2021 PSU Virtual Visiting Professor Talk

SUSTAINABLE CHEMICAL PROCESS DESIGN & DECISION MAKING

AP Ir. Dr.-Ing. Mohamad Rizza Othman PEng CEng MIChemE
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INSTRUCTOR BACKGROUND

Mohamad Rizza Othman
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Education

- Dr.-Ing. (TU Berlin). 2011
- M.Sc. (UTM). 2005
- B.Sc. (UTM). 2003

Professional Affil. & Cert.

- PEng (BEM)
- CEng (UK)
- MIChemE
- Certified Aspen Plus User

Management

- Deputy Director (Strategic Planning & Quality)
- Acting Deputy Dean (R&D) FTKKP
- Founder Competence Centre SISPI
- Former Head of ProSES RG

Education & Research

- Process sustainability, modelling, simulation, safety and control
- 28 papers, 40 conferences & 9 exhibitions
- Invited talks i.e., NUS, MPOB, IChemE and AspenTech

Competence Centre for Smart Integration System in Process Industries (CC-SISPI)

- Established in early 2020 from a grant by MOHE
- Focuses on providing technical training, short courses & certification for students, staff, engineers & technologist in process industries.
- Equipment: -
  - Upstream Production Integrated Pilot Plant
  - L, F & P Control Self-Assembly Training Rig
  - Portable Temperature Control Lab System
  - USB HART Interface
  - Workstations

UNIVERSITI MALAYSIA PAHANG (UMP)

- UMP was established as a technical university in 2002.
- It has two campuses located in Gambang and Pekan, Pahang.
- Ranked as one of the best in Research and Innovation within the classifications of Malaysia Technical University Network (MTUN) and Non-Research University (Non-RU).

5 STARS	801-1000	#129 ASIA
QS RATES FOR EXCELLENCE 2018	QS WORLD UNIVERSITY RANKINGS 2022	QS WORLD UNIVERSITY RANKINGS 2022

OUTCOMES

1. Describe the concept of sustainability, applications, and importance particularly in chemical industries.
2. Describe the concept DfS (Design for Sustainability) in chemical process design and various methods to assess them.
3. Perform steps to use analytic hierarchy process (AHP) technique for solving multi criteria problem.
4. Perform sustainability assessment and AHP for selection of sustainable process design

OUTLINE

1. Introduction to Sustainability
2. Sustainability Assessment
3. Design for Sustainability (DfS)
4. Introduction to Analytical Hierarchy Process (AHP)

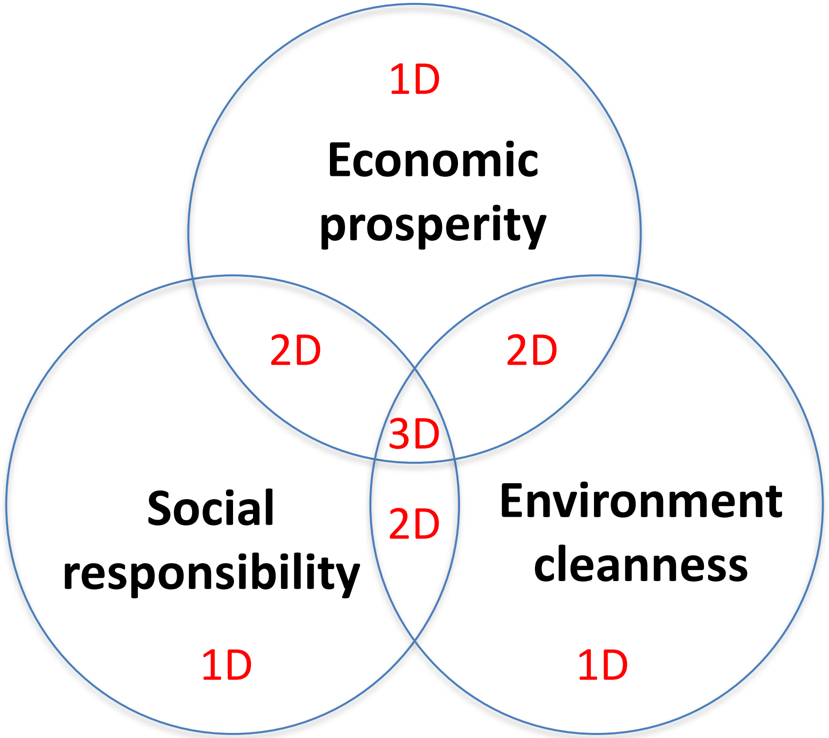
Definition of Sustainability

- General definition:-

"… development must meet the needs of the present without compromising the ability of future generations to meet their own needs".

The Brundtland Commission

- The development of sustainability increases and broaden the definition.
- New terms emerges i.e., cleaner production, pollution prevention, pollution control, and minimization of resource usage, eco-design etc.
- The Triple Bottom Line (TBL) is commonly used to describe organizational sustainability based on 3 principles of sustainability; economic, environmental and society.



3 Dimensions of Sustainability

Sustainability Principles

- Economic principles embrace terms:-
  - Environmental Accounting
  - Eco-efficiency
  - Ethical Investments
- Societal principles composed of terms such as:-
  - Social Responsibility that refers to safe, respectful, liberal, equitable and equal human development, contributing to humanity and the environment.
  - Health and safety refers to the working environment and includes responsibilities and standards.
  - Reporting is about sharing the progress, results and planning with the general public.
- Environmental/ecological describe environmental/ecological performance to minimize the use of hazardous or toxic substances, resources and energy. Environmental terms include:-
  - Renewable resources, resource minimization, source reduction, recycling, reuse, repair, regeneration, recovery, remanufacturing, purification, end-of-pipe, degradation etc.

Sustainability Development Goals (SDG)

- Decades of development started in June 1992, at the Earth Summit in Rio de Janeiro, Brazil,
- The 2030 Agenda for Sustainable Development provides a shared blueprint for peace and prosperity for people and the planet, now and into the future.
- At its heart are the 17 Sustainable Development Goals (SDGs).

"… ending poverty and other deprivations must go hand-in-hand with strategies that improve health and education, reduce inequality, and spur economic growth – all while tackling climate change and working to preserve our oceans and forests."


SUSTAINABLE DEVELOPMENT GOALS
17 GOALS TO TRANSFORM OUR WORLD
1 NO POVERTY
2 ZERO HUNGER
3 GOOD HEALTH AND WELL-BEING
4 QUALITY EDUCATION
5 GENDER EQUALITY
6 CLEAN WATER AND SANITATION
7 AFFORDABLE AND CLEAN ENERGY
8 DECENT WORK AND ECONOMIC GROWTH
9 INDUSTRY, INNOVATION AND INFRASTRUCTURE
10 REDUCED INEQUALITIES
11 SUSTAINABLE CITIES AND COMMUNITIES
12 RESPONSIBLE CONSUMPTION AND PRODUCTION
13 CLIMATE ACTION
14 LIFE BELOW WATER
15 LIFE ON LAND
16 PEACE, JUSTICE AND STRONG INSTITUTIONS
17 PARTNERSHIPS FOR THE GOALS
SUSTAINABLE DEVELOPMENT GOALS

Example of sustainability efforts and activities in the process industry.

What can the chemical industry do to maintain or enhance the 'stock' of the following resources, or 'capitals'	As a business, accountable to shareholders	As a provider of products and services	As a significant member of the community where it operates
NATURAL The resources and services provided by natural world	• Eliminate the use of non-renewable energy • Use energy efficiently • Use water efficiently • Use raw materials efficiently • Audit supply chain performance • Eliminate waste • Operate to a consistently high global standard of environmental and social performance • Increase resource productivity	• Develop products that reduce energy use of customers • Develop products that copy natural processes • Improve biodegradability • Remove toxicity • Eliminate persistent compounds • Design products for reuse and recycling • Service models replace products	• Protect and enhance biodiversity • Commit to long-term carbon neutrality • Eliminate noise and odour • Eliminate visual intrusion • Eliminate negative impacts of local air quality
HUMAN The energy, motivation, capacity for relationships, and intelligence of individuals	• Implement (continuous) employee training and development schemes • Develop leadership • Implement diversity and inclusiveness programmes • Protect health and safety of employees • Provide opportunities for personal growth	• Eliminate negative health and safety impacts of products • Design products that meet human needs and enhance quality of life	• Foster local employment • Develop employee volunteering programmes • Engage in dialogue • Protect human rights
SOCIAL The social groupings that add value to individuals (e.g. families, communities, parliaments, universities)	• Encourage local procurement • Ensure that employees understand company vision, policies and programmes. • Support and encourage progressive regulation	• Communicate information related to product performance, risks and appropriate use. • Assist consumers to understand the impact of their actions and consumption patterns.	• Sustainability performance is openly and accurately communicated • Develop partnerships with the local community • Involved in education programmes • Community investment programme aligned to sustainable development
MANUFACTURED The "stuff" that already in terms of infrastructure n terms of the tools, machines, roads, buildings in which we live and work, and so on.	• Maximise process efficiency • Reduce volumes of throughput (energy, raw materials etc) for each unit of output) • Audit supply chain performance	• Infrastructure encourages product reuse and recycling	• Provide communities with appropriate access to and use of physical assets. For example, community groups provided with use of office space etc outside of normal working hours. • Continued investment in the maintenance and development of infrastructure that reduces risk of negative impact on the community.
FINANCIAL The money, stocks etc. that enable us to put a value on, and buy and sell, the above resources and ways that value can more accurately represent the real 'cost' of using them.	• Makes acceptable financial returns • Account for total cost of activities encompassing both intangibles, risk and externalities • Shift the focus of management compensation from short term financial performance to include areas of sustainability performance	• Total cost accounting is reflected along value chain • Create economically viable products • Research and development priorities aligned to sustainability objectives	• Contribute to local economies through appropriate taxation in all areas of operation. • Eliminate corruption • Philanthropy aligned to strategic vision of company • Systematically avoid any "legacy effects" associated with operations and products

Assessment Indicators

- Screening tools or indicators are useful to assess/measure product or process sustainability performance.
- Currently there is no standard method for measuring sustainability.
- Most indicator works independently.
- Assessment tools were developed that integrate the individual indicators to assess/measure sustainability.
- Indicators can be categorized as hard (quantitative) and soft (qualitative).

Hard (Quantitative)	Soft (Qualitative)

• Measurable & quantifiable.
• Represented by formulars/equations and resulted numerical values.
• Example :
  • Net present value (NPV)
  • Life cycle analysis (LCA)
  • WAR algorithm
  • Fault tree analysis (FTA)
  • IChemE Metrics
  • Emergy
  • etc.
	• Based on human knowledge & experience.
	• Important in process assessment and decision making.
	• Example :
	  • What if? Analysis
	  • Cause-consequences diagram
	  • Industrial hygiene reviews
	  • etc.

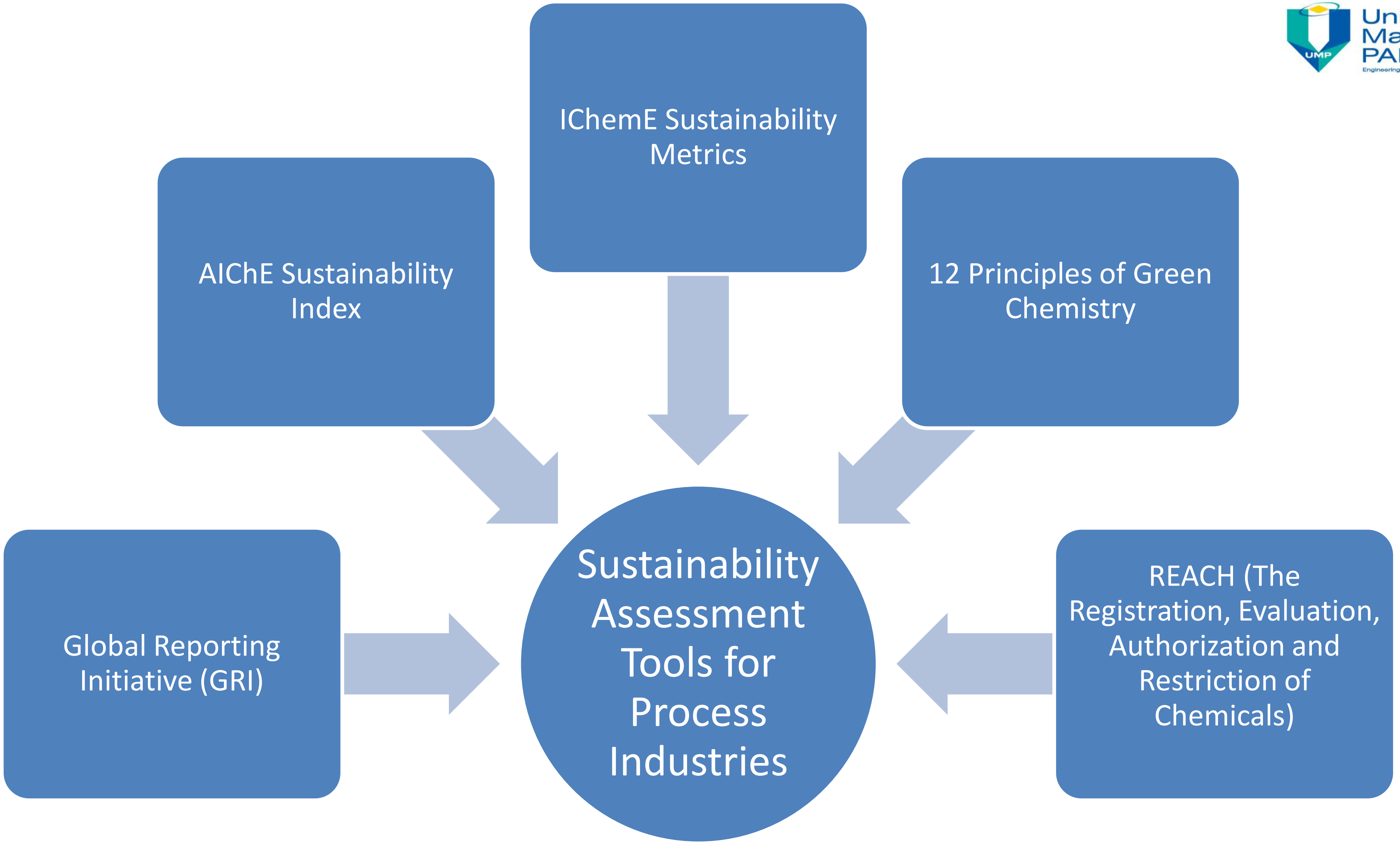
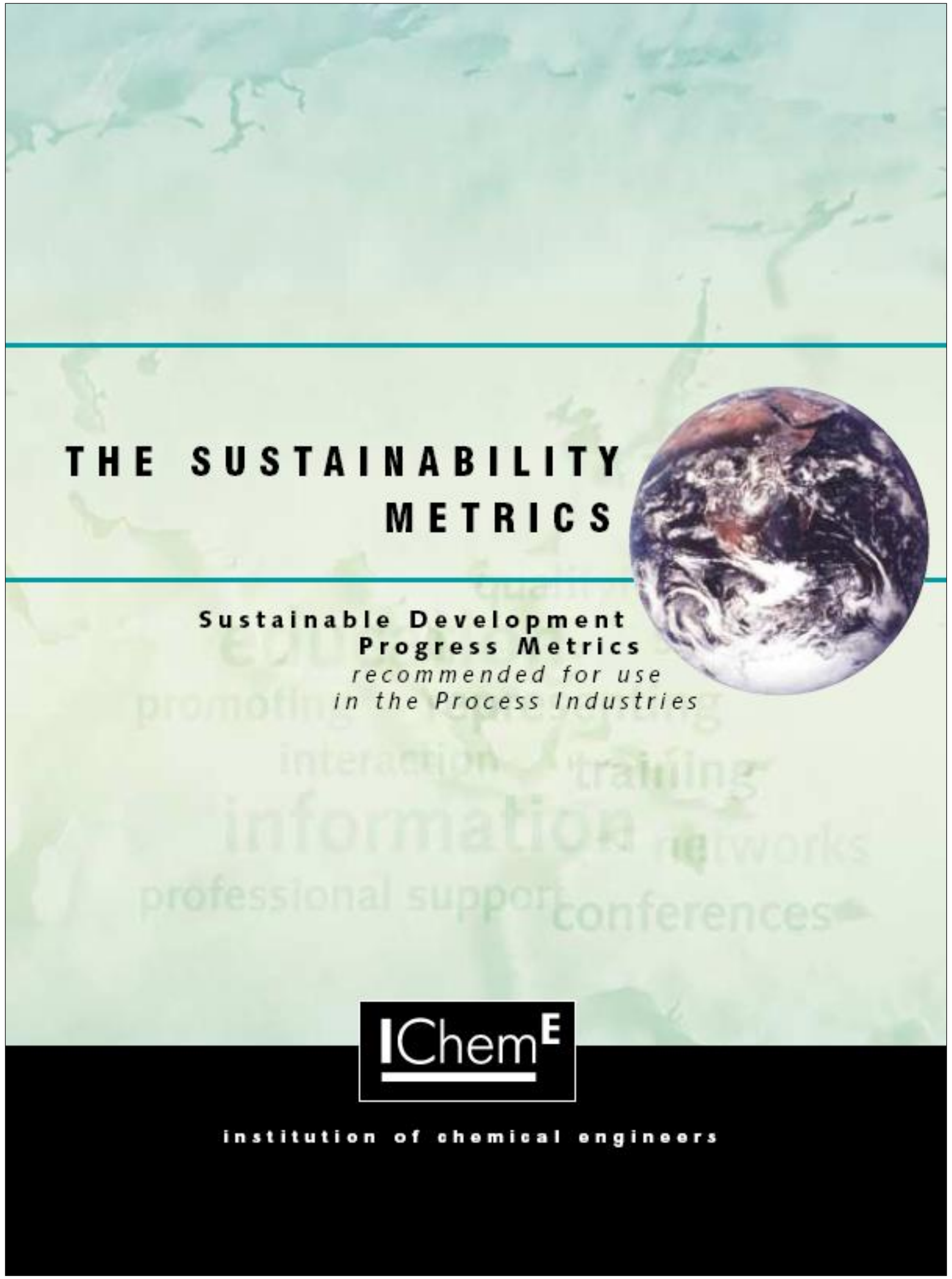

IChemE Sustainability Metrics
AIChE Sustainability Index
12 Principles of Green Chemistry
Global Reporting Initiative (GRI)
Sustainability Assessment Tools for Process Industries
REACH (The Registration, Evaluation, Authorization and Restriction of Chemicals)

Table 1: Main principles/evaluation guidelines of reviewed assessment methods [5, 12–16].

	GRI	AIChE	IChemE	Green Chemistry
Environmental performance	**Materials** **Energy** Water Biodiversity Emissions **Effluents and waste** Products and services Compliance Transport Suppliers	(i) **Resource use** (a) **Energy** (b) **Materials** (c) **Renewables** (d) Water **GHG emissions** **Waste**, wastewater Compliance management Value chain management	**Resource usage** (i) **Energy** (ii) **Material** (iii) Water (iv) Land **Emissions, effluents, and waste**	**Prevent waste** **Use renewable feedstock** Avoid chemical derivatives **Catalysts** Product degradability
Economic performance	**Economic performance** Market presence Procurement practices	(i) **Sustainability innovation** (ii) Strategic commitment to sustainability	**Profit**, value, tax (i) Investments	**Maximise atom economy** **Increase energy efficiency**
Social performance	Labor practices (i) Employment (ii) **Health and safety** (iii) **Innovation and knowledge potential** (iv) Diversity and equality society (i) Acceptability and social dialogue Human rights	Social responsibility (i) Stakeholder partnership (ii) Social investment (iii) Image in the community Product stewardship (i) assurance system (ii) risk communication (iii) legal proceedings	Workplace (i) Employment (ii) **Health and safety** society	**Less hazardous chemical syntheses** **Safer chemicals, products, solvents, and reactions** **Accident prevention and real time analysis**

IChemE Sustainability Metrics

- Develop by IChemE to help companies to set targets and develop internal standards and to monitor their sustainability progress in time.
- Divided into environmental, economic, and social indicators.
- Environmental indicators concentrate on:-
  - How much resource are use i.e., energy, material, water.
  - Impacts to atmospheric, aquatic, and land caused by emissions, effluents, and waste.
- Economic indicators concentrate on:-
  - Profit gained
  - Value added
  - Taxes paid
  - Investments made
- Social indicators consider:-
  - the employment situation
  - health and safety at work
  - impacts to society

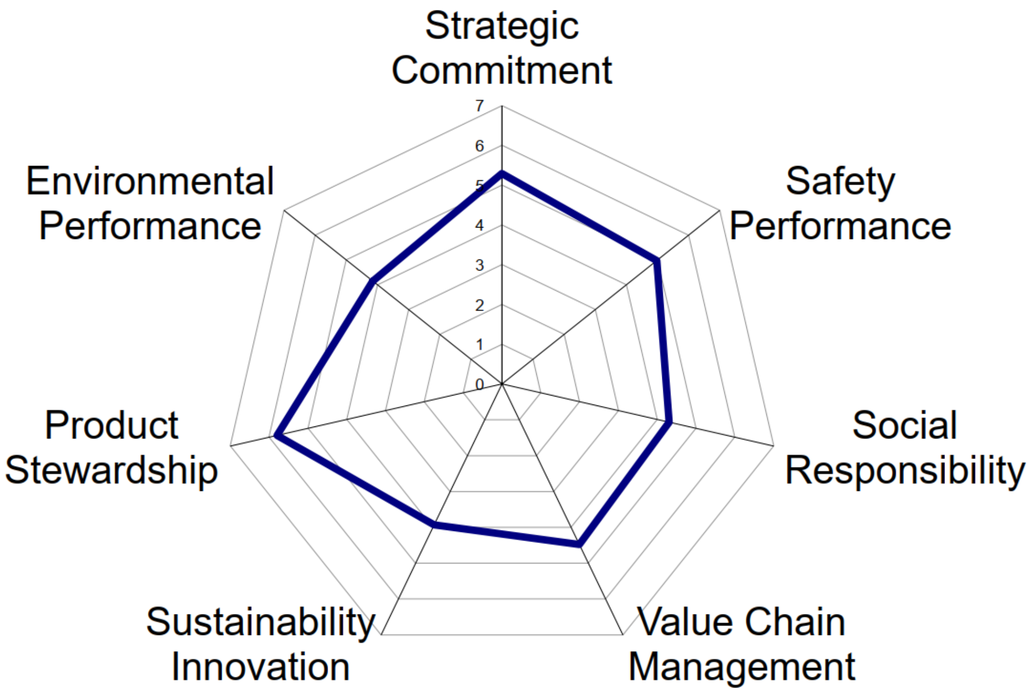


AIChE Sustainability Index

AIChE
The Global Home of Chemical Engineers

- Uses 7 key metrics to show sustainability efforts to the community, shareholders, customers and peers.
- The metrics developed are simple, understandable, easy to reproduce, and comparable.

