Sustainable Chemistry Measurements

Green and Sustainable Chemistry: Is there a difference?

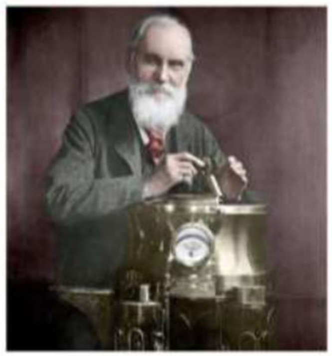
- Sustainable Chemistry: maintenance and continuation of ecologically sound development; must fulfil the meta-principle that “ *human activities should not exceed critical eco-system capacity such as resource depletion, ecological degradation and transgression of local, regional and planetary boundaries*”

- Green Chemistry : Design, synthesis, manufacture and use of chemicals and chemical processes that have little or no pollution potential or environmental risk and are both economically and technologically feasible

B. R. Bakshi, et. al., ACS Sustainable Chemistry and Engineering, 2018, 6, 3632; O.Hutzinger, Environ. Sci & Pollut. Res., 1999, 6, 123

Why do we need to measure?

"To measure is to know"



"If you cannot measure it, you cannot improve it."

William Thomson, 1st Baron Kelvin (1824–1907)
British physicist and engineer

- The first step is to measure whatever can be easily measured. This is fine.
- The second step is to disregard that which cannot be easily measured or to give it an arbitrary quantitative value. This is artificial and misleading.
- The third step is to presume that what can not be measured easily is not important. This is blindness.
- The fourth step is to say that what can not be easily measured really does not exist. This is suicide

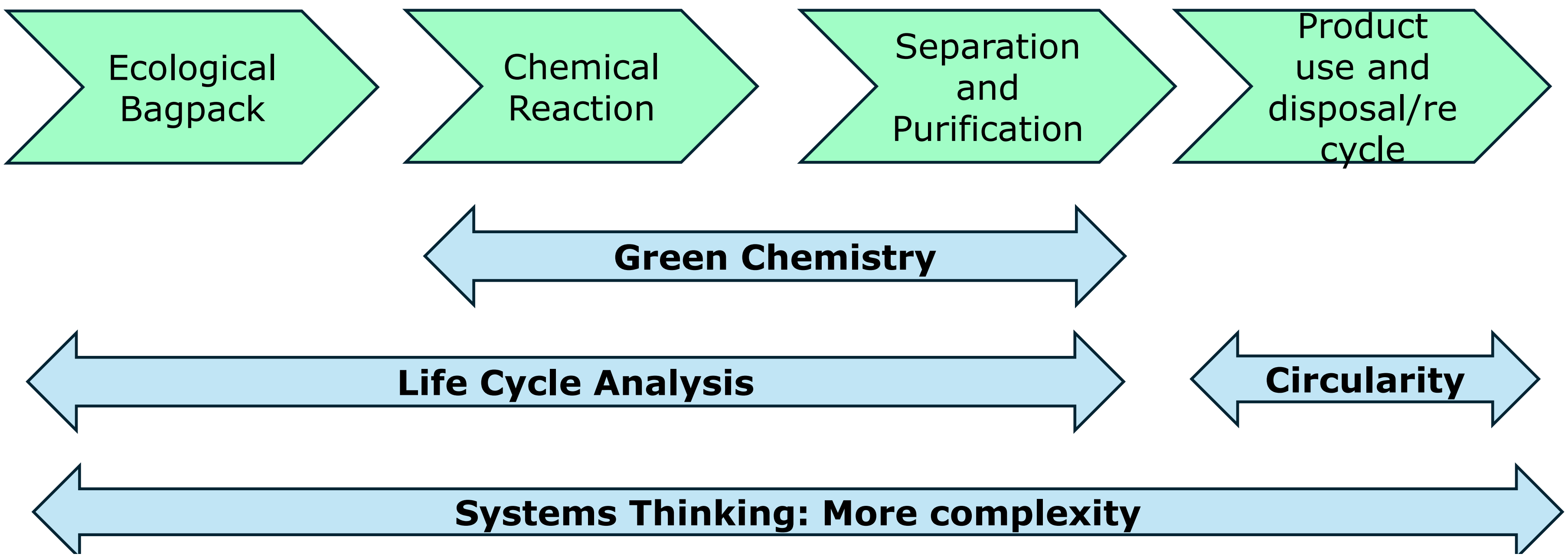
Daniel Yankelovich, " Corporate Priorities: A continuing study of the new demands on business",1972.

McNamara Fallacy

The tendency to make the measurable important rather than making the important measurable.

Scope of Sustainability Assessments

- Green Chemistry Metrics helps optimize linear production chains **(A Chemist’s View)**
- Life Cycle Analysis quantifies the whole-of-life environmental (energy and material) impacts **(A Regulator’s View)**
- Circular Economy provides an umbrella framework for transforming whole systems and presents a real world picture outside the factory gate **(A Society’s View)**



Green Chemistry Metrics

Percent (Chemical) Yield:

$$\text{Chemical Yield} = \frac{\text{mols (g) pdt obtained}}{\text{mols (g) pdt possible}} x100\%$$

Atom Economy *(Barry Trost, , Science, 1991, 254, 1471):*

$$\text{Atom Economy} = \frac{MW_{\text{desired pdt}}}{\square\, MW_{\text{starting materials}}} x100\%$$

- ✓ How much of the reactants remain in the final product
- ✓ Does not account for solvents, reagents, catalysts, reaction yield, and reactant molar excess

Calculation Atom Economy

$$H_3C{-}CH_2{-}CH_2{-}CH_2{-}OH + Na{-}Br + H_2SO_4 \longrightarrow H_3C{-}CH_2{-}CH_2{-}CH_2{-}Br + NaHSO_4 + H_2O$$

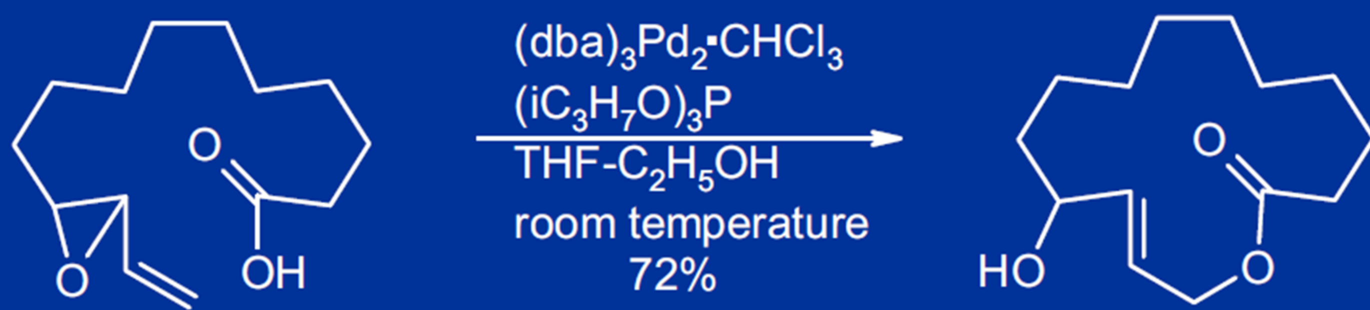
1 2 3 4 5 6

Reagents Formula	Reagents FW	Utilized Atoms	Weight of Utilized Atoms	Unutilized Atoms	Weight of Unutilized Atoms
1 C_4H_9OH	74	4C,9H	57	HO	17
2 NaBr	103	Br	80	Na	23
3 H_2SO_4	98	-----	0	2H,4O,S	98
Total 4C,12H,5O,BrNaS	275	4C,9H,Br	137	3H,5O,Na,S	138

Palladium catalysts

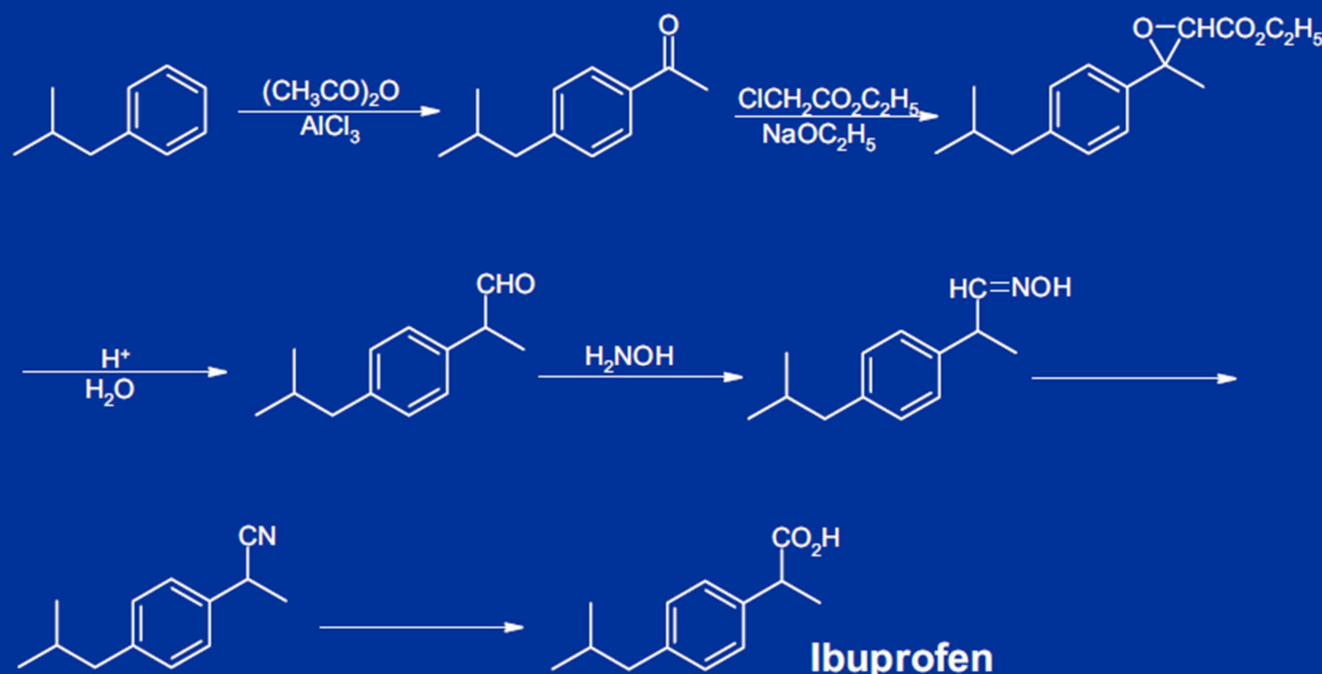
- Allylic alkylations with high atom economy

