Chapter 8

Methods for Design and Evaluation of Sustainable Processes and Industrial Systems

8.1. Introduction

8.1.1. *Concept of sustainable development in process engineering*

The concept of sustainable development is based on the creation of goods and services using processes and non-polluting systems, which preserve the energy resources and raw materials while being economically viable. The social demands relate not only to the continuity of employment but also ensure complete safety of a process for operators, consumers, and the public. The need and desire for continuous innovation, which characterize the industries of material and energy processing, must therefore be applied to the search for a new industrial socio-economics. The "eco-efficiency" period, which aims at promoting a more "efficient" use of raw materials and energy in order to simultaneously reduce the economic costs and the environmental impact of production must be followed by an era of "eco-design", where environmental parameters are taken into consideration right from the design of the product and process. "Eco-design" thus appears to be the operational contribution of sustainable development.

In this context, process engineering must play an important role for two main reasons: (i) the production induced by this type of industry, which contributes significantly to the national income, is essential for the modern society: the development of the society depends on the chemical industry and vice versa; (ii) many environmental issues are either directly related to such processes or to the

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use of chemical products through impacts on water, air, and soil. The chemical industry develops products for multiple consumer markets, which have to be manufactured, used, and recycled by specific, safe, and economically viable processes. It is therefore necessary to improve the existing processes and to invent new ones that avoid waste production at the source rather than collecting and processing the produced waste, thus going from a curative approach to a preventive approach (see Figure 8.1).

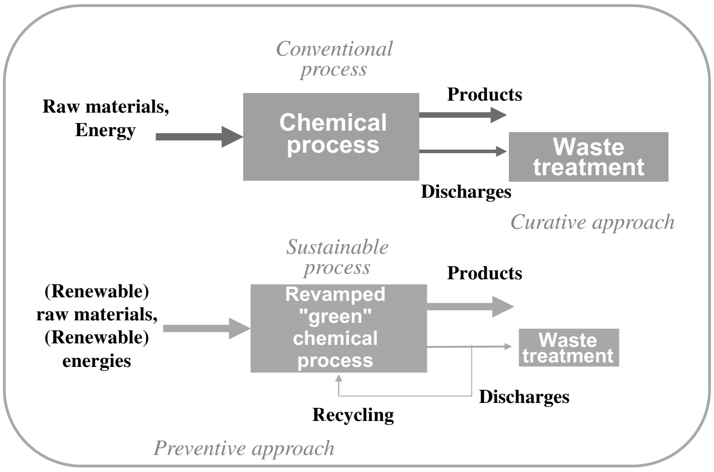

Figure 8.1. *Curative approach versus preventive approach in process design*

This vision, which takes into account the product–process lifecycle and expands the scope of investigation, involves a systemic approach (see Figure 8.2). It is part of the concerns of the “roadmaps” published in the last 10 years. These concerns are stated through the 12 principles of green chemistry [ANA 98], 12 principles of green engineering [ANA 03], challenges for engineering outlined by the American National Academy of Engineering [NAE 08], or the roadmap of the *IChemE 21st Century Chemical Engineering* (*IChemE roadmap, UK, 2007*) [ICH 07].

8.1.2. *Indicators, indices, and metrics of sustainable development in process engineering*

The main objective of this chapter is to present the methods and tools to assess the performance of processes towards the criteria of sustainable development that could be applied in the preliminary stages of their design. The economy, society, and the environment are the three pillars of sustainable development. They are interdependent.

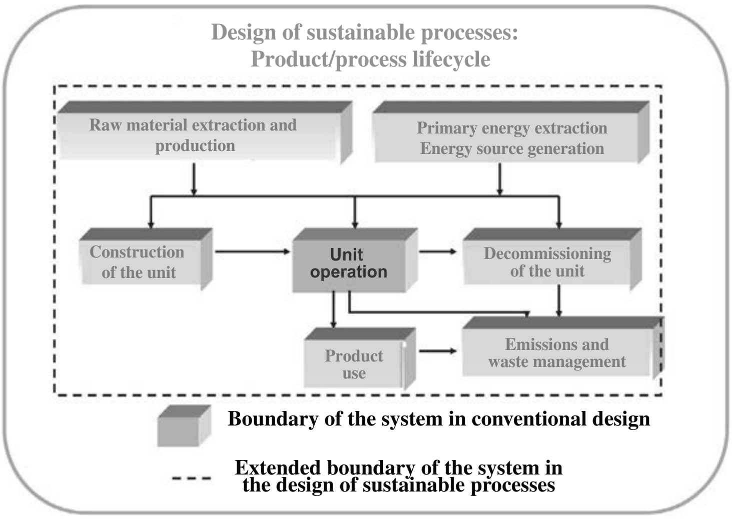

Figure 8.2. *System approach and boundary of the system in conventional design process*

