Part II

Tools

Biorefineries and Chemical Processes: Design, Integration and Sustainability Analysis, First Edition.
Jhuma Sadhukhan, Kok Siew Ng and Elias Martinez Hernandez.

Companion Website: http://www.wiley.com/go/sadhukhan/biorefineries

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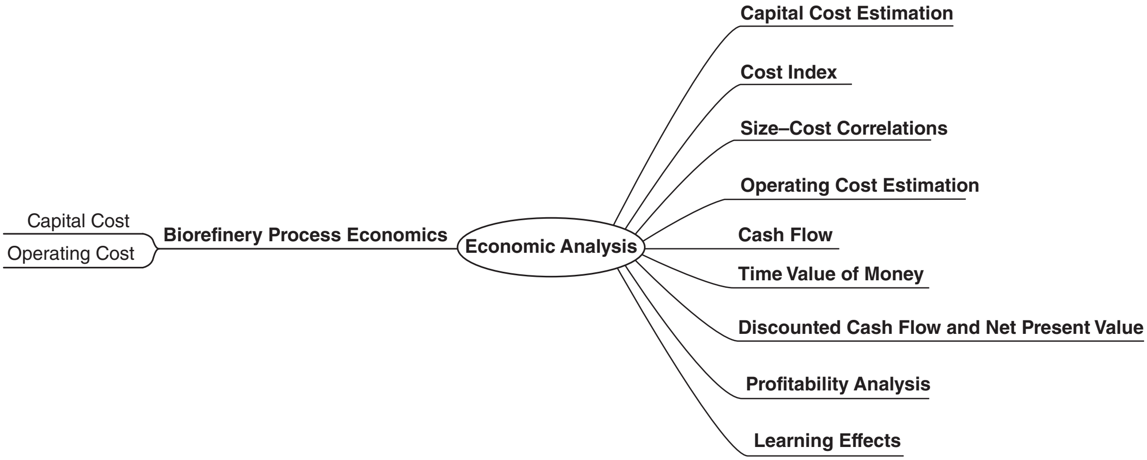
Economic Analysis



Structure for Lecture Planning

2.1 Introduction

Process economics is one of the crucial aspects for evaluation of process designs. It is often the main criterion in justifying the feasibility of a new design or modification of a plant. Many biomass based technologies are not yet widely employed. This is primarily attributed to the high capital investment and operating costs associated with these technologies, and thus they are less competitive compared to the fossil fuel based technologies. Therefore, it is highly essential to master the skills of performing a proper economic evaluation of a biorefinery plant design in order to gain deeper insights and achieve a better outcome in terms of economics and optimal designs.

This chapter discusses the fundamental concepts of economics germane to chemical engineering process design (Section 2.2) and the methodology for performing economic analysis of process technologies (Section 2.3). The correlation and cost data information of biorefinery design options (Section 2.4) are also shown.

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The learning outcomes from this chapter are as follows.

- To assimilate the fundamental economic terminologies and concepts.
- To perform a capital and operating costs evaluation using the standard techniques, equations, graphs, cost correlations and factors.
- To use economic criteria such as economic potential and netback to justify the economic viability of a design.

2.2 General Economic Concepts and Terminology

2.2.1 Capital Cost and Battery Limits

Capital cost is the cost for building a plant. It can be categorized into two parts: direct and indirect capital costs. Direct capital costs refer to the purchased and installation costs of equipment for constructing a plant. The cost data and correlation for standard equipment can be obtained from various sources including (1) website: *Matches' Process Equipment Cost Estimates*, www.matche.com; (2) reference books: *Coulson & Richardson's Chemical Engineering Design Volume 6, Product & Process Design Principles* and *Guide to Capital Cost Estimating* published by the Institute of Chemical Engineers (IChemE); (3) peer-reviewed archived journals. Most of the equipment costs provided in the literature are the free-on-board (f.o.b.) purchased cost. This means that the delivery cost of equipment is not included. The equipment cost is also influenced by various factors, namely, material of construction, pressure and temperature. These factors need to be considered for each piece of equipment by multiplying the correction factors. The geographical location of a plant is also a highly influential factor for the capital cost due to variations in local regulations, labor, taxes, cost of transportation, etc. A correction factor, if available, should be applied to account for such variations.

Battery limit is used to classify direct capital cost. Inside battery limits (ISBL) comprise the cost of purchasing and installation of major process equipment such as reactors, separators and gas turbines, etc. Other supporting facilities such as utilities and services are considered as outside battery limits (OSBL). Indirect capital costs refer to the design and engineering costs for building a site, contractor's fees and contingency allowances (costs forecasted for some unforeseen circumstances). These are estimated by taking a certain factor on top of the direct capital costs. Working capital should also be included in the capital cost evaluation. It is the cost required for the acquisition of raw materials during the initial start-up stage of a plant, until the plant becomes productive or makes money.

2.2.2 Cost Index

The cost data of equipment obtained for a year is only valid for that particular year. Costs vary with time. Therefore, the cost index method is applied, as shown below for updating the cost taken from previous years and to be used in the current cost analysis:

$$C_{pr} = C_o \left(\frac{I_{pr}}{I_o} \right) \tag{2.1}$$

where

C_{pr} is the present cost
C_o is the original cost
I_{pr} is the present index value
I_o is the original index value.

Many methods to estimate the cost index are available, such as the Chemical Engineering Plant Cost Index (CEPCI), the Marshall and Swift (M&S) Equipment Cost Index, the Nelson-Farrar–(NF) Refinery Construction Cost Index and the Engineering New-Record (ENR) Construction Cost Index. These include the cost index for equipment, labor, engineering and supervision, etc. The Chemical Engineering Plant Cost Index (CEPCI) and the Marshall and Swift (M&S) Equipment Cost Index are used for the cost estimation of biorefineries. Both cost indices are published monthly in *Chemical Engineering*. Figure 2.1 shows the annual CEPCI from year 1996 to 2010.

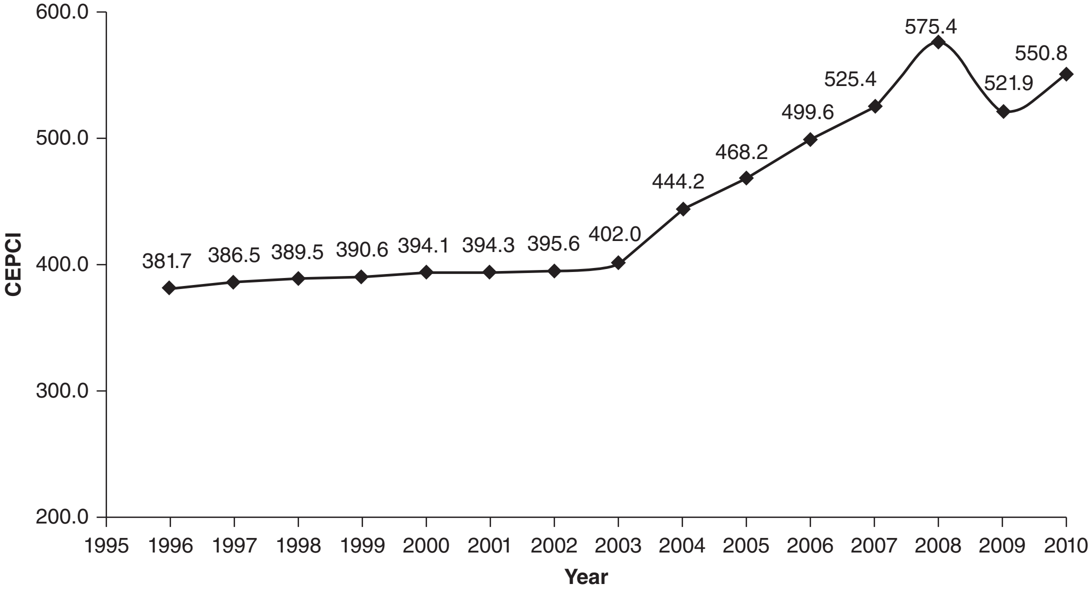

Figure 2.1 *Annual Chemical Engineering Plant Cost Index (CEPCI) from year 1996 to 2010.*

Exercise 1. Calculate the capital cost of two boiler units in year 2010 (CEPCI: 550.8), if the capital cost of one unit was \$0.345 million in year 1998 (CEPCI: 389.5).

Solution to Exercise 1. Using Equation (2.1), the capital cost of one boiler in year 2010 is

$$\begin{aligned} C_{pr} &= C_o\left(\frac{I_{pr}}{I_o}\right) \\ &= 0.345 \times \left(\frac{550.8}{389.5}\right) \\ &= \$0.488 \text{ million} \end{aligned}$$

Hence, two boilers cost: 2 × \$0.488 million = **\$0.976 million** in year 2010.

2.2.3 Economies of Scale

A scaling factor R is applied to estimate the cost of a system based on the known cost of the system for a different size, as shown below. This relationship assumes that the equipment or unit operations can be scaled up/down. The maximum size limit is normally given and multiple units have to be taken into account if the size of the unit exceeds the maximum size.

$$\frac{COST_{size2}}{COST_{size1}} = \left(\frac{SIZE_2}{SIZE_1}\right)^R \tag{2.2}$$

where

$SIZE_1$ is the capacity of the base system
$COST_{size1}$ is the cost of the base system
$SIZE_2$ is the capacity of the system after scaling up/down
$COST_{size2}$ is the cost of the system after scaling up/down
R is the scaling factor.

Exercise 2. Calculate the capital cost of two water gas shift reactors in million $ for a flow rate of 942 kmol h^{-1} through each reactor. The known capital cost of $40.59 million was obtained for a flow rate of 15 600 kmol h^{-1} through one reactor. The scaling factor is 0.85.

Solution to Exercise 2. Using Equation (2.2), the capital cost of one water gas shift reactor in million $ is as follows:

$$\frac{COST_{size2}}{COST_{size1}} = \left(\frac{SIZE_2}{SIZE_1}\right)^R$$

$$COST_{size2} = 40.59 \times \left(\frac{942}{15600}\right)^{0.85} = \$3.73 \text{ million}$$

Hence, the capital cost of two water gas shift reactors is 2 × 3.73 = **$7.46 million**.

2.2.4 Operating Cost

The operating costs can be classified into two main categories: fixed and variable operating costs. Fixed operating costs are independent of the production rate and quantity, in contrast to variable operating costs. These include the costs of maintenance, labor, taxation, insurance, royalties, etc. Fixed operating costs are estimated using factors that are normally based on indirect capital costs. Variable operating costs consist of the costs of raw materials, utilities, etc. The sum of fixed and variable operating costs is the direct production costs (DPCs) of a plant. Other costs such as the costs of research and development, sales expenses and general overheads are added as % of DPC to obtain the total operating cost.

Variable operating costs include the costs of raw materials (e.g., feedstock, catalyst, solvent, etc.) and utilities (e.g., electricity, steam, cooling water, etc.). The costs of raw materials and prices of products are highly volatile, vary with time and thus have the largest impact on the economic performance of a plant in most cases. These values can be obtained from business information providers such as *ICIS Pricing* and *IHS Chemical Week*. The costs of utilities also contribute to a major part of the variable operating costs. These costs vary across organizations. Thus to obtain relevant results, specific information must be collected from associated utility providers.

Table 2.1 shows the factors associated with the fixed cost and other DPC specifications.

Table 2.1 *Cost estimation of fixed operating cost. (Reproduced with permission from Sinnott (2006)[1]. Copyright © 2006, Elsevier: Butterworth-Heinemann.)*

No.	Specification	Cost Estimation
	Fixed Operating Costs	
1	Maintenance	5–10% of indirect capital cost
2	Personnel	See "labor cost" in Section 2.4.2
3	Laboratory costs	20–23% of (2)
4	Supervision	20% of (2)
5	Plant overheads	50% of (2)
6	Capital charges	10% of indirect capital cost
7	Insurance	1% of indirect capital cost
8	Local taxes	2% of indirect capital cost
9	Royalties	1% of indirect capital cost
Direct Production Cost (DPC) = Variable + Fixed Operating Costs		
10	Sales expense	20–30% of DPC
11	General overheads	
12	Research and development	
	Total operating cost = 1.2 or 1.3 times the DPC	

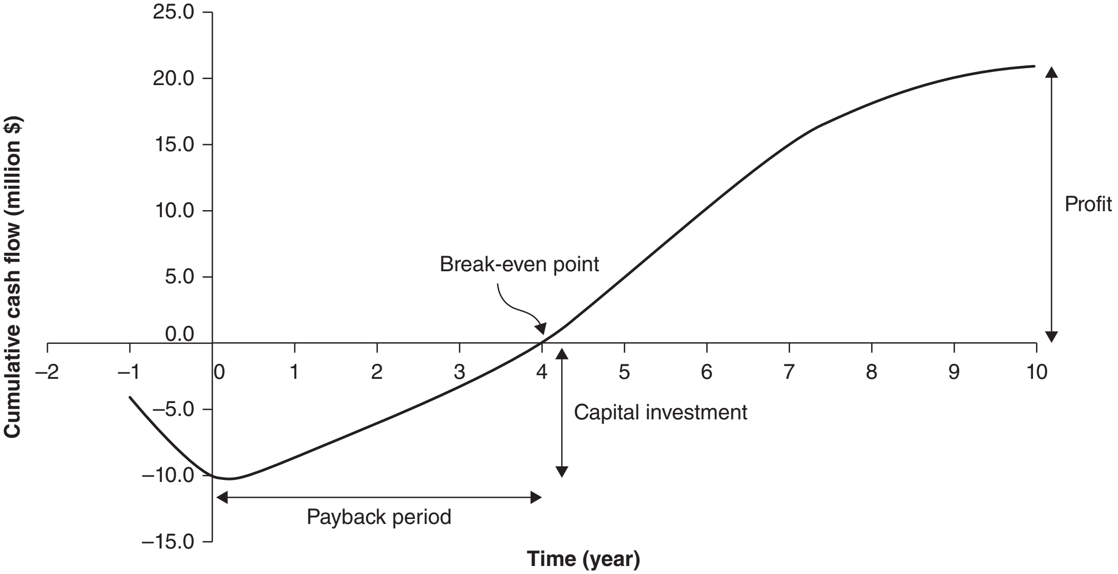

Figure 2.2 Typical cash flow diagram.

2.2.5 Cash Flows

An organization runs its everyday business by relying on a sustainable cash flow. It is thus crucial to understand the input and output of the money flows within an organization. A cash flow diagram, Figure 2.2, shows the capital investment during the initial start-up period (year −1 and 0) and the net cash flow. The net cash flow accounts for the earnings and expenditure over a project lifetime. The process begins at the end of year 0, with a variable yet increasing income until the profits stabilize at around a net cash flow. This relates to the equipment lifespan, increasing production costs and also the market value of the products. The cumulative cash flow remains negative until all the capital investment is reimbursed; this period of time is known as the *payback period*. The cumulative cash flow becomes positive as soon as the plant receives a net positive cash flow from selling products (starting from year 4 in the figure). Having a shorter payback period corresponds to an economically more viable design.

2.2.6 Time Value of Money

The "time value of money" reflects that the present value of money is worthier than the future value of money. For example, \$100 cash that you receive today would have the same amount as the \$100 you would receive after two years, but the "worthiness" of the money is different. If you invest \$100 in a bank at present, you will eventually be getting more than \$100 after two years, due to the addition of the interest paid by the bank. The relationship between present and future values is shown by

$$PV = \frac{FV}{(1+r)^n} \tag{2.3}$$

where

PV is the present value
FV is the future value
r is the discount rate or interest rate
n is the number of years of investment.

By taking an interest rate of 15% each year, an initial investment of \$100 (present value) will become $\$100 \times (1 + 0.15)^2 = \$132.25$ (future value) after two years. The present value is lower than the future value since the money at present is more valuable than in the future. This is the reason for using the discount rate to predict the "worthiness" of the future money in the present context.

Did you know?

If you win a lottery, it is better to redeem the whole lump sum of money now rather than receiving numerous payments over a few years. This is because the value of the money at present is greater than in the future and the money will depreciate over time. Your money will "shrink"!

2.2.7 Discounted Cash Flow Analysis and Net Present Value

A discounted cash flow (*DCF*) analysis is a method to evaluate the economic potential of an investment, where the projected future value of the cash flow based on capital investment is converted into its present value by applying a discount rate. This analysis considers the aforementioned time value of money.

The cumulative discounted cash flow is expressed as the net present value (*NPV*) in the *DCF* analysis. *NPV* is calculated using the following equation, where C_f is the cash flow in a particular year and T_{PL} is the plant life:

$$NPV = \sum_{n=0}^{n=T_{PL}} \frac{C_f}{(1+r)^n} \tag{2.4}$$

An example of *DCF* analysis is shown in Table 2.2. In this example, the capital investment is assumed to be \$10 million and the cost is distributed over two years, that is, year −1 and 0, by 40% and 60% of the total capital investment, respectively.

In general, *NPV* also serves as an indicator for the profit of a project and thus deciding the feasibility of a particular project; for example, $NPV > 0$ means that the project can bring profits, $NPV < 0$ will result in a loss while $NPV = 0$ represents neither gain nor loss. See Equation (6.7) for a further discussion on calculation of the DCF analysis.

Table 2.2 *An example of DCF analysis for a plant life of 10 years and annual discount rate of 15%.*

Year	Cash Flow (million \$)	Discounted Cash Flow (million \$)	*NPV* (million \$)
−1	−4.0	−4.0	−4.0
0	−6.0	−6.0	−10.0
1	1.5	1.3	−8.7
2	2.5	1.9	−6.8
3	2.8	1.8	−5.0
4	3.2	1.8	−3.1
5	5.0	2.5	−0.6
6	5.0	2.2	1.5
7	5.0	1.9	3.4
8	3.0	1.0	4.4
9	2.0	0.6	4.9
10	1.0	0.2	5.2

Did you know?

Discounted cash flow is strongly associated with our everyday lives. The calculations of the repayments of home mortgage, car loan and credit card are a few applications of discounted cash flow analysis.

Exercise 3. Andy is applying for a housing mortgage from a bank. He intends to borrow $300 000 where the current annual interest rate offered is 4.0%. The repayment period he has chosen is 30 years with a fixed rate scheme. How much does Andy have to pay monthly? The financial advisor of the bank suggested that he should choose a repayment period of 20 years. What is the benefit of having a shorter repayment period?

Solution to Exercise 3. There are 360 payments in total that need to be made over a 30 year period, that is, 1 year = 12 months. Monthly interest rate is 4/12 = 0.333%.

Method 1. By using the *DCF* method shown in Table 2.2, applying Equation (2.4) and setting $NPV = 0$ at the end of 30 years

or

Method 2. Using the PMT function in Excel, that is, = PMT(0.04/12, 360, −300 000)

Note that the PMT function is a Financial function in Excel that can be used for calculating the periodic payment for a loan based on constant payments and a constant interest rate.

or

Method 3. Using formula

$$\text{Monthly instalment, } M = \frac{P \times r \times (1+r)^N}{[(1+r)^N] - 1} = \frac{P \times \left(\frac{i}{q}\right) \times \left(1 + \frac{i}{q}\right)^N}{\left[\left(1 + \frac{i}{q}\right)^N\right] - 1} \tag{2.5}$$

where

P is the principal of the loan
$r = i/q$, i is the annual interest rate and q is the number of payments a year
N is the number of payments in total.

$$\text{Monthly instalment, } M, \text{ for 30 years} = \frac{300\,000 \times \left(\frac{0.04}{12}\right) \times \left(1 + \frac{0.04}{12}\right)^{360}}{\left[\left(1 + \frac{0.04}{12}\right)^{360}\right] - 1} = \$1432.25$$

There are a total 240 payments that need to be made over the 20 years period, that is, 1 year = 12 months. The monthly interest rate is 4/12 = 0.333%.

$$\text{Monthly instalment, } M \text{ for 20 years} = \frac{300\,000 \times \left(\frac{0.04}{12}\right) \times \left(1 + \frac{0.04}{12}\right)^{240}}{\left[\left(1 + \frac{0.04}{12}\right)^{240}\right] - 1} = \$1817.94$$

The monthly repayment for the 30 years period is estimated to be **\$1432.25**.
If the 20 years repayment period is chosen, the monthly repayment would be **\$1817.94**.
Total interest paid can be determined using

$$\text{Total interest paid, } I_T = (M \times n \times q) - P \tag{2.6}$$

$$\text{Total interest paid, } I_T \text{ for 30 years} = (1432.25 \times 30 \times 12) - 300\,000 = \$215\,610$$

$$\text{Total interest paid, } I_T \text{ for 20 years} = (1817.94 \times 20 \times 12) - 300\,000 = \$136\,305.60$$

The total amount of interest paid over 30 years and 20 years are **\$215 610** and **\$136 305.60**, respectively. Therefore, the financial advisor was right! A shorter repayment period will incur less amount of interest. In this case, **\$79 304.40** savings can be achieved.

Note that the monthly instalment is also known as the EMI (equated monthly instalment). Sometimes, processing fees are included, for example, for a mortgage payment. This should be accounted as part of the loan. The APR (annual percentage rate) is normally used as an indicator to compare among different schemes with different interest rates and processing fees.

2.2.8 Profitability Analysis

A profitability analysis is essential to justify the economic feasibility of a project. This can be carried out using various methods and measures, depending on the level of details required. During the preliminary stage of a project, the time value of money is not considered. The approximate quantitative indicators at the preliminary stage are payback time, return on investment and total annualized cost.

Payback time is the period from the start of a project until the time when all capital investment is recovered from selling of products (breakeven), shown in Figure 2.2. Intuitively, a shorter payback time is preferred. However, the usefulness of the payback time as an indicator is limited since it is only valid up to the break-even point. The economic performance after the break-even point cannot be measured using this indicator.

Return on investment (*ROI*) is a common profitability measure of a project, defined as the ratio of the annual income over a project life to the total capital investment, shown below. *ROI* gives a sense of the efficiency of an investment being made:

$$ROI = \frac{\text{Annual income}}{\text{Capital investment}} \times 100\% \tag{2.7}$$

The discounted cash flow rate of return (DCFRR) is essentially the interest rate that makes the *NPV* zero at the end of a project. The DCFRR is a way to measure the performance of utilizing a capital for projects, but does not give any indication of the profit, unlike the *NPV*. The DCFRR can be calculated using Equation (2.4) through the trial-and-error method (e.g., using the Solver function in Excel or the iteration method) or the graphical method.

The total annualized cost includes capital and operating costs in most of the cases, shown in the following equation. The annualized capital cost can be estimated using a fixed interest rate over the plant life. The operating cost is estimated by assuming operating hours in a year.

$$\text{Total annual cost} = \text{Annualized capital cost} + \text{Annual operating cost} \tag{2.8}$$

A more rigorous profitability analysis considering the time value of money is desirable in the detailed process design stage. Economic criteria such as economic potential, netback and cost of production can be applied.

Economic potential (*EP*) is the economic margin and can be evaluated using the following equation when values of products, feed, capital cost and operating cost are available. To obtain an annualized capital cost with the consideration of time value of money, the DCFRR needs to be calculated using Equation (2.4) by setting $NPV = 0$.

$$EP = \text{Value of products} - (\text{Value of feed} + \text{Annualized capital cost} + \text{Annual operating cost}) \tag{2.9}$$

Netback indicates the value of a feedstock from its products selling and can be determined using the following equation. Product prices, capital cost and operating cost except the feedstock cost are known. The market price or cost of the feedstock thus must be less than the netback to result in a positive economic margin.

$$\text{Netback} = \text{Value of products} - (\text{Annualized capital cost} + \text{Annual operating cost}) \tag{2.10}$$

Cost of production of a product is a meaningful indicator when comparing the economic viability between various production routes. It is used when the value of a product is not known, especially when a new product is synthesized or a conventional product is generated from a nonconventional feedstock. The cost of production is calculated from

$$\text{Cost of production} = \frac{\text{Value of feed} + \text{Annualized capital cost} + \text{Annual operating cost}}{\text{Production rate}} \tag{2.11}$$

2.2.9 Learning Effect

The cost of a new and developing technology such as fast pyrolysis of biomass and gasification of biomass is usually very high in the beginning of the development stage. The cost of the technologies decreases as more plants are built and productivity increases due to more experience gain by organizations. This effect is known as a *learning curve* or *experience curve* or *progress curve* or *learning by doing effect*, as shown in Figure 2.3.

The trend of the learning curve can be described by

$$y = a x^{-b} \tag{2.12}$$

where y is the cost of the xth unit, a is the cost of the first unit, x is the cumulative number of units and b is a parameter shown as $b = \log$ (progress ratio)/log 2.

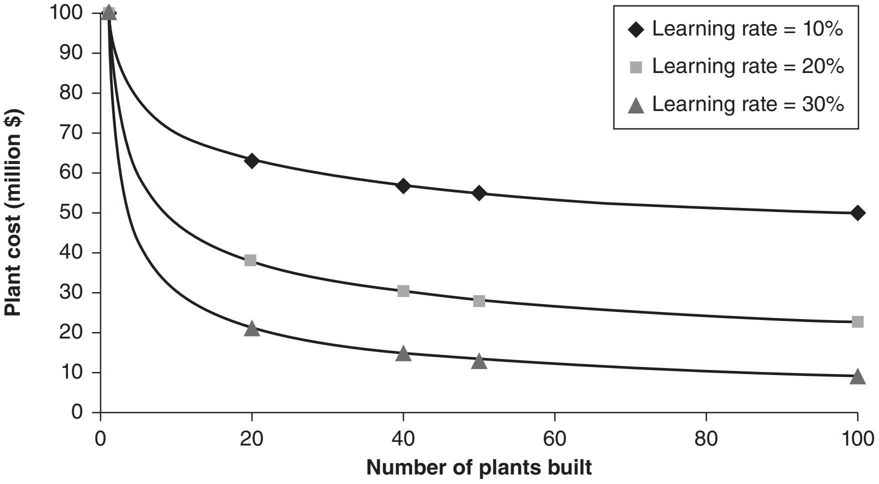

Figure 2.3 Learning curve effect.

The learning rate is shown by

$$\text{Learning rate} = 1 - (\text{Progress ratio}) \tag{2.13}$$

The rates of learning vary across different organizations. The factors influencing the rate of learning are crucial and particular attention has to be paid to enhance the performance and economics of the plant. A few factors have been identified as follows:

- Organization forgetting
- Employee turnover
- Transfer of knowledge
- Failure to control other factors such as economies of scale.

The learning curve effect and the learning rate can be easily understood by visualizing the teaching and learning environment in a classroom. If there are 30 students in a classroom, the amount of material that can be assimilated varies from individual to individual, assuming they have no background knowledge on a particular subject and the time of learning is the same. In this case, the method of learning, individual ability and attitude are variables.

2.3 Methodology

2.3.1 Capital Cost Estimation

There is extensive published literature reporting the correlations for estimating the cost of standard equipment, for example, heat exchangers, boilers, turbines, pumps, etc. This information is normally enough for carrying out a chemical plant economics evaluation. However, for a plant undergoing development, such as the biorefinery systems, much of the cost data is unavailable, not readily accessible or may be proprietarily to organizations. Therefore, the costs of equipment may need to be estimated based on existing methodologies or vendor quotes of similar equipment. The Aspen Icarus process evaluator is widely used for an equipment cost estimation in industry. The software may not be available with academic and small organizations; hence spreadsheet based economic evaluation is more convenient and still preferable.

The approach for estimating the equipment cost presented here has avoided using a cost chart that may lead to inconsistent results. A set of established information on equipment costs for biorefinery systems is used as the base cost and the suggested methodology is to scale up or down according to the desired capacity. The base costs and scale factors are collected from various sources[2–7].

The capital cost can be estimated using different methods, that is, order of magnitude estimate, study estimate, preliminary estimate, definitive estimate and detailed estimate. These methods need information at different levels of detail, hence leading to different levels of accuracy. A capital cost estimation by the order of magnitude results in an accuracy of 30–50%. The definitive and detailed estimates require Aspen Icarus software and also a vendor's quote, and thus are more complicated. For these reasons, study and preliminary estimates are preferable since they involve moderate complexity while giving accuracy at a reasonable level. The recommended capital cost estimation approaches are Guthrie's[8] and Lang's[9] methods, able to achieve an accuracy of 20–30%. These approaches should be used for a new design and more time should be allowed to complete the evaluation since many details are required, that is, a complete flowsheet with mass and energy balances, equipment sizing, etc.

The recommended approach for estimating capital costs is shown as follows:

1. Generate a list of equipment and estimate the size of each piece of equipment. The size information in terms of flow rates and power requirements (e.g., for pumps and compressors, etc.) can be obtained directly from simulation. However, some equipment require additional sizing procedures, such as weight of vessel and heat transfer area of the heat exchanger.
2. By applying the concept of economies of scale (Equation (2.2)), the base cost of equipment with a specific size is scaled up/down to obtain the cost of equipment for a desired size. Refer to Table 2.3 (gasification and hydrocracking systems) and Table 2.4 (bioethanol system) for information on base sizes, base costs and scale factors.
3. If the desired size of equipment exceeds the maximum size given, multiple units have to be assumed.

4. Apply the correction factors to the cost of equipment (where relevant) depending upon the material of construction, pressure and temperature.
5. The estimated cost of a piece of equipment can be obtained for different years. Therefore it has to be updated to the cost at the current year, by adopting Equation (2.1) and the cost index in Figure 2.1.
6. Estimate the total capital investment of the system, either based on the individual factor method (Guthrie's method) or the overall factor method (Lang's method).
   a. Guthrie's method. The cost of equipment is given in terms of the f.o.b. purchased cost. Apply individual installation factors for each unit operation to determine the total capital investment.
   b. Lang's method. The cost of equipment is given in terms of the f.o.b. purchased cost. Assume 10% delivery charges as a preliminary estimation. Calculate the total installed cost of equipment using an overall Lang factor based on the plant type, shown in Table 2.5.

For technologies at an early development stage, the estimated cost is normally very high. The learning curve effect (Equation (2.12)) can be taken into account to forecast the future cost of a system and to obtain a reasonable estimation of the cost. A reasonable reference point is the cost of building the tenth plant ($x = 10$ in Equation (2.12)) and a progress ratio of 0.8 can be used as a preliminary estimation.

Remarks. The Golden Rule: an estimated capital cost of a facility is unlikely to give its actual value. No matter how sophisticated the capital cost estimation method is, it will never be accurate. It is not possible to apply the same values for different locations and time. However, an estimated cost needs to be reasonable. Aspen Icarus is widely accepted and has been a standard in the chemical industry due to its strength in performing sizing and costing of equipment. Vendor's quotes are more up-to-date, yet it is still unreliable at some point due to several factors such as the seller-and-buyer relationship, contemporary supply and demand, etc. It is advisable to use the same basis throughout a capital cost evaluation of equipment in a plant so that the same degree of accuracy can be attained. A sensitivity analysis should be carried out to examine the effects of inaccuracies on results.

2.3.2 Profitability Analysis

The economic feasibility of a plant can be examined using the economic criteria mentioned in Section 2.2. A systematic approach is provided as a guideline to evaluate the economic performance of a plant up to a reasonably detailed level, as follows:

1. Evaluate the capital cost using the procedures given in Section 2.3.1. The annualized capital cost is calculated using the discounted cash flow (*DCF*) analysis (Section 2.2.7), by assuming a reasonable plant life.
2. Evaluate the annual operating cost. Variable operating costs such as biomass feedstock and transportation costs are shown in Tables 2.6 and 2.7, respectively, and the costs of chemicals and utilities can be obtained conveniently elsewhere. The cost factors for fixed operating costs are shown in Table 2.1.
3. Select an indicative economic measure, that is, economic potential, netback and cost of production, and determine the economic performance of the plant.

2.4 Cost Estimation and Correlation

The correlations for estimating the capital and operating costs of biorefinery systems are shown in Sections 2.4.1 and 2.4.2, respectively.

2.4.1 Capital Cost

The parameters required for estimating the equipment cost (base scales, base costs and scale factors) of gasification, hydrocracking and bioethanol systems[2–7] are shown in Tables 2.3 and 2.4, respectively. The installation factors for

Table 2.3 *Equipment cost correlation – gasification and hydrocracking systems*[2–4,6,7].

Item No.	Component	Base cost (million \$)	Scale Factor	Base Size	Capacity	Maximum Size	Installation Factor	Base Year
A. Pretreatment								
A.1	Conveyers	0.35	0.8	33.5	wet t h^{-1} biomass feed	110	1.86	2001
A.2	Grinding	0.41	0.6	33.5	wet t h^{-1} biomass feed	110	1.86	2001
A.3	Storage	1.0	0.65	33.5	wet t h^{-1} biomass feed	110	1.86	2001
A.4	Dryer	7.6	0.8	33.5	wet t h^{-1} biomass feed	110	1.86	2001
A.5	Iron removal	0.37	0.7	33.5	wet t h^{-1} biomass feed	110	1.86	2001
A.6	Feeding system	0.41	1.0	33.5	wet t h^{-1} biomass feed	110	1.86	2001
B. Gasification System								
B.1	Gasifier BCL[a]	16.3	0.65	68.8	dry t h^{-1} biomass feed	83	1.69	2001
B.2	Gasifier IGT[b]	38.1	0.7	68.8	dry t h^{-1} biomass feed	75	1.69	2001
C. Syngas Cleaning								
C.1	Tar cracker	3.1	0.7	34.2	m^3 s^{-1} gas input	52	1.86	2001
C.2	Cyclones	2.6	0.7	34.2	m^3 s^{-1} gas input	180	1.86	2001
C.3	Gas cooling	6.99	0.6	39.2	kg s^{-1} steam generation		1.84	2001
C.4	Baghouse filter	1.6	0.65	12.1	m^3 s^{-1} gas input	64	1.86	2001
C.5	Condensing scrubber	2.6	0.7	12.1	m^3 s^{-1} gas input	64	1.86	2001
C.6	Hot gas cleaning	30	1.0	74.1	m^3 s^{-1} gas input		1.72	2001
D. Syngas Processing								
D.1	Steam reformer	9.4	0.6	1390	kmol h^{-1} gas input		2.3	2001
D.2	Autothermal reformer	4.7	0.6	1390	kmol h^{-1} gas input		2.3	2001
D.3	Shift reactor	36.9	0.85	15.6	Mmol h^{-1} $CO+H_2$ input		1.0	2001
D.4	Selexol CO_2 removal	54.1	0.7	9909	kmol h^{-1} CO_2 removed		1.0	2001
E. Product Synthesis and Upgrading								
E.1	Solid bed FT gas phase 60 bar	25.3	1.0	100	MW (HHV) FT produced		1.3	2001
E.2	Slurry phase FT 60 bar	36.5	0.72	131	MW (HHV) FT produced		1.0	2001
E.3	FT product upgrading	233	0.7	286	m^3 h^{-1} FT produced		1.0	2001
E.4	Gas phase methanol synthesis reactor	7	0.6	87.5	t h^{-1} MeOH produced		2.1	2001
E.5	Liquid phase methanol synthesis reactor	3.5	0.72	87.5	t h^{-1} MeOH produced		2.1	2001
E.6	Methanol product upgrading	15.1	0.7	87.5	t h^{-1} MeOH produced		2.1	2001
F. Combined Cycle								
F.1	Gas turbine + HRSG	18.9	0.7	26.3	MW$_e$ electrical output		1.86	2001
F.2	Steam turbine and steam system	5.1	0.7	10.3	MW$_e$ electrical output		1.86	2001
G. Common Process Machinery								
G.1	Compressor	11.1	0.85	13.2	MW$_e$ compression work		1.72	2001
H. Separation Unit								
H.1	Oxygen plant	44.2	0.85	41.7	t h^{-1} O_2 produced		1.0	2001
H.2	Pressure swing adsorption (PSA) unit[c]	28	0.7	9600	kmol h^{-1} throughput		1.69	2001
H.3	Membrane[c]	21.6	0.8	17	t h^{-1} H_2 recovered		1.0	2001
I. Pyrolysis Unit								
I.1	Pyrolyzer (circulating fluidized bed)	3.392	0.7	500	t d^{-1} biomass feed		2.47	2003
J. Refinery Unit								
J.1	Hydrocracker unit[d]	30	0.65	2250	bbl d^{-1} pyrolysis oil feed		2.47	2005
J.2	Separation[e]	2.28	0.65	2250	bbl d^{-1} pyrolysis oil feed		1.0	2007

[a] Gasifier BCL (Batelle Columbus) is an indirect, air-blown and atmospheric gasifier.

[b] Gasifier IGT (Institute of Gas Technology) is a direct, oxygen-blown and pressurized gasifier.

[c] Pressure swing adsorption unit and membrane are employed for hydrogen recovery process.

[d] Hydrocracker unit consists of fired heater, hydrocracker vessel, feed/product exchanger, air cooler, trim cooler, high and low pressure flash.

[e] Separation units include fractionators, splitters, reboilers, condensers and reflux drums.

Notes:

FT: Fischer–Tropsch (c.f. Chapter 14).

HRSG: heat recovery steam generator.

HHV: higher heating value (c.f. Section 10.2.2).

Table 2.4 *Equipment cost correlation – bioethanol system*[5].

