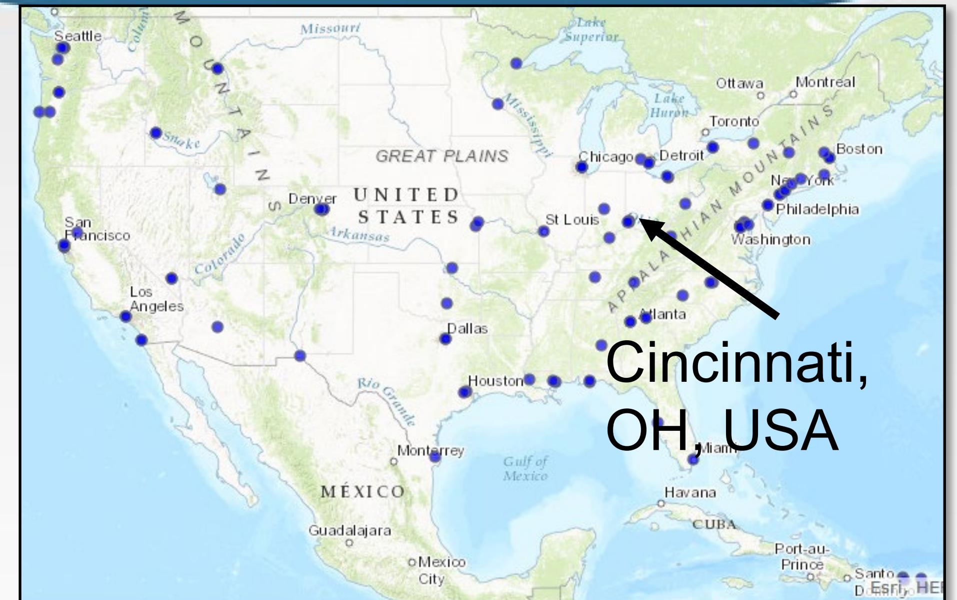

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- Office of Research and Development (ORD)
- Center for Environmental Solutions and Emergency Response

Some research areas:
Life cycle assessment, impact assessment, and sustainable chemistry

http://savecincinnati.com/images/cincinnati%20skyline.jpg

http://www.rwdconsultingllc.com/wp-content/uploads/2014/01/EPA_ohio1.jpg

Contents

- Sustainable Development
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- GREENSCOPE Tool
- Design for Sustainability and GREENSCOPE Evaluation
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- EPA Information and Opportunities

Sustainable Development

- This concept was placed in 1987
- “Our common future” report from the World Commission on Environment and Development (WCED):

“Development that meets the needs of the present without compromising the ability of future generations to meet their own needs.”

- This is the most widely accepted definition of sustainable development across the world

Sustainable Development Goals

17 Goals with 169 associated targets which are integrated and indivisible (From 2015 to 2030)

http://www.un.org/sustainabledevelopment/wp-content/uploads/2015/09/Icons-FINAL.png

Sustainable Development Goals, 1 - 8:
Specific targets to be achieved by 2030

1. End poverty in all its forms everywhere
2. End hunger, achieve food security and improved nutrition and promote sustainable agriculture
3. Ensure healthy lives and promote well-being for all at all ages
4. Ensure inclusive and quality education for all and promote lifelong learning
5. Achieve gender equality and empower all women and girls
6. Ensure access to water and sanitation for all
7. Ensure access to affordable, reliable, sustainable and modern energy for all
8. Promote inclusive and sustainable economic growth, employment and decent work for all

http://www.un.org/ga/search/view_doc.asp?symbol=A/RES/70/1&Lang=E

Sustainable Development Goals, 9 - 17

9. Build resilient infrastructure, promote sustainable industrialization and foster innovation
10. Reduce inequality within and among countries
11. Make cities inclusive, safe, resilient and sustainable
12. Ensure sustainable consumption and production patterns
13. Take urgent action to combat climate change and its impacts
14. Conserve and sustainably use the oceans, seas and marine resources
15. Sustainably manage forests, combat desertification, halt and reverse land degradation, biodiversity loss
16. Promote just, peaceful and inclusive societies
17. Revitalize the global partnership for sustainable development

http://www.un.org/ga/search/view_doc.asp?symbol=A/RES/70/1&Lang=E

Goal 7. Ensure access to affordable, reliable, sustainable and modern energy for all by 2030

7.1 Ensure universal access to affordable, reliable and modern energy services

7.2 Increase substantially the share of renewable energy in the global energy mix

7.3 Double the global rate of improvement in energy efficiency

7.a Enhance international cooperation to facilitate access to clean energy research and technology, including renewable energy efficiency and advanced and cleaner fossil-fuel technology

7.b Expand infrastructure and upgrade technology for supplying modern and sustainable energy services for all in developing countries

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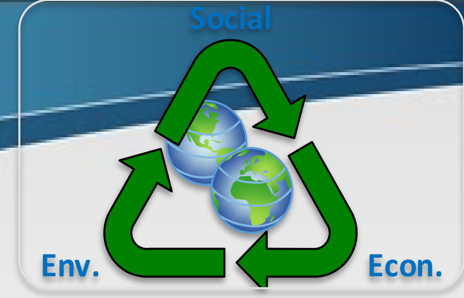
Sustainability for Chemical Processes, 1/2

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

Sustainability for Chemical Processes, 2/2



- Guidelines to achieve quality of life improvements
  - without affecting the availability of ecological goods & services
- Assess and address environmental, social, and economic aspects affected by industry
  - identify which system components are affected
  - localize process and product aspects which generate effects
  - redesign relevant processes and products & demonstrate system improvements
- Minimize or eliminate the environmental impacts and maximize the social/economic benefits

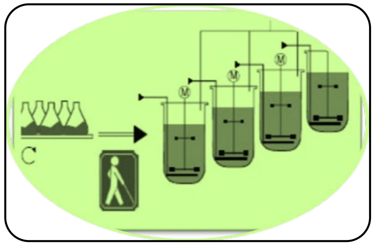
Needs of Industry to Incorporate Sustainability

Current environmental and social challenges toward more sustainable development

- Sustainable chemical process & products: meet economic, social, and environmental benefits

Join efforts to incorporate sustainability principles

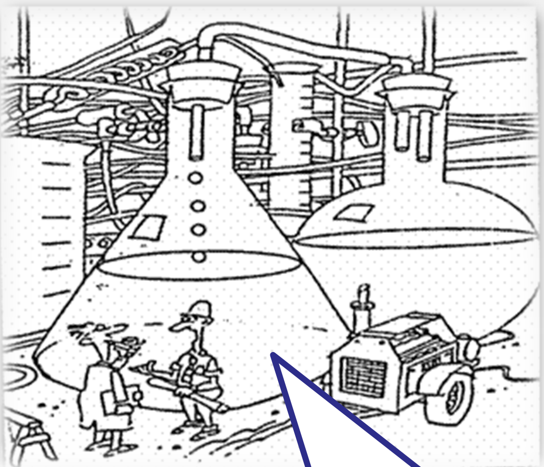
- Efficient material transformation
- Less energy consumption and waste generation
- Clean processes, optimum social and economic benefits



Sustainability from the lab to the manufacturing plant

Easy to scale-up manufacturing equipment and processes

Sustainability From the Lab to the Manufacturing Plant



We've got a few problems going from lab scale to full scale commercial

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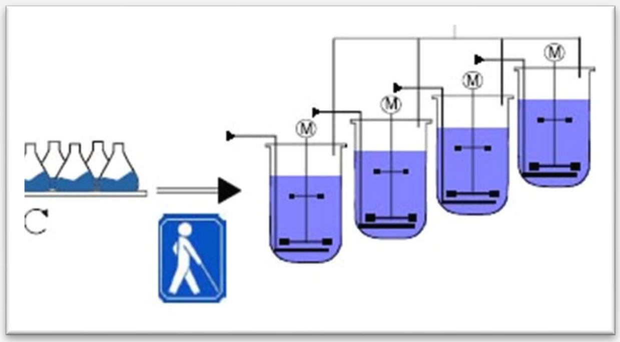

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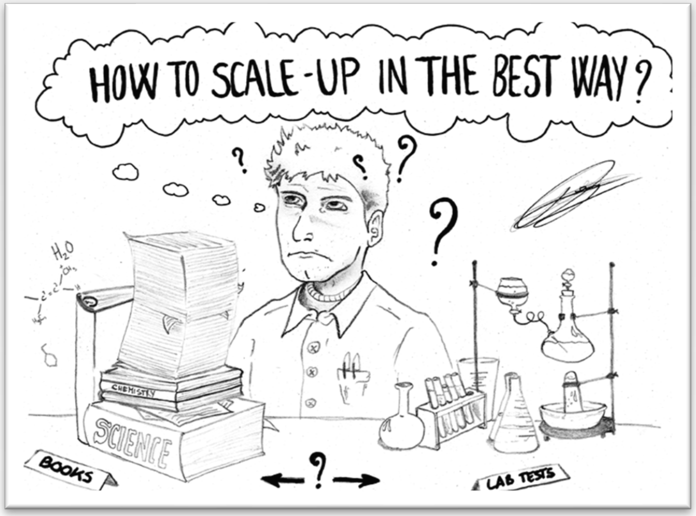

