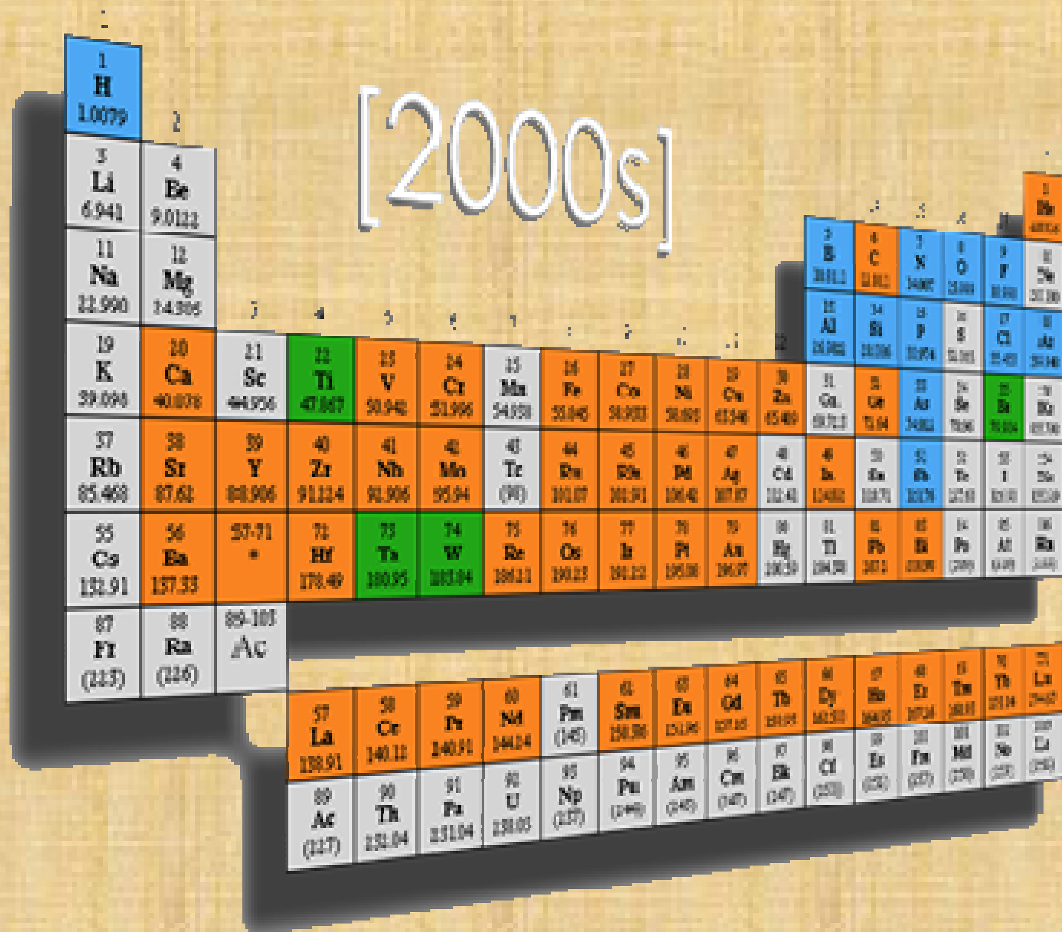
Sustainability Analysis for Products and Processes

Subhas K. Sikdar
National Risk Management Research Laboratory
U.S. Environmental Protection Agency
Cincinnati, OH 45268
Sikdar.subhas@epa.gov

Nanotech Product Categories

- Appliances
  - Batteries
  - Heating, cooling and air conditioning
  - Kitchen appliances
  - Laundry and clothing care
- Automotive
  - Exterior
  - Maintenance & accessories
  - Watercraft
- Crosscutting
  - Coatings
- Electronics & computers
  - Audio/video/display
  - Cameras & film
  - Computer hardware/mobile devices/communication equipment
- Health & fitness
  - Clothing
  - Personal care/cosmetics/sunscreen
  - Sporting goods
- Children's goods
  - Toys and games
- Home & Garden
  - Cleaning
  - Construction materials
  - Home furnishing
  - Luggage
  - Luxury
  - Paints
  - Pet products

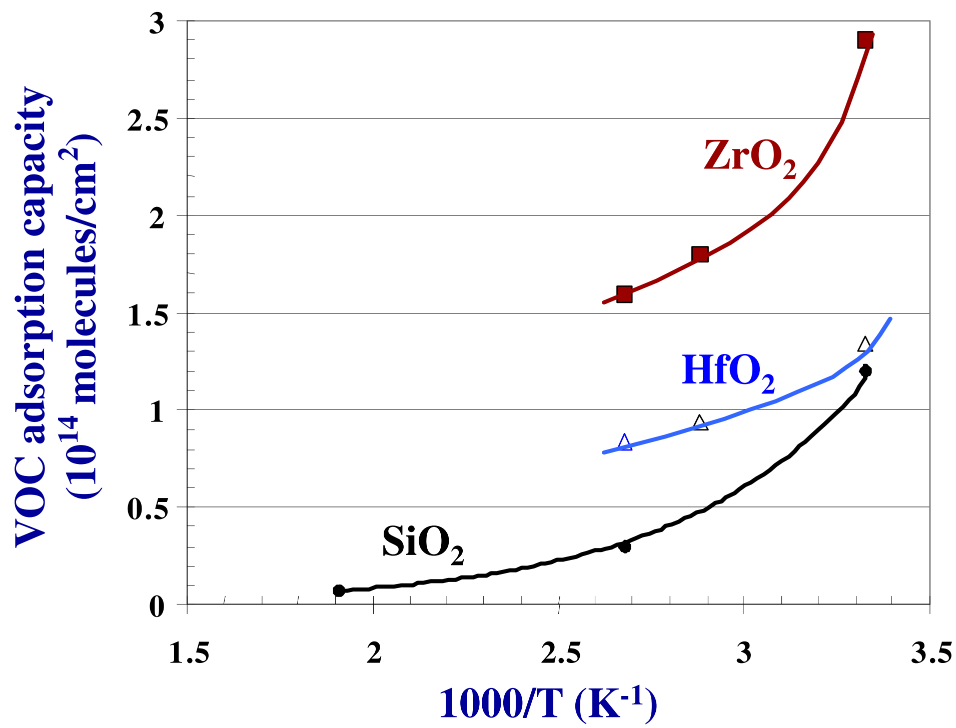


Extensive use of elements from the Periodic Table in the Semiconductor Industry

Courtesy of Prof. Farhang Shadman, University of Arizona, Tucson

Risk is not necessarily from the nanoparticles themselves but what might be on them

a) Nano-particles in the gas phase
15ppb VOC; 40 nm particles



b) Nano-particles in the wastewater

- **10 ppb of Cu^{++} in CMP wastewater results in $3x10^6$ ppb of adsorbed copper on 90 nm CeO_2 nano-particles**
- **10 ppb of PFOS in wastewater results in $2.8x10^4$ ppb of contaminated 10 nm carbon nano-particles**

Courtesy of Prof. Farhang Shadman, University of Arizona, Tucson

Types of Risk Enquiry

1. **Risk from exposure to nanoparticles**

   - impact on humans during manufacturing practices

   - impact on ecosystems during dispersion resulting from products in their life cycle in the environment

2. **Risk from exposure to consumer products**

   - direct exposure to humans

   - to ecosystems after disposal

Sustainability analysis of nanotech products is no different than that of any other product

Sustainability issues associated with modern products and processes

OUTLINE

Purpose:

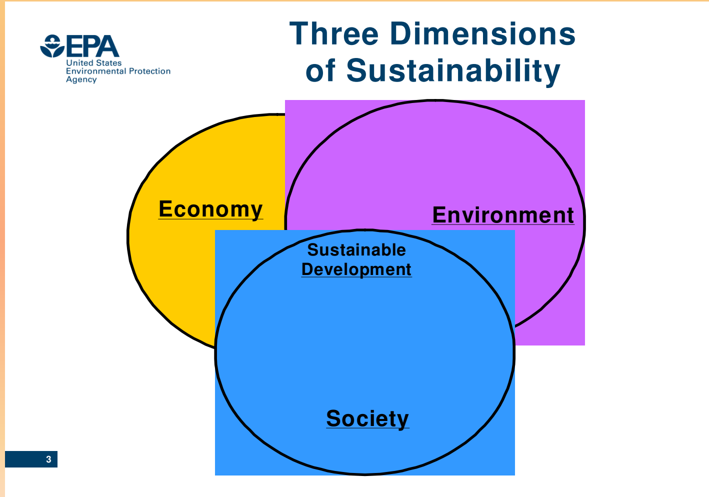
Incorporating Sustainability Considerations into Products/Processes

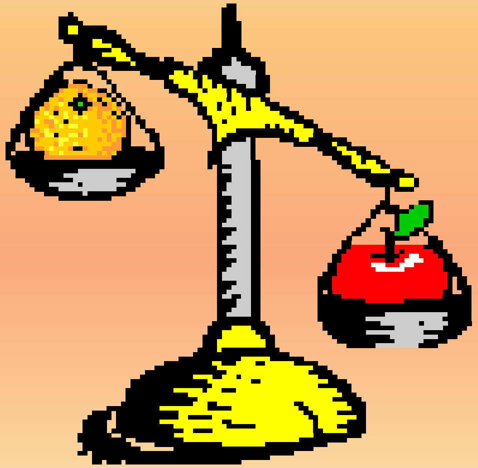
Sustainability Analysis:

- **Engineering Definition**
- **Systems and LCA thinking**
- **Sustainability metrics, classification, selection for Processes**
- **Consolidation of metrics for easy decision making for sustainability**

President's Council for Sustainable Development

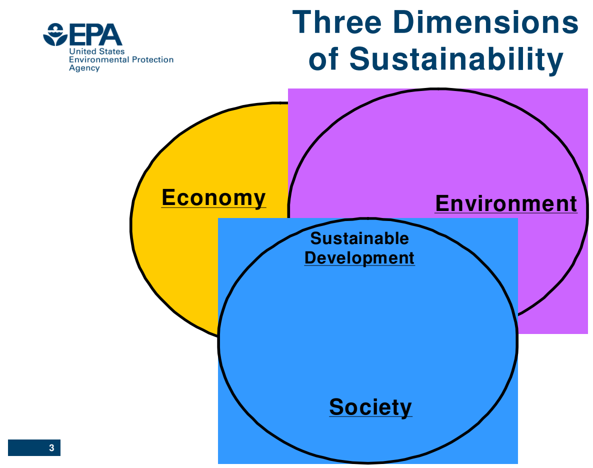
- Sustainable development is an evolving process that improves the economy, the environment, and society for the benefit of current and future generations.





WCED (Bruntlund) idea of sustainable development

Economic development (i.e. by technology application) with decreasing environmental impact and improving societal benefit



An Engineering Definition:

For a man-made system, sustainable development is continual improvement in one or more of the three domains of sustainability, i.e., economic, environmental, and societal without causing degradation in any one of them, either now or in the future, when compared, with quantifiable metrics, to a similar system it is intended to replace.

P.S. Even though continual improvement simultaneously in all domains provides a practical approach, this is still a high bar. In practice, an overall improvement is feasible.

SYSTEM-SURROUNDING PARADIGM

System: maximum space over which the process owner has control

Sustainability Analysis is essentially an accounting of what the system is doing to itself and to the surrounding in terms of environmental, societal, and economic impacts, and how these impacts can be minimized

Corollary: Maximization of benefits with cost minimization

Differences between Environmental Impact Assessment (EIA) and Sustainability

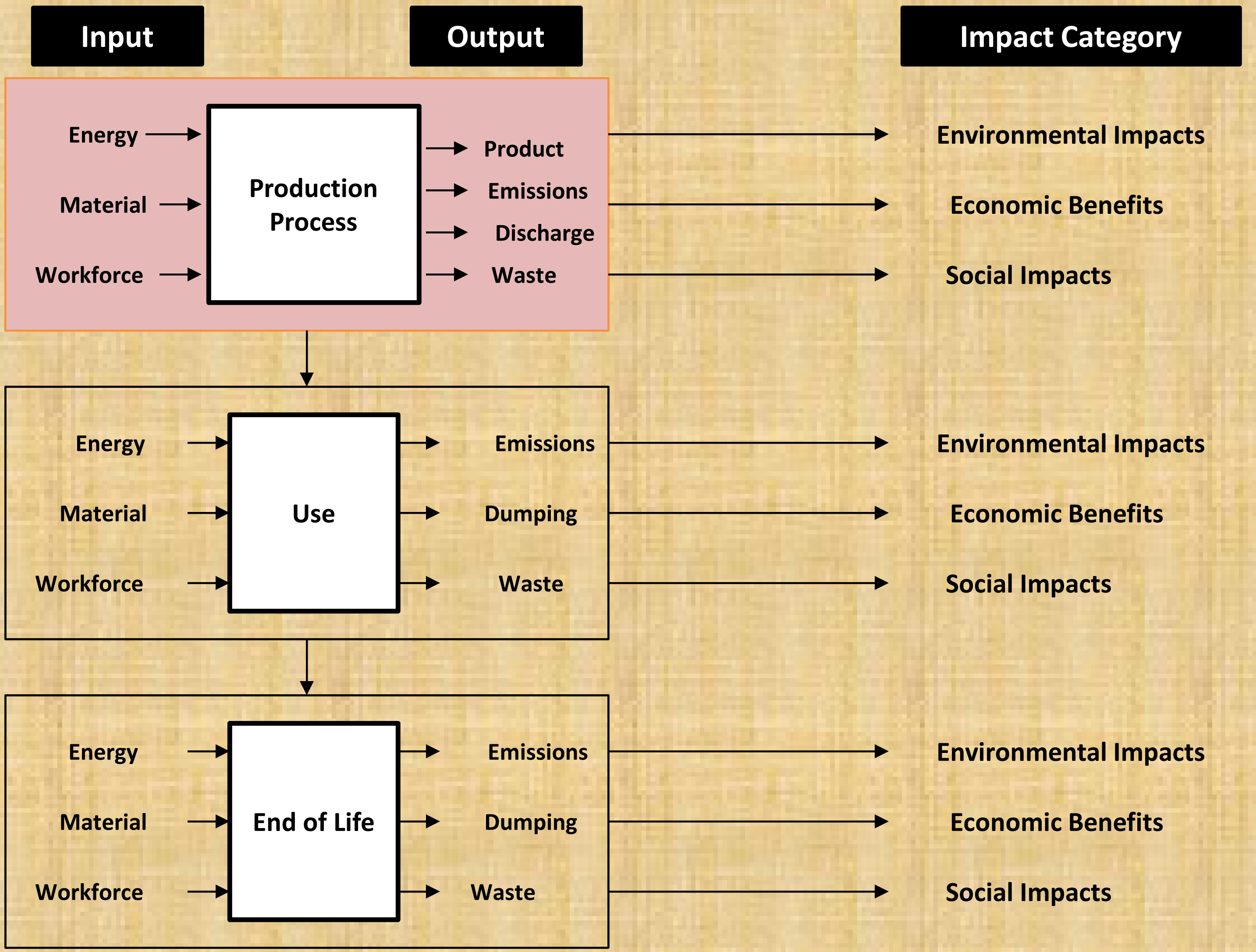
- Estimation of all applicable environmental impacts in quantitative terms
- Assessment is in absolute terms
- Can be done on an LCA basis
- Decision on cost-benefit term

- Estimation of all applicable environmental, economic, and societal impacts in comparison to a reference case
- No absolute in sustainability
- Should be done on an LCA basis
- Decision on overall quantitative desirability compared to the reference

Engineering Approaches to Sustainability

- **Impact accounting:** on a life cycle basis
- **Analysis:** comparative among processes, or over time
- **Reference system:** the one to supersede
- **A single aggregate index composed of applicable metrics:** to be used in the comparative study