Trost, Stanford University



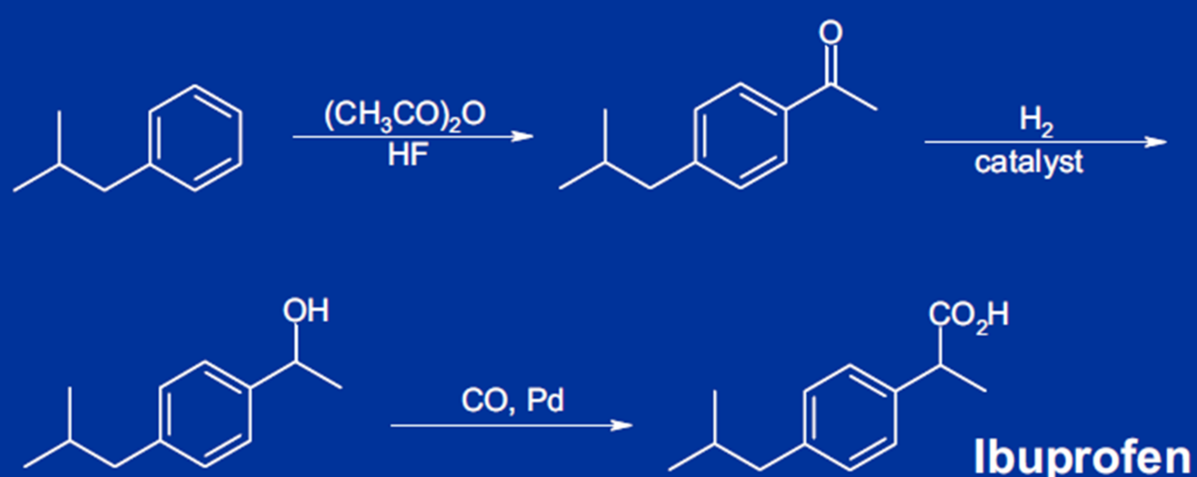
100% atom economy

- Traditional synthesis of ibuprofen
  - 6 stoichiometric steps
  - <40% atom utilization

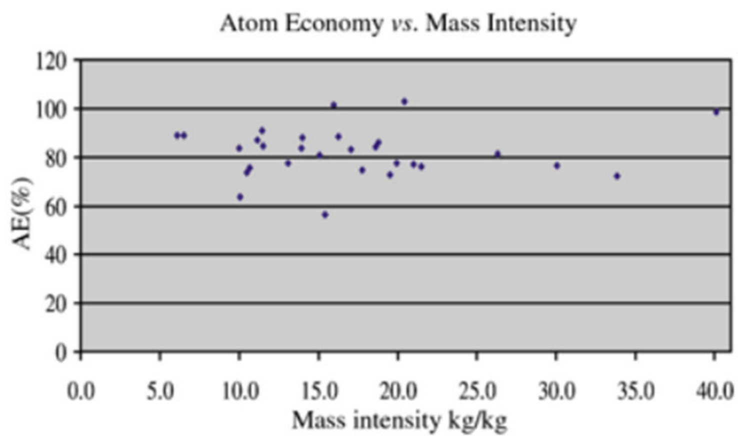


- Catalytic synthesis of ibuprofen
  - 3 catalytic steps
  - 80% atom utilization (99% with recovered acetic acid)

BHC



Other Green Chemistry Parameters



- **Process Mass Intensity:** PMI = $\dfrac{\text{Mass of all materials used [kg]}}{\text{Mass of desired products [kg]}}$
- **Atom Efficiency:**

* Reagents +reactants + catalysts + solvents + work-up chemicals

$$\text{Atom Efficiency} = (\%\ \text{Yield})(\text{Atom Economy})$$

✓ Applicable to individual steps

✓ Assumes the use of stoichiometric quantities of starting materials and disregards solvents and other chemicals that do not appear in the stoichiometric equation

Other Green Chemistry Parameters

Process
React benzyl alcohol (10.81 g, 0.10 mol, FW 108.1) with *p*-toluenesulfonyl chloride (21.9 g, 0.115 mol, FW 190.65) in toluene (500 g) and triethylamine (15 g, FW 101) to give the sulfonate ester (FW 262.29) isolated in 90% yield (0.09 mol, 23.6 g)

Mass intensity = (10.81 + 21.9 + 500 + 15)/23.6 = 23.2 g/g
Reaction mass efficiency = 23.6/(10.81 + 21.9) × 100 = 70.9%
Atom economy = 262.29 / (108.1 + 190.65 + 101) × 100 = 65.8%

The atom economy is < 100% due to formation and neutralisation of the HCl by-product. The reaction mass efficiency also takes into account the 90% yield and the need for a 15% molar excess of *p*-toluenesulfonyl chloride.

E-Factor and C-Factor

- **E-Factor** *(R.A. Sheldon, Chem.& Ind., 1992. 903) :*

$$\text{E - Factor} = \frac{\text{Total Waste (Kg)}}{\text{Product (Kg)}}$$

  - ✓ Typically split into 2 sub-categories: organic & aqueous waste
  - ✓ Higher E factor implies greater negative environmental impact
  - ✓ Applicable to multi-step processes

- **C-Factor** *(C.H.C Christenson, et.al.,ChemSusChem, 2009, 2, 1152) :*

$$\text{C-Factor} = \frac{Total\ Mass\ of\ Carbon\ Dioxide\ Emitted}{Mass\ of\ Product\ Formed}$$

E-factor and C-Factor

Industry Sector	Tons per annum	E Factor
Oil refining and Petrochemicals	10^6 to 10^8	<0.1
Commodity Chemicals	10^4 to 10^6	<1-5
Fine Chemicals	10^2 to 10^4	5- to <50
Specialty Chemicals and Pharmaceuticals	10 to 10^2	25 to <100

R.A. Sheldon, Chem. & Ind., 1992, 903

Environmental Impact on Waste

- Mass efficiency metrics do not provide a weightage to wastes depending on the nature of the waste
- All wastes do not have the same environmental impact. e.g., I kg of NaCl does not have the same impact as 1 kg of dichloromethane or I kg of a chromium (VI) compound
- This deficiency can be overcome by introducing the term "environmental quotient" (E x Q), where "Q" is an arbitrary "unfriendliness" factor or weighting factor
- Many approaches to estimating "Q" values for organic reactions have been developed over the years

Environmental Assessment Tool for Organic Synthesis (EATOS) (M. Eissen and J.O. Metzger, Chem. Eur. J.2002, 8, 3580 (Software can be downloaded at http://www.metzger.chemie.unioldenburg.de/eatos/english.htm
Ecoscale , a semi empirical quantitative tool to select an organic preparation based on economical and ecological parameters, Beilstein J. Org. Chem. 2006, 2, 1

Toxicity and Safety Matrices

- **Hazard Metric**

Hazard = 1 - $\frac{\sum Hazard_{coeff} \times Mass_{Materials}}{Mass\ of\ all\ materials}$

Hazard Coefficient parameter is obtained from Material Safety Data Sheets (MSDS) in terms of harmful materials, irritant, corrosive, explosive and flammable

- **Toxicity Metric**

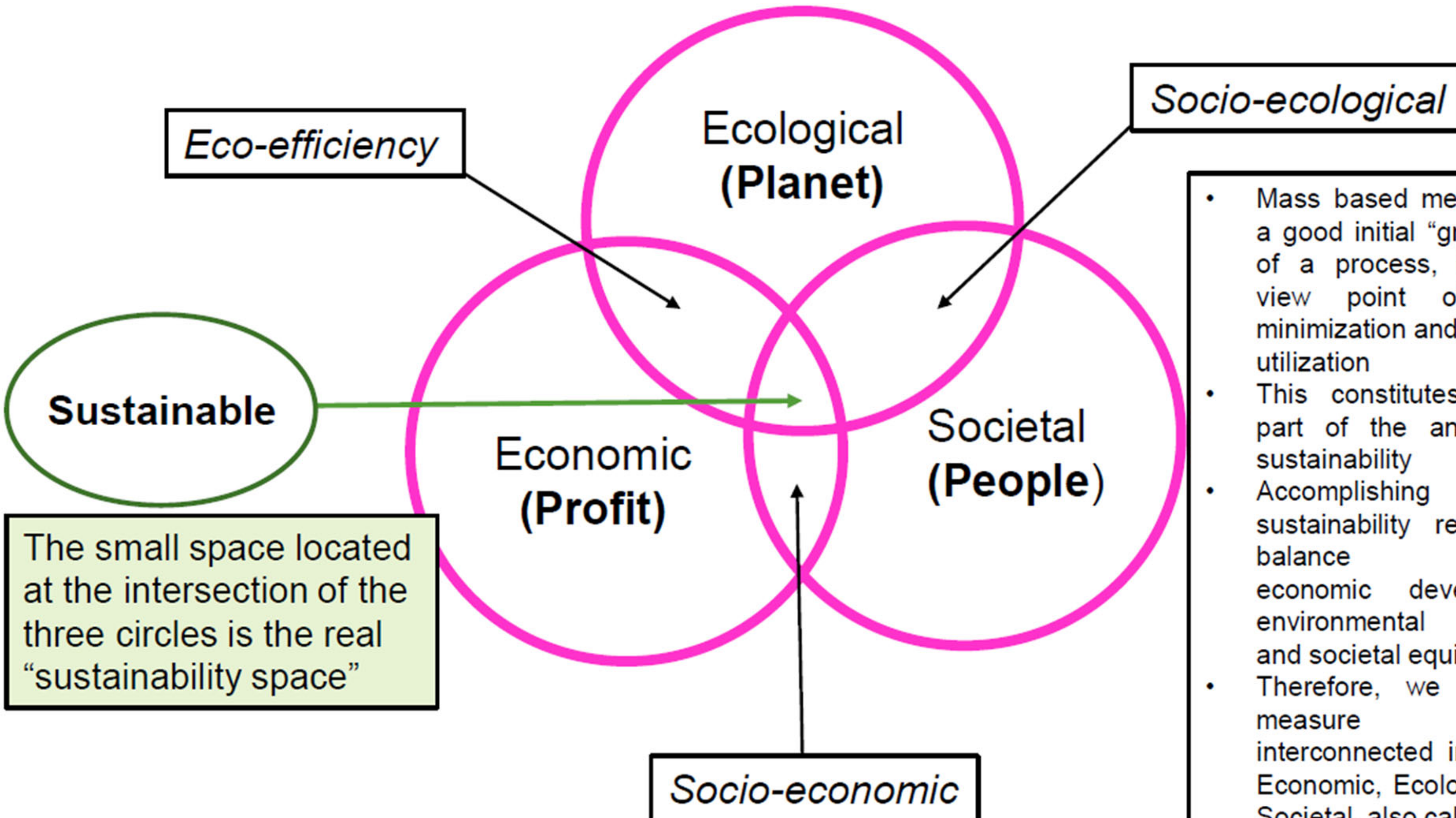
Toxicity = 1- $\frac{\sum (Toxicity_{Coeff} \times Mass_{Materials})}{Mass\ of\ all\ materials}$

Toxicity Coefficient parameter is also obtained from MSDS

- **Risk**

Risk = F_n [Hazard or Toxicity Coefficient x Exposure Time]

H. Kerras, et.al.,10th International Renewable Energy Congress, IEEE, 2019,doi: 10.1019/IREC



- Mass based metrics give a good initial "greenness" of a process, from the view point of waste minimization and resource utilization
- This constitutes only a part of the analysis of sustainability
- Accomplishing true sustainability requires a balance between economic development, environmental impact, and societal equity
- Therefore, we have to measure three interconnected indicators: Economic, Ecological and Societal, also called 3 P's

Carbon Footprint

- Interest in the carbon footprint has been driven by concerns about anthropogenic climate change due to emission of greenhouse gases and their increasing atmospheric concentration.
- In addition to CO_2, other major greenhouse gases (GHGs) include methane, nitrous oxide, and various chlorofluorocarbon (CFC) and hydrochlorofluorocarbon (HCFC)
- Since the contribution of each GHG to radiative forcing is different, to determine the overall impact all GHG emissions are represented in terms of carbon dioxide equivalents (CO2eq).