Item No.	Component	Base Cost (million $)	Scale Factor	Base Size	Capacity	Maximum Size	Installation Factor	Base Year
A. Pretreatment								
A.1	Mechanical	4.44	0.67	83.3	dry t h^{-1} biomass feed	83.3	2.00	2003
A.2	Mill	0.37	0.7	50	wet t h^{-1} biomass feed		1.00	2003
A.3	Dilute acid	14.1	0.78	83.3	dry t h^{-1} biomass feed		2.36	2003
A.4	Steam explosion	1.41	0.78	83.3	dry t h^{-1} biomass feed		2.36	2003
A.5	Liquid hot water	5.62	0.78	83.3	dry t h^{-1} biomass feed		2.36	2003
A.6	Ion exchange	2.39	0.33	83.3	dry t h^{-1} biomass feed		1.88	2003
A.7	Overliming	0.77	0.46	83.3	dry t h^{-1} biomass feed		2.04	2003
B. Hydrolysis and Fermentation								
B.1	Cellulase production (SSF)	1.28	0.8	50	kg h^{-1} cellulase produced	50	2.03	2003
B.2	Seed fermenters (SSF+SSCF)	0.26	0.6	3.53	t h^{-1} ethanol produced	3.53	2.20	2003
B.3	C5 fermentation (SSF)	0.67	0.8	1.04	t h^{-1} ethanol produced	1.04	1.88	2003
B.4	Hydrolyze-fermentation (SSF)	0.67	0.8	1.04	t h^{-1} ethanol produced	1.04	1.88	2003
B.5	SSCF	0.67	0.8	1.04	t h^{-1} ethanol produced	1.04	1.88	2003
B.6	CBP	0.67	0.8	1.04	t h^{-1} ethanol produced	1.04	1.88	2003
C. Upgrading								
C.1	Distillation and purification	2.96	0.7	18.466	t h^{-1} ethanol produced	18.466	2.75	2003
C.2	Molecular sieve	2.92	0.7	18.466	t h^{-1} ethanol produced	18.466	1.00	2003
D. Residuals								
D.1	Solids separation	1.05	0.65	10.1	dry t h^{-1} solids	10.1	2.20	2003
D.2	(An)aerobic digestion	1.54	0.6	43	t h^{-1} wastewater	43	1.95	2003

Notes:
SSF: simultaneous saccharification and fermentation.
SSCF: simultaneous saccharification and co-fermentation.
CBP: consolidated bioprocessing.

Table 2.5 *Typical Lang factors of various plants for estimating capital investment based on the delivered cost of equipment*[9].

Plant	Solid Processing	Solid–Fluid Processing	Fluid Processing
Direct Cost			
Delivered cost of equipment	1.00	1.00	1.00
Installation	0.45	0.39	0.47
Instrumentation and control	0.18	0.26	0.36
Piping	0.16	0.31	0.68
Electrical systems	0.10	0.10	0.11
Buildings (including services)	0.25	0.29	0.18
Yard improvements	0.15	0.12	0.10
Service facilities	0.40	0.55	0.70
Total direct cost, C_D	**2.69**	**3.02**	**3.60**
Indirect Cost			
Engineering and supervision	0.33	0.32	0.33
Construction expenses	0.39	0.34	0.41
Legal expenses	0.04	0.04	0.04
Contractor's fee	0.17	0.19	0.22
Contingency	0.35	0.37	0.44
Total indirect cost, C_{ID}	**1.28**	**1.26**	**1.44**
Working capital	0.7	0.75	0.89
Total capital investment, C_{TCI}	**4.67**	**5.03**	**5.93**

individual equipment are required in Guthrie's method. These factors have taken into account the direct and indirect cost components, but with different assumptions compared to the Lang factor and also working capital is not included. The Lang factors depending upon plant types are shown in Table 2.5.

2.4.2 Operating Cost

The variable operating costs of biorefinery systems include the costs of raw materials (e.g., feedstock, chemical, catalyst, etc.), utilities (e.g., electricity, steam, etc.) and transportation. These are highly dependent on process specification and preferences. Most of the prices of chemicals can be easily obtained from published literature and online resources. Therefore, only the biomass prices (Table 2.6) and its transportation costs (Table 2.7) are shown for year 2007[10].

Table 2.6 *Estimated prices of various biomass feedstocks. (Reproduced with permission from Department of Trade and Industry (2007)[10].)*

Biomass	Central Price ($ GJ^{-1})	Price Range ($ odt^{-1})	($ GJ^{-1})
Forestry woodfuel-chips	5	120	4.0–6.0
Forestry woodfuel-logs	4	80	3.0–5.0
Energy crops			
Short rotation coppice (SRC)	7	140	6.0–8.0
Miscanthus	6	106	5.0–7.0
Arboricultural arisings	5	98	4.0–6.0
Straw	4	70	3.0–5.0
Waste wood (clean)	5	98	4.0–6.0
Waste wood (contaminated)	2	40	1.0–3.0
Pellets to power/industry/commercial from woodfuel	9	180	8.0–10.0
Pellets to power/industry/commercial from SRC	11	220	10.0–12.0
Pellets to power/industry/commercial from miscanthus	10	200	9.0–11.0
Pellets to domestic (including delivery)	14	280	12.0–16.0
Imported biomass (including delivery)	9	180	7.0–11.0

Note: odt = oven dry tonne.

Table 2.7 *Estimated average transportation costs for different biomass feedstocks. (Reproduced with permission from Department of Trade and Industry (2007)[10].)*

	Transportation Cost ($ GJ^{-1})		
Application	Energy Crops	Woodfuel	Straw
Power generation			
1% co-firing, 2000 MW	NA	0.60 (17)	0.60 (17)
5% co-firing, 2000 MW	1.0 (35)	NA	1.60 (52)
10% co-firing, 2000 MW	1.32 (49)	NA	NA
30 MW dedicated	0.72 (24)	0.74 (25)	0.76 (28)
Heat			
0.1–10 MW of heat generation	0.60 (17)	0.60 (17)	NA
CHP			
0.1–10 MW of electricity generation	0.60 (17)	0.60 (17)	NA
> 10 MW of electricity generation	0.72 (24)	0.74 (25)	0.76 (28)

Note: Numbers in parentheses are estimated average transport distance in km. NA = not assessed.

Table 2.8 *Personnel requirement for chemical processing plants. (Reproduced with permission from Seider et al. (2010)[11]. Copyright © 2010, John Wiley & Sons, Ltd.)*

Process	Number of Personnel per Processing Step
Continuous	
i. Fluids processing	1
ii. Solids–fluids processing	2
iii. Solids processing	3
Batch/semi-batch	
i. Fluids processing	2
ii. Solids–fluids processing	3
iii. Solids processing	4

The cost of labor/personnel is difficult to estimate since it is dissimilar from one organization to another. Furthermore, it varies across different chemical sectors (e.g., petroleum and pharmaceutical), different countries and even different locations. Additionally, the personnel position also determines the salary that they earn. For preliminary estimation purposes, the following approach can be used to estimate the cost of labor.

Step 1. Calculate the number of personnel per shift using Equation (2.14)

The operating labor requirement is related to the number of processing steps depending on the process, as shown in Table 2.8. The number of personnel per processing step is also shown:

$$\begin{aligned}\text{Number of personnel per shift} &= \text{Number of processing steps}\\ &\quad\times \text{Number of personnel per processing step}\end{aligned} \tag{2.14}$$

The number of personnel per processing step should be doubled when the size of the continuous process is large, that is, greater than 1000 t d^{-1} of product[11].

Step 2. Calculate the cost of personnel using Equation (2.15)

$$\begin{aligned}\text{Cost of personnel } (\$\ y^{-1}) &= \text{Number of personnel per shift} \times 5 \text{ shifts} \times 40 \text{ hours/week} \times 52 \text{ weeks/year}\\ &\quad\times \text{hourly wages } (\$\ h^{-1})\end{aligned} \tag{2.15}$$

Assume 5 shifts per day are required. Each personnel works 40 hours per week and there are 168 hours per week. In addition, consider other factors such as sick leaves, holidays, etc.

The Bureau of Labor Statistics in the US Department of Labor estimated that the mean hourly wages for a chemical engineer in year 2008 is at the rate of $42.67 (€29) per hour.

2.5 Summary

This chapter shows the generic economic analysis concept and fundamental teaching and learning tools for chemical engineering process economics. The time value of money and discounted cash flow are among the important aspects in an economic evaluation. The methods for analyzing capital cost and operating cost have been outlined and translated into easy-to-follow procedures, accompanied by cost estimation correlation and data.

2.6 Exercises

Refer to the ***Online Resource Material, Chapter 2 – Additional Exercises and Examples***, the solutions to all Exercise problems.

1. A company is planning to start a methanol production plant via thermochemical conversion of biomass. The plant encompasses the following main equipment:
- Dryer
- Gasifier (direct, oxygen-blown and pressurized)
- Oxygen plant
- Tar cracker
- Water gas shift reactor
- Methanol synthesis reactor (gas phase)

Process specifications and assumptions:
- Biomass feed = 150 dry t h^{-1}
- Moisture content of biomass = 30 wt%
- Oxygen requirement in gasifier = 0.45 kg kg^{-1} dry biomass feedstock
- Yield of product gas from gasification = 100 kmol t^{-1} dry biomass feedstock
- Standard molar volume of gas = 22.414 m^3 $kmol^{-1}$
- Mole fraction of components in product gas

$$CO = 0.15;\ H_2 = 0.20$$

- Higher heating value (HHV) of

$$\text{Biomass} = 20\,\text{MJ kg}^{-1}$$

$$\text{Methanol} = 23\,\text{MJ kg}^{-1}$$

- Output efficiency = 45% based on HHV
  - a. Calculate the purchased cost of each individual piece of equipment and hence the total purchased cost of equipment of the methanol production system.
  - b. Calculate the total capital investment of the methanol production plant by applying Guthrie's method.
  - c. The cost of equipment is valid in year 2001. Estimate the total cost of equipment in year 2010 using the Chemical Engineering Plant Cost Index.

2. The methanol production plant requires steam and electricity to run the process. It has been estimated that 2.0 kg of steam per kg of methanol produced is needed for the whole system while 235 kW h of electricity per tonne of O_2 are needed for the oxygen plant.
- a. Calculate the utility cost required per annum for this plant using the results calculated from Question 1.
- b. If heat integration is applied on this plant, steam can be generated through heat exchange with process streams. The steam requirement can then be partially satisfied by the steam generated on site. It has been estimated that 40% of the imported steam can be reduced. Calculate the % cost saving from heat integration relative to the steam import scenario.

Assumptions:
- 8000 operating hours per year
- Cost of imported steam = \$15 t^{-1}
- Cost of imported electricity = \$0.1 kW h^{-1}

3. The company is at the stage of choosing between two plant options, X and Y. The finance department has provided an estimation of the annual cash flow for a period of 10 years, shown in Table 2.9. Evaluate both options with respect to:
- a. Payback time.
- b. Return on investment.

Table 2.9 Cash flow for two plant options.

	Cash Flow (million $)	
Year	Option X	Option Y
−1	−40.0	−40.0
0	−60.0	−60.0
1	30.0	5.0
2	40.0	15.0
3	50.0	25.0
4	65.0	40.0
5	70.0	50.0
6	75.0	65.0
7	85.0	75.0
8	90.0	75.0
9	90.0	80.0
10	90.0	80.0

c. Discounted cash flow and net present value for each year. Assume an annual discount rate of 10%.
d. Discounted cash flow rate of return.
e. Suggest the preferred option based on the results obtained from (a), (b) and (c) and (d).
f. Illustrate the effect of having different annual discount rates, that is, 5% and 20%, on the overall economic performance of the preferred option in *NPV* versus time plot and draw conclusions based on the trend.

4. By using the results obtained from Questions 1 and 2(b), show the netback calculation to estimate the value of the biomass feedstock. Assume a DCFRR of 15% for the annualized capital cost.

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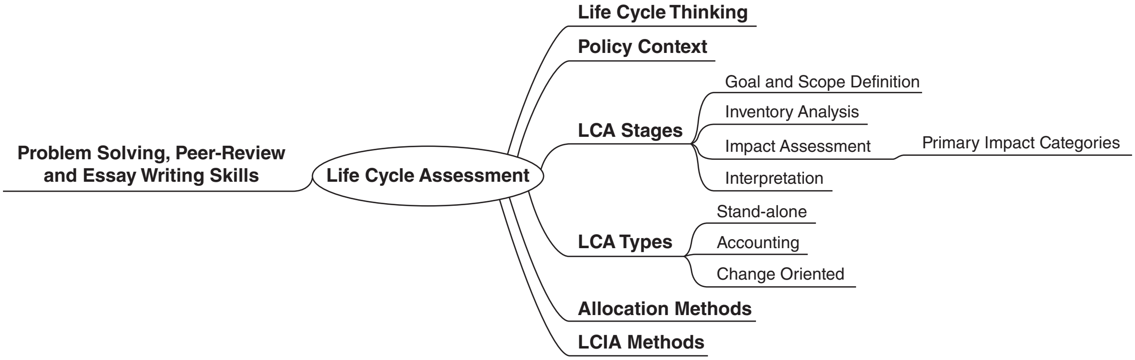
4

Life Cycle Assessment



Structure for Lecture Planning

4.1 Life Cycle Thinking

Life cycle thinking (*LCT*) includes analysis of whole system environmental impacts from primary material and energy resource extraction to end of life (*cradle to grave*), much beyond a chemical plant's material and energy efficiency. A system that includes primary resource extraction to manufacturing of products or *upto the plant gate* is called a *cradle to gate* system. If one part of a system has positive impacts, other parts of the system are likely to have negative impacts. System thinking is imperative for environmental sustainability. Environmental sustainability relates to the impact assessments due to emissions to air, water and land and avoidance of emissions by improved process configurations, feedstocks, products and supply chain distributions.

An example is whether a particular nuclear power generation plant can give more energy than it consumes; there is a need to go beyond the generation facilities and consider impacts of other aspects involved such as uranium mining, transportation, associated research and even the marketing services. The systematic process design and development study for one single step can be extended to the formulation of all steps in a product life cycle, raw material acquisition, manufacturing, logistics and, after consumption, reuse, recycling and landfill, etc. Figure 4.1 shows the basic building stages for the production of a product, from raw material extraction through manufacturing to end of life reuse and recycling. However, Figure 4.1 does not include life cycle impacts associated with the construction materials of the

Biorefineries and Chemical Processes: Design, Integration and Sustainability Analysis, First Edition.
Jhuma Sadhukhan, Kok Siew Ng and Elias Martinez Hernandez.

Companion Website: http://www.wiley.com/go/sadhukhan/biorefineries

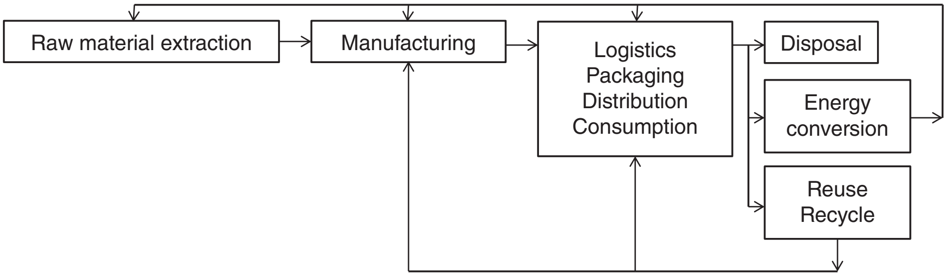


Figure 4.1 *Basic building stages for the production of a product.*

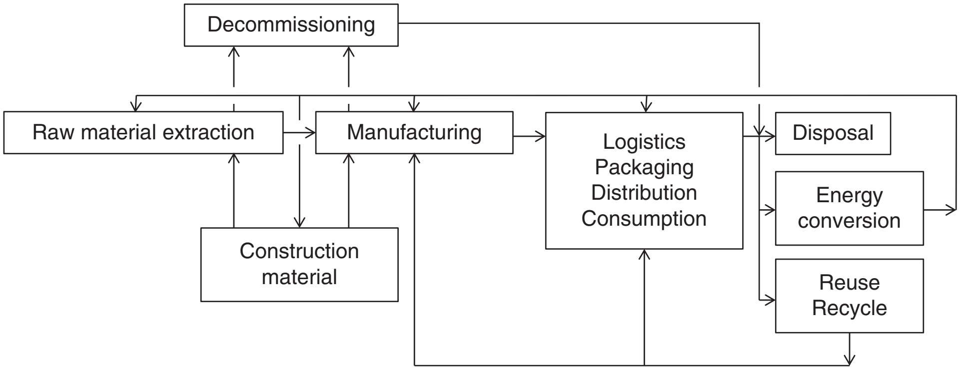


Figure 4.2 *Life cycle stages of a cradle to grave system.*

manufacturing plants. Figure 4.2 shows the complete life cycle stages of a system. Figure 4.2 shows that the emissions from the construction materials life cycles should be included in a life cycle assessment (LCA) study of a manufactured product.

The LCA is a holistic environmental impact assessment tool for cradle to grave systems that systematizes the assessment in a standardized way and format. LCA studies are data intensive. A whole system in Figure 4.2 can be divided into two parts, foreground and background systems, such as in Figure 4.3. This division is primarily applied to minimize the data

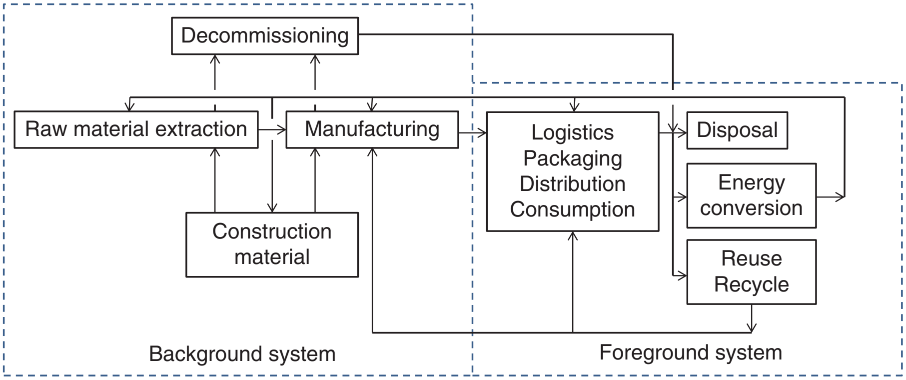


Figure 4.3 *Foreground and background systems.*

need. A decision maker primarily deals with one or some parts of a system, known as *foreground* system. The rest of the cradle to grave system is the *background* system for the decision maker. For the background system the life cycle inventory analysis data may be collected, compared and reconciled for incorporation into the foreground system. The foreground system is of central focus in terms of design, optimization and decision making.

Figure 4.3 shows an example of the foreground system with the rest presented as the background system. Which part of the system is the foreground system depends on the concerned decision maker. In this case, the decision maker is primarily dealing with the product logistics, such as a local authority trying to influence waste recycling as a better policy than landfilling, by taking the LCA approach. Whilst the foreground and the background systems are highly interactive and influenced by each other in terms of environmental impacts, the decision maker may just be concerned with the detailed evaluation of the foreground system, which can include raw material extraction and manufacturing, instead.

Uncertainties in data exist all the way in entire value chains; henceforth, structured approaches are recommended and guidelines are provided for making the most of LCA tools and for the best use of LCA results. Here, the focus is to first get familiar with the LCA approach generically followed by specific practical examples to help in applying LCA to biorefinery problems. The LCT spans not only across the whole lifetime of a process or product but also how the product or process is connected with other networks of products and processes. The networks may span across different geographic regions and hence value or supply chain analysis becomes part of the problem. Thus LCT-inspired problem formulation may take account of interacting products and process network design and decision making across supply chains in different geographic regions as well as time scale. Figure 4.4 shows an example of interacting networks of products and processes[1]. The primary raw material and energy for all kinds of products or processes under consideration come from reserves of coal, crude oil, natural gas and minerals from soil. Soil or land and water are also important resources. These resources contribute to the development of any product shown for cement, iron, electricity and heat, interdependent on each other by the constraints on resource availability. There are also demand side constraints for various products. Policies need to be in place to ensure that supply and demand are constantly balanced without damage to the environment, so as to retain resource reserves and reduce pollutant emissions to land, water and air. In this chapter, the

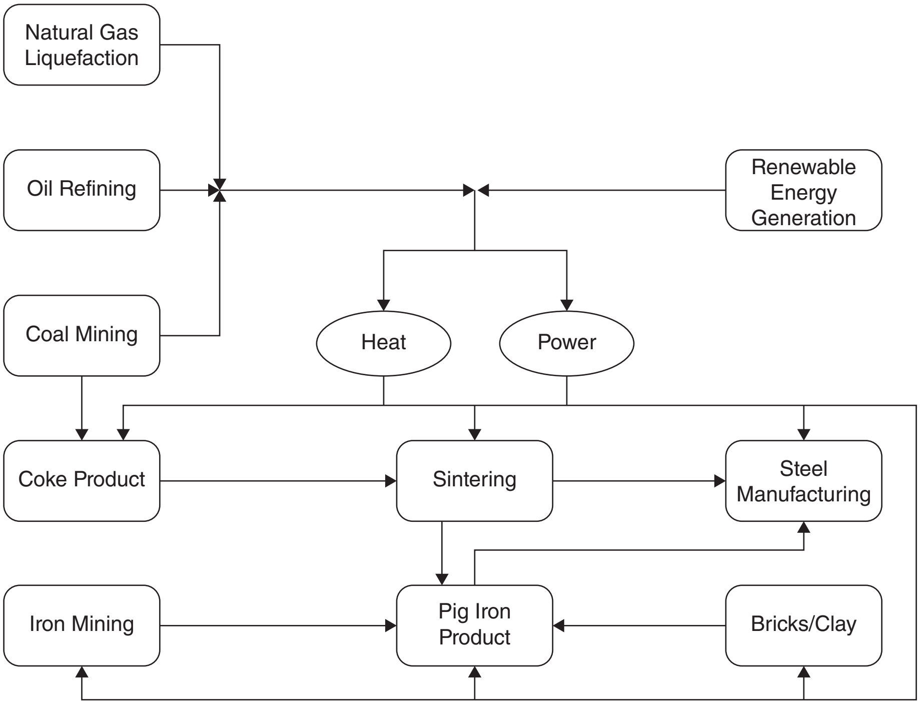


Figure 4.4 *Interacting networks of products and processes.*

focus is to discuss LCA for analyzing interactions between engineering systems and the environment through assessments of resource depletion and pollutant emissions. The learning objectives can be subdivided as follows.

1. Find the likely environmental impacts.
2. Structure pollutants under various impact characterizations.
3. Impact assessments.
4. Compare impacts between materials.

4.2 Policy Context

The policy landscapes are fast evolving by being more concerned about whole system impacts, such as the extended producer policy in which a producer's responsibility for a product is extended to the postconsumer stage of a product's life cycle, defined by OECD (2005)[2]. In this context, the decision maker must also systematically present the whole system impacts; hence the knock-on effects in the background system due to any changes in the foreground system and vice versa must be analyzed for any product or process development.

Modern lifestyle is chemical dependent. Chemicals contribute to household activities (energy appliances, clothes, food, beverages, polymers), pharmaceutical, petrochemical, agrochemical, industrial, etc. Throughout life cycles, chemicals have environmental impacts under various categories. Chemicals may cause global warming, stratospheric ozone layer depletion, acid rain, leaching to soil and water bodies (eutrophication), etc. These various environmental impact categories are commonly known as environmental impact characterizations, which is used in this text. In a broad sense, chemicals contribute to land, atmosphere and water environmental impacts. One of the earliest recognitions of environmental pollutions was by Dangerous Substances Directives, as follows, to regulate discharges to water bodies[3]. Because the earth's water body is connected through rain and soil water absorption, pollutants spread very quickly by water.

The Environmental Protection Act 1990 – for discharges from severe pollutants from industrial processes.
The Water Resources Act 1991 – for discharges to water.
The Water Industry Act 1991 – for discharges to sewer.

These first set of Directives were to limit the concentration and/or the total amount of priority pollutant categories, also known as List I substances, given in Table 4.1.

4.3 Life Cycle Assessment (LCA)

In the 1960s, the life cycle assessment (LCA) technique was applied to energy analysis; however, a group of researchers were commissioned by Coca Cola Amatil around the same period to study the resources and environmental profile of the different packaging materials they used for their products[3]. The impacts of pollutants turned out to be more severe than estimated. The majority of chemicals is related to one or more categories of environmental pollutants. Understanding the impacts of chemicals under various environmental categories or characterizations can help identifying and eliminating them at their sources, if possible at the first instance. If not, chemicals must be treated and regulated before their discharge to the environment.

By the mid-1980s the multicriteria systematic analysis had spread to include many more products. Different terms were used to describe these studies, the term Life Cycle Assessment was proposed and agreed upon at a workshop held by the Society of Environmental Toxicology and Chemistry (SETAC) at Vermont, USA, in 1990. SETAC have since published various guides and advice material on LCA simplification and methods.

The definition of Life Cycle Assessment as given by the *International Organization for Standardization* (ISO) in 1997 is:

> Compilation and evaluation of the inputs, outputs and the potential environmental impacts of a product system throughout its life cycle.

According to *ISO standards 14040, 14041 and 14044*, the LCA is carried out in four phases: Goal and Scope definition, Inventory analysis, Impact Assessment and Interpretation[4–6]. All these phases are interdependent as a result of one phase

Table 4.1 *List I of priority pollutant categories.*

1. Organohalogen compounds	For example, CCl_4 used as refrigerant, fire extinguisher, degreasing and dry cleaning agent. Its use declined in recent times due to its effect on stratospheric ozone depletion.
2. Organophosphorous compounds	Phosphates in fertilizer (though insoluble in water) can adhere to soil particles and erode into water bodies.
3. Organotin compounds	Chemicals of hydrocarbons and tin (Sn) generally used as a heat stabilizer in polyvinyl chloride, biocide, wood preservative, antibiofouling agent. Their toxic effects are detrimental to marine lives (1 ng L^{-1})
4. Compounds with carcinogenic properties in aquatic environment	Polycyclic aromatic hydrocarbons have toxic and carcinogenic properties and occur by natural and anthropogenic activities.
5. Mercury and its compounds	Organic mercury is more harmful than inorganic mercury, for human body (brain, nervous system and kidney and more harmful for youngsters). Occurs from rain, rock, soil, thermochemical process of coal and smelting processes.
6. Cadmium and its compounds	Categorized as Category 2 carcinogen by National Occupational Health and Safety Commission. Exposure limit in work place 0.01 mg m^{-3} and 0.002 mg m^{-3} for drinking water. They are present in ores, coal and other fossil fuels and in products, tobacco, fertilizer, PVC, petrol, tires, electronic components, batteries, textile dyes and ceramic glazes.
7. Mineral oils and hydrocarbons of petroleum origin	Fossil hydrocarbons in oil and petrochemical products have environmental impacts in all categories.
8. Synthetic substance in water	Pesticides, solvents and water-borne chemicals are the biggest threat to the fresh water supply and damaging to human reproductive systems.

determining the execution of the next phase. Figure 4.5 shows the different phases involved in an LCA study. Figure 4.6 illustrates the documents published by the ISO and an example of a life cycle management framework developed by 3M, 1997, for the assessments of risks and opportunities throughout the various stages of a product's life cycle.

Life cycle stages include compiling inventories over the complete supply chain, providing a service or product extending from the "cradle" of primary resources – fossil and metal ores, for example – through to the "grave" of recycling or safe disposal; the term "life cycle" also includes the service life of the capital goods needed for a product or process. In the sequence of steps conventionally followed in carrying out an LCA, compiling the material and energy balance is termed

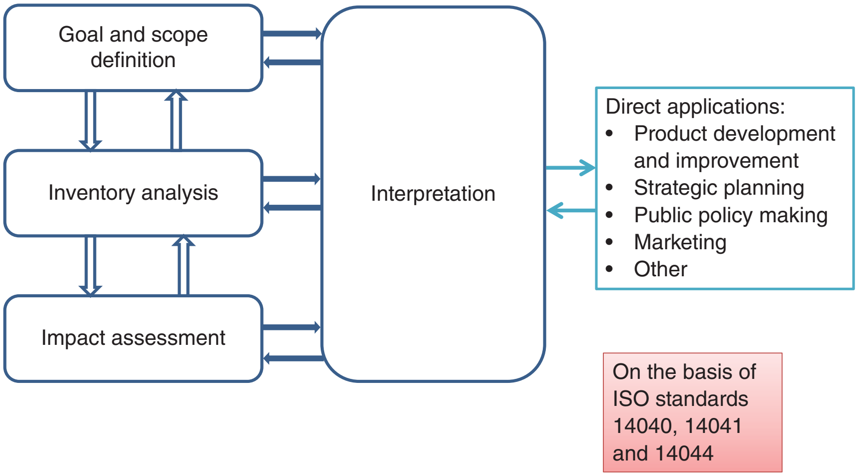


Figure 4.5 *LCA study stages*$^{4-6}$.

June 1997	ISO 14040 Life cycle assessment – principles and framework
October 1998	ISO14041 Life cycle assessment – goal and scope definition and inventory analysis
March 2000	ISO 14042 Life cycle assessment – life cycle impact assessment
March 2000	ISO 14043 Life cycle assessment – life cycle interpretation
2002	ISO/TS14048 Life cycle assessment – data documentation format

				Customer needs	
LCM stage impact	Material acquisition	R&D operations	Manufacturing operations	Use	Disposal
Environment					
Energy/Resources					
Health					
Safety					

Figure 4.6 *(above) LCA documents published by the International Organization for Standardization (ISO). (below) 3M, 1997, developed a Life Cycle Management framework for the assessment of risks and opportunities throughout the various stages of a product's life cycle.*

the *Inventory* phase. Apart from the extended system boundary, an inventory analysis differs from a conventional material and energy balance analysis by the need to include trace flows of species whose environmental significance is large, for example, because they have high human or ecotoxicity. There are two terminologies often used in LCA, LCI and LCIA. LCI refers to *Life Cycle Inventory* and LCIA refers to *Life Cycle Impact Assessment*. A study is not an LCA study when the study includes a goal and scope definition and inventory analysis, but not the impact assessment. This is then referred to as an LCI analysis. An LCIA includes an impact assessment, but not necessarily the interpretation. The LCA must include transparent and systematic discussions on all four stages.

It is more common to find chemicals with more profound (or primary) effects on one or more impact characterizations than others (secondary, tertiary, etc.), more commonly known as mid-point and end-point impacts. Pollutants with primary impacts are included in an impact characterization. Several pollutants have mid-point impacts on various characterizations. However, only primary effects of pollutants are considered to avoid double counting in most LCA studies. In Section 4.8, the various life cycle impact assessment (LCIA) methodologies are shown. A study can include a combination of primary, mid- and end-point impacts. Inclusion of mid- or end-point impacts in the LCIA methodology calls for robust reasons for doing so.

The effect of greenhouse gases (GHGs) such as CO_2, CH_4, N_2O, CFC (chlorofluorocarbon), etc., emissions on various levels is explained[3]. These gases absorb solar infrared radiation. Different gases have different abilities to absorb radiation. These gases create a GHG effect in sending the radiation to the earth's surface (Figure 4.7). Earth then absorbs some of this radiation energy and sends back the rest to the atmosphere. This exchange of radiative force between earth and GHGs in the atmosphere is regarded as a primary effect. The change in radiative force is expected to change the global temperature level, known as global warming and regarded as a secondary effect. The global warming effect is not uniform on the earth's surface, causing ice to melt, raised sea levels and severe weather patterns. These effects are known as tertiary effects. Once again, the consequences of tertiary effects on human health and ecological systems vary from place to place. The result may be changes in biodiversity in various ecosystems and impacts on food availability, agricultural patterns, society and economics. Having long chains of cause and effect, describing the environmental effects in a quantitative manner all the way through to the effects on the later stages in geographically segregated regions becomes impossible. As a result, LCIA is mostly done at a primary impact level or mid-point level (see Section 4.8: LCIA Methods).

The global warming potential (GWP) of a gas is determined by the infrared absorption capacity of the gas, which is related to the chemical structure and physicochemical properties of the gas. Similarly, all other impact characterizations depend on physicochemical properties of chemicals. Governed by molecular properties of chemicals, different chemicals have different levels of environmental impact characterizations. Over a 100 year period, methane gas has 25 times more GWP than carbon dioxide gas. Therefore, factors are used to provide an environmental impact characterization in relative

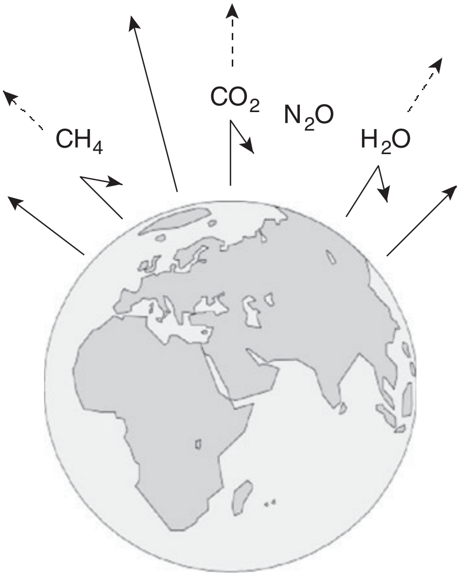


Figure 4.7 GWP impact of GHGs.

terms compared to a base chemical with an assumed value of 1 in the environmental impact characterization. Hence, methane gas has a global warming impact characterization factor of 25, over a 100 year period, implying that one unit mass of methane gas has 25 times more intensive global warming impact than the unit mass of carbon dioxide.

Quantities are then associated with each pollutant impacting on every category. These factors are called equivalence factors/equivalents/potentials/category indicators (according to the ISO standard)/characterization factors. Characterization factors are more commonly used in this text. The characterization factors depend on physicochemical properties of pollutants and are provided in relative terms compared to a base pollutant (assumed to have a value of 1 in an impact category). As shown, CO_2 is a base pollutant for the GWP impact category, that is, its GWP impact characterization factor is 1. All other pollutant GWPs are presented relative to CO_2. The GWP of CH_4 is 25 CO_2 equivalent and that of chlorofluorocarbons (CFCs) is 5000 CO_2 equivalent, over a 100 year lifespan.

Their units are represented in terms of: CO_2 equivalent, for example, kg CO_2 equivalent. Various notations used are CO_2 eq., CO_2-eq., etc.

The GHGs have different lifespans and therefore a basis of 25, 100 and 500 years is generally assumed over which the total GWP is predicted.

The volatile organic compounds (VOCs) are carbon containing compounds that take part in photochemical reactions. The VOCs do not include carbon dioxide, carbon monoxide, carbonic acid, metallic carbide, carbonates and ammonium carbonates. VOCs react with NO_x in the presence of sunlight to produce ozone and photochemical pollutants, such as peroxyacetyl nitrate (PAN), formaldehyde and acetic acid in the lower atmosphere. These pollutants and ozone in the lower atmosphere are responsible for urban smog and ground level ozone formation and are classified under photochemical oxidant creation potential.

NO_x (excluding N_2O) has primary effects on acidification and eutrophication potential impact categories. All these environmental impacts discussed are around ecological consequences. Most chemical pollutants also have primary impacts on human health. Depletion of quality and quantity of resources, for example, fossil energy, mineral and ores in earth, land and water, is also a reality and must be considered with due importance, in the context of growing population, energy demands and needs for sustainable lifestyles. Broadly, there are three classifications of environmental impacts of chemicals: resource use, human health and ecological consequences. Table 4.2 shows the most common impact characterizations responsible for environmental consequences that can be assessed. Table 4.3 shows the links between the various types of inventory stressors and their primary and secondary environmental impacts[3].

Table 4.2 Broad impact characterizations.

Resource Use	Human Health	Ecological Consequences
1. Energy (can also be subdivided into fossil and renewable)	1. Toxicological impacts	1. Global warming
2. Water	2. Nontoxicological impacts	2. Ozone depletion
3. Land	3. Work environment impacts	3. Acidification
4. Abiotic (ores) depletion		4. Eutrophication
		5. Photochemical oxidant creation
		6. Aquatic, human, terrestric ecotoxicity
		7. Biodiversity

In evaluating the environmental impact characterization factors, no geographical segregation is considered. Henceforth, assessment of the environmental impact characterization factors, generally restricted up to the primary and mid-point levels of impacts can be applied to analyze life cycle impacts of any products or process systems, irrespective of geographic locations. The following sections explain the various calculation stages of the LCA.

4.4 LCA: Goal and Scope Definition

The goal and scope definition is the first step of LCA. A decision maker sets out objectives of interest for LCA study. The objectives need to be consistent with the intended application. The goal and scope definition involves identification of:

1. Functional unit
2. System definition
3. System boundaries

This phase also includes product definition, coproduct and waste utilization routes, any allocation method considered, LCIA methodology selected, database sources, year and geographic location.

> The functional unit is the unit of analysis for the study, and it provides a basis for comparison if more than one alternative is being studied. It should be defined in terms of the **service(s)** provided by any product, process, or activity under analysis.

An example often used to describe a *functional unit* is use of nappies by two babies. Nappies can be used up at various rates. In order to obtain average representative rates of use, the rates can be calculated based on uses over six months or longer. A functional unit can then be presented as the mass of nappies used in six months by each baby.

To compare between two or more washing liquids, the *functional unit* can be the mass of washing done per unit mass of a washing liquid. The functional unit of a system to be studied is associated with the service provided, for comparison

Table 4.3 Inventory stressors and environmental impacts.