Environmental, Economic, and Societal Impacts from a Life Cycle Basis



Paths to Sustainability

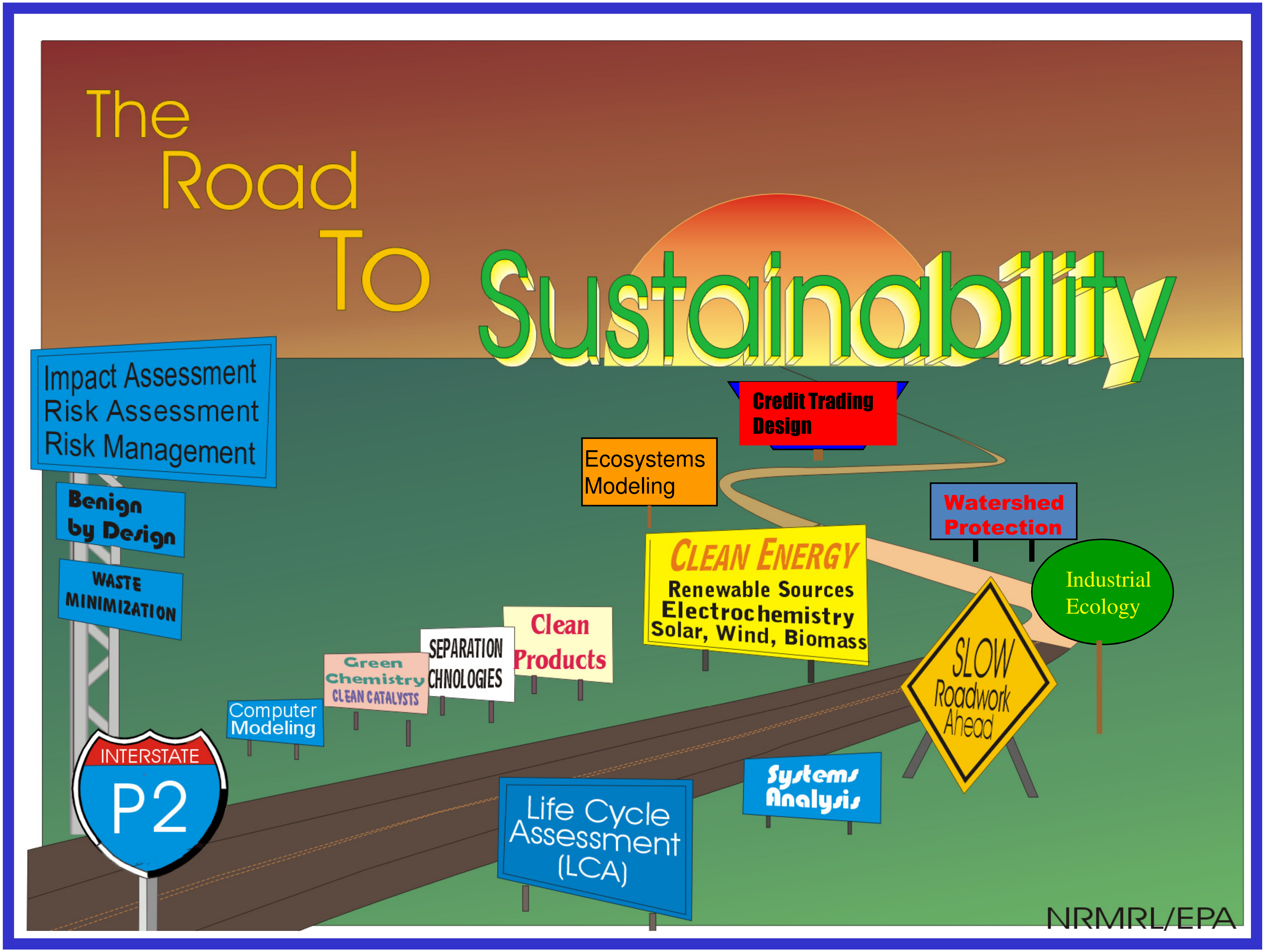
Two schools of thoughts

1. **Incremental improvement in the journey towards sustainable development:**

   Think globally, Act locally

2. **Radical changes for attaining an envisioned outcome:**

   Think globally, Act globally



The Road To Sustainability
Impact Assessment
Risk Assessment
Risk Management
Benign by Design
WASTE MINIMIZATION
INTERSTATE
P2
Computer Modeling
Green Chemistry
CLEAN CATALYSTS
SEPARATION
CHNOLOGIES
Clean Products
Ecosystems Modeling
Credit Trading Design
CLEAN ENERGY
Renewable Sources
Electrochemistry
Solar, Wind, Biomass
Watershed Protection
Industrial Ecology
SLOW Roadwork Ahead
Life Cycle Assessment (LCA)
Systems Analysis
NRMRL/EPA

Scale and Nesting of Sustainable Systems

Five levels of scales for sustainable systems:

Level I: Global Systems (e.g. global CO2 budgeting)
Level II: National Systems (energy system, material flow)
Level III: Regional Systems (e.g. watersheds, Brownfields)
Level IV: Business Systems (e.g. business networks, waste exchange networks)
Type V: Sustainable technologies (e.g. green materials, sustainable products)

System-Surrounding Paradigm

Sustainability analysis is essentially an accounting of what impacts (environmental, economic, and societal) the system is causing to itself and to the surrounding, and how these impacts can be minimized.

I: Global Scale
(e.g. global CO2 budgeting)

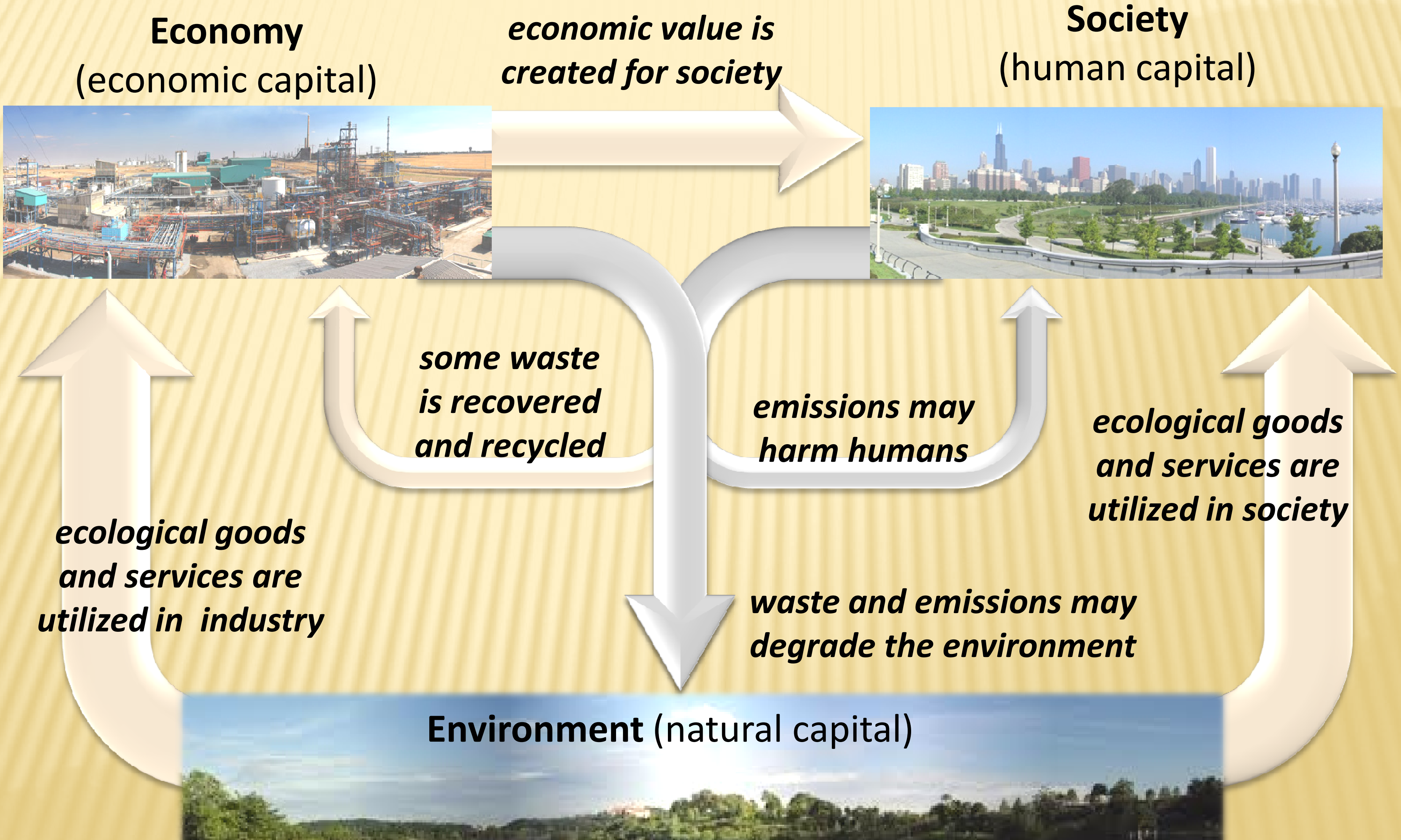
II. National Scale (e.g. energy)

III: Regional Scale
(e.g. watersheds)

IV: Business or Institutional Scale
(e.g. eco-industrial park)

V: Sustainable Technologies Scale
(e.g. sustainable products)

A SYSTEMS VIEW OF SUSTAINABILITY



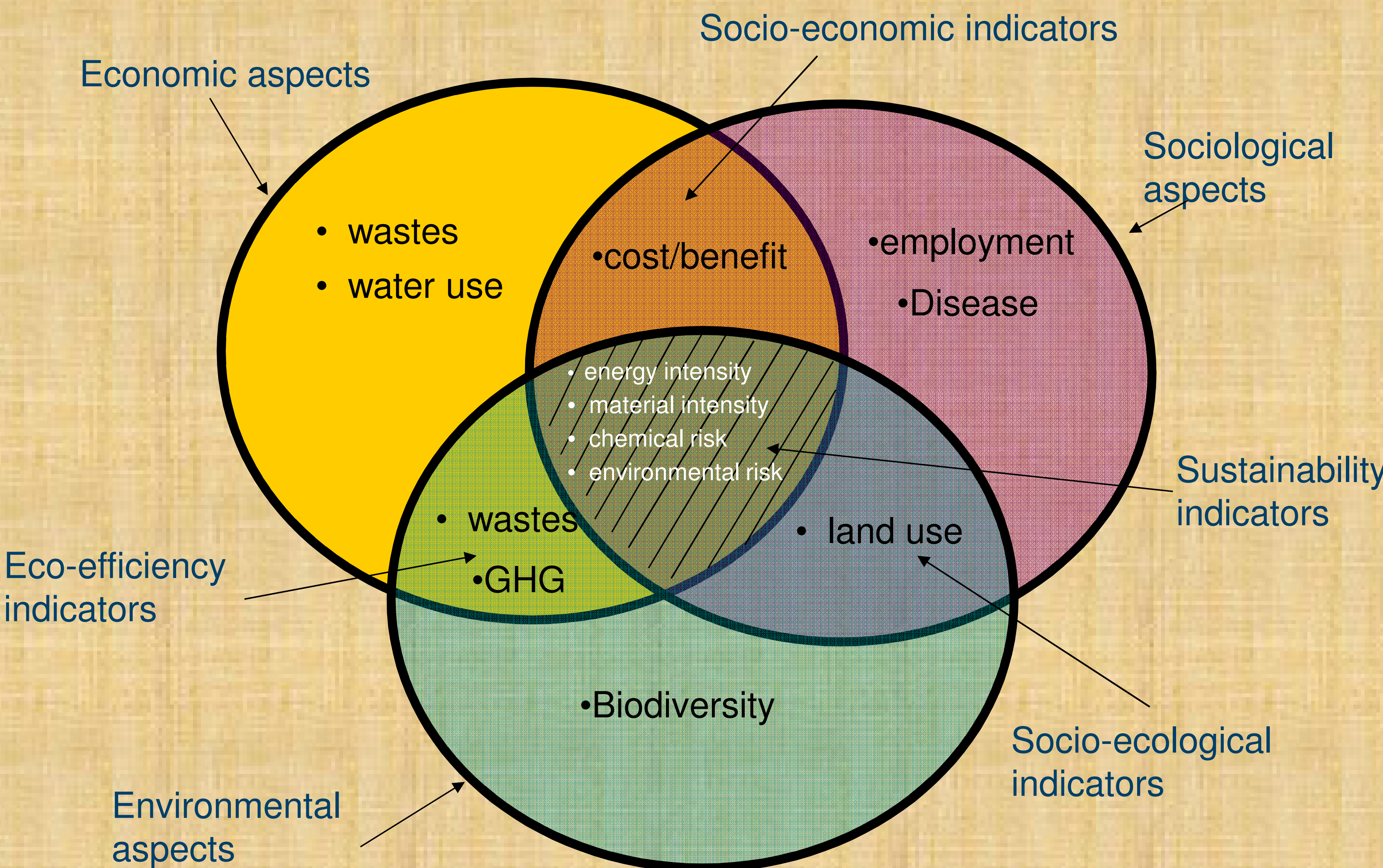
Courtesy of Joseph Fiksel, Ohio State University