		GWP for given time horizon		
Common name	Chemical formula	20-yr	100-yr	500-yr
Carbon dioxide	CO_2	1	1	1
Methane	CH_4	72	25	7.6
Nitrous oxide	N_2O	289	298	153
CFC-11	CCl_3F	6730	4750	1620
Carbon tetrachloride	CCl_4	2700	1400	435
HCFC-22	$CHClF_2$	5160	1810	549
HFC-134a	CH_2FCF_3	3830	1430	435
Sulfur hexafluoride	SF_6	16,300	22,800	32,600
Methyl chloride	CH_3Cl	45	13	4

Calculation Carbon Footprint

Example: A life cycle inventory consists of the following emissions: 20 kg of CO2, 0.001 kg of CFC-11, 0.5 kg of N2O, and 2 kg of NO2. Determine the GWP using a 100-year time horizon. The GWP of these emissions is

		GWP for given time horizon		
Common name	Chemical formula	20-yr	100-yr	500-yr
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Methane	CH_4	72	25	7.6
Nitrous oxide	N_2O	289	298	153
CFC-11	CCl_3F	6730	4750	1620
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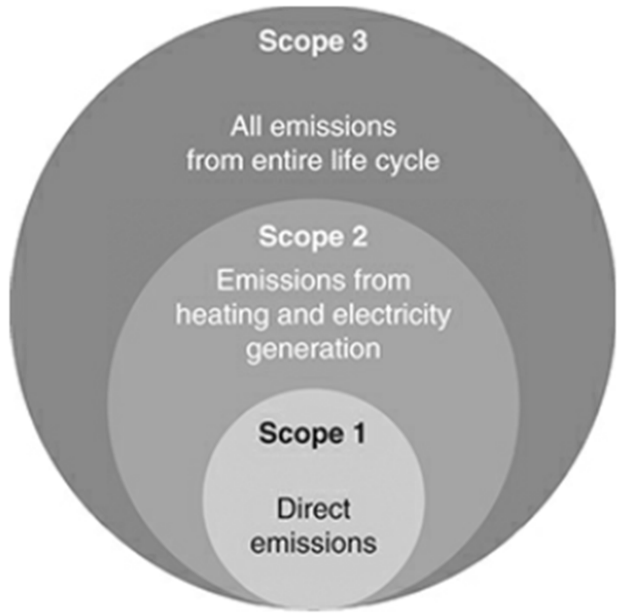
Methyl chloride	CH_3Cl	45	13	4

$$\begin{aligned} \text{GWP} &= (20 \times 1) + (0.001 \times 4750) + (0.5 \times 298) \\ &= 173.8 \text{ kg } CO_2\text{eq} \end{aligned}$$

Scope of Carbon Footprint Calculations



- The boundary of carbon footprint calculations is often classified as Scope 1, 2, or 3.
- Scope 1 is a narrow boundary that considers direct GHG emissions from only selected processes
- Scope 2 includes GHG emissions in generating the electricity and those caused by the heating that is used in the processes included in Scope 1
- Scope 3 is the full life cycle GHG emissions.

Table 11.3 Carbon footprint in gCO2eq/kWh of some pathways for generating electricity in the USA [6].

Item	C footprint
Coal – fluidized bed	1144
Coal – integrated gasification combustion cycle	903
Coal – pulverized	989
Coal – supercritical	768
Natural gas – natural gas combined cycle	449
Natural gas – natural gas combustion turbine	588
Nuclear – boiling water reactor	13
Nuclear – light water reactor	9
Nuclear – pressurized water reactor	12
Wind – offshore and onshore	11
Hydropower	7
Geothermal – enhanced geothermal system	25
Geothermal – flash steam	56
Concentrated solar power – dish	22
Concentrated solar power – tower	33
Concentrated solar power – trough	27
Photovoltaic – monocrystalline Si, ground-mounted	40
Photovoltaic – monocrystalline Si, rooftop	40
Photovoltaic – polycrystalline Si, ground-mounted	69
Photovoltaic – polycrystalline Si, rooftop	46
Biopower – agricultural residues	37
Biopower – animal wastes	40
Biopower – forest residues	34
Biopower – herbaceous crops	50
Biopower – mill wastes	15
Biopower – other wastes	51
Biopower – urban wastes	37
Biopower – woody crops	43
Biopower – cofiring	48
Biopower – direct combustion	35
Biopower – gasification	47

Water Footprint

- The water footprint approach provides insight into the direct and indirect dependence of products, processes, and other systems on water
- Such insight is increasingly important, particularly for water-intensive activities in water-stressed regions of the world.
- The water footprint relies on the concept of virtual water, which is the water used to make a product or service.
- Water use is defined as the water in the product and the water that cannot be used directly for any other purpose.
- For example, the virtual water use in thermal power is mainly due to evaporative losses and leaks, and the virtual water in a beverage is the water contained in it.

use in the region.

Example 11.4 The production of 1 kg of product E withdraws 200 liters of water from a river, and returns 150 liters at a downstream location. The manufacture of 1 kg of this product also requires 0.2 kg of A, 5 kg of B, and 1 kg of C. These resources, A, B, and C, use 100, 10, and 80 liters of water per kilogram, respectively. Determine the virtual water required for making 1 kg of E, and its water footprint.

Solution

Since the virtual water includes only the direct water use, the virtual water requirement of E is $V_E = 200 - 150 = 50$ liters.

The water footprint of E considers both the direct and indirect use. We may define a boundary that includes the resources A, B, and C needed to make product E but ignores activities beyond these resources. Then, the water footprint of E may be calculated as follows:

$$
\begin{aligned}
F_{W,E} &= 50 + (0.2 \times 100) + (5 \times 10) + (1 \times 80) \\
&= 200 \text{ liters}
\end{aligned}
$$

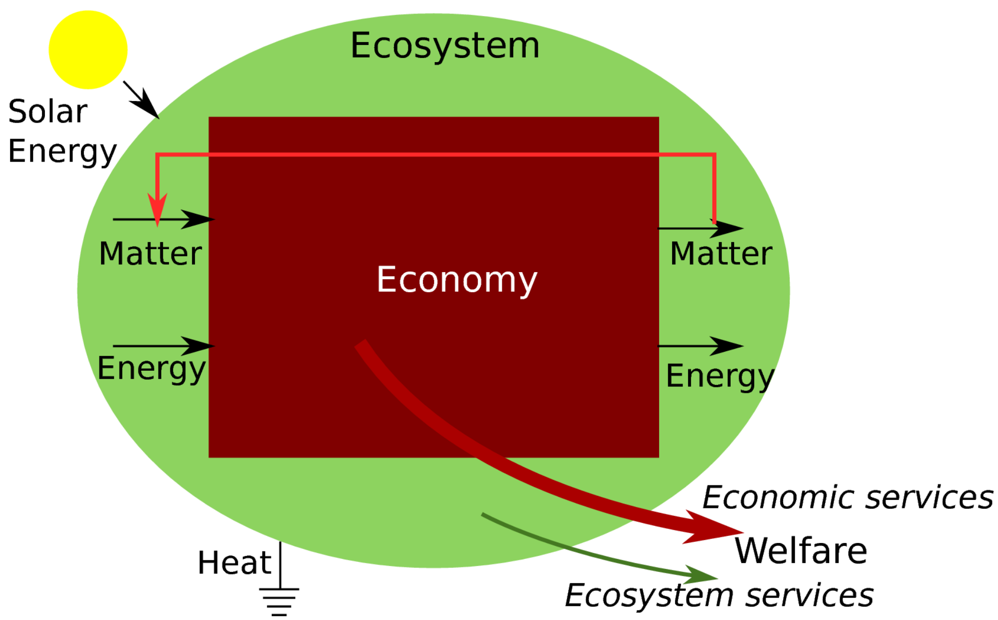
To account for different sources of water and changes in quality, most water footprint calculations consider the following three categories of water.

Water Footprint for Selected Products

Item	Quantity	Water footprint (L)
Apple	1 (150 g)	125
Banana	1 (200 g)	160
Beef	1 kg	15,415
Beer	1 glass (250 ml)	74
Corn ethanol	1 liter	2854
Cheese	1 kg	3178
Chicken meat	1 kg	4325
Cotton	1 shirt (250 g)	2495
Leather (bovine)	1 kg	17,093
Pizza	1 pizza	1259
Pork	1 kg	5988
Rice	1 kg	2497

Measuring Material and Energy Flows

- Our present economy is dependent on a massive inward flow of natural resources. This is followed by a reverse flow of economically spent and dilute matter back to the ecosphere.
- Sustainability problems are determined largely by these economy-ecosphere material and energy flows which is predominantly linear in fashion today



*How do we **measure** the in-flow and the out-flow and establish a material/energy balance ?*

Motivation – Why Energy Footprint?

- Energy is required for all activities – ecological and industrial – a universal currency

- All systems involve transformation of energy

- Can analysis of energy flow help in improving processes and life cycles?

- Can an energy footprint help?