Strategic commitment	Stated sustainability commitments, reporting, corporate goals and programs
Environmental Performance	Resource use, GHG, other emissions, compliance
Safety Performance	Employee safety, process safety, plant security
Product stewardship	Assurance system, risk communication, legal proceedings
Social responsibility	Stakeholder partnership, social investment, image in community
Sustainability Innovation	R&D spending, innovation for sustainability, integration into process, results
Value Chain Management	EMS, supply chain management



Remarks

- Multiple indicators should include the effect of preference while single indicator is difficult to track individual improvement.
- The assessment objectives affect the boundaries and selection of indicators.
- Indicators for early process design assessment should use simple algorithm and less data extensive but still maintain its relevancy.
  – Economic performance i.e., NPV, DCFRR
  – Environmental performance i.e., WAR algorithm
  – Social performance i.e., Hard (qualitative) indicator
- As proses development progresses complex indicators are applicable.

Our early work on Sustainable Process Design & Decision Making

7870 Ind. Eng. Chem. Res. 2010, 49, 7870–7881

A Modular Approach to Sustainability Assessment and Decision Support in Chemical Process Design

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In chemical and allied industries, process design sustainability has gained public concern in academia, industry, government agencies, and social groups. Over the past decade, a variety of sustainability indicators have been introduced, but with various challenges in application. It becomes clear that the industries need urgently practical tools for conducting systematic sustainability assessment on existing processes and/or new designs and, further, for helping derive the most desirable design decisions. This paper presents a systematic, general approach for sustainability assessment and design selection through integrating hard (quantitative) economic and environmental indicators along with soft (qualitative) indicators for social criteria into design activities. The approach contains four modules: a process simulator module, an equipment and inventory acquisition module, a sustainability assessment module, and a decision support module. The modules fully utilize and extend the capabilities of the process simulator Aspen Plus, Aspen Simulation Workbook, and a spreadsheet, where case model development, data acquisition and analysis, team contribution assessment, and decision

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Process systems engineering

FOLLOW

TITLE	CITED BY	YEAR
A modular approach to sustainability assessment and decision support in chemical process design MR Othman, JU Repke, G Wozny, Y Huang Industrial & Engineering Chemistry Research 49 (17), 7870-7881	141	2010
Prioritizing HAZOP analysis using analytic hierarchy process (AHP) MR Othman, R Idris, MH Hassim, WHW Ibrahim Clean Technologies and Environmental Policy 18 (5), 1345-1360	31	2016
Introducing sustainability assessment and selection (SAS) into chemical engineering education MR Othman, L Hady, JU Repke, G Wozny Education for Chemical Engineers 7 (3), e118-e124	19	2012
Kinetic based simulation of methane steam reforming and water gas shift for hydrogen production using aspen plus UI Amran, A Ahmad, MR Othman Chemical Engineering Transactions 56, 1681-1686	16	2017
Process fault detection using hierarchical artificial neural network diagnostic strategy	13	2007

NPV & DCFRR

- Pintarič and Kravanja (2006) suggested net present value (NPV) and discounted cash flow rate of return (DCFRR) as economic indicators as it favored by entrepreneurs.
- NPV & DCFRR reflect a comprehensive economic assessment of the overall project's economic life cycle.
- NPV provide profitability measurement whereas DCFRR reflect the highest, after-tax interest or discount rate at which the project can just break even.

$$NPV = \sum_{m=1}^{n} \frac{C_{A,m}}{(1+r)^m} - C_{TCI}$$

C_A = total annual income cash flow after the base year for year m

r = interest rate (%)

n = project life time after the base year

C_{TCI} = total capital investment

DCFRR = r or r_{ROR} when NPV = 0.

$r_{ROR} >> r_{ir}$ is more preferred.

$$0 = \sum_{m=1}^{n} \frac{C_{A,m}}{(1+r)^m} - C_{TCI}$$

Example

- Calculate NPV when r = 8%

$$NPV = \sum_{m=1}^{n} \frac{C_{A,m}}{(1+r)^m} - C_{TCI}$$

- Calculate DCFRR

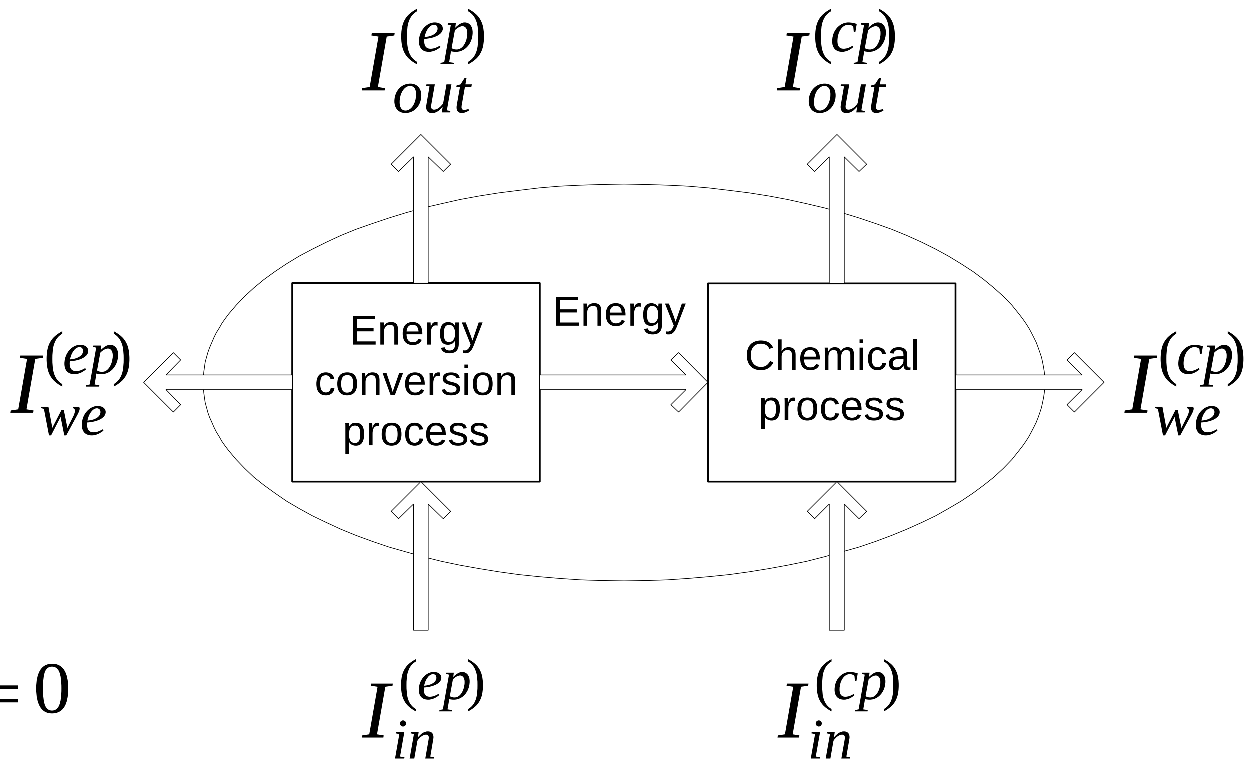
$$0 = \sum_{m=1}^{n} \frac{C_{A,m}}{(1+r)^m} - C_{TCI}$$

- Which is better?

Period	Cash flow 1, $	Cash flow 2, $
0	-1000	-1000
1	475	400
2	400	425
3	330	390
4	270	150
5	200	250
NPV	**379.3**	**324.7**
DCFRR	**23.9%**	**21.4%**

WAR (Waste Reduction) Algorithm

- Introduced by Young and Cabezas (1999) for assessing environmental impact at early process design stage.
- Simple to use algorithm and easy to find data.



$$I_{in}^{cp} + \cancel{I_{in}^{ep}} - I_{out}^{cp} - I_{out}^{ep} - \cancel{I_{we}^{cp}} - \cancel{I_{we}^{ep}} + I_{gen}^{t} = 0$$

Energy source is assumed in solid

Can be neglected due to small amount

Overall expression is reduced to:-

$$I_{gen}^{t} = I_{out}^{cp} - I_{in}^{cp} + I_{out}^{ep}$$

$$I_{in}^{cp} = \sum_{h}^{cp} I_{h,in} = \sum_{h}^{cp} M_{h,in} \sum_{c} x_{c,h} \psi_c + \ldots$$

$$I_{out}^{cp} = \sum_{h}^{cp} I_{h,out} = \sum_{h}^{cp} M_{h,out} \sum_{c} x_{c,h} \psi_c + \ldots$$

$$I_{out}^{(ep)} = \sum_{h}^{ep} I_{h,out}$$

$$I_{out}^{(ep)} = \sum_{m,n}^{ep} \left[\sum_{m}^{stream-gas} E_{m,in}^{Direct} + \sum_{n}^{stream-gas} \alpha E_{n,in}^{Indirect} \right] \sum_{g} EF_{g}^{m,n} \psi_c$$

M_h = the mass flow rate of the stream *h*

$x_{c,h}$ = mass fraction of component *c* in stream *h*

ψ_c = PEI of component *c* associated with impact categories

ψ_{we} = PEI of energy emission

E^{cp} = rate of energy emission

I_{in}^{ep} = PEI combustion source

I_{out}^{ep} = PEI of energy output

E = energy requirement

m = direct energy streams requirement

n = indirect energy streams requirement

EF = emission factor for gas pollutants *g* (in kg *g*/kWh for coal-fired power plants, see table below)

α = ratio of electrical energy to steam energy for plant utilities produced through burning the same amount of coal.

ψ_{we} = PEI of energy emission

Gas pollutants	EF, kg/kWh
SO_x	0,00272
NO_x (NO_2,NO)	0,00181
CO_2	0,3719
HCl	$9,0 \times 10^{-5}$
Methane	0,4763
Mercury (Hg)	$4,944 \times 10^{-9}$

Summing all the energy requirements of the system i.e. compressors, reboilers, heat exchangers,
cooling and reboiler pumps, refrigeration units, turbines, etc.

Energy source
- Direct energy (electricity)
- Indirect energy (steam)

Impact Category : Global Atmospheric

Global warming potential (GWP)	• *Extent of chemical C absorbs infrared radiation over its atmospheric lifetime / Extent of CO_2 absorbs infrared radiation over its atmospheric lifetime*
Ozone depletion potential (ODP)	• $(C + Ozone = O_2)_R / (CFC + Ozone = O_2)_R$
Acidification potential (AP)	• *Rate of release of H^+ promoted by chemical C / Rate of release of H^+ promoted by SO_2*
Photochemical oxidation (or smog formation) potential (PCOP)	• $(C + OH\cdot)_R / (C_2H_4 + OH\cdot)_R$

* These data can be obtained from Heijungs et al. (1992)

Impact Category : Local toxilogical

HTPI & TTP

- Human toxicity potential by ingestion (HTPI)
- Terrestrial toxicity potential (TTP)
- LD50

ATP

- Aquatic toxicity potential (ATP)
- LC50

HTPE

- Human toxicity potential by inhalation/dermal exposure (HTPE)
- TWA-TLV

* These data can be obtained from MSDS data from different source such as OSHA, NIOSH, ACGIH etc.

Environmental indicators definition:-

$$I_{out}^{(t)} = I_{out}^{(cp)} + I_{out}^{(ep)}$$

Total rate of PEI output (TRO) - Identify an appropriate site for a plant (a plant with low should be located in an ecologically sensitive area).

$$\hat{I}_{out}^{(t)} = \frac{I_{out}^{(cp)} + I_{out}^{(ep)}}{\sum_{p}^{prodStreams} \dot{P}_p}$$

Total rate of PEI output/product (TOP) - measures the efficiency of material utilization by a specific process per unit mass of products; it decreases when the mass rate of PEI emitted decrease or/and when product mass flow rate increase.

$$I_{gen}^{(t)} = I_{out}^{(cp)} - I_{in}^{(cp)} + I_{out}^{(ep)}$$

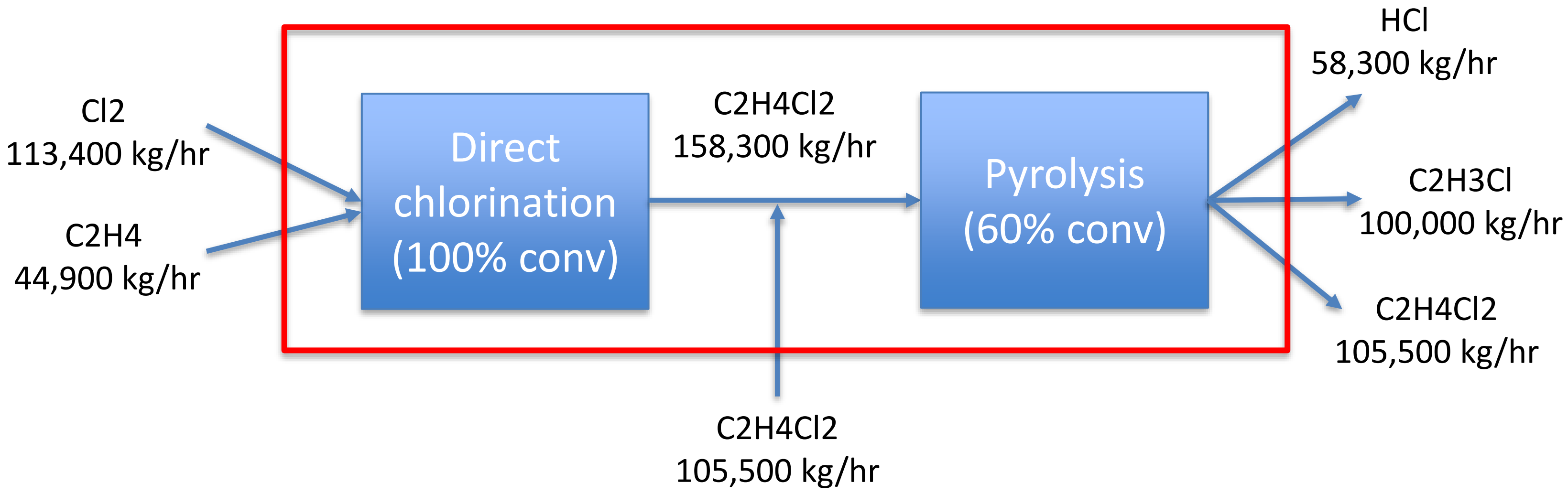
Total rate of PEI generated (TRG) - useful in comparing processes based on how fast they generate impact.

$$\hat{I}_{gen}^{(t)} = \frac{I_{out}^{(cp)} - I_{in}^{(cp)} + I_{out}^{(ep)}}{\sum_{p}^{prodStreams} P_p}$$

Total rate of PEI generated/product (TGP) - is used for comparing processes and products based on the amount of new potential environmental impact generated in product manufacturing.

****Obviously, the lower the PEI, the more desirable the process.**

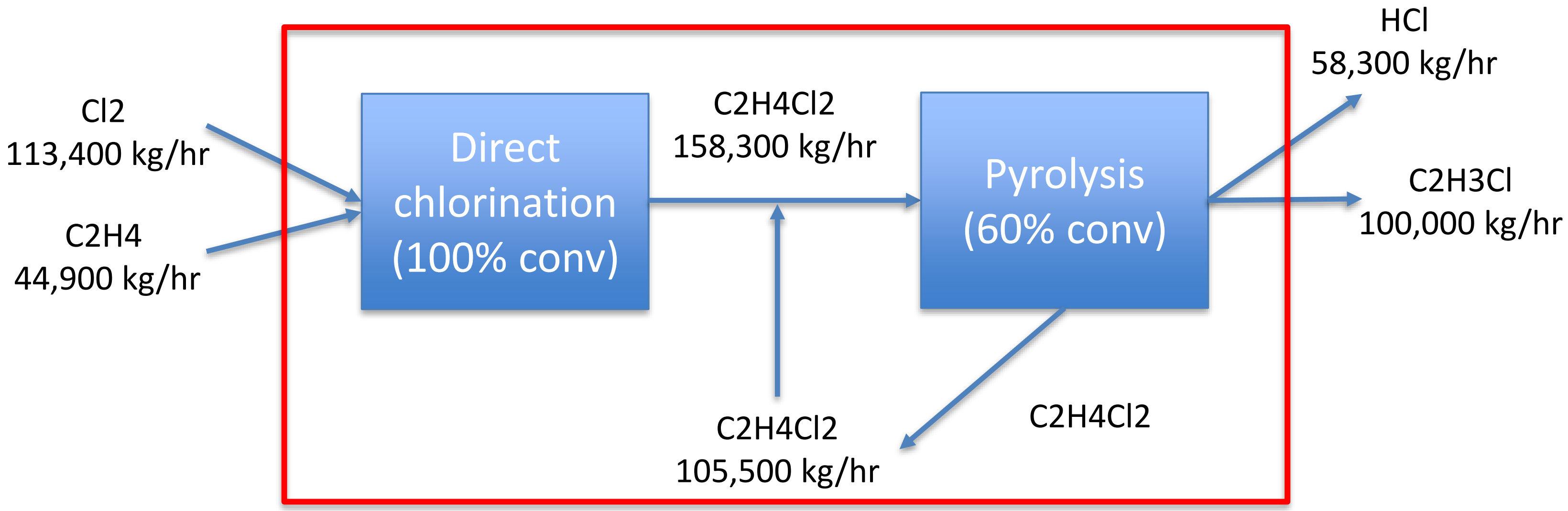
Example VC production – before recycle



Component	Input, kg/hr	Output, kg/hr
Chlorine, Cl_2	113400	
Ethylene, C_2H_4	44900	
1,2-dichloroethane, $C_2H_4Cl_2$	105500	105500
Hydrogen chloride, HCl		58300
VC, C_2H_3Cl		100000
Energy		60000 kW

Component	PEI (GWP)	Input		Output	
		kg/hr	PEI	kg/hr	PEI
Chlorine, Cl2	1.1	113400	124740	-	-
Ethylene, C2H4	1.3	44900	58370	-	-
1,2 dochloroethane, C2H4Cl2	1.5	105500	158250	105500	158250
Hydrogen chloride, HCl	1.9	-	-	58300	110770
VC, C2H3Cl	1.7	-	-	100000	170000
TOTAL PEI (GWP)			**341360**		**439020**
Gas pollutants	**EF, kg/kWh**	**PEI (GWP)**		**Output**	
Energy, kWh	60000			**kg/hr**	**PEI**
SOx	0.00272	1.2		163.2	195.84
NOx (NO2,NO)	0.00181	1.4		108.6	152.04
CO2	0.3719	1.6		22314	35702.4
HCl	9.0 x 10-5	1.1		5.4	5.94
Methane	0.4763	1.1		28578	31435.8
Mercury (Hg)	4.944 x 10-9	1.1		0.000297	0.000326
TOTAL PEI (GWP)					**67492.02**

Example VC production – after recycle



Component	Input, kg/hr	Output, kg/hr
Chlorine, Cl2	113400	
Ethylene, C2H4	44900	
1,2-dichloroethane, C2H4Cl2		
Hydrogen chloride, HCl		58300
VC, C2H3Cl		100000
Energy		65000 kWh

Component	PEI (GWP)	Input		Output	
		kg/hr	PEI	kg/hr	PEI
Chlorine, Cl2	1.1	113,400	124,740	-	-
Ethylene, C2H4	1.3	44,900	58,370	-	-
1,2 dochloroethane, C2H4Cl2	1.5	-	-	-	-
Hydrogen chloride, HCl	1.9	-	-	58,300	110,770
VC, C2H3Cl	1.7	-	-	100,000	170,000
TOTAL PEI (GWP)			**183,110**		**280,770**
Gas pollutants	**EF, kg/kWh**	**PEI (GWP)**		**Output**	
Energy, kWh	65000			**kg/hr**	**PEI**
SOx	0.00272	1.2		176.8	212.16
NOx (NO2,NO)	0.00181	1.4		117.65	164.71
CO2	0.3719	1.6		24173.5	38677.6
HCl	9.0 x 10-5	1.1		5.85	6.435
Methane	0.4763	1.1		30959.5	34055.45
Mercury (Hg)	4.944 x 10-9	1.1		0.000321	0.000353
TOTAL PEI (GWP)					**73116.36**