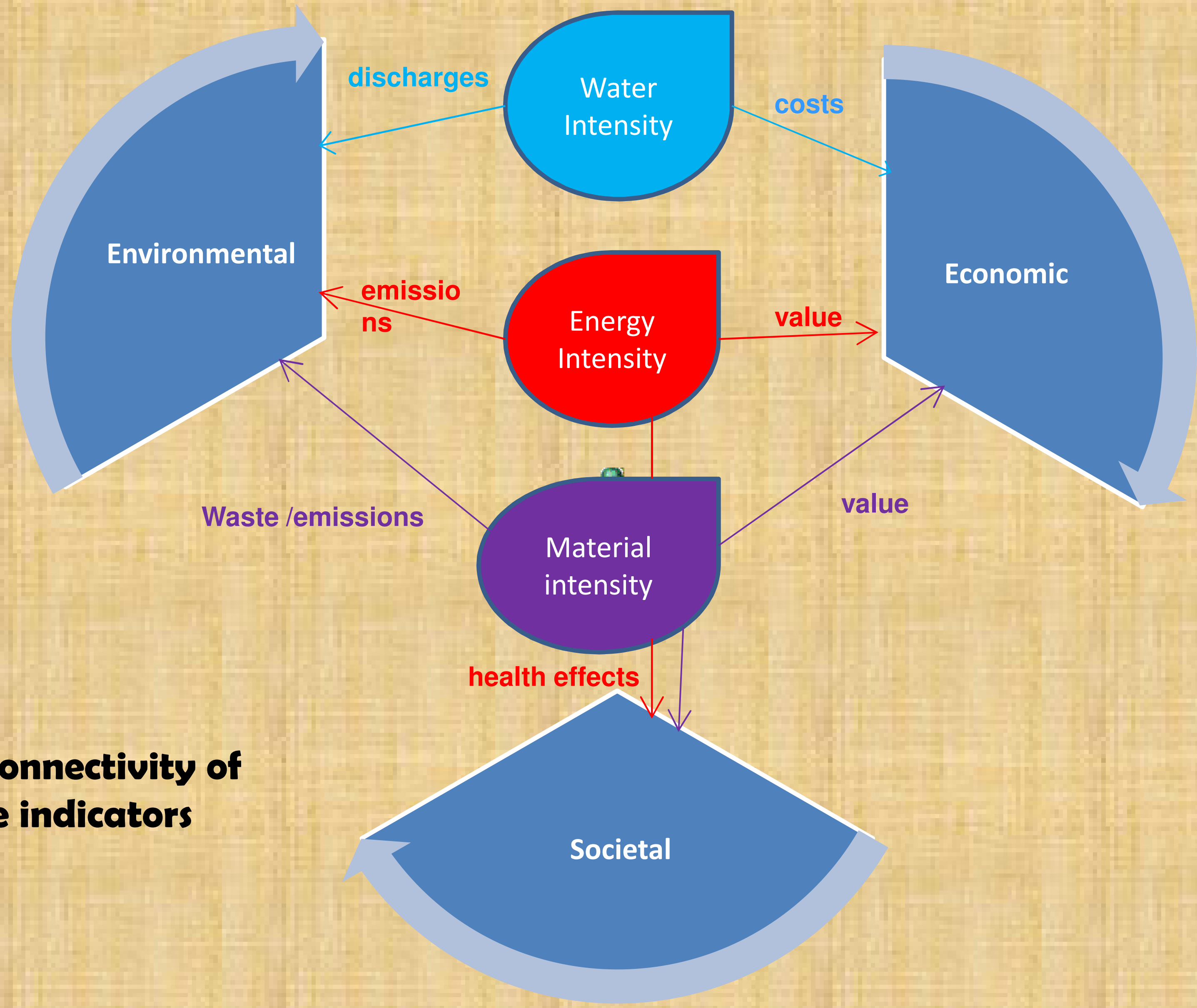
Metrics for Sustainability

- Sustainability metrics (or indicators) need to be chosen for each problem system. Indicators can be grouped into three categories:

Group I:	One dimensional: economic, ecological, societal
Group II:	Two dimensional: socio-economic, eco-efficiency, and socio-ecological
Group III:	Three dimensional: sustainability

Sustainability as the intersection of three domains





Interconnectivity of The indicators

The system analysis must satisfy the following

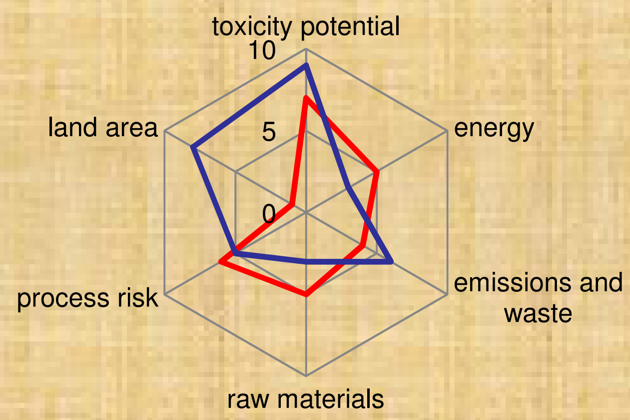
- Must be comparative to a reference system
- Must be based on life cycle of material, energy, and cost through the appropriate supply chain
- Must consider quantitative measure to represent environmental, economic, and societal domains
- Must identify the necessary and sufficient number of critical metrics that characterize the system
- Must lead to a decision of better or worse than the reference system, preferably with a single aggregate metric (or index)

Sustainability Analysis with Metrics

One way is to present sustainability results on a spider diagram for two states of a system or two similar systems

But, for too many metrics and/or two many alternatives, visual comparison is impossible, and dealing with too many numbers is difficult

BASF Eco-efficiency metrics



Euclidean Distance:

$$D_e = \sqrt{\left(\sum_{i=1}^{n} c_i{}^2 \left(x_i - x_{i0} \right)^2 \right)}$$

Where
D_e (t, x_i) is relative sustainability of a candidate from a designated reference n Dimensional point
x_i is the value of metric i for candidate (process, product etc.)
X_{io} is the value of metric i for the reference point
c_i is the weighting factor for metric i
n is the number of metrics used

P.S. If necessary, $x_i - x_{i0}$ can be normalized to render them dimensionless

Consolidation of Metrics

For metrics m_1, m_2, ---------, applied to a base case X and a new case Y, we introduce the composite measure D as

$$\mathbf{D} = \left(\prod_{i}^{n} \left[c_i \left(y_i / x_i \right) \right] \right)^{1/n}$$

Where c_i is the weighting factor ($0< c_i$) for metric i

y_i is the value of metric i for Y

x_i is the value of metric i for X (x_i or $y_i \neq 0$ or ∞)

and n is the number of metrics used.

• Idea based on geometric mean of the ratios (dimensionless) of the values of the metrics between the two states being representative of the difference between the two states X and Y. The geometric can be looked upon as the statistical distance between the two states.