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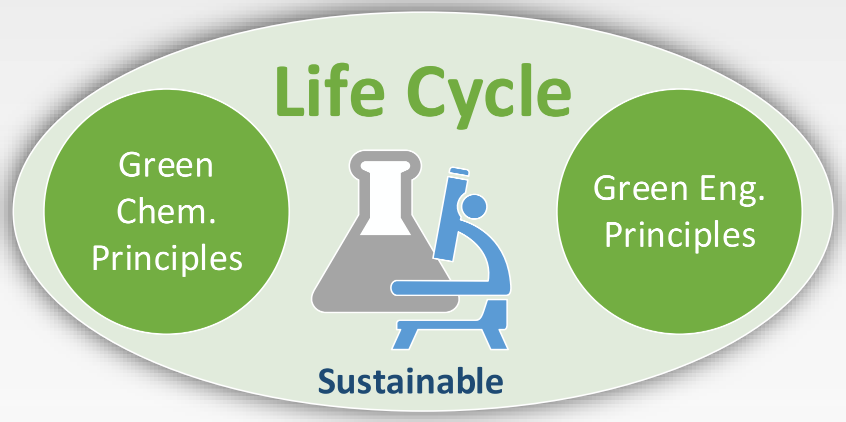
How to Achieve Sustainability (1/2)?

- Sustainability is characterized by:
  - Efficient energy and material use
  - Less waste generation
  - Clean and simple processes
  - Optimum social and economic benefits
- Sustainable chemicals should be safer, nonhazardous, with zero or reduced environmental impacts, and renewables-based
- Design modifications of existing and new chemical products and processes
  - Example: comparing different reagents for producing the same valuable product

How to Achieve Sustainability (2/2)?



- Design modifications of existing and new chemical products and processes
- Developed under Green Chemistry and Green Engineering principles
- Life Cycle Assessment consideration

Green Chemistry & Green Engineering Principles

Green Chemistry Pocket Guide

The 12 Principles of Green Chemistry

Provides a framework for learning about green chemistry and designing or improving materials, products, processes and systems.

1. Prevent waste
2. Atom Economy
3. Less Hazardous Synthesis
4. Design Benign Chemicals
5. Benign Solvents & Auxiliaries
6. Design for Energy Efficiency
7. Use of Renewable Feedstocks
8. Reduce Derivatives
9. Catalysis (vs. Stoichiometric)
10. Design for Degradation
11. Real-Time Analysis for Pollution Prevention
12. Inherently Benign Chemistry for Accident Prevention

www.acs.org/greenchemistry

ACS Chemistry for Life™

ACS Green Chemistry Institute®

1.Inherent Rather Than Circumstantial
Designers need to strive to ensure that all materials and energy inputs and outputs are as inherently nonhazardous as possible.

2.Prevention Instead of Treatment
It is better to prevent waste than to treat or clean up waste after it is formed.

3.Design for Separation
Separation and purification operations should be designed to minimize energy consumption and materials use.

4.Maximize Efficiency
Products, processes, and systems should be designed to maximize mass, energy, space, and time efficiency.

5.Output-Pulled Versus Input-Pushed
Products, processes, and systems should be "output pulled" rather than "input pushed" through the use of energy and materials.

6.Conserve Complexity
Embedded entropy and complexity must be viewed as an investment when making design choices on recycle, reuse, or beneficial disposition.

7.Durability Rather Than Immortality
Targeted durability, not immortality, should be a design goal.

8.Meet Need, Minimize Excess
Design for unnecessary capacity or capability (e.g., "one size fits all") solutions should be considered a design flaw.

9.Minimize Material Diversity
Material diversity in multicomponent products should be minimized to promote disassembly and value retention.

10.Integrate Material and Energy Flows
Design of products, processes, and systems must include integration and interconnectivity with available energy and materials flows.

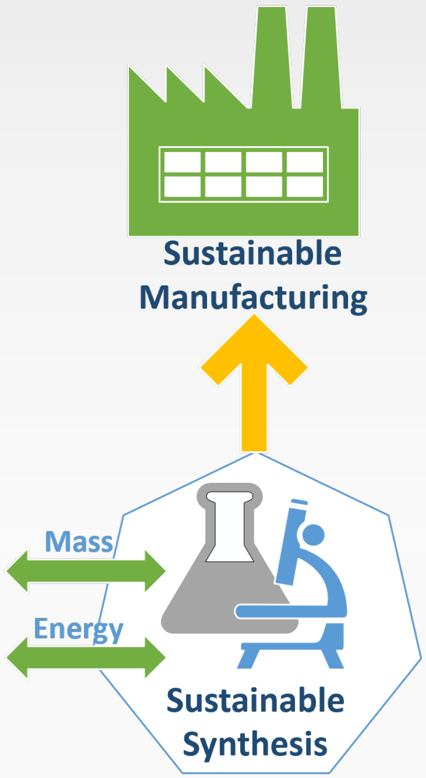
11.Design for Commercial "Afterlife"
Products, processes, and systems should be designed for performance in a commercial "afterlife."

12.Renewable Rather Than Depleting
Material and energy inputs should be renewable rather than depleting.

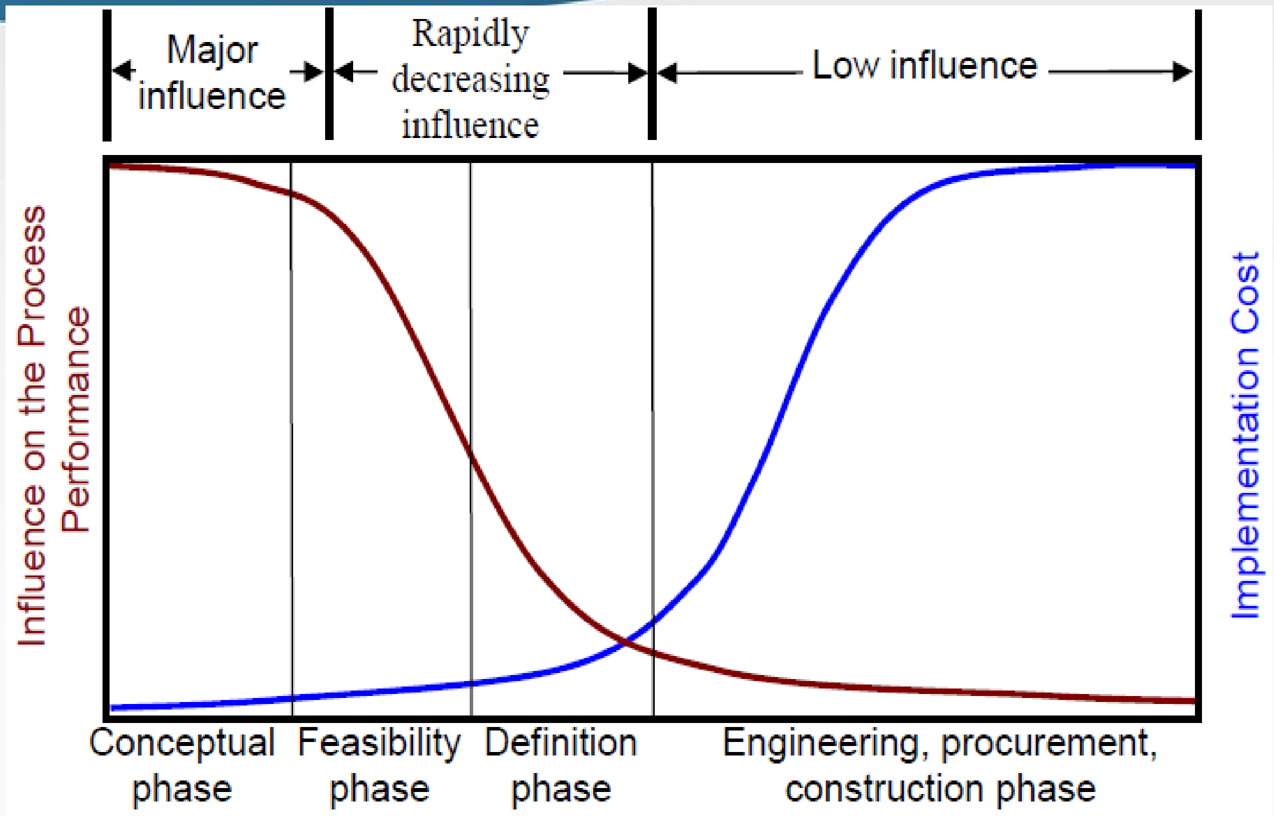
http://www.acs.org/content/dam/acsorg/greenchemistry/resources/the-12-principles-of-green-chemistry-pocket-guide.pdf
http://www.acs.org/content/acs/en/greenchemistry/what-is-green-chemistry/principles/12-principles-of-green-engineering.html