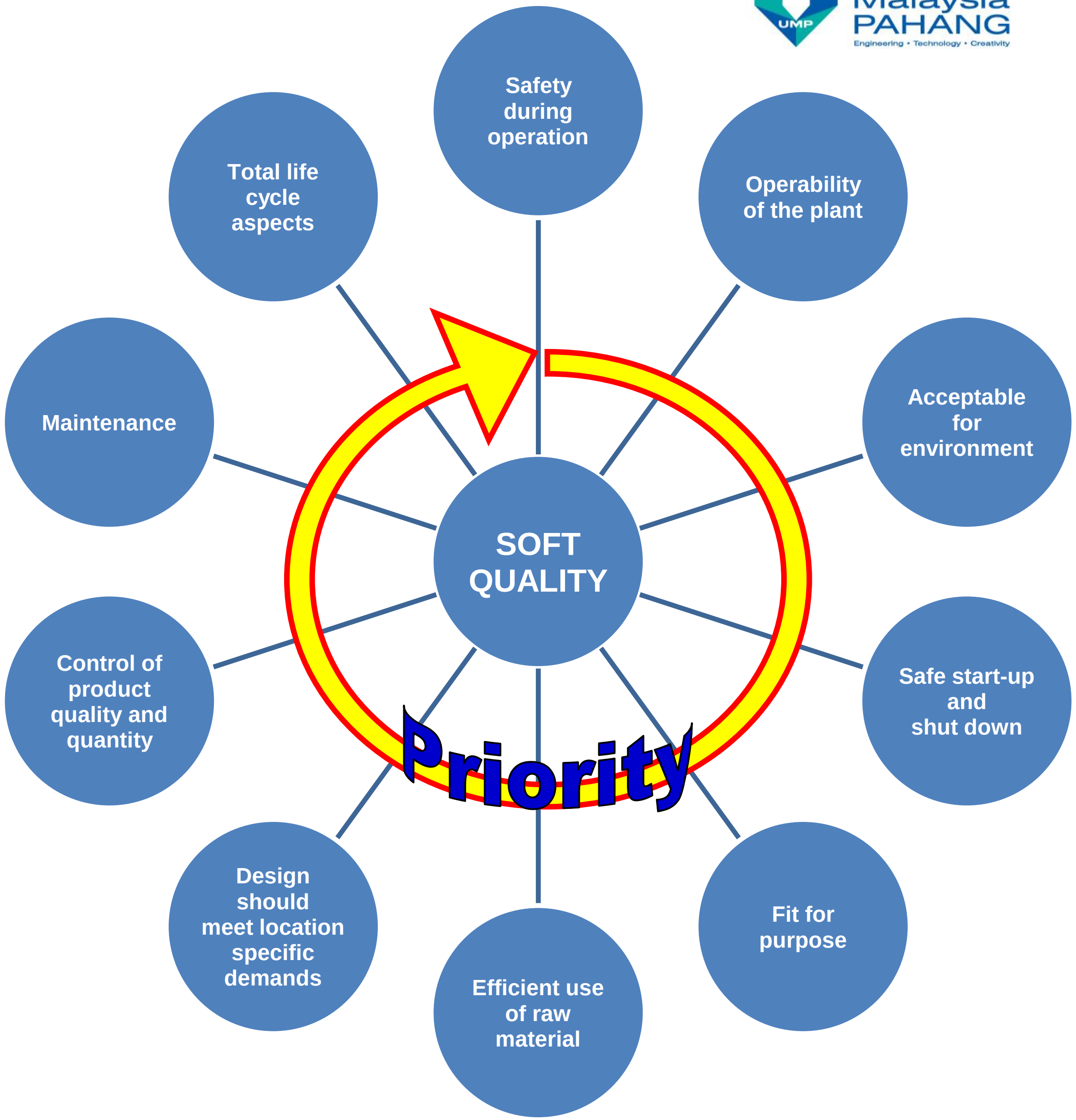
Comparison of PEI based on GWP

Parameter	PEI before recycle	PEI after recycle
TOTAL MASS IN	**341,360**	**183,110**
TOTAL MASS OUT	**439,020**	**280,770**
TOTAL ENERGY OUT	**67492.02**	**73116.36**
TOTAL OUT (MASS OUT + ENERGY OUT)	**506,512**	**353,886**
TOTAL OUT/PRODUCT	**5.1**	**3.5**
TOTAL PEI (OUT – IN + ENERGY)	**165152**	**170776**

- Red color indicate favorable option.
- Each parameter has its own definition and should be consider based on the assessment objectives.
- Final decision making should consider other criteria i.e., economic potential and social aspects.

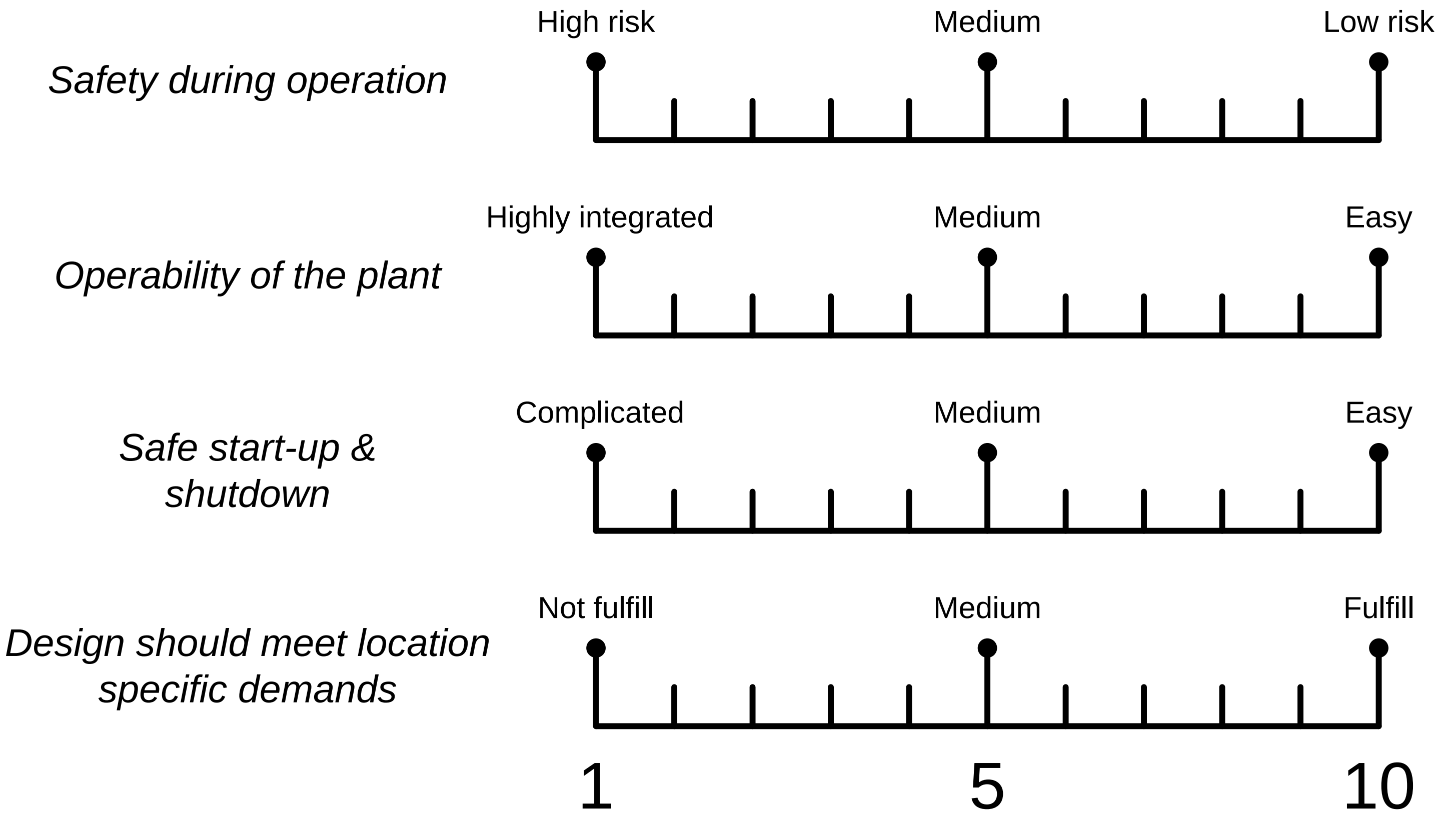
Social Indicators

- IChemE social indicators (quantitative)
  – Reflects company's attitude to treatment of its own employees, suppliers, contractors and customers and also its impact on society at large.
  – Irrelevant at early design stage esp. for back driven data.
- Herder and Weijnen (1998) define quality indicators for early design decision making.
  – Utilize the heuristics knowledge.
  – Provide a rapid assessment without the need for extensive data search.



In our work (Othman et.al., 2010), 4 of them are adopted. As a guideline, each of the indicators is defined below. Although not very rigid, they should be useful to guide decision makers.

Indicators	Definition
Safety during operation	The condition or state of being safe; free from danger or hazard; exemption from hurt, injury, or loss. Evaluation of hazards and risks associated to, but not limited, chemical compounds, reactions, unit operations and equipments and operating conditions should include in the assessment.
Operability of the plant	The condition where the plant is able to operate feasibly. Assessment should consider the operation feasibility by workers and also control systems of the plant especially if tightly integrated and also in the presence of process variations and uncertainties.
Safe start-up and shutdown	Start-up means the act or process of setting into operation or motion while shut down means cease to operate or cause to cease operating. The degree of difficulties of the procedure depends on the system complexity and workers capability.
Design should meet location specific demands	Local demands may include technology transfer, employment, affect to other related industries, local regulations and policies, legal proceedings etc.



- Because of heuristics assessment a scaling system is proposed.
- Although not very specific, it acts as a general guideline to assess various types of chemical processes.

Approach for DfS (Design for Sustainability) in Process Industries

- Process synthesis
- Process intensification
- Process retrofit
- Process optimization

Process Synthesis

- Refers to steps to “process creation” in a reliable, environmentally friendly, safe and economical manner, and at high yield with little or no waste.
- Shows how to create a synthesis tree with its many promising flowsheets.
- For each of the most promising alternative in the synthesis tree, a base-case design is created.

Vinyl Chloride Production

5 synthesis routes

1. Direct chlorination of ethylene:

$$C_2H_4 + Cl_2 \rightarrow C_2H_3Cl + HCl$$

Advantages

- Occurs spontaneously at a few hundred C

Disadvantages

- Does not give high yield of VC without simultaneously producing large amounts of by-products such as dichloroethylene
- Half of the expensive Cl2 is consumed to produce HCl by-product which may not be sold easily.

2. Hydrochlorination of acetylene:

$$C_2H_2 + HCl \rightarrow C_2H_3Cl$$

Advantages

- Provides good conversion (98%) in the presence of HgCl2 catalyst at atmospheric pressure.
- These are fairly moderate reaction conditions, and hence, this reaction deserves further study.

Disadvantages

- Flammability limit of C2H2 (2.5 -> 100%)

Vinyl Chloride Production

5 synthesis routes

3. Thermal cracking of $C_2H_4Cl_2$ from chlorination of C_2H_4:

$$C_2H_4 + Cl_2 \rightarrow C_2H_4Cl_2$$
$$C_2H_4Cl_2 \rightarrow C_2H_3Cl + HCl$$
$$\overline{C_2H_4 + Cl_2 \rightarrow C_2H_3Cl + HCl}$$

Advantages

- Conversion of ethylene to 1,2-dichloroethane in exothermic reaction is around 98% at 90 C and 1 atm with a Friedel-Crafts catalyst such as FeCl3.
- This intermediate is converted to VC by thermal cracking according to endothermic reaction which occurs spontaneously at 500 C with conversion as high as 65%.

Disadvantages

- Half of the expensive Cl2 is consumed to produce HCl by-product which may not be sold easily.

4. Thermal Cracking of $C_2H_4Cl_2$ from Oxychlorination of C_2H_4:

$$C_2H_4 + 2HCl + \tfrac{1}{2}O_2 \rightarrow C_2H_4Cl_2 + H_2O$$
$$C_2H_4Cl_2 \rightarrow C_2H_3Cl + HCl$$
$$\overline{C_2H_4 + HCl + \tfrac{1}{2}O_2 \rightarrow C_2H_3Cl + H_2O}$$

Advantages

- High exothermic reaction achieves 95% conversion to C2H4Cl2 in the presence of CuCl2 catalyst, followed by pyrolysis as in route 3.
- Excellent candidate when cost of HCl is low.

Disadvantages

- Economics dependent on cost of HCl.

Vinyl Chloride Production

5 synthesis routes

5. Balanced Process for Chlorination of Ethylene:

$$C_2H_4 + Cl_2 \rightarrow C_2H_4Cl_2$$

$$C_2H_4 + 2HCl + \tfrac{1}{2}O_2 \rightarrow C_2H_4Cl_2 + H_2O$$

$$2C_2H_4Cl_2 \rightarrow 2C_2H_3Cl + 2HCl$$

$$2C_2H_4 + Cl_2 + \tfrac{1}{2}O_2 \rightarrow 2C_2H_3Cl + H_2O$$

Advantages

- Combinations of route 3 and 4
- All Cl2 converted to VC
- No by products

Economic Evaluation of Alternative Pathways

- Route 1 is eliminated due to its low selectivity.
- The other routes to be compared in terms of gross profit.

Chemical Bulk Prices

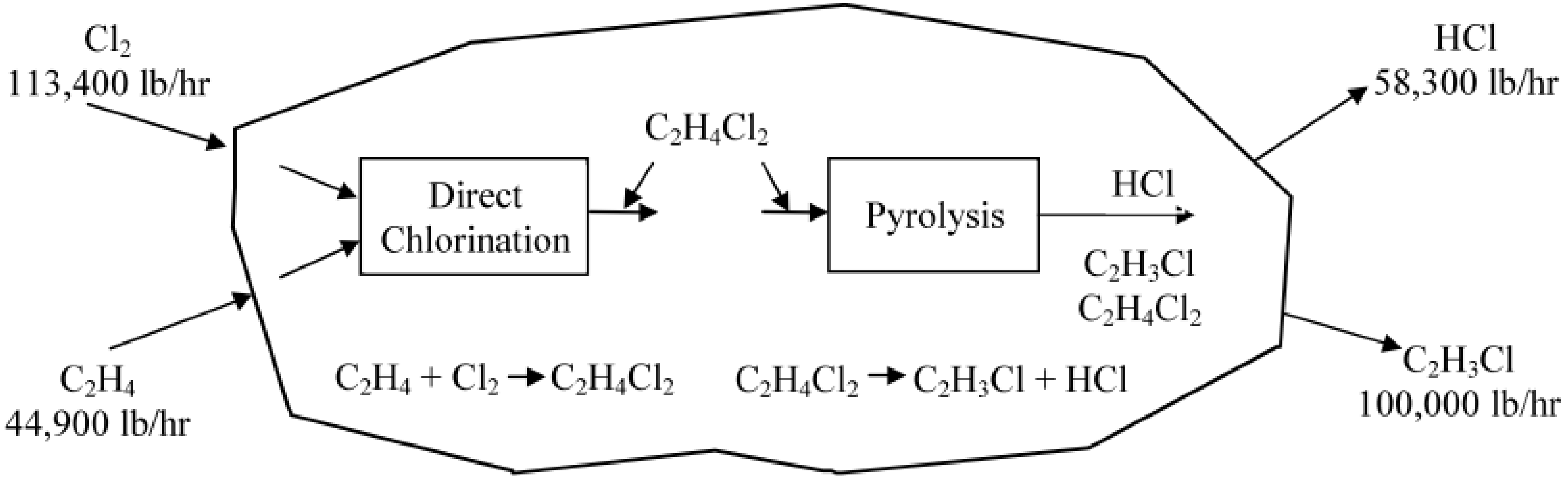
Chemical	Cost (cents/lb)
Ethylene	30
Acetylene	80
Chlorine	18
Vinyl chloride	35
Hydrogen chloride	25
Water	0
Oxygen (air)	0

Reaction path 3	C_2H_4	+	Cl_2	=	C_2H_3Cl	+	HCl
lb-mole	1		1		1		1
Molecular weight	28.05		70.91		62.50		36.46
Amount (lb)	28.05		70.91		62.50		36.46
lb/lb of vinyl chloride	0.449		1.134		1		0.583
cents/lb	30		18		35		25

Gross profit = 35(1) + 25(0.583) - 30(0.449) - 18(1.134) = 15.69 cents/lb VC

Reaction Path	Overall Reaction	Gross Profit (cents/lb of VC)
2	$C_2H_2 + HCl = C_2H_3Cl$	-16.00
3	$C_2H_4 + Cl_2 = C_2H_3Cl + HCl$	15.69
4	$C_2H_4 + HCl + \frac{1}{2}O_2 = C_2H_3Cl + H_2O$	6.96
5	$2C_2H_4 + Cl_2 + \frac{1}{2}O_2 = 2C_2H_3Cl + H_2O$	11.32

Preliminary Flowsheet for Route 3

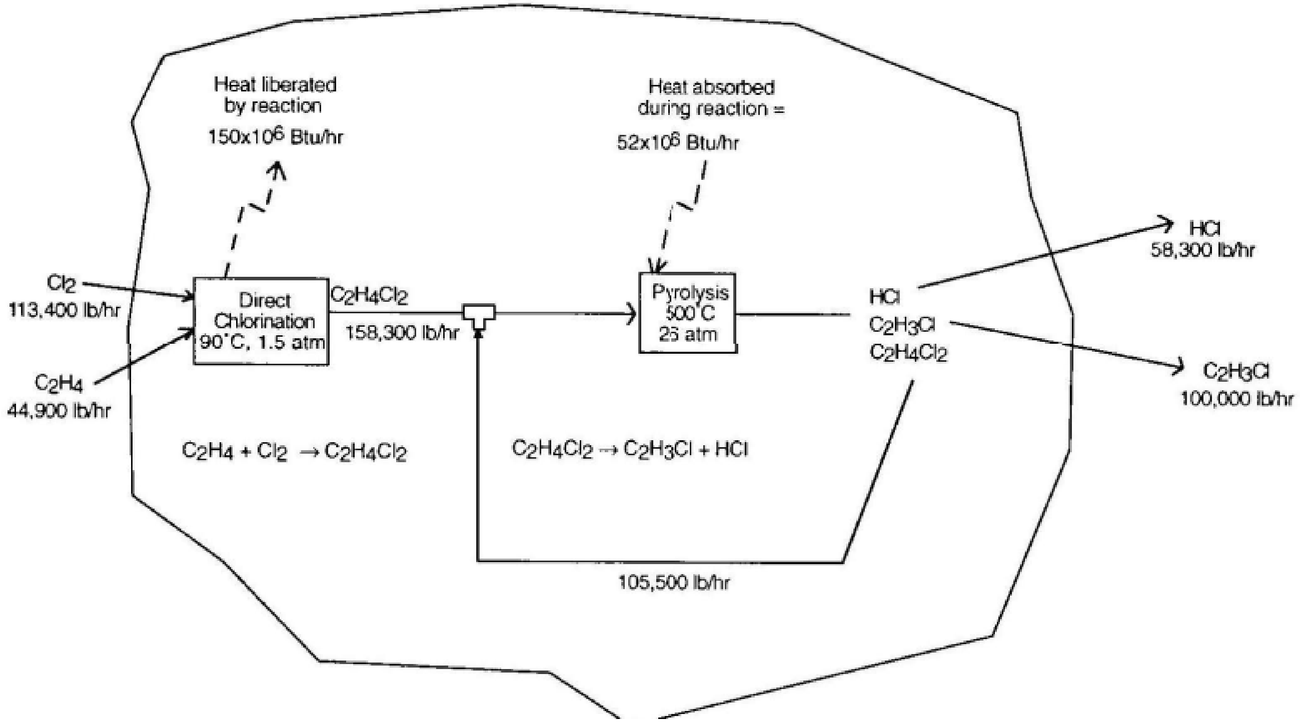


- 800 MM lb/year @ 330 days/y $\Rightarrow$ 100,000 lb/hr VC
- On the basis of this principal sink, the HCl sink and reagent sources can be computed (each flow is 1,600 lbmol/h)
- Next step involves distributing the chemicals by matching sources and sinks.