Inventory Stressor	Initial Impact	Secondary Impact
Acid emission	Acid rain	Acidified lakes
Photochemical oxidants	Smog	Health impairment
Nutrients	Eutrophication	Bogs
Greenhouse gases	Global warming	Sea level rise
Ozone depletors	Ozone depletion	Skin cancer
Toxic chemicals	Toxic effect	Health impairment
Solid waste	Land consumption	Habitat destruction
Chemicals to groundwater	Groundwater impact	Health impairment
Fossil fuel use	Resource depletion	

Table 4.4 *Transferable forms for comparison of LCA results between competing systems.*

Item	Basis: 1	CPE (MJ)	GWP (g CO_2 eq.)
N fertilizer (urea)	kg	49.25	2940
P fertilizer (triple superphosphate)	kg	18.81	1160
K fertilizer	kg	5.6	380
Diesel	MJ	1.114	74.4
Electricity mix	MJ	2.597	173.4
Natural gas (NG)	MJ	1.016	61.2
Liquified petroleum gas (LPG)	MJ	1.06	76.4
Fuel oil	MJ	1.11	94.9
Hexane	kg	37.5	861
Methanol	kg	12.872	2836
Hydrogen	kg	183.2	11888
Soy meal	kg	4.13	726

with other systems. Issues of durability and maintenance should be taken into account for a realistic comparison between the same functional products.

In a goal and scope definition, system boundaries, LCIA methods and purpose must be defined with clear justifications. These will relate to audience and uses of a study. Assumptions, data availability, limitations and the quality of data are important to acknowledge for a system definition. It is important to recognize important impact categories for assessment at an early stage of an LCA. The supply of any component if changed from one region to another can affect impacts in accompanying categories. Thus, geographic regions need to be mentioned. System boundaries can show life cycle stages of productions and any transport involved.

Table 4.4 shows an example of *transferable form* for comparison. To compare between nitrogen fertilizers, a common basis of the mass of nitrogen in a fertilizer rather than the mass of the fertilizer should be selected. If the fertilizer (e.g., urea) is not in the pure form, then 1 kg of nitrogen can be selected as a basis for comparison between N based fertilizers. The unit that is highly dependent on the type of system or functionality to compare can be chosen to reflect the function or service for which a product has been produced. For example, 1 MJ of energy output from each of diesel, electricity, natural gas, LPG and fuel oil products may be compared in terms of the cumulative primary energy (CPE) use and GWP over 100 years. Likewise, if hydrogen rich gases produced from various flowcharts are to be compared for environmental impacts, the amounts of individual gas streams containing 1 kg of hydrogen can be taken as a basis. Thus, 1 kg of hydrogen production is the common basis (functional unit) for comparison of environmental impacts between various gas streams.

Figure 4.8 shows the boundary of an integrated crop and residue based biorefinery system. Assumptions, data availability, limitations and the quality of data are important to acknowledge for a system definition. It is important to recognize important impact categories for assessment in LCA that can be done at any stage and included in the goal and scope definition later. Assumptions and applicability of data over geographic regions and time scales must also be defined. The supply of any component if changed from one region to another may affect impacts in accompanying categories. Generally, 20 years and 100 years of time horizons are chosen for environmental impact assessment. In Figure 4.8, the system boundary shown considers the subsoil preparation outside the boundary, because the subsoil preparation occurs once before a given crop can be grown annually, when a steady state can be assumed, which is further explained in the section on land use.

Various cradle to grave system boundaries, such as for anaerobic digestion of sewage sludge for agricultural and energy generation applications, solar organic photovoltaic (OPV) glass manufacturing system and solar OPV cell manufacturing system, which can be considered within the goal and scope definition of the corresponding systems, are shown in Figures 4.9(a) to (c). The boundaries here are shown for the interactions between systems and the environment in terms of material and energy resource depletion and emissions to the environment. This is the convention followed in process engineering. However, in LCA, it is unnecessary to show such interactions between systems and the environment, because interactions are common: material resource (including land and water), primary energy resource and emissions to atmosphere, water and land.

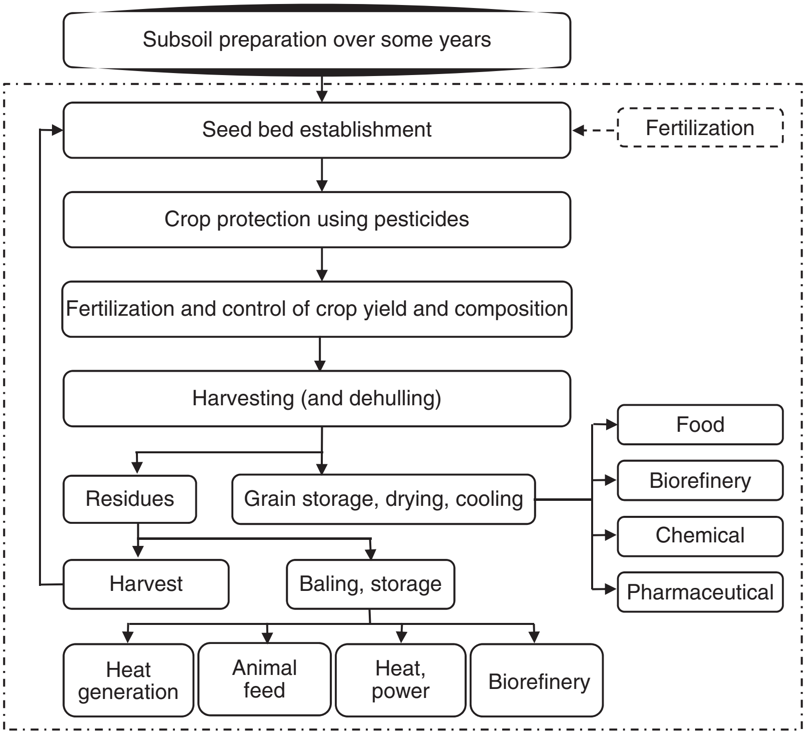


Figure 4.8 *Boundary of an integrated crop and residue based biorefinery system.*

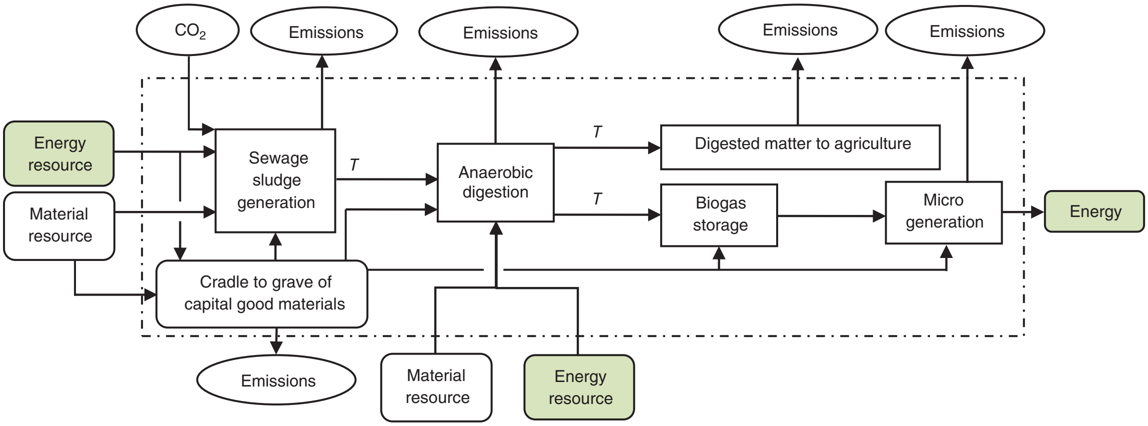


Figure 4.9(a) *Interactions between anaerobic digestion of sewage sludge system and the environment for LCA. T stands for transport.*

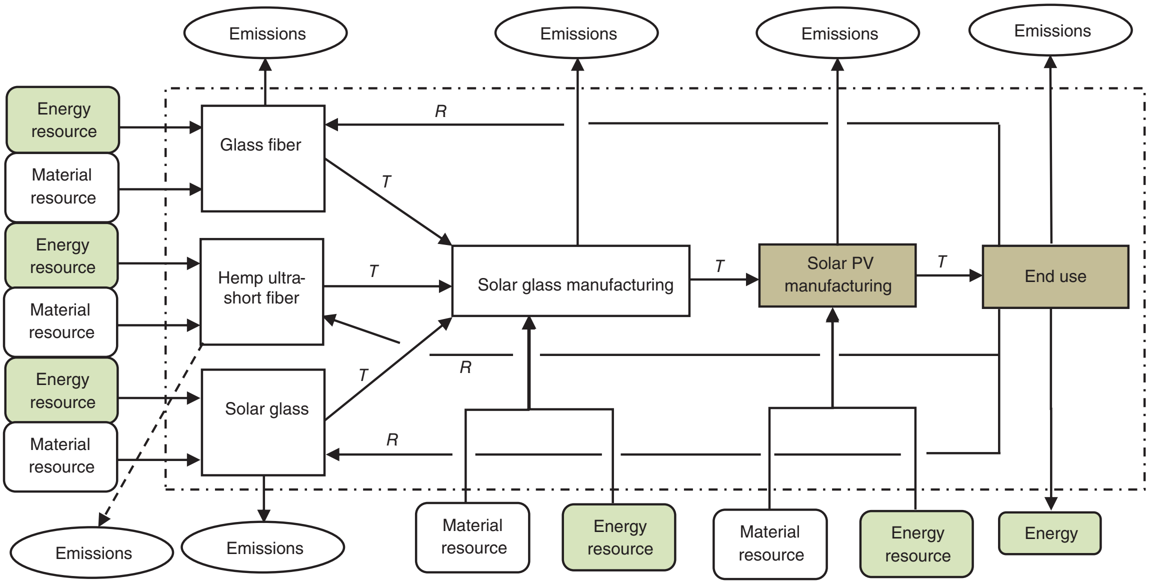


Figure 4.9(b) *Interactions between solar organic photovoltaic (OPV) glass manufacturing system and the environment for LCA. T stands for transport. R stands for recycle. T and R also cause resource depletion and environmental emissions. Only a part of the impacts from the "Solar PV manufacturing" and "End use" blocks that is due to solar glass manufacturing is considered within the system boundary.*

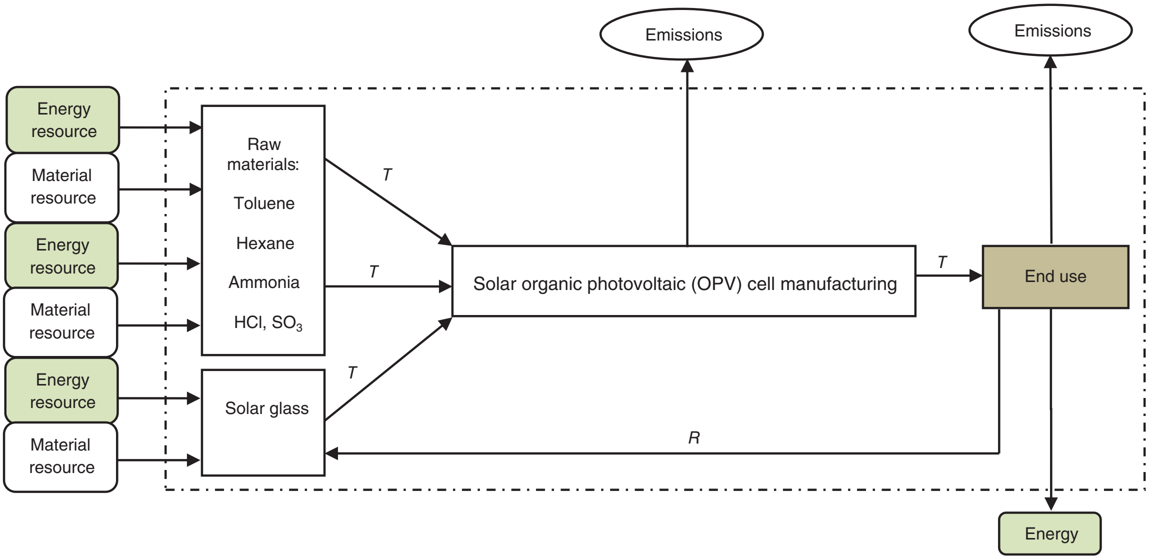


Figure 4.9(c) *Interactions between solar OPV cell manufacturing system and the environment for LCA. T stands for transport. R stands for recycle. T and R also cause resource depletion and environmental emissions.*

4.5 LCA: Inventory Analysis

The inventories are stressors or pollutants causing environmental impacts under various categories. Their analysis is about inlet and outlet mass and energy flow analysis. The inventory analysis is to identify each block of a process life cycle, for example, Figures 4.1 to 4.3, and to quantify the material and energy inputs and outputs for each of these stages.

The inventory analysis includes the following steps, detailed definition of the system, data collection, allocation and quantification of the environmental burdens. Each of the steps in the flowchart in Figures 4.1 to 4.3 can be expanded to look into substeps and to establish the mass and energy flows in and out of the boxes from/to the environment. Further, the compositions of streams emitted to water, land and air must be estimated for the assessment of impacts under various categories. This step may involve simulation/data collection/modeling of each box (e.g., fertilization and control of the crop yield step in Figure 4.8). The environmental burdens (B_j) can be quantified for each step, shown as

$$B_j = \sum bc_{j,i} x_i \tag{4.1}$$

where $bc_{j,i}$ is the burden j from the process i, while x_i is the mass or energy flow associated with that activity. The calculation is further explained by using example problems from biorefinery systems.

Broadly, there are three categories of environmental impacts: resource use, human health and ecological consequences (Table 4.2). They include:

1. Global impacts (global warming, ozone depletion, eutrophication, aquatic ecotoxicity)
2. Regional impacts (acidification)
3. Local impacts (photochemical oxidant creation, biodiversity).

These impact categories are further discussed in the Impact Assessment section.

Various LCI databases exist: Ecoinvent, ILCD/ELCD (ILCD: International reference Life Cycle Data system and ELCD: European reference Life Cycle Database), US-LCI, national ones such as in Australia and older ones include Buwal, IDEMAT, etc. In order to make an LCA study report transparent, the year of data publication, data source and the geographical relevance should be included. The data sets are adaptable and to bridge a gap may exist for process blocks.

Exercise 1. Draw a flowchart schematic with an inventory analysis for a wheat bioethanol plant consisting of processes shown in Table 4.5. The feedstock and raw material consumption rates on a daily basis and production specifications of various processes are shown in Table 4.5[7].

Table 4.5 *Basis for wheat bioethanol process flowsheet mass balance for Exercise 1. (Reproduced with permission from Sadhukhan et al. (2008)[7]. Copyright © 2013, Elsevier.)*

Process Unit	Feedstock	Product	Other Raw Materials	Specification
Milling (hammer)	Wheat: 340 kt	Milled wheat	–	–
Liquefaction	Milled wheat	Liquified grain	Process water	625.6 kt
			Sodium hydroxide	1.70 kt
			Calcium chloride	0.41 kt
			α-Amylase	0.28 kt
Saccharification	Liquified grain	Fermenter feed	Sulfuric acid	0.73 kt
			Glucoamylase	0.37 kt
Fermenter	Fermenter feed	Fermenter product: 88.27% CO_2 rich stream	Yeast	0.07 kt
CO_2 recovery	CO_2 rich stream	CO_2: 90%	–	–
Centrifugation	fermenter product	Ethanol rich stream: 74.68% Waste stream	–	–
Ethanol production	Ethanol rich stream	Ethanol: 17.934%	–	–
Rotary dryer	Waste stream	DDGS: 38.59%	–	–

Solution to Exercise 1. Figure 4.10 shows the flowchart schematic with an operational inventory analysis of a wheat bioethanol plant consisting of processes shown in Table 4.5.

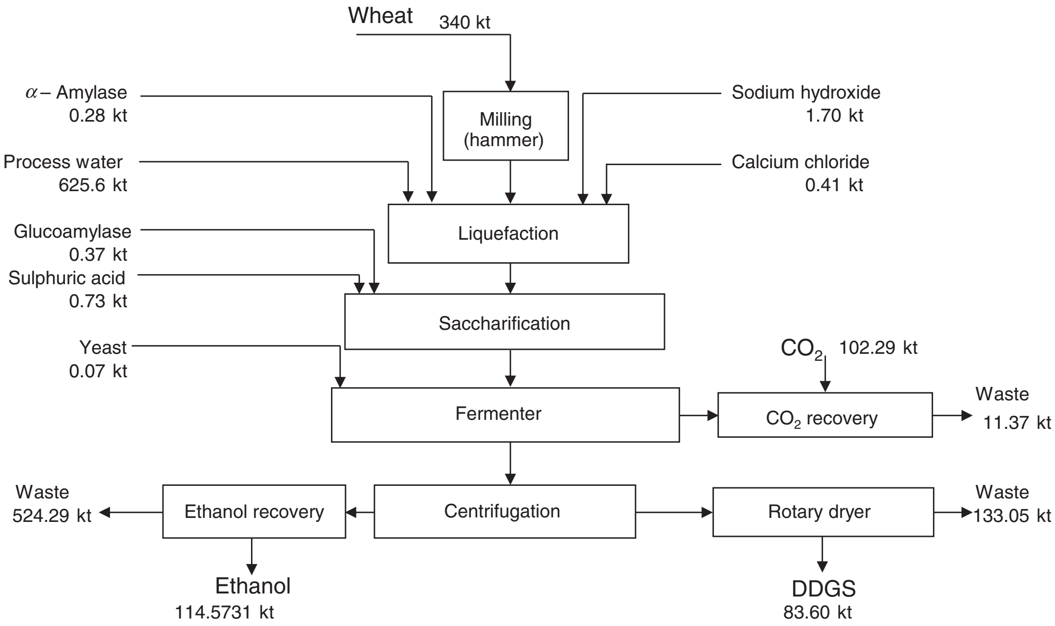


Figure 4.10 *Inventory analysis of wheat to bioethanol production plant operation. (Reproduced with permission from Sadhukhan et al. (2008)[7]. Copyright © 2013, Elsevier.)*

Exercise 2. The mass and energy distribution for a wheat bioethanol and straw combined heat and power (CHP) system in the UK is given in Table 4.6[8].

a. Complete the wheat bioethanol and straw CHP system mass and energy balance for a functional unit of 1 hectare of land use for the cultivation, shown in Figure 4.11(a). Sketch the system with completed operational inventory data.

Table 4.6 *Stream data for Exercise 2. (Reproduced with permission from Martinez-Hernandez et al. (2013)[8]. Copyright © 2013, Elsevier.)*

Subsystem	Product	Yield	LHV (GJ t^{-1})
Wheat cultivation	Wheat	6.96 t DM ha^{-1}	18.6
	Straw[a]	3.49 t ha^{-1}	14.6
Bioethanol plant	Ethanol	0.34 t t^{-1} (DM wheat basis)	26.7
	DDGS	0.25 t t^{-1} (DM wheat basis)	18.2
Straw CHP plant (processes 60% of the total straw cultivated)	Electricity	1060 kW h t^{-1} (straw basis)	
	Heat	567 kW h t^{-1} (straw basis)	

[a] Total amount of straw cultivated before soil retention; 40% of this amount is retained in the soil for enriching nutritional value.
DDGS: dried distillers grains and solubles.
DM: dry matter.
LHV: lower heating value (*c.f.* Section 10.2.2).
1 GJ = 304.2 kW h based on 8000 operating hours per year. This is based on the following calculation: 1 GJ = $\frac{10^6}{3600} \times \frac{365 \times 24}{8000}$ kW h.

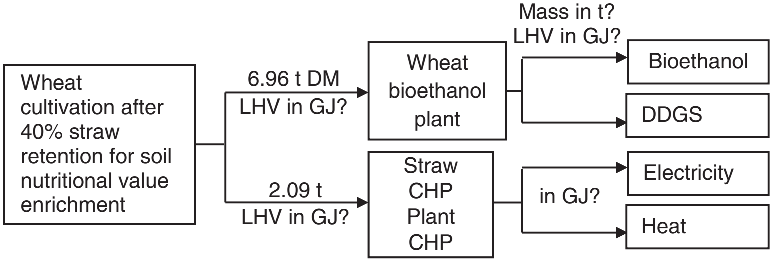


Figure 4.11(a) *Development of wheat bioethanol and straw CHP system mass and energy balance.*

b. Repeat the calculation for a functional unit of 100 t d^{-1} of bioethanol production. Sketch the mass and energy flow diagram. Calculate the land use for the production of 100 t d^{-1} of wheat bioethanol in the UK.
c. Calculate the energy efficiency of the straw based CHP plant.
d. Calculate the energy efficiency of the wheat bioethanol plant, if only bioethanol is used as an energy product.
e. In 2010 in the UK, there were 1.2 million hectares of land available for wheat cultivation. The CHP requirement from the biomass in the UK was 48.2 PJ y^{-1} (1 petajoule = 10^{15} joule). Estimate the percentage contribution potential of CHP from the available wheat straw.

Solution to Exercise 2

a. Figure 4.11(b) shows the completed mass and energy balance on the flowchart on the basis of 1 hectare.
b. Hint: the basis a functional unit of 100 t d^{-1} of ethanol production. Multiply all the mass and energy values in Figure 4.11(a) by 42.26 (obtained from 100/2.37). The UK land requirement for the production of 100 t d^{-1} of wheat bioethanol is 42.26 hectares.
c. The energy efficiency of the straw based CHP plant = 37% (obtained from the energy balance in Figure 4.11(b): $(7.3 + 3.9)/30.6 \times 100$).
d. The energy efficiency of the wheat bioethanol plant is 49%, if bioethanol is only used as an energy product (obtained from the energy balance in Figure 4.11(b): $63.2/129.5 \times 100$). All the energy inputs and outputs other than the wheat energy input and bioethanol energy output are neglected.
e. The UK straw CHP generation per unit land is 11.2 GJ per hectare (Figure 4.11(b)). Thus, the excess straw CHP energy yield is: $11.2 \times 1.2 = 13.44$ PJ y^{-1} from 1.2 million hectares of land available for wheat cultivation. The percentage contribution potential of CHP from the available wheat straw towards UK's total CHP requirement of 48.2 PJ y^{-1} is 28%.

Process simulation can also be used for data extraction for an inventory analysis. An example of the use of Aspen Plus, a process simulator, for the impact assessment of a bio-oil based methanol and a bio-oil based Fischer–Tropsch (FT) liquid synthesis plant[9,10] is shown as follows in Exercise 3.

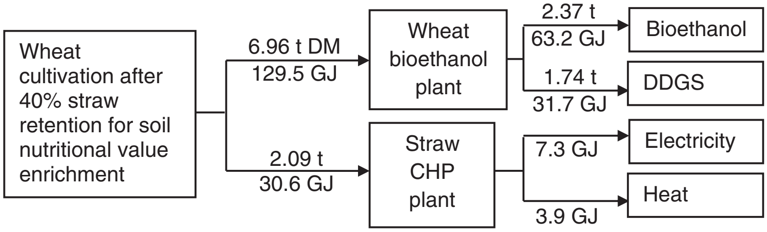


Figure 4.11(b) *A wheat bioethanol and straw CHP system mass and energy balance on the basis of 1 hectare land use.*

Exercise 3. The inventory analysis of a bio-oil based methanol and a bio-oil based Fischer–Tropsch (FT) liquid synthesis plant is shown in Figure 4.12. The details of these process simulations and technoeconomic analyses are available in Ng and Sadhukhan (2011)[9,10] and Sadhukhan and Ng (2011)[11]. A portion of CO_2, 0.75 kg per kg of bio-oil separated by Sulfinol unit (from the "Heat recovery, Water gas shift and Gas cleaning block" in Figure 4.12) is capture-ready and, therefore, is not accounted for in the plant GWP impact. CO_2 along with water vapor and nitrogen (in air) in the exhaust gas is emitted to the atmosphere after combined heat and power (CHP) generation. Calculate the GHG impact from the exhaust gas for the given plant capacity.

Mass fraction of exhaust gas	Methanol synthesis	FT synthesis	GHG impact kg CO_2 eq.
CO_2	0.16	0.17	1
H_2O	0.15	0.13	0.08218
N_2	0.69	0.7	
Exhaust gas, kt d^{-1}	57	37	
GHG impact, kt CO_2 eq. d^{-1}	9.9	6.7	

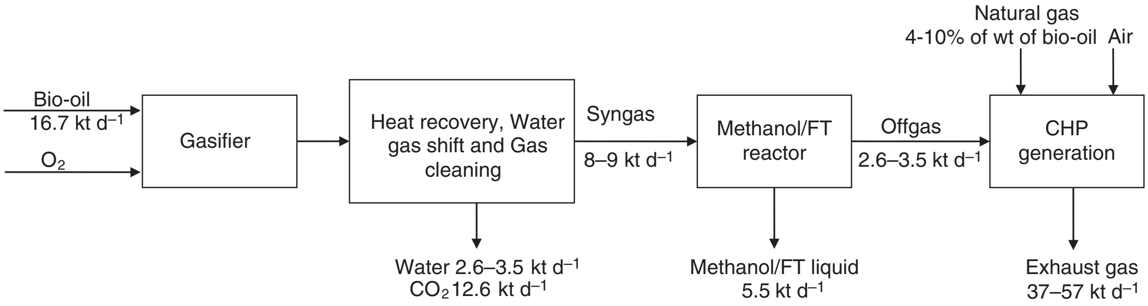


Figure 4.12 *Simulation results of kt CO_2 eq. d^{-1} bio-oil based methanol and a bio-oil based Fischer–Tropsch (FT) liquid synthesis plants for the impact assessment. The GHG impact (in kt CO_2 eq. d^{-1}) from the exhaust gas for the given plant capacity calculated is shown in the inset table.*

Solution to Exercise 3. Figure 4.12 shows the problem data and the inset table shows the solution in terms of the GHG impact from the exhaust gas.

The mass fractions and flow rates of the exhaust gases from the methanol and FT liquid synthesis centralized plants are shown in Figure 4.12. CO_2 and water vapor contribute to the GWP by a total of $(57 \times 0.16 + 57 \times 0.15 \times 0.08218) =$ 9.9 kt CO_2 eq. d^{-1} or $(9.9/16.7) = 0.6$ kg CO_2 eq. kg^{-1} of bio-oil and 6.7 kt CO_2 eq. d^{-1} or 0.4 kg CO_2 eq. kg^{-1} of bio-oil from methanol and FT synthesis centralized plants, respectively.

Exercise 4. A biomass boiler can use straw/wood/RDF (refuse-derived fuel) fuels to produce 50 MW energy output. The ultimate analyses of the fuels are shown in Tables 4.7 to 4.9, respectively. If the fuels are fully combusted in the presence of a stoichiometric amount of oxygen, estimate the composition and the GWP of the exhaust gas resulting from the combustion of the fuels. Assume that nitrogen, sulfur and chlorine present in the fuels do not contribute to the GHG emissions. Assume that ash is removed completely in the solid phase from the biomass boiler.

Solution to Exercise 4. To calculate the emissions resulting from the process operation, mass balance and energy efficiency are used in the first place. The basis assumed in this case is 50 MW of energy output.

Table 4.7 *Proximate and ultimate analyses of straw. (Reproduced with permission from Sadhukhan et al. (2009)[12]. Copyright © 2009, American Chemical Society.)*

Proximate Analysis (wt%)		Ultimate Analysis (wt%)	
Moisture	8.5	C	36.57
Volatile matter	64.98	H	4.91
Fixed C	17.91	O	40.7
Ash	8.61	N	0.57
LHV, MJ kg^{-1}	14.6	S	0.14

Table 4.8 *Proximate and ultimate analyses of wood[12].*

Proximate Analysis (wt%)		Ultimate Analysis (wt%)	
Moisture (after long storage)	25	C	51.8
		H	5.7
Ash (dry basis)	1.1	O	40.9
LHV (dry basis), MJ kg^{-1}	19.3	N	0.1

Table 4.9 *Proximate and ultimate analyses of RDF.*

Proximate Analysis (wt%)		Ultimate Analysis (wt%)	
Moisture	50	C	45.5
Volatile matter	79.6	H	5.8
Fixed C	10	O	37.8
Ash	10.5	N	0.3
		S	0.2
LHV, MJ kg^{-1}	17.73	Cl	0.4

An energy efficiency value should be assumed to determine the biomass feed flow rate from its lower heating value (LHV). The energy efficiency that is calculated using the equation below is found to be 40–45% for combined heat and power (CHP) generation from a biomass[12]:

$$\text{Energy efficiency of CHP generation from biomass} = \frac{\text{Output energy generation}}{\text{Energy input in biomass}} \tag{4.2}$$

Based on a realistic assumption of an energy efficiency of 0.4 of the biomass CHP plant, the mass flow rates of straw (LHV = 14.6 MJ kg^{-1}), wood (19.3 MJ kg^{-1}) and RDF (17.73 MJ kg^{-1}) biomass feedstocks required are calculated as follows.

Assume 8000 operating hours per year. Then

$$\frac{50}{0.4\times 14.6}\times 3600\times \frac{8000}{365}\times \frac{1}{1000} = 675\ \text{t d}^{-1}\ \text{straw feedstock}$$

$$\frac{50}{0.4\times 19.3}\times 3600\times \frac{8000}{365}\times \frac{1}{1000} = 511\ \text{t d}^{-1}\ \text{wood feedstock}$$

$$\frac{50}{0.4\times 17.73}\times 3600\times \frac{8000}{365}\times \frac{1}{1000} = 556\ \text{t d}^{-1}\ \text{RDF feedstock}$$

However, the energy efficiency is not a flat number for any type of biomass feedstock. For more precise results, a rigorous process simulation must be undertaken to determine the energy efficiency for specific biomass processing plants for a range of given operating conditions.

Table 4.10 *Emissions to atmosphere, land and water from the operation of 50 MWe of electricity generation plant for the three types of biomass.*

Emissions to:	Pollutant[1] or Component[2]	Straw (t d^{-1})	Wood (t d^{-1})	RDF (t d^{-1})
Atmosphere	[1]CO_2	906	728	923
	[2]N_2	1029	1110	2050
Land	[2]S	0.9	0	1.1
	[1]Ash	58	6	58
Water	[1]Effluent	35.6	32.4	28.9
	Total oxygen (air) requirement	649 (2786)	548 (2350)	719 (3085)

Hence, the following emissions result from the fuel combustion into 50 MW energy generation:
Straw: 906 t CO_2 d^{-1}
Wood: 728 t CO_2 d^{-1}
RDF: 923 t CO_2 d^{-1}

Table 4.10 shows the emissions to atmosphere, land and water from the operation of 50 MWe of an electricity generation plant using mass balance based on the three types of biomass selected. The exhaust gas has primarily carbon dioxide and steam generated from carbon and hydrogen combustion, respectively. Several other assumptions are required.

Nitrogen present in the biomass leaves along with the exhaust gas as gaseous nitrogen. Hence there is no atmospheric emission impact associated with the processing of nitrogen embedded in the biomass body. Though the impact of nitrogen and other GHGs will be significant, if inventories for fertilizer production for biomass growth are considered.

Sulfur present in the biomass is converted into hydrogen sulfide that is generally removed during gas clean-up. Hence, the exhaust gas is free of any sulfur compound. The hydrogen sulfide removed is finally recovered as metallic sulfur using the Claus process. Hence, there is no associated sulfur emission in the exhaust gas from the operation of a biomass boiler.

Land emission from a biomass CHP plant operation results from the ash present in the biomass. A small percentage of the land emissions can be leached into the aqueous body. Metallic components present in the biomass can also be emitted to land and water.

Component Balance

Carbon. The carbon content of the biomass (C in weight %, obtained from the ultimate analysis given in Tables 4.7 to 4.9) is converted into carbon dioxide. The molar mass of carbon dioxide is 44 and that of carbon is 12.

$$CO_2 \text{ mass flow rate in t d}^{-1} = \frac{(C)}{100} \times \frac{44}{12} \times \text{Biomass feedstock mass flow rate in t d}^{-1} \tag{4.3}$$

Sulfur. Sulfur (S in weight % in Tables 4.7 to 4.9) in a biomass feedstock is recovered as a solid product using the sulfur recovery unit via the production of hydrogen sulfide.

$$\text{S mass flow rate in t d}^{-1} = \frac{(S)}{100} \times \text{Biomass feedstock mass flow rate in t d}^{-1} \tag{4.4}$$

Ash. Ash (*Ash* in weight % in Tables 4.7 to 4.9) in a biomass feedstock is disposed to land.

$$\text{Ash mass flow rate in t d}^{-1} = \frac{(\text{Ash})}{100} \times \text{Biomass feedstock mass flow rate in t d}^{-1} \tag{4.5}$$

Water. Hydrogen present (H in weight % in Tables 4.7 to 4.9) in a biomass is combusted to generate steam. This steam and moisture present (H_2O in weight % in Tables 4.7 to 4.9) in the body of a biomass give rise to condensate after energy recovery.

$$\text{Effluent purge flow rate in t d}^{-1} = 0.1 \times \left(\frac{(H)}{100} \times \frac{18}{2} + \frac{(H_2O)}{100}\right) \times \text{Biomass feedstock mass flow rate in t d}^{-1} \tag{4.6}$$

Some negligible amount of hydrogen is used up by the sulfur and chlorine present in the biomass. After effluent purge (10% by mass of the condensate), the remaining condensate is recovered as boiler feed water (BFW). An equal amount of fresh BFW is required to make up for the lost amount. Moisture can also emit with the exhaust gas in some process configurations without heat recovery from the exhaust gas. Some industrial systems still adopt this to maintain a required chimney length for releasing exhaust gas to the atmosphere. The downside of such a process is the lost opportunity for heat recovery, resulting in lower energy efficiency. The molar mass of water is 18 and that of hydrogen is 2.

Oxygen. The oxygen required is calculated from the balance of stoichiometric oxygen required for the combustion of carbon and hydrogen present in the biomass and the oxygen available (O in weight % in Tables 4.7 to 4.9) in the biomass.

$$\text{Oxygen required in t d}^{-1} = \left(\frac{(\text{H})}{100} \times \frac{16}{2} + \frac{(\text{C})}{100} \times \frac{32}{12} - \frac{(\text{O})}{100}\right) \times \text{Biomass feedstock mass flow rate in t d}^{-1} \tag{4.7}$$

The source of oxygen is air.

$$\text{Air required in t d}^{-1} = \frac{\text{Oxygen required in t d}^{-1}}{32} \times \frac{(0.79 \times 28 + 0.21 \times 32)}{0.21} \tag{4.8}$$

The atomic mass of oxygen required to combust 1 mole of hydrogen (molar mass = 2) into 1 mole of water is 16. The molar mass of oxygen to combust 1 mole of carbon (molar mass = 12) into 1 mole of carbon dioxide is 32. Assume that air consists of 79 volume or molar % of nitrogen and rest of oxygen. Molar mass of nitrogen is 28 and that of oxygen is 32. A part of the oxygen is produced from the air separation unit (ASU).

For straw:

$$\text{Oxygen produced from the ASU in t d}^{-1} = 0.5 \times \text{Biomass feedstock mass flow rate in t d}^{-1} \tag{4.9}$$

For wood:

$$\text{Oxygen produced from the ASU in t d}^{-1} = 0.67 \times \text{Biomass feedstock mass flow rate in t d}^{-1} \tag{4.10}$$

For RDF:

$$\text{Oxygen produced from the ASU in t d}^{-1} = 0.61 \times \text{Biomass feedstock mass flow rate in t d}^{-1} \tag{4.11}$$

Nitrogen. The source of nitrogen outlet from a biomass based energy generation plant to the atmosphere is that supplied with the air and that present in the biomass feedstock (N in weight % in Tables 4.7 to 4.9), shown in the following equation:

$$\begin{aligned}&\text{Nitrogen outlet flow rate in t d}^{-1}\\ &= \frac{\left(\text{Oxygen required in t d}^{-1} - \text{Oxygen produced from the ASU in t d}^{-1}\right)}{32} \times \frac{0.79 \times 28}{0.21}\\ &+\frac{(\text{N})}{100} \times \text{Biomass feedstock mass flow rate in t d}^{-1}\end{aligned} \tag{4.12}$$

Chlorine in the case of RDF can be removed during process clean-up.

Exercise 5. Biomass gasification processes are commonly integrated to gas turbine for combined heat and power (CHP) generation. Figure 4.13 shows a biomass integrated gasification combined cycle (BIGCC) flowsheet configuration.

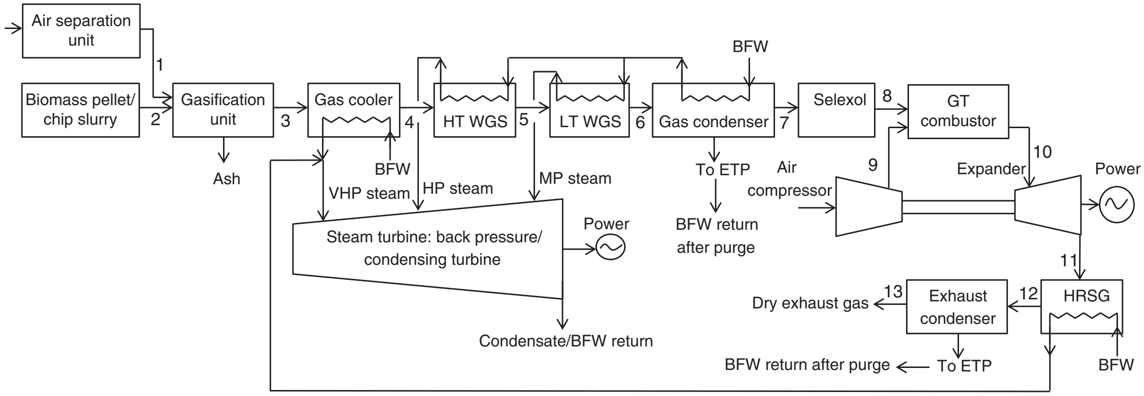


Figure 4.13 *Biomass integrated gasification combined cycle (BIGCC) flowsheet configuration. BFW, boiler feed water; ETP, effluent treatment plant; GT, gas turbine; HRSG, heat recovery steam generator; HP, high pressure; MP, medium pressure; VHP, very high pressure.*

Simulate the BIGCC process flowsheet based on the process models shown in Table 4.11[10]. Table 4.12 shows the correlations for the yields of products: gas, tar and char from biomass primary pyrolysis or devolatilization[12]. Primary pyrolysis or devolatilization is a common occurrence as soon as biomass comes in contact with the hot bed in the gasifier. Biomass breaks down into gas, tar and char products. Gas and tar are steam gasified into a product gas. Char could be combusted in a separate combustor to supply the reforming heat in the gasifier. Alternatively, char could be gasified in the same gasifier. The product gas from the steam gasifier after purification mainly consisting of carbon monoxide and hydrogen is called syngas.