Early Consideration of Sustainability in the Chemical Synthesis (2/1)

- Early consideration of sustainability in the chemical synthesis is independent of the production scale
- Sustainability achievements at the lab would be reflected at manufacturing stage
  – Scalability limitations (material demand, conversion, energy needs, cost and revenues, etc.)
  – Accounted when developing novel synthesis routes

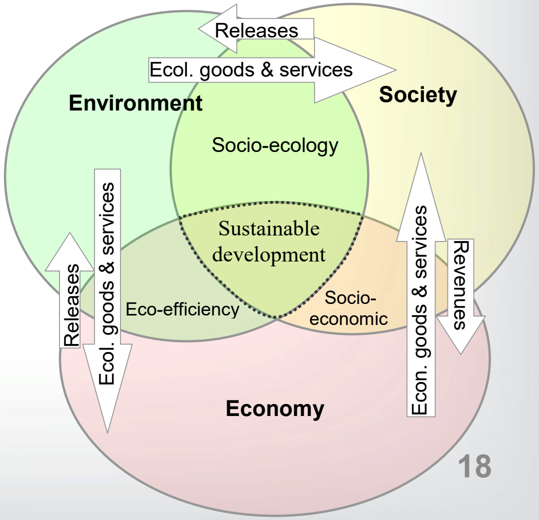


Early Consideration of Sustainability in the Chemical Synthesis (2/2)



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

Sustainability Assessment



Quantitative Sustainability Assessment

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

GREENSCOPE
- Sustainability indicators
- Dimensionless scale

Sustainability indicator results
- Trends
- Clear visualization

Potential sustainable process

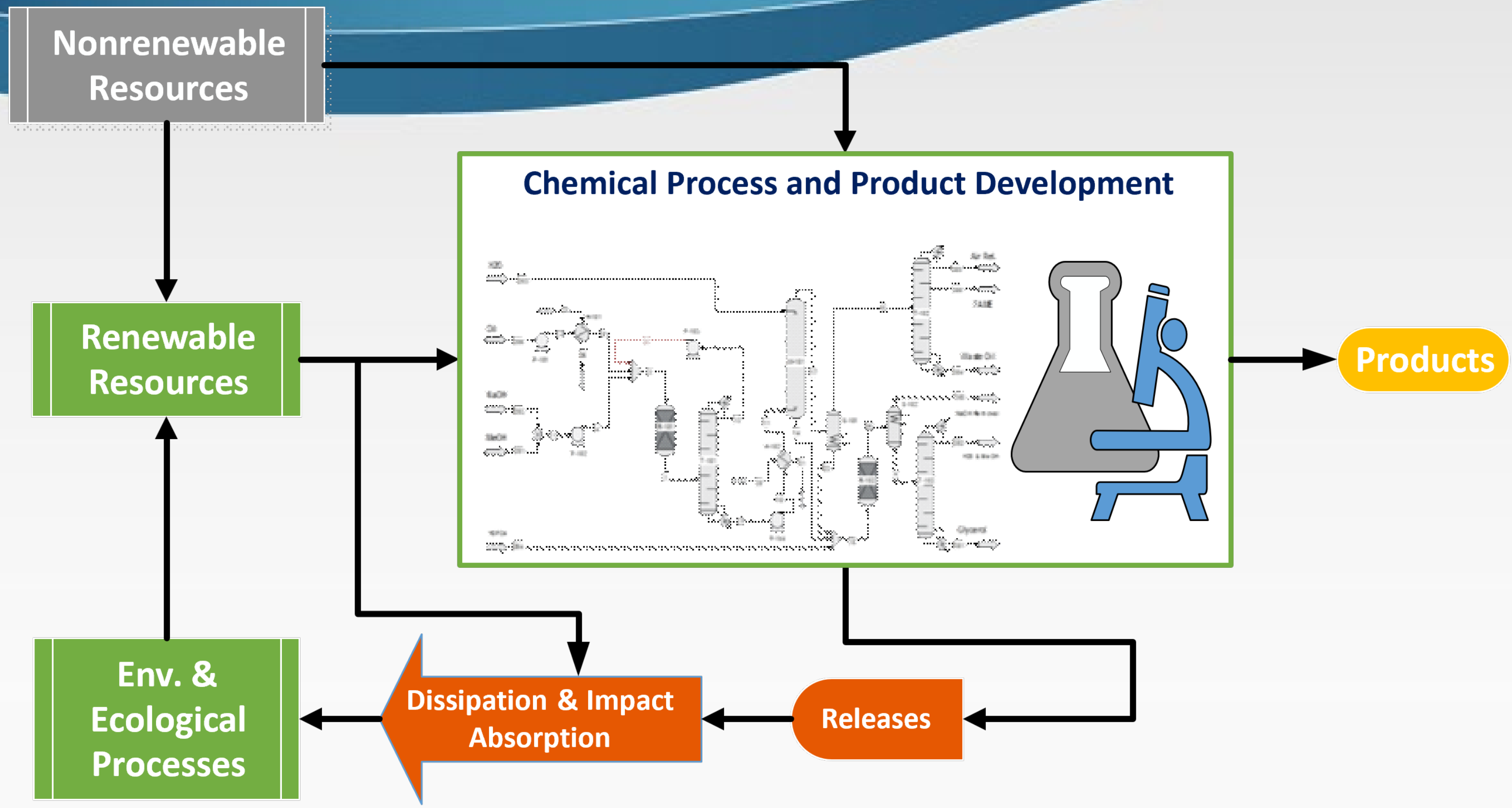
Qualitative Approaches
Apply all of them?
Levels of implementation?
A “win-win” situation?
Multiobjective function

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

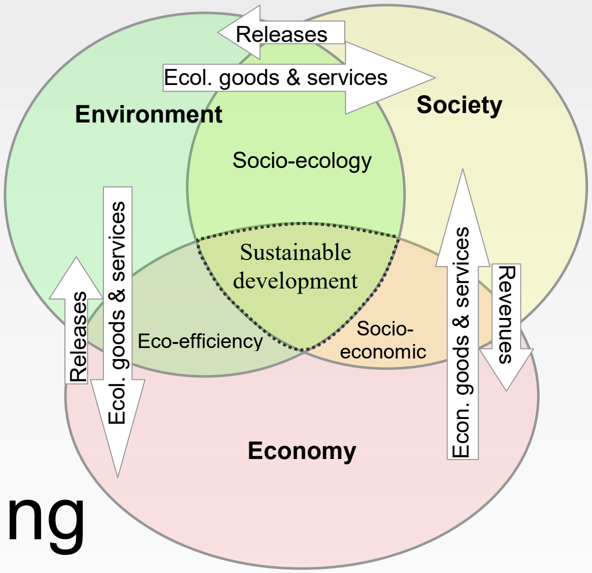
Sustainability for Chemical Synthesis



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

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

The GREENSCOPE Tool and Indicators

- Clear, practical, and user-friendly approach
- Monitor & predict sustainability at any process design stage
- Capable of calculating 139+ different indicators
- User can choose which indicators 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

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

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 costs	•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

GREENSCOPE Indicators: Example

Specific hazardous raw materials input

$$m_{\text{haz. mat. spec.}} = \frac{m_{\text{haz. mat.}}}{\text{Mass of product}}$$

$$m_{\text{haz. mat. spec.}} = \frac{\sum_{i=1}^{I} m^{\bullet\,\text{in}}_{\text{haz. mat.},i}}{m^{\bullet}_{\text{product}}}$$

Sustainability Value

Best, 100%	Worst, 0%
0	all inputs are hazardous

$m^{\bullet}_{\text{product}}$: mass flow of product *i* , kg
$m^{\bullet\,\text{in}}_{\text{haz.mat.},i}$: mass flow rate of the hazardous component *i*, kg

Global warming potential

$$\text{GWP} = \frac{\text{Total mass of } CO_2 \text{ equivalent produced}}{\text{Total mass of product}}$$

$$\text{GWP} = \frac{\sum_{i=1}^{I} m_i^{\bullet\text{out}} \times \text{PF}_{\text{CO2}, i}}{m^{\bullet}_{\text{product}}}$$