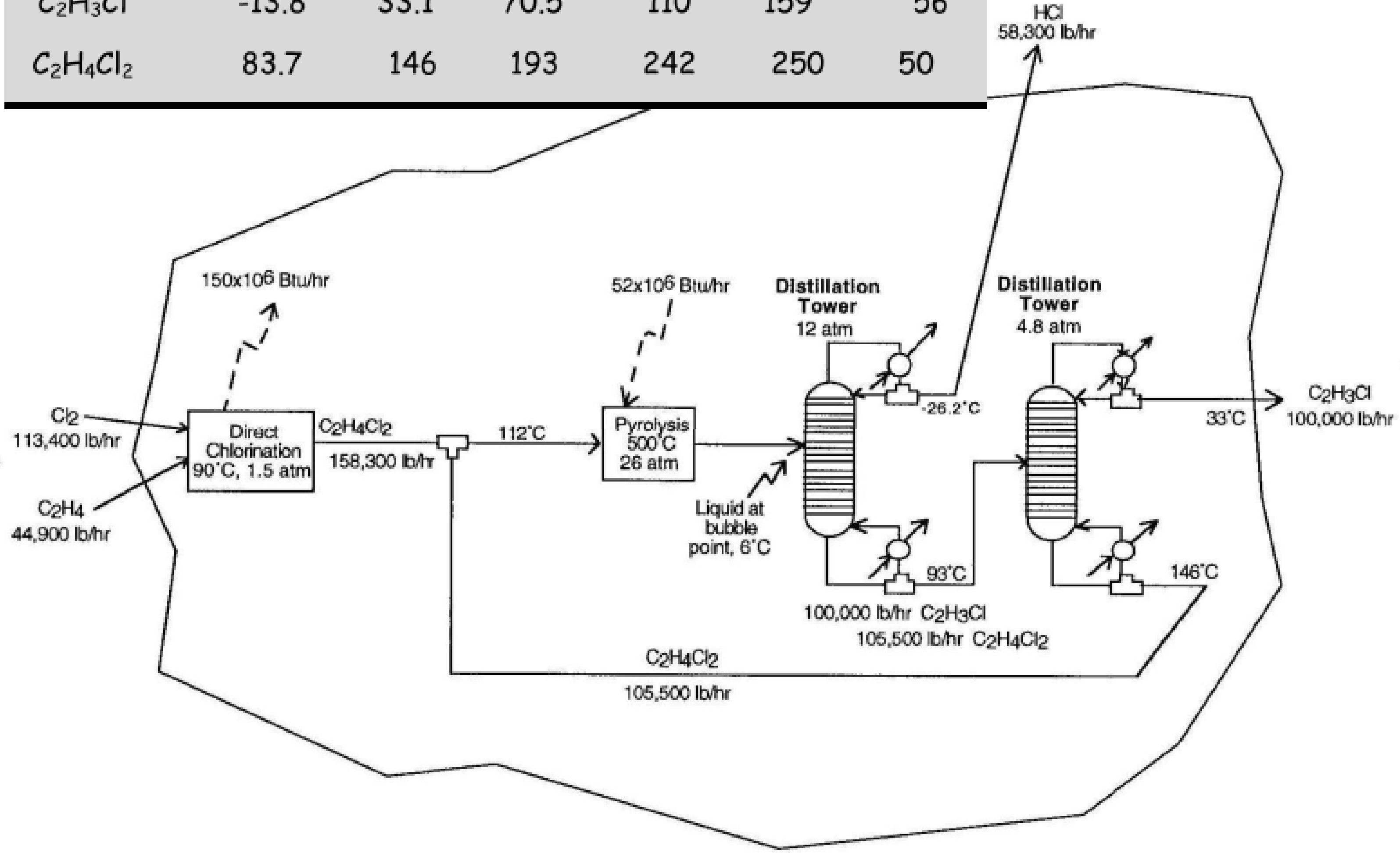
Distribution of Chemicals

- Only 60% of the $C_2H_4Cl_2$ is converted to C_2H_3Cl with a byproduct of HCl, according to Eqn. (2.4).
- To satisfy the overall material balance, 158,300 lb/h of C_2H_4Cl must produce 100,000 lb/h of C_2H_3Cl and 58,300 lb/h of HCl.
- But a 60% conversion only produces 60,000 lb/h of VC.
- The additional $C_2H_4Cl_2$ needed is computed by mass balance to equal: [(1 - 0.6)/0.6] x 158,300 or 105,500 lb/h.
- Its source is a recycle stream from the separation of C_2H_3Cl from unreacted $C_2H_4Cl_2$, from a mixing operation, inserted to combine the two sources, to give a total 263,800 lb/h.

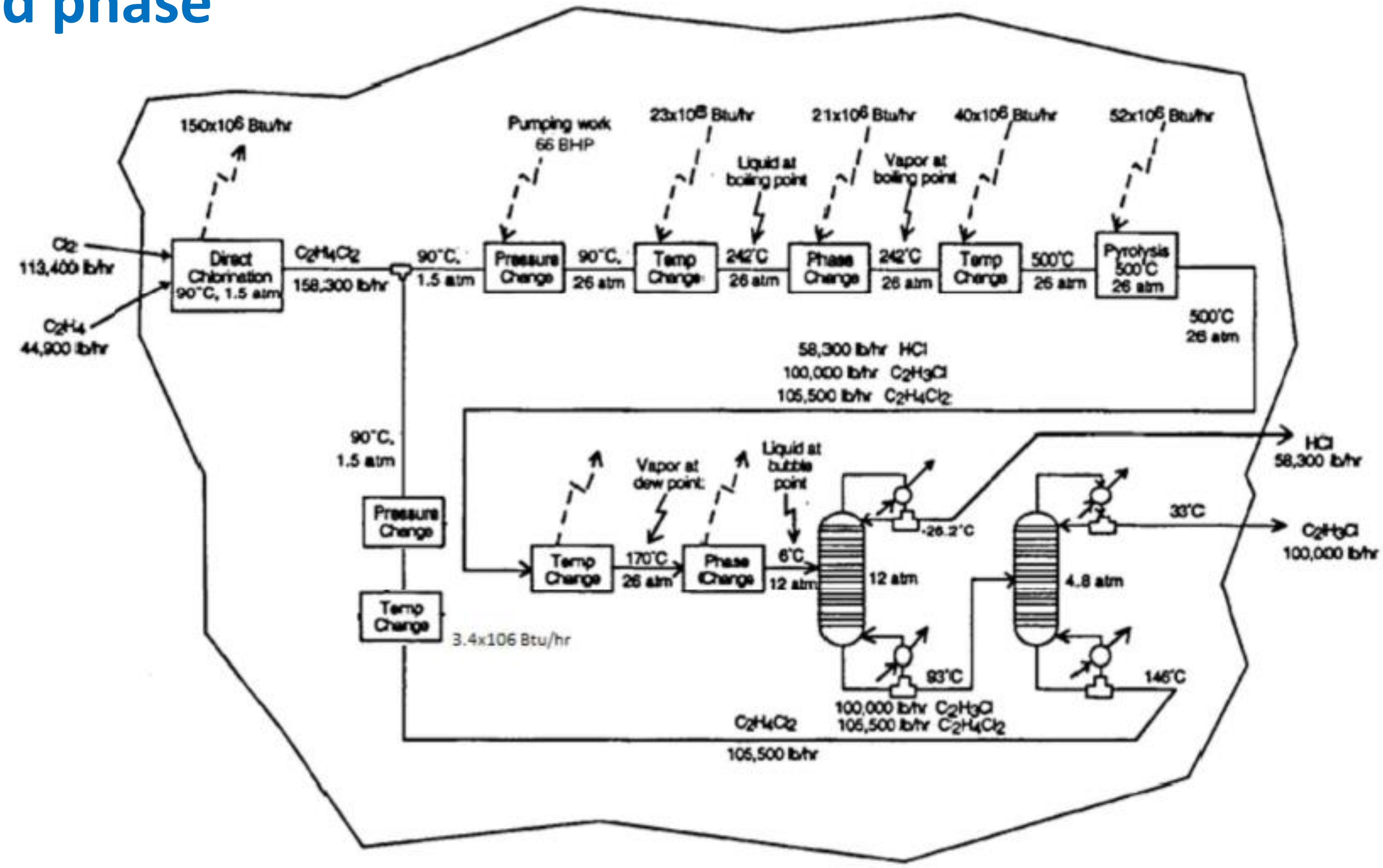
- The effluent stream from the pyrolysis operation is the source for the C_2H_3Cl product, the HCl by-product, and the $C_2H_4Cl_2$ recycle.



	Boiling point (°C)				Critical constants	
Chemical	1 atm	4.8 atm	12 atm	26 atm	T_c,°C	P_c, atm
HCl	-84.8	-51.7	-26.2	0	51.4	82.1
C_2H_3Cl	-13.8	33.1	70.5	110	159	56
$C_2H_4Cl_2$	83.7	146	193	242	250	50



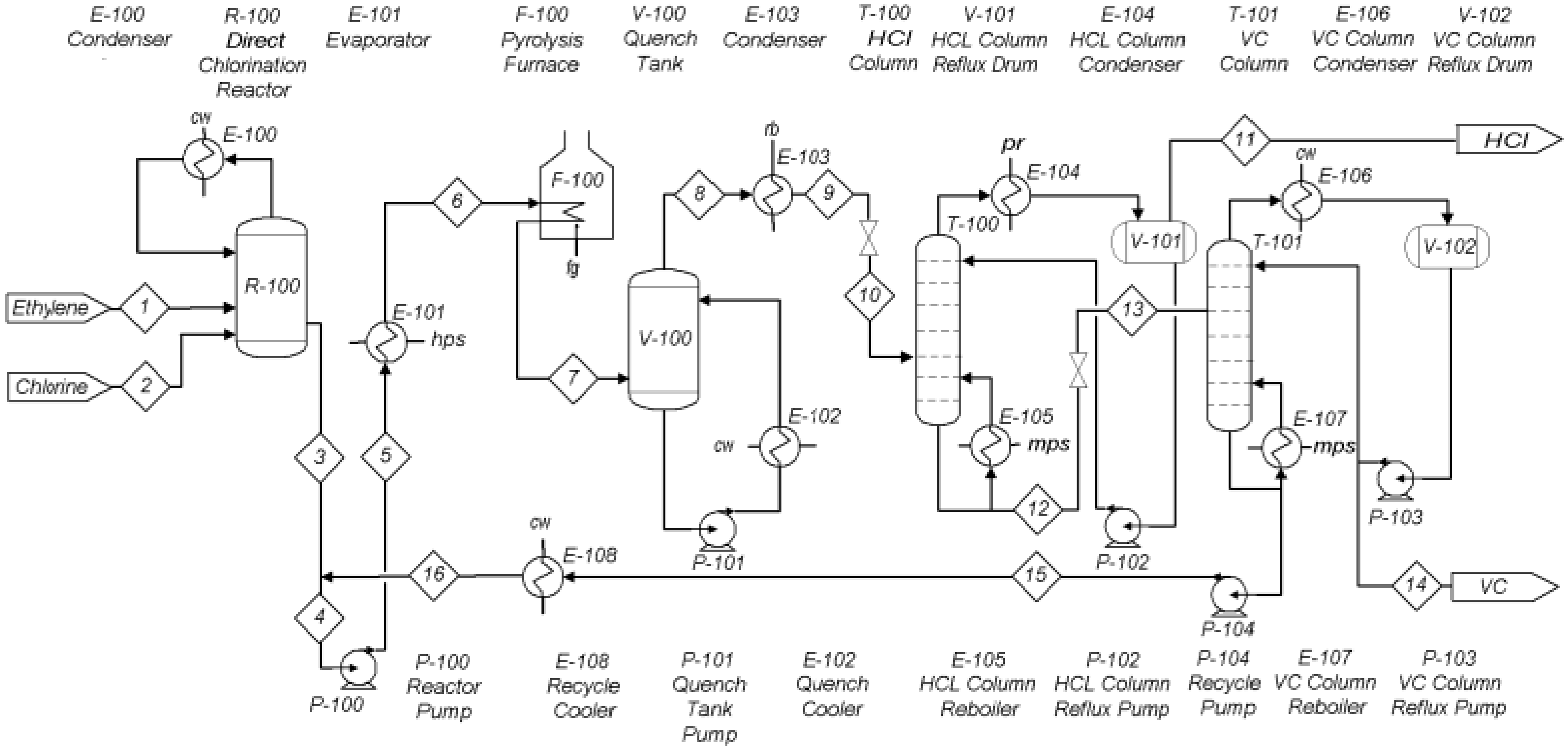
T, P and phase



150x10⁶ Btu/hr
Pumping work
66 BHP
23x10⁶ Btu/hr
21x10⁶ Btu/hr
40x10⁶ Btu/hr
52x10⁶ Btu/hr
Liquid at boiling point
Vapor at boiling point
Cl2
113,400 lb/hr
C2H4
44,900 lb/hr
Direct Chlorination
90°C, 1.5 atm
C2H4Cl2
158,300 lb/hr
90°C, 1.5 atm
Pressure Change
90°C, 26 atm
Temp Change
242°C
26 atm
Phase Change
242°C
26 atm
Temp Change
500°C
26 atm
Pyrolysis
500°C
26 atm
500°C
26 atm
58,300 lb/hr HCl
100,000 lb/hr C2H3Cl
105,500 lb/hr C2H4Cl2
90°C,
1.5 atm
Pressure Change
Temp Change
3.4x106 Btu/hr
Vapor at dew point
Liquid at bubble point
Temp Change
170°C
26 atm
Phase Change
6°C
12 atm
12 atm
-26.2°C
HCl
58,300 lb/hr
33°C
4.8 atm
C2H3Cl
100,000 lb/hr
93°C
146°C
100,000 lb/hr C2H3Cl
105,500 lb/hr C2H4Cl2
C2H4Cl2
105,500 lb/hr

Base Case Design

Develop one or two of the more promising flowsheets from the synthesis tree for more detailed consideration.



Process Intensification

- Any chemical engineering development that leads to a substantially smaller, cleaner, safer, and more energy efficient technology.
- Process Intensifying involve
  - Equipment: special designs that optimize critical parameters (e.g., heat transfer, mass transfer), and
  - Methods: multiple processing steps are integrated into a single unit operation or alternative energy sources are used.
- Advantages
  - reducing energy usage
  - lowering equipment costs, and
  - shrinking the required footprint of a given production facility.

Steps for Process Intensification

Process review

- Literature reviews
- Technology evaluations
- Generation MEB
- Identify process flow diagrams

Process evaluation

- Identify improvements in capital costs, energy usage, and process footprint of design alternatives.

Comparison

- Identify performance and operational difference between intensified process and conventional equipment.

Pilot plant setup

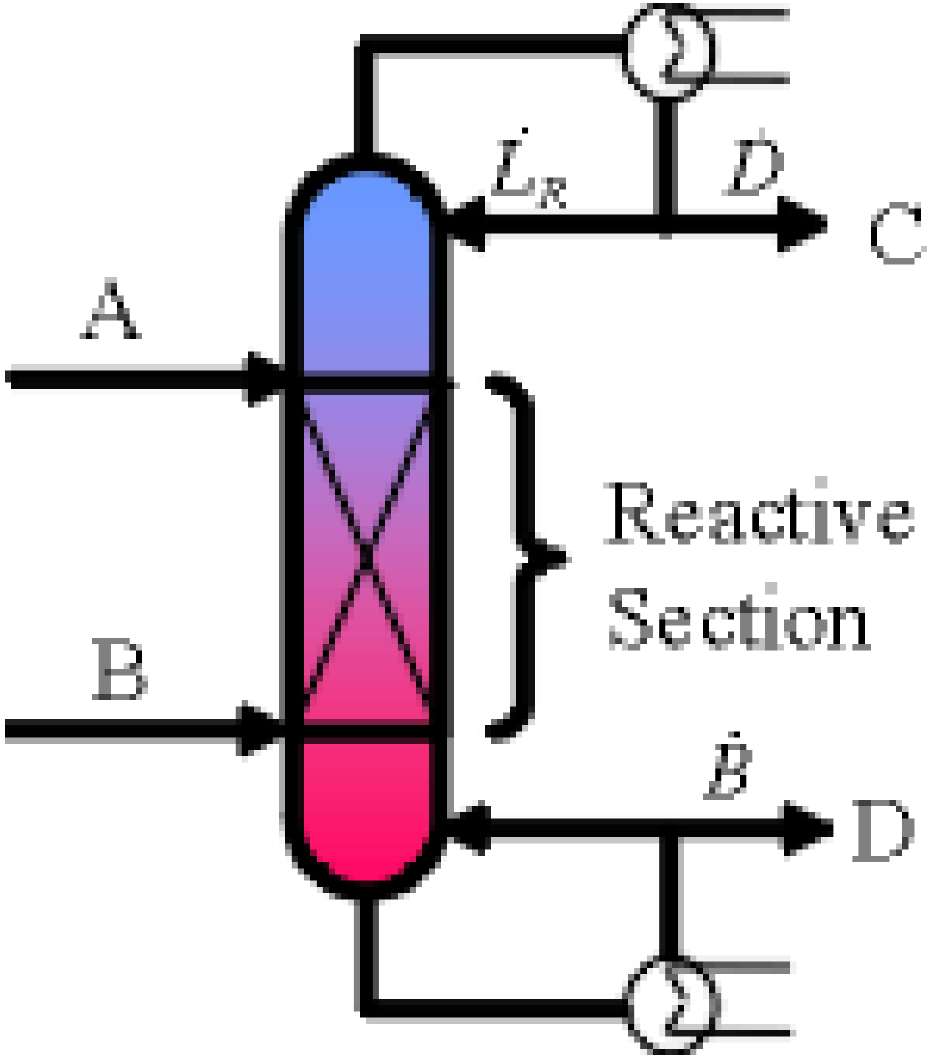
- Determine optimal process conditions and help with later scale-up of the intensified process.

Experience

- Process engineer and fabricator needs to be highly experienced to build reliable test units using non-conventional technologies.

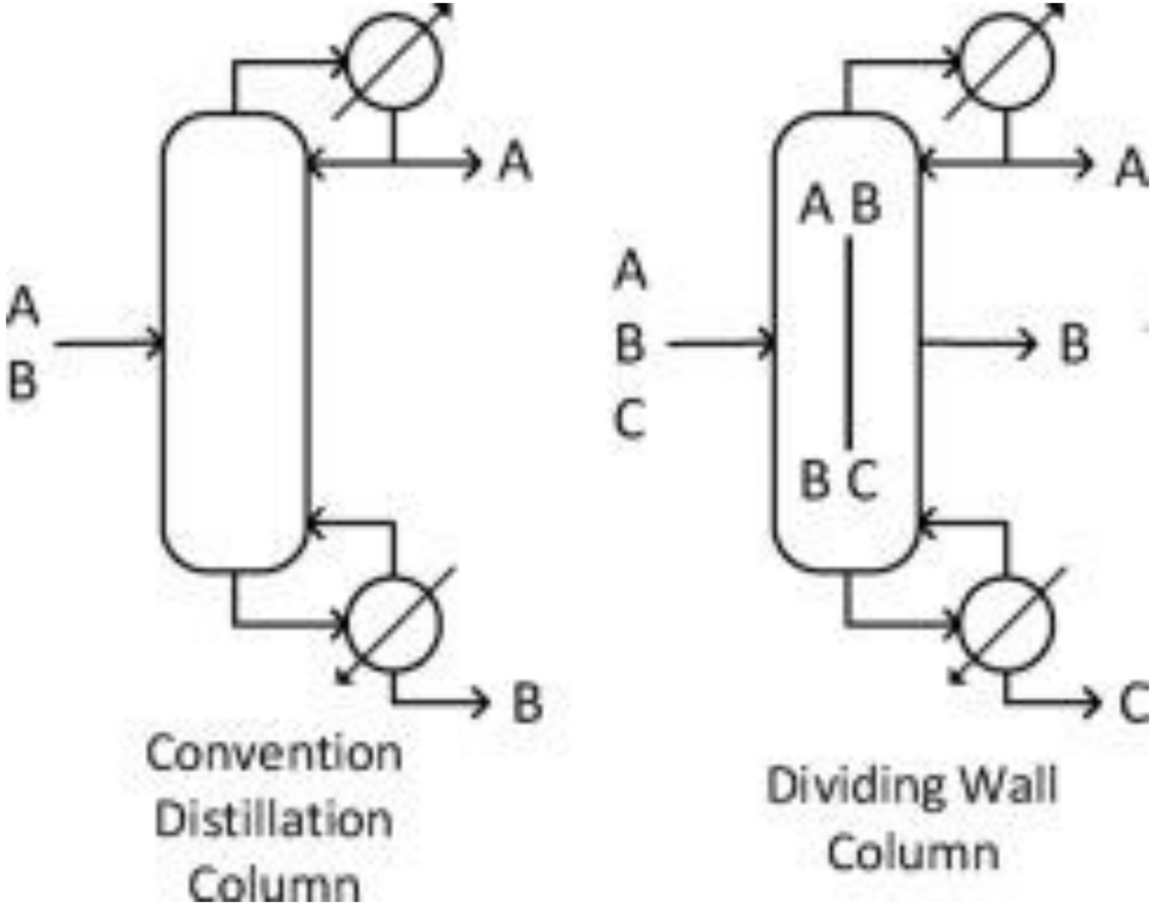
Example – Reactive Distillation

- Reactive distillation combines chemical reactor and distillation column into a single unit.
- RD can lead to a 20-80% reduction in capital costs and/or energy usage (Harmsen, 2010).
- Applications included production of MTBE, acetates (methyl, ethyl, and butyl), hydrolysis reactions, methylal synthesis etc.
- Over 150 RD units are operating at commercial scale in the last 30 years.



Example – DWC

- Dividing Wall Columns (DWC) has been used for the past 18 years.
- Advantage for separating multicomponent mixtures with reduced cost and energy consumption.
- For ternary mixtures only a single DWC is needed compared to 2 DC using conventional distillation.
- DWC are expected to become the standard in the chemical industry in the next decades because of promising cost and energy savings.