The first classification of criteria proposed in [AZA 04] is illustrated in Figure 8.3. Let us note that several sustainable development criteria are often considered routinely in conventional design, especially the microeconomic criteria (e.g. costs and profits), and some environmental (e.g. energy consumption and water), or social criteria (e.g. employee health and safety).

Economic criteria	Environmental criteria	Social criteria
Capital cost Operating costs Profitability Decommissioning costs Added value Taxes, including "green taxes" (e.g. carbon tax?) Investments (e.g. prevention of pollution, health, safety, decommissioning) Potential costs of environmental liability	Use of energy Use of water Water discharges Solid waste Biotic resource depletion Global warming Ozone layer depletion Acidification Summer fog Eutrophication Human toxicity Ecotoxicity	Number of employees Health and safety of personnel Health and safety of customers Nuisance (odor, noise, visual impact and transportation) Social acceptance

Figure 8.3. *Classification of sustainable development criteria in process design according to [AZA 04]*

It is generally accepted that sustainability results from a balance between the three components. The selection of an appropriate set of indicators for assessing sustainability is essential for a comparative analysis between the different versions of a process. In order to provide a method applicable for the analysis of systems with respect to the sustainability aspect, a typology of indicators is proposed in [SID 03a], classifying the three dimensions of sustainable development into three distinct hierarchical groups: (i) 1D indicators providing information on a single dimension: economic, ecological, or social; (ii) 2D indicators simultaneously providing information on two dimension: socio-ecological, socio-economical, or economic-ecological components; and (iii) 3D indicators leading to information on the three dimensions.

For the sake of illustration, let us consider the amount of non-renewable energy used to produce a unit quantity of final product, a criterion taken into account in the metrics proposed by the AIChE [BEA 02]. This criterion does not only provide information on a single branch coming under the economic, environmental, or societal aspect. These three dimensions are implicitly integrated. This is a 3D indicator. If we know the manufacturing cost, this indicator provides information on both the economic and social aspects and is called a 2D indicator.

The goal is not to exhaustively identify all the metrics proposed and applicable to the chemical industry processes, but rather to put the emphasis on the most important ones in relation to a decision-making objective.

It is useful to distinguish beforehand among the indicator, index, and metrics. An indicator is a tool for simplification, quantification, and communication of information; it is the first level of basic data analysis. Ideally, according to the classification by [SID 03b], an indicator of sustainable development should satisfy the three components simultaneously. However, the construction and selection of such indicators are not direct and have hence been the subject of numerous studies (see for example [SEG 02]). A good indicator must meet several requirements related to the technical soundness, the relevance towards the stakeholders, the cost towards data collection, reliability, spatial and temporal boundaries, ease of interpretation, access to a comparison standard, and the ability to show trends in the evolution over time. However, a reliable indicator can be difficult to interpret, thus failing in its function of communication. In most cases, the indicator assessment involves either a standardization or a comparison with a predefined value, to facilitate its interpretation (e.g. the percentage of renewable energy used with respect to the national average). An indicator is therefore an observable variable, which is used to characterize the complexity of a phenomenon. The term index refers to a synthetic indicator built by aggregating other basic indicators.

The other way to characterize the different aspects of a complex phenomenon is to use a set of indicators within a metric. The utility of a metric is necessarily related to the number of indicators: an insufficient number is likely to misrepresent the phenomenon and a large number may make the implementation cost prohibitive.

The advantage of a single index instead of a collection of indicators thus lies in the ease of communication (e.g. ecological footprint). However, we can also notice many drawbacks: loss of details and accuracy due to the combination of parameters with different orders of magnitudes and levels of accuracy, and usage of conversion ratios to express all the variables with the same units.