Determine the mass and energy inventories of the BIGCC plant operations for straw, wood chip and refuse-derived fuel (RDF). The proximate and ultimate analyses of straw, wood and RDF are shown in Tables 4.7 to 4.9, respectively.

The solution of this exercise problem is given in the ***Online Resource Material in the Companion Website: Case Study 1.***

4.6 LCA: Impact Assessment

In this phase, the results from the inventory analysis are used to evaluate the potential of different environmental impacts. The inventory data are converted into environmental effects by multiplying a flux of an inventory with an impact characterization factor. The impact characterization factor of an environmental load (or substance or chemical or pollutant) indicates its intensity to an impact category with respect to a reference substance. For example, methane's GWP impact characterization factor of 25 g CO_2 equivalent means that methane has 25 times more GWP compared to carbon dioxide. Various methodologies for LCIA exist, detailed in Section 4.8. Different extents of effects, such as primary, mid- and end-points, normalization, weighting and valuation are used in different LCIA methodologies. Different impact categories are also included in different LCIA methodologies. The assessment is done on the basis of the scope and goal defined for the study. The impact assessment can be carried out using the following steps:

1. Classification
2. Characterization
3. Normalization
4. Valuation.

In classification, inventory data are assigned to different impact categories. Various pollutants resulting from an inventory analysis are classified under various impact categories.

Table 4.11 BIGCC flowsheet modeling. (Reproduced with permission from Sadhukhan et al. (2009)[12]. Copyright © 2009, American Chemical Society.)

Unit Names	Modeling Framework	Process Specification
Gasification	Estimate pyrolysis or devolatilization product yield using EXCEL spreadsheet based model shown in Table 4.12. Use RGibbs reactor in Aspen Plus for the gasification of pyrolysis product into product gas.	Temperature = 900–950 °C. Desired product decides the system and the gasification operating pressure. Pressure = near atmospheric when integrating to fuel cell or 25–30 bar for combined cycle integration and fuel and chemical production.
Air compressor	Compressor Isentropic model in Aspen Plus.	Desired product decides the system and compressors' operating pressure. Isentropic efficiency = 75%.
Gas cooler and heat recovery steam generator (HRSG)	Cooler in Aspen Plus.	Temperature is just above the dew point of the gas/flue gas at the system/gasification pressure, such that single-phase gas still leaves the cooler/HRSG without requiring special design of the gas cooler/HRSG.
Gas or exhaust condenser	Flash2, two-phase flash separator in Aspen Plus.	Keep at or lower than the dew point of the gas, so as to dry the gas from the water present in the gas. After purification in the effluent treatment plant (ETP) and 10% purge, the rest of the water is recovered as boiler feed water (BFW).
High temperature water gas shift reactor (HT WGS)	REquil: Rigorous Equilibrium reactor based on stoichiometric approach in Aspen Plus.	Temperature = 450 °C at the system pressure. The water gas shift reaction is as follows: $CO + H_2O \rightleftharpoons CO_2 + H_2$
LT (low temperature) WGS	REquil in Aspen Plus.	Temperature = 350 °C at the system pressure.
Gas clean-up and carbon capture and storage; air separation unit	Sep2: two-outlet component separator based on component purity, flow, etc., for the site flowsheet simulation in Aspen Plus. Individual processes (such as Selexol) can be simulated in detail.	Specify the mole fraction of the component to be separated as 1 in the outlet pure gas.
Gas turbine (GT) combustor	REquil in Aspen Plus.	1300 °C temperature at the system pressure. This temperature restricts the NO_x emission. The combustion reactions of syngas include the following: $CO + 0.5O_2 \rightleftharpoons CO_2$ $H_2 + 0.5O_2 \rightleftharpoons H_2O$ $CH_4 + 2O_2 \rightleftharpoons CO_2 + 2H_2O$
GT expander	Turbine Isentropic model in Aspen Plus.	Exit pressure = Near atmospheric but allowing pressure drop across HRSG. Isentropic efficiency = 75–90%.
Steam gasifier in allothermal gasification	RGibbs reactor in Aspen Plus. Gas and tar yields from the spreadsheet based pyrolysis or devolatilization product yield modeling (Table 4.12) are to be entered as feedstock to the steam gasifier model in Aspen Plus.	Temperature = 900–950 °C. Desired product decides the system and the gasification operating pressure. Pressure = near atmospheric (when integrating to fuel cell) or 25–30 bar (IGCC, fuel and chemical production).
Char combustor cooler	Cooler in Aspen Plus.	Temperature is above the dew point of the flue gas at atmospheric pressure, such that single-phase gas still leaves the cooler without requiring special design of the cooler.
Direct quench	Flash2, two-phase flash separator in Aspen Plus.	Kept at or lower than the dew point of the gas, so as to dry the gas from the water present in the gas. After effluent treatment and 10% purge, the rest of the water is recovered as BFW.
Char combustor in allothermal gasification	RGibbs reactor in Aspen Plus. Char yield from the spreadsheet based pyrolysis or devolatilization product yield model entered as feedstock to the char combustor model in Aspen Plus.	About 50 °C higher temperature than steam gasifier to maintain the temperature gradient and supply exothermic heat of the combustion reaction to the steam gasifier.

Table 4.12 *Correlations for the yields of products: gas, tar and char from biomass primary pyrolysis or devolatilization*[12].

Component	kg per kg biomass
Total devolatilization	0.96
Total gas	0.48
H_2	0.00
CH_4	0.02
C_2	0.12
CO	0.22
CO_2	0.03
H_2O	0.08
Tar	Total devolatilization – Total gas
Char	1 – Total devolatilization

The characterization factors are assigned to them according to their relative contributions to the environmental impacts. For example, for calculating the GWP, the contribution of methane or any other GHG is given in relation to the impact of CO_2. Some of the impact categories are the GWP over 20, 50 or 100 years, eutrophication potential (EP), acidification potential (AP), ozone depletion, human toxicity and aquatic toxicity. The environmental impact can be calculated using.

$$E_k = \sum\nolimits_{j=1}^{J} ec_{k,j} B_j \tag{4.13}$$

where $ec_{k,j}$ is the relative contribution of burden B_j (j is the index for pollutant; J is the total number of pollutants) to environmental impact E_k (k is the index for impact category.

In normalizing, impacts are represented with respect to the total emissions in certain areas or over a period of time. This can be useful to assess the potential effects of the activity on a regional or global environment. However the normalization results are not always reliable due to lack of reliable data for many impacts.

Valuation is the final step of impact assessment wherein relative importance of each impact is determined on the basis of a value or weight assigned to it. The environmental impacts (EI) can be aggregated into a single environmental impact function, shown as

$$EI = \sum\nolimits_{k=1}^{K} w_k E_k \tag{4.14}$$

where w_k is the relative importance of E_k and K is the total number of environmental impact strategies.

The commonly occurring pollutants from power plants are carbon dioxide, methane, chlorofluorocarbons (CFCs), VOCs, nitrous oxide, nitrogen oxides (NO_x) and sulfur dioxide. Figure 4.14 shows commonly occurring atmospheric pollutants and their characterization factors, resulting in various environmental impacts. The characterization factors depend on physicochemical properties of pollutants and are provided in relative terms compared to a base pollutant (assumed a value of 1 in an impact category). For example, CO_2 is a base pollutant for the GWP impact category, that is, its GWP characterization factor is 1.

One of the most effective sets of primary impact characterizations and their units, developed by CML, are shown in the following list from the Institute of Environmental Sciences, Leiden University, Netherlands. A spreadsheet with the primary impact characterization factors of all tested chemicals is freely available from their website. Various other

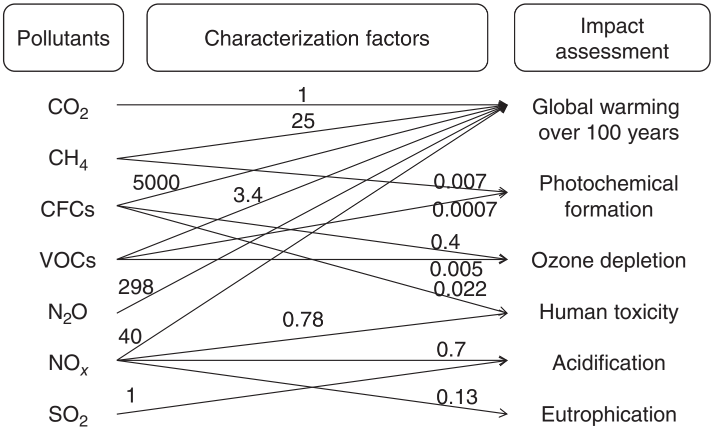


Figure 4.14 *Pollutants with characterization factors resulting in various environmental impacts.*

sources of characterization factors are available[13–20]. 1,4-Dichlorobenzene (DCB) is used as the base chemical for the toxicity categories. The various impact categories for assessment are discussed thereafter.

Resources
1. Abiotic depletion element (kg Sb equivalent)
2. Abiotic depletion fossil (MJ)

Emissions
1. Global warming potential (kg CO_2 equivalent)
2. Acidification potential (kg SO_2 equivalent)
3. Eutrophication potential (kg phosphate equivalent)
4. Ozone layer depletion potential (kg R-11 equivalent; chlorofluorocarbon-11 or CFC-11 or refrigerant-11)
5. Photochemical oxidant creation potential (kg ethylene equivalent)
6. Freshwater aquatic ecotoxicity potential (kg DCB equivalent)
7. Human toxicity potential (kg DCB equivalent)
8. Marine aquatic ecotoxicity potential (kg DCB equivalent)
9. Terrestric ecotoxicity potential (kg DCB equivalent)

4.6.1 Global Warming Potential

The global warming potential (GWP) of all pollutants is presented relative to CO_2. The GWP of a pollutant is the ratio between the infrared absorption by the pollutant and the infrared absorption by an equal amount of CO_2. The GWP of CFCs is 5000 over a 100 year lifespan. Their units are also represented in terms of CO_2 equivalent, for example, kg CO_2 equivalent. The GHGs have different lifespans and therefore a basis of 20, 100 and 500 years is generally assumed over which the total GWP is predicted. In evaluating the environmental impact characterization factors, there is no geographical segregation considered. Henceforth, these environmental impact characterization factors, generally restricted up to the primary level of impacts, can be applied to analyze life cycle impacts of any products or process systems, irrespective of geographic locations. The following section provides an assessment of environmental impact characterization factors using example problems. The other important impact categories of global importance for biorefinery systems are explained as follows.

4.6.2 Land Use

Land is an important resource used for renewable energy supply. Biomass uses land for energy and value-added productions. Even though the second generation residues use much less land than the first generation crops, there are land implications during their growth phase. Imagine an agricultural residue, for example, straw, husk, corn stover, sugarcane, etc., is used for energy generation. Without land, these residues cannot be grown. These residues should be used for value-added productions: bulk, fine and specialty chemicals, for which there is no alternative sustainable carbon source. For energy generation, however, land use could be reduced by tidal, hydro, wind, solar, geothermal, etc., alternative to biomass. Municipal wastes have least implication of land use amongst all lignocellulose or waste biomasses.

The type of land differs widely within a geographical boundary. High to low grass lands are used for animal grazing and high fertile lands are used for arable feed crops. Poultry and pigs live on arable crops and therefore rely on fertility of arable lands graded as 3a, while grass lands belong to grade 2. Land use for organically grown systems is more due to building of fertility of the land. From an energy efficiency and environmental impact point of view, the objective is to maximize energy yield, for example, in joules per unit land used, for example, per hectare. Exercise 2 shows the energy yield calculation per unit land use. Sustainable energy crops must use lesser land compared to lignocellulose.

However, fertilizers are needed for growing any kind of crops, arable or energy crops. Fertilizer production and emissions are the hot spots of biomass production systems. The key to successful biorefineries is to mitigate these hot spots and minimize land use for biomass growth and land transformation from it. Both the type of land used and the fertilization application decide the energy or crop yield per unit land used. Thus, within the subject of land use, the steps involved in the agriculture of crops are highlighted from input–output with respect to system boundaries and environmental footprint perspectives. An illustration of the steps involved in the agriculture of arable crops is shown in Figure 4.8. A measure of land use refers to the crop or energy yield per unit land use during a steady-state period of an agricultural system shown within the boundary in Figure 4.8.

Outside this boundary, to prepare a land for agriculture for the first time, the subsoil nutritional value is enriched by nitrogen (N), phosphorus (P) and potassium (K) fertilizer applications. During this time, the input and output of N, P, K around the land are not in balance. Once the land reaches the required maximum nutritional stage for seed bed establishment, a steady state or equilibrium is reached, when N, P, K inputs to the land (fertilizer applications) and outputs from the land (fixation within a plant body and emission to the atmosphere in the case of nitrogen) are in balance. During this time, crops stabilize to steady yields. This is the time for crop rotation. Amongst N, P, K fertilizers, P and K fertilizers remain in solid forms. Hence, these solids form the basis of constitution of higher plants and animals and eventually at the end of their life cycles through various chemicals and species they return to mining extraction, sea bed, etc., via sludge.

However, nitrogen may be emitted as the atmospheric nitrogen gas as well as in eight various forms of NO_x, of which nitrous oxide (N_2O), nitric oxide (NO) and nitrogen dioxide (NO_2) are the more commonly occurring ones. Because of denitrification of the soil, nitrogen fertilizer is applied periodically during a crop rotation period to keep up with the soil nitrogen balance. Once a crop is harvested, dehulled to recover grain, the grain is stored, dried, cooled and transported to various application points. A similar process applies to agricultural residues after dehulling from harvested grains. A part of the residues dehulled from the grain is bedded into the soil to particularly retain the soil carbon balance and other nutritional balances for the next phase of seed bed establishment. Additional fertilizer may be needed at this point to keep the steady balance of N, P, K. Also herbicide is used for crop protection over a rotation.

Figure 4.15 shows the cumulative primary energy and the GWP impacts from a *Jatropha* agricultural system. The inventory refers to the production of 4.21 t of *Jatropha* fruit per hectare of land.

Impacts from fertilizers are the most notoriously known for any agricultural system. The biggest hot spot identified from an agricultural system impact assessment is the application of fertilizer, still primarily sourced from fossil resources.

The field emissions due to NO_x, mainly N_2O, followed by NO and NO_2, and seed conditioning are the second worst impact hot spots. Because of the prominent effect of nitrogen oxides on the environment, many scientists look at the nitrogen footprint, especially for agricultural systems (due to the application of fertilizers), separately from other GHG emissions, but analogous to the carbon footprint to get an idea of the magnitude of the problem.

The GWP, carbon footprint and nitrogen footprint can be estimated from an inventory analysis, shown in the following exercise problem, for two types of fertilizers.

Exercise 6. Calculate the GWP impact and the carbon and nitrogen footprint for two types of fertilizers, ammonium nitrate and urea, for the data shown in Table 4.13.

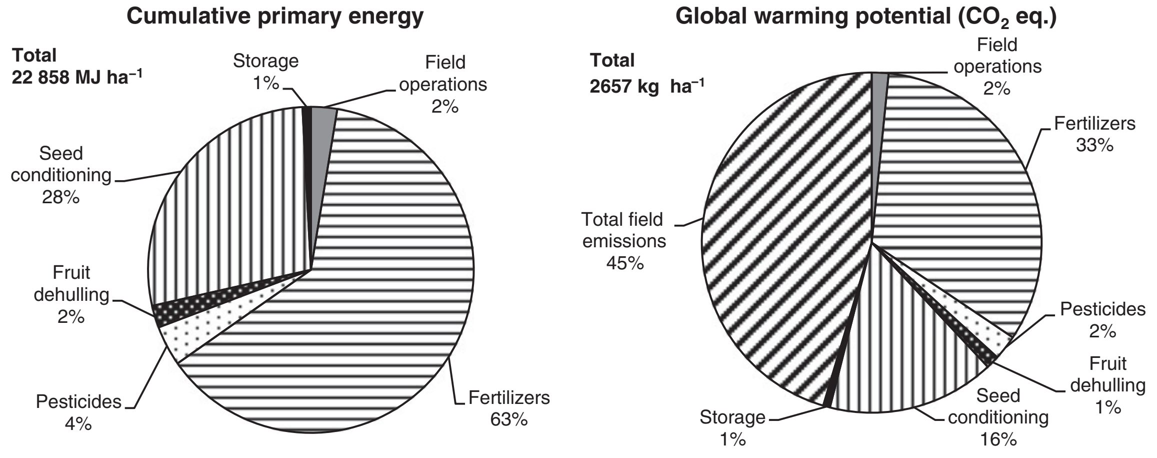


Figure 4.15 *Impact assessment of* Jatropha *fruit agricultural system for hot spot analysis on the basis of 1 hectare of land use.*

Table 4.13 *Pollutant emission data for ammonium nitrate and urea fertilizers and the characterization factors of the pollutants.*

Impact characterization factor	Pollutants					
	N_2O (kg)	CO_2 (kg)	VOC (kg)	CH_4 (kg)	NO_2 (kg)	CO (kg)
Global warming potential 100 years kg CO_2 eq.	298	1	3.4	25		1.9
Pollutant emissions	N_2O as nitrogen (kg)	CO_2 (kg)	VOC (kg)	CH_4 (kg)	NO_2 (kg)	CO (kg)
Ammonium nitrate as per kg nitrogen	0.005592	2.241140	0.000132	0.007007	0.002030	0.000690
Urea as per kg nitrogen	0.000008	2.713971	0.000123	0.008618	0.002310	0.000810

Solution to Exercise 6

GWP of ammonium nitrate

$$= \left(298 \times 0.005592 \times \frac{28+16}{28}\right) + (1 \times 2.241140) + (3.4 \times 0.000132) + (25 \times 0.007007) + (1.9 \times 0.000690)$$

$$= 5.0\ \mathrm{CO_2}\ \text{eq. per nitrogen, kg kg}^{-1}$$

GWP of urea

$$= \left(298 \times 0.000008 \times \frac{28+16}{28}\right) + (1 \times 2.713971) + (3.4 \times 0.000123) + (25 \times 0.008618) + (1.9 \times 0.000810)$$

$$= 2.9\ \mathrm{CO_2}\ \text{eq. per nitrogen, kg kg}^{-1}$$

Carbon footprint of ammonium nitrate

$$= [(1 \times 2.241140) + (3.4 \times 0.000132) + (25 \times 0.007007) + (1.9 \times 0.000690)] \times \frac{12}{44}$$

$$= 0.66\ \text{carbon per nitrogen, kg kg}^{-1}$$

Carbon footprint of urea

$$= [(1 \times 2.713971) + (3.4 \times 0.000123) + (25 \times 0.008618) + (1.9 \times 0.000810)] \times \frac{12}{44}$$
$$= 0.8 \text{ carbon per nitrogen, kg kg}^{-1}$$

Nitrogen footprint of ammonium nitrate

$$= 0.005592 + \left(0.00203 \times \frac{14}{14 + 32}\right)$$
$$= 0.0062 \text{ nitrogen per nitrogen, kg kg}^{-1}$$

Nitrogen footprint of urea

$$= 0.000008 + \left(0.002310 \times \frac{14}{14 + 32}\right)$$
$$= 0.0007 \text{ nitrogen per nitrogen, kg kg}^{-1}$$

Regarding land use impacts, there are three terms frequently used,

1. *Land use.* This is a measure of the actual use of land per unit yield of biomass, sometimes referred to the dry matter (DM) of the biomass. Its unit is m^2 per kg yield of biomass or m^2 per kg yield of DM of biomass.
2. *Land transformation.* It is a value lower than the value of land use. A fraction of the total land used for a given service (bioenergy production) can be transformed from one type to another, for example, cutting forest into a forest road for transporting timber. The land transformation constantly happens due to production of food, fiber and energy.

   The land transformation can be contributed by a range of activities on arable land, forest, construction, dump sites, industrial, mineral extraction, pasture and meadow, sea and ocean, permanent crop, shrub land, tropical rain forest, rail, road, urban and artificial water bodies and courses. Figure 4.16 shows an overview of the types of land transformation.

   A decision must be made in terms of selecting the feedstock with minimum land use for a required service, for example, heat and power production. The unit of land use or land transformation can be:

   m^2 per m^3 of biomass produced,
   m^2 per kg of biomass produced,
   m^2 per MJ of biomass calorific value,
   m^2 per MJ of net energy production.

3. *Land occupation.* Land transformation data can be converted into land occupational data, by multiplying the land transformation with the number of years for which the land is used after transformation. Hence, the unit for land occupational data is:

   m^2 year per m^3 of biomass produced,
   m^2 year per kg of biomass produced,
   m^2 year per MJ of biomass calorific value,
   m^2 per MJ of net energy production.

On the basis of inventory data of 1 kg of wheat grain production and corresponding straw production, the land occupation is 0.159 m^2 year per kg of wheat grain production; 99% of this land occupation is in the arable nonirrigated land and the remaining 1% is in forest, intensive, normal. Taking account of the yearly rotation of the crop, the land transformation for 1 kg of wheat grain and corresponding straw production is 0.159 m^2 per kg of wheat grain.

Table 4.14 shows % contributions of various categories in Figure 4.16 in land occupation for wood production. The value of land transformation varies between 0.89 m^2 m^{-3} for soft wood to 1.89 m^2 m^{-3} for hard wood, respectively. If the lifetime of the infrastructure used is assumed as 100 years, the land occupation is 89 m^2 year per m^3 of soft wood and 189 m^2 year per m^3 of hard wood, respectively.

The land use of soft and hard wood is 7.5–13.5 m^2 m^{-3}.

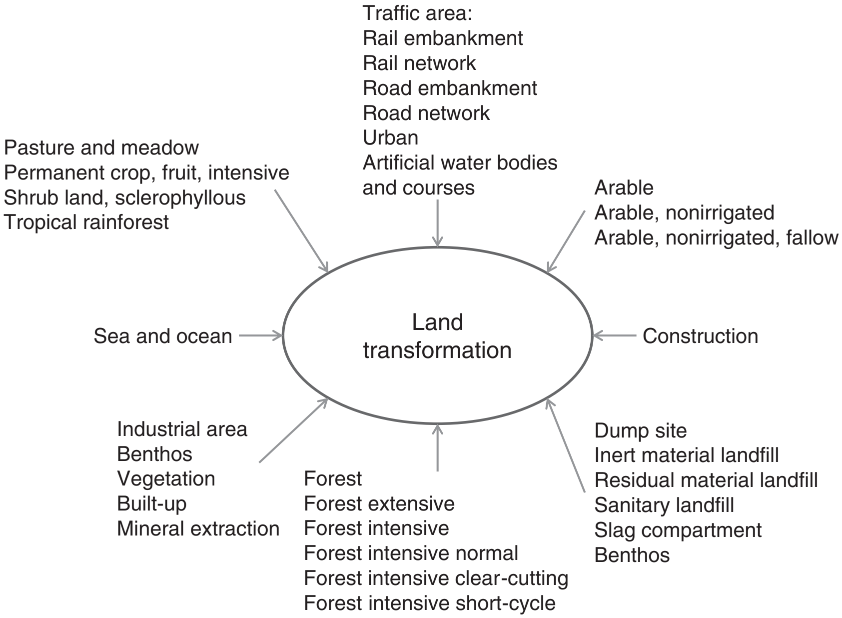


Figure 4.16 *Overview of land transformation types.*

Table 4.14 *The % contributions of various categories in Figure 4.16 in land occupation for wood production.*

Arable	0.00
Arable, nonirrigated	0.06
Arable, nonirrigated, fallow	0.00
Construction site	0.04
Dump site	0.50
Dump site, benthos	0.01
Forest, intensive	3.28
Forest, normal	87.52
Forest, short-cycle	0.00
Industrial area	0.18
Industrial area, benthos	0.00
Industrial area, built-up	0.84
Industrial area, vegetation	0.15
Mineral extraction site	1.49
Permanent crop, fruit, intensive	0.00
Shrub land, sclerophyllous	0.13
Traffic area, rail embankment	0.02
Traffic area, rail network	0.02
Traffic area, road embankment	0.95
Traffic area, road network	0.49
Urban, discontinuously built	0.00
Water bodies, artificial	0.39
Water courses, artificial	0.18

4.6.3 Resource Use

The implication of resource depletion must be understood, mainly that nonrenewables are compared to global reserves when using them for energy commodity productions. Nonrenewable resources including fossil resources, minerals and clays can only be regenerated within human lifetimes. The heaviest to lightest fossil resources are coal (also tar and heavy oils) > medium to light crude oils > natural gas. Unlike renewable resources, solar, wind and tidal, the nonrenewable resources are not continuously regenerated and are depleted over time. Therefore, the depletion of their reserves must be within control all the time and included in environmental impact characterization. The evaluation of the environmental impact characterization factors of nonrenewable resources is dependent on the energy efficiency of their conversion processes. The lower heating value (LHV: an indication of the transferable calorific value) of a nonrenewable resource and the efficiency of conversion processes into useful energy commodities can be multiplied to evaluate the output energy generation. Therefore, if the desired output energy and efficiency of conversion process are known, the nonrenewable resource depletion can be calculated.

Energy resource input (in MJ) × Efficiency of conversion process systems (in fraction) = Output energy generation (in MJ)

Like all other impacts, engineers need to understand the implication of resource depletion, mainly of nonrenewables, compared to global reserves when using them for energy commodity productions.

Exercise 7. Twenty-five million households with an annual average total heating and electricity demands (in the ratio of 2:1) of 172 15 kW h y^{-1} per household are to be supplied by coal and natural gas based energy systems, given in Table 4.15. It is proposed to build city level centralized and household–community level decentralized energy conversion systems. This high level analysis is aimed at assessing whether the resources available are adequate for meeting the household energy demand for two scenarios, the lowest cost scenario and the lowest GHG emission scenario. The LHV of coal and natural gas, the conversion system efficiency into electricity or heat generations, maximum resource supplies, cost ratio of systems compared to the lowest cost technology option and the GHG emission reduction potential are given in Table 4.15. The conversion systems under consideration are electricity generation without carbon capture and storage (CCS) using coal, heat generation using natural gas, electricity generation using natural gas and electricity generation with CCS using coal, from the lowest to the highest cost technology options, respectively. Determine the lowest cost scenario and the lowest GHG emission scenario in terms of the use of resource mix to meet the total household electricity and heat demands (1 PJ = 10^{15} J; 1 MT = 10^6 tonne).

Table 4.15 *Coal and natural gas data to supply household energy.*

	LHV (MJ kg^{-1})	Conversion into	Efficiency (%)	Resource Supply, (MT y^{-1})	Cost Ratio	GHG Emission Reduction (%)
Coal	28	Electricity without CCS	70	<40	1	0
		Electricity with CCS	36	<15	5	90
Natural gas	50	Heat	90	<14	2	40
		Electricity	70	<14	3	30
Electricity		Heat	90			

Solution to Exercise 7. The household electricity and heat demands on a yearly basis are calculated as follows:

Total household electricity and heat demands = $\left(25\times10^{6}\right)\times 17215\times\frac{1000\times3600}{10^{15}} = 1549$ PJ y^{-1}

Total household electricity demand = $1549\times\frac{1}{3} = 516$ PJ y^{-1}

Total household heat demand = $1549\times\frac{2}{3} = 1033$ PJ y^{-1}

The maximum energy resource supply constraints from the lowest to the highest cost technology options are as follows:

Coal energy used for electricity generation without CCS = 40 × 28 = 1120 PJ y^{-1}
Natural gas energy used for heat generation = 14 × 50 = 700 PJ y^{-1}
Natural gas energy used for electricity generation = 14 × 50 = 700 PJ y^{-1}
Coal energy used for electricity generation with CCS = 15 × 28 = 420 PJ y^{-1}

Lowest Cost Scenario. For the lowest cost energy resource use scenario, electricity generation from coal without CCS is selected first, as the lowest cost option, to meet the entire electricity demand of households of 516 PJ y^{-1}.

The total potential for electricity generation from coal at 70% efficiency is 1120 × 0.7 = 784 PJ y^{-1}. After meeting the household electricity demand of 516 PJ y^{-1}, the balance of electricity available from coal without CCS, 268 PJ y^{-1}, is converted into 241 PJ y^{-1} of heat at an efficiency of 90%, assuming that the cost of heat generation from electricity is not considerable.

This consumes all 1120 PJ y^{-1} of coal available.

The balance of heat (1033 − 241 = 792 PJ y^{-1}) is supplied by a natural gas based heat generation system at first, followed by heat from a natural gas electrification system. The maximum amount of natural gas energy available for direct heat generation is 700 PJ y^{-1} and can generate 630 PJ y^{-1} of heat, at 90% energy efficiency. Thus, the remaining household heat demand of 162 PJ y^{-1} is to be supplied from the natural gas based electricity system.

Natural gas consumed for meeting the rest of the heat requirements (162 PJ y^{-1}) via electrification is $162/(0.7 \times 0.9) =$ 257 PJ y^{-1}.

Natural gas remaining after meeting the heat requirement via electrification is 700 – 257 = 443 PJ y^{-1}.

The total amount of natural gas resources used is then 700 + 257 = 957 PJ y^{-1}. The coal to natural gas resource mix used to meet the total household heat and electricity demands is 1.2:1.

Table 4.16 shows the resource supply in terms of energy contents, output heat and electricity generations for households, energy efficiencies and the GHG emission reduction potential compared to the case of the coal energy system without CCS, where all GHGs are emitted to the atmosphere.

The evaluation shows that due to the mix of natural gas by 46% with the rest as coal, as the resources used, the overall GHG emission is reduced by 19% based on the output energy distribution. Overall 75% of energy efficiency is obtained. Note that the actual efficiency would be lower and GHG emission would be higher due to transmission losses, not taken into account in this high level analysis. The cost ratio shown is calculated on the basis of energy resource use as follows:

$$\frac{738 + 382 + 700 \times 2 + 257 \times 3}{2077} = 1.58$$

Lowest GHG Emission Scenario. For electricity generation, the order of preference of technologies for the lowest GHG emission scenario is the electricity generation from coal with CCS and electricity generation from natural gas, respectively.

For the heat supply, the order of preference for the lowest GHG emission scenario is as follows: heat generation from natural gas, heat generation from natural gas based electricity and electricity from coal with CCS systems, respectively.

Table 4.16 *Resource supply, output heat and electricity generations for households, energy efficiency and cost ratio, for the lowest cost resource use scenario.*

	Resource (PJ y^{-1})	Generation (PJ y^{-1})	Efficiency (%)	GHG Emission Reduction (%)	Cost Ratio
Coal without CCS electricity	738	516	70	0	1
Coal without CCS electricity – heat	382	241	63	0	1
Natural gas – heat	700	630	90	40	2
Natural gas electricity – heat	257	162	63	30	3
Total	2077	1549	75	19	1.58

Table 4.17 *Resource supply, output heat and electricity generations for households, energy efficiency and cost ratio, for the lowest cost resource use scenario.*

	Resource ($PJ\ y^{-1}$)	Generation ($PJ\ y^{-1}$)	Efficiency (%)	GHG Emission Reduction (%)	Cost Ratio
Coal with CCS electricity	420	151	36	90	5
Natural gas electricity	522	365	70	30	3
Natural gas – heat	700	630	90	40	2
Natural gas electricity – heat	178	112	63	30	3
Coal without CCS electricity – heat	461	291	63	0	1
Total	2281	1549	68	32	2.66

The resource use, output heat and electricity production for the household supply, efficiency, GHG emission reduction potential and cost implications for the lowest GHG emission scenario are shown in Table 4.17. The natural gas use as a resource compared to coal is higher by 1.6 times, for achieving the lowest emission energy scenario. Following the approach for the lowest cost scenario, try working out the solution for the lowest GHG emission scenario.

The GHG emission reduction potential is improved by 32% based on the output energy generation, with a cost implication (ratio) of 2.66 (based on the resource energy used). Only 10% of the output energy can be supplied from a 90% decarbonization technology, coal electricity generation with CCS.

4.6.4 Ozone Layer Depletion

The upper atmosphere called the stratosphere contains ozone that absorbs ultraviolet (UV) rays of the sun, which otherwise would have reached the lower atmosphere and surface of the earth. The ozone layer depletion implies thinning of the stratospheric ozone. UV rays cause skin cancer and endanger polar species. Destruction of ozone creates ozone holes (thinnest ozone layers) at the North and South Poles. The ozone layer depletion is a global problem and hence a global solution is required. NO_x emission is partly responsible for decomposing stratosphere ozone into oxygen:

$$\begin{aligned} O_3 + NO &\rightarrow NO_2 + O_2 \\ 2NO_2 &\rightarrow N_2O_4 \\ 2NO_2 &\rightarrow 2NO + O_2 \end{aligned} \tag{4.15}$$

The stratospheric ozone layer is also destroyed by halocarbons, for example, CCl_4, $CHCl_3$, CFCs that occur naturally by volcanic eruption, marine species and wood fire. This reaction occurs through chlorine, chlorine oxide or halogen radical formations. Catalyzed by these radicals, ozone breaks down into the oxygen molecule, which is not good for the upper atmosphere:

$$\begin{aligned} Cl\cdot + O_3 &\rightarrow ClO\cdot + O_2 \\ ClO\cdot + O &\rightarrow Cl\cdot + O_2 \end{aligned} \tag{4.16}$$

Trichlorofluoromethane, commonly presented as CFC-11, is known to display the highest stratospheric ozone depletion potential. CFC-11 used to be widely applied as a refrigerant due to its phase changing behavior at relatively low pressures compared to other refrigerants. However, due to the presence of chlorine and its associated damaging effect on the environment, its use was banned.

The stratospheric ozone depletion potential is well established for chlorinated and brominated compounds. However, this potential for other halocarbons is yet to be established. The convention is to present the stratospheric ozone depletion potential for any chemical relative to that of the CFC-11 assumed stratospheric ozone depletion potential of 1. If all other CFCs are grouped together, their stratospheric ozone depletion potential is ~0.4 in 100 years, relative to CFC-11. It is seen that CFC-11 has the highest stratospheric ozone depletion potential. Hence, all other chemicals have fractional

Table 4.18 Inventory analysis in kg of chemicals, for ozone layer depletion on the basis of 1 kg of wheat grain production and corresponding straw production. (Reproduced with permission from GaBi and Ecoinvent database[21].)

Benzene	4.4311×10^{-14}
Butadiene	4.1979×10^{-14}
Cadmium	2.2211×10^{-17}
Carbon dioxide, fossil	6.9965×10^{-9}
Carbon monoxide, fossil	8.2181×10^{-12}
Chromium	1.1106×10^{-16}
Copper	3.7758×10^{-15}
Dinitrogen monoxide	6.6634×10^{-14}
Ethylene oxide	4.0579×10^{-13}
Formaldehyde	3.4984×10^{-13}
Hydrogen chloride	1.9102×10^{-15}
Lead	4.4423×10^{-17}
Mercury	1.5548×10^{-19}
Methane, fossil	1.1106×10^{-13}
Nickel	1.5548×10^{-16}
Nitrogen oxides	3.1095×10^{-11}
Non-methane volatile organic compounds	1.4903×10^{-12}
Particulates, <2.5 μm	8.4403×10^{-14}
Selenium	2.2211×10^{-17}
Sulfur dioxide	2.2211×10^{-12}
Water	2.7541×10^{-9}
Zinc	2.2211×10^{-15}

stratospheric ozone depletion potentials relative to that of CFC-11 eq. The ozone depletion rate of these substances is considerable over the short term; hence their remediation must also mean controlling the emission of these substances.

Exercise 8. The inventory analysis of wheat cultivation includes the processes of soil cultivation, sowing, weed control, fertilization, pest and pathogen control, harvest and grain drying. Machine infrastructure and a shed for machine sheltering are included. Inputs of fertilizers, pesticides and seed as well as grain transports in the EU regional processing centre (10 km) are considered. The direct emissions on the field are also included.

Table 4.18 shows the cultivation inventory data of various chemicals that have impacts on ozone layer depletion[21]. The basis of inventory data is 1 kg of wheat grain production and a corresponding straw production. The same basis used in Exercise 2, 6.96 t of wheat grains per hectare and corresponding 3.49 t of straw per hectare production, can be assumed.

Figure 4.17 shows the group impact characterization factor of the chemicals in terms of kg CFC-11 eq. over a 5 to 40 year span. For the equation shown, y is the ozone depletion potential impact characterization factor of the chemicals in terms of kg CFC-11 and x is the number of years. The coefficient of determination (defined as $R^2 = 1 -$ SSQ/summation of square (SSQ) of variance) close to 1 shows a very good fit of the empirical equation given.

a. Calculate the total impact potential of the chemicals in kg CFC-11 eq. over a 100 year span generated from 1 kg of wheat grain production and corresponding straw production by extrapolation of the group impact characterization factor.
b. Calculate the impact potential of the chemicals in kg CFC-11 eq. over a 100 year span based on the characterization factor calculated in (a) from 1 kg of straw production. An economic allocation to impact potentials with an allocation factor of 92.5% to wheat grains can be assumed[21].