Shifting the reference point to

(1) Place all data in the positive side for calculating D_e

(2) To avoid zero and infinity in calculating D

$$\mathbf{D_e} = \sqrt{\sum_i^n \left[c_i \frac{(y_i - x_{i0})}{(y_i - x_{i0})_{\max}} \right]^2}$$

$$\mathbf{D} = \left(\prod_i^n \left[c_i (y_i' / x_i') \right] \right)^{1/n}$$

$$y_i' = y_i - (x_{i0} - C_{offset})$$

$$x_i' = x_i - (x_{i0} - C_{offset})$$

Finding the minimum number of indicators for sustainability analysis

- The Principle of Parsimonious Parameterization: necessary and sufficient number of indicators for sustainability analysis

- Use of Principal Component Analysis on the indicator data space constructing an Eigenvalue Problem:

  $A x = \lambda x$ where A is the n x n indicator corelation matrix, x is an n dimensional eigenvector (called principal component) corresponding to eigenvalue λ

- Use of Partial Least Squares (PLS) and Variable importance in Projection (VIP) method to determine the least number of indicators that will provide reliable D_e or D data for comparing relative sustainability of options

Hierarchical Analysis

- Step 1: Select the metrics to be used

Hierarchical Analysis

- **Step 1:** Select the metrics to be used
- **Step 2:** Classify them in 3D, 2D, and 1D metrics

Hierarchical Analysis

- **Step 1:** Select the metrics to be used
- **Step 2:** Classify them in 3D, 2D, and 1D metrics
- **Step 3:** Map on the Venn diagram to detect possible omissions

Hierarchical Analysis

- Step 1: Select the metrics to be used
- Step 2: Classify them in 3D, 2D, and 1D metrics
- Step 3: Map on the Venn diagram to detect possible omissions
- Step 4: Compute the values of the chosen metrics (3D, 2D, 1D) for comparative analysis

Hierarchical Analysis

- **Step 1:** Select the metrics to be used
- **Step 2:** Classify them in 3D, 2D, and 1D metrics
- **Step 3:** Map on the Venn diagram to detect possible omissions
- **Step 4:** Compute the values of the chosen metrics (3D, 2D, 1D) for comparative analysis

- "Strong Sustainability": Examine for sustainability improvement against the definition that when at least one metric improves, the other metrics do not decline (Pareto optimality)

Hierarchical Analysis

- Step 1: Select the metrics to be used
- Step 2: Classify them in 3D, 2D, and 1D metrics
- Step 3: Map on the Venn diagram to detect possible omissions
- Step 4: Compute the values of the chosen metrics (3D, 2D, 1D) for comparative analysis

- "Strong Sustainability": Examine for sustainability improvement against the definition that when at least one metric improves, the other metrics do not decline (Pareto optimality)

- Step 5: "Weak Sustainability" (Real World): Compute Aggregate Index (D or D_e) for alternatives for relative sustainability decisions.

Hierarchical Analysis

- **Step 1:** Select the metrics to be used
- **Step 2:** Classify them in 3D, 2D, and 1D metrics
- **Step 3:** Map on the Venn diagram to detect possible omissions
- **Step 4:** Compute the values of the chosen metrics (3D, 2D, 1D) for comparative analysis

- "Strong Sustainability": Examine for sustainability improvement against the definition that when at least one metric improves, the other metrics do not decline (Pareto optimality)

- **Step 5:** "Weak Sustainability" (Real World): Compute Aggregate Index (D or D_e) for alternatives for relative sustainability decisions.
- **Step 6:** Prioritize metrics using Principal Component Analysis-Identification Protocol (PCA-VIP) to arrive at the number of necessary and sufficient metrics.

Hierarchical Analysis

- **Step 1:** Select the metrics to be used
- **Step 2:** Classify them in 3D, 2D, and 1D metrics
- **Step 3:** Map on the Venn diagram to detect possible omissions
- **Step 4:** Compute the values of the chosen metrics (3D, 2D, 1D) for comparative analysis

- "Strong Sustainability": Examine for sustainability improvement against the definition that when at least one metric improves, the other metrics do not decline (Pareto optimality)

- **Step 5:** "Weak Sustainability" (Real World): Compute Aggregate Index (D or D_e) for alternatives for relative sustainability decisions.
- **Step 6:** Prioritize metrics using Principal Component Analysis- Variable Identification Protocol (PCA-VIP) to arrive at the number of necessary and sufficient metrics.
- **Step 7:** Redo the D (or D_e) analyses using metrics of step 6

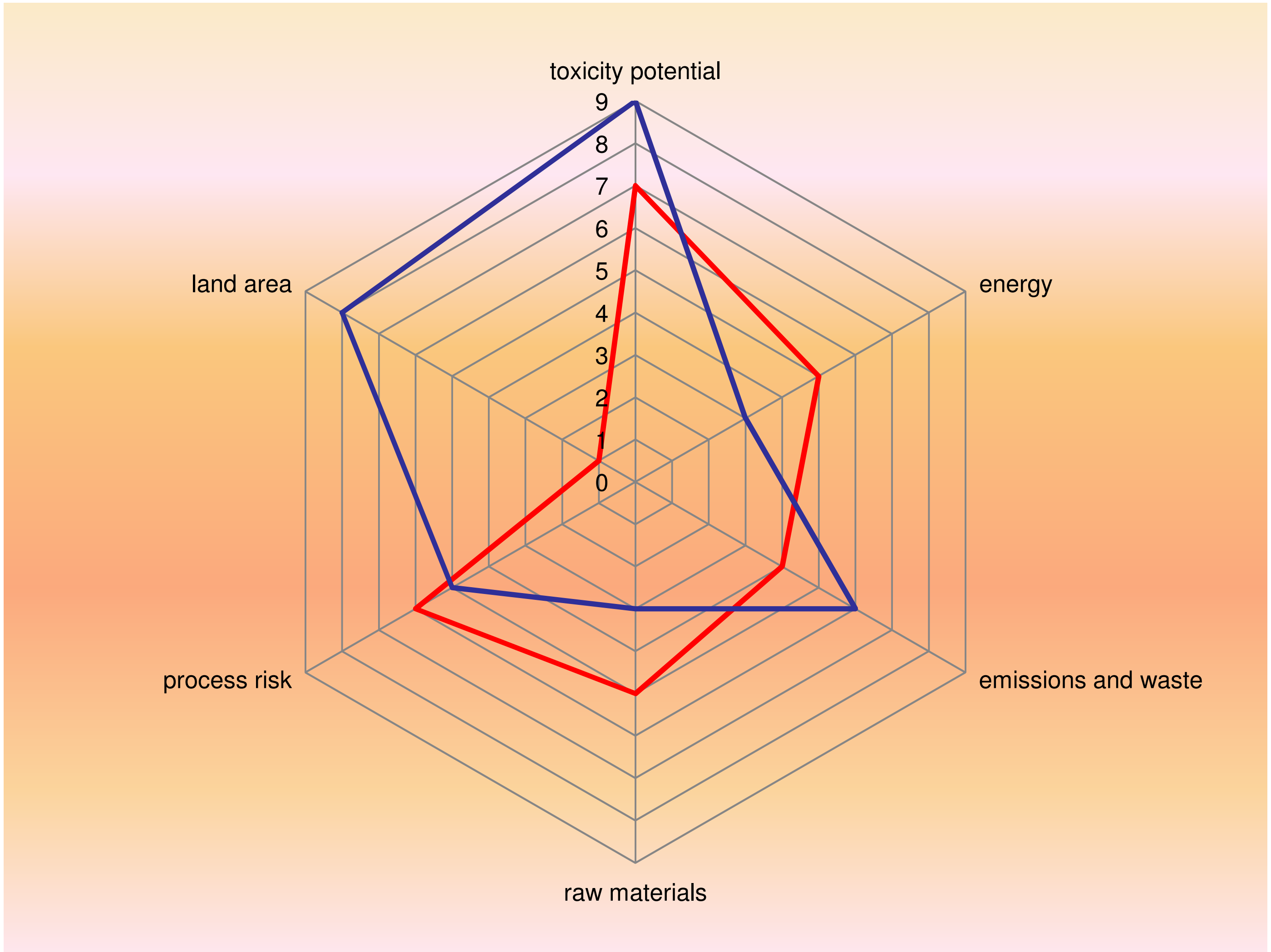
Hierarchical Analysis

- **Step 1:** Select the metrics to be used
- **Step 2:** Classify them in 3D, 2D, and 1D metrics
- **Step 3:** Map on the Venn diagram to detect possible omissions
- **Step 4:** Compute the values of the chosen metrics (3D, 2D, 1D) for comparative analysis

- "Strong Sustainability": Examine for sustainability improvement against the definition that when at least one metric improves, the other metrics do not decline (Pareto optimality)

- **Step 5:** "Weak Sustainability" (Real World): Compute Aggregate Index (D or D_e) for alternatives for relative sustainability decisions.
- **Step 6:** Prioritize metrics using Principal Component Analysis-Variable Identification Protocol (PCA-VIP) to arrive at the number of necessary and sufficient metrics.
- **Step 7:** Redo the D (or D_e) analyses using metrics of step 6

Potential outcome: The analysis will help in finding conditions that improve Aggregate Index to targeted values (process development)