This chapter exclusively considers the currently available approaches to assess the sustainability of processes and new or existing systems. It lists the most significant examples of indicators, indices, or metrics used in process industries. Economic indicators, widely used in the traditional process design methods will not be presented in detail. Readers can refer to reference books in this field (e.g. [CHA 01]). The design methods based on these indicators will complement this chapter.

8.2. AIChE and IChemE metrics

In order to analyze the sustainability of a process, we should first mention the two metrics developed by the AIChE (1D) and IChemE (3D), which consider indicators that are particularly adapted to the process domain and to a production system. The works conducted in Canada (*Canada's National Round Table on the Environment and the Economy*) [NRT 99] can be mentioned first. These works recommend eco-efficiency measurements, which are defined by ratios, with resource uses or environmental impacts as numerators and value creation as denominators or vice versa.

8.2.1. *AIChE metrics*

Following these principles, the eco-efficiency metrics have been refined to be applied on the operational level by the *American Institute of Chemical Engineers* (AIChE, www.aiche.org/cwrt/projects/sustain.htm) in collaboration with a not-for-profit organization, *BRIDGES* to *Sustainability Institute* (formerly known as *BRIDGES to Sustainability*).

The metrics proposed in terms of eco-efficiency (a basic version is presented in Table 8.1), comprises the six following aspects:

– material consumption: the usage of materials, notably non-renewable materials, and materials with finite resources, affects the availability of resources and leads to environmental degradation during raw material extraction and during conversion as discharges;

– energy consumption: apart from the aspects related to its availability and use as a resource, the use of energy leads to varied environmental impacts. For example, the combustion of fossil fuels has an impact on global warming, oxidation of photochemical ozone, and acidification;

– water consumption: fresh water is essential for life and almost for all economic activities. As there is an increase in anthropogenic demands and a depletion of water resources in some regions of the world, water consumption is a key factor;

– emission of polluting products;

– solid waste;

– land use: the soil is considered to be a finite resource, which provides varied ecological and socio-economic services. However, the definition of an indicator seems to be complicated and does not appear explicitly in the basic metrics.

Denominator = Mass of products or Sales or Added value	Material intensity	$\dfrac{\textit{Mass of raw materials} - \textit{mass of products}}{\textit{Denominator}}$
	Energy intensity	$\dfrac{\textit{Net amount of energy (in primary energy equivalent)}}{\textit{Denominator}}$
	Water intensity	$\dfrac{\textit{Volume of fresh water used}}{\textit{Denominator}}$
	Effluents (gases, liquids)	$\dfrac{\textit{Total mass of effluents}}{\textit{Denominator}}$
	Solid waste	$\dfrac{\textit{Total mass of solid waste}}{\textit{Denominator}}$
	Polluting effects	*Global Warming* *Depletion of the ozone layer* *Photochemical pollution* *Air acidification* *Eutrophication potential*

Table 8.1. *Basic metrics of the AIChE [BEA 02]*

The choice of ratios to express the metrics facilitates on the one hand the comparison between several options and, on the other hand, the choice of the process during the decision-making phase. As the indicator decreases, the generated impact decreases per unit of value created.

Heuristics and decision rules have been developed and tested on industrial pilots involving more than 50 processes of the chemical industry from the data of the *Process Economic Program* (PEP) of the SRI International (Menlo Park, California) [BEA 02]. The indicator values have been calculated for standard flowsheets. Some examples are presented in Table 8.2.

Product	**Process**	**Material intensity** /lb prod. (lb/lb)	**Energy** /lb prod (10^3 BTU/lb)	**Water** /lb prod. (gal/lb)	**Toxic effluents targeted** /lb prod. (lb/lb)	**Pollutants + CO_2** /lb prod. (lb/lb)	**Pollutants + CO_2** /lb prod. (lb/lb)
Acetic acid	Carbonylation of methanol	0.062	1.82	1.24	0	0	0.133
Acrylic acid	Ammoxidation of propylene	0.493	5.21	3.37	0.015	0.008	0.966
Maleic anhydride	Partial oxidation of n-butane	0.565	0.77	1.66	0	0	2.77
Sulfuric acid	From sulfur dioxide: pyrometallurgy	0.002	0.073	0.57	–0.65	–0.63	–0.04
Sulfuric acid	From sulfur	0.001	–0.87	0.7	0.002	0.002	0.002

Negative values used for the components indicate that the discharges from other processes are used as raw materials.
Water and air are not used in calculating the use of the material.
Negative values used for energy indicate that the process produces energy.