Solution to Exercise 8

a. Adding all the inventory analysis data of the chemicals, for ozone layer depletion on the basis of 1 kg of wheat grain production and corresponding straw production, shown in Table 4.18, the total inventory obtained is

$$9.79 \times 10^{-9}\ \text{kg}$$

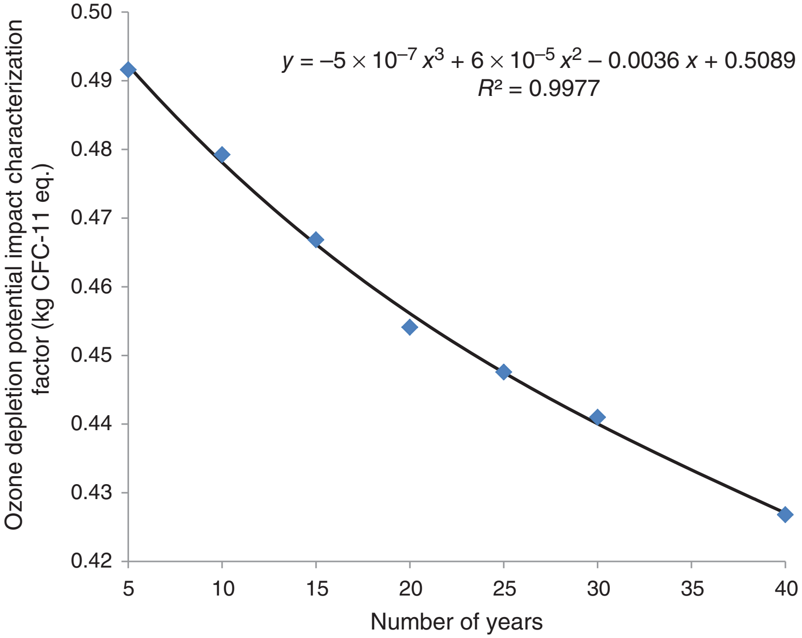


Figure 4.17 *Group impact characterization factor of the chemicals in terms of kg CFC-11 eq. over a 5 to 40 year span.*

By substituting 100 years in the place of x in the equation shown in Figure 4.17, the ozone depletion potential impact characterization factor (y) is calculated as

$$0.25 \text{ kg CFC-11 eq.}$$

The total impact of the chemicals in kg CFC-11 eq. over a 100 year span from 1 kg of wheat grain production and corresponding straw production is

$$9.79 \times 10^{-9} \times 0.25 = 2.44 \times 10^{-9} \text{ kg CFC-11 eq.}$$

Though extrapolation is perfectly feasible for the set of data provided, the reliability of the characterization factor obtained by extrapolation must be examined from physicochemical data and atmospheric science.

b. A kg of straw produced per kg of wheat = 3.49/6.96 = 0.5 kg.

Hence, 1.5 kg of wheat grain and straw produce 2.44×10^{-9} kg CFC-11 eq.

Hence, 1 kg of wheat grain and straw produce 1.63×10^{-9} kg CFC-11 eq.

Out of 1.63×10^{-9} kg CFC-11 eq. a $(1 - 0.925) = 0.075$ fraction can be allocated to the straw.

The ozone depletion potential impact of chemicals in kg CFC-11 eq. over a 100 year span, generated from 1 kg straw production is $1.63 \times 10^{-9} \times 0.075 = 1.22 \times 10^{-10}$ kg CFC-11 eq.

4.6.5 Acidification Potential

Sulfur and nitrogen oxides, SO_x and NO_x (except N_2O, which contributes to GWP), are generated from chemical processes and inefficient combustion processes. In addition, carbon oxides emit from the processes. These gaseous emissions dissolve in atmospheric moisture to form sulfurous, sulfuric, nitrous, nitric and carbonic acids, reducing the natural pH from 5–6 to 2–4 (acidic).

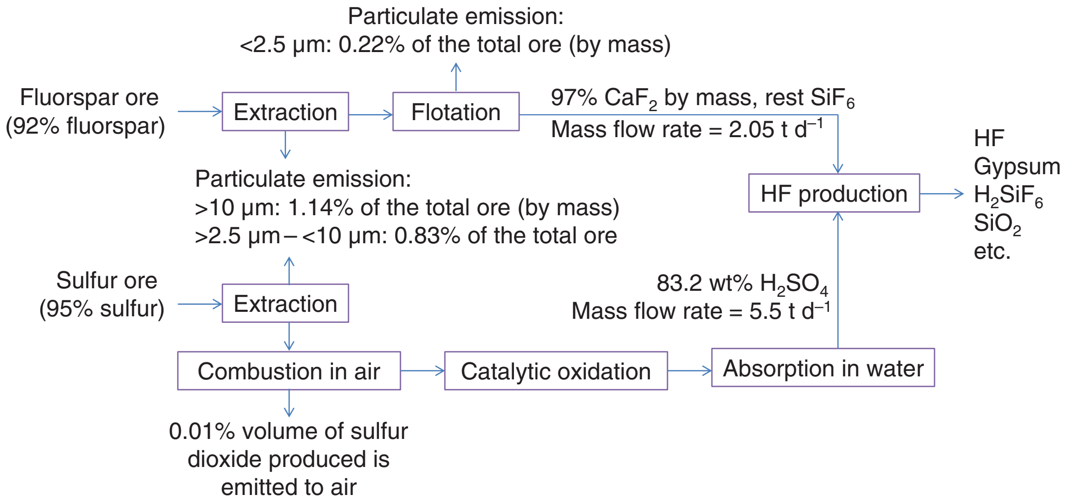


Figure 4.18 *Flow chart from sulfur and fluorspar ore extraction to the production of hydrogen fluoride and other products at the plant gate. The total ore includes both the fluorspar and sulfur ores.*

Acid rain or acidification is a regional problem as acidic clouds can travel. Scandinavia's acid rain is caused by emissions from the UK, Germany and France. The effect is acidification of water that damages water life, water quality, plant life and forests and causes dead lakes and streams. Buildings, particularly of marble and sandstone materials, can also corrode.

The acidifying chemicals commonly generate H^+ ions, responsible for lowering of atmospheric pH. The acid rain potential of a chemical is presented by the maximum number of H^+ ions that can be produced per unit mole of the chemical. In environmental impact potential terms, this potential of a chemical is presented relative to that of sulfur dioxide (SO_2). Sulfur takes part in a number of reactions. It is an important element for a number of chemicals, such as sulfuric acid, sulfites, gypsum, etc. The smelting process that recovers copper from ores can also emit sulfur compounds. When fuels or even desulfurized fuels are processed, sulfur present in the body is emitted mainly in oxidized form, SO_2. Sulfur compounds in gaseous forms, especially sulfur oxides, cause acid rain. Though there is a maximum acid rain potential for every chemical, the actual acid rain effect depends on many factors, such as the buffering capacity of soil and water, sunlight, temperature and moisture content of the atmosphere and air entrapment.

Exercise 9. Hydrogen fluoride is the main component for Teflon (polytetrafluoroethylene) production; 80% of the world's hydrogen fluoride is produced by reaction between extracted fluorspar containing 97% CaF_2 and the rest of SiF_4 by mass and sulfuric acid with a mass concentration of 83%, shown below in Equation (4.17). Gypsum ($CaSO_4.2H_2O$) can be produced as a by-product from the reaction. The SiF_4 present reacts with excess water to produce hexafluoride silica acid and silica, shown below in Equation (4.18). Figure 4.18 shows the flow chart from the extraction of sulfur and fluorspar

Table 4.19 *Molar mass of chemicals.*

Chemical	CaF_2	H_2SO_4	$CaSO_4$	HF	SiF_4	H_2SiF_6	SiO_2	H_2O
Full name	Calcium fluoride	Anhydrous sulfuric acid	Calcium sulfate	Hydrogen fluoride	Silicon tetrafluoride	Hexafluorosilicic acid	Silica	Water
Molar mass	78.07	98	136	20.01	104.08	144.09	60.08	18

Table 4.20 *Molar and mass flow rates of the reactants consumed and products produced by the two reactions in Equations (4.17) and (4.18).*

Reaction	Reactant Consumed				Product Produced			
	kmol d^{-1}	t d^{-1}	kmol d^{-1}	t d^{-1}	kmol d^{-1}	t d^{-1}	kmol d^{-1}	t d^{-1}
Reaction 1 in Equation (4.17)	CaF_2		H_2SO_4. $2H_2O$		Gypsum		HF	
	25.5	1.9885	25.5	3.413	25.5	4.381	51	1.0205
Reaction 2 in Equation (4.18)	SiF_4		H_2O		H_2SiF_6		SiO_2	
	0.591	0.0615	0.394	0.0071	0.394	0.0568	0.197	0.0118

ores to the production of hydrogen fluoride and other products at the plant gate. The required reaction conversion and yield data are also shown. Table 4.19 shows the molar masses of the chemicals involved in the process.

$$CaF_2 + H_2SO_4.2H_2O \rightarrow CaSO_4.2H_2O + 2HF \tag{4.17}$$

$$3SiF_4 + 2H_2O \rightarrow 2H_2SiF_6 + SiO_2 \tag{4.18}$$

a. Calculate the inlet and outlet mass flow rates of the flowchart in Figure 4.18.
b. Determine the relevant environmental impact characterizations from the resulting emissions.

Solution to Exercise 9. Calculate the mass of the fluorspar ore assuming 92% of it is the fluorspar:

$$= 2.05/0.92 = 2.23 \text{ t d}^{-1}$$

The ore extraction processes are assumed to give an ideal split of 100%. This assumption will not affect the impact on land as after extraction the residual ore goes back to the land. Hence, the net effect is the depletion of the fluorspar and sulfur from the land. They are amongst the most abundant elements on the earth.

Calculate the mass of sulfur ore using the mass balance, starting from the reactant consumptions in the reactions in Equations (4.17) and (4.18).

Assume complete conversion of CaF_2 and SiF_4 in the two respective reactions. Table 4.20 shows the amounts of reactants consumed and the amounts of products produced by the two reactions.

Assume complete conversion of sulfur dioxide into sulfur trioxide in the catalytic oxidation in the reaction

$$SO_2 + 0.5O_2 \rightarrow SO_3 \tag{4.19}$$

Assume complete sulfur trioxide absorption into water to form sulfuric acid, shown as

$$SO_3 + 3H_2O \rightarrow H_2SO_4.2H_2O \tag{4.20}$$

Doing a backward calculation from the amount of H_2SO_4 solution (at 83.2% in weight basis), the molar flow rate of SO_2 produced from sulfur ore is (1 kmol of H_2SO_4 weighs 98 kg and requires 1 kmol of SO_3, which requires 1 kmol of SO_2, according to Equations (4.19) and (4.20)):

$$\frac{5.5 \times 0.832 \times 1000}{98} = 46.7 \text{ kmol d}^{-1}$$

The mass flow rate of sulfur ore required (assuming that 0.01% by volume of sulfur dioxide is emitted to air, the ore contains 95% sulfur by mass and a 100% split in the extraction process) is

$$\frac{46.7}{0.9999 \times 1000} \times \frac{32}{0.95} = 1.573 \text{ t d}^{-1}$$

(The atomic mass of sulfur is 32.)

Table 4.21 *Product distribution corresponding to unit mass production of HF.*

HF	Gypsum	H_2SiF_6	SiO_2	Anhydrous H_2SO_4
1	4.3	0.056	0.012	2.04

HF is the precursor to many important compounds including pharmaceuticals and polymers such as Teflon. However, upon contact with moisture it forms corrosive hydrofluoric acid. The gas can also cause blindness. Hence, an important aspect of further research will be to find a replacement safer precursor. The results in Table 4.21 will allow comparison with a substitute product and process.

Calculate the total amount of ore:

$$(2.23 + 1.573) = 3.8\ \mathrm{t\,d^{-1}}$$

Particulate emissions (calculated based on the total ore including both the fluorspar and sulfur ores):

$$<2.5\ \mu\mathrm{m}:\ 8.4\ \mathrm{kg\ d^{-1}}$$
$$>2.5\ \mu\mathrm{m} - <10\ \mu\mathrm{m}:\ 31.6\ \mathrm{kg\ d^{-1}}$$
$$>10\ \mu\mathrm{m}:\ 43.3\ \mathrm{kg\ d^{-1}}$$

Sulfur dioxide emission to air:

$$\frac{46.7 \times 0.0001}{0.9999 \times 1000} \times 64 = 0.3\ \mathrm{kg\ d^{-1}}$$

(The molar mass of sulfur dioxide is 64.)
The acidification potential of the flowchart is:

$$0.3\ \mathrm{kg\ SO_2\ equivalent}$$

In addition to the products shown in Table 4.20, there will be unreacted anhydrous sulfuric acid:

$$2.08\ \mathrm{t\ d^{-1}}$$

Residual ore (including the particulates present) from fluorspar ore from the extraction process:

$$0.18\ \mathrm{t\,d^{-1}}$$

Residual ore (including the particulates present) from sulfur ore from the extraction process:

$$0.08\ \mathrm{t\,d^{-1}}$$

On the basis of the unit mass flow rate of HF produced, the product distribution is as shown in Table 4.21.

4.6.6 Photochemical Oxidant Creation Potential

This impact is also known as urban smog, brownish colored air, commonly found in modern cities, especially where air is trapped in a basin, for example, Los Angeles, Mexico City, etc. Photochemical pollutants have harmful effects on living tissue and on buildings. Together, the formation of ozone in the lower atmosphere, the troposphere, adds to detrimental impacts on ecological and human health.

The volatile organic compounds react with NO_x in the presence of sunlight to produce ozone and photochemical pollutants in the lower atmosphere. Photochemical pollutants include peroxyacetyl nitrate (PAN), formaldehyde, acetic acid, etc. These pollutants are named as photochemical pollutants, because their formations are catalyzed by sunlight. These pollutants and ozone, known as photochemical oxidant, in the lower atmosphere are extremely detrimental to health and the environment. The photochemical oxidant creation potential is expressed in terms of the ethylene equivalent.

VOCs are carbon containing compounds that take part in photochemical reactions. VOCs do not include carbon dioxide, carbon monoxide, carbonic acid, metallic carbide, carbonates and ammonium carbonates. VOCs are responsible for urban smog and ground level ozone formation. When there is a mixture of VOCs, the concentration-average photochemical oxidant creation potential of the mixture is estimated.

The various photochemical reaction products they contribute to are also very harmful to health and the environment. High levels of these pollutants cause breathing difficulties and bring on asthma attacks, which can be fatal. Warm weather and still air can exacerbate the problem. Therefore, VOC emissions must be controlled and regulated. The photochemical oxidants are formed when NO_x, VOC and sunlight are present. Therefore, regional effects must be considered in estimating the photochemical oxidant creation potential. See Web Chapter 1 for VOC measurements and mitigation pathways.

4.6.7 Aquatic Ecotoxicity

The effect of manufactured chemicals on aquatic organisms at subcellular, organism, population, community and ecosystem levels is commonly known as aquatic ecotoxicity. There are two main ways of measuring concentration levels of toxic chemicals, at the mark of mortality by 50% of test organisms within a specified time and a specific effect grown by 50% in test organisms within a specified time. Wastewater and sewage treatment discharges are the core causes of aquatic ecotoxicity. PCBs (polychlorinated biphenyls), DDT (dichlorodiphenyltrichloroethane) and dioxins are the main chemical constituents causing aquatic ecotoxicity. As can be noted, some of the toxicities are more human health related than others, with profound impacts on the environment. Thus, human toxicity is differentiated from ecotoxicity, which includes aquatic as well as terrestrial toxicities.

Within aquatic toxicity, both freshwater and marine water toxicities are included. This differentiation is to structure primary impacts of chemicals relevant to different impact characterizations as precisely as possible. The more exhaustive the division the more targeted are the estimations of the environmental impact characterizations of the chemicals. To express toxicity, a critical volume approach is sometimes adopted. The critical volume is the volume of water needed (in the case of aquatic toxicity) to dilute a pollutant to an acceptable or safe limit. At some other times, a toxicity can be measured in terms of the kg of DCB equivalent.

It can be interpreted that a global consensus needed to be agreed to decide on environmentally safe limits for various pollutants to mitigate the toxicity impact potential. The physicochemical properties are also counted to evaluate the primary impacts to aquatic, terrestrial and human bodies. Similar to other characterizations, there is a base chemical, DCB, against which the primary level of toxicity for other chemicals is defined.

4.6.8 Eutrophication Potential

Eutrophication is a result of leaching of soil nutrients into a water body, particularly applicable for biorefinery systems, because of the application of nutrients to agricultural land. It is caused by nutrients, mainly nitrates and phosphates, leaching into a water body. The sources are agricultural, animal and sewage activities. The fertilizers applied in agriculture can be transmitted with rain through soil into the water body. As a result of eutrophication, there is an increase in biomass, for example, algal bloom, on the surface of water bodies, preventing light reaching inside the water bodies. As living creatures, fish lives are endangered. When algae start dying, aerobic bacteria use up dissolved oxygen to decompose algae. Increasing biological oxygen demand (BOD) indicates decreasing dissolved oxygen in water bodies. Nitrates (in fertilizers) are able to enter water bodies easily, because of their high water solubility. Phosphates (also in fertilizers), though water insoluble, can adhere to soil particles eroding into water bodies. All pollutants leaching into a water body have one common characteristic, dissolved oxygen reduction in the water. Thus, the eutrophication potential of a substance can be interpreted in terms of its ability to reduce the dissolved oxygen content in fresh water, with respect to a base chemical, phosphate in this case.

As seen in an agricultural system, nitrogen fertilization is crucial to plant growth, which proportionally increases with increasing nitrogen fertilizer intake. This implies that nitrate leaching into a water body is due to agricultural activity. The main source of phosphate, however, is the sewage discharge. After the treatment of black water (e.g., sewage discharge) and grey water (e.g., water returned from other household activities) the resulting sludge is generally embedded within the sea bed. Given that phosphate is water insoluble, the sea bed discharge of sludge was seen to be a reasonable thing to do. However, soil eroded into water and phosphate content in fresh water increased over the years. One of the ways for reducing phosphate leaching into fresh water is to deposit sludge in deep rocks for mineral formation. It is thus implied that the eutrophication potential is directly linked with human activity, for example, agricultural practices and effluent treatment strategies, etc.

4.6.9 Biodiversity

Amongst all impact categories, biodiversity is the end-point in the cause and effect chain of environmental impacts and directly affects nature. Biodiversity was introduced at the United Nations Conference on Environment and Development in Rio de Janeiro in 1992 (Rio Earth Summit). The International Convention on Biological Diversity was agreed amongst 150 countries and moved to halve the loss of biodiversity, wildlife and habitats. Responsibility at national level includes an action plan and programmes to reduce biodiversity loss of species under their jurisdiction. The UK Biodiversity Action Plan implemented in 1994 focused on the delivery of actions for conservation and protection of priority/targeted species and habitats (1150 species and 65 habitats in 2007–2011). Biodiversity assessment relies on analysis and understanding the whole cause and effect chain of environmental impacts. For example, the aquatic ecotoxicity and marine ecotoxicity can be measured. Their effect can be death to marine life or even species extinction. The latter is the end effect of a cause, ecotoxicity, and a direct effect on nature. An end effect analysis is not straightforward, requiring longer term qualitative as well as quantitative dimensions and multidisciplinary interventions. Often LCA studies are done up to the primary impact characterizations and biodiversity but other end-point impacts are not included because of the evaluation uncertainty.

4.7 LCA: Interpretation

This is the final phase of LCA, where the results of inventory analysis and impact assessment are gathered together with an aim to improve system performance and suggest possible changes. Interpretation of an LCA study includes identification of major burdens, impacts, hot spots; identification of areas with a scope for improvement; sensitivity analysis; robustness of results; evaluation and recommendations. Reliability and applicability of the data are a major issue, for which sensitivity must be analyzed for variability and uncertainty in the data used. Furthermore, there are various issues around the LCA methodology.

Even for primary effect assessments, different characterization factors have been suggested by different research groups, though with little variation. Some works undertake normalization to understand the relative importance and magnitude of the environmental benefits/damages of the technology or product and thereby compare the reliability of such studies, which must be carefully assessed. Characterization and normalization must be drawn on common references and may be related to a given community, country or region over a period of time. After normalization, results are given in the same unit and all the normalized indicator results corresponding to each impact category can be added. A single score for each technology or product is then obtained. It is an effective tool for comparisons of environmental benefits and business generation, if undertaken reliably and responsibly. LCA studies can be of a stand-alone, accounting (consequential) and change oriented (attributional) type. The sets of questions that can be answered using the three different types of LCA follow.

The following chapter discusses the data uncertainty analysis and LCA interpretation.

4.7.1 Stand-Alone LCA

- Product/process/systems/network focused.
- What is the environmental impact of a product/process/system/ …?
- What are the relevant impact characterizations of a product/ … ? What are the key pollutants?
- What are the input parameters that have the maximum impact on the key pollutant emissions and on the relevant impact characterizations?
- Analyze the sensitivity of the significant input parameters on the key pollutant emissions and on the relevant impact characterizations and decide the bounds of their acceptable values.
- What are the limits of the pollutants and what are the optimal design and operating conditions to keep the pollutants within their limits?
- What are the key observations that can be communicated to the policy makers, design and decision makers?
- The approach is stand-alone; hence no comparison is made with an existing product/ … . This implies that the product / … can be functionally different.
- It is a useful attribute of the LCA study that the hot spots and the causes for hot spots are identified and remedial actions are made to mitigate impacts.

4.7.2 Accounting LCA

- This type is about replacement of an existing product/process/systems/network. Hence LCA is to provide a comparison of a decision today with existing ones, retrospectively. This implies that the new product/ … is intended to replace a similar functionality product/ … . A comparison can be made between a number of different products with similar functionality or providing similar services.
- If a product/ … is replaced by another type of product/ …, how can the impact under a given characterization be improved?
- Identify the areas of major improvements with the least cost achievable.
- What would be an appropriate policy measure if a particular product or production route is held responsible for a major impact under a characterization?
- A typical example is the recycling of extracted material in the place of virgin material. What are the additional environmental impacts of using recycled material in place of virgin material? Compare the consequential impacts between landfill disposal and the material being recycled. Take account of the additional material use from construction to decommissioning to process the recycled material in the place of virgin material. Produce the entire flowchart and indicate the impact hot spots.
- The standard set of sensitivity analysis questions can be answered.

4.7.3 Change Oriented LCA

- The change oriented LCA is useful in making comparisons between products/activities prospectively. This is therefore used in making choices of products and processes, while considering growing environmental concerns and policies.
- This LCA is effective in the minimization of resource use, waste management and ways of reusing the materials after the end of product life.
- Thus it allows a comparison amongst a number of options to govern a whole system decision from resource selection through the conversion process decision making to the product end of life, prospectively.
- While the stand-alone LCA is just the beginning of an exercise, the accounting and change oriented LCAs are more appropriate to answer a number of relevant sustainable business development questions.

4.7.4 Allocation Method

The allocation of impact to different products utilizing the same processes and pathways is a difficult decision for an LCA study. The allocation can be done using the by economic value (if market prices are known). If products are functionally the same, allocation by unit functional value or allocation by substitutions/contributions to the service concerned can be useful. In the case of energy production, allocation of impacts by energy values of products is a rational way. Table 4.22 shows the environmental impact allocation to two main products from wheat cultivation, grain and straw. The allocation

Table 4.22 *Allocation of environmental impacts from wheat cultivation. ARU, abiotic resource use.*

Functional Unit	CPE (MJ)	GWP (kg CO_2 eq.)	EP (kg PO_4^{3-} eq.)	AP (kg SO_2 eq.)	ARU (kg Sb eq.)
ha^{-1} grain	18335	3426	16.1	15.8	10.8
ha^{-1} straw	632	77	0.2	0.2	0.30
Total (ha^{-1})	18967	3503	16.3	16.0	11.1
t^{-1} grain	2634	492	2.3	2.3	1.5
t^{-1} straw	181	22	0.1	0.1	0.1
y^{-1} grain	3.16×10^9	5.91×10^8	2.77×10^6	2.72×10^6	1.85×10^6
y^{-1} straw	1.09×10^8	1.33×10^7	4.17×10^4	4.25×10^4	5.26×10^4
Total (y^{-1})	3.27×10^9	6.04×10^8	2.81×10^6	2.76×10^6	1.91×10^6
Land use	Grade 2	Grade 3a	Grade 3b	Grade 4	
ha y^{-1}	151685	172370	186159	193054	
ha t^{-1} grain	0.13	0.14	0.16	0.16	

was done by their relative economic values. Hence, wheat had a bigger burden than straw. Also, note the choices of functional units for comparison with other cultivation systems.

Refer to the ***Online Resource Material in the Companion Website: Case Studies 1 to 4*** for LCA based problem solving approaches for industrial systems.

4.8 LCIA Methods

A number of LCIA methods exist to predict impact under various categories. A method can focus on the primary impact characterizations, such as, by CML. However, the LCIA methods can also include combinations of primary as well as mid- or end-point impacts. A cause–effect chain is created using characterization factors to predict the mid-point and end-point impacts. Needless to say, the latter approaches introduce more uncertainties in LCIA modeling results.

In this book, the CML 2010 method has primarily been used (http://www.cml.leiden.edu/research/industrialecology/researchprojects/finished/new-dutch-lca-guide.html) for comparisons, for example, between biorefinery configurations, feedstock selections, product selections by avoided emissions and focusing on the primary impact characterizations.

The EC-ILCD International Reference Life Cycle Data System and ELCD European Reference Life Cycle Database are available on http://lca.jrc.ec.europa.eu/lcainfohub/index.vm.

ILCD recommendations (http://lct.jrc.ec.europa.eu/pdf-directory/ILCD-Handbook-General-guide-for-LCA-DETAIL-online-12March2010.pdf) include primary as well as mid-point estimations as follows. For some primary impacts, such as the eutrophication potential, the method provides individual impact values in kg N or S equivalent (terrestrial) and in kg P equivalent (for water). For some others, such as the abiotic depletion potential, the combined resource depletion in terms of fossil and mineral reserves is shown.

The USA-TRACI “Tool for the Reduction and Assessment of Chemical and Other Environmental Impacts” method is available on http://www.epa.gov/nrmrl/std/traci/traci.htm and http://www.gabi-software.com/support/gabi/gabi-lcia-documentation/life-cycle-impact-assessment-lcia-methods/traci/. The method provides primary as well as mid-point characterizations. In addition to some of the CML primary categories, but often in different units except GWP, mid-point impacts to human health are estimated.

The various methodologies are in-built and offered by commercially available LCA software, recommended to use. The units used for various impact characterizations included under ILCD recommendations, CML 2001 – November 2010, TRACI and ReCiPe in GaBi, are shown in four parts in Table 4.23[21].

Table 4.23(a) *Units for various impact characterizations under ILCD recommendations.*

Impact Characterization	Accepted Unit
Climate change	kg CO_2 equivalent
Ozone depletion	kg CFC-11 equivalent
Human toxicity, cancer effects	CTUh (comparative toxic unit for human)
Human toxicity, non-cancer effects	CTUh
Particulate matter, respiratory inorganics	kg PM2.5 equivalent
Ionising radiation, human health	Human exposure efficiency relative to U^{235}
Photochemical ozone formation	kg NMVOC (non-methane volatile organic compounds) equivalent
Acidification	kg N or S equivalent
Eutrophication, terrestrial	kg N or S equivalent
Eutrophication, aquatic	Fraction of nutrients reaching end compartment
Ecotoxicity	CTUe (comparative toxic unit for ecosystem)
Resource depletion, water	Water stress index (WSI)
Resource depletion, mineral, fossil and renewable	kg Sb equivalent

Table 4.23(b) *Units for various impact characterizations under CML 2001 – November 2010.*

Impact Characterization	Accepted Unit
Global warming potential	kg CO_2 equivalent
Acidification depletion potential	kg SO_2 equivalent
Eutrophication potential	kg phosphate equivalent
Ozone layer depletion potential	kg CFC-11 equivalent
Abiotic depletion potential, elements	kg Sb equivalent
Abiotic depletion potential, fossil	MJ
Freshwater aquatic ecotoxicity potential	kg DCB equivalent
Human toxicity potential	kg DCB equivalent
Marine aquatic ecotoxicity potential	kg DCB equivalent
Photochemical ozone creation potential	kg ethylene equivalent
Terrestric ecotoxicity potential	kg DCB equivalent

Table 4.23(c) *Units for various impact characterizations under TRACI.*

Impact Characterization	Accepted Unit
Global warming potential	kg CO_2 equivalent
Acidification depletion potential	kg H^+ equivalent
Eutrophication potential	kg N equivalent
Ozone layer depletion potential	kg CFC-11 equivalent
Ecotoxicity air	PAF (potentially affected fraction) m^3 day kg^{-1}
Ecotoxicity soil	PAF m^3 day kg^{-1}
Ecotoxicity water	PAF m^3 day kg^{-1}
Human health cancer air	Cases
Human health cancer soil	Cases
Human health cancer water	Cases
Human health non-cancer air	Cases
Human health non-cancer soil	Cases
Human health non-cancer water	Cases
Human health criteria air	kg PM10 equivalent
Smog air	kg O_3 equivalent

Table 4.23(d) *Units for various impact characterizations under ReCiPe.*

Impact Characterization	Accepted Unit
Climate change	kg CO_2 equivalent
Terrestrial acidification	kg SO_2 equivalent
Freshwater eutrophication potential	kg P equivalent
Ozone depletion potential	kg CFC-11 equivalent
Fossil depletion	kg oil equivalent
Freshwater ecotoxicity	kg DCB equivalent
Ionizing radiation	kg U235 equivalent
Marine ecotoxicity	kg DCB equivalent
Marine eutrophication	kg N equivalent
Metal depletion	kg Fe equivalent
Natural land transformation	m^2
Particulate matter formation	kg PM10 equivalent
Photochemical oxidant formation	kg NMVOC equivalent
Terrestrial ecotoxicity	kg DCB equivalent
Water depletion	m^3

CML2001 - Dec. 07, Experts IKP (Central Europe)
CML2001 - Dec. 07, Experts IKP (Northern Europe)
CML2001 - Dec. 07, Experts IKP (Southern Europe)
CML2001, Experts IKP (Central Europe)
CML2001, Experts IKP (Northern Europe)
CML2001, Experts IKP (Southern Europe)
CML96, Expert judgement, IKP
CML96, Experts, IKP
CML96, Policy long term, IKP
CML96, Policy short term, IKP
CML96, Policy, IKP
CML96, Population, IKP
CML96, Survey Europe, IKP
CML96, Survey Germany, IKP
CML96, Sustainable development, IKP
EDIP 1997, Env. imp. eval. (PET W, EU 2004)
EDIP 1997, Ress. eval. (PR W 2004)
EDIP 1997, Toxicity eval. (PET EU 2004)
EDIP 1997, Waste eval. (PET DK 2000)
EDIP 2003, Env. imp. eval. (PET W, EU 2004)
EI95
EI95 (incl. ionizing radiation, RF)
EI99, EE (Egalitarian approach)
EI99, HA (Hierarchist approach)
EI99, II (Individualist approach)
PE LCIA Survey 2012 (Europe; CML and ReCiPe)
PE LCIA Survey 2012 (Global; CML, ReCiPe and Traci)
PE LCIA Survey 2012 (North-America; Traci)

Figure 4.19 *A comprehensive list of LCIA methodologies.*

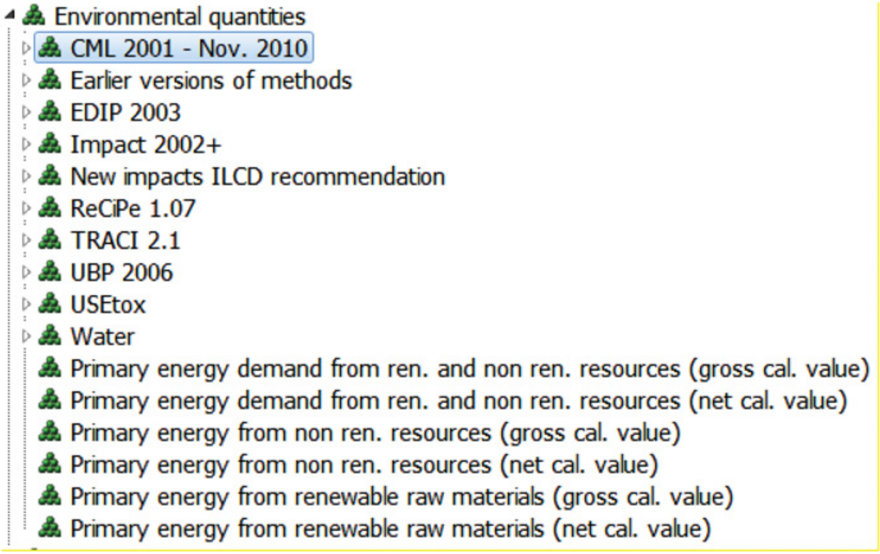
Figure 4.19 shows a comprehensive list of LCIA methodologies and regions applied for, which include CML, EDIP, EI and the PE LCIA survey, offered in GaBi 6, from PE International. The most recent LCIA methodologies are shown in Figure 4.20 (a) to (h). Each of the LCIA methodologies is then elaborated to show the impact characterizations, under the methodology shown in Figure 4.20.

Foundation Concepts Quiz (20 marks in total)

Problem 1. Carries 5 Marks

Consider the emissions from the conversion of two feedstocks, shown on the basis of the weight percentage in Table 4.24.

1. Calculate the global warming potential of the emissions from the two feedstocks. (2.5 marks)
2. Calculate the CO_2 credit gain by environmentally better performing feedstock compared to inferior feedstock. (2.5 marks)

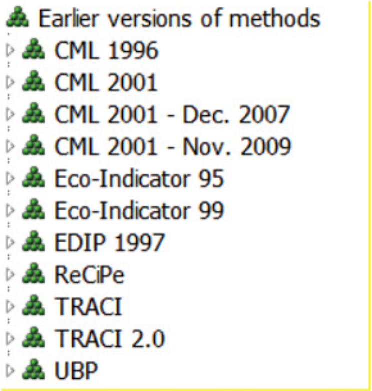


- Environmental quantities
  - CML 2001 - Nov. 2010
  - Earlier versions of methods
  - EDIP 2003
  - Impact 2002+
  - New impacts ILCD recommendation
  - ReCiPe 1.07
  - TRACI 2.1
  - UBP 2006
  - USEtox
  - Water
  - Primary energy demand from ren. and non ren. resources (gross cal. value)
  - Primary energy demand from ren. and non ren. resources (net cal. value)
  - Primary energy from non ren. resources (gross cal. value)
  - Primary energy from non ren. resources (net cal. value)
  - Primary energy from renewable raw materials (gross cal. value)
  - Primary energy from renewable raw materials (net cal. value)

Figure 4.20 *LCIA methodologies and their impact characterizations available in LCA software (a to h).* ***(a)*** *LCIA methodologies available in LCA software.*

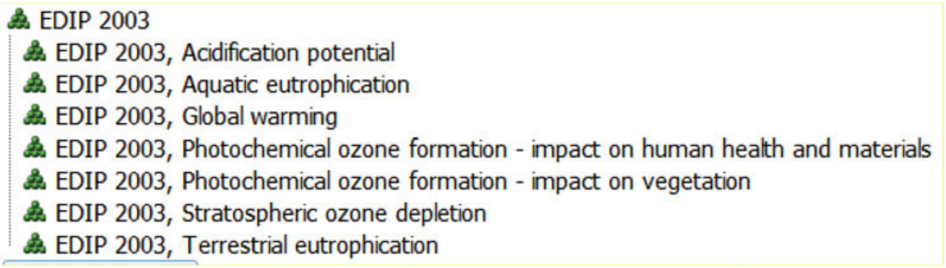
- CML 2001 - Nov. 2010
  - CML2001 - Nov. 2010, Abiotic Depletion (ADP elements)
  - CML2001 - Nov. 2010, Abiotic Depletion (ADP fossil)
  - CML2001 - Nov. 2010, Acidification Potential (AP)
  - CML2001 - Nov. 2010, Eutrophication Potential (EP)
  - CML2001 - Nov. 2010, Freshwater Aquatic Ecotoxicity Pot. (FAETP inf.)
  - CML2001 - Nov. 2010, Global Warming Potential (GWP 100 years)
  - CML2001 - Nov. 2010, Global Warming Potential, excl biogenic carbon (GWP 100 years)
  - CML2001 - Nov. 2010, Human Toxicity Potential (HTP inf.)
  - CML2001 - Nov. 2010, Marine Aquatic Ecotoxicity Pot. (MAETP inf.)
  - CML2001 - Nov. 2010, Ozone Layer Depletion Potential (ODP, steady state)
  - CML2001 - Nov. 2010, Photochem. Ozone Creation Potential (POCP)
  - CML2001 - Nov. 2010, Terrestric Ecotoxicity Potential (TETP inf.)