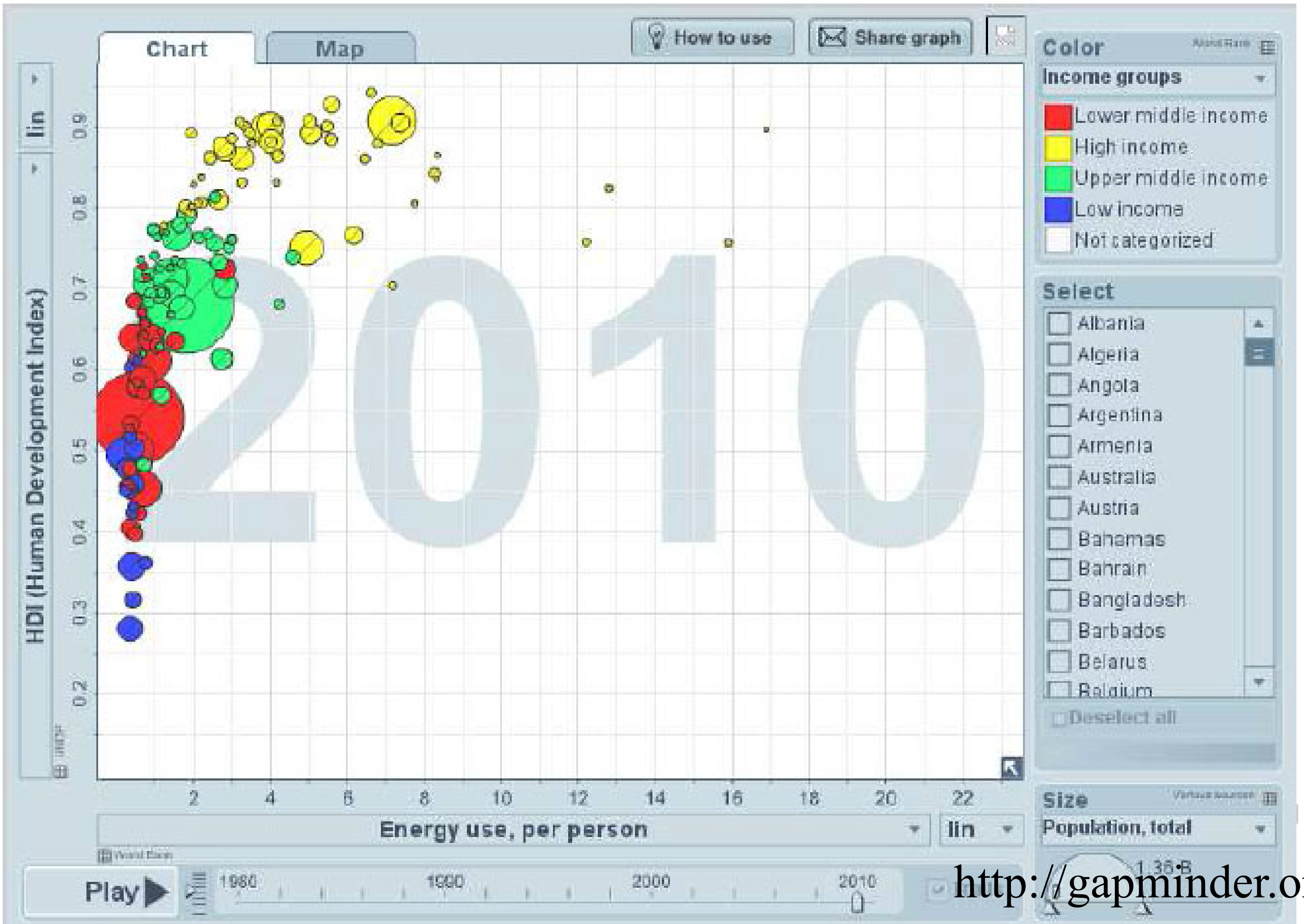
What is Energy?

- Term created by Aristotle (384-322 B.C.) by joining $\epsilon\nu$ (in) and $\epsilon\rho\gamma o\nu$ (work)
- Aristotle said that every object's existence is maintained by energeia related to the object's function
- Energy is used in the context of force, power, and in many other ways
- Most common definition
  - "Energy is the capacity for doing work"
- Many types of energy
  - Kinetic, gravitational, chemical, nuclear, electrical, thermal
- Can convert from one form to another

Calculations

- Thermal energy, enthalpy
  - $\Delta H = mc_p\Delta \mathrm{T}$
- Kinetic
  - $E_k = 0.5mv^2$
- Potential
  - $E_p = mgh$
- Chemical, heat of reaction
  - ΔH_r
- Energy Efficiency = (Energy output) / (Energy input)

Energy and Human Well-Being



http://gapminder.org

Energy Flows and Equations

- $E_f + E_{pr} = E_p + E_w$
- Efficiency, $\eta = E_p/(E_f+E_{pr})$
- Energy return on investment, EROI = E_p/E_{pr}
- Net energy, $E_{net} = E_p - E_{pr}$

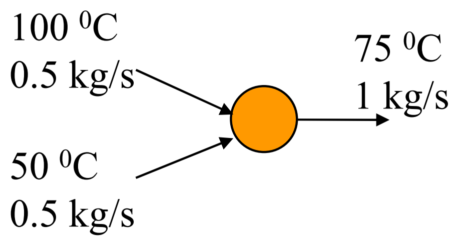
Different Types of Energy

Activity	Feedstock energy, E_f	Product energy, E_p	Processing energy, E_{pr}
Coal Mining	Coal under ground	Coal above ground	Energy for bringing coal above ground from the mine
Refining crude oil			
Cheetah hunting a gazelle			

Example

- Thermal mixing process

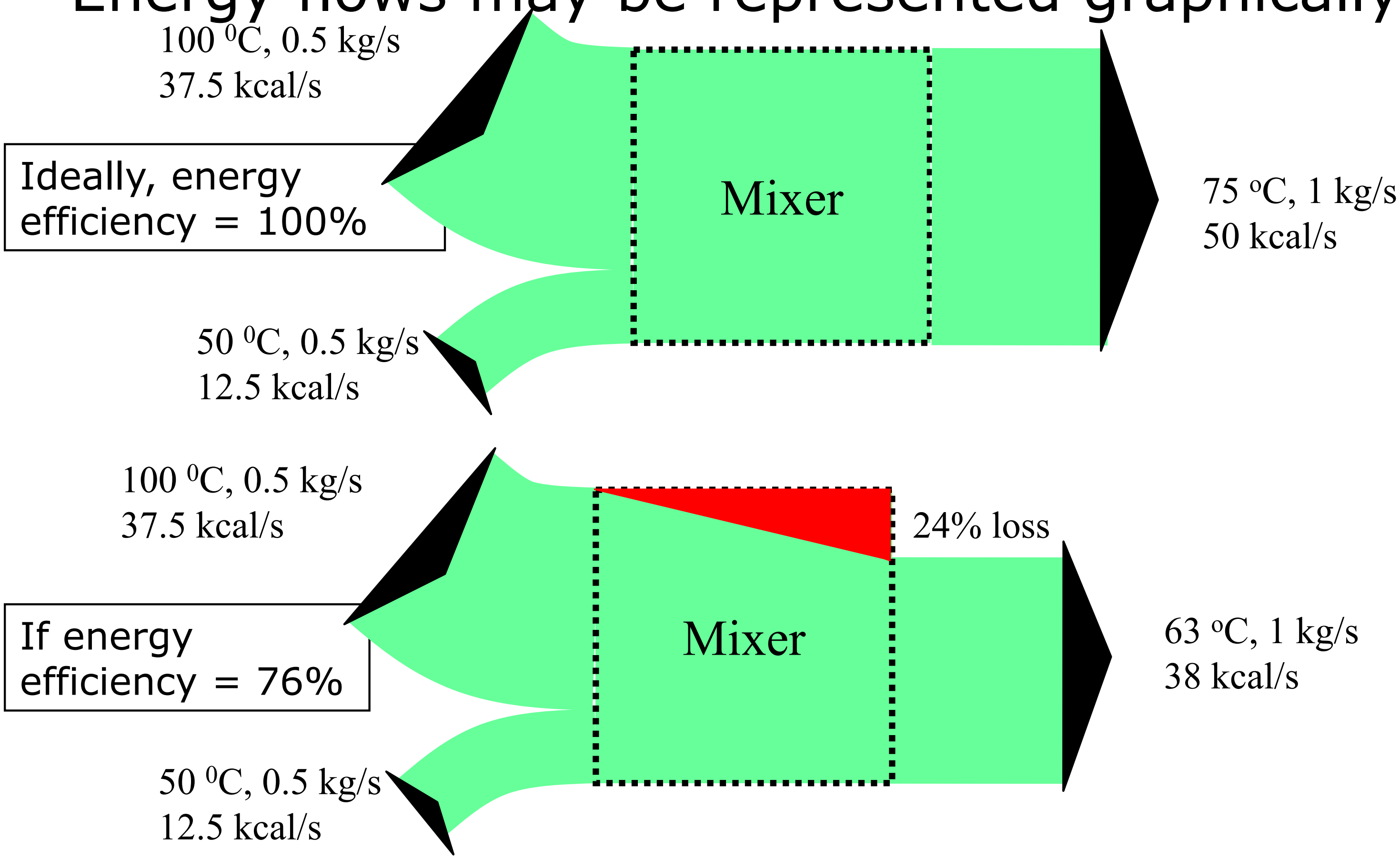
  0.5 kg/s of water at 100 ^oC and 1 atm is mixed adiabatically and isobarically with 0.5 kg/s of water at 50 ^oC and 1 atm