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ADVANCING OLEOCHEMICAL FRACTIONATION: AN OUTLOOK ON ENERGY & ECONOMIC EVALUATION USING ASPEN PLUS

MOHAMAD RIZZA OTHMAN & NORUL MALAKIAH SIDEK

18 – 20 MAY 2021

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ADVANCING OLEOCHEMICAL FRACTIONATION: FROM MODELLING WORK TO PILOT PLANT

Ir. Dr.-Ing. Mohamad Rizza Othman

Universiti Malaysia Pahang | Beyond OPTIMIZE '21

Decision Making Support

- How do you make decision for multicriteria?
- What method do you use?
- Selection of biodiesel process
  - Alkali-based process (Case 1)
  - Supercritical MeOH (Case 2)

Assessment criteria/elements

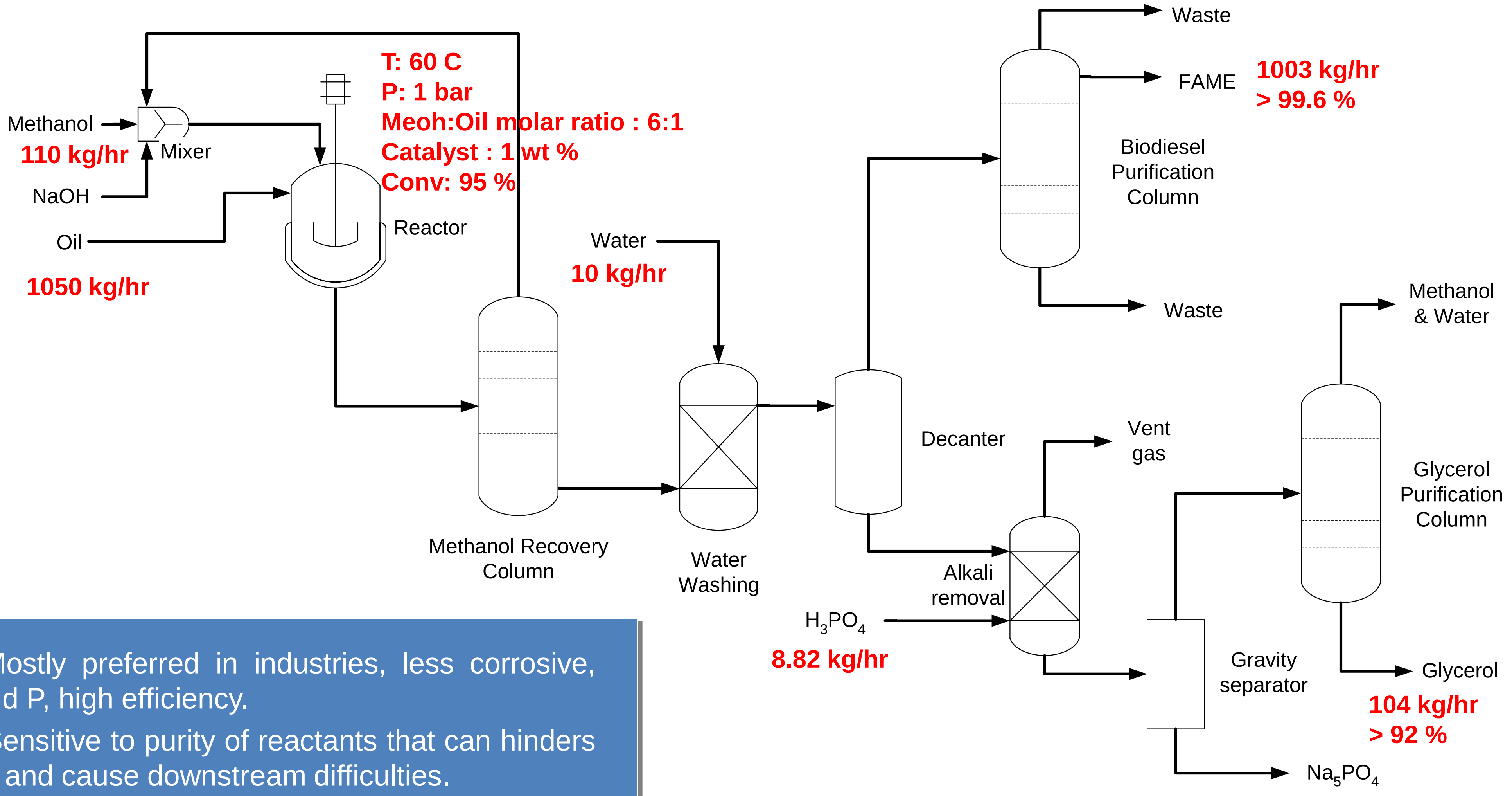
Decision methodology

Decision makers

Engineers, managers, operators etc.

Biodiesel process - Alkali-based process (Case 1)

* Zhang et al. (2003), Myint and El-Halwagi (2008) & West et al. (2008)

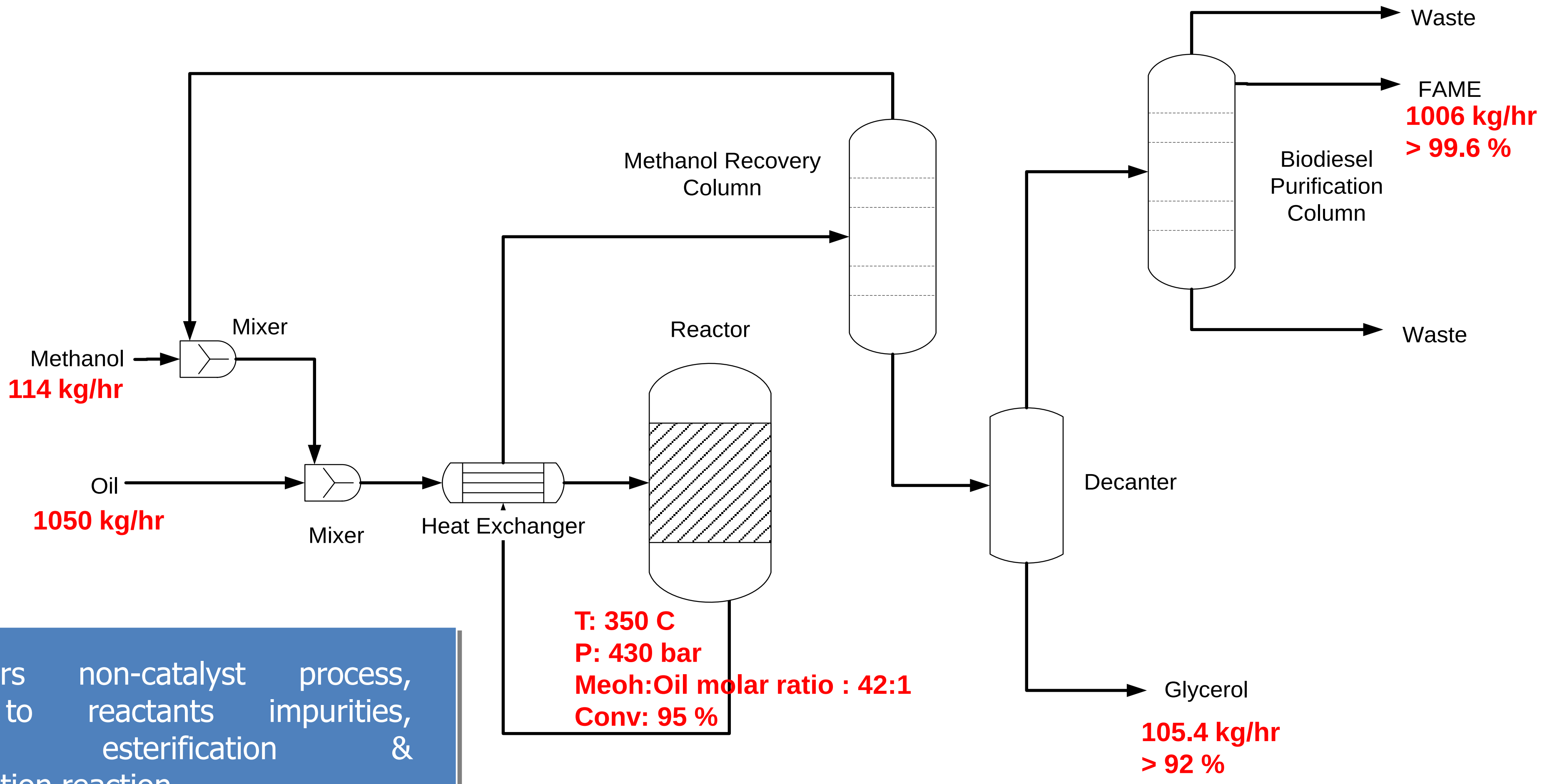


Pros: Mostly preferred in industries, less corrosive, low T and P, high efficiency.

Cons: Sensitive to purity of reactants that can hinders reaction and cause downstream difficulties.

Biodiesel process – Supercritical MeOH (Case 2)

* Lim et al. (2009), West et al. (2008) & van Kasteren & Nisworo, (2007)



Pros: Offers non-catalyst process, insensitive to reactants impurities, simultaneous esterification & transesterification reaction.

Cons: Require high operating T and P.

Decision Making – Conventional way

Indicator, *j*	Value, *v*	
	Case 1	Case 2
NPV, $	2,028 k	2,640 k
DCFRR, %	28,7	23,5
Total rate PEI output	1793	2649
Total PEI output/product	1,62	2,39
Total rate PEI gen.	1670	2540
Total PEI gen./product	1,51	2,29
Safety during operation	5	3,5
Plant operability	5	6
Safe startup and shutdown	5	3
Design meet local specific demand	10	10
TOTAL		

Higher value – higher desirability (LVHD)

Lower value – higher desirability (HVHD)

Decision Making – Conventional way

Indicator, *j*	Value, *v*		Method 1*	
	Case 1	Case 2	Case 1	Case 2
NPV, $	2,028 k	2,640 k		
DCFRR, %	28,7	23,5		
Total rate PEI output	1793	2649		
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Safety during operation	5	3,5		
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Safe startup and shutdown	5	3		
Design meet local specific demand	10	10		
TOTAL				

* Symbolic approach

Decision Making – Conventional way

Indicator, *j*	Value, *v*		Method 1*	
	Case 1	Case 2	Case 1	Case 2
NPV, $	2,028 k	2,640 k	✓	✓✓
DCFRR, %	28,7	23,5	✓✓	✓
Total rate PEI output	1793	2649	✓✓	✓
Total PEI output/product	1,62	2,39	✓✓	✓
Total rate PEI gen.	1670	2540	✓✓	✓
Total PEI gen./product	1,51	2,29	✓✓	✓
Safety during operation	5	3,5	✓✓	✓
Plant operability	5	6	✓	✓✓
Safe startup and shutdown	5	3	✓✓	✓
Design meet local specific demand	10	10	✓	✓
TOTAL			17 x ✓	12 x ✓

* Symbolic approach

Decision Making – Conventional way

$$V_{N_{HVND}}^{j} = \frac{v^j}{\sum_{a=1}^{m} v^j} \qquad V_{N_{LVND}}^{j} = \frac{1/v^j}{\sum_{a=1}^{m} 1/v^j}$$

a = design alternative

m = number of design

j = indicator

V_N = normalized value

v = assessment value

	…alue, v		Method 1*		Method 2**	
	…1	Case 2	Case 1	Case 2	Case 1	Case 2
	…k	2,640 k	✓	✓✓		
		23,5	✓✓	✓		
		2649	✓✓	✓		
		2,39	✓✓	✓		
		2540	✓✓	✓		
		2,29	✓✓	✓		
		3,5	✓✓	✓		
		6	✓	✓✓		
Safe startup and shutdown	5	3	✓✓	✓		
Design meet local specific demand	10	10	✓	✓		
TOTAL			17 x ✓	12 x ✓		

* Symbolic approach ** Normalized score approach

Decision Making – Conventional way

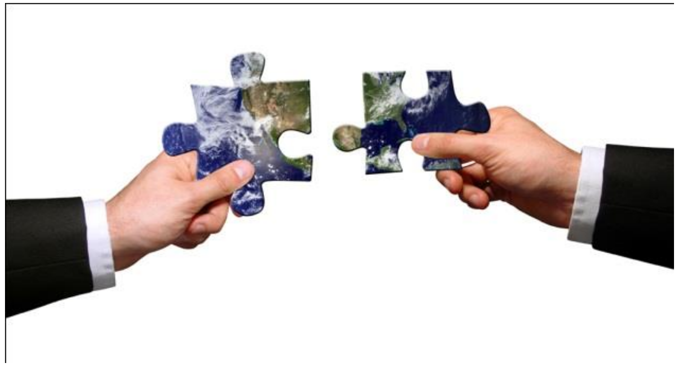
- Remarks…
  - Does not consider the quantitative difference between the values.
  - Does not consider the assessor's preferability towards certain criteria or indicator.
  - Does not consider the importance/priority of the elements.

			Method 1*		Method 2**	
			Case 1	Case 2	Case 1	Case 2
			✓	✓✓	0,43	0,57
			✓✓	✓	0,55	0,45
			✓✓	✓	0,6	0,4
			✓✓	✓	0,6	0,4
			✓✓	✓	0,6	0,4
			✓✓	✓	0,6	0,4
Safety during operation	5	3,5	✓✓	✓	0,59	0,41
Plant operability	5	6	✓	✓✓	0,45	0,55
Safe startup and shutdown	5	3	✓✓	✓	0,63	0,38
Design meet local specific demand	10	10	✓	✓	0,5	0,5
TOTAL			17 x ✓	12 x ✓	5,55	4,46

* Symbolic approach ** Normalized score approach

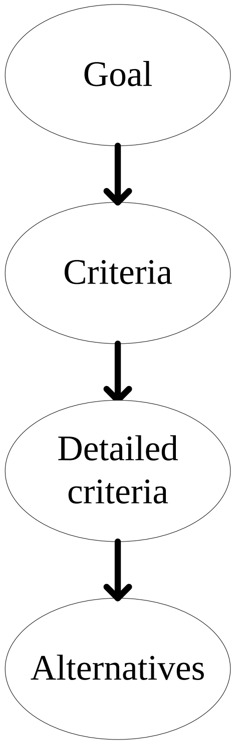
Analytic hierarchy process (AHP)

- Decision making should be: -
  - Systematic
  - Comprehensive
  - Justifiable
- AHP (Saaty, 1980) is suitable because:-
  - Provide a systematic and simple approach.
  - Hierarchy-based
  - Offer multiple and specific criteria for decision inclusion.
  - Accept team work participation.


AHP : Procedure

1. Problem decomposition → 2. Pairwise comparison → 3. Weights ranking → 4. Evaluation

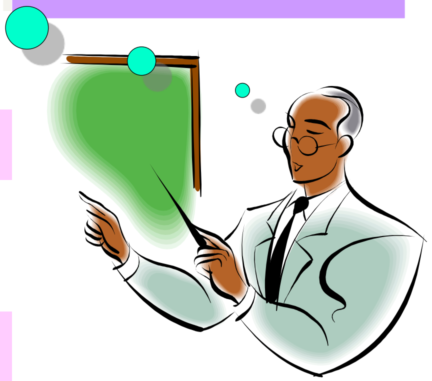


- Uni-directional hierarchical structure.
- Advantages of hierarchical design:-
  - Describe how changes in priority affects the system.
  - Give great detail of information of the system structure.
  - Natural systems assembled hierarchically.
  - They are stable and flexible.
- Can range from simple to complex decision tree depends on the problem complexities.
- Problem model must be well define to give a justifiable and accurate decision.

AHP : Procedure

1. Problem decomposition → 2. Pairwise comparison → 4. Evaluation

Let's go to the biodiesel design selection problem



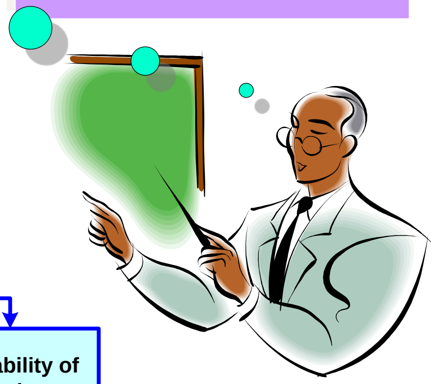
Criteria	Indicator
Economy	▸ Net present value (NPV) ▸ Discounted cash flow rate of return (DCFRR)

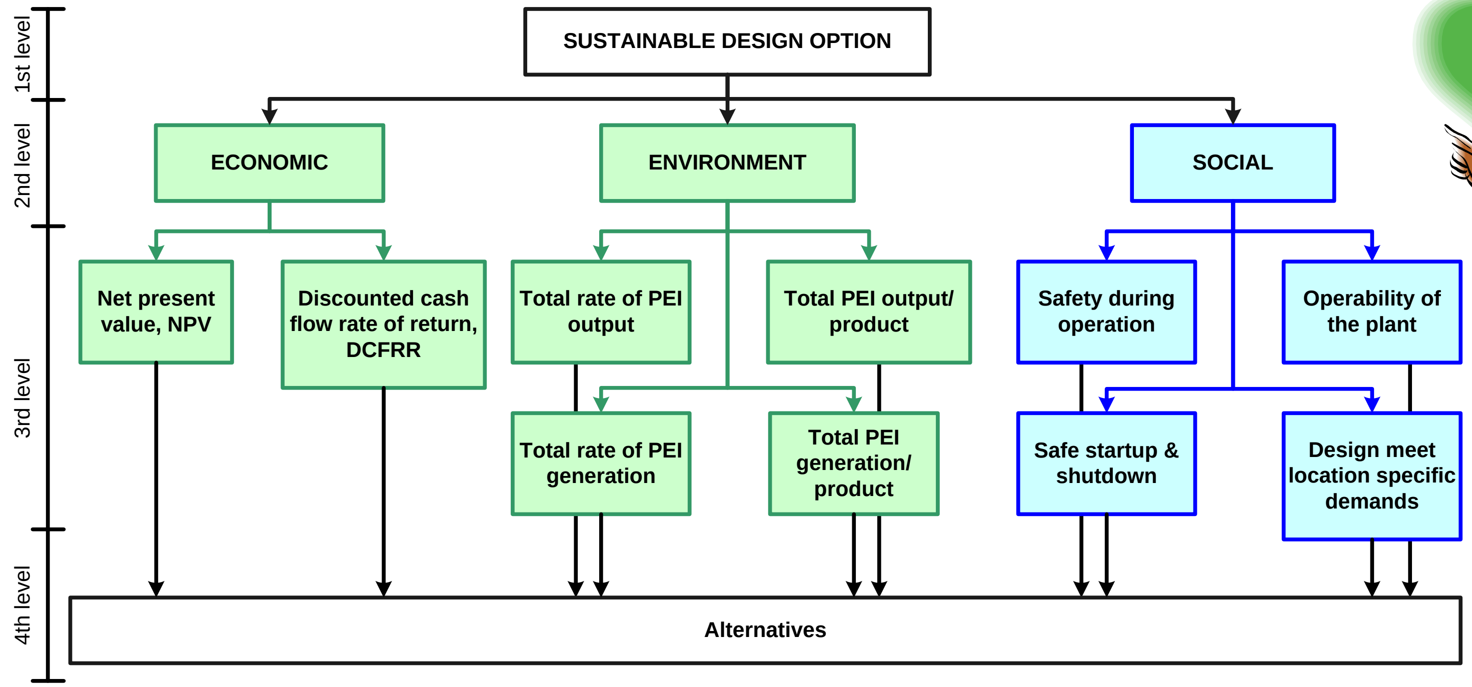
Environment	▸ WAR algorithm
	  ▸ Total rate PEI output
	  ▸ Total PEI output/product
	  ▸ Total rate PEI gen.
	  ▸ Total PEI gen./product

Social	▸ Safety during operation ▸ Plant operability ▸ Safe startup and shutdown ▸ Design meet local specific demands

AHP : Procedure

1. Problem decomposition
2. Pairwise comparison
3. Let's go to the biodiesel design selection problem
4. Evaluation





- **Hard (quantitative) assessment**
  Utilization of process simulators for quantitative assessment.
- **Soft (qualitative) assessment**
  Allow contribution from heuristic type of knowledge and experience.

AHP : Procedure

1. Problem decomposition → **2. Pairwise comparison** → 3. Weights ranking → 4. Evaluation

Pairwise comparison for the 2nd level

GOAL	Econ.	Env.	Social
Econ.	1	A_{12}	A_{13}
Env.	$1/A_{12}$	1	A_{23}
Social	$1/A_{13}$	$1/A_{23}$	1

Quantitative scale	Qualitative indicator	Explanation
1	Equal Importance	Two activities contribute equally to the objective
2	Weak or slight	
3	Moderate importance	Experience and judgement slightly favour one activity over another
4	Moderate plus	
5	Strong importance	Experience and judgement strongly favour one activity over another
6	Strong plus	
7	Very strong or demonstrated importance	An activity is favoured very strongly over another; its dominance demonstrated in practice
8	Very, very strong	
9	Extreme importance	The evidence favouring one activity over another is of the highest possible order of affirmation
2, 4, 6, 8	Intermediate values	
1/3	Weakly less important	May be difficult to assign the best value but when compared with other contrasting activities the size of the small numbers would not be too noticeable, yet they can still indicate the relative importance of the activities.
1/5	Moderately less important	
1/7	Strongly less important	
1/9	Absolutely less important	
1/2, 1/4, 1/6, 1/8	Intermediate value etc.	

- Comparing 2 components with respect to a control criterion using weights scale (see Table).
- Identify a value of A_{ij}, which denotes the importance of the *i*-th element (left) compared to the *j*-th element (top) with respect to their relative importance towards their control criterion.
- >1 = Base criterion more important than the paired criteria
- <1 = Inverse importance
- A reciprocal value is assigned to the inverse comparison, $a_{ji} = 1/a_{ij}$.

AHP : Procedure

1. Problem decomposition → 2. Pairwise comparison → 3. Weights ranking → 4. Evaluation

- To aid the comparison process series of questions can be use such as: -

  "When considering sustainable process design, what is the relative importance of economic feasibility when compared to environmental friendliness?'

Economic is ***???*** *than environment friendliness.*

1/9	1/8	1/7	1/6	1/5	1/4	1/3	1/2	1	2	3	4	5	6	7	8	9

Pairwise comparison for the 2nd level

GOAL	Econ.	Env.	Social
Econ.	1	A_{12}=2	A_{13}=1,5
Env.	1/A_{12}=0,5	1	A_{23}=0,75
Social	1/A_{13}=0,667	1/A_{23}=1,333	1

Quantitative scale	Qualitative indicator	Explanation
1	Equal Importance	Two activities contribute equally to the objective
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1/5	Moderately less important	
1/7	Strongly less important	
1/9	Absolutely less important	
1/2, 1/4, 1/6, 1/8	Intermediate value etc.	