Table 8.2. *Application of the AIChE metrics for a few key processes in the chemical industry [ALL 07]*

8.2.2. *IChemE metrics*

Significant efforts to establish the sustainable development metrics have also been made by IChemE (UK) [ICH 03] by adding the economic and social metrics to the metrics focused on environmental aspects. The indicators are specifically grouped into environmental, economical, and social categories. The list is particularly suitable for a production site. The environmental indicators are related to resources or to categories of environmental impacts.

Metrics involves two types of quantitative indicators, i.e. the environmental burdens and impacts. The first group includes the use of material and energy, emissions in air and water, and the amount of solid waste. It is obtained from the flowsheet and material and energy balances. The information obtained from the burdens can then be used to calculate environmental impacts.

As mentioned above, most of the indicators of the metrics are calculated as ratios to provide an impact measurement regardless of the scale of the operation. They are based on a simple rule: the process gets more efficient as the indicator decreases.

They involve both the process inputs (use of resources) and outputs (emissions, effluents, discharges, products, and services). They involve a subset of the impact factors used in environmental science, which are the most significant towards process industries, for the calculation of environmental burdens.

The environmental burden (EB), caused by the emission of a range of substances, is calculated by adding the weighted emissions of each substance. The potential factor of the impact is identified as the impact factor of each substance. Let us note that a substance may contribute differently to different environmental burdens and have different impact factors:

$$FE_i = \sum M_N FP_{i,N} \qquad [8.1]$$

where FE_i denotes the environmental burden i, M_N is the mass of the emitted substance N, and $FP_{i,N}$ is the impact potential factor of the substance N related to the environmental burden i.

Environmental burdens are determined with respect to a reference substance (e.g. SO_2 for atmospheric acidification).

This approach involves a total of 49 indicators. However, the life span of chemical products in various environments is not taken into account. In addition, the indicator on human health (normalized with respect to benzene) is limited to carcinogenic effects. The set of indicators is given in Table 8.3.

We present all the social and economic criteria proposed by the IChemE in Tables 8.4 and 8.5.

Environmental criteria	**Emissions, effluents, and discharges**	**Water**	Ecotoxicity with respect to aquatic life (metals) (*in te/y copper equivalent*) Ecotoxicity with respect to aquatic life (other substances) (*in te/y formaldehyde equivalent*) Eutrophication (*in te/y* PO_4^{3-} *equivalent*) Aquatic acidification (*in te/y* H^+ *released equivalent*) Aquatic oxygen demand (*in te/y oxygen equivalent*)
		Air	Air acidification (*in te/y* SO_2 *equivalent*) Carcinogenic effect (*in te/y Benzene equivalent*) Ozone Layer Depletion (*in te/y CFC-11 equivalent*) Global warming (*in te/y* CO_2 *equivalent*) Photochemical pollution (*in te/y* C_2H_4 *equivalent*)
	Use of Resources	**Energy**	Total net primary energy use = input – output (*GJ/year*) % Total net primary energy from renewable sources Total primary energy (*kJ/kg product*) Total primary energy per unit of added value (*kJ/€*)
		Material	Total quantity of raw materials used (*per kg of product, kg/kg*) Total quantity of raw materials used (*per unit of added value kg/€*) Fraction of raw materials recycled in the plant (*kg/kg*) Fraction of raw materials recycled by consumers (*kg/kg*) Hazardous raw materials (*per kg of product, kg/kg*)
		Water	Net consumption of water used (*per kg of product, kg/kg*) Net consumption of water used (*per unit of added value, kg/€*)
		Land	Land Use (m^2) Waste (*Tons of waste*)

Table 8.3. *Environmental criteria recommended by the IChemE*

Social criteria	**Employment situation**	Benefices as percentage of payroll (*%*)
		Employee turnover (*%*)
		Number of promotions/number of employees (*%*)
		Working hours lost percent of total hours worked (*%*)
		Income + benefit ratio (top 10% / bottom 10%)
	Health and safety	Lost time accident frequency
		Expenditures on illness and accident prevention/payroll expense (€/€)
	Company	Number of stakeholder meetings per unit of added value (/€)
		Indirect community benefit per unit of added value (€/€)
		Number of complaints per unit of added value (/€)
		Number of legal actions per unit of added value (/€)