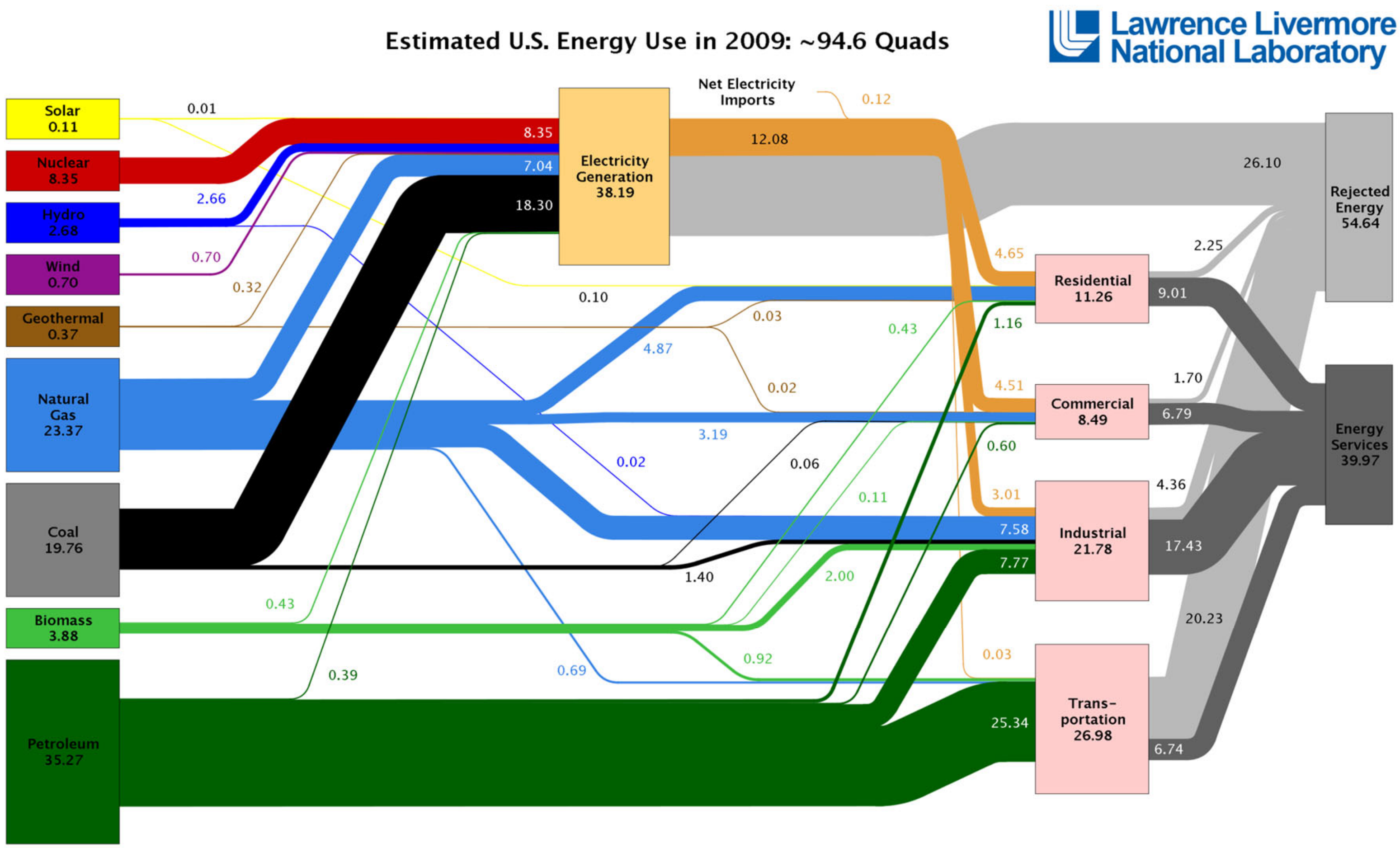
- Reference is 25 ^oC, 1 atm
- $H_{hot} = m_1C_p(T_1\text{-}T_{ref})$ = 37.5 kcal/s
- H_{cold} = 12.5 kcal/s
- H_{mix} = 50 kcal/s
- Ideal energy efficiency = 100%

Sankey Diagram

- Energy flows may be represented graphically



U.S. Energy Use



Source: LLNL 2010. Data is based on DOE/EIA-0384(2009), August 2010. If this information or a reproduction of it is used, credit must be given to the Lawrence Livermore National Laboratory and the Department of Energy, under whose auspices the work was performed. Distributed electricity represents only retail electricity sales and does not include self-generation. EIA reports flows for non-thermal resources (i.e., hydro, wind and solar) in BTU-equivalent values by assuming a typical fossil fuel plant "heat rate." The efficiency of electricity production is calculated as the total retail electricity delivered divided by the primary energy input into electricity generation. End use efficiency is estimated as 80% for the residential, commercial and industrial sectors, and as 25% for the transportation sector. Totals may not equal sum of components due to independent rounding. LLNL-MI-410527

Energy Return on Investment

- Energy is needed for converting feedstock into desired product
- EROI = Energy in Product / Processing Energy
- Net Energy = Energy in Product – Processing Energy
- EROI should be more than one for being energetically "profitable"
- EROI of 10 indicates 10 J produced for every J used in processing

EROI of Fuels

- EROI of selected fuels (approximate)
  - Crude Oil (1930) 100
  - Crude Oil (2000) 20
  - Coal (1950) 100
  - Coal (2000) 80
  - Gasoline 8
  - Corn ethanol 1.2
  - Oil Shale 3
  - Coal Liquefaction 2
  - Shale gas >70

From Cleveland, C. J., *Energy*, 30, 769-782, 2005

EROI of Fuels

Resource	Year	Region	EROI
Oil and gas production	1950	USA	100
Oil and gas production	1970	USA	20
Oil and gas production	1999	Global	35
Oil and gas production	2006	Global	18
Oil and gas production	2010	China	10
Natural gas	1993	Canada	38
Natural gas	2000	Canada	26
Natural gas	2009	Canada	20
Coal	1950	USA	100
Coal	2000	USA	80
Coal	2007	USA	60
Shale oil	*	*	5
Shale gas	*	*	>70
Nuclear	n/a	USA	5-15
Hydropower	n/a	n/a	>100
Wind	n/a	n/a	18
Photovoltaic	n/a	n/a	6-12
Gasoline	n/a	n/a	8
Sugarcane ethanol	n/a	n/a	0.8-10
Corn ethanol	n/a	n/a	0.8-1.6

Features of Energy Analysis

- Pros
  - Appealing approach because energy is the common currency in all systems
  - Can be used for analysis of systems at any scale – equipment, life cycle, economy, ecosystem
  - Relatively easy to understand
  - Easier to calculate than LCA
- Cons
  - Is energy all that matters?
  - What about material use?
  - Primary focus is on fossil fuels – is that adequate?
  - Does energy really represent the “capacity for doing work”?
  - Can different types of energy be added?

Quality of Energy

- Net energy analysis adds fuel content of crude oil, coal and natural gas
- What are the implications of adding these fuel values?
  - Substitutability between these fuels
  - Is a joule of coal equivalent to a joule of crude oil or natural gas?
- How to account for differences in quality of resources?

Quality of Energy

- Would you prefer 1 kW of work or 1 kW of heat?
- How about 1 kW water at 80 ^{o}C vs. 1 kW water at 50 ^{o}C?
- Some intuitive facts
  - Work can be converted to heat completely (no loss)
  - Can heat be converted back to work without loss?
- No, heat cannot be converted to work without loss
  - Work increases molecular motion (randomness) due to heat
  - The randomness cannot be put back in order without additional work
- Heat is a lower *quality* of energy than work
- As temperature decreases, heat becomes less useful
- Difference between heat and work is captured by concept of *entropy*

The Concept of Exergy

- Exergy is the *maximum* energy available for doing work
  - Also called availability
- It is “entropy free” energy
- Measured with respect to a reference state
  - Ambient environment is popular reference state for environmental applications
- In general,
  - $B = (H - H_0) - T_0(S - S_0)$

This equation looks similar to the equations for free energy. So is exergy the same as free energy?

Exergy and Free Energy

$$B = (H - H_0) - T_0(S - S_0)$$

Exergy. If the reference state is the environment, the above equation calculates exergy.

Temperature: 25 °C, Pressure: 1 atm, Minerals: Concentration of first kilometer of Earth's crust, Other materials: Concentration of sea water

Gibbs free energy. If the reference state is the final state of a chemical reaction, and pressure and volume are held constant along the path toward this state, then above equation becomes the Gibbs free energy.

Life-Cycle Assessment: Motivation

- Methods discussed so far focus on either univariate measures or aggregate metrics
- Do not consider all emissions, resource use and their impact

Approach	Multivariate?	Resources?	Emissions?	Ecosystem Services?
C footprint	No	No	GHG	No
H_2O footprint	No	Water	Gray water	No
Energy	Partially	Fossils	No	No
Exergy	Partially	Materials & Energy	No	Partially
LCIA	Yes, hierarchical	Many	Many	No (being developed)

Life Cycle Assessment (LCA)

- LCA is a process to asses the environmental impact of a product in all stages of its " From acquisition of raw materials through production and use to end of life treatment and disposal or recycling (cradle to grave)"
- Includes mass and energy balances, and environmental impact categories, such as, global warming potential, ozone depletion, acidification, eutrophication, smog formation, human and eco toxicity
- The methodology for LCA is available as a standard, ISO 14040 2006
- Use of the Standard builds trust and credibility of the assessment
- It is a widely used decision making tool both by Government and industry, especially the regulatory bodies
- Conducting full LCA is both time and cost intensive and will require high quality of data. This can be done only at the end of the design stage of a product and its manufacturing

Steps in LCA Analysis

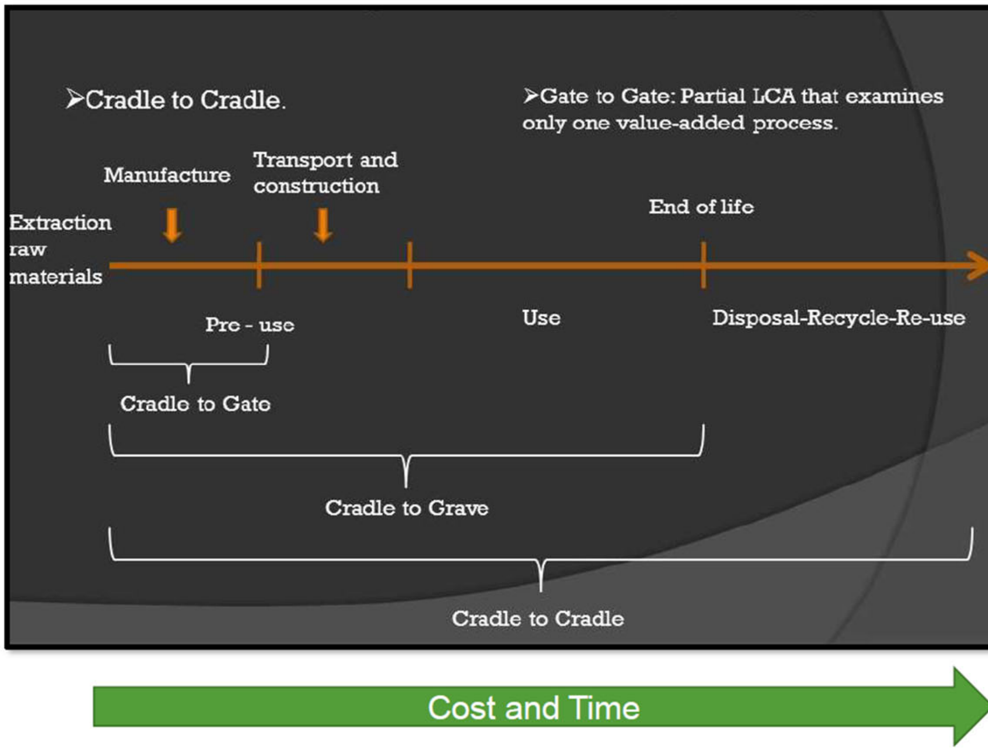
LCA is an iterative process consisting of four phases:

1. Definition of goal, system boundaries and scope
2. Inventory analysis, material flow analysis, environmental impact of chemicals
3. Impact assessment
4. Interpretation

Conducting full scale cradle to grave LCA in the development phase of a process is generally difficult