AHP : Procedure

1. Problem decomposition → **2. Pairwise comparison** → 3. Weights ranking → 4. Evaluation

- To aid the comparison process series of questions can be use such as: -

  "When considering sustainable process design, what is the relative importance of economic feasibility when compared to environmental friendliness?'

Economic is ***equally important*** *than environment friendliness.*

1/9	1/8	1/7	1/6	1/5	1/4	1/3	1/2	1	2	3	4	5	6	7	8	9

Pairwise comparison for the 2nd level

GOAL	Econ.	Env.	Social
Econ.	1	A_{12}=2	A_{13}=1,5
Env.	$1/A_{12}$=0,5	1	A_{23}=0,75
Social	$1/A_{13}$=0,667	$1/A_{23}$=1,333	1

Quantitative scale	Qualitative indicator	Explanation
1	Equal Importance	Two activities contribute equally to the objective
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6	Strong plus	
7	Very strong or demonstrated importance	An activity is favoured very strongly over another; its dominance demonstrated in practice
8	Very, very strong	
9	Extreme importance	The evidence favouring one activity over another is of the highest possible order of affirmation
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1/9	Absolutely less important	
1/2, 1/4, 1/6, 1/8	Intermediate value etc.	

AHP : Procedure

1. Problem decomposition → **2. Pairwise comparison** → 3. Weights ranking → 4. Evaluation

- To aid the comparison process series of questions can be use such as: -

  "When considering sustainable process design, what is the relative importance of economic feasibility when compared to environmental friendliness?'

*Economic is **moderately important** than environment friendliness.*

1/9	1/8	1/7	1/6	1/5	1/4	1/3	1/2	1	2	3	4	5	6	7	8	9

Pairwise comparison for the 2nd level

GOAL	Econ.	Env.	Social
Econ.	1	$A_{12}=2$	$A_{13}=1,5$
Env.	$1/A_{12}=0,5$	1	$A_{23}=0,75$
Social	$1/A_{13}=0,667$	$1/A_{23}=1,333$	1

Quantitative scale	Qualitative indicator	Explanation
1	Equal Importance	Two activities contribute equally to the objective
2	Weak or slight	
3	Moderate importance	Experience and judgement slightly favour one activity over another
4	Moderate plus	
5	Strong importance	Experience and judgement strongly favour one activity over another
6	Strong plus	
7	Very strong or demonstrated importance	An activity is favoured very strongly over another; its dominance demonstrated in practice
8	Very, very strong	
9	Extreme importance	The evidence favouring one activity over another is of the highest possible order of affirmation
2, 4, 6, 8	Intermediate values	
1/3	Weakly less important	May be difficult to assign the best value but when compared with other contrasting activities the size of the small numbers would not be too noticeable, yet they can still indicate the relative importance of the activities.
1/5	Moderately less important	
1/7	Strongly less important	
1/9	Absolutely less important	
1/2, 1/4, 1/6, 1/8	Intermediate value etc.	

AHP : Procedure

1. Problem decomposition → 2. Pairwise comparison → 3. Weights ranking → 4. Evaluation

- To aid the comparison process series of questions can be use such as: -

  "When considering sustainable process design, what is the relative importance of economic feasibility when compared to environmental friendliness?'

Economic is ***moderately less important*** *than environment friendliness.*

1/9	1/8	1/7	1/6	1/5	1/4	1/3	1/2	1	2	3	4	5	6	7	8	9

- Decision makers' knowledge, experience, and judgment ability are critical in weight assignment.

Pairwise comparison for the 2nd level

GOAL	Econ.	Env.	Social
Econ.	1	A_{12}=2	A_{13}=1,5
Env.	1/A_{12}=0,5	1	A_{23}=0,75
Social	1/A_{13}=0,667	1/A_{23}=1,333	1

Quantitative scale	Qualitative indicator	Explanation
1	Equal Importance	Two activities contribute equally to the objective
2	Weak or slight	
3	Moderate importance	Experience and judgement slightly favour one activity over another
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1/5	Moderately less important	
1/7	Strongly less important	
1/9	Absolutely less important	
1/2, 1/4, 1/6, 1/8	Intermediate value etc.	

AHP : Procedure

1. Problem decomposition → 2. Pairwise comparison → **3. Weights ranking** → 4. Evaluation

Pairwise comparison for the 2nd level

GOAL	Economy	Environment	Social
Economy	1	3	2
Environment	0,333	1	0,5
Social	0,5	2	1

1. Sum the values in each column of the pairwise comparison matrix

$$matrix, w = \begin{bmatrix} 1 & 3 & 2 \\ 0,333 & 1 & 0,5 \\ 0,5 & 2 & 1 \end{bmatrix}$$
$$0,933 \quad 6 \quad 3,5$$

2. Divide each element in a column by the sum of its respective column. The resultant matrix is referred to as the normalized pairwise comparison matrix.

$$w = \begin{bmatrix} 1/0,933 = 1,072 & 3/6 = 0,5 & 2/3,5 = 0,571 \\ 0,357 & 0,167 & 0,143 \\ 0,536 & 0,333 & 0,286 \end{bmatrix}$$

3. Sum the elements in each row of the normalized pairwise comparison matrix, and divide the sum by the n elements in the row. These final numbers provide an estimate of the relative priorities for the elements being compared with respect to its upper level criterion.

$$w = \begin{bmatrix} 1,072 & + & 0,5 & + & 0,571 \\ 0,357 & + & 0,167 & + & 0,143 \\ 0,536 & + & 0,333 & + & 0,286 \end{bmatrix} = \begin{bmatrix} 2,143 \\ 0,667 \\ 1,155 \end{bmatrix}$$
$$3,965$$

$$eigenvector, p_w = \begin{bmatrix} 2,143/3,965 = 0,54 \\ 0,17 \\ 0,29 \end{bmatrix}$$

AHP : Procedure

1. Problem decomposition → 2. Pairwise comparison → **3. Weights ranking** → 4. Evaluation

Pairwise comparison for the 2nd level

GOAL	Economy	Environment	Social
Economy	1	3	2
Environment	0,333	1	0,5
Social	0,5	2	1

1. Another way of solving *w* is through multiplication of matrix **A** with **A** itself at Step 1 as shown below:

$$matrix, w^2 = \begin{bmatrix} 1 & 3 & 2 \\ 0{,}333 & 1 & 0{,}5 \\ 0{,}5 & 2 & 1 \end{bmatrix} \times \begin{bmatrix} 1 & 3 & 2 \\ 0{,}333 & 1 & 0{,}5 \\ 0{,}5 & 2 & 1 \end{bmatrix}$$

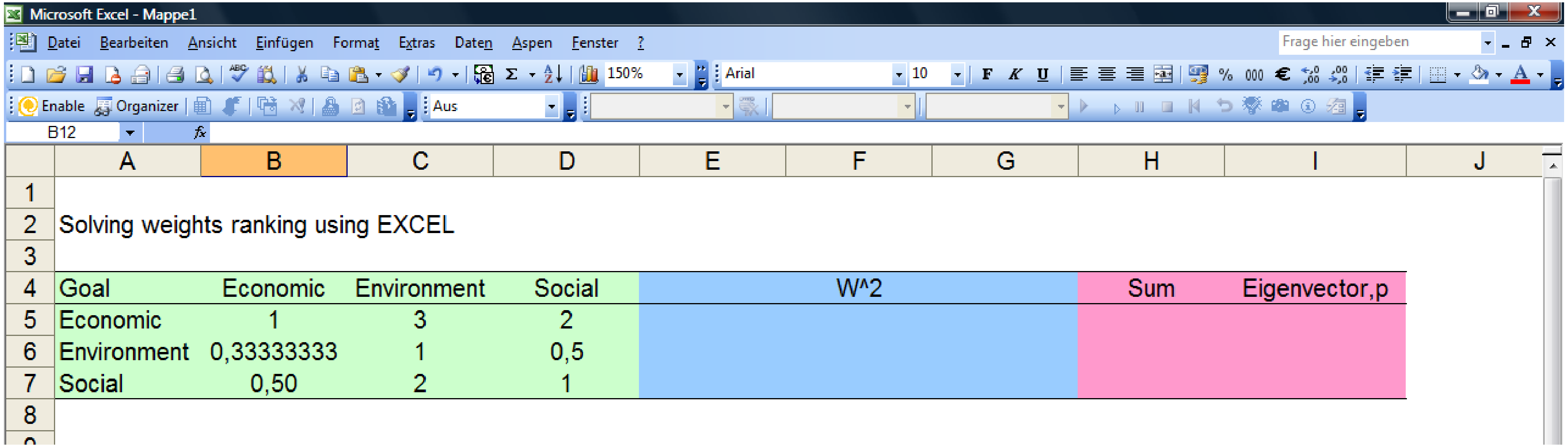
2. The next step is the same as Step 2 and 3 to obtain the relative priorities and will result in the same value as in the previous method.

AHP : Procedure

1. Problem decomposition → 2. Pairwise comparison → **3. Weights ranking** → 4. Evaluation

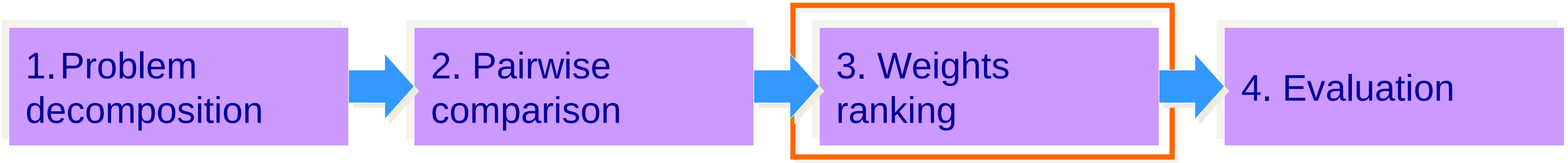
Using excel to solve weights ranking.

1. Create a block comprising the pairwise matrix, ***W*** for the designated control criterion.

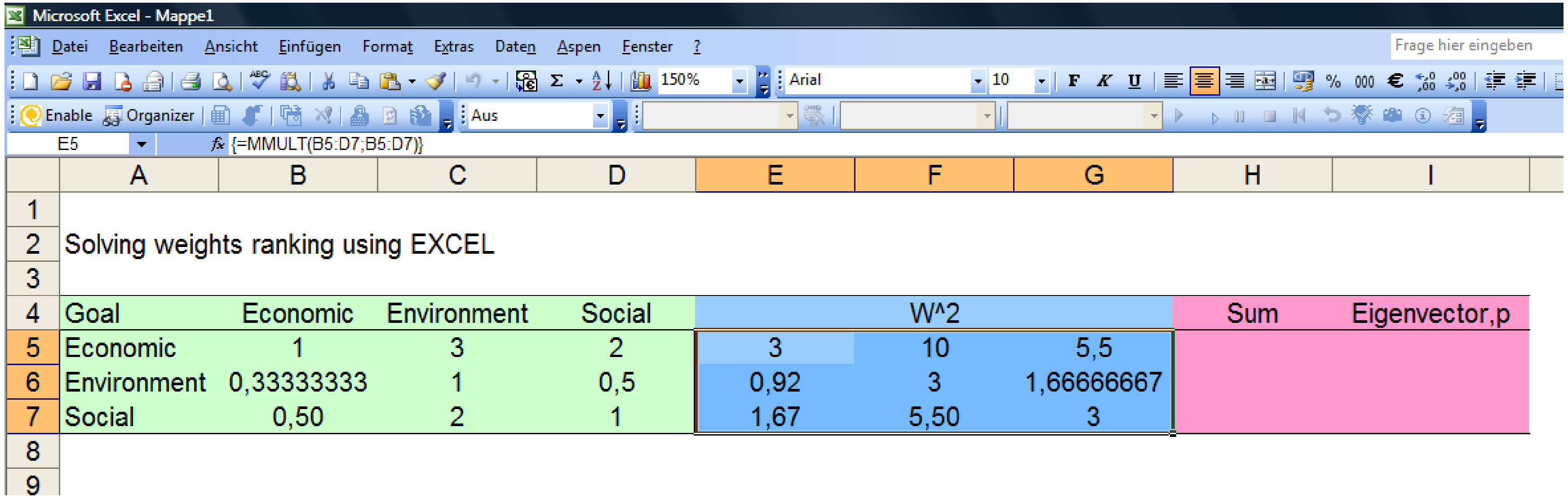


Goal	Economic	Environment	Social	W^2			Sum	Eigenvector,p
Economic	1	3	2					
Environment	0,33333333	1	0,5					
Social	0,50	2	1					

AHP : Procedure



2. Create another block for calculating ***W*²** which has the same dimension as ***W***.
3. Perform matrix multiplication,
   - Select the corresponding row and column for which to insert the calculation result. In this case E5:G7.
   - =MMULT(*Matrix1*;*Matrix2*)
   - =MMULT(*B5:D7*;*B5:D7*)
   - and press Ctrl+Shift+Enter



	A	B	C	D	E	F	G	H	I
1									
2	Solving weights ranking using EXCEL								
3									
4	Goal	Economic	Environment	Social		W^2		Sum	Eigenvector,p
5	Economic	1	3	2	3	10	5,5		
6	Environment	0,33333333	1	0,5	0,92	3	1,66666667		
7	Social	0,50	2	1	1,67	5,50	3		
8									
9									

AHP : Procedure

1. Problem decomposition → 2. Pairwise comparison → **3. Weights ranking** → 4. Evaluation

4. For each criteria add the resulted matrix value of its corresponding row as in the 'Sum' column.
5. Add the 'Sum' column.
6. Normalize each sum with respect to the total sum to obtain the eigenvector, p which is the prioritization fraction.

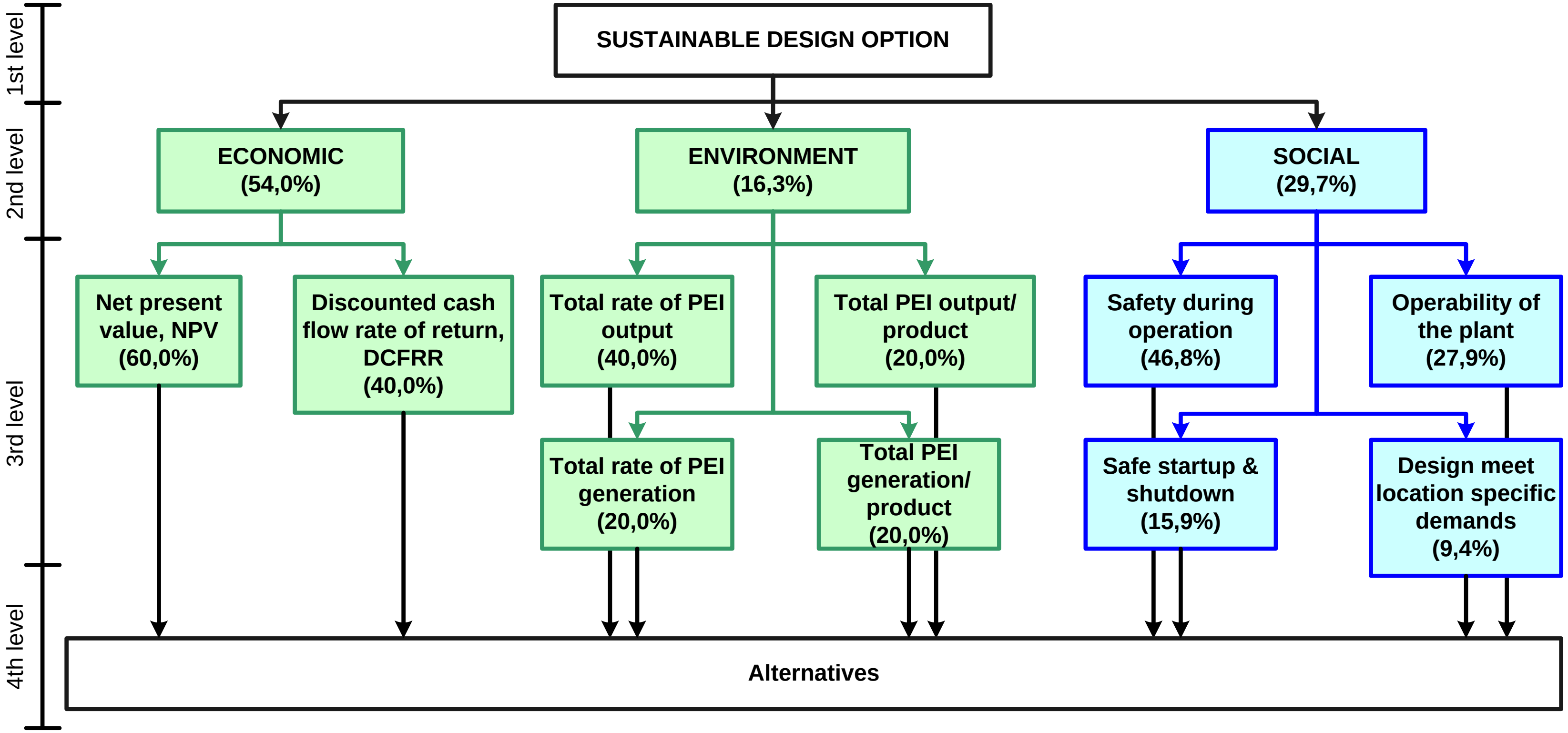
Microsoft Excel - Mappe1

Solving weights ranking using EXCEL

Goal	Economic	Environment	Social		W^2		Sum	Eigenvector,p
Economic	1	3	2	3	10	5,5	18,50	0,540
Environment	0,33333333	1	0,5	0,92	3	1,66666667	5,58	0,163
Social	0,50	2	1	1,67	5,50	3	10,17	0,297
							34,25	

AHP : Procedure

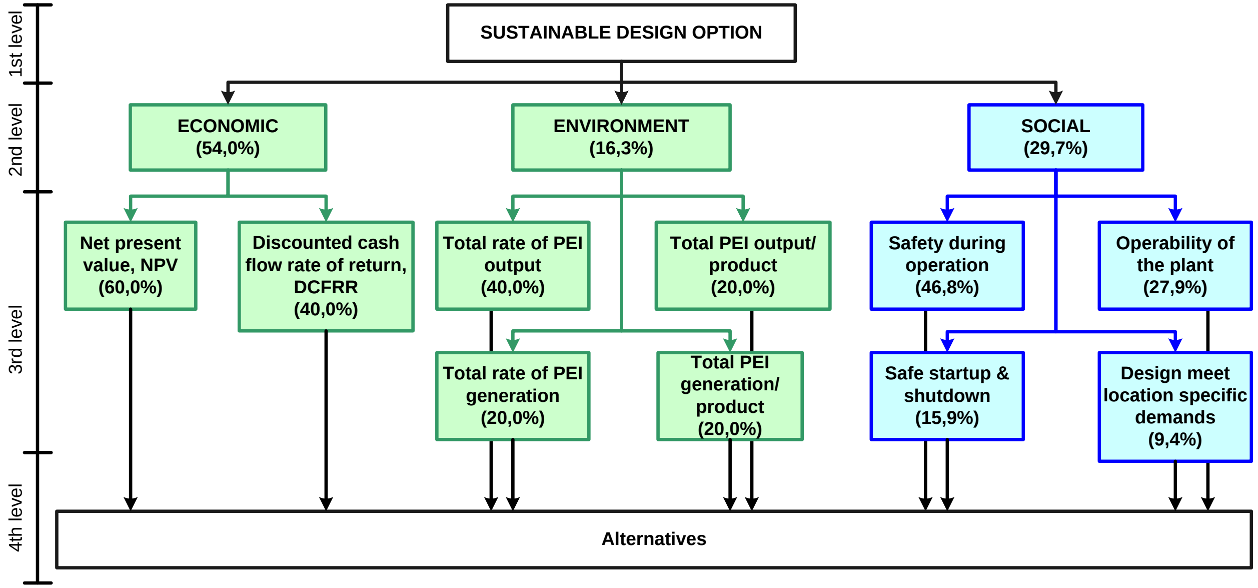
1. Problem decomposition → 2. Pairwise comparison → 3. Weights ranking → 4. Evaluation



AHP : Procedure

1. Problem decomposition → 2. Pairwise comparison → 3. Weights ranking → **4. Evaluation**

- The selection of best alternatives depends on the summation of all the score index, *I* for an alternative, *a* for each designated criteria, *i*. The equation for calculating *I* (4 level decision hierarchy) is defined by,



$$I_{a,i} = p_i n_{ij} V_{N,ij}$$

i = criteria

j = indicator

$V_{N,ij}$ = *normalized assessment value*

p_i = eigenvector for criteria i

n_{ij} = eigenvector for indicator j of criteria i

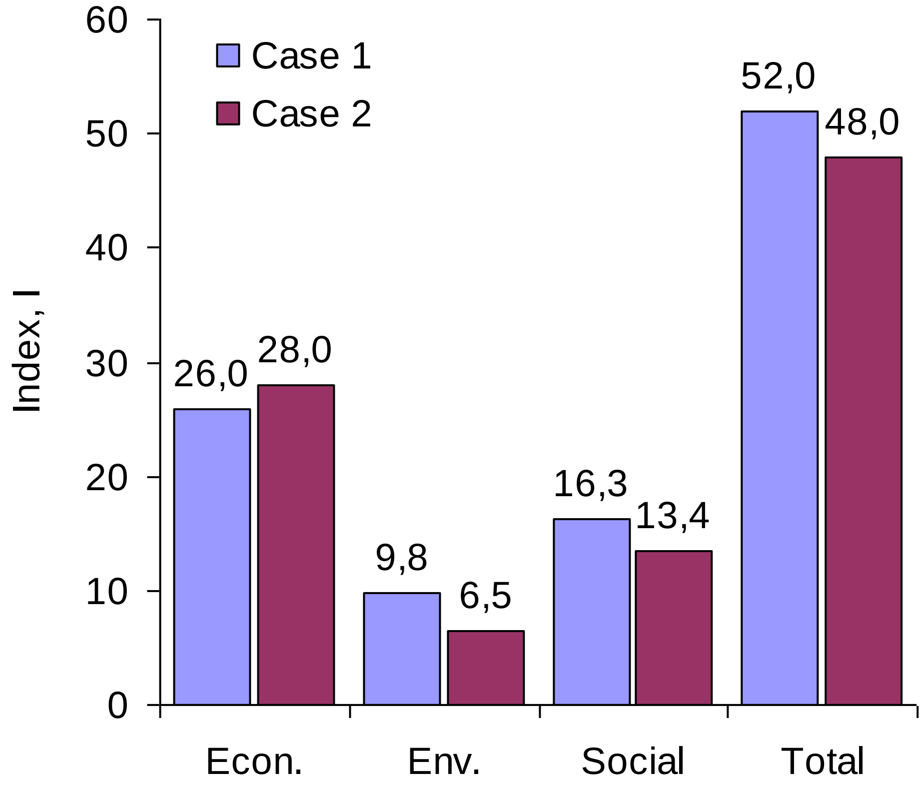
AHP : Procedure

1. Problem decomposition → 2. Pairwise comparison → 3. Weights ranking → **4. Evaluation**

i	*p*	*j*	*n*	Value, *v*		Norm. value, V_N		Index, *I*	
				C1	C2	C1	C2	C1	C2
Econ.	0.540	NPV	0.60	2,028 k	2,640 k	0.434	0.566	0.14	0.18
		DCFRR	0.40	28.7	23.5	0.550	0.450	0.12	0.10
Env.	0.163	Total rate PEI output	0.40	1793	2649	0.596	0.404	0.04	0.03
		Total PEI output/product	0.20	162	2.39	0.596	0.404	0.02	0.01
		Total rate PEI gen.	0.20	1670	2540	0.603	0.397	0.02	0.01
		Total PEI gen./product	0.20	1.51	2.29	0.603	0.397	0.02	0.01
Social	0.297	Safety during operation	0.468	5	3.5	0.588	0.412	0.08	0.06
		Plant operability	0.279	5	6	0.455	0.545	0.04	0.05
		Safe startup and shutdown	0.159	5	3	0.625	0.375	0.03	0.02
		Design meet local specific demand	0.094	10	10	0.500	0.500	0.01	0.01
TOTAL								0.52	0.48

AHP : Procedure

1. Problem decomposition → 2. Pairwise comparison → 3. Weights ranking → **4. Evaluation**



- AHP elucidate the same result as the conventional method.
- But what's different are: -
  - It provide a clear elucidation of the results.
  - It gave numerical results based on quantitative and qualitative data.
  - DM preference were included in the assessment.
  - Highlights the importance of each elements.