Table 8.4. *Social criteria recommended by the IChemE*

Economic criteria	**Profit, value, tax**	Value added (€*/year*)
		Value added per unit of sales value (€/€)
		Value added per direct employee (€*/year*)
		Gross margin per direct employee (€*/year*)
		Return on average capital employed (*%/year*)
		Taxes paid, as percentage of the net profit before tax (*%*)
	Investment	Percentage of increase (decrease) in capital employed (*%/year*)
		R & D expenditures as % of sales (*%*)
		Employees with a post-A-level qualification (*%*)
		New appointments/number of direct employees (*%/year*)
		Training expenditure as percentage of payroll expenditure (*%*)
		Ratio of indirect jobs/number of direct employees
		Donations in percentage of net profit before tax (*%*)

Table 8.5. *Economic criteria recommended by the IChemE*

8.2.3. *Using sustainable development metrics*

Sustainable development metrics can be used at different levels in the support process for decision making:

– evaluation of technical (variety of raw materials, options of process improvements, etc.) or financial (variety of suppliers, etc.) alternatives;

– comparison of industrial units;

– identification of environmental impacts of an industrial unit.

They can also be used for communication with the stakeholders.

We note that sustainable development metrics are becoming more and more complex by both their content and methodology [TAN 06]. The example of the two previous metrics shows that the choice of appropriate indicators depends on the specificities of the concerned industrial sector or even the product types. According to [LAP 04], indicators should reflect the by-products, discharges, and emissions characterizing the process or the product, but also the necessary resources to provide a service. It is therefore difficult to provide a universal list of indicators. It seems more sound to analyze and explain the choice of indicators in a few typical situations. In this way, two industrial examples are reported in the literature:

– example of GlaxoSmithKline (GSK): the use of a sustainable development metrics within this pharmaceutical company is described by [CON 05]. In order to adapt the metrics for its own requirements, GSK has developed a specific "green" metrics, including indicators related to the atom economy, carbon efficiency (CE), and reaction mass efficiency (RME) or the solvent recovery energy. The CE indicator takes into account the efficiency and amount of carbon in the reactants, which is incorporated in the final product. CE takes into account the yield and the amount of carbon in the reactants that is incorporated into the final product. RME takes into account yield, the actual molar quantities of reactants, and atom economy. Examples of calculation are proposed in [CON 02];

– example of BASF: an eco-efficiency analysis developed within BASF is described in detail in [SAL 02] and [SCH 05]. On the basis of the lifecycle assessment method, the approach uses the metrics based on the usage of resources and calculations of environmental impacts, health, and safety. The use of a standardization and weighting method to generate an environmental performance index was illustrated through examples (notably the production of indigo or ibuprofen). The approach was extended to cover the aspects of "socio-efficiency" by including the social aspects of sustainable development [SCH 04], and by developing a software tool SEEbalance [SCH 04]. The methodology was applied initially during product and process development phases. It was then implemented for the development of industrial and communication strategies towards industrial customers and other partners in the value chain.

Nowadays, there is still a lack of management and metric tools for sustainable development: the BRIDGESworks™ Metrics software [TAN 04] is one of them. It is clear that such tools will help to take into account sustainability criteria, especially if they are integrated into the global system of information management of the company. Hence, such an approach will encourage the lifecycle thinking throughout the product's lifecycle.

8.3. Potential environmental impact index (*waste reduction algorithm*)

As it is difficult to provide all the information required for calculating the indicators of a metrics, at the preliminary design stage of a process, some studies have focused on the development of an environmental balance.

The method, commonly cited in the literature and identified by the term Waste Reduction Algorithm (WAR), is based on the concept of environmental balance, which is similar to material and energy balances. This is not a lifecycle assessment tool: the approach is essentially based on the process and generation of associated utilities within the lifecycle of the product and does not include the other phases, i.e. raw material acquisition, distribution, usage, and recycling of the product (see Figure 8.4).