Sustainability Value

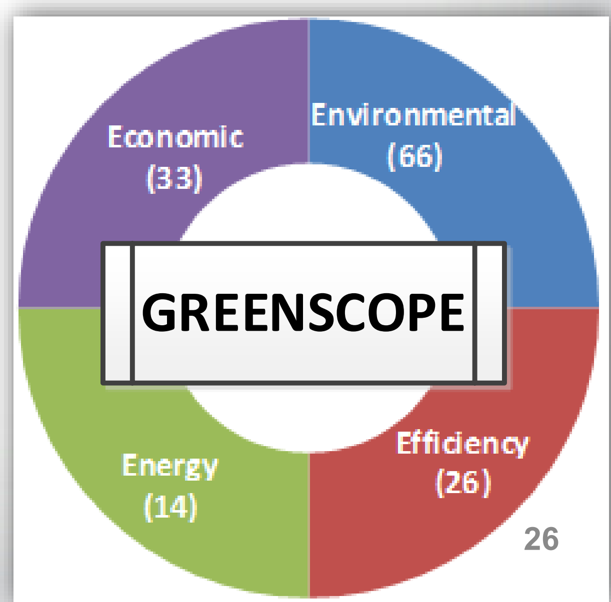
Best, 100%	Worst, 0%
1	any waste released has a potency factor at least equal to one

$m_i^{\bullet\,\text{out}}$: output mass flow rate of the component *i*, kg

$\text{PF}_{\text{CO2}, i}$: potency factor of the component *i* for the global warming burden, kg CO_2/kg *i*

$m^{\bullet}_{\text{product}}$: mass flow of product *i* , kg

Design for Sustainability and GREENSCOPE Evaluation



Maleic Anhydride Production Process: Conventional Approach

- MA is produced at industrial scale for applications in coatings and polymers:
  - Unsaturated polyester resin, production of fumaric and malic acid, lube oils as an additive, and maleic copolymers
- Currently, two main production routes:
  - Benzene oxidation or other aromatic compounds
    - Environmental concerns, increasing price of benzene
  - Gas phase oxidation of n-butane
    - Availability of n-butane as a feedstock
    - Nonrenewable material

Maleic Anhydride Production Process: A. Conventional Approach

- Major components in the MA process
  - Feedstock supply (benzene or n-butane), catalyst manufacture, air compression, reaction system, MA recovery/refining and off gas incineration
- Catalyst fixed bed reactor
  - Vanadium-phosphorus-oxide (VPO) for n-butane
  - V_2O_5-MoO_3 for benzene
- Multiple parallel and in-series oxidization reactions not only to MA, but also to CO and CO_2
- A large amount of water is produced
- Highly exothermic reactions

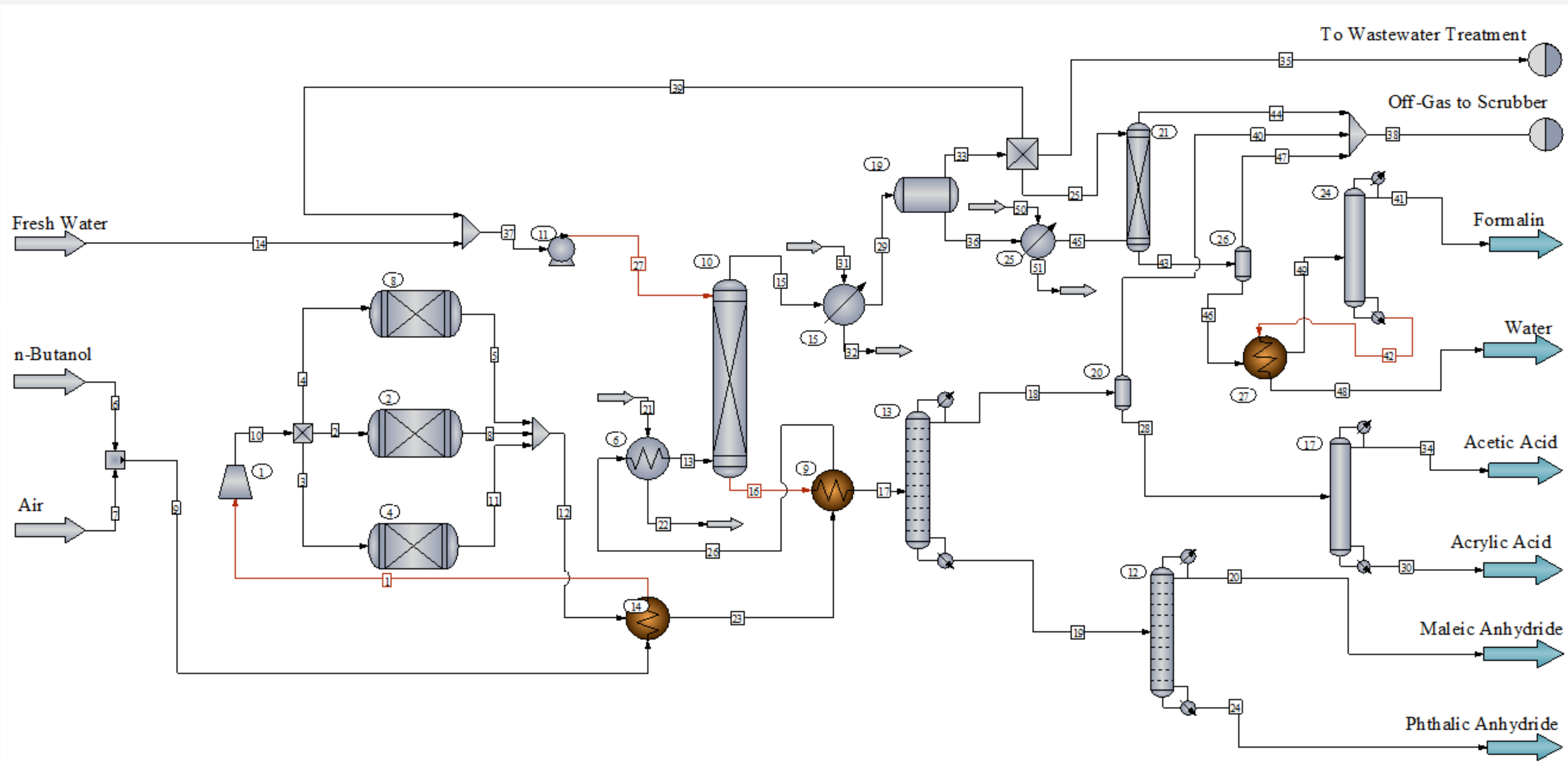
Maleic Anhydride Production Process: B. Bio-based Approach

- Feedstock: Bio-butanol with air
  - Gas phase reaction, no solvent used
- Catalyst fixed bed reactor
  - Catalyst: Vanadyl pyrophosphate
  - Air in excess is compressed, heated and mixed with the feedstock before being fed to the reactor
  - 3 s residence time
- T: 340 °C; P: 1 bar
- Multiple oxidization reactions:
  - MA, CO, CO_2, H_2O, phthalic anhydride, acetic acid, acrylic acid, and other "lights", such as formaldehyde, butenes, lighter hydrocarbons

Maleic Anhydride from Bio-butanol CHEMCAD Process Simulation

- Bio-butanol
- 98% butanol conversion
- Products: maleic anhydride, acetic acid, acrylic acid, phthalic anhydride, formalin
- Utilities: steam, electricity, cooling water
- Liquid, & air releases