Concluding remarks

In this lecture you have been thought: -

- The concept of sustainability and its indicators used to assess chemical industries.
- The methodology of performing decision making using AHP.

Outlook

- Including interaction or dependency among the elements in the decision model using analytic network process (ANP).
- Study the effect of different decision models towards decision making.
- Application to various scenario in chemical industries e.g., supply chain.
- Introduction to chemical engineering education.

THE SUSTAINABILITY METRICS

Sustainable Development Progress Metrics
recommended for use in the Process Industries

IChemE

institution of chemical engineers

FOREWORD

I am pleased that the IChemE Sustainable Development Progress Metrics are now ready for issue. The document is the result of three years work and debate by a number of individuals drawn from industry, academia and consultancy. The people on the attached list deserve all our thanks for their contributions and particularly their perseverance.

The emphasis in our work has been to produce a practical tool for practicing engineers using as far as possible information already available. Our aim has also been to develop a wider understanding of sustainability within the process industry sector.

I very much hope that you will find the metrics useful in measuring your company's progress towards a more sustainable operation and that you will share your experience via IChemE so that we can all learn to improve.

Bill Tallis
Chairman
Sustainable Development Working Group

SUSTAINABILITY WORKING PARTY

Adisa Azapagic
Alan Howard
Alan Parfitt
Bill Tallis
Charles Duff
Clive Hadfield
Colin Pritchard
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Judith Hackitt
Miles Seaman
Richard Darton
Richard Rathbone
Roland Clift
Steve Watson
Steven Elliot

SUSTAINABLE DEVELOPMENT PROGRESS METRICS

Recommended for use in the Process Industries

SUMMARY

The Institution of Chemical Engineers sees sustainable development as the most significant issue facing society today. Engineering for sustainable development means providing for human needs without compromising the ability of future generations to meet their needs. The impact of industry on sustainability can be summarised in the "triple bottom line", covering the three components - environmental responsibility, economic return (wealth creation), and social development. For industry to guide its activities towards greater sustainability, more engineers need to have the tools to assess the operations with which they are concerned. This publication therefore introduces a set of indicators that can be used to measure the sustainability performance of an operating unit. These metrics will help engineers address the issue of sustainable development. They will also enable companies to set targets and develop standards for internal benchmarking, and to monitor progress year-on-year.

Sustainable Development Progress Metrics has been produced by the Sustainable Development Working Group of The Institution of Chemical Engineers.

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SUSTAINABLE DEVELOPMENT PROGRESS METRICS

Recommended for use in the Process Industries

CONTENTS

1 INTRODUCTION

The Institution of Chemical Engineers (IChemE), a learned society representing 25,000 chemical engineers worldwide, sees sustainable development as the most significant issue facing society today. The IChemE's approach to sustainable development is encapsulated in the London Communiqué of 1997 (a statement signed by the leaders of 18 chemical engineering societies throughout the world): "We will work to make the world a better place for future generations" and to "provide the processes and products which will give the people of the world shelter, clothing, food and drink, and which keep them in good health". The IChemE has thus been working, with other bodies, to encourage progress to a more sustainable world through the activities of its members and the organizations for which they work.

The laws of conservation of mass and energy are basic principles utilised by engineers. However the results of manipulating the resources of the planet through these principles have consequences for the global eco-system. Engineering for sustainable development means providing for human needs without compromising the ability of future generations to meet their needs. It is clear that we have to be less profligate in our use of non-renewable resources if the planet is to be fit for future generations to live on. We must also be more aware of the consequences of our activities for society at large.

The process industries have made significant progress over the last decade, particularly in improving their efficiency of production and their environmental performance, and the IChemE has lent support to this improvement. However, moving towards the goal of sustainability requires us also to examine and improve other aspects that have not traditionally been given much attention, at least by practicing engineers.

Broadly, the impact of industry can be summarised in the "triple bottom line", covering the three components of sustainable development which are environmental responsibility, economic return (wealth creation), and social development.

Many companies now recognize and monitor these three parallel strands, using their assessment to guide their product, process and personnel development and to secure their position in the rapidly changing climate of environmental legislation and stakeholder concerns. IChemE would like to encourage more companies to follow this lead, which requires more engineers to have the tools to assess the sustainability of operations with which they are concerned.

This publication therefore introduces a set of indicators that can be used to measure sustainability performance of an operating unit. If comparable statistics are gathered from a number of operations, they can be aggregated to present a view of a larger operation, on a company, industry or regional basis for example. The operating unit envisaged is a process plant, a group of plants, part of a supply chain, a whole supply chain, a utility or other process system.

We believe that these metrics will help engineers address the issue of sustainable development, and learn about the broader impact of company operations. They will also enable companies to set targets and develop standards for internal benchmarking, and to monitor progress year-on-year.

The IChemE would welcome your comments on these metrics, which we hope to develop in the light of experience with their use.

2 REPORTING FORMAT

Companies in the processing sector are encouraged to report their performance according to the standards recommended by the Global Reporting Initiative (Sustainability Reporting Guidelines, www.globalreporting.org). The format recommended here is consistent with that of the GRI. Naturally the contents of the report will depend on the scope of the operations under consideration, but it is important that even for small operating units the wider implications and impacts are considered.

The report should include the following.

1 **Profile.**
Definition of reporting unit, its boundaries and activities. Any significant changes over reporting period.

2 **Summary.**
Key indicators - environmental, economic and social - which give a balanced overview of the report. Other important comments, conclusions and plans.

3 **Vision and strategy.**
Short-term and long-term actions planned for the unit, to move to greater sustainability. Explanation of how these harmonise with company policy. Identification of specific targets.

4 **Policy and organization.**
Description of policies and organisation, management structure, stakeholder interactions – how these impact on unit performance. Statement on compliance with ISO 14001, EMAS, Responsible Care, etc. Procedures for monitoring sustainability performance of suppliers, contractors and outsourced activities in general.

5 **Performance.**
In this section the metrics are reported. It will be helpful also to note historical trends, targets, and factors affecting performance, as an aid to interpretation.

Although designed for internal use, companies are encouraged to publish their progress metrics report, in whole or in part, to demonstrate their commitment to sustainable development. The IChemE will be pleased to receive the information collected by each Company, on a confidential basis not for publication. These data will help us to monitor the usefulness of our metrics, and to develop future recommendations for best practice.

Respondents sending data to IChemE are kindly requested to use the Report Form (Appendix C). This can be completed with the aid of the explanatory notes and working tables found in section 3 of this report.

3 THE METRICS

The metrics are presented in the three groups

3.1 Environmental indicators
3.2 Economic indicators
3.3 Social indicators

which reflect the three components of sustainable development.

Not all the metrics we suggest will be applicable to every operating unit. For some units other metrics will be more relevant and respondents should be prepared to devise and report their own tailored metrics. Choosing relevant metrics is a task for the respondent. Nevertheless, to give a balanced view of sustainability performance, there must be key indicators in each of the three areas (environmental, economic, social).

Most products with which the process industries are concerned will pass through many hands in the chain *resource extraction – transport – manufacture – distribution – sale – utilization – disposal – recycling – final disposal.* Suppliers, customers and contractors all contribute to this chain, so in reporting the metrics it is important that the respondent makes it clear where the boundaries have been drawn.

As with all benchmarking exercises, a company will receive most benefit from these data if they are collected for a number of operating units, over a number of years, on a consistent basis. This will give an indication of trends, and the effect of implementing policies.

A note on ratio indicators

Most of the progress metrics are calculated in the form of appropriate ratios. Ratio indicators can be chosen to provide a measure of impact independent of the scale of operation, or to weigh cost against benefit, and in some cases they can allow comparison between different operations. For example, in the environmental area, the *unit of environmental impact* per unit of *product or service value* is a good measure of eco-efficiency. The preferred unit of product or service value is the value added (see section 3.2.1), and this is the scaling factor generally used in this report. However, the value added can sometimes be difficult to estimate accurately, so surrogate measures such as net sales, profit, or even mass of product may be used. Alternatively, a measure of value might be the worth of the service provided, such as the value of personal mobility, the value of improved hygiene, health or comfort. But a well-founded and consistent method of estimating these 'values' must be presented.

3.1 Environmental indicators

These metrics should give a balanced view of the environmental impact of inputs – resource usage, and outputs – emissions, effluents and waste and the products and services produced.

3.1.1 Resource usage

(a) Energy

Imports

	Energy Value	Conversion factor	Primary Energy Value	Quantity used/y	Usage rate GJ/y
Electricity	kJ	a)	kJ		
Fuel Oil	kJ/kg	1	kJ/kg		
Gas	kJ/kg	1	kJ/kg		
Coal	kJ/kg	1	kJ/kg		
Steam	kJ/kg	a)	kJ/kg		
Other (specify)	kJ/kg	a)	kJ/kg		
Total					

Export

	Energy Value	Conversion factor	Primary Energy Value	Quantity used/y	Usage rate GJ/y
Electricity	kJ	a)	kJ		
Fuel Oil	kJ/kg	1	kJ/kg		
Gas	kJ/kg	1	kJ/kg		
Coal	kJ/kg	1	kJ/kg		
Steam	kJ/kg	a)	kJ/kg		
Other (specify)	kJ/kg	a)	kJ/kg		
Total					

Note

The Energy Value is multiplied by the Conversion factor to give the Primary Energy Value. It thus corrects for the efficiency of generation and supply of the secondary energy source, to yield comparable figures for the primary energy usage rate. The Conversion factors are available from the suppliers of the energy and will vary from provider to provider.

Total Net Primary Energy Usage rate = Imports – Exports ________________ **GJ/y**

Percentage Total Net Primary Energy sourced from renewables ________________ **%**

Total Net Primary Energy Usage per kg product ________________ **kJ/kg**

Total Net Primary Energy Usage per unit value added ________________ **kJ/£**

(b) Material (excluding fuel and water)

Total raw materials used, including packaging	________________	te/y
Raw material recycled from other company operations	________________	te/y
Raw material recycled from consumer	________________	te/y
Raw material used which poses health, safety or environmental hazard (describe hazard)	________________	te/y

Total raw materials used per kg product	________________	**kg/kg**
Total raw materials used per unit value added	________________	**kg/£**
Fraction of raw materials recycled within company	________________	**kg/kg**
Fraction of raw materials recycled from consumers	________________	**kg/kg**
Hazardous raw material per kg product	________________	**kg/kg**

(c) Water

Water used in cooling	________________	te/y			
Water used in process	________________	te/y			
Other water used	________________	te/y	Total	________________	te/y
Water recycled internally				________________	te/y
Net water consumed = Total used – recycled				________________	te/y

Net water consumed per unit mass of product	________________	**kg/kg**
Net water consumed per unit value added	________________	**kg/£**

(d) Land

Land occupied by operating unit	________________	m^2 (include land needed for ALL activities)
Other land affected by unit's activities	________________	m^2 (describe effect)
Total land	________________	m^2
Land restored to original condition	________________	m^2/y

Total land occupied+affected for value added a)	________________	**m^2/(£/y)**
Rate of land restoration (restored per year /total) b)	________________	**(m^2/ y)/m^2**

Notes

a) Land affected might be, eg land used in mining raw material or in dumping waste product.

b) The areas of land occupied and affected are those at the start of the reporting period, and the land restored is that area restored during the reporting period.

3.1.2 Emissions, effluents and waste

The environmental impact categories chosen are a sub-set of those used internationally in environmental management, selected to focus on areas where the process industry's activities are most significant. The environmental burden approach (developed by ICI) is a scientifically sound way to quantify environmental performance. It draws on developments in environmental science to estimate potential environmental impact, rather than merely stating quantities of material discharged.

The environmental impact arising from use of the product must be separately assessed under the appropriate environmental impact headings and reported, see 3.1.3 (a).

Note on the calculation method (for further details see appendices A and B)

The Environmental Burden (EB) caused by the emission of a range of substances, is calculated by adding up the weighted emission of each substance. The weighting factor is known as the "potency factor". Note that because a single substance will contribute differently to different Burdens, each substance will have a number of different potency factors.

$$EB_i = \Sigma W_N \times PF_{i,N}$$

where EB_i = ith environmental burden

W_N = weight of substance N emitted, including accidental and unintentional emissions

$PF_{i,N}$ = potency factor of substance N for ith environmental burden.

The ratio indicator is then found by dividing the Environmental Burden by the value added.

(a) Atmospheric impacts (see appendix A for calculation of Environmental Burdens)

Atmospheric acidification burden per unit value added [a)]	__________	**te/£**
Global warming burden per unit value added [b)]	__________	**te/£**
Human Health burden per unit value added [c)]	__________	**te/£**
Ozone depletion burden per unit value added [d)]	__________	**te/£**
Photochemical ozone burden per unit value added [e)]	__________	**te/£**

Notes

a) Atmospheric acidification. EB is te/y sulphur dioxide equivalent.

b) Global warming. EB is te/y carbon dioxide equivalent.

c) Human health (carcinogenic) effects. EB is te/y benzene equivalent.

d) Stratospheric ozone depletion. EB is te/y CFC-11 equivalent.

e) Photochemical ozone (smog) formation. EB is te/y ethylene equivalent.

(b) Aquatic impacts (see appendix B for calculation of Environmental Burden)

Aquatic acidification per unit value added [a)]		______________	**te/£**
Aquatic oxygen demand per unit value added [b)]		______________	**te/£**
Ecotoxicity to aquatic life per unit value added [c)]	**(i) metals**	______________	**te/£**
	(ii) other	______________	**te/£**
Eutrophication per unit value added [d)]		______________	**te/£**

Notes

a) Aquatic acidification. EB is te/y of released H+ ions.

b) Aquatic oxygen demand. EB is te/y oxygen.

c) Ecotoxity to aquatic life. EB is (i) te/y copper equivalent, and (ii) te/y formaldehyde equivalent.

d) Eutrophication. EB is te/y phosphate equivalent.

(c) Impacts to Land

Total Hazardous Solid Waste Disposal ______________ te/y (describe hazard)

Total Non-Hazardous Solid Waste Disposal ______________ te/y

Hazardous solid waste per unit value added	______________	**te/£**
Non-hazardous solid waste per unit value added	______________	**te/£**

3.1.3 Additional environmental items

Also report where appropriate

a) Duty of care with respect to products and services produced. Environmental impact and mitigating steps taken. This to include issues concerning long-term environmental or health problems arising from process or product, for which the solution is not yet known.

b) Issues concerning environmental impact of plant construction and decommissioning.

c) Compliance. Magnitude and nature of penalties for non-compliance with any local, national or international environmental regulations or agreements.

d) Impacts on protected areas (Sites of Special Scientific Interest, proposed Special Areas of Conservation, National Parks). Impacts on local biodiversity or important habitats.

e) Issues concerning long-term supply of raw materials from non-renewable resources.

f) Other possible relevant metrics.

3.2 Economic indicators

A key element of sustainability is the success of industry in creating wealth. The economic indicators go somewhat further than conventional financial reporting in describing the creation of wealth or value, and in reporting its distribution and reinvestment for future growth. Both human and financial capital are considered. The social consequences of economic activity are explored further in section 3.3.

3.2.1 Profit, value and tax

Sales	________	£/y
Cost of goods, raw materials and services purchased	________	£/y
Value added	________	£/y (see note a)
Gross margin	________	£/y (see note b)
Net income before tax	________	£/y (NIBT)
Taxes (total paid to all taxing authorities)	________	£/y

Value added [a)]	________	**£/y**
Value added per unit value of sales	________	**£/£**
Value added per direct employee	________	**£/y**
Gross margin [b)] per direct employee	________	**£/y**
Return on average capital employed	________	**%/y**
Taxes paid, as percent of NIBT	________	**%**

Notes

a) Value added by the operation is the value of sales less the cost of goods, raw materials (including energy) and services purchased.

b) Gross margin is the value of sales minus all variable costs.

3.2.2 Investments

(a) Direct

Average capital employed (plant, associated infrastructure, stocks, working capital etc.)	________	£
Increase (decrease) in capital employed	________	£/y
Research and Development expenditure	________	£/y
Average number of direct employees (full-time equivalents)		
Number of new employees appointed	________	/y
Number of employees with at least 2 years of post-school education	________	(defined in note a)
Total wages expense	________	£/y
Total benefits expense	________	£/y
Payroll expense = wages + benefits Total	________	£/y
Total training expense for direct employees	________	£/y

Percentage increase (decrease) in capital employed	________	**%/y**
R&D expenditure as % sales	________	**%**
Employees with post-school qualification a)	________	**%**
New appointments/number of direct employees	________	**%/y**
Training expense as percentage of payroll expense	________	**%**

Note

a) Technicians and graduates and others who have had at least two years of education or training after leaving secondary school. They should possess a vocational qualification, degree, or similar.

(b) Indirect

Number of indirect jobs wholly dependent on operating unit (external, not on company payroll. Full-time equivalents.)	________	
Investment in education (non-employee) at all levels (schools, colleges, universities and other educational programmes)	________	*£/y*
Other philanthropy and charitable gifts and donations	________	*£/y*

Ratio of indirect jobs a)/number of direct employees	________	
Investment in education b)/employee training expense	________	**£/£**
Charitable gifts as percentage of NIBT c)	________	**%**

Notes

a) The number of indirect jobs includes contractors with supply or other contract, and also includes workers servicing the operation in any way, or in the local community, whose jobs would disappear or diminish if the operation ceased. This could include teachers, shopkeepers, transport workers, accountants etc. Report full-time equivalents.

b) This item refers to support of educational institutions and programmes not specifically for the benefit of employees. Employee education comes under the heading of training, see above.

c) This metric is a measure of the investment in the community.

3.2.3 Additional economic items

Also report where appropriate

a) Other possible relevant metrics.

3.3 Social indicators

Indicators of social performance reflect the company's attitude to treatment of its own employees, suppliers, contractors and customers, and also its impact on society at large. Good social performance is important in ensuring a company's license to operate over the longer term.

3.3.1 Workplace

(a) Employment situation

Number of employees who have resigned or been made redundant	______________	/y
Number of direct employees promoted	______________	/y
Working hours lost through absence	______________	/y
(all unplanned causes - strikes, sickness, absenteeism etc but not holiday or training)		
Indicative wage and benefit package for highest-paid 10% of employees	______________	£/y
Indicative wage and benefit package for lowest-paid 10% of employees	______________	£/y

Benefits as percentage of payroll expense	______________	%
Employee turnover (resigned+redundant/number employed)	______________	%
Promotion rate (number of promotions/number employed)	______________	%
Working hours lost as percent of total hours worked	______________	%
Income+benefit ratio (top 10%/bottom 10%)	______________	

(b) Health and safety at work

Lost time accident frequency (number per million hours worked)	______________	
Expenditure on illness and accident prevention/payroll expense	______________	**£/£**

3.3.2 Society

Number of meetings with external stakeholders concerning company operations	______	/y
Indirect benefit to the community resulting from presence of operating unit	______	£/y
Number of complaints registered from members of the public concerning the process or products	______	/y
Number of successful legal actions taken against company or employees for work-related incidents or practices	______	/y

Number of stakeholder [a)] meetings per unit value added	______	/£
Indirect community benefit [b)] per unit value added	______	£/£
Number of complaints per unit value added	______	/£
Number of legal actions per unit value added [c)]	______	/£

Note

a) External stakeholders include customers, residents and other community groups, local government, non-governmental organizations (NGO's). This metric represents company efforts in communicating with external stakeholders.

b) A major social benefit arising from the presence of a successful process industry unit is the dissemination of skills and know-how which are used in the community to create wealth and enhance quality of life. It is difficult to quantify these benefits, but estimates may be made. We suggest to include items such as

i) Net value to community of freely published information and know-how

ii) Net value to community of training given to contractors and suppliers

iii) Net value to community of training given to (ex-)employees.