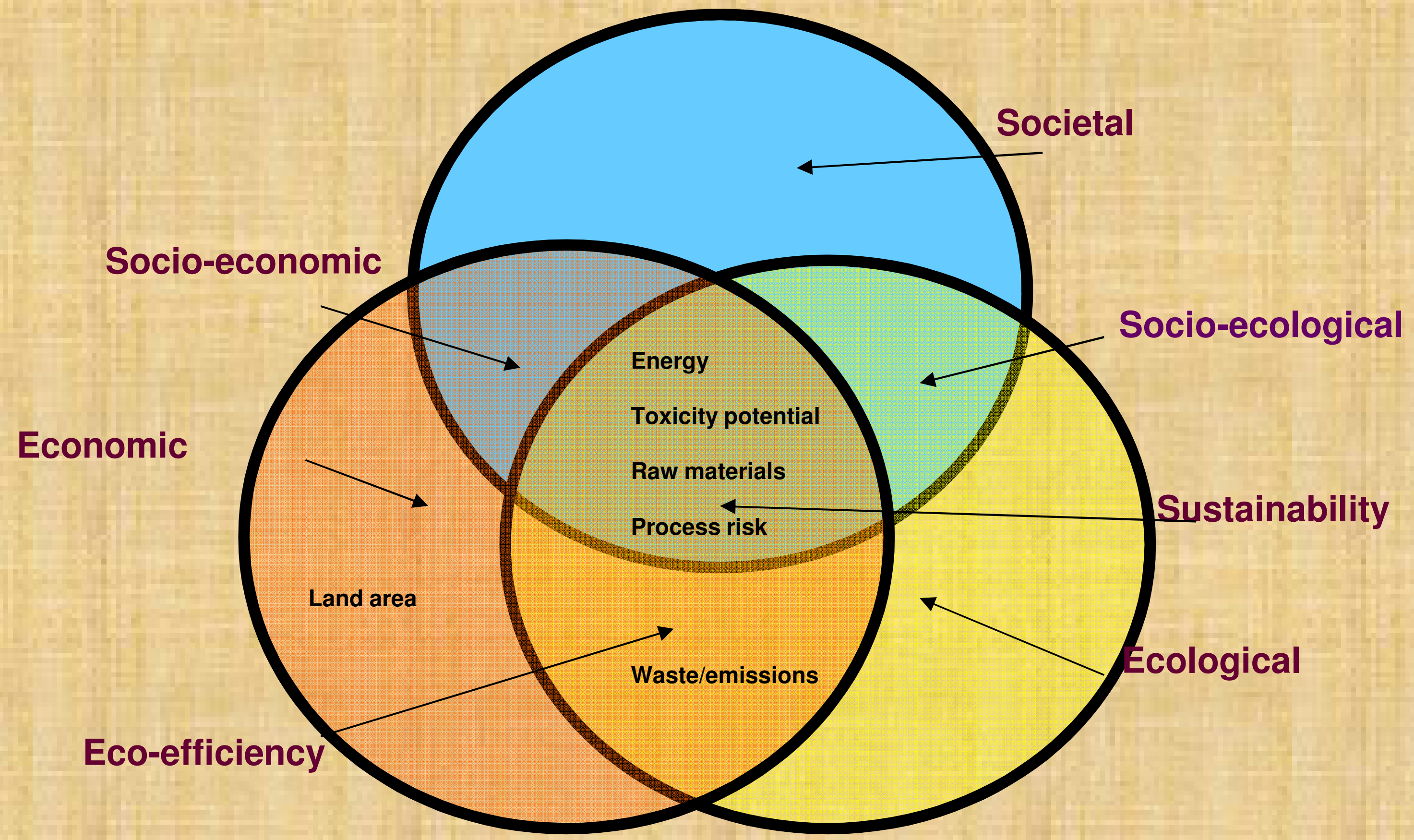
toxicity potential
energy
emissions and waste
raw materials
process risk
land area
9
8
7
6
5
4
3
2
1
0

BASF: five coating formulation

Environmental Fingerprints of alternate Curing Processes
Shonnard, Kirchner, and Saling, ES&T: 2003, 37, 5340-5348

- **Processes:**
  - Aqueous Coating
  - 2C-PU Coating
  - AC-Coating
  - NC-Coating
  - UV-Coating
- **Metric Used**
  - Energy consumption
  - Raw material consumption
  - Risk potential
  - Toxicity potential
  - Emissions into media
  - Land area

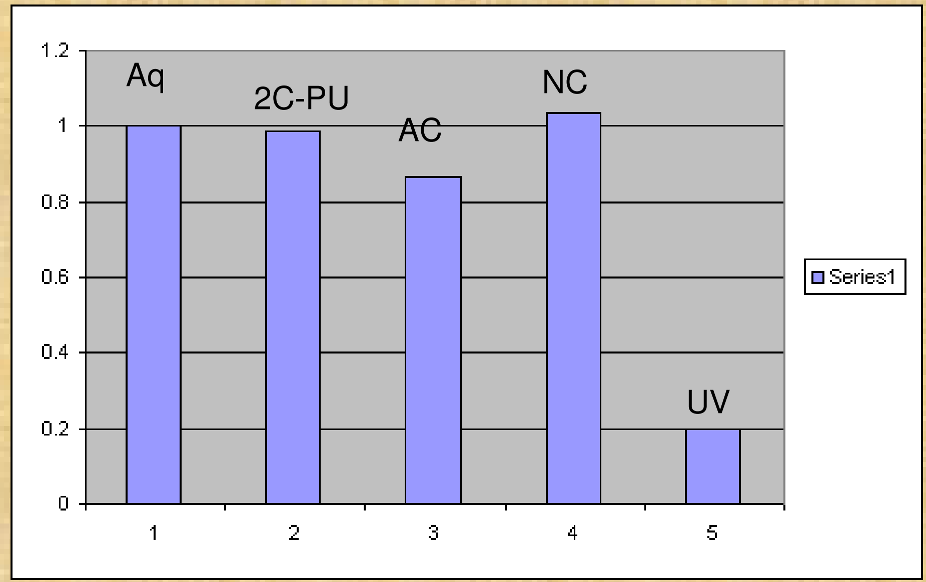
Sustainability of Engineered Processes



Mapping the BASF Metrics

Environmental Fingerprints of alternate Curing Processes
Shonnard, Kirchner, and Saling, ES&T: 2003, 37, 5340-5348

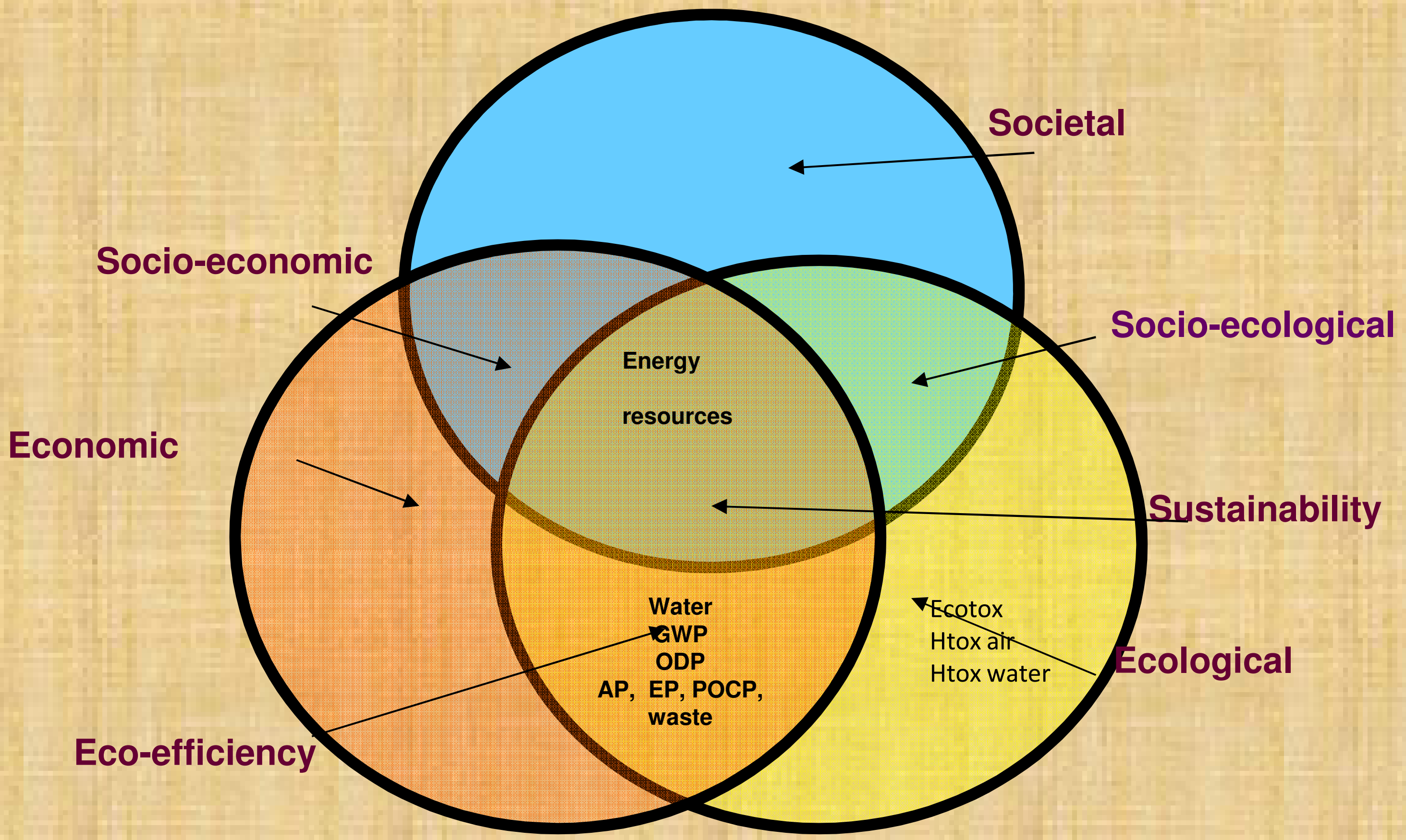
Process	Aggregated metric, D	Metrics used:
Aqueous coating:	1.0	energy consumption, raw matl consumption, risk potential, toxicity potential, emissions into media, land area
2 C-PU Coating	0.987	
AC-Coating	0.868	
NC-Coating	1.034	
UV-Coating	0.196	