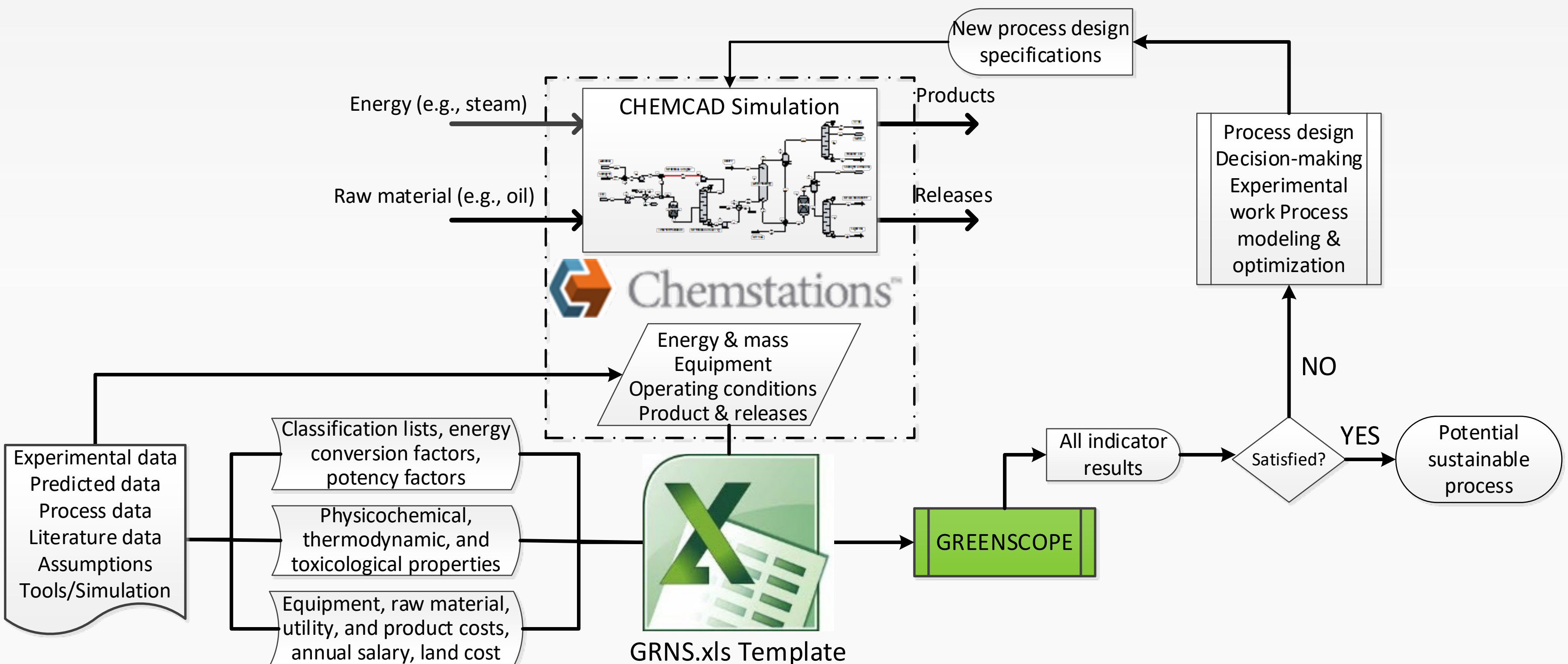
INPUTS



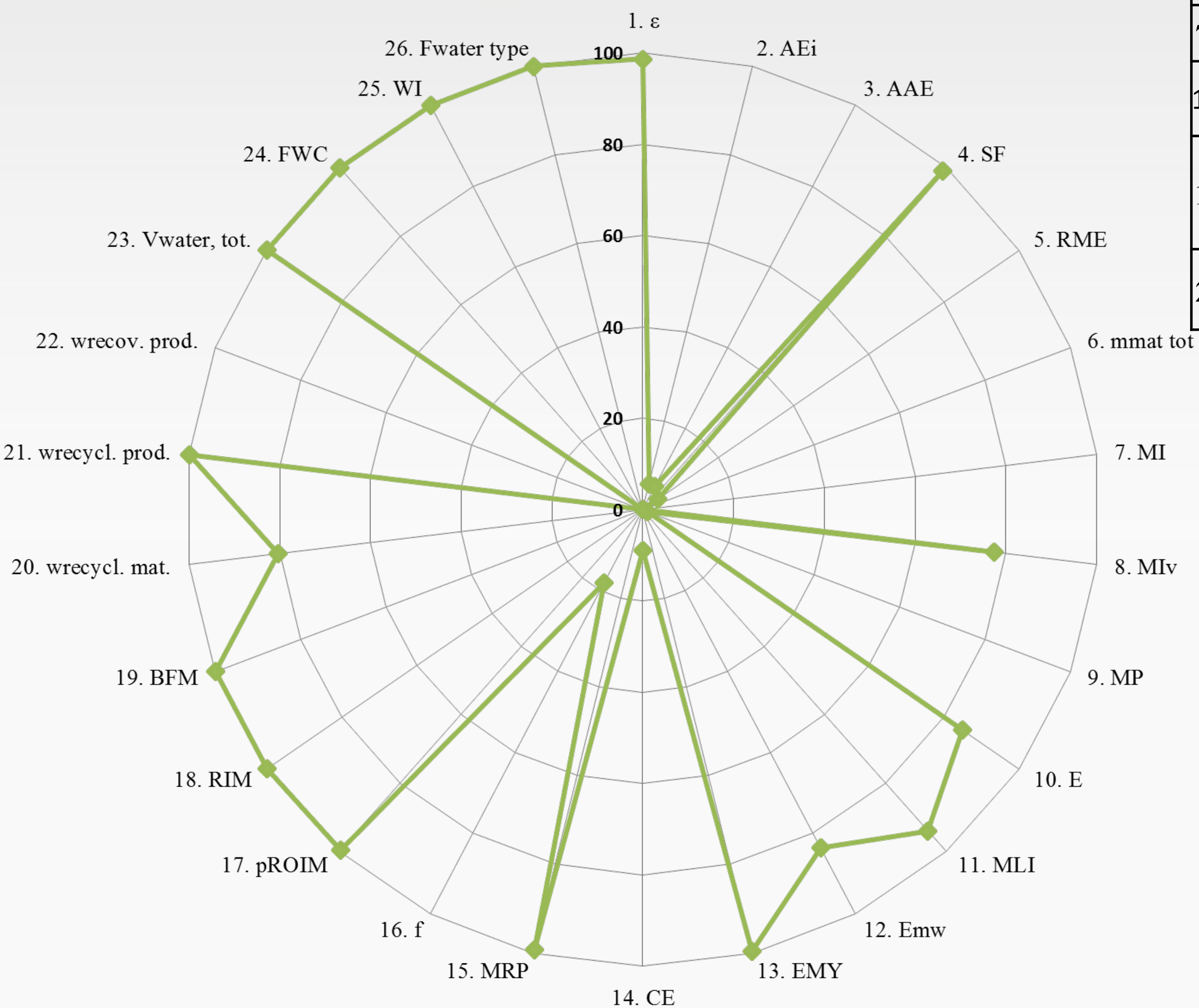
OUTPUTS

Sustainability Assessment & Design: GREENSCOPE Tool

- Sustainability quantitative assessment
- Individual or multiple process comparisons
- Key factors, areas for improvements, optimal tradeoffs