Figure 4.20(b) *Primary impact characterizations included in CML 2001 – November 2010.*



- Earlier versions of methods
  - CML 1996
  - CML 2001
  - CML 2001 - Dec. 2007
  - CML 2001 - Nov. 2009
  - Eco-Indicator 95
  - Eco-Indicator 99
  - EDIP 1997
  - ReCiPe
  - TRACI
  - TRACI 2.0
  - UBP

Figure 4.20(c) *Earlier versions of LCIA methods.*

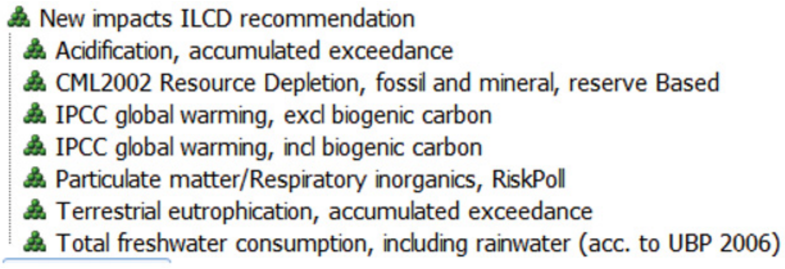


- EDIP 2003
  - EDIP 2003, Acidification potential
  - EDIP 2003, Aquatic eutrophication
  - EDIP 2003, Global warming
  - EDIP 2003, Photochemical ozone formation - impact on human health and materials
  - EDIP 2003, Photochemical ozone formation - impact on vegetation
  - EDIP 2003, Stratospheric ozone depletion
  - EDIP 2003, Terrestrial eutrophication

Figure 4.20(d) *Primary impact characterizations included in EDIP 2003.*

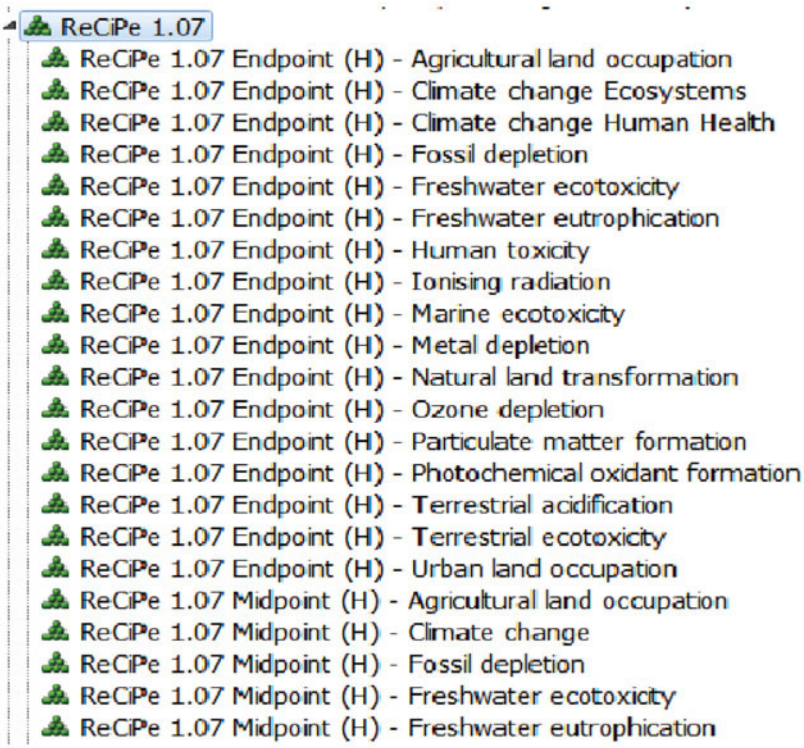
- Impact 2002+
  - I02+ v2.1 - Aquatic acidification - Midpoint
  - I02+ v2.1 - Aquatic ecotoxicity - Midpoint
  - I02+ v2.1 - Aquatic eutrophication - Midpoint
  - I02+ v2.1 - Carcinogens - Midpoint
  - I02+ v2.1 - Global warming 500yr - Midpoint
  - I02+ v2.1 - Ionizing radiation - Midpoint
  - I02+ v2.1 - Land occupation - Midpoint
  - I02+ v2.1 - Mineral extraction - Midpoint
  - I02+ v2.1 - Non-carcinogens - Midpoint
  - I02+ v2.1 - Non-renewable energy - Midpoint
  - I02+ v2.1 - Ozone layer depletion - Midpoint
  - I02+ v2.1 - Photochemical oxidation - Midpoint
  - I02+ v2.1 - Respiratory effects - Midpoint
  - I02+ v2.1 - Terrestrial acidification/nutrification - Midpoint
  - I02+ v2.1 - Terrestrial ecotoxicity - Midpoint

Figure 4.20(e) *Mid-point impact characterizations included in Impact 2002+.*



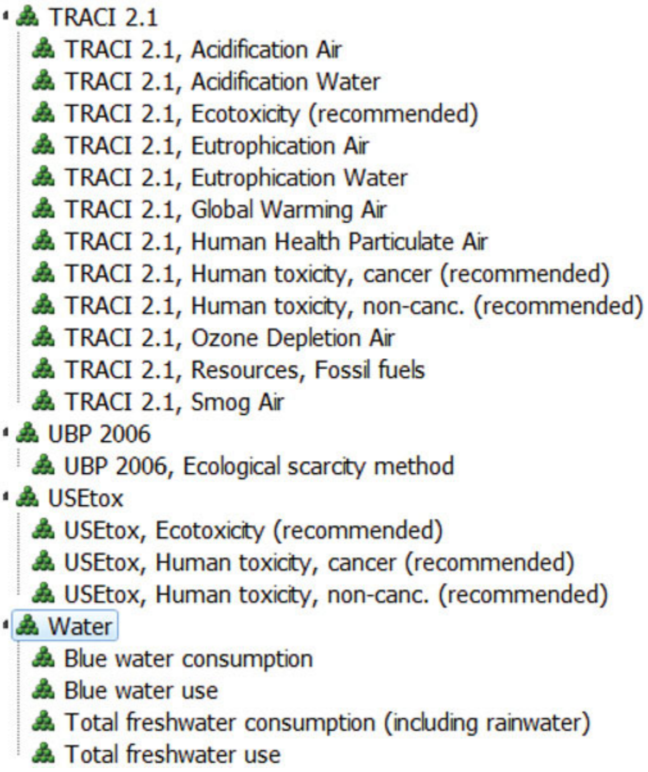
New impacts ILCD recommendation
- Acidification, accumulated exceedance
- CML2002 Resource Depletion, fossil and mineral, reserve Based
- IPCC global warming, excl biogenic carbon
- IPCC global warming, incl biogenic carbon
- Particulate matter/Respiratory inorganics, RiskPoll
- Terrestrial eutrophication, accumulated exceedance
- Total freshwater consumption, including rainwater (acc. to UBP 2006)

Figure 4.20(f) *New impacts recommended in ILCD.*



ReCiPe 1.07
- ReCiPe 1.07 Endpoint (H) - Agricultural land occupation
- ReCiPe 1.07 Endpoint (H) - Climate change Ecosystems
- ReCiPe 1.07 Endpoint (H) - Climate change Human Health
- ReCiPe 1.07 Endpoint (H) - Fossil depletion
- ReCiPe 1.07 Endpoint (H) - Freshwater ecotoxicity
- ReCiPe 1.07 Endpoint (H) - Freshwater eutrophication
- ReCiPe 1.07 Endpoint (H) - Human toxicity
- ReCiPe 1.07 Endpoint (H) - Ionising radiation
- ReCiPe 1.07 Endpoint (H) - Marine ecotoxicity
- ReCiPe 1.07 Endpoint (H) - Metal depletion
- ReCiPe 1.07 Endpoint (H) - Natural land transformation
- ReCiPe 1.07 Endpoint (H) - Ozone depletion
- ReCiPe 1.07 Endpoint (H) - Particulate matter formation
- ReCiPe 1.07 Endpoint (H) - Photochemical oxidant formation
- ReCiPe 1.07 Endpoint (H) - Terrestrial acidification
- ReCiPe 1.07 Endpoint (H) - Terrestrial ecotoxicity
- ReCiPe 1.07 Endpoint (H) - Urban land occupation
- ReCiPe 1.07 Midpoint (H) - Agricultural land occupation
- ReCiPe 1.07 Midpoint (H) - Climate change
- ReCiPe 1.07 Midpoint (H) - Fossil depletion
- ReCiPe 1.07 Midpoint (H) - Freshwater ecotoxicity
- ReCiPe 1.07 Midpoint (H) - Freshwater eutrophication

Figure 4.20(g) *End- and mid-point impact characterizations included in ReCiPe.*



- TRACI 2.1
  - TRACI 2.1, Acidification Air
  - TRACI 2.1, Acidification Water
  - TRACI 2.1, Ecotoxicity (recommended)
  - TRACI 2.1, Eutrophication Air
  - TRACI 2.1, Eutrophication Water
  - TRACI 2.1, Global Warming Air
  - TRACI 2.1, Human Health Particulate Air
  - TRACI 2.1, Human toxicity, cancer (recommended)
  - TRACI 2.1, Human toxicity, non-canc. (recommended)
  - TRACI 2.1, Ozone Depletion Air
  - TRACI 2.1, Resources, Fossil fuels
  - TRACI 2.1, Smog Air
- UBP 2006
  - UBP 2006, Ecological scarcity method
- USEtox
  - USEtox, Ecotoxicity (recommended)
  - USEtox, Human toxicity, cancer (recommended)
  - USEtox, Human toxicity, non-canc. (recommended)
- Water
  - Blue water consumption
  - Blue water use
  - Total freshwater consumption (including rainwater)
  - Total freshwater use

Figure 4.20(h) *Primary impact characterizations included in TRACI, UBP, USEtox and Water.*

Problem 2. Carries 10 Marks

A comparison of the environmental impact assessment results between anaerobic digestion and natural gas based production systems is shown in Figures 4.21 to 4.28. Neglect the differences due to geographic locations (CH in the figures refers to Switzerland and RNA refers to North America, according to the geographical codes used in GaBi software, http://www.gabi-software.com/support/gabi/geographical-codes/ and <u-so> or <p-agg> indicates the impact potential from that process block only).

1. Calculate the credit gain by environmentally better performing feedstock compared to inferior feedstock in each impact category shown. (2 marks)

Table 4.24 *Emissions from the conversion of two feedstocks on the basis of weight percentage.*

Chemical	Feedstock 1 (weight%)	Feedstock 2 (weight%)	GWP Characterization Factor
CO_2	80	65	1
CH_4	10	30	25
CFC	0.05	0	5000
N_2O	4	5	298
NO	5.95	0	40

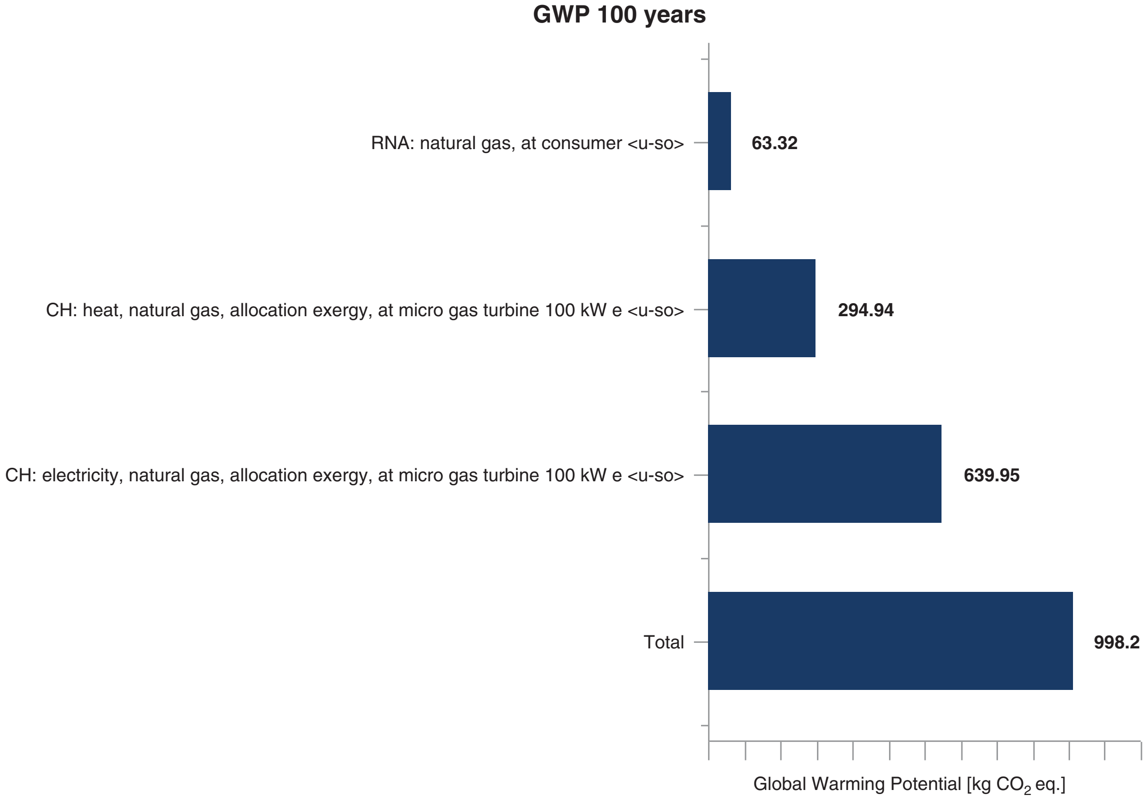


Figure 4.21 *GWP from natural gas based CHP generation system (basis 11 340 MJ energy content in natural gas).*

2. Give the reason for the credit gained by biogas compared to natural gas or otherwise, for each of the categories shown. (3 marks)
3. State the hot spot for each feedstock under each category. (2 marks)
4. Explain how these hot spots may be mitigated. (3 marks)

Problem 3. Carries 5 Marks

A biomass integration gasification combined cycle plant is required to produce 50 MW e output. The biomass feedstock can be wheat straw, waste wood and refuse-derived fuel (RDF), which is produced by shredding and dehydrating municipal solid waste. Their ultimate analyses are shown in Table 4.25.

1. Name the impact categories that can be evaluated to create a hierarchy of biomass feedstocks from most to least beneficial ones. Assume that the toxicity potentials in all categories are comparable between feedstocks. Given that the data generation is a huge constraint in the LCA study, your list must not consist of more than three most important impact categories. (1.5 marks)
2. Give the reasoning for your above selection. (3.5 marks)

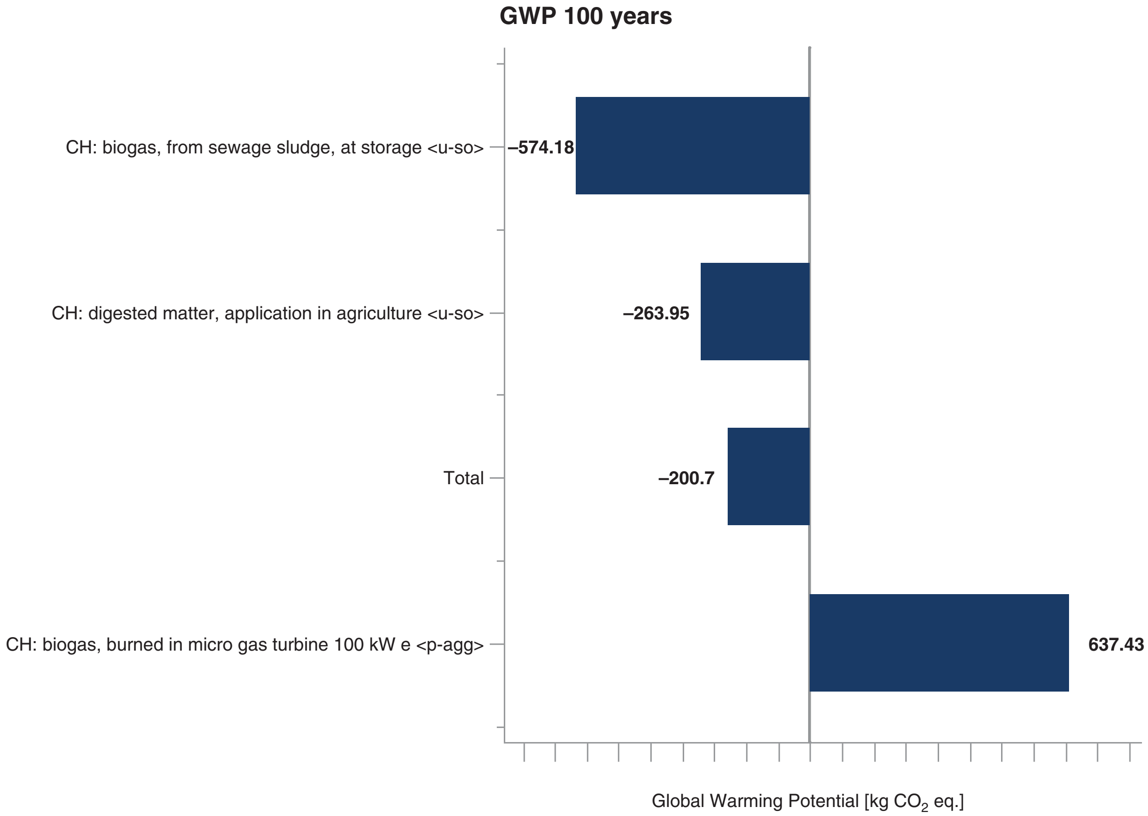


Figure 4.22 *GWP from anaerobic digestion based production system (basis 11 340 MJ energy content in biogas).*

Test of Peer Review Skill

The LCA study is proving to be effective for LCA studies. Amongst the various environmental impact categories, the most important issues considered are the global warming potential impact saving, land use and water footprint. Various journals provide numerous LCA studies of biorefinery systems. Though not exhaustive, the following list of journals can be searched for biorefinery LCA papers. Select studies under topic areas, such as Bioethanol, Biorefinery, Polygeneration, CHP, Sustainability and LCA and test your review skills.

- Nature journals: http://www.nature.com/siteindex/index.html
- Science: http://www.sciencemag.org/magazine
- Environmental Science and Technology
- Energy and Environmental Science
- Water Research
- Journal of Power Sources
- Applied Energy
- Biomass and Bioenergy
- Atmospheric Environment

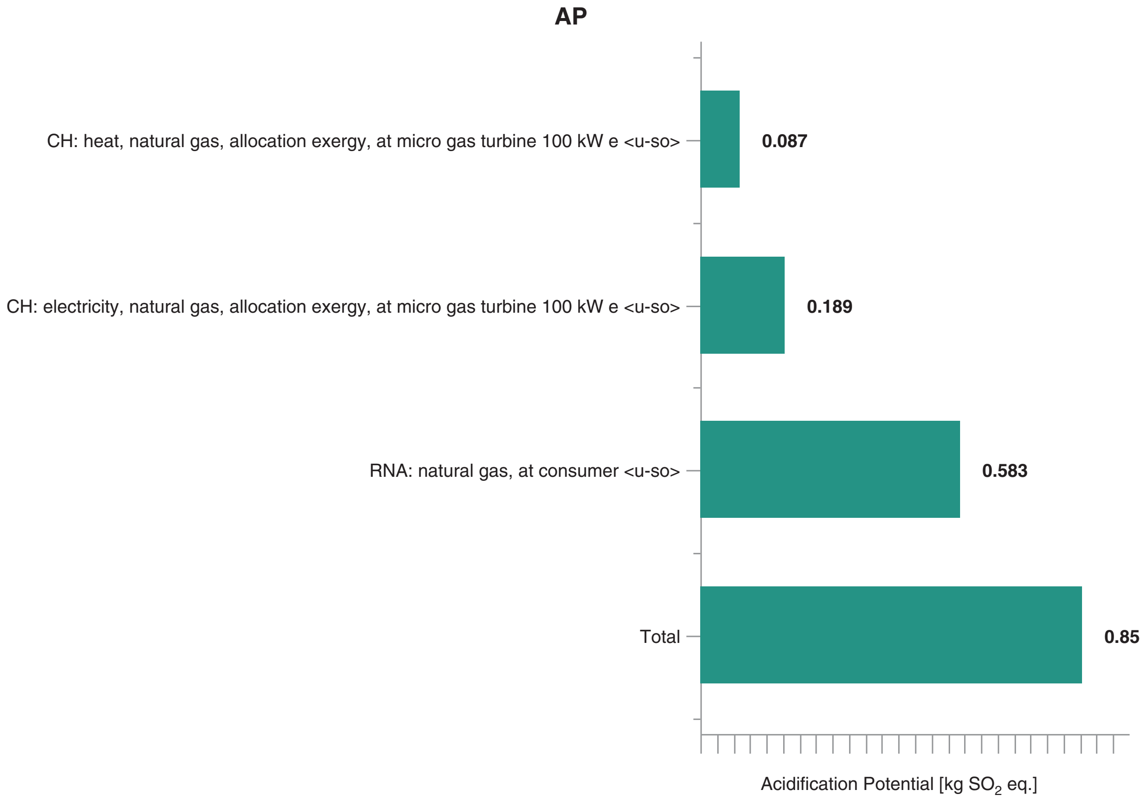


Figure 4.23 *Acidification potential (AP) from natural gas based CHP generation system (basis 11 340 MJ energy content in natural gas).*

- Ecological Economics
- International Journal of Life Cycle Assessment
- Journal of Industrial Ecology
- Energy
- Energy Policy
- Environmental Science and Pollution Research
- Journal of Environmental Management
- Water Resources Management
- Renewable and Sustainable Energy Review
- Solar Energy
- Resources, Conservation and Recycling
- International Journal of Energy Research
- Journal of Cleaner Production
- Technological Forecasting and Social Change
- Energy and Buildings
- Sustainable Development
- Chemical Engineering Research and Design
- Industrial and Engineering Chemistry Research

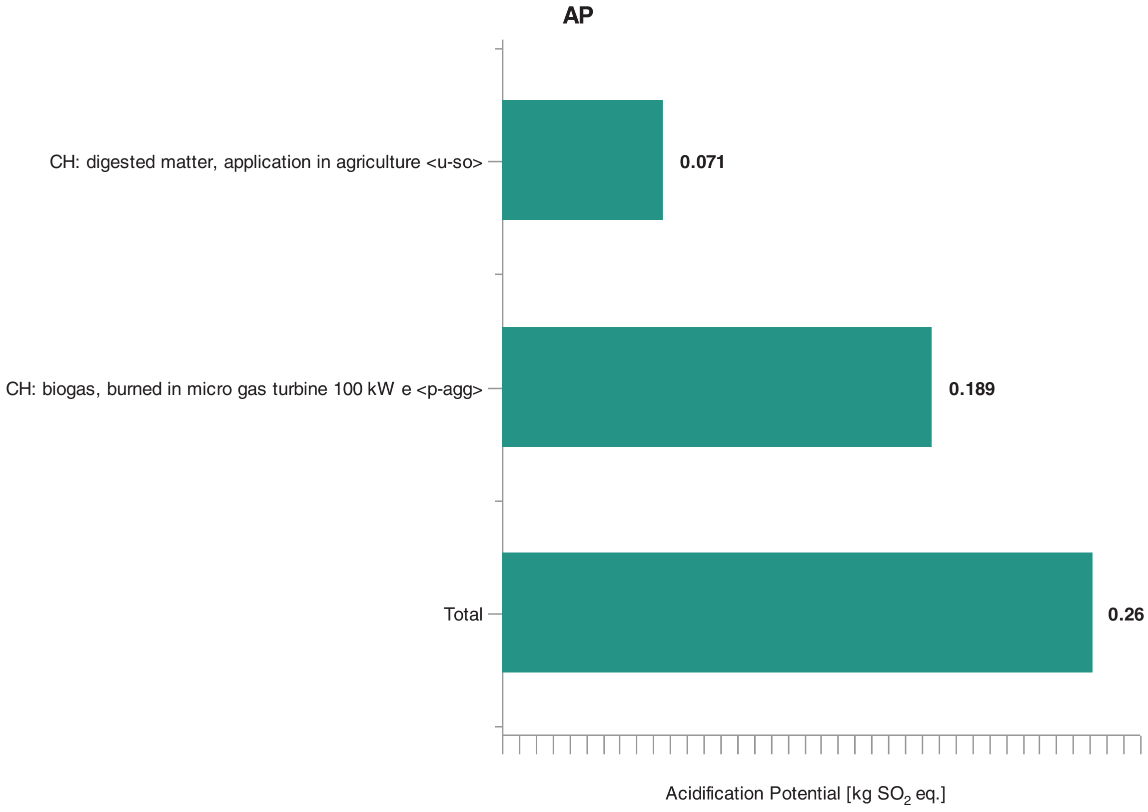


Figure 4.24 *Acidification potential (AP) from anaerobic digestion based production system (basis 11 340 MJ energy content in biogas).*

- Sustainability
- Journal of Applied Microbiology
- Critical Reviews in Environmental Science and Technology

Answer to the Following Questions

Goal and Scope Definition

Are the boundaries defined for the systems appropriate? What other blocks/subsystems could have been added (or otherwise) within the boundaries to make differences in impact assessment values and interpretation?

A biorefinery LCA publication may show the use of various units to present results, such as, per land use, per mass, per energy and per annual bases. Explain the reason for using each unit.

Which other impact categories might have been relevant for the study? Remember “less” is “more” when a study is complete, transparent and coherent. LCA study results should also be in transferable form such that these can be used/adapted and cited in another study (an example is shown in Table 4.4).

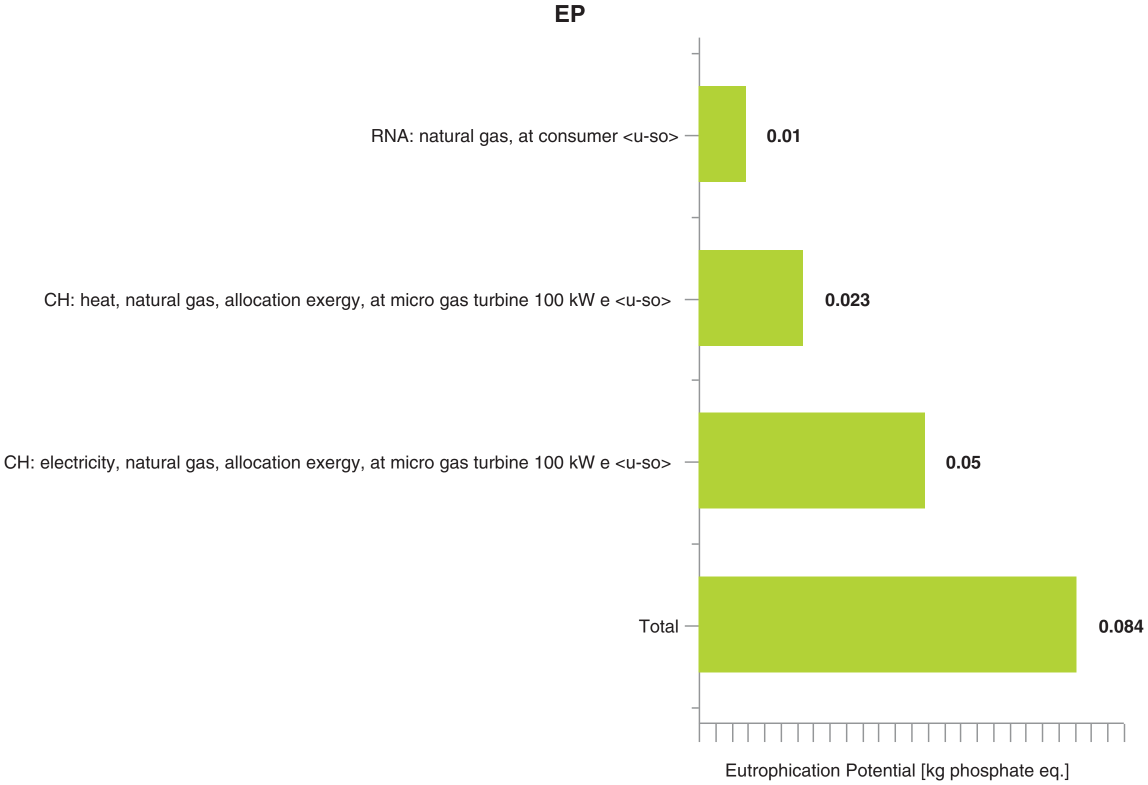


Figure 4.25 *Eutrophication potential (EP) from natural gas based CHP generation system (basis 11 340 MJ energy content in natural gas).*

Inventory Analysis

What are the advantages in showing inventories around various internal boundaries in the system (i.e., cultivation, processing and then for each unit operation)?

What are the advantages and disadvantages of using simulation results, databases from software such as GaBi and primary social science research data?

Interpretation

Are the results clearly shown? Are the expected results clearly stated in the goal and scope definition?

Is this a stand-alone, accounting (consequential) or change oriented (attributional) type of study?

How would you like to improve the presentation of the sensitivity analysis results?

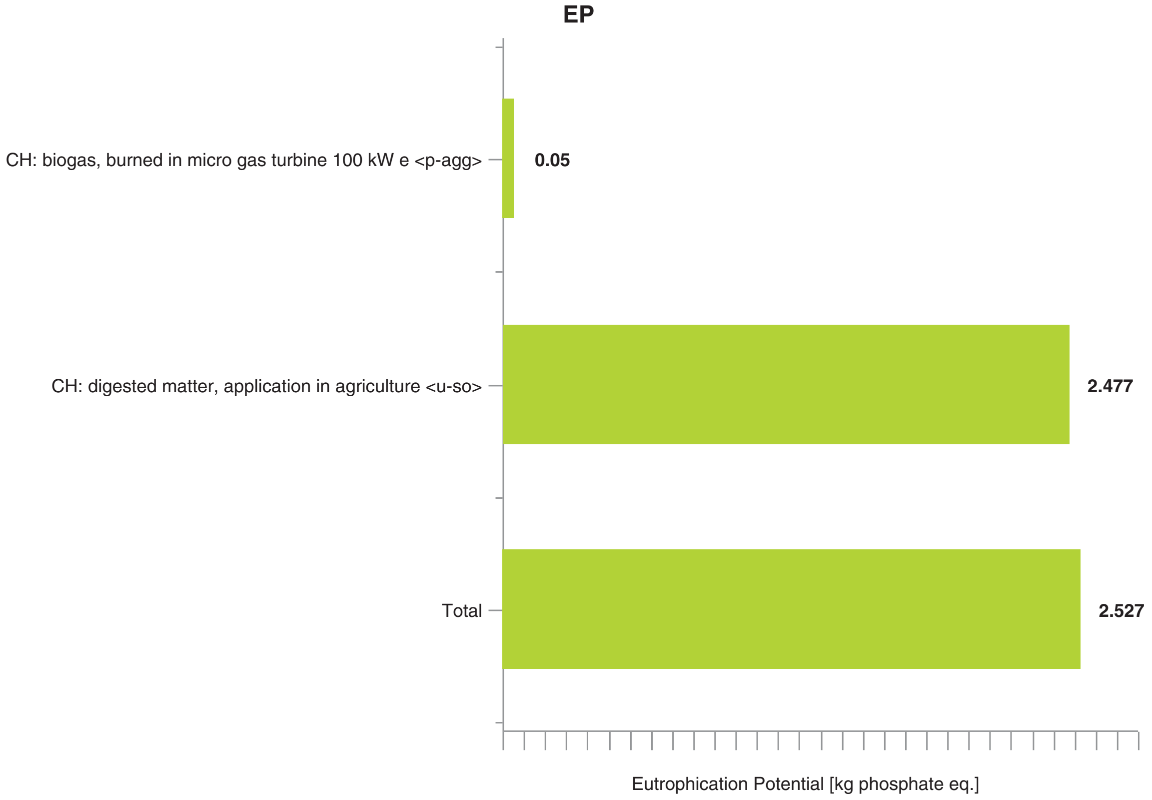


Figure 4.26 *Eutrophication potential (EP) from anaerobic digestion based production system (basis 11 340 MJ energy content in biogas).*

Essay writing (100 marks)

Task

Write a research paper on LCA studies of **your chosen case study or one of the following topics**. It is important that your research refers to a variety of sources, of which a significant proportion should be peer-reviewed journal papers. Answers must be fully referenced using the author–date (Harvard) system. The report may contain solutions for the following issues as appropriate. The list is not exhaustive and only meant to provide a guidance. Please include any other issues as you consider appropriate.

- Identify alternative technology options.
- Select one or two technologies to do LCA in detail.
- Identify system boundary and functional units (suitable for making comparisons with other systems).
- State assumptions and limitations.
- Identify hot spots in alternative technology options.
- Identify key pollutants.
- Identify geographic locations and any associated transport.
- Identify utility requirements (e.g., electricity and heat, etc.) and sources of them.
- Discuss hot spots, types of pollutants and ways to remedy in detail (see the next chapter).
- Make comparison with other equivalent systems for environmental sustainability.

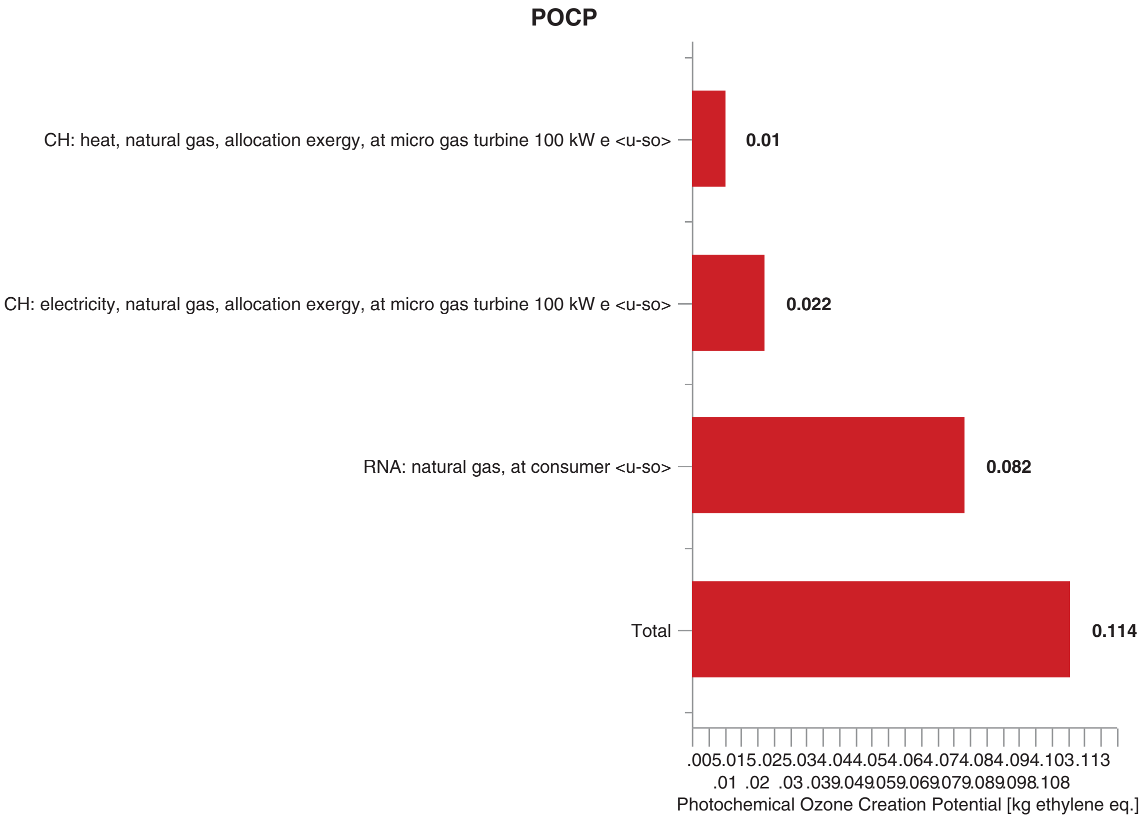


Figure 4.27 *Photochemical oxidant creation potential (POCP) from natural gas based CHP generation system (basis 11 340 MJ energy content in natural gas).*

- Report critical input parameters and sensitivity analysis results.
- Include critical analysis of the quality of results and LCA done by you and others in the field.
- Report results ***in transferable form.***
- Include techno-economic and socio-economic analyses as appropriate.
- Discuss policy drivers and barriers; learning points from the case study; action and policy recommendations.
- Discuss key benefits and challenges of the application of LCA.

Option 1. LCA of solar photovoltaic for electricity generation.
Option 2. LCA of energy generation from wastewater sludge.
Option 3. LCA of energy generation from municipal solid wastes.
Option 4. LCA of biofuel production from waste wood.
Option 5. LCA of composite/polymer production from biomass, with applications in aeronautics, automotive industry, construction, etc.

For your own case study:

Describe how LCA can be applied to a specific case. This can be, for example, a specific substance, or a specific product or service or technology.