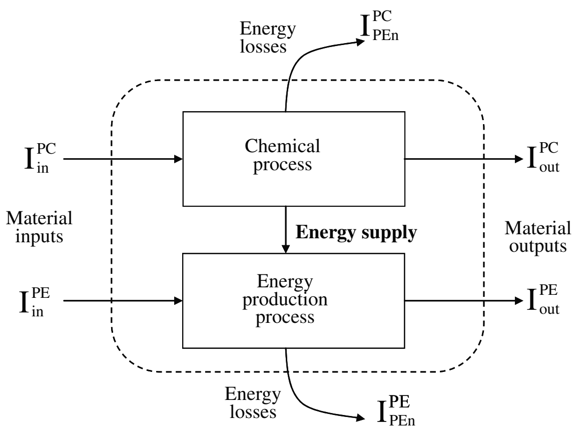

Figure 8.4. *Recognition of energy in the WAR algorithm (according to [YOU 00])*

This method is used in the design phase of a process and uses the process information (flow rates and mass fractions), as well as the toxicological data to calculate the environmental impact of a process. It requires the use of a flowsheeting software tool. This American method was developed within the EPA (*Environmental Protection Agency, National Risk Management Research Laboratory*) to take into account the environmental aspect from the preliminary design phase of the process.

8.3.1. *Theory of the potential environmental impact*

The approach is based on the calculation of the potential environmental impact (PEI) of a process, which results from an environmental balance. This type of balance must be carried out during the design phase of a process, as the material and energy balances.

The result of the PEI balance is the calculation of an impact index (I) that provides a quantitative measurement of the impact of a process discharge. This methodology consists of minimizing the PEI for a process rather than minimizing the amount of waste generated by the process.

The concept of potential environmental impact of the WAR algorithm is based on the traditional mass and energy balances. The key points of the method are briefly recalled below (see the article by [CAB 99] for a complete presentation).

In steady state:

$$I_{in}^{PC} + I_{in}^{PE} - I_{out}^{PC} - I_{out}^{PE} - I_{PEn}^{PC} + I_{Gen}^{PE} = 0 \qquad [8.2]$$

where I_{in}^{PC} and I_{out}^{PC} are, respectively, the input and output rates of the PEI for the chemical process; I_{in}^{PE} and I_{out}^{PE} are, respectively, the input and output rates of the PEI for the energy production process. I_{PEn}^{PC} and I_{PEn}^{PE} are respectively the PEI outputs associated with the energy losses of the chemical and energy production processes.

Young [YOU 99] considers that the fugitive emissions are negligible compared with those relative to the amounts of energy consumed and produced by the process (I_{PEn}^{PC} and I_{PEn}^{PE} are neglected). In addition, the impact of input flow rates in the energy production process I_{in}^{PE} is neglected.

Equation [8.2] is simplified to give:

$$I_{in}^{PC} - I_{out}^{PC} - I_{out}^{PE} = 0 \qquad [8.3]$$

This balance can be written as:

$$I_{in}^{(t)} - I_{out}^{(t)} + I_{Gen}^{(t)} = 0 \qquad [8.4]$$

$I_{in}^{(t)}$ is defined as the total potential environmental impact that lies in the material inputs of the process, including the product development and energy generation process, which is estimated exclusively by the impacts within the chemical process I_{in}^{PC}.

$I_{out}^{(t)}$ is defined as the total potential environmental impact that lies in the material outputs of the process, including the product development and energy generation process, which is estimated by the impact that comes from both the chemical process I_{out}^{PC} and the energy production unit I_{out}^{PE}.

The input potential environmental impact index $I_{in}^{(t)}$ can be approximated as follows:

$$I_{in}^{(t)} = \sum_{i}^{Cat\ Approx.} \alpha_i I_{i,in}^{(t)} = \sum_{i}^{Cat\ Approx.} \alpha_i \sum_{j}^{flow\ rate} M_{j,in} \sum_{k}^{Comps} x_{kj} \psi_{ki}^{s} + ... \qquad [8.5]$$

α_i denotes a weighting factor assigned to the category of potential environmental impact (PEI) i, $I_{i,in}^{(t)}$ denotes the input PEI index for the category i, $M_{j,in}$ is the mass flow of product j (either input or output), x_{kj} is the mass fraction of component k in product j, and ψ_{ki}^{s} represents the standardized value of the environmental impact of a component for one of the identified impact categories i.

Let us note that the weighting factors α_i are used to combine the impact categories into a single index and represent the relative importance attributed to an impact by the designer. Most of the studies listed in the bibliography attribute equivalent values to the weighting factors.