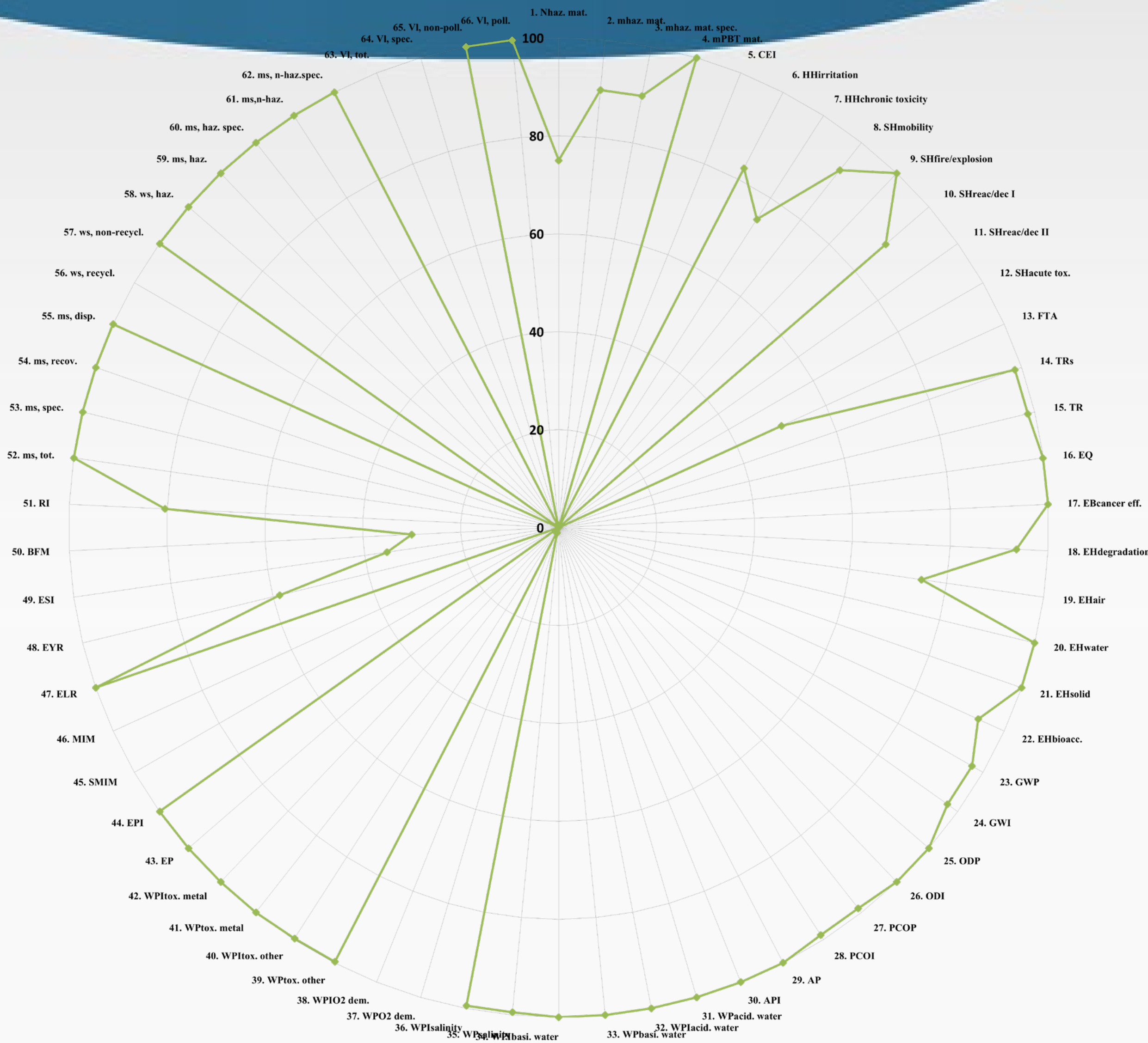


Efficiency Indicator Results



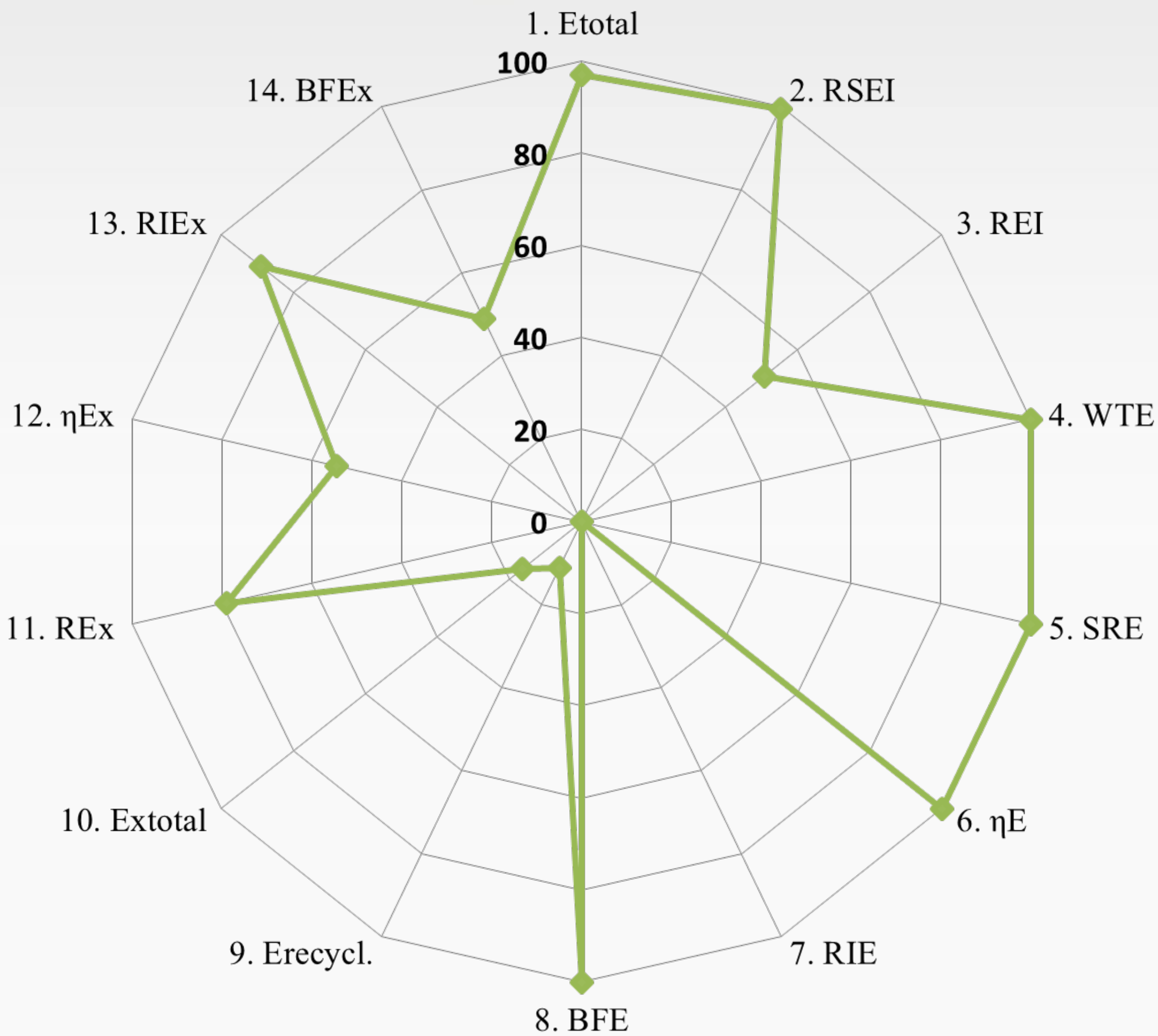
Indicator	Description	Sust. (%)
2. AE_i	Atom economy	5.8
7. MI_v	Value mass intensity	0
15. MRP	Material recovery parameter	0
17. $pROI_M$	Physical return on investment	99.4
23. $V_{water, tot.}$	Total water consumption	100

Environmental Indicator Results



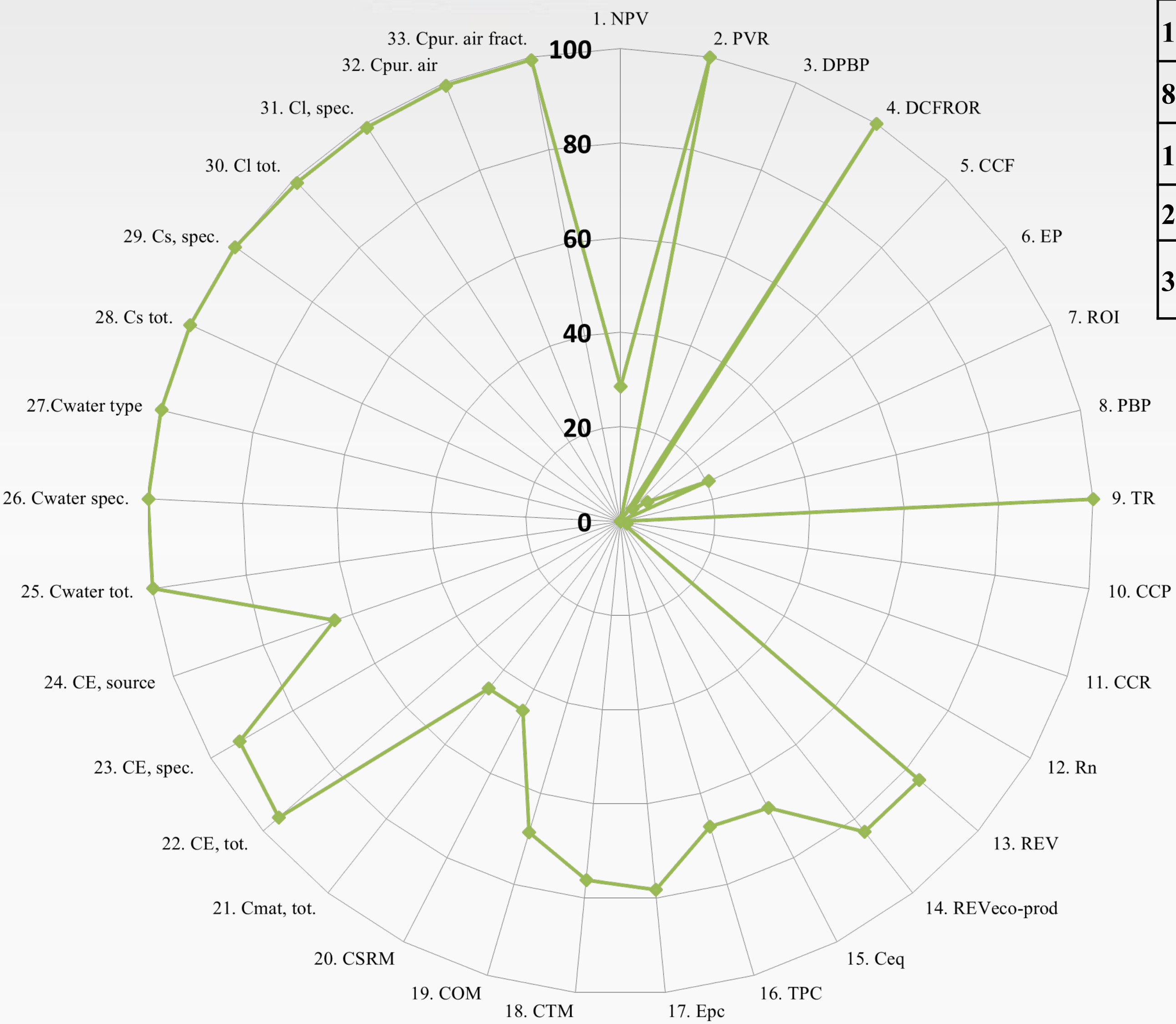
Indicator	Description	Sust. (%)
1. $N_{\text{haz. mat.}}$	Number of hazardous materials input	75
6. $\text{HH}_{\text{irritation}}$	Health hazard, irritation factor	68.5
10. $\text{SH}_{\text{reac/dec I}}$	Safety hazard, reaction / decomposition I	88.3
22. $\text{EH}_{\text{bioacc.}}$	Environmental hazard, 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