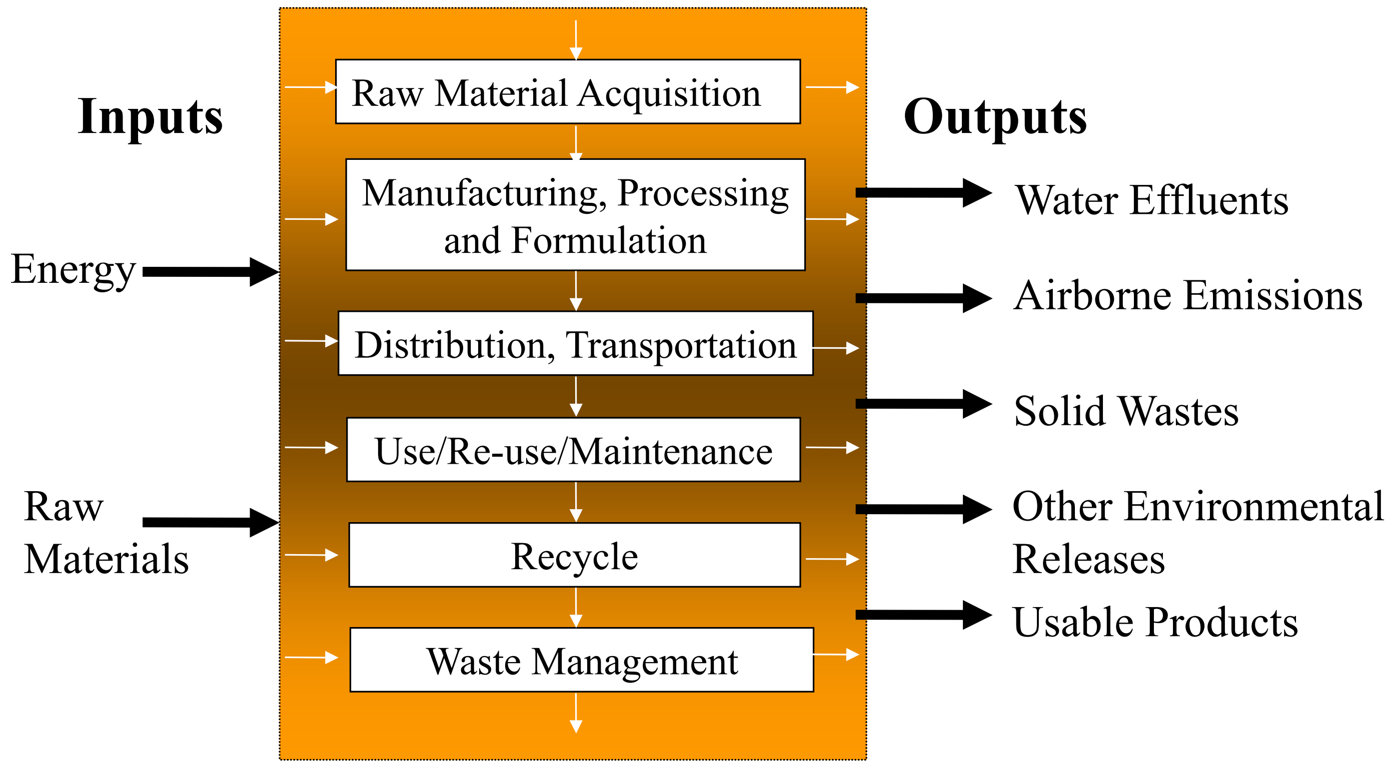
One can limit the LCA to a chemical process (gate to gate)