Fender Case Study
- Impact Assessment results - total

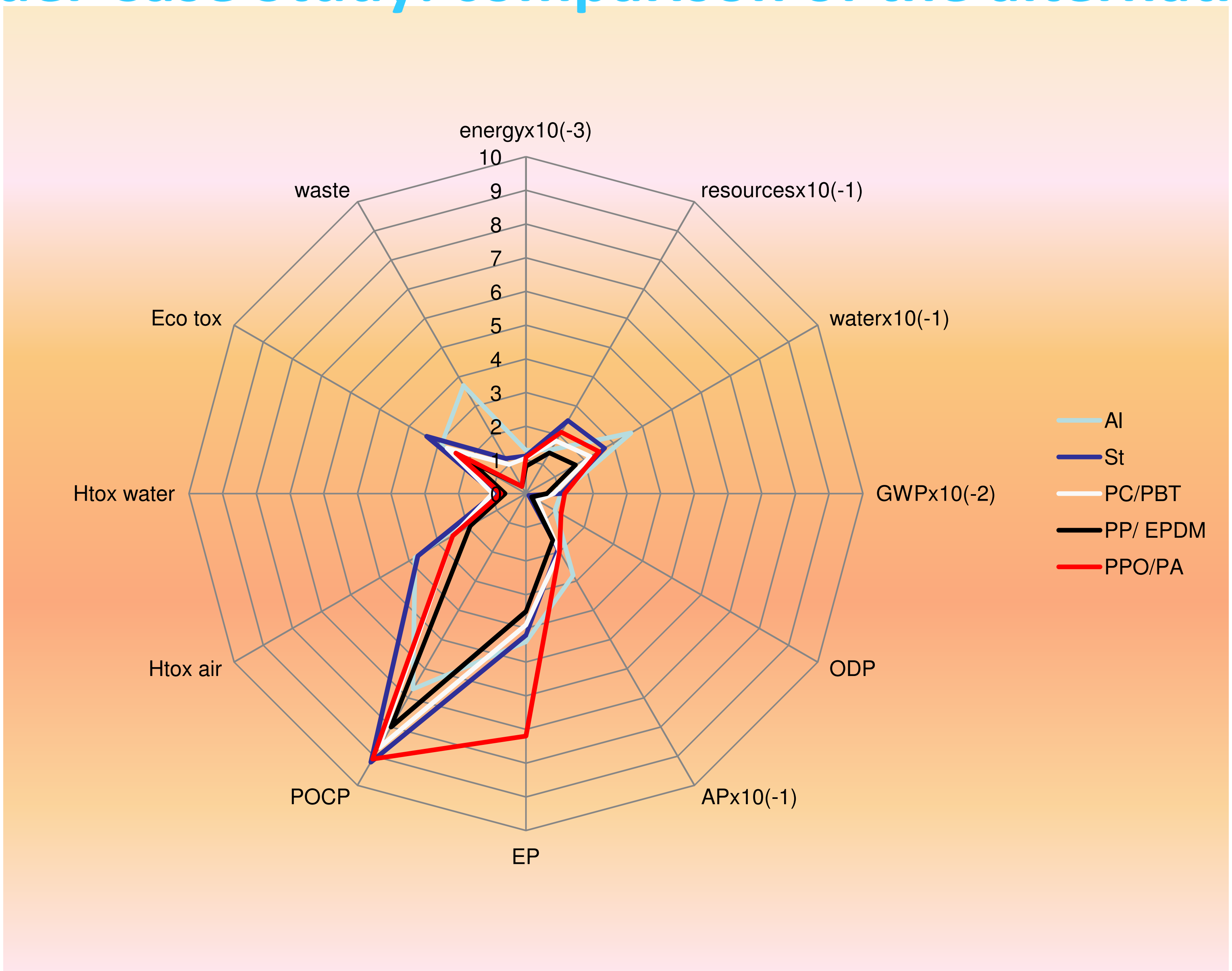
	Al	St	PC/PBT	PP/ EPDM	PPO/PA
energy	**1290**	***1120***	1060	810	1080
resources	15	**25**	18	***14***	21
water	**36**	27	22	**17**	25
GWP	104	105	83	**62**	**115**
ODP	1	**0.1**	0.4	0.2	**1.2**
AP	**28**	19	20	***16***	20
EP	4.4	4.2	3.9	***3.5***	**7.2**
POCP	**6.7**	**9.2**	8.7	8	9.1
Htox air	**3.8**	3.7	2.5	***1.9***	2.5
Htox water	0.66	0.92	**0.99**	**0.62**	0.74
Eco tox	2.9	**3.4**	2.7	**1.9**	2.4
waste	**3.7**	1.2	1	**0.25**	**0.25**

Sustainability of Engineered Processes

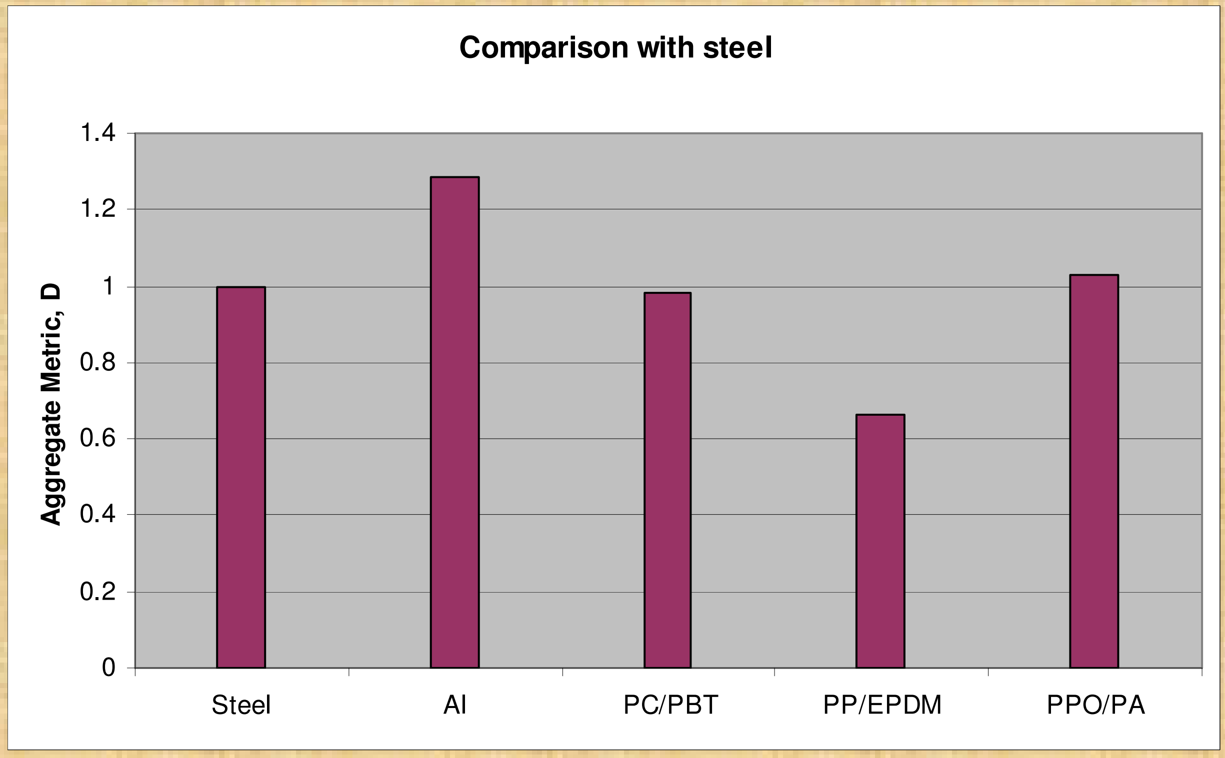


Mapping the fender Metrics

Fender Case Study: comparison of the alternatives



Automobile Fender Study D Results



Case: Automotive Shredder Residue Treatment (Catholique U, Leuven)

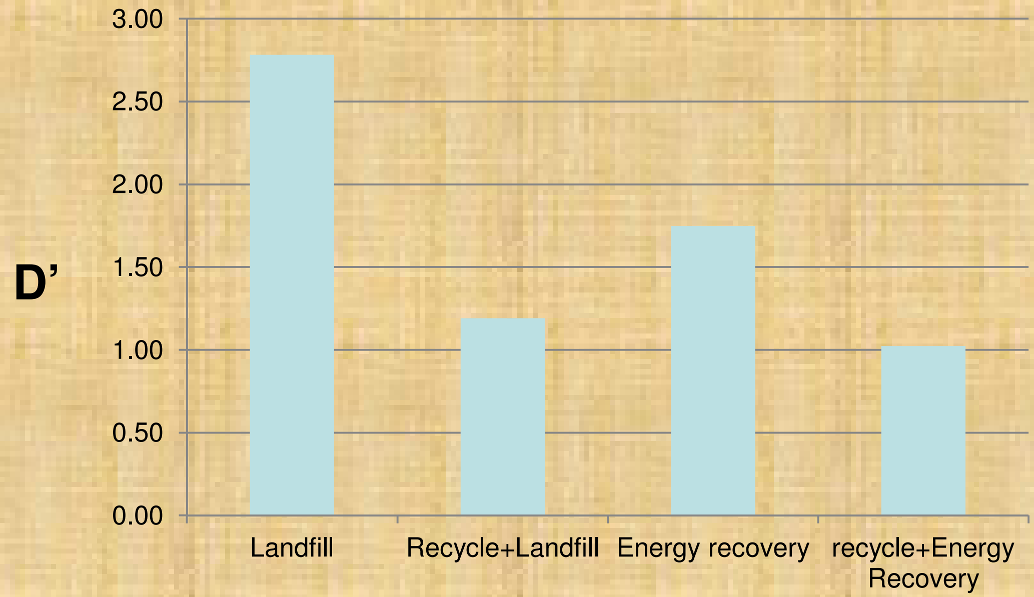
(where improvement is described as negative)