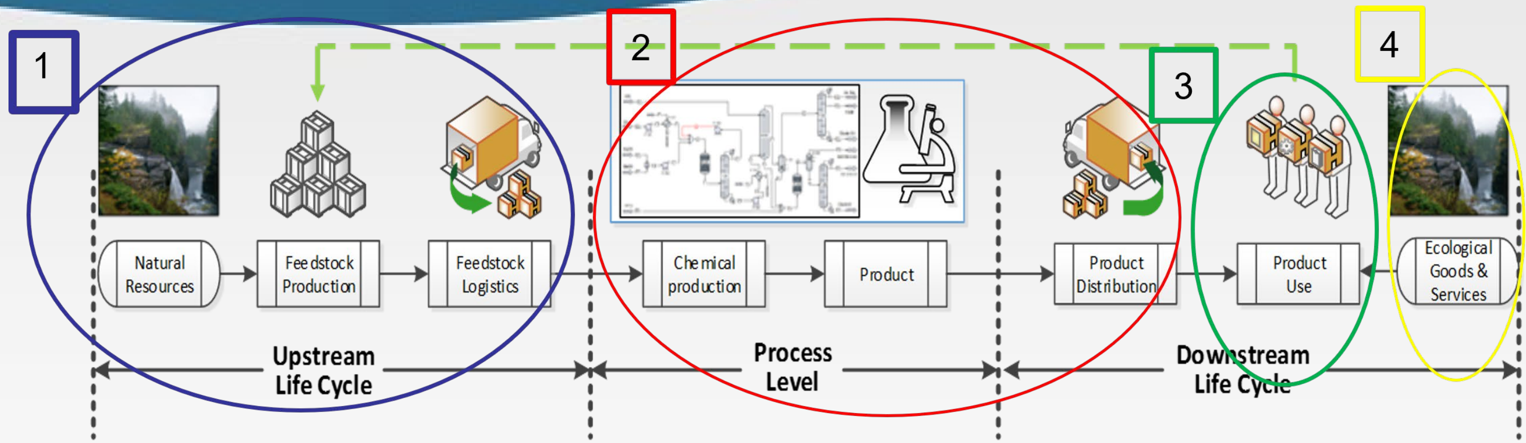
Life Cycle Inventory Results: GREENSCOPE Tool

Compound #	Compound Name	CAS Number	0: Waste; 1: Product; 2: Feedstock; 3: Catalyst; 4: Global reagent/Solvent; 5: Other (drying agent, additive, solvent, washing agent, etc.)	Input (kg/h)	Output (kg/h)	Net output waste, kg/h	Net product flow, kg/h
1	N-Butanol	71-36-3	2	7412.300	7.376	2.838	4.54
2	Maleic Anhydride	108-31-6	1	0	890.546	0.000	890.55
3	Water	7732-18-5	4	250.000	5488.405	1811.729	3676.68
4	Carbon Monoxide	630-08-0	0	0	1017.527	1017.527	0.00
5	Carbon Dioxide	124-38-9	0	0	1598.754	1598.754	0.00
6	Phthalic Anhydride	85-44-9	1	0	1345.182	0.000	1345.18
7	Acrylic Acid	79-10-7	1	0	2617.892	0.000	2617.89
8	Acetic Acid	64-19-7	1	0	1088.059	249.033	839.03
9	Nitrogen	7782-44-7	5	50425.200	50425.206	50425.206	0.00
10	Oxygen	7727-37-9	2	14399.551	6407.793	6407.793	0.00
11	(E)-2-Butene	107-01-7	0	0	509.528	508.586	0.94
12	Formaldehyde	50-00-0	1	0	1090.707	146.153	944.55

Utility type	Utility flow rate needs, kg/h, m^3/h, MJ/h, or kWh/h
Medium pressure steam @10 barg 184° C, 1/kg	9385.6599
Moderately low T Refrigerated water, T_{in} = 5 ° C T_{out} = 15° C, 1/kg	2232940.6935
Electricity (kWh/h)	1980.1353

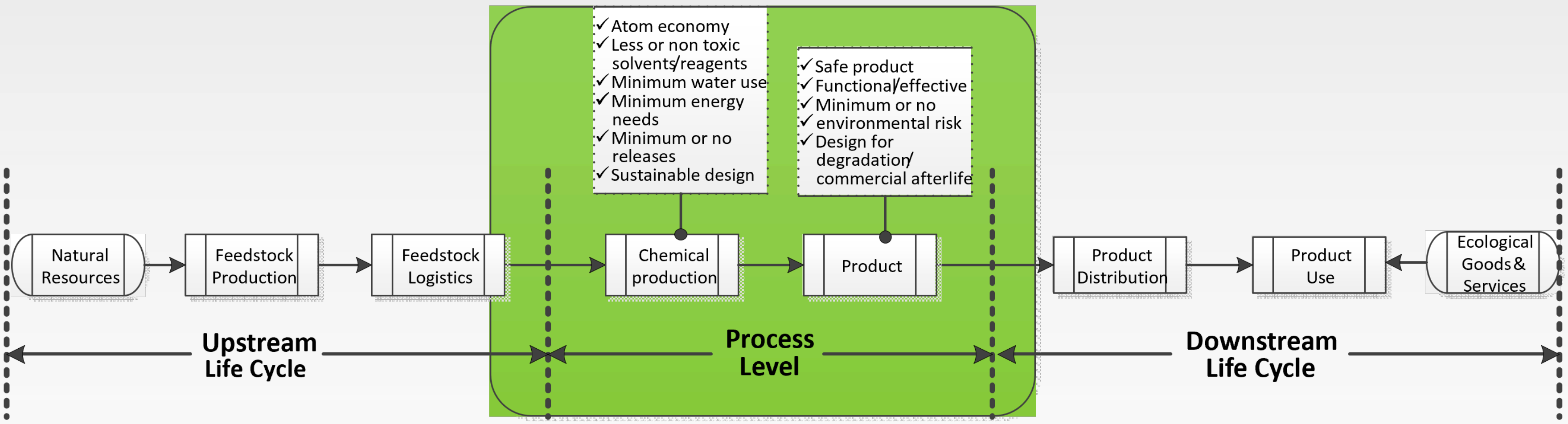
Life Cycle of Chemicals & Sustainability

Global Sustainability Assessment



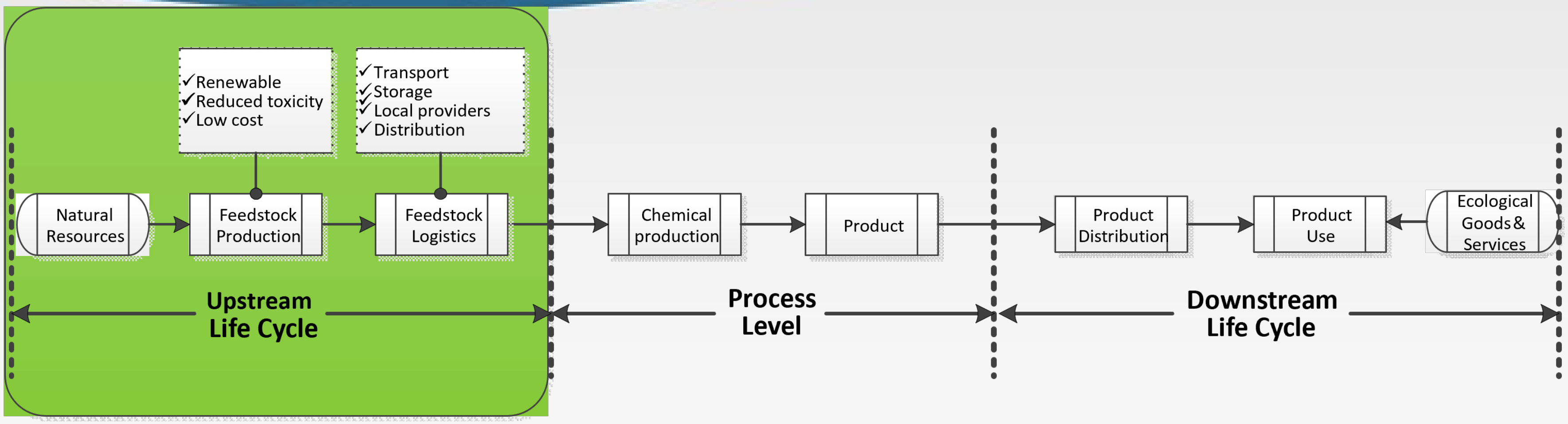
1. **Raw material acquisition**: removal of feedstocks and energy sources from the planet
2. **Manufacturing**: Valuable product production from the feedstocks and its delivery
3. **Use**: actual use, reuse, and maintenance of the product, energy requirements & releases
4. **End-of-life**, energy requirements & releases, material management options