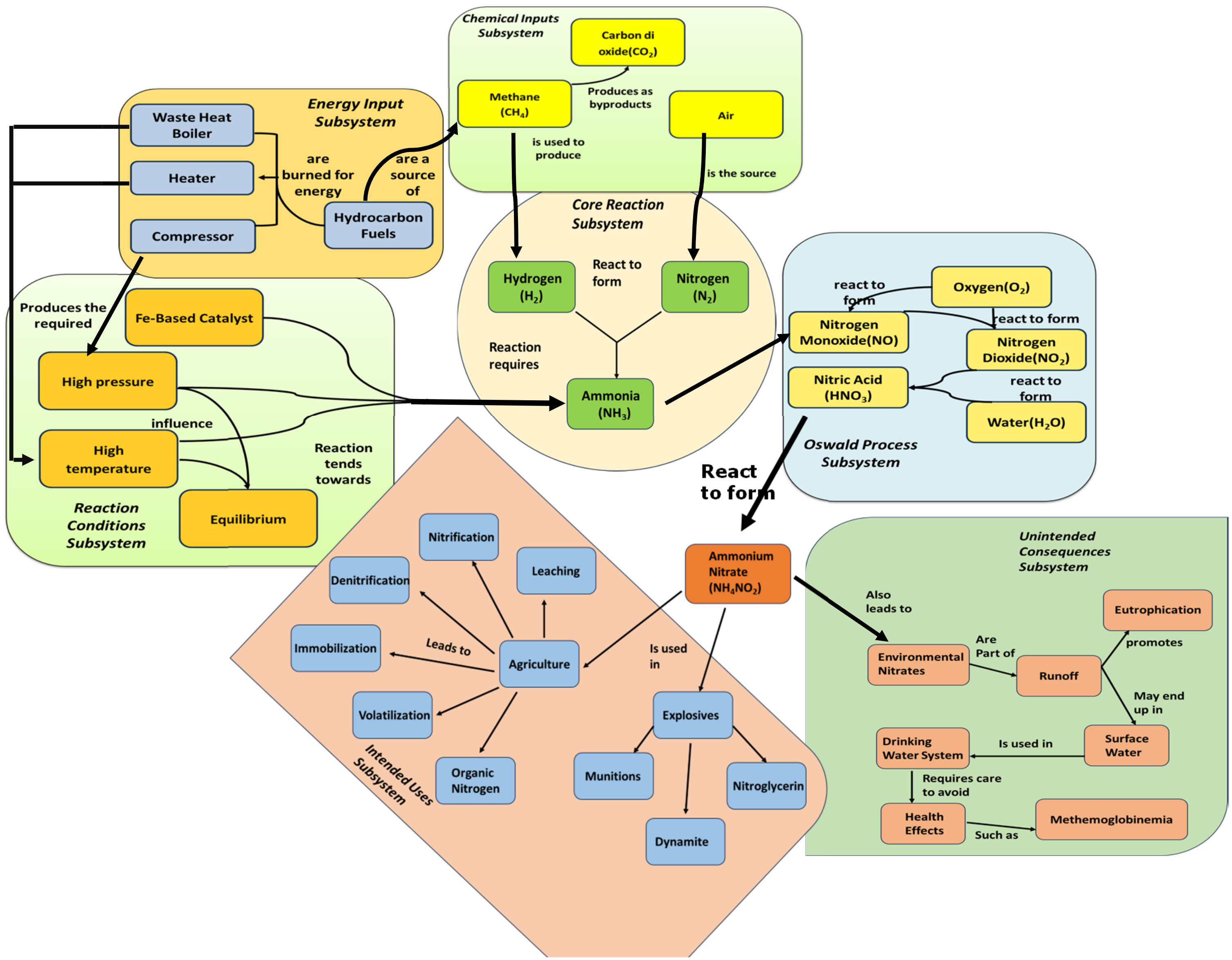
LCA: Scope and System Boundaries



- Gate to Gate
- Cradle to Gate
- Cradle to Grave
- Cradle to Cradle

Step 2: Inventory Analysis



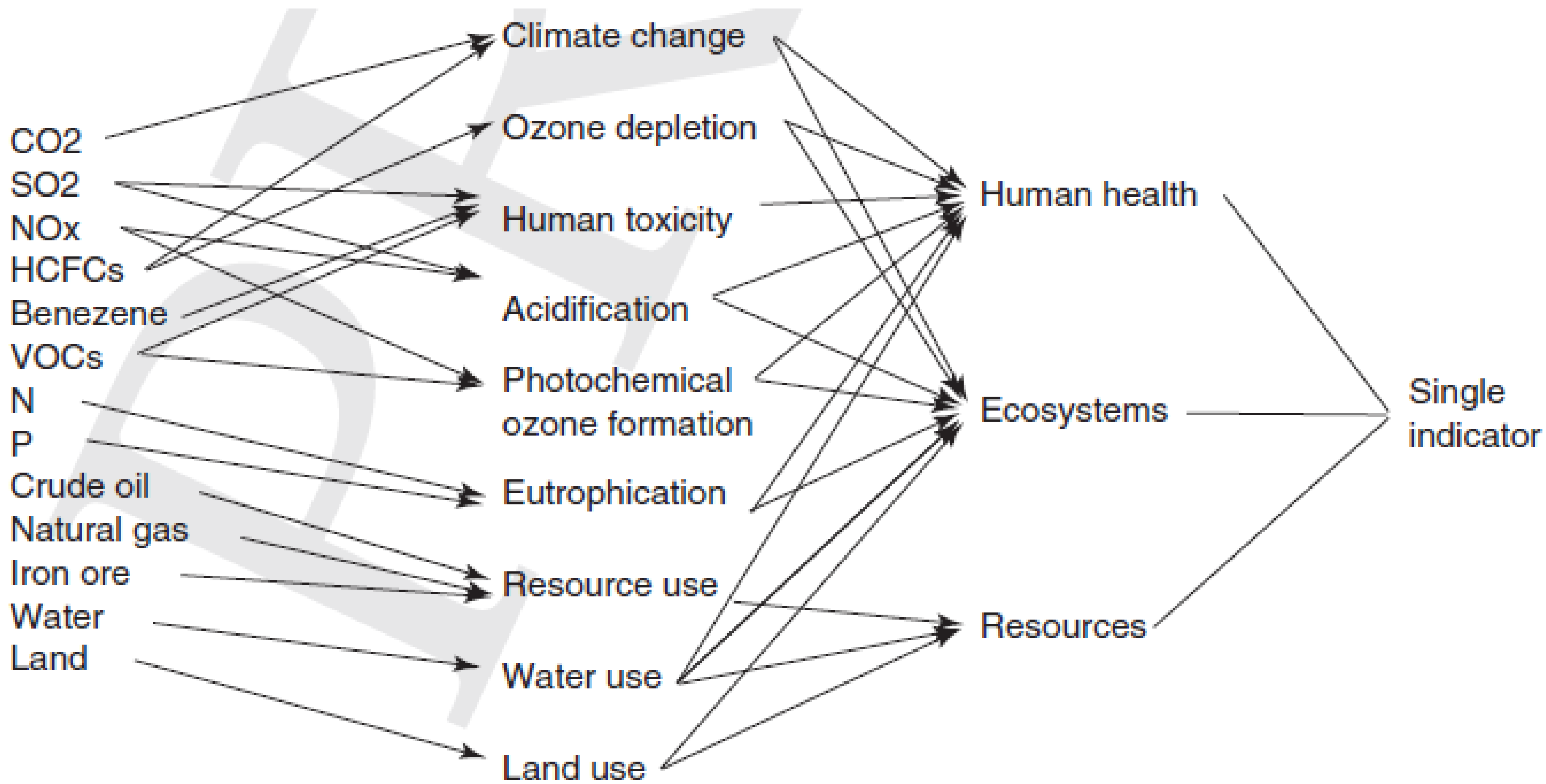


Chemical Inputs Subsystem
Carbon di oxide(CO_2)
Methane (CH_4)
Produces as byproducts
Air
is used to produce
is the source
Energy Input Subsystem
Waste Heat Boiler
Heater
Compressor
are burned for energy
are a source of
Hydrocarbon Fuels
Core Reaction Subsystem
Hydrogen (H_2)
React to form
Nitrogen (N_2)
Reaction requires
Ammonia (NH_3)
Oswald Process Subsystem
react to form
Oxygen(O_2)
react to form
Nitrogen Monoxide(NO)
Nitrogen Dioxide(NO_2)
Nitric Acid (HNO_3)
react to form
Water(H_2O)
React to form
Produces the required
Fe-Based Catalyst
High pressure
influence
High temperature
Reaction tends towards
Equilibrium
Reaction Conditions Subsystem
Ammonium Nitrate (NH_4NO_2)
Intended Uses Subsystem
Nitrification
Leaching
Denitrification
Immobilization
Leads to
Agriculture
Volatilization
Organic Nitrogen
Is used in
Explosives
Munitions
Nitroglycerin
Dynamite
Unintended Consequences Subsystem
Also leads to
Eutrophication
promotes
Environmental Nitrates
Are Part of
Runoff
May end up in
Surface Water
Drinking Water System
Is used in
Requires care to avoid
Health Effects
Such as
Methemoglobinemia

Sustainability Matrices Categories

Category	Measurement Unit
Net mass of materials used	kg
Net energy used	MJ
Green house gas equivalent	kg CO_2 equivalent
Fossil fuel used for material manufacture	kg
Acidification potential	kg SO_2 equivalent
Eutrophication potential	kg PO_4^{-3} equivalent
Photochemical ozone creation potential	kg ethylene equivalent
Total organic carbon (TOC) load in waste water	

Life Cycle Impact Assessment



Limitations of LCA

- Compiling life cycle inventory data can be expensive and time consuming
- Unavailability of data and uncertainties in assumption can impact the conclusions
- LCA needs us to choose one of the impact categories. Choosing another set of impact category can lead to another view of sustainability
- The results will depend upon the weightage method used to calculate a single environmental score; this could be subjective
- LCA does not consider social and economic impacts

Because of these complexities, it may be difficult to determine the best performing alternative in a comparative context. Outcomes of LCA must be supplemented by other decision making tools

https://www.levistrauss.com/wp-content/uploads/2015/03/Full-LCA-Results-Deck-FINAL.pdf

Life Cycle of Levi's Jeans

Impact Categories

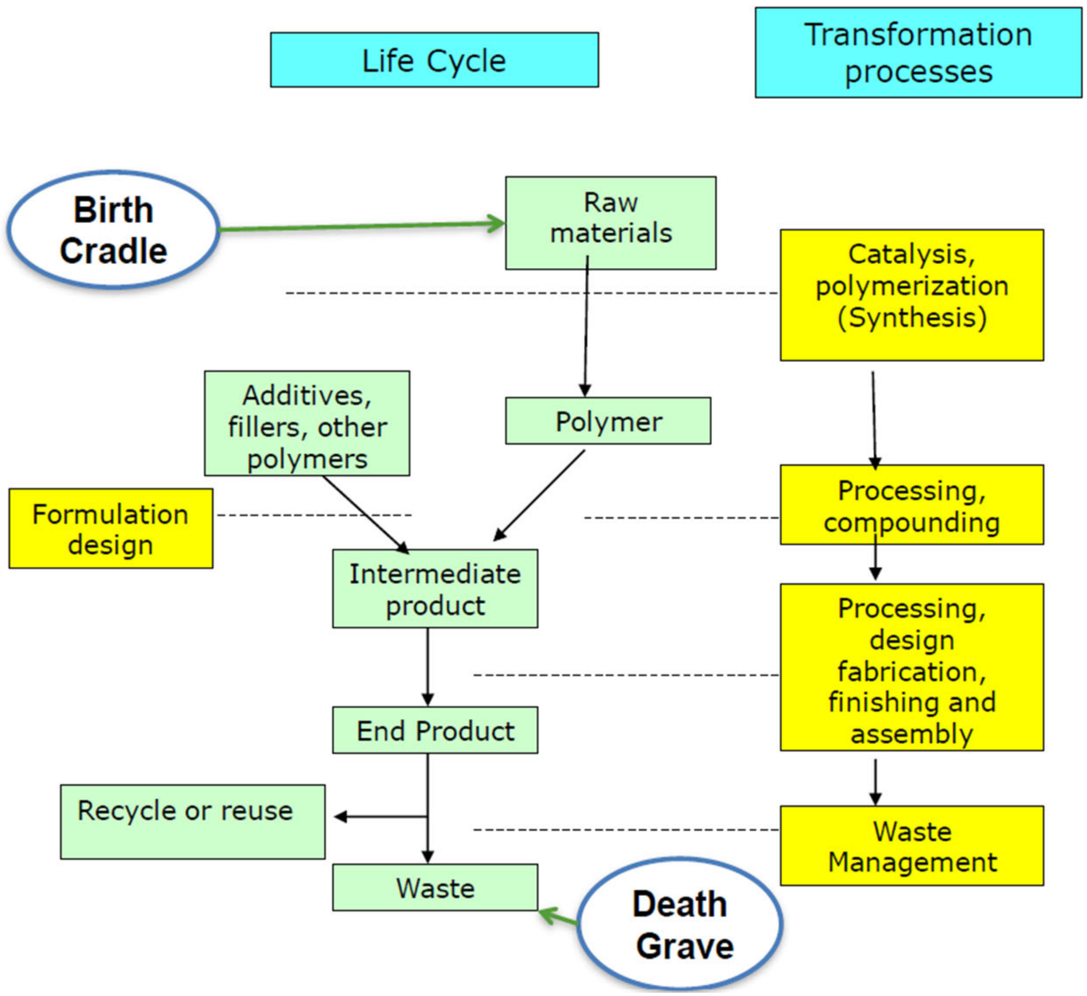
- Climate change
- Fresh water intake from the environment
- Water consumption: Net water taken minus water returned to the same watershed at the same quality
- Eutrophication: Oxygen depletion in fresh water environment
- Land Occupation: Land occupied to support the product
- Abiotic depletion: A measure of depletion of natural resources

Life Cycle Impact

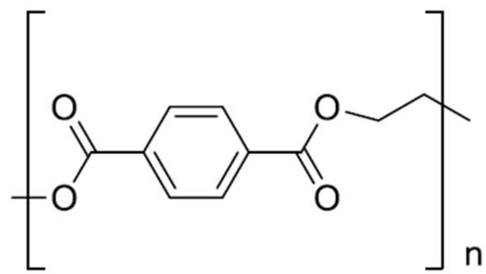
The entire life time of a one pair of jean equates to

Climate Change 33.4 kg of CO_2 equiv	• 69 miles driven by an average car in the US • 246 hours of TV on a plasma big screen
Water Consumed 3,781 liters	Three days of one US household's water needs
Eutrophication 48.9 g of PO_4 equiv	The total amount of phosphorous found in 1700 tomatoes
Land Occupation: 12 m^2/ year	Seven people standing with arms outstretched would form one side of a square of this size

Life-Cycle and Transformation



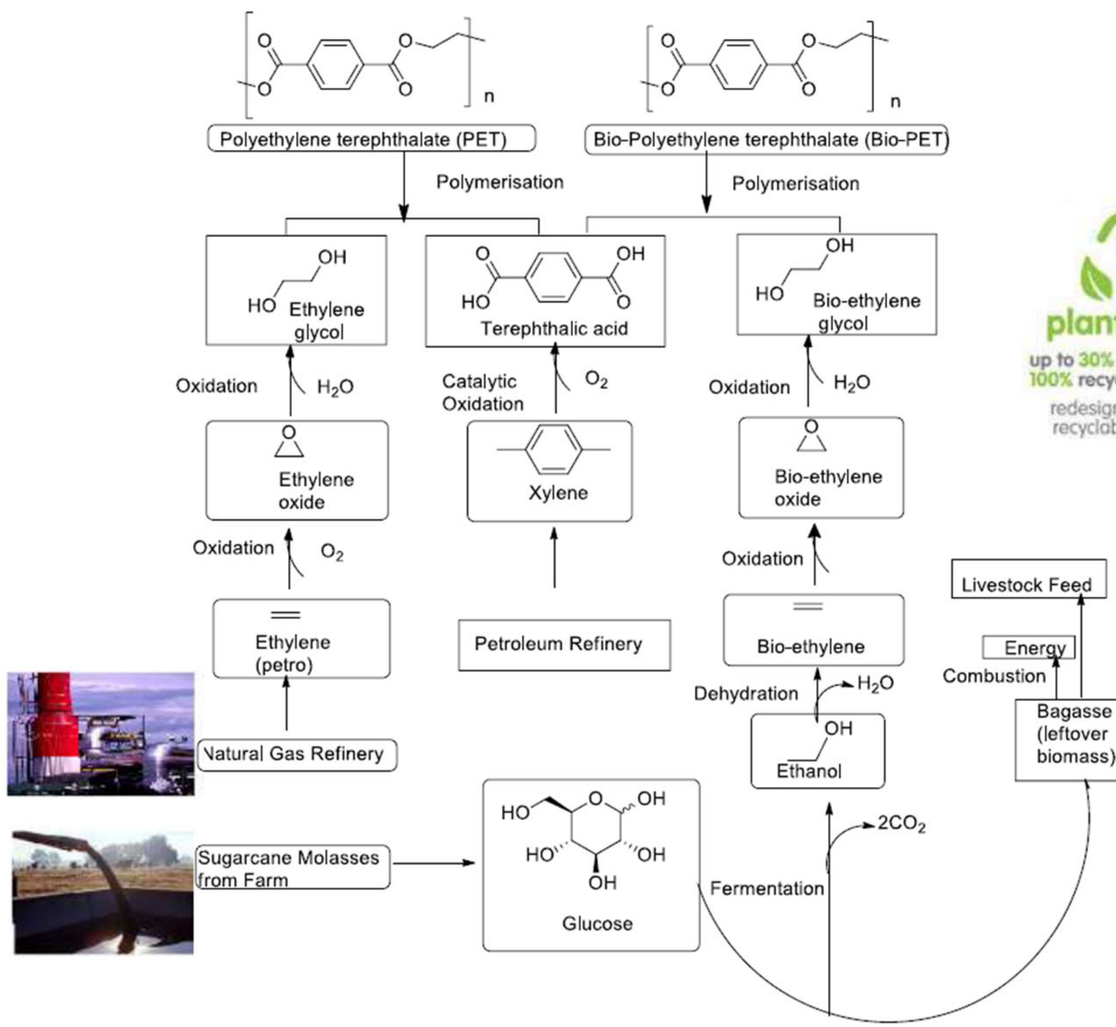
PET: POLY(ETHYLENETEREPHTHALATE)



Purified Terephthalic Acid (PTA) and Mono-Ethylene Glycol (MEG) Content : 67.8 and 32.2 wt%

- One among the "Top Ten" Synthetic Polymers
- Accounts for about 25 % of world polymer production
- Global demand: Over 75 million tons
- Applications: Packaging films, fibers (filament and staple), PET bottle

Bio-PET: Are they Sustainable?



plantbottle
up to 30% plant-based
100% recyclable bottle
redesigned plastic, recyclable as ever.