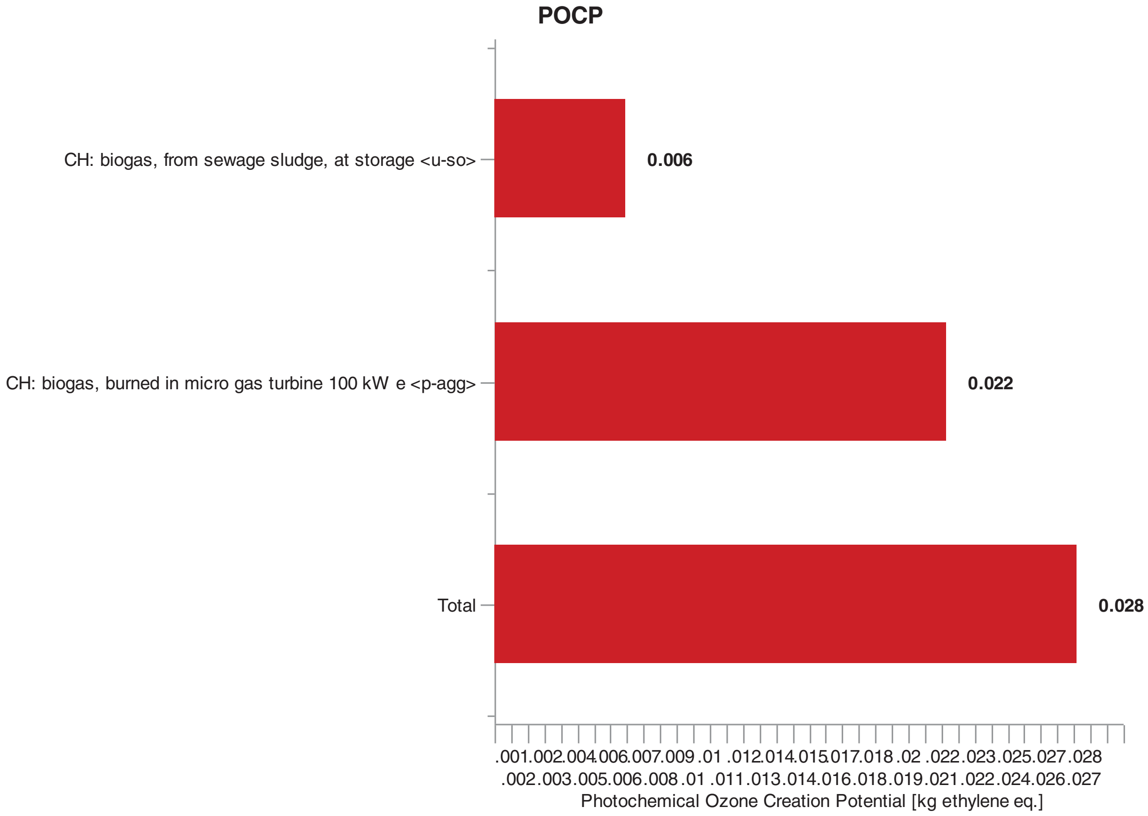


Figure 4.28 Photochemical oxidant creation potential (POCP) from anaerobic digestion based production system (basis 11 340 MJ energy content in biogas).

Format

- The content of paper should not exceed 5000 words (this excludes title, abstract, table of contents, reference list and appendix mainly used to show calculations).
- Use standard report format (including abstract, table of contents, headings, subheadings, reference list).

Table 4.25 Biomass composition in weight %.

Component in weight %	Straw	Wood	RDF
C	18.66	29.94	35.25
H	4.91	4.28	5.77
O	40.7	30.69	37.59
N	0.57	0.075	0.298
S	0.14	0	0.199
Cl	0	0	0.398
Moisture	8.5	25	0
Fixed C	17.91	8.92	10
Ash	8.61	1.1	10.5
Lower heating value (MJ kg^{-1})	14.6	19.3	17.73

Criteria for Assessment

- Demonstrated understating of LCA and LCT (25%).
- Appreciation of the application of theory to practice in the selected case (25%).
- Evidence of research to develop arguments, and the clarity and comprehensiveness of the arguments (35%).
- Overall structure, quality of the writing and presentation as well as the appropriate use and citing of reference materials (15%).

4.9 Future R&D Needs

Investment for biorefineries should be justified by a more holistic evaluation of social consequences (the agricultural focus may be shifted to energy crops rather than food crops due to subsidies and business cases that would fuel further to the energy demand), economic impacts (food price is likely to increase and affordability is likely to decrease) and long-term environmental implications on land, water and biosphere. It is imperative to compare land to energy yields, life cycle costs and environmental, economic and social sustainability between various energy systems with similar functional products. It is imperative to have an understanding of the value implications across supply chains that are global in some connections, complemented by bottom-up LCA approaches. Crop cultivation mapping on temporal and spatial scales using LCA is also a useful exercise. Research effort in the overall process and energy integration and enhancement of efficiency of integrated biorefinery systems is not apparent. Thus current deployment of process integration and life cycle approaches for the maximization of energy efficiency and minimization of life cycle inventories will be highly relevant for sustainable application of biorefineries.

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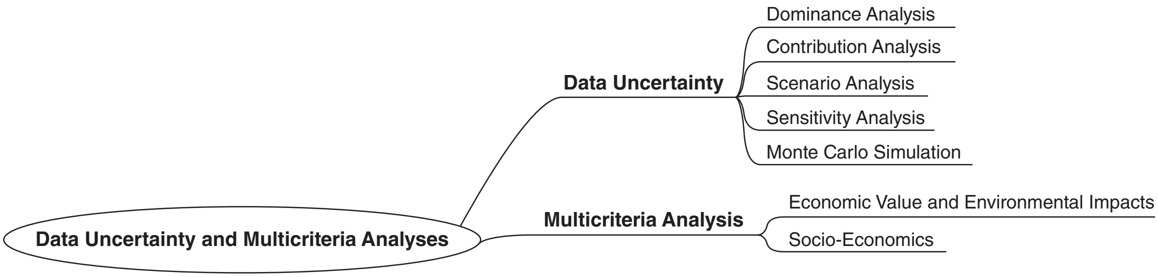
5

Data Uncertainty and Multicriteria Analyses



Structure for Lecture Planning

5.1 Data Uncertainty Analysis

LCA (Chapter 4) results have a number of data uncertainties. A transparent approach aims to track the uncertainties in data and reduce the effects of uncertainties in data. Data uncertainty in LCA can result from imprecise measurements of inventories, average or even outdated data using proxies and incomplete data. Various assumptions are made when deducing life cycle inventories (LCI), such as linear correlations and averaged data over time and across regions. During life cycle impact assessments (LCIAs), model approximations can result from average characterization factors deduced from simple biogeochemical models. Missing characterization factors for certain substances and interactions between substances are also approximated. Data uncertainties result from normalization, weighting and valuation stages.

Uncertainties can result due to choices of:

1. Functional units, systems boundaries.
2. LCI.
3. LCIA.
4. Allocation approaches for multioutput and for recycling processes.

Biorefineries and Chemical Processes: Design, Integration and Sustainability Analysis, First Edition.
Jhuma Sadhukhan, Kok Siew Ng and Elias Martinez Hernandez.

Companion Website: http://www.wiley.com/go/sadhukhan/biorefineries

When all errors are accumulated for data interpretation, the errors can be large. Most LCA results present spatially and temporally averaged data and in this approach resulting errors are also difficult to comprehend. Data uncertainty can be managed by probabilistic or stochastic approaches such as Monte Carlo simulation, and also some deterministic ways such as scenario analysis and sensitivity analysis.

The LCA results include the following aspects:

1. Dominance analysis
2. Contribution analysis
3. Testing robustness of the results
   - Scenario analysis
   - Sensitivity analysis
   - Monte Carlo simulations

5.1.1 Dominance Analysis

A dominance analysis is about hot spot analysis due to environmental activities. The analysis shows what activity has the highest value in an impact category. Dominance analysis results can be shown in various ways. The pie charts in Figure 5.1 show examples of the sequence of activities from the most to the least detrimental activities for the environment. Cumulative primary energy depletion and global warming, acidification and abiotic depletion potential categories are shown[1]. The agricultural system shown is for UK wheat, comprising the FO: Field Operations, F & P: Fertilizers and Pesticides, Dir. & Ind. FE: Direct and Indirect Field Emissions, GC: Grain Conditioning.

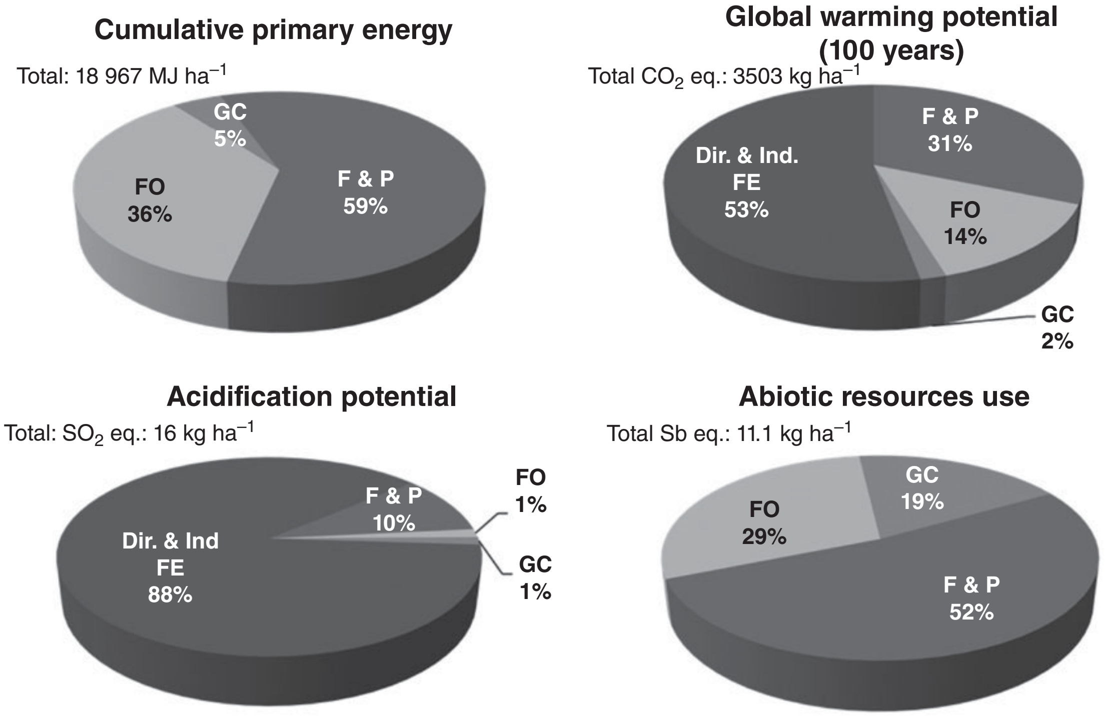


Figure 5.1 An example of dominance analysis results. (Reproduced with permission from Martinez-Hernandez et al. (2013)[1]. Copyright © 2013, Elsevier.)

The activities, from the highest to the lowest impacts are as follows:

Cumulative primary energy:

$$F \,\&\, P > FO > GC$$

Global warming potential:

$$\text{Dir. \& Ind. FE} > F \,\&\, P > FO > GC$$

Acidification potential:

$$\text{Dir. \& Ind. FE} > F \,\&\, P > FO/GC$$

Abiotic resource use:

$$F \,\&\, P > FO > GC$$

Note that the total values of the impact characterizations are shown on a per hectare basis. This is a transferable form to compare with other equivalent systems, such as first generation crops.

A Sankey diagram is another way to present the hot spot analysis from various activities. In a Sankey diagram, the thickness of a link joining a source to a sink process is proportional to the environmental impact from the source process. A much thicker line from a source process than a line entering to the process shows that the process is environmentally more detrimental. The line thickness increases from upstream to downstream processes as environmental impacts are aggregated. The life cycle global warming potential (GWP) (as CO_2 equivalent) in g MJ^{-1} of two integrated whole *Jatropha* fruit biorefinery systems producing heat and power and (a) biodiesel or (b) green diesel is shown in Figure 5.2. The combustion processes have the highest GWP impacts, followed by the integrated biomass gasification combined cycle (IBGCC) plants producing methanol or hydrogen.

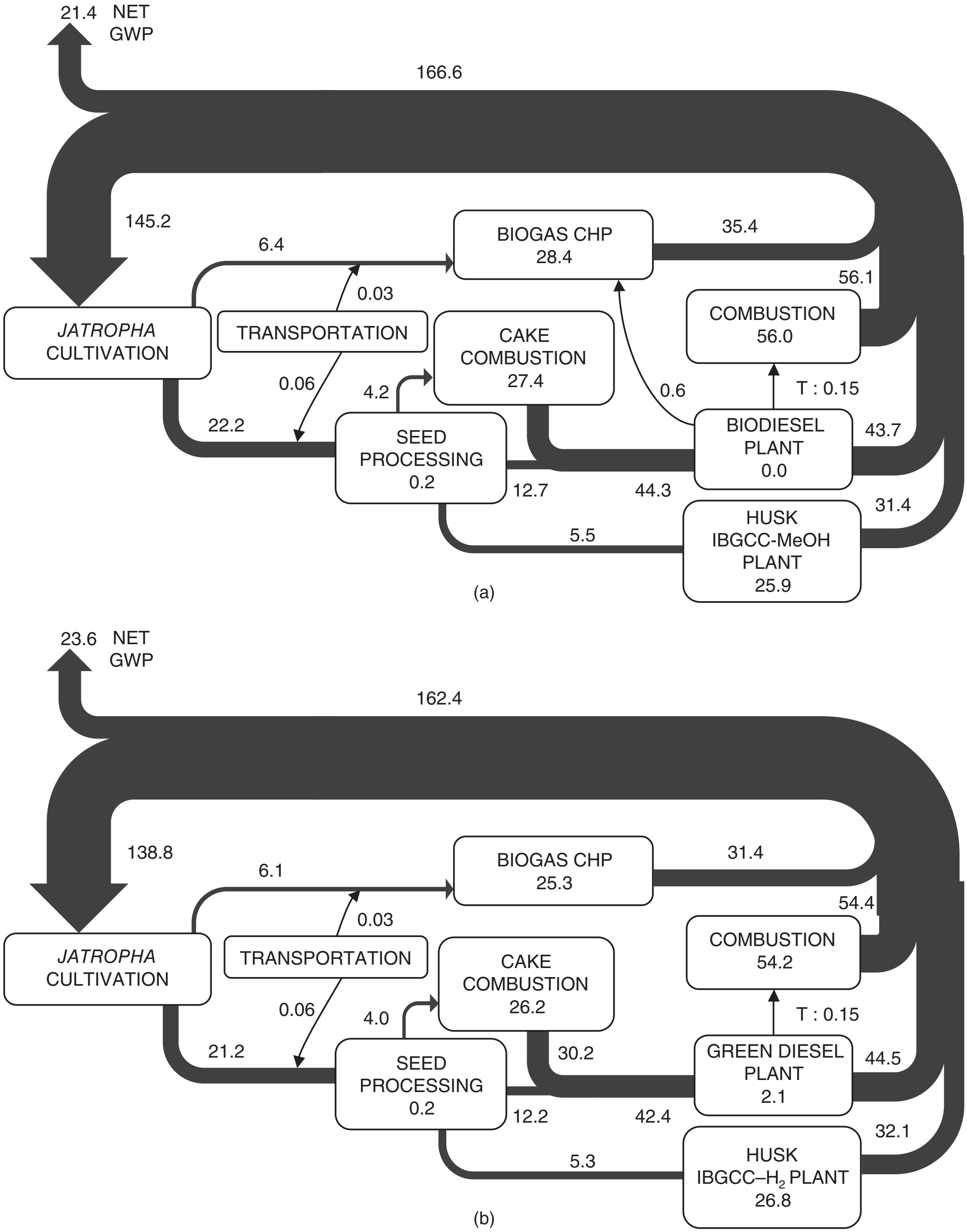
5.1.2 Contribution Analysis

Chemicals causing higher environmental impacts must be identified and replaced with environmentally better performing similar functionality chemicals. This is also a hot spot analysis, but one related to chemicals or loads or polluting substances rather than activities as in the case of dominance analysis. Thus contribution analysis is carried out to track back pollutants to their origins and minimize their emissions from the origin.

Figure 5.3 shows an example of a contribution analysis. The outlet pollutants include carbon dioxide, nitrous oxide and methane in kg per tonne of sewage sludge. These flow rates do not account for the GWP impact characterization factors, such as 298 CO_2 equivalent for nitrous oxide and 25 CO_2 equivalent for methane. You are recommended to use CO_2 equivalent values on the y-axis for direct comparisons, through a contribution analysis. Note that the outlet carbon dioxide quantities do not take account of the inlet carbon dioxide capture during biomass production.

Figure 5.4 shows the contribution analysis of nonrenewable and renewable energy resources for the production of biogas for micro generation (electricity and heat generations) and digested matter for agricultural application (fertilizer production) from sewage sludge anaerobic digestion (AD). Tracking back the GHG emissions, the primary energy resources such as natural gas (by 61%), crude oil (by 5%) and hard coal and lignite (each by 2%), out of a total of 2468.5 MJ of energy input, were found to be responsible. The functional unit is 1000 kg of sewage sludge AD into 315 N m^3 of biogas and 700 kg of digested matter productions. If natural gas is replaced with a renewable energy source, the GHG emissions will be reduced. Note that the organic substance, primary forest and wind and solar energy use is close to zero. Hence, increasing their inputs to the AD system, in particular solar and wind energy, will reduce the environmental emissions. Tracking the routes between primary resources and end uses through conversion processes is essential. The pollutants causing impact hot spots, pollutants with larger impact reduction potentials and the primary resources of pollutants need to be identified. Primary resources causing depletion of energy or material reserves of the earth and emissions can be replaced with better alternatives that reduce these environmental impacts.

A contribution analysis is very useful for identifying resource (elements and fossil) use. The input resources required for the production of polyethylene terephthalate for 1 cm^2 solar organic photovoltaic (OPV) cell fabrication, extracted from Ecoinvent 2.0 and BUWAL databases, are shown in Table 5.1.



(a)

(b)

Figure 5.2 *Sankey diagram for GWP (as CO_2 equivalent) flows in g MJ^{-1} in two integrated whole* Jatropha *fruit biorefinery systems producing heat and power and (a) biodiesel or (b) green diesel.*

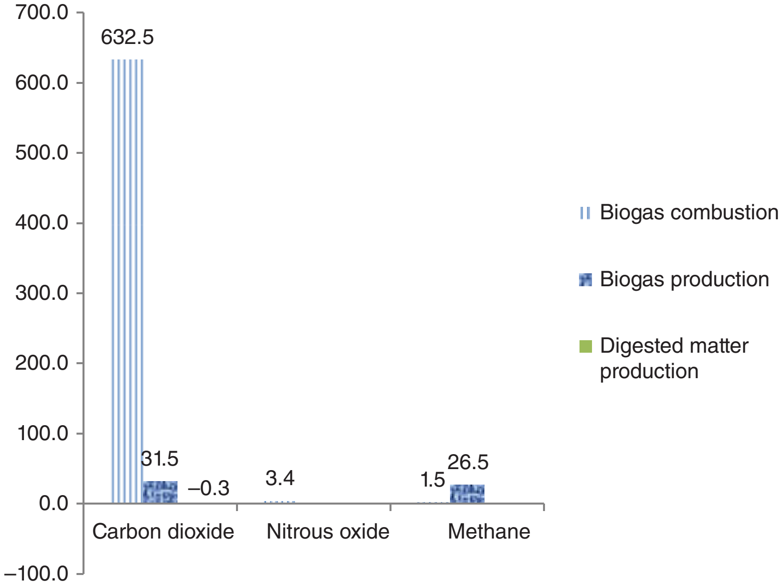


Figure 5.3 *Contribution analysis in kg per tonne of sewage sludge (which environmental load contributes the most).*

5.1.3 Scenario Analysis

At first, independent variables are fixed at certain values for an LCIA. Independent variables can be varied to generate numerous scenarios. One or more independent variables can be varied at the same time. A sensitivity analysis refers to variations in estimated impact potentials due to unit changes in independent variables or due to standard deviations from mean values of independent variables. Independent variables, one or more at a time, can be examined for a sensitivity

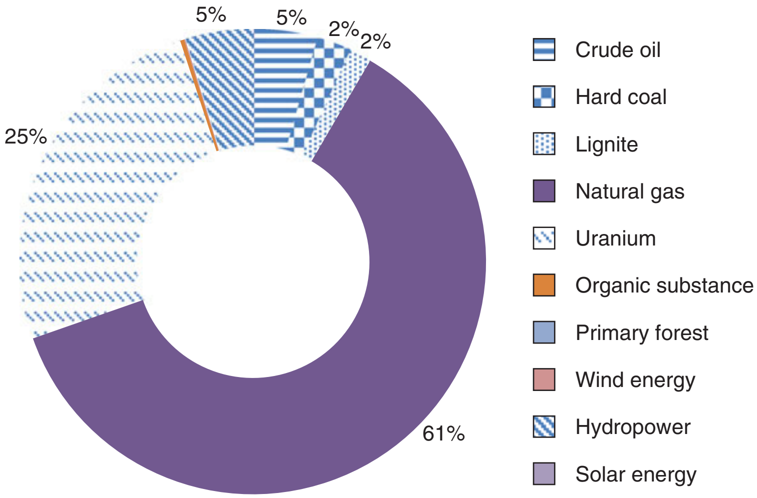


Figure 5.4 *Contribution analysis of nonrenewable and renewable energy resource use for the production of biogas for micro generation (electricity and heat generations) and digested matter for agricultural application.*

Table 5.1 Resource depletion from the manufacture of a solar OPV cell. Some databases were obtained from BUWAL (Bundesamt für Umwelt, Wald und Landschaft).

Crude oil free wellhead [crude oil (resource)]	1.07 kg
Raw natural gas (BUWAL) [natural gas (resource)]	0.576 kg
Primary energy from hydropower (BUWAL) (renewable energy resources)	0.5 MJ
Raw hard coal (BUWAL) [hard coal (resource)]	0.13 kg
Raw brown coal (BUWAL) [lignite (resource)]	0.11 kg
Process and cooling water [operating materials]	0.017 kg
Sodium chloride (rock salt) [nonrenewable resources]	0.0049 kg
Iron ore [nonrenewable resources]	0.0005 kg
Bauxite [nonrenewable resources]	0.0003 kg
Limestone (calcium carbonate) [nonrenewable resources]	0.00025 kg
Quartz sand (silica sand; silicon dioxide) [nonrenewable resources]	2.00×10^{-5} kg
Uranium free ore (BUWAL) [uranium (resource)]	1.60×10^{-6} kg

analysis on the environmental impacts. More sensitive independent variables displaying greater chances of variations from their mean values can be selected for further analyses. A number of scenarios can be evaluated using extreme bounds of independent variables and combinations of their values within feasible ranges.

An example of 1 tonne of epoxy resin production from biomass is shown in Table 5.2. Hexane and nitrogen mass flow rates are the two key input independent variables to the LCIA model. Their values are varied within feasible ranges to examine their combined effects on the GWP estimates from the LCIA model. The base value of GWP is 518.46 kg CO_2 equivalent from 1 tonne of epoxy resin production; 3 kg of hexane and 13 kg of nitrogen mass inputs to the system, for example, achieve a GWP reduction by 25%. As can be seen, the hexane mass flow rate can be varied between 3 kg and 99 kg and the nitrogen mass flow rate between 5 kg and 15 kg. For various combinations of their input values within these ranges, impact potentials can be evaluated. This method is called a scenario analysis. Two extreme scenarios can be created: maximum GWP reduction by 25% and minimum GWP reduction by 8% from the base impact value. A number of other scenarios result in 19% and 14% reductions in GWP. One or both flow rates can be varied at the same time.

Table 5.2 Hexane and nitrogen mass flow rates for various reductions from the base value of GWP impact.

Hexane Mass Flow Rate (kg)	Nitrogen Mass Flow Rate (kg)	GWP (100 years) Reduction (%)
3	13	25
12	12	
31	10	
60	7	
78	5	
18	15	19
27	14	
37	13	
46	12	
65	10	
93	7	
46	15	14
55	14	
65	13	
74	12	
93	10	
89	14	8
99	13	

5.1.4 Sensitivity Analysis

To do a sensitivity analysis with respect to an independent parameter, a range is specified and variations in LCI and LCIA are estimated for the range. An example is shown in Figure 5.5. A sewage sludge AD system producing biogas for micro generation (electricity and heat generations) and digested matter for fertilizer production is studied for the sensitivity analysis. The independent variable is the biogas volumetric production rate. All other flow rates are dependent on the biogas volumetric production rate. These include digested matter mass flow rate, electricity and heat generation, etc. The biogas volumetric production rate is varied by ±25% standard deviation from the mean value and the LCIA are examined. The variations in the LCIA from their mean values are shown in Figure 5.5. The plot was generated using the graph:stock:high–low–close (this applies as maximum-minimum-mean) option in the Excel spreadsheet. Note that the values are not shown in absolute terms, but in relative terms. Thus, the base value is taken as 100; the mean value is marked at ~100. The minimum and maximum values are thus below and above 100, respectively. The difference between maximum and mean values is the positive standard deviation from the mean value. The difference between minimum and mean values is the negative standard deviation from the mean value. The difference between maximum and minimum values is defined as the range.

Impact categories include the acidification potential (AP) in kg SO_2 equivalent, eutrophication potential (EP) in kg phosphate equivalent, freshwater aquatic ecotoxicity potential (FAETP) in kg 1,4-dichlorobenzene (DCB) equivalent, global warming potential (GWP) in kg CO_2 equivalent, human toxicity potential (HTP) in kg DCB equivalent, marine aquatic ecotoxicity potential (MAETP) in kg DCB equivalent, photochemical oxidant creation potential (POCP) in kg ethylene equivalent and terrestric ecotoxicity potential (TETP) in kg DCB equivalent.

The maximum range is obtained for the POCP, 38.2%, from 80.92 to 119.12. Its standard deviation is thus ±19.1% from its mean value. The high–low–close stock graphical choice in the Excel spreadsheet was used to create this range: 119.12 (high)–80.92 (low)–100.02 (close). This graph shows the sensitive impact categories with greater ranges. Thus, POCP is the most sensitive and MAETP is the least sensitive impact category. MAETP is the least sensitive impact

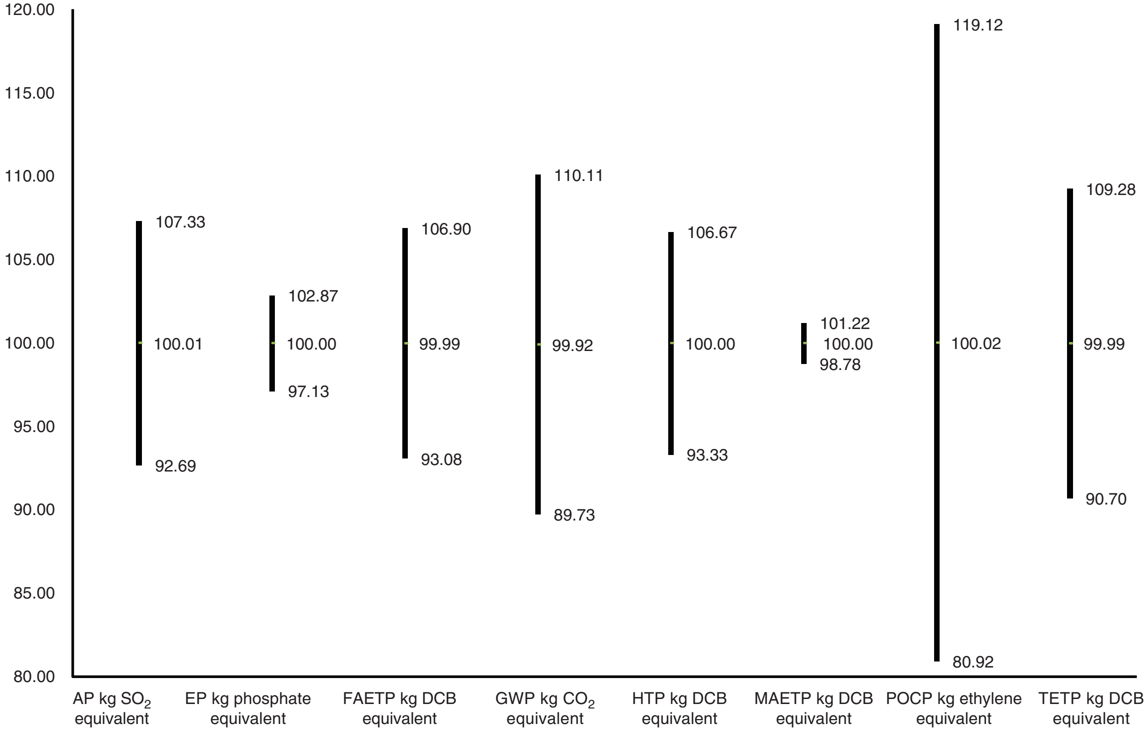


Figure 5.5 *Sewage sludge to micro generation and digested matter: range of variations from the mean values due to ±25% standard deviation in the independent variable (biogas volumetric production rate).*

category due to its very large value and narrow range. The most to the least sensitive life cycle impact categories are as follows:

POCP > GWP > TETP > AP > FAETP > EP > MAETP

5.1.5 Monte Carlo Simulation

Sensitivity analysis can be undertaken for a multiparametric decision making problem using a Monte Carlo simulation combined LCA (MCLCA) approach. With MCLCA important impact characterizations can be selected and optimized to make a choice between various technologies. In Monte Carlo simulation, values of independent variables within their specified standard deviations from their mean values can be randomly selected during a simulation run. All the primary impact characterizations are calculated for the selected set of values of independent variables. At the end of all Monte Carlo simulation runs, the chances or probabilities of occurrence at various values of an impact characterization are counted and plotted (on the *y*-axis) against percentage standard deviations from mean value of the impact characterization (on the *x*-axis). This results in the probability distribution curve of an impact category. Highly sensitive categories show wider probability distributions. Narrow probability distribution curves imply less sensitive categories.

Intergovernmental Panel on Climate Change (IPCC) Guidelines for National Greenhouse Gas Inventories; Geneva, Switzerland, 2006, recommended a Monte Carlo simulation to estimate and mitigate uncertainty in impact assessments[2]. The methodology can be adapted according to the LCA goal and scope definition. Figure 5.6 shows the steps involved in an uncertainty analysis using a Monte Carlo simulation. The MCLCA approach consists of three main steps:

1. Develop equations or models for the LCI in terms of independent and uncertain input variables to the model.
2. Select a standard deviation and probability distribution function for each independent variable.

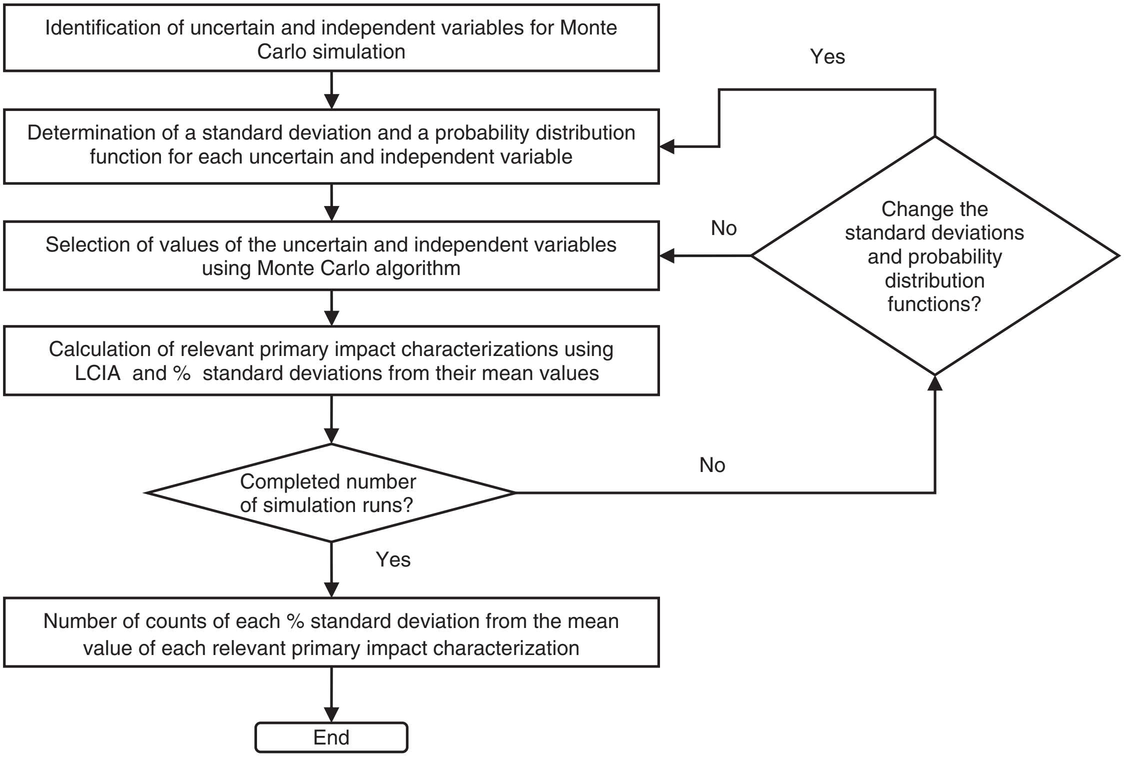


Figure 5.6 *Monte Carlo simulation framework integrated with LCA.*

3. Monte Carlo simulation run. Using the Monte Carlo algorithm (for random number generation), a set of values of independent variables within their given distributions is randomly selected. Determine the LCIA. At the end of a large number of specified simulation runs, count the occurrence of an impact characterization at the estimated values.
4. Repeat the Monte Carlo simulation runs, steps 2 to 3, until enough number of runs is completed for obtaining smooth distribution trends of the LCIA. Calculate the mean value and standard deviations from the mean value for each impact category.
5. Count the chances of occurrence of each model predicted impact characterization by the % standard deviation from their mean values. Ensure that there are enough simulation runs to obtain a smooth and representative probability distribution curve for an impact category.

LCA is data intensive. A dispersed data set makes MCLCA computationally intensive. There lies uncertainty in primary raw material and energy flow data assimilation and in an inventory analysis. A large number of Monte Carlo simulation runs ensures that the approximation can be made more accurately. Monte Carlo simulation runs of ~5000 are recommended in the IPCC Guidelines[2].

The equation below shows the formula for calculating the standard deviation, σ, of n data points: $x_1, x_2, x_3, \ldots, x_{n-1}, x_n$, with respect to their average or mean value, $\bar{x}$:

$$\sigma = \sqrt{\frac{\sum_i (x_i - \bar{x})^2}{n}} \tag{5.1}$$

The values of independent variables are generated using their given probability distribution functions. The simplest form of probability distribution function is the uniform probability distribution function. Three other most common forms of probability distribution functions are the normal or Gaussian, lognormal and triangular.

Equations (5.2a) to (5.2c) below show their respective correlations in terms of mean, standard deviation and values of the variable (x_i):

Normal or Gaussian probability distribution function =

$$f(x_i) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(x_i - \bar{x})^2}{2\sigma^2}\right)^{\pi} \tag{5.2a}$$

Lognormal probability distribution function =

$$f(x_i) = \frac{1}{x_i\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(\ln x_i - \bar{x})^2}{2\sigma^2}\right)^{\pi} \tag{5.2b}$$

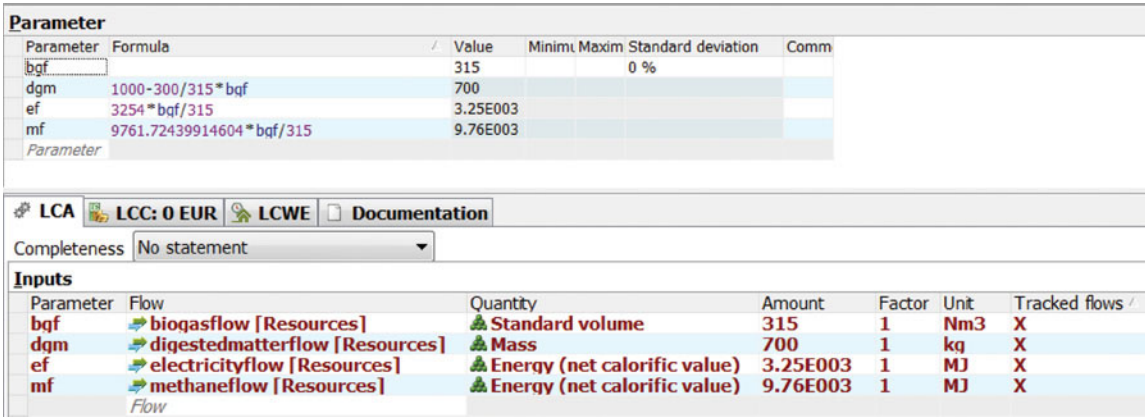
Triangular probability distribution function =

$$f(x_i) = \left\{ \begin{array}{c} 0(x_i \le a; x_i \ge c) \\ \dfrac{2(x_i - a)}{(b-a)(c-a)}(a < x_i < b) \\ \dfrac{2(c - x_i)}{(c-a)(c-b)}(b \le x_i < c) \end{array} \right\} \tag{5.2c}$$

where

a = minimum value of x
b = modal value of x
c = maximum value of x

A sewage sludge AD plant can be operated to maximize the output energy generation via biogas production. An AD plant also coproduces digested matter for agricultural application. The biogas and digested matter yields are related by the mass balance for a given sewage sludge mass throughput through an AD plant. As the biogas yield increases, the energy generation increases and digested matter yield decreases, lowering the fertilizer production rate and vice versa. Hence, one



Parameter

Parameter	Formula	Value	Minimu	Maxim	Standard deviation	Comm
bgf		315			0 %	
dgm	1000-300/315*bgf	700				
ef	3254*bgf/315	3.25E003				
mf	9761.72439914604*bgf/315	9.76E003				
Parameter						

Completeness: No statement

Inputs

Parameter	Flow	Quantity	Amount	Factor	Unit	Tracked flows
bgf	biogasflow [Resources]	Standard volume	315	1	Nm3	X
dgm	digestedmatterflow [Resources]	Mass	700	1	kg	X
ef	electricityflow [Resources]	Energy (net calorific value)	3.25E003	1	MJ	X
mf	methaneflow [Resources]	Energy (net calorific value)	9.76E003	1	MJ	X
	Flow					

Figure 5.7 *Screenshot from GaBi, to define the independent and dependent parameters involved in an AD plant LCA study.*

of the mass yields of biogas and digested matter can be considered as an independent variable and the other can be shown as a function of the independent variable. The following example and data analysis show a systematic decision making about the transfer coefficient of sewage sludge for energy generation an against agricultural application. The problem can be formulated for sensitivity analysis, Monte Carlo simulations, etc., and solved in a spreadsheet environment or any other software supporting such analyses.