Global Sustainability: Implementing Improvements at Process Level



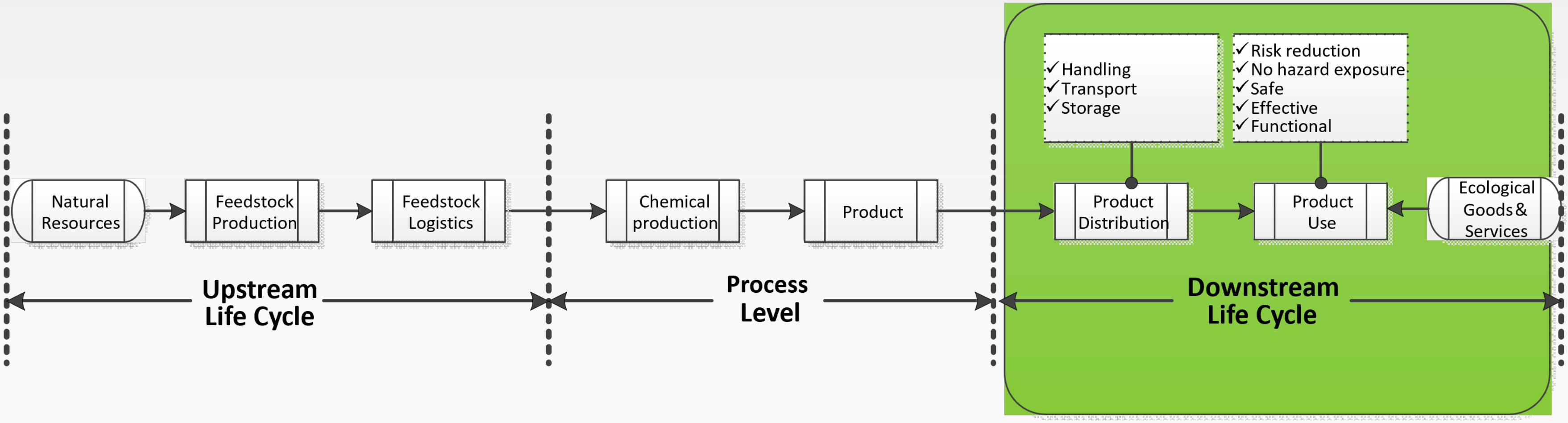
- Elimination of waste treatment units, decreasing capital and manufacturing costs
- No energy load for waste treatment units
- Reduce recycling
- Simplify separation / purification systems

Global Sustainability: Implementing Improvements at Process Level - Upstream



- Reduce resource depletion, feedstock processing and the need for extra raw materials used for intermediate steps
- Reduce # of feed components & increased capital utilization
- Decrease need for separation agents
- Decrease need for upstream energy-related inputs (processes)

Global Sustainability: Implementing Improvements at Process Level - Downstream



- Less hazardous chemical syntheses: reduction of hazard risks
- Design for energy efficiency: minimize high temperature releases, reduce GHG emissions

EPA

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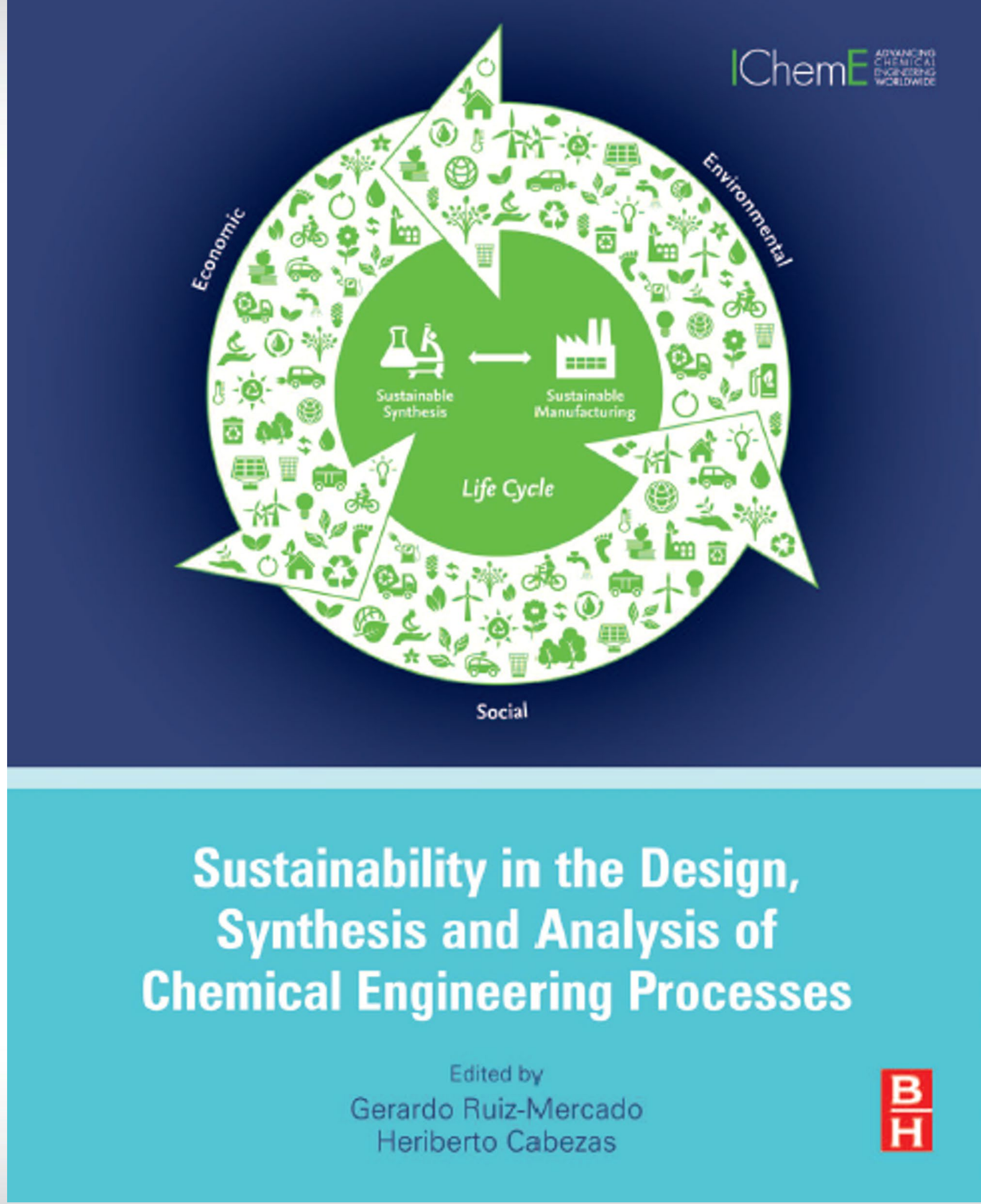

Many Student & Professional Opportunities!

GREAT PLACE TO WORK!

EPA Careers - https://www.epa.gov/careers

https://www.usajobs.gov/Search/Results?a=EP00

52 opportunities on 03/11/2024

Student Opportunities

- PATHWAYS Program
  - Internship Employment Program (current students)
  - Recent Graduate Program (BS, MSc, PhD)
  - Presidential Management Fellowship Program
  - All may lead to permanent positions

https://www.epa.gov/careers/student-internships

https://www.usajobs.gov/Help/working-in-government/unique-hiring-paths/students/

Fellowships and post-doctoral opportunities

- EPA Office of Research & Development Post-Doctoral Research Program
  - Full benefits and a salary commensurate with qualifications
  - Learn more about it: http://cfpub.epa.gov/ordpd/
- National Academy of Sciences/National Research Council Resident Research Associateship Program
  - Post-doctoral, mid-career technical professionals, and assistant Professor level
  - https://www.epa.gov/careers/fellowships-scholarships-and-post-doctoral-opportunities#nas
- Oak Ridge Institute for Science and Education (ORISE) Fellowships
  - Opportunities are available year-round to science and engineering undergrads, grad students, recent grads, post-docs, faculty
  - https://orise.orau.gov/epa/current-research-opportunities.html
  - https://orise.orau.gov/internships-fellowships/index.html

ORISE Research opportunity: Life Cycle and Sustainability Analyses for Designing Chemical Circular Economy Routes, ask @ ruiz-mercado.gerardo@epa.gov

Questions?

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Recommended Sites:

EPA Careers - https://www.epa.gov/careers

USAJOBS Pathways info - https://www.usajobs.gov/StudentsAndGrads