Impact Comparison

	Atom Economy, %	Carcinogens, kg benzene eqv/L	Non-Carcinogens, kg toluene eqv/L	Respiratory Effects, kgPM2.5 eqv/L	Ecotoxicity, kg benzene eqv/L	Cumulative Energy Demand, MJ Eqv/L	% Renewable Material	Distance of feedstocks
Polymer								
PET	**80**	**1.1×10^{-2}**	**62.9**	**4.9×10^{-3}**	**5.72**	**123.8**	**0**	**Intern**
Bio-PET	**62**	**1.3×10^{-2}**	**72.7**	**5.7×10^{-3}**	**6.98**	**146.2**	**15**	**Intern**

Environ. Sci. Technol., 44, 8264 (2010)

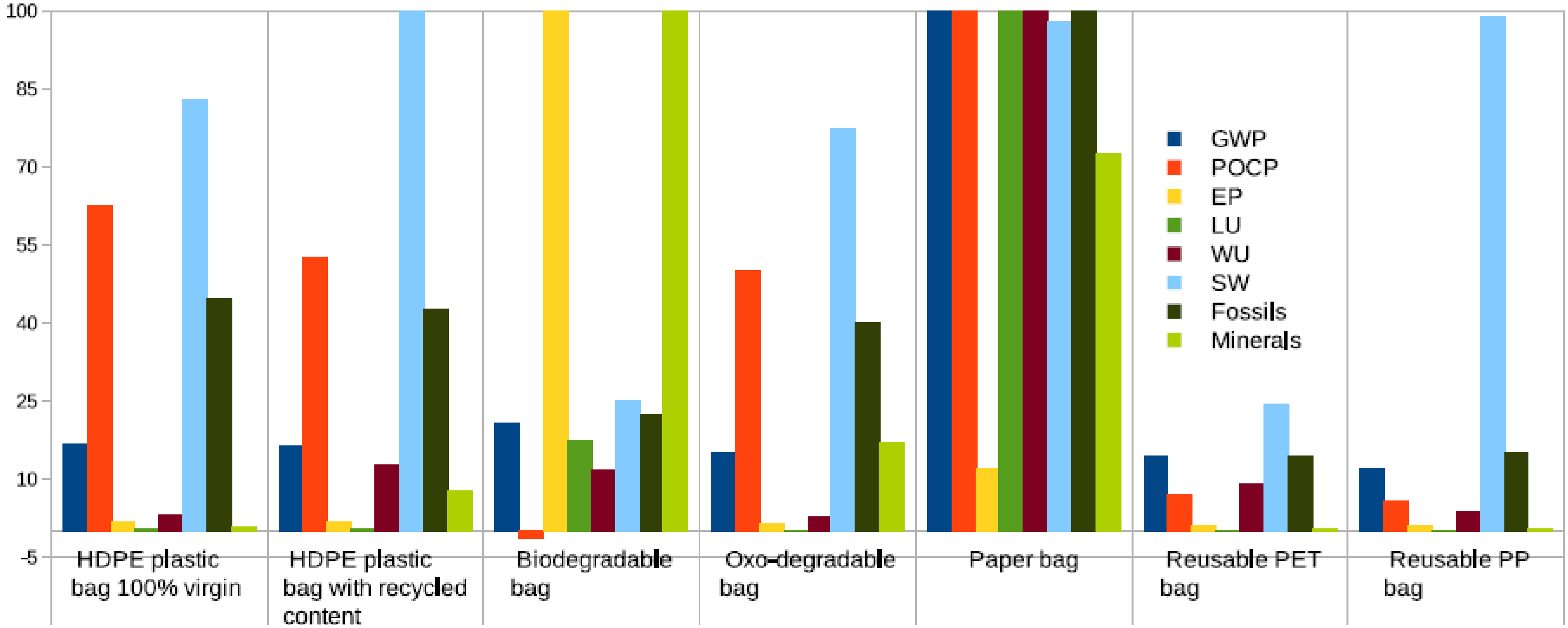
- Switching to renewable resources results in increases in impact categories:
  - -eutrophication
  - -human health impacts
  - -eco-toxicity

- The impact result from increased use of fertilizer and pesticide, increased land use requirement for agricultural production, as well as, from fermentation and other chemical processing steps

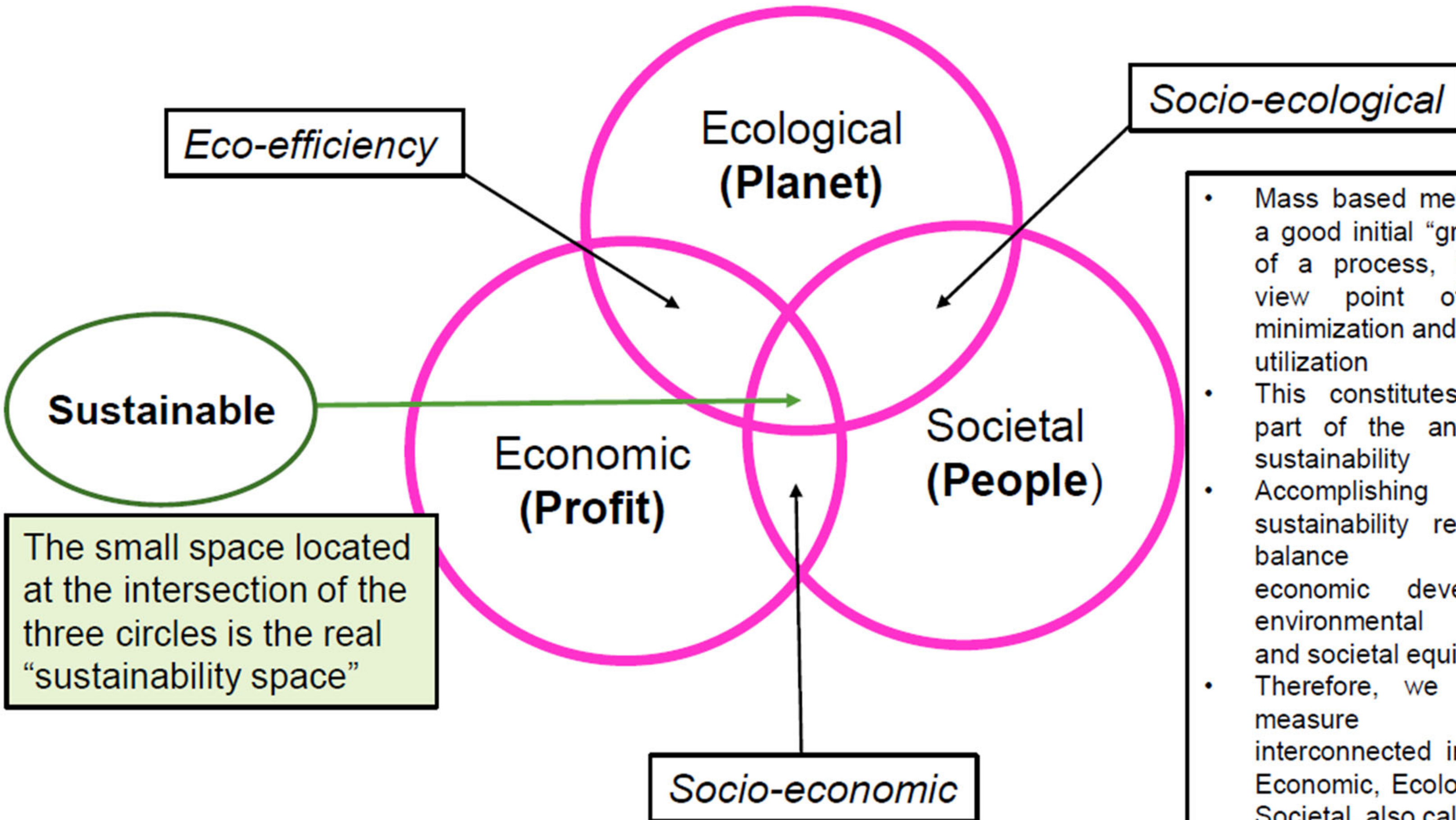
LCA of Grocery Sacks

Impact category	Unit	HDPE plastic bag 100% virgin	HDPE plastic bag with recycled content	Biodegradable bag	Oxo-degradable bag	Paper bag	Reusable PET bag	Reusable PP bag
GWP	kg CO_2e	7.52	7.35	9.19	6.69	44.74	6.47	*5.43*
POCP	kg C_2H_4e	0.045	0.038	*-0.001*	0.036	0.072	0.005	0.004
EP	kg PO_4e	0.005	0.005	0.278	0.004	0.033	*0.003*	*0.003*
LU	Ha a	6.6E-6	5.9E-6	3.5E-4	*9.2E-7*	2.0E-3	2.0E-6	1.3E-6
WU	kL H_2O	0.013	0.053	0.050	*0.012*	0.423	0.038	0.016
SW	kg	2.74	3.31	0.83	2.56	3.24	*0.81*	3.27
Fossils	MJ s	19.93	19.07	9.96	17.94	44.77	*6.46*	6.65
Minerals	MJ s	8.44E-5	7.79E-4	1.02E-2	1.73E-3	7.42E-3	3.39E-5	*2.50E-5*

LCA of Grocery Sacks



- Comparing grocery sacks after normalizing each impact category to 100
- Which sack is best?



- Mass based metrics give a good initial "greenness" of a process, from the view point of waste minimization and resource utilization
- This constitutes only a part of the analysis of sustainability
- Accomplishing true sustainability requires a balance between economic development, environmental impact, and societal equity
- Therefore, we have to measure three interconnected indicators: Economic, Ecological and Societal, also called 3 P's