Figure 5.7 shows a screenshot from GaBi, LCA software from PE International, to define the independent and dependent variables of an AD plant. Independent variables do not have any formula, while the dependent variables are formulated in terms of independent variables. In the figure, the biogas volumetric flow rate, presented by the symbol `bgf`, is shown as the independent variable carrying no formula in the formula bar. The dependent variables: digested matter mass flow rate, electricity generation and methane calorific value, using the symbols `dgm`, `ef` and `mf`, respectively, are shown as a function of `bgf`. The correlations are linear with respect to `bgf`. A Monte Carlo simulation is then undertaken with:

(a) 5000 runs,
(b) ±25% standard deviations and normal distributions in `bgf`.

The probability distribution of the global warming potential impact with respect to its mean value in ±100% standard deviation scale is shown in Figure 5.8. For example, the probability of the global warming potential occurring at the

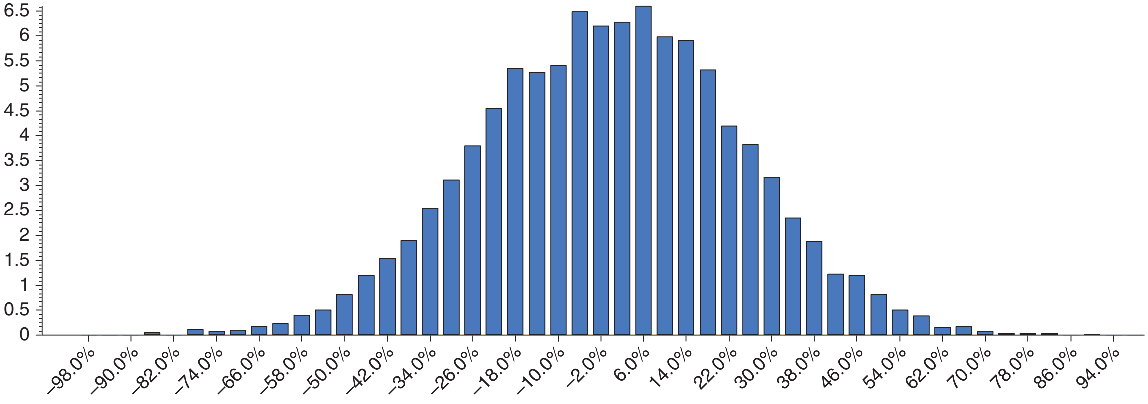


Figure 5.8 *Probability distribution of the global warming potential impact in ±100% standard deviation scale from the mean.*

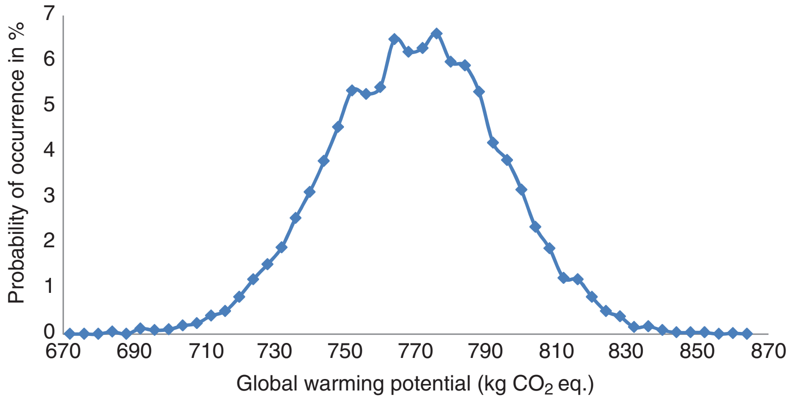


Figure 5.9 *Probability distribution against the global warming potential impact values.*

mean value is ~6.3%. The peak probability, ~6.6%, occurs at the standard deviation of ±6%. The summation of all the probabilities across the ±100% standard deviation scale is 100. The resulting distribution corresponds to the normal distribution.

It is also possible to generate the data points or actual impact values from a probability distribution curve in Figure 5.8, using Equation (5.1). The probability distribution against the actual impact values can then be plotted, such as in Figure 5.9. The mean global warming potential is 768 kg CO_2 equivalent. The number of data points or clusters is 49.

The probability distributions of FAETP, HTP and TETP with respect to standard deviations are shown in Figure 5.10. As TETP displays a wider distribution it has a greater chance of change from the mean value. Figure 5.11 similarly shows that the probability of occurrence of MAETP at the mean value is 98% and hence the probability of reduction (or increase) in the MAETP mean value is only 2%. This is due to the MAETP's very high absolute mean value in the order of 10^4 magnitudes in kg DCB equivalent. EP also shows a narrow distribution, but it is wider than that of MAETP. This analysis thereby helps to screen out the most sensitive set of impact categories for further investigation. For the given example, the GWP showing wider distribution is the most sensitive impact category. The MAETP showing the narrowest

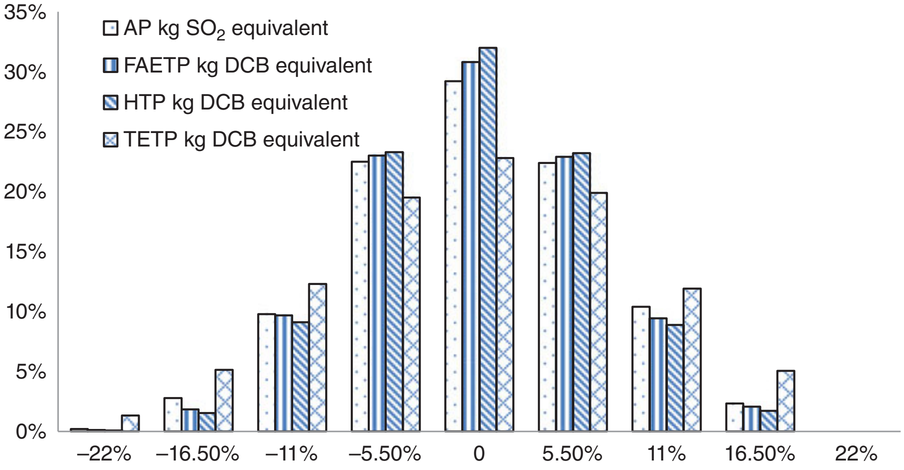


Figure 5.10 *Acidification, freshwater aquatic ecotoxicity, human toxicity and terrestric ecotoxicity potentials (AP, FAETP, HTP and TETP) impact probability distributions (y axis) with respect to standard deviations (x axis) from their mean values.*

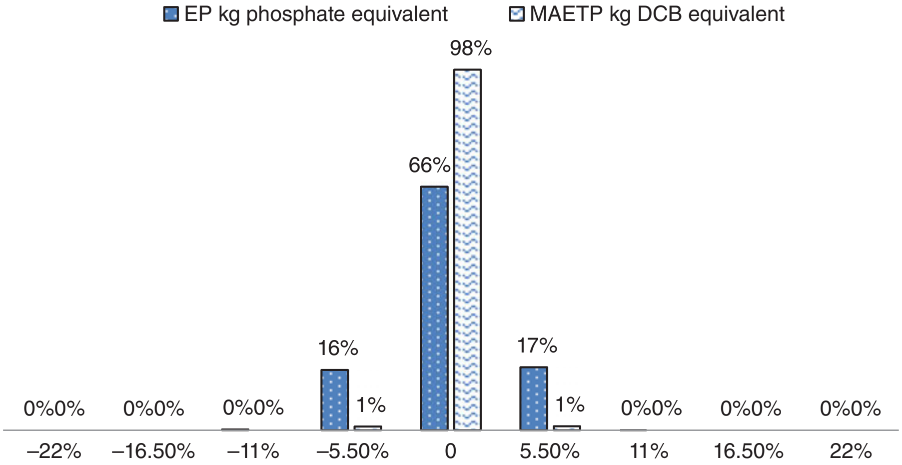


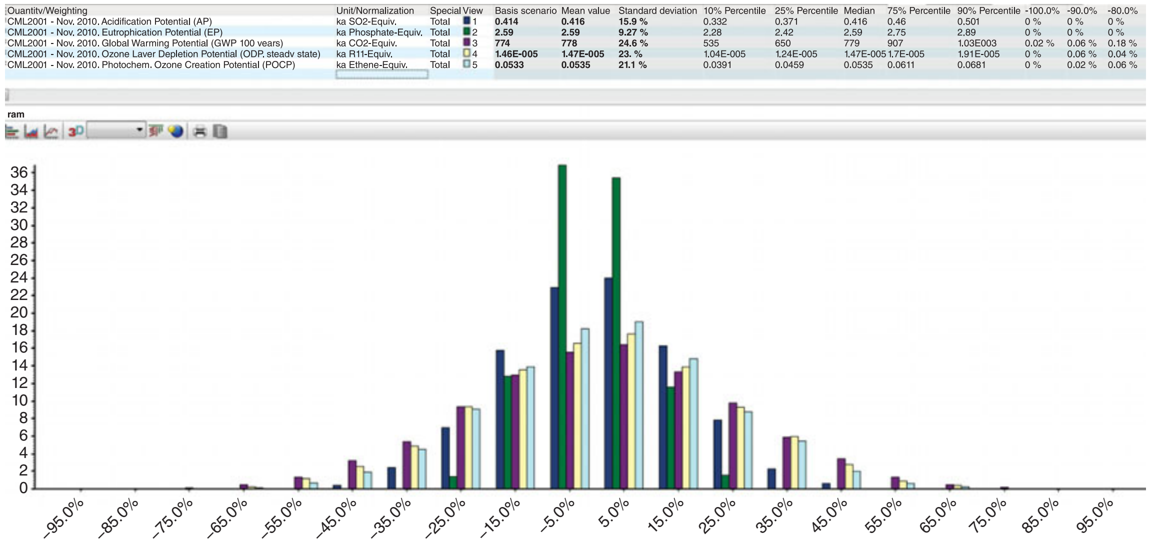
Figure 5.11 *Probability distributions (y axis) of marine aquatic ecotoxicity potential (MAETP) and eutrophication potential (EP) with respect to standard deviations (x axis) from their mean values.*

distribution is the least sensitive impact category. The least sensitive categories also imply that they will not be affected by model uncertainties.

Figure 5.12 shows the probability distribution versus the standard deviation from the mean value of various impact categories using GaBi software.

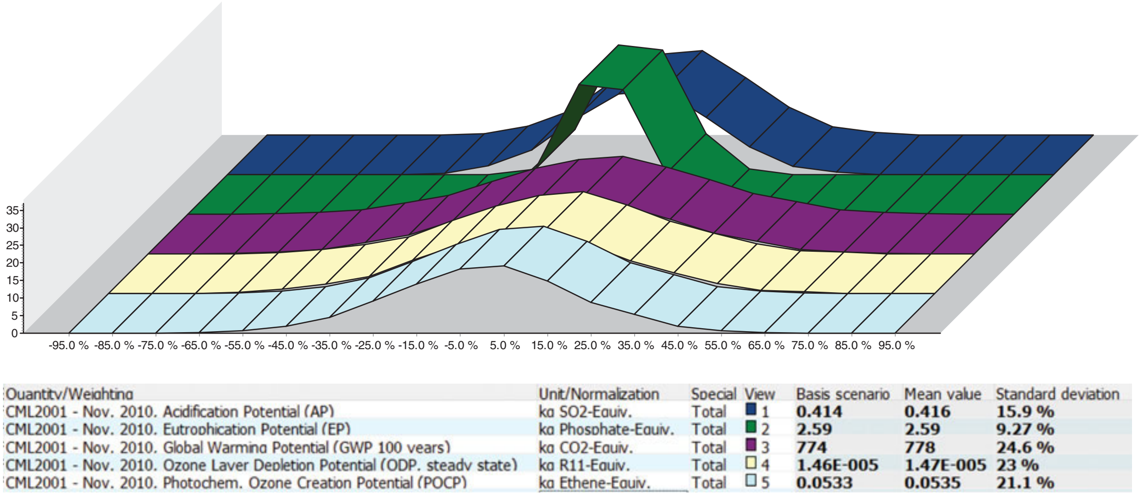
The recommended specifications for the Monte Carlo simulation are:

(a) 5000 runs
(b) Normal distributions and standard deviations by ±25% of independent variables
(c) Capture ±100% standard deviations scale for the impact characterizations.



Quantity/Weighting	Unit/Normalization	Special	View	Basis scenario	Mean value	Standard deviation	10% Percentile	25% Percentile	Median	75% Percentile	90% Percentile	-100.0%	-90.0%	-80.0%
CML2001 - Nov. 2010. Acidification Potential (AP)	kg SO2-Equiv.	Total	1	**0.414**	**0.416**	**15.9 %**	0.332	0.371	0.416	0.46	0.501	0 %	0 %	0 %
CML2001 - Nov. 2010. Eutrophication Potential (EP)	kg Phosphate-Equiv.	Total	2	**2.59**	**2.59**	**9.27 %**	2.28	2.42	2.59	2.75	2.89	0 %	0 %	0 %
CML2001 - Nov. 2010. Global Warming Potential (GWP 100 years)	kg CO2-Equiv.	Total	3	**774**	**778**	**24.6 %**	535	650	779	907	1.03E003	0.02 %	0.06 %	0.18 %
CML2001 - Nov. 2010. Ozone Layer Depletion Potential (ODP, steady state)	kg R11-Equiv.	Total	4	**1.46E-005**	**1.47E-005**	**23. %**	1.04E-005	1.24E-005	1.47E-005	1.7E-005	1.91E-005	0 %	0.06 %	0.04 %
CML2001 - Nov. 2010. Photochem. Ozone Creation Potential (POCP)	kg Ethene-Equiv.	Total	5	**0.0533**	**0.0535**	**21.1 %**	0.0391	0.0459	0.0535	0.0611	0.0681	0 %	0.02 %	0.06 %

Figure 5.12 *Probability distribution versus standard deviation from the mean value of various impact categories using GaBi software.*



Quantity/Weighting	Unit/Normalization	Special	View	Basis scenario	Mean value	Standard deviation
CML2001 - Nov. 2010, Acidification Potential (AP)	kg SO2-Equiv.	Total	🟦 1	**0.414**	**0.416**	**15.9 %**
CML2001 - Nov. 2010, Eutrophication Potential (EP)	kg Phosphate-Equiv.	Total	🟩 2	**2.59**	**2.59**	**9.27 %**
CML2001 - Nov. 2010, Global Warming Potential (GWP 100 years)	kg CO2-Equiv.	Total	🟪 3	**774**	**778**	**24.6 %**
CML2001 - Nov. 2010, Ozone Layer Depletion Potential (ODP, steady state)	kg R11-Equiv.	Total	☐ 4	**1.46E-005**	**1.47E-005**	**23 %**
CML2001 - Nov. 2010, Photochem. Ozone Creation Potential (POCP)	kg Ethene-Equiv.	Total	☐ 5	**0.0533**	**0.0535**	**21.1 %**

Figure 5.13 *3D plots of probability distributions of impact characterizations given in Figure 5.12.*

Figure 5.13 shows the 3D plots of probability distributions of impact characterizations given in Figure 5.12.

The following list is the summary of MCLCA approach:

- Standard deviations from mean values and nature of distributions are specified for independent variables.
- Values of independent variables can be randomly selected within the given specifications during a simulation run.
- All the primary impact characterizations are calculated for the randomly selected set of values of independent variables.
- Another set of values of independent variables are randomly selected within their specified ranges. This is called a Monte Carlo simulation run. Several runs (~5000) are repeated.
- The total number of runs is specified and the above steps are repeated until all the runs are completed.
- At the end of all Monte Carlo simulation runs, the probability distribution of each impact characterization for various percentage standard deviations from the mean value is counted. The impact characterizations that can be reduced by adjusting values of independent variables show a wider probability distribution and vice versa.

5.2 Multicriteria Analysis

Sustainable development calls for a multicriteria analysis, including social, economic and environmental impact assessments. While LCA is a tool for environmental sustainability analysis, social and economic impacts can also be assessed over life cycles. These are called social LCA (SLCA) and life cycle cost (LCC), respectively. Similar to LCA, SLCA and LCC show corresponding hot spots and ways of mitigation. The hot spots can span across the time scale (life cycle) as well as geographic regions (supply chains). The SLCA and LCC can be applied in the same way as LCA, for accounting (consequential) and change oriented (attributional) systems, discussed in Chapter 4.

Figure 5.14 shows the desirable domain for multicriteria analysis combining LCA, SLCA and LCC tools. Table 5.3 shows the various SLCA categories. The analysis proceeds in the same way, from primary through mid-point to end-point impacts. The analysis is to help decision making about sustainable supply chains by eliminating hot spots and mitigating potential negative or rebound impacts.

SLCA, an evolving tool, is discussed in 2009 UNEP/SETAC *Guidelines for Social Life Cycle Assessment* for SLCA; http://socialhotspot.org/user-portal-2/portal-info also “offers an online database that allows users to browse data on social risks by sector, country, or risk theme. There are choices of 227 countries and 57 economic sectors. The data

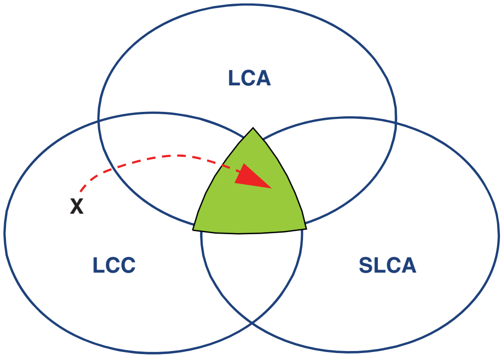


Figure 5.14 *Multicriteria analysis combining LCA, SLCA and LCC tools.*

comprehensively addresses social issues on human rights, working conditions, community impacts and governance issues, via a set of nearly 150 risk indicators grouped within 22 themes. Risks are also expressed, whenever relevant, by country and sector." LCC is implemented using a net present value and discounted cash flow analysis; this is discussed in Chapters 2, 6 and 7.

5.2.1 Economic Value and Environmental Impact Analysis of Biorefinery Systems

The biorefinery system shown in Figure 5.15 has biomass production, product manufacturing, end use and construction materials' life cycle process blocks. The two commonly used system boundaries include cradle to grave and cradle to gate with and without the carbon dioxide sequestration or capture by biomass and biorefinery products' end use blocks, respectively. Each block causes primary resource depletion (input) and emission impacts (output) that are accounted for in the LCA.

The contribution analysis of a biorefinery system shows typical characteristics in the environmental impact against an added cost profile. Raw materials, energy, raw materials for plant installations (capital good raw materials) and emissions are the four main loads interacting between biorefinery systems and the environment. Their environmental impacts decrease in the following sequence:

Emissions > Raw materials > Energy (provided that the energy required by the biorefinery systems can be supplied from renewable sources) > Capital good raw materials

Table 5.3 *SLCA categories.*

Labor Rights	Health and Safety	Human Rights	Governance	Community Infrastructure
1. Child labor	1. Injuries	1. Indigenous rights	1. Legal systems	1. Medical facilities
2. Forced labor	2. Toxics	2. Conflicts	2. Corruption	2. Drinking water
3. Excessive working time	3. Hazards	3. Gender equity		3. Sanitation
4. Wage assessment		4. Human health		4. Children education
5. Poverty				
6. Migrant labor				
7. Freedom of association				
8. Unemployment				
9. Labor laws				

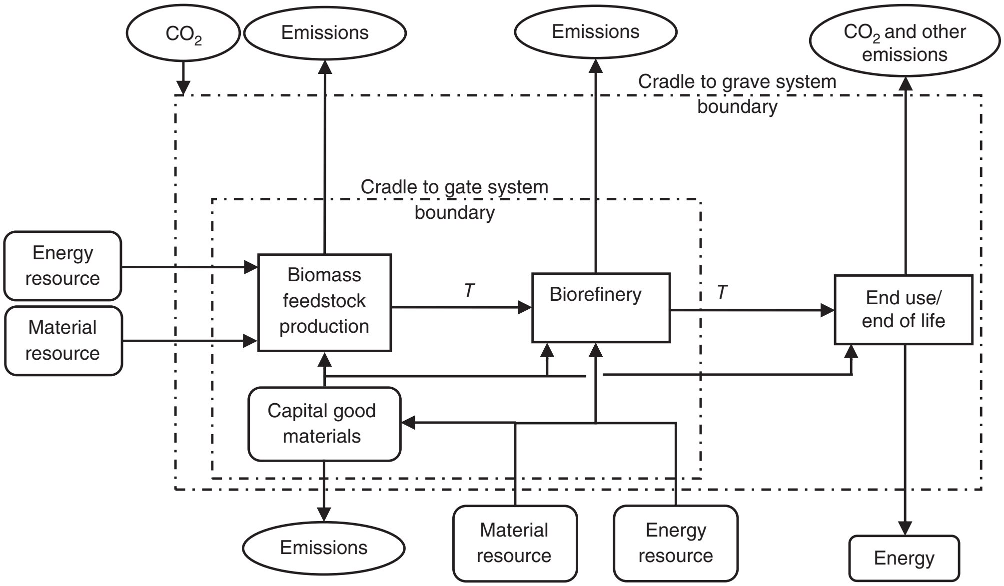


Figure 5.15 *A biorefinery system has biomass production, product manufacturing, end use and construction materials' life cycle process blocks. T shows where the transportation of materials is involved.*

The sequence for annualized costs is different from the sequence for environmental impacts and is shown as follows:

Biomass feedstock > Energy > Raw materials (excluding biomass feedstock) > Capital good raw materials > Emissions

These observations are shown by a generic plot of the environmental impact versus annual added cost of biorefinery systems in Figure 5.16. The cradle to gate biorefinery system has four main loads to analyze for LCA, as follows, shown by numbers 1 to 4 in the figure:

1. Raw materials
2. Energy
3. Capital good raw materials
4. Emissions

Figure 5.16 shows a horizontal line for higher emissions from a fossil based equivalent conversion system that the biorefinery system is designed to replace. The environmental impact from the biorefinery system is shown by the y axis value of point 4. The added cost of production is shown by the x axis value of point 3 or 4 (assuming that emissions do not add cost to the plant). A biorefinery cradle to gate plant may prove to be unsustainable if the target for emission reduction is higher than its current level of emission reduction and if the market price of its products is lower than their added cost of production.

The following lines are thus shown in Figure 5.16:

- Emission from fossil based equivalent product
- Emission reduction target by policy
- Cost of production
- Market price of product

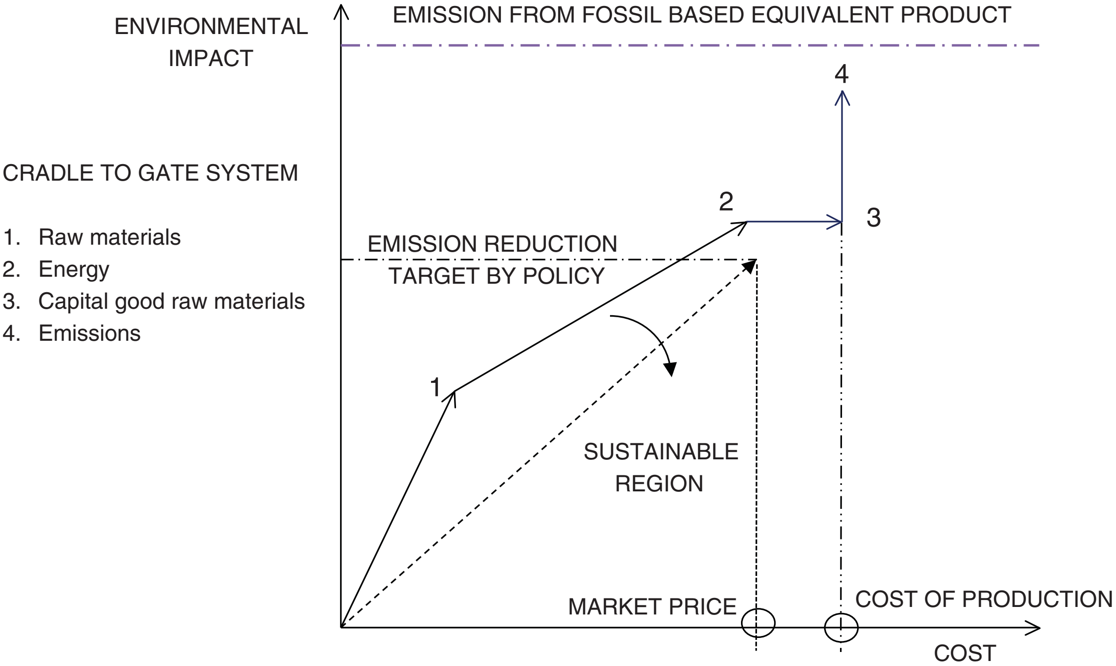


Figure 5.16 Added cost and environmental impact (contribution analysis) of biorefinery cradle to gate systems.

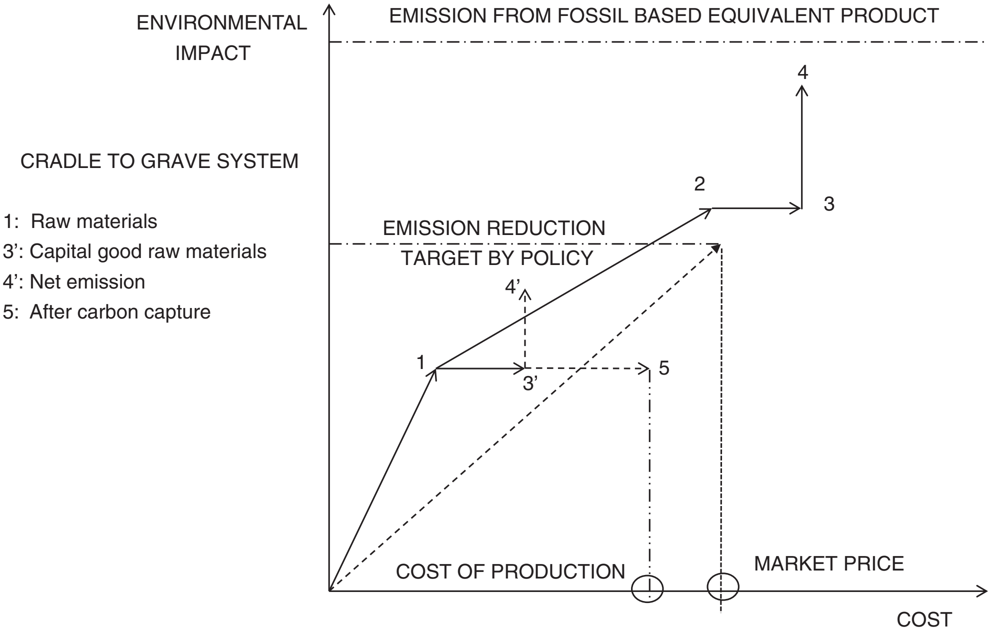


Figure 5.17 Added cost and environmental impact (contribution analysis) of biorefinery cradle to grave systems.

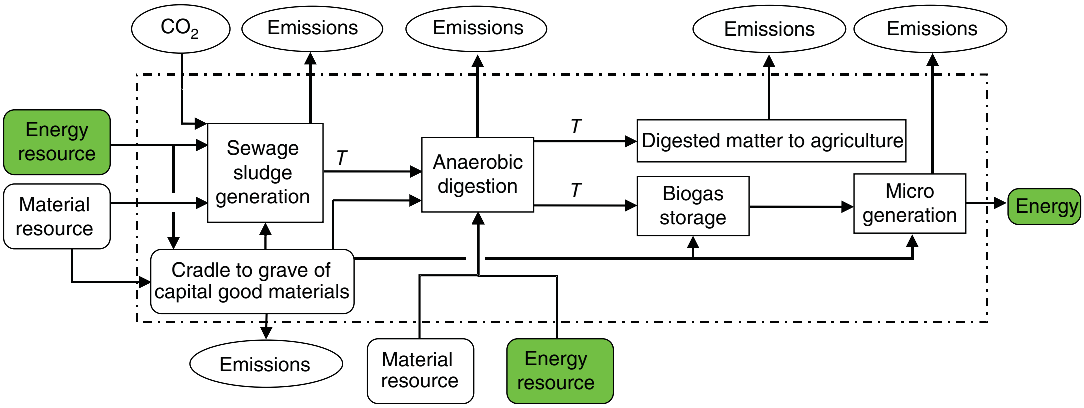


Figure 5.18 *Cradle to grave anaerobic digestion of sewage sludge system for LCA. T stands for transport.*

The target will be to operate the plant below the diagonal and within the lower triangle of the rectangle created by the horizontal line for the “Emission reduction target by policy” and the vertical line for the “Market price” of the product.

A cradle to grave biorefinery system analysis can show a reduction in emissions due to capture of carbon dioxide during biomass production. In addition, the energy balance over the entire cradle to grave system should show net energy production rather than consumption via biomass exploitation. Thus, line 1–2 does not exist in the cradle to grave biorefinery system’s added economic value and environmental impact (contribution analysis) profile in Figure 5.17. Line 1–3′ shows the capital good raw material. Line 3′–4′ shows the new net emission after carbon capture (by biomass during production), reduced from line 3–4 for the cradle to gate system. If the entire emission is captured by added investment, line 3′–5 can be created. Therefore, any emission reduction will be accomplished by added costs. The cradle to grave biorefinery system operating at points 4′ and 5, lower than the emission reduction target and product market price, is sustainable.

Further, see the combined economic value and environmental impact analysis calculations in Chapter 7.

Further Challenge Exercise 1. Draw the added cost and environmental impact (contribution analysis) profiles of the following systems in Figures 5.18 to 5.20. Develop hypotheses as necessary.

5.2.2 Socioeconomic Analysis

A socioeconomic analysis is done to estimate the number of job creations and any challenges and barriers associated with an industrial activity. The social performance needs to be compared with other similar systems, in order for an industrial system to operate over the long term. The IChemE provides a metrics to organize the socioeconomic data in the categories of workplace and society:

http://nbis.org/nbisresources/metrics/triple_bottom_line_indicators_process_industries.pdf

These are adaptable to biorefinery systems analysis. Furthermore, the following categories are recommended for biorefinery supply chains.

1. Employment and social well-being: average, highest paid and lowest paid indicative wages and benefit packages
2. Profit as a percentage of payroll expenses
3. External trade
4. Energy security
5. Resource conservation
6. Social acceptability

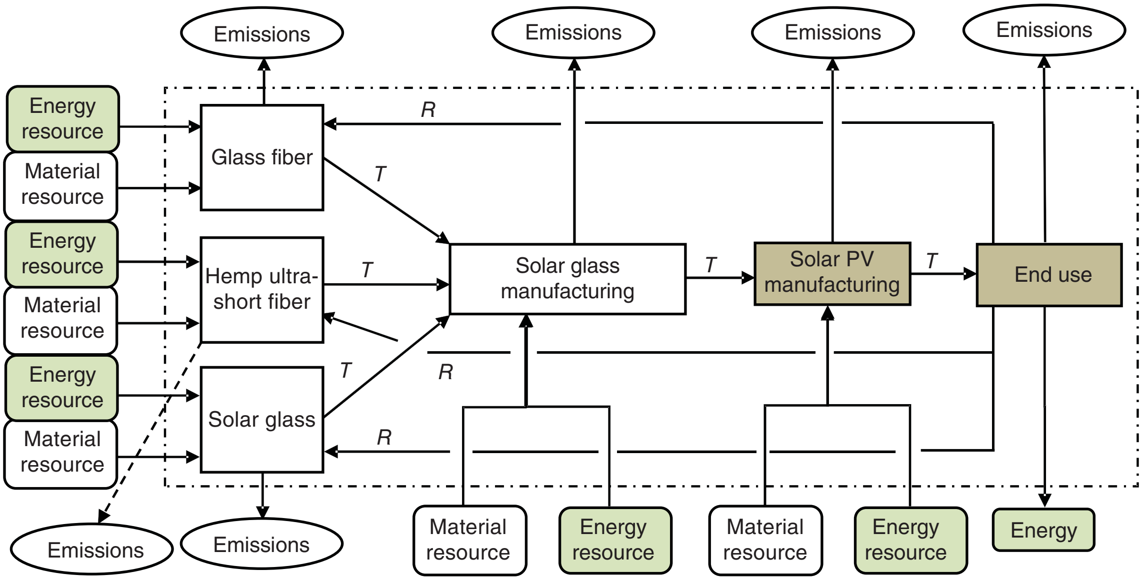


Figure 5.19 *Cradle to grave solar organic photovoltaic (OPV) glass manufacturing system for LCA. T stands for transport. R stands for recycle. T and R also cause resource depletion and environmental emissions. Only a part of "Solar PV manufacturing" and "End use" block impacts due to solar glass manufacturing needs to be considered within the system boundary.*

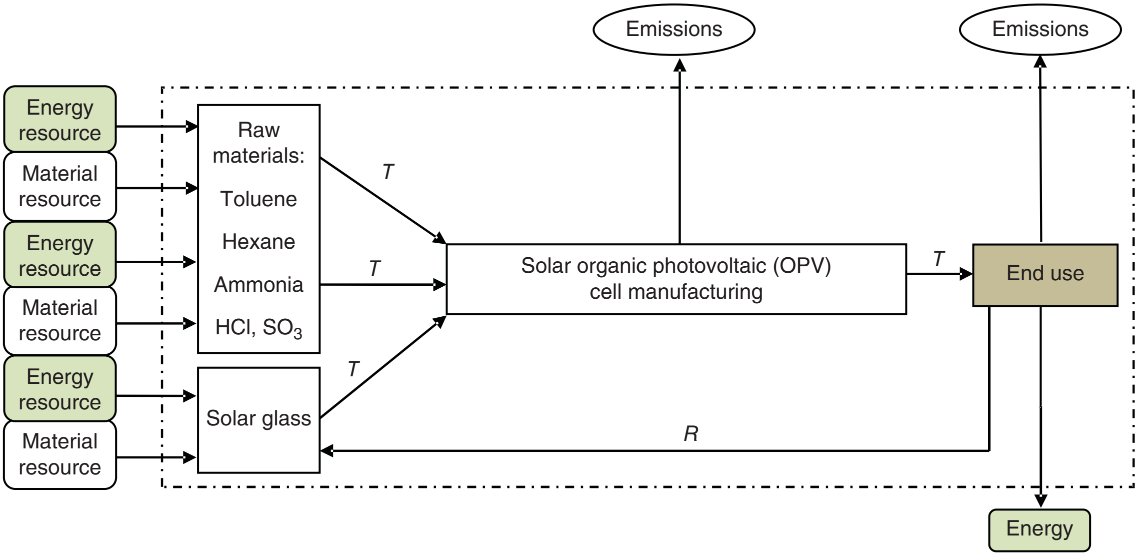


Figure 5.20 *Cradle to grave solar OPV cell manufacturing system for LCA. T stands for transport. R stands for recycle. T and R also cause resource depletion and environmental emissions. Only a part of "End use" block impacts due to solar cell manufacturing needs to be considered within the system boundary.*

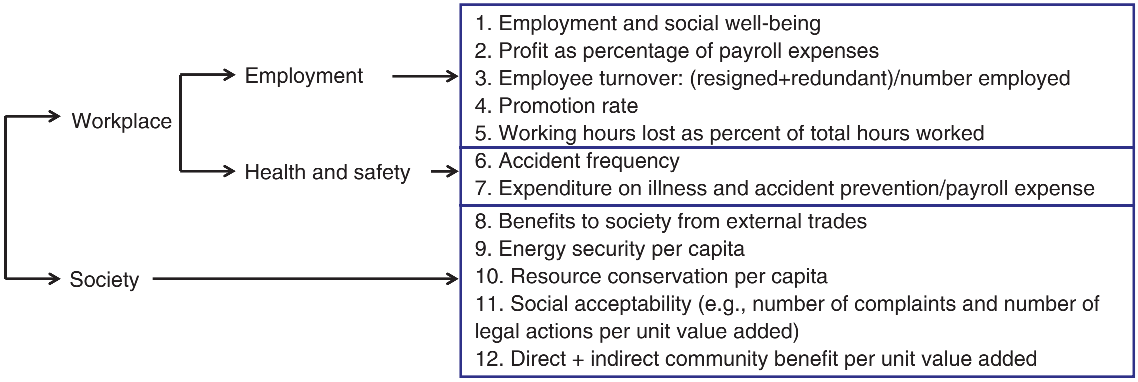


Figure 5.21 *Recommended socioeconomic indicators for biorefinery systems.*

Figure 5.21 shows the recommended structure of the socioeconomic indicators for biorefinery systems.

5.3 Summary

This chapter shows important ways to present LCA results, such that interpretation is accessible. The chapter also outlines multicriteria methods, as well as the incorporation of technoeconomics and socioeconomics in the analysis. Biorefinery sustainability must be assessed using LCA, technoeconomics and socioeconomics. Data uncertainty analysis, sensitivity analysis and Monte Carlo simulations are essential to minimize errors in estimation, to find more important indicators, activity and inventory hot spots. Though these tools are shown to apply for LCA results interpretation, these can also be used for technoeconomic and socioeconomic analyses.

References

1. E. Martinez-Hernandez, M.H. Ibrahim, M. Leach, P. Sinclair, G.M. Campbell, J. Sadhukhan, Environmental sustainability analysis of UK whole-wheat bioethanol and CHP systems, *Biomass Bioenergy*, **50**, 52–64 (2013).
2. *IPCC Guidelines for National Greenhouse Gas Inventories*, Intergovernmental Panel on Climate Change, Geneva, Switzerland, 2006.