These estimates of value should not include direct benefits which have already been included in section 3.2.2. Value may be estimated by considering what it has cost the company to generate the benefit on the one hand, and what society might be willing to pay for it on the other.

c) This metric is a measure of antisocial behaviour.

3.3.3 Additional items

Also report where appropriate

a) Issues concerning discrimination, concerning women and minorities or indigenous communities, the number in senior and middle management; programmes to improve employability including focused education or training, and mentoring.

b) Incidents of child labour, forced labour or violation of human rights, on the part of the company, its suppliers or contractors, and public protest concerning such issues. Report positive steps taken in this regard.

c)Performance of suppliers and contractors relative to criteria for their selection. Incidents of non-compliance with sustainability requirements, eg Responsible Purchasing.

d) Other possible relevant metrics.

APPENDIX A

ENVIRONMENTAL BURDENS FOR EMISSIONS TO AIR

Atmospheric Acidification

Substance	Potency Factor PF	Emissions	
		Tonnes W	EB value = W x PF
SO_2	1		
Ammonia	1.88		
HCl	0.88		
HF	1.6		
NO_2	0.7		
H_2SO_4 mist	0.65		
Total			

The potential of certain released gases to form acid rain and acids to water is the potency factor for atmospheric acidification. The unit of Environmental Burden is te/y sulphur dioxide equivalent.

Global Warming

Substance	Potency Factor PF	Emissions	
		Tonnes W	EB value = W x PF
Carbon dioxide	1		
Carbon monoxide	3		
Carbon tetrachloride	1,400		
Chlorodifluoromethane, R22	1,700		
Chloroform	4		
Chloropentafluoroethane, R115	9,300		
Dichlorodifluoromethane, R12	8,500		
Dichlorotetrafluoroethane, R114	9,300		
Difluoroethane	140		
Hexafluoroethane	9,200		
Methane	21		
Methylene chloride	9		
Nitrous Oxide	310		
Nitrogen Oxides (NOx)	40		
Pentafluoroethane, R125	2,800		
Perfluoromethane	6,500		
Tetrafluoroethane	1,300		
Trichloroethane (1,1,1)	110		
Trichlorofluoromethane, R11	4,000		
Trichlorotrifluoroethane, R113	5,000		
Trifluoroethane, R143a	3,800		
Trifluoromethane, R23	11,700		
Volatile Organic Compounds	11		
Total			

These potency factors are based on a 100-year integrated time horizon. The unit of Environmental Burden is te/y carbon dioxide equivalent – the global warming potential.

Human Health (carcinogenic) Effects
Unlike Global Warming, there are no internationally accepted potency factors for Human Health. For this reason, carcinogenic effects are offered as a default set but companies are encouraged to use other sets if they are more appropriate.

The potency factor for this category in the table below has been derived from the reciprocal of the Occupational Exposure Limits (OEL) set by the UK Health and Safety Executive. The OEL for benzene has been chosen as the normalizing factor for this category. For other chemicals take the OEL in mg m-3, calculate the reciprocal and divide it by the reciprocal of the OEL for benzene (0.0625) i.e. $PF_{substance} = (OEL_{benzene}/OEL_{substance})$.

Chemicals with an OEL greater than 500 mg m^{-3} will have a minimal impact on the total weighted impact.

The unit of Environmental Burden is te/y benzene equivalent.

Substance	CAS Number	Potency Factor PF	Emissions	
			Tonnes W	EB value = W x PF
Acrylamide	79-06-1	53.3		
Acrylonitrile	107-13-1	3.6		
Antimony & compounds except stibine, as Sb	7440-36-0	32		
Arsenic & compounds except arsine, as As	7440-38-0	160		
Azodicarbonate	123-77-3	16		
Benzene	71-43-2	1		
Berylium & Compounds		8000		
Bis (chloromethyl) ether	542-88-1	3200		
Buta-1,3-diene	106-99-0	0.73		
Cadmium & Compounds		640		
Cadmium oxide fume	1306-19-0	640		
Carbon disulphide	136-23-6	0.5		
1-Chloro-2,3-epoxypropane	106-89-8	8.4		
Chromium (VI) compounds		320		
Cobalt & Compounds		160		
Cotton dust		6.4		
1,2-dibromoethane	106-93-4	4.1		
1,2-dichloroethane	107-06-2	0.76		
Dichloromethane	75-09-2	0.05		
2-2′-Dichloro-4,4′-methylene dianiline (MbOCA)	101-14-4	3200		
Diethyl sulphate	64-67-5	50		
Dimethyl sulphate	77-78-1	3.8		
2-Ethoxyethanol	110-80-5	0.43		
2-Ethoxyethyl acetate	111-15-9	0.3		
Ethylene oxide	75-21-8	1.7		
Formaldehyde	50-00-0	6.4		
Grain dust		1.6		
Hardwood dust		3.2		
Hydrazine	30-07-2	533.3		
Iodomethane	74-88-4	1.3		
Isocyanates, all		800		
Maleic anhydride	108-31-6	16		
Man-made mineral fibre		3.2		
2-Methoxyethanol	109-86-4	1		
2-Methoxyethyl acetate	110-49-6	0.64		
4-4′-methylenedianiline	101-77-9	200		
Nickel & inorganic compounds		160		

2-Nitropropane	79-46-9	0.8		
Phthalic anhydride	85-44-9	4		
Polychlorinated biphenyls (PCB)	1336-36-3	160		
Propylene oxide	75-56-9	1.33		
Rubber fume		26.7		
Rubber process dust		2.6		
Silica respirable crystalline		53.3		
Softwood dust		3.2		
Styrene	100-42-5	0.04		
o-Toluidine	95-53-4	18		
Triglycidyl isocyanurate (TGIC)	2451-62-9	160		
Trimellite anhydride	552-30-7	400		
Vinylidene chloride	75-35-4	0.4		
Wool process dust		1.6		
Softwood dust		3.2		
Total				

Stratospheric Ozone Depletion
The potency factor for this category is based on the potential to deplete ozone in the upper atmosphere relative to chlorofluorocarbon – 11 (ODP - the ozone depletion potential). The unit of Environmental Burden is te/y CFC-11 equivalent (CFC-11 is trichlorofluoromethane).

Substance	Potency Factor PF	Emissions	
		Tonnes W	EB value = W x PF
CFC - 11	1.0		
CFC - 12	1.0		
CFC - 113	0.8		
CFC - 114	1.0		
CFC - 115	0.6		
CFC - 13	1.0		
CFC - 111	1.0		
CFC - 112	1.0		
CFC - 212	1.0		
CFC - 213	1.0		
CFC - 214	1.0		
CFC - 215	1.0		
CFC - 216	1.0		
CFC - 217	1.0		
halon-1211	3.0		
halon-1301	10.0		
halon-2402	6.0		
Carbon tetrachloride	1.1		
1,1,1-trichloroethane	0.1		
Methyl bromide	0.7		
HCFC-21	0.04		
HCFC-22	0.055		
HCFC-31	0.02		
HCFC-121	0.04		

HCFC-122	0.08		
HCFC-123 (3)	0.02		
HCFC-124 (3)	0.022		
HCFC-131	0.05		
HCFC-132	0.05		
HCFC-133	0.06		
HCFC-141	0.07		
HCFC-141b (3)	0.11		
HCFC-142	0.07		
HCFC-142b (3)	0.065		
HCFC-151	0.005		
HCFC-221	0.07		
HCFC-222	0.09		
HCFC-223	0.08		
HCFC-224	0.09		
HCFC-225	0.07		
HCFC-225ca (3)	0.025		
HCFC-225cb (3)	0.033		
HCFC-226	0.1		
HCFC-231	0.09		
HCFC-232	0.1		
HCFC-233	0.23		
HCFC-234	0.28		
HCFC-235	0.52		
HCFC-241	0.09		
HCFC-242	0.13		
HCFC-243	0.12		
HCFC-244	0.14		
HCFC-251	0.01		
HCFC-252	0.04		
HCFC-253	0.03		
HCFC-261	0.02		
HCFC-262	0.02		
HCFC-271	0.03		
Total			

Photochemical Ozone (smog) Formation

Potency factors for this category are obtained from the potential of substances to create ozone photochemically. The unit of Environmental Burden is te/y ethylene equivalent.

Substance	Potency Factor PF	Emissions	
		Tonnes W	EB value = W x PF
Alkanes			
Methane	0.034		
Ethane	0.14		
Propane	0.411		
n-Butane	0.6		
i-Butane	0.426		

n-Pentane	0.624		
i-Pentane	0.598		
n-Hexane	0.648		
2-Methylpentane	0.778		
3-Methylpentane	0.661		
2,2-Dimethylbutane	0.321		
2,3-Dimethylbutane	0.943		
n-heptane	0.77		
2-Methylhexane	0.719		
3-Methylhexane	0.73		
n-Octane	0.682		
2-Methylheptane	0.694		
n-Nonane	0.693		
2-Methyloctane	0.706		
n-Decane	0.680		
2-Methylnonane	0.657		
n-Undecane	0.616		
n-Dodecane	0.577		
Cyclohexane	0.595		
Methyl cyclohexane	0.732		
Alkenes			
Ethylene	1.0		
Propylene	1.08		
1-Butene	1.13		
2-Butene	0.99		
2-Pentene	0.95		
1-Pentene	1.04		
2-Methylbut-1-ene	0.83		
3-Methylbut-1-ene	1.18		
2-Methylbut-2-ene	0.77		
Butylene	0.703		
Isoprene	1.18		
Styrene	0.077		
Alkynes			
Acetylene	0.28		
Aromatics			
Benzene	0.334		
Toluene	0.771		
o- Xylene	0.831		
m-Xylene	.08		
p- Xylene	0.948		
Ethylbenzene	0.808		
n-Propylbenzene	0.713		
i-Propylbenzene	0.744		
1,2,3-Trimethylbenzene	1.245		
1,2,4- Trimethylbenzene	1.324		
1,3,5- Trimethylbenzene	1.299		
o-Ethyltoluene	0.846		
m-Ethyltoluene	0.985		
p-Ethyltoluene	0.935		

3,5-Dimethylethylbenzene	1.242		
3,5-Diethyltoluene	1.195		
Aldehydes			
Formalhyde	0.554		
Acetaldehyde	0.65		
Propionaldehyde	0.755		
Butyraldehyde	0.77		
i-Butyraldehyde	0.855		
Valeraldehyde	0.887		
Benzaldehyde	-0.056*		
Ketones			
Acetone	0.182		
Methylethylketone	0.511		
Methyl- i -butylketone	0.843		
Cyclohexanone	0.529		
Alcohols			
Methyl alcohol	0.205		
Ethyl alcohol	0.446		
i-Propanol	0.216		
n-Butanol	0.628		
i-Butanol	0.591		
s-Butanol	0.468		
t-Butanol	0.191		
Diacetone alcohol	0.617		
Cyclohexanol	0.622		
Esters			
Methyl acetate	0.046		
Ethyl acetate	0.328		
n-Propyl acetate	0.481		
i-Propyl acetate	0.291		
n-Butyl acetate	0.511		
s-Butyl acetate	0.452		
Organic Acids			
Formic acid	0.003		
Acetic acid	0.156		
Propionic acid	0.035		
Ethers			
Butyl glycol	0.629		
Propylene glycol methyl ether	0.518		
Dimethyl ether	0.263		
Methyl- t -butyl ether	0.268		
Halocarbons			
Methyl chloride	0.035		
Methylene chloride	0.031		
Methylchloroform	0.002		
Tetrachloroethylene	0.035		
Trichloroethylene	0.075		
Vinyl chloride	0.272		
1,1-Dichloroethylene	0.232		
cis 1,2- Dichloroethylene	0.172		

trans 1,2- Dichloroethylene	0.101		
Other Pollutants			
Nitric oxide	-0.427*		
Nitrogen dioxide	0.028		
Sulphur dioxide	0.048		
Carbon monoxide	0.027		
Total			

* *The negative values imply the ability to reduce photochemical ozone production.*

APPENDIX B

ENVIRONMENTAL BURDENS FOR EMISSIONS TO WATER

Aquatic Acidification

Substance	Potency Factor PF	Emissions	
		Tonnes W	EB value = W x PF
Sulphuric acid	0.02		
Hydrochloric acid	0.027		
Hydrogen fluoride	0.05		
Acetic acid	0.02		
Total			

The potency factor is the mass of hydrogen ion released by unit mass of acid i.e. the number of hydrogen ions released divided by the molecular weight. The unit of Environmental Burden is te/y of H+ ions released.

The calculation of the H+ ion is the preferred method of deriving the potency factor in this category, however measured pH values may also be used.

Aquatic Oxygen Demand

Substance	Potency Factor PF	Emissions	
		Tonnes W	EB value = W x PF
Acetic acid	1.07		
Acetone	2.09		
Ammonium nitrate in solution	0.8		
Ammonium sulphate in solution	1		
Chlorotrifluoroethane	0.54		
1,2 – Dichloroethane (EDC)	0.81		
Ethylene	1		
Ethylene glycol	1.29		
Ferrous ion	0.14		
Methanol	1.5		
Methyl methacrylate	1.5		
Methylene Chloride	0.47		
Phenol	2.38		
Vinyl chloride	1.28		
Total			

The Stoichiometric Oxygen Demand (StOD) has been chosen as the potency factor. It represents the maximum potential of emissions to water to remove dissolved oxygen that would otherwise support fish and other aquatic life. StOD is expressed as tonnes of oxygen required per tonne of substance. The unit of Environmental Burden is te/y oxygen.

An alternative potency factor is Chemical Oxygen Demand (COD).

Calculation of the Stoichiometric Oxygen Demand (StOD)
From knowledge of the chemical structure, calculate the empirical formula as follows:

$C_cH_hN_nCl_{Cl}Na_{Na}O_oP_pS_s$

Then calculate the StOD in te O_2 per te of substance from the equation:

StOD = 16(2c+0.5(h-Cl)+2.5n+3s+2.5p+0.5Na - o)/Molecular Weight

This equation assumes that nitrogen is oxidized and eventually released as the nitrate ion (NO_3-). It is assumed that carbon is mineralized to CO_2, hydrogen (H) to H_2O, phosphorus (P) to P_2O, sodium (Na) to Na_2O, sulphur (S) to SO_2 and halides (represented by Cl) to their respective acids. The compounds described after oxidation are those specified by international convention for calculating oxygen demand.

For example, Acetic acid CH_3COOH with a molecular weight of 60

StOD = 16(2´2 + 0.5´4 - 2)/60 = 1.07 te O_2 per te acetic acid

Another example, Phenol C6H5OH with a molecular weight of 94

StOD = 16(2´6 + 0.5´6 - 1)/94 = 2.38 te O_2 per te of phenol

For ionic species the calculation must take into account the charge of the ionic unit. For the ammonium ion (NH4+), for example, we remove an H+ ion and calculate on the NH3, so that the ionic balance is not disturbed.

StOD = 16(0.5x3 + 2.5x1)/17 = 3.76 te O_2 per te of ammonia

= 3.56 te O_2 per te of ammonium ion

Ecotoxicity to Aquatic Life
(values for sea water conditions)

(i) Metals

Substance	Potency Factor PF	Emissions	
		Tonnes W	EB value = W x PF
Arsenic	0.2		
Cadmium	2.0		
Chromium	0.33		
Copper	1		
Iron	0.005		
Lead	0.2		
Manganese	0.1		
Mercury	16.67		
Nickel	0.17		
Vanadium	0.05		
Zinc	0.125		
Total			

The potency factor is equal to the reciprocal of the Environmental Quality Standard (EQS) divided by the reciprocal of the EQS of copper. The unit of Environmental Burden is te/y copper equivalent.

(ii) Other Substances

Substance	Potency Factor PF	Emissions	
		Tonnes W	EB value = W x PF
Ammonia	0.24		
Benzene	0.17		
Carbon tetrachloride	0.42		
Chloride	0.5		
Chlorobenzene	1.0		
Chloroform	0.42		
Cyanide	1.0		
1,2-Dichloroethane (EDC)	0.5		
Formaldehyde	1.0		
Hexachlorobenzene	166.67		
Hexachlorobutadiene	50		
Methylene chloride	0.5		
Nitrobenzene	0.25		
Nitrophenol	0.5		
Toluene	0.125		
Tetrachloroethylene (PER)	0.5		
Trichloroethylene (TRI)	0.5		
Xylenes	0.17		
Total			

The above potency factors are equal to the reciprocal of the Environment Quality Standard (EQS) divided by the reciprocal of the EQS of formaldehyde. The unit of Environmental Burden is te/y formaldehyde equivalent.

Eutrophication

Substance	Potency Factor PF	Emissions	
		Tonnes W	EB value = W ´ PF
NO_2	0.2		
NO	0.13		
NO_x	0.13		
Ammonia	0.33		
Nitrogen	0.42		
PO_4 (III-)	1		
Phosphorus	3.06		
COD	0.022		
Total			

Eutrophication is defined as the potential for over-fertilisation of water and soil, which can result in increased growth of biomass. The species above are those considered to be responsible for eutrophication. The unit of Environmental Burden is te/y phosphate equivalent.

APPENDIX C

REPORT FORM

Name of company and unit:	
Contact person:	Job Title:
Address:	
Phone and fax numbers:	Email address:

Period covered by the report:

Signed:
Place:
Date:

This page containing company information will be kept by IChemE separately from the following report. The reported data and metrics will thus be anonymous, providing respondents themselves do not reveal their identity in the report.

Report

1	Profile: statement attached	Yes ❑	No ❑
2	Summary: statement attached	Yes ❑	No ❑
3	Vision and strategy: statement attached	Yes ❑	No ❑
4	Policy and organisation: statement attached	Yes ❑	No ❑
5	Performance: statement attached	Yes ❑	No ❑

Metrics should be reported below.

Resource usage

Total Net Primary Energy Usage rate = Imports – Exports	________	GJ/y
Percentage Total Net Primary Energy sourced from renewables	________	%
Total Net Primary Energy Usage per kg product	________	kJ/kg
Total Net Primary Energy Usage per unit value added	________	kJ/£
Total raw materials used per kg product	________	kg/kg
Total raw materials used per unit value added	________	kg/£
Fraction of raw materials recycled within company	________	kg/kg
Fraction of raw materials recycled from consumers	________	kg/kg
Hazardous raw material per kg product	________	kg/kg

Describe hazard

Net water consumed per unit mass of product	________	kg/kg
Net water consumed per unit value added	________	kg/£
Total land occupied+affected for value added	________	$m^2/(£/y)$

Describe effect

Rate of land restoration (restored per year /total)	________	$(m^2/y)/m^2$

Emissions, effluents and waste

Atmospheric acidification burden per unit value added	________	te/£
Global warming burden per unit value added	________	te/£
Human Health burden per unit value added	________	te/£
Ozone depletion burden per unit value added	________	te/£

Photochemical ozone burden per unit value added	____________	te/£
Aquatic acidification per unit value added	____________	te/£
Aquatic oxygen demand per unit value added	____________	te/£
Ecotoxicity to aquatic life per unit value added (i) metals	____________	te/£
(ii) other	____________	te/£
Eutrophication per unit value added	____________	te/£
Hazardous solid waste per unit value added	____________	te/£

Describe hazard

Non-hazardous solid waste per unit value added	____________	te/£

Additional environmental items
Statement attached Yes ❑ No ❑

Profit, value and tax

Value added	____________	£/y
Value added per unit value of sales	____________	£/£
Value added per direct employee	____________	£/y
Gross margin per direct employee	____________	£/y
Return on average capital employed	____________	%/y
Taxes paid, as percent of NIBT	____________	%

Investments

Percentage increase (decrease) in capital employed	____________	%
R&D expenditure as % sales	____________	%
Employees with post-school qualification	____________	%
New appointments/number of direct employees	____________	%
Training expense as percentage of payroll expense	____________	%
Ratio of indirect jobs/number of direct employees		
Investment in education/employee training expense	____________	£/£
Charitable giving as percentage of NIBT	____________	%

Additional economic items
Statement attached Yes ❑ No ❑

Workplace

Benefits as percentage of payroll expense ____________ %

Employee turnover (resigned+redundant/number employed) ____________ %

Promotion rate (number of promotions/number employed) ____________ %

Working hours lost as percent of total hours worked ____________ %

Income+benefit ratio (top 10%/bottom 10%)

Lost time accident frequency (number per million hours worked)

Expenditure on illness and accident prevention/payroll expense ____________ £/£

Society

Number of stakeholder meetings per unit value added ____________ /£

Indirect community benefit per unit value added ____________ £/£

Number of complaints per unit value added ____________ /£

Number of legal actions per unit value added ____________ /£

Additional social items

Statement attached Yes ❑ No ❑

Produced by the Sustainable Development Working Group of the Institution of Chemical Engineers

The leading professional body

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