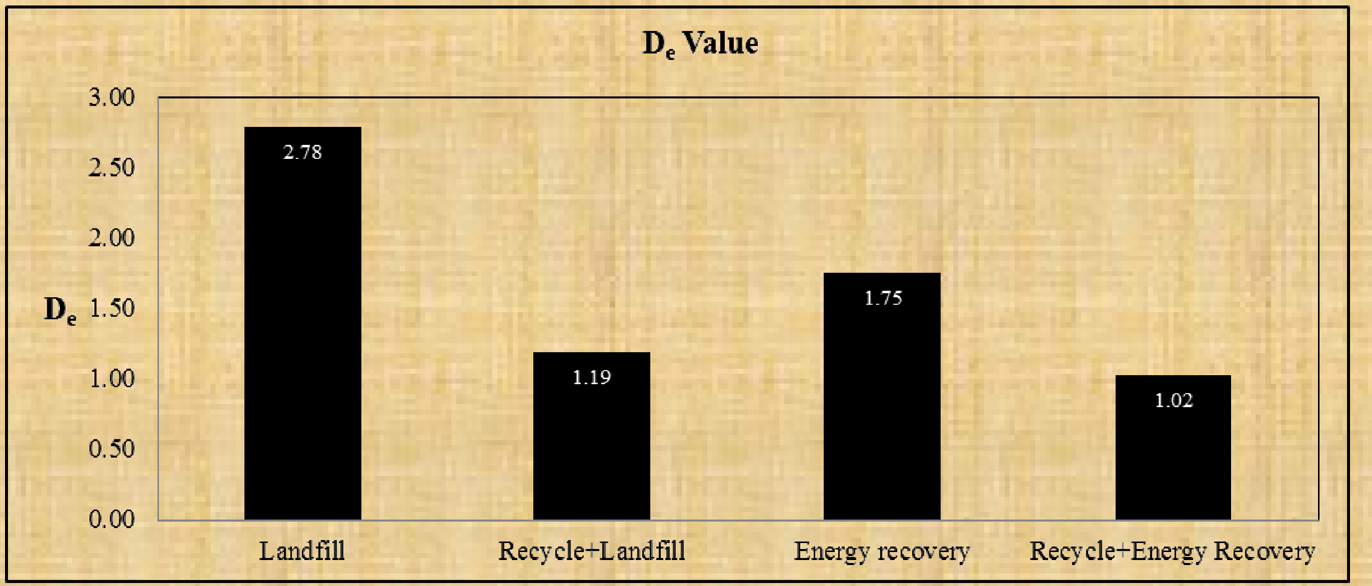
Treatment strategy	EI	MI	WC	LU	GW		HT		TC
y					ST	LT	ST	LT	
Landfill	1.8	3.6	1.7	8.7	637	3844	472	533	106
Recycle+Landfill	-13.1	-408	-4.3	-3.6	-641	1614	-675	-2617	161
Energy recovery	-24.6	-48.2	-5.2	-11.5	841	841	12	-383	133
recycle+Energy Recovery	-26	-438	-7.8	-14.6	-325	-325	-812	-3000	177
Minimum	-26	-438	-7.8	-14.6	-641	-325	-812	-3000	106
y'									
Landfill-Minimum	27.8	441.6	9.5	23.3	1278	4169	1284	3533	0
Recycle+Landfill-Minimum	12.9	30	3.5	11	0	1939	137	383	55
Energy recovery-Minimum	1.4	389.8	2.6	3.1	1482	1166	824	2617	27
recycle+Energy Recovery-Minimum	0	0	0	0	316	0	0	0	71
Maximum	27.8	441.6	9.5	23.3	1482	4169	1284	3533	71

Normalized										Root Square D'
Landfill	1	1	1	1	0.86235	1	1	1	0	2.78
Recycle+Landfill	0.464029	0.067935	0.36842	0.472103	0	0.4651	0.1067	0.108406	0.774648	1.19
Energy recovery	0.05036	0.882699	0.27368	0.133047	1	0.279683	0.64174	0.74073	0.380282	1.75
recycle+Energy Recovery	0	0	0	0	0.21323	0	0	0	1	1.02

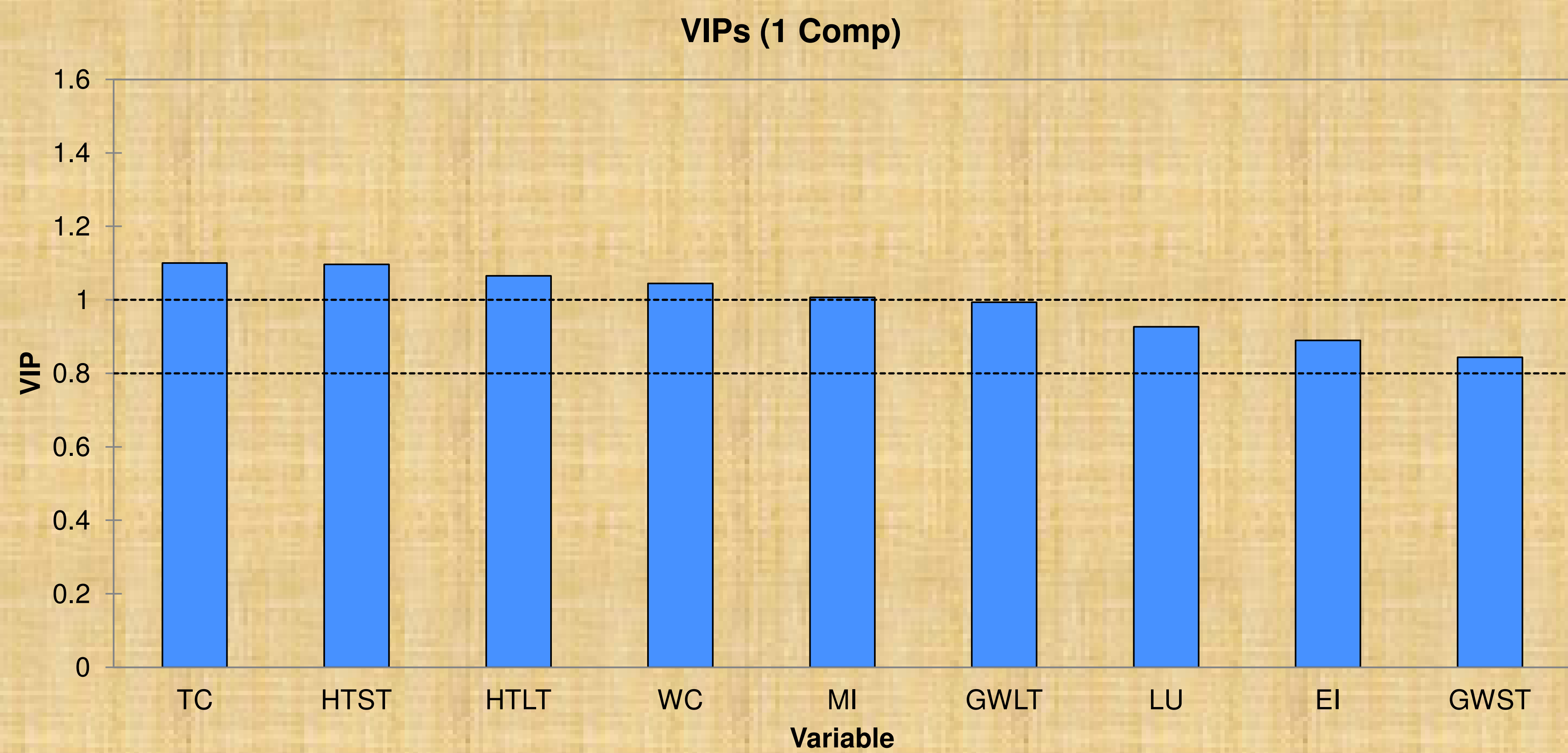
Best-->Worst **D,B,C,A**

Relative Sustainability of the Automotive Shredder Residue options




D_e Value
3.00
2.50
2.00
D_e
1.50
1.00
0.50
0.00
2.78
1.19
1.75
1.02
Landfill
Recycle+Landfill
Energy recovery
Recycle+Energy Recovery

PLS-VIP



The PLS-VIP score shows that TC has the maximum contribution to overall sustainability.
TC, HTST, HTLT, WC and MI are the important variables in that order for their contribution to overall sustainability. All variables have VIP scores more than 0.8.

Sustainability Analysis for Products and Processes

Subhas K. Sikdar
National Risk Management Research Laboratory
U.S. Environmental Protection Agency
Cincinnati, OH 45268
Sikdar.subhas@epa.gov

SNO Conference, November, 2012