Similar reasoning is applied to determine an output potential environmental impact index:

$$I_{out}^{(t)} = \sum_{i}^{Cat\ Approx.} \alpha_i I_{i,out}^{(t)} = \sum_{i}^{Cat\ Approx.} \alpha_i \sum_{j}^{flow\ rate} M_{j,out} \sum_{k}^{Comps} x_{kj} \psi_{ki}^{s} + ... \qquad [8.6]$$

Finally, two types of environmental indices are used to assess the environmental nature of a process: an index based on time PEI/h or on production PEI/kg of a product, i.e.:

$$\hat{I}_{out}^{(t)} = \frac{I_{out}^{(t)}}{\sum_{p}^{products} P_p} \qquad [8.7]$$

In this expression, $\hat{I}_{out}^{(t)}$ represents the output PEI index expressed in PEI/kg of a product and P_p denotes the mass flow of current p.

A similar transformation is performed to convert the environmental impact generation index in terms of PEI/kg:

$$\hat{I}_{gen}^{(t)} = \frac{I_{gen}^{(t)}}{\sum_{p}^{products} P_p} \qquad [8.8]$$

The objective of the WAR algorithm is to provide a means for comparing the potential environmental impact between process design alternatives: as the index becomes lower, the process becomes more environmental friendly.

8.3.2. *Categories of environmental impacts*

The toxicological data are classified into eight environmental impact categories: global warming potential, acidification potential, ozone depletion potential, photochemical oxidation or *smog*-forming potential, human toxicity potential by ingestion and inhalation, and aquatic and terrestrial toxicity potentials. A brief description of these impacts is given below and illustrated in Figure 8.5. The classification of these impact categories is based on a study by [HEI 92]. These categories have been proposed to highlight the most representative indicators in the field of process design. These indicators can be classified into two domains: global atmospheric domain and local toxicity domain (see Table 8.6).

The global warming potential (GWP) is an index that compares the contribution of greenhouse gas emissions to global warming with that of carbon dioxide (CO_2), over a given period.

Carbon dioxide (CO_2) being the reference index, its GWP is equal to 1. The GWP takes into account the measurement of radiative forcing capacity (amount of infrared that a substance can absorb, a_i in Wm^{-2}) induced by a molecule with concentration C_i in the atmosphere in ppm. This is followed by the integration of the radiative forcing capacity over a given period of time (usually 100 years):

$$GWP_i = \frac{\int_0^n a_i C_i dt}{\int_0^n a_{co_2} C_{co_2} dt} \qquad [8.9]$$

$$X + ... \rightarrow \alpha H^+ + ... \qquad [8.10]$$

X denotes the chemical substance initiating the acidification, and the molar stoichiometric ratio α represents the ratio of the number of moles of H^+ per mole of X. Acidification is usually expressed in terms of mass (η_i, mole H^+/kg):

$$\eta_i = \frac{\alpha_i}{M_i} \qquad [8.11]$$

where M_i denotes the molecular weight of X (kg i/mole i). As mentioned before, a reference compound SO_2 is used to express the acidification potential:

$$AP_i = \frac{\eta_i}{\eta_{SO_2}} \qquad [8.12]$$

The acidification potential (AP) of a compound is related to the number of moles of H^+ created by the number of moles of compound according to the reaction.

Local toxicological		**Global atmospheric impact**	**Regional atmospheric impact**
Impact on man	**Ecological**		
– Human toxicity potential by ingestion (HTPI) – Human toxicity potential by inhalation or dermal exposure (HTPE)	– Aquatic toxicity potential (ATP) – Terrestrial toxicity potential (TTP)	– Global warming potential (GWP) – Ozone depletion potential (ODP)	– Acidification potential (AP) – Photochemical oxidation potential or “smog”-forming potential (PCOP)

Table 8.6. *Environmental impact categories used in the WAR algorithm*

Ozone depletion potential (ODP) in the stratosphere is based on the calculation of the variation in time and space of O_3 concentration (δ [O_3]) due to the emission of a specific gas with respect to the same amount for a reference compound, trichlorofluoromethane (CFC-11, CCl_3F).

The photochemical oxidation potential or smog-forming potential (*Photochemical Oxidation Potential*, PCOP) quantifies the contribution to the smog phenomenon (photochemical oxidation of certain gases, which produces ozone). It is expressed in equivalent ethylene, C_2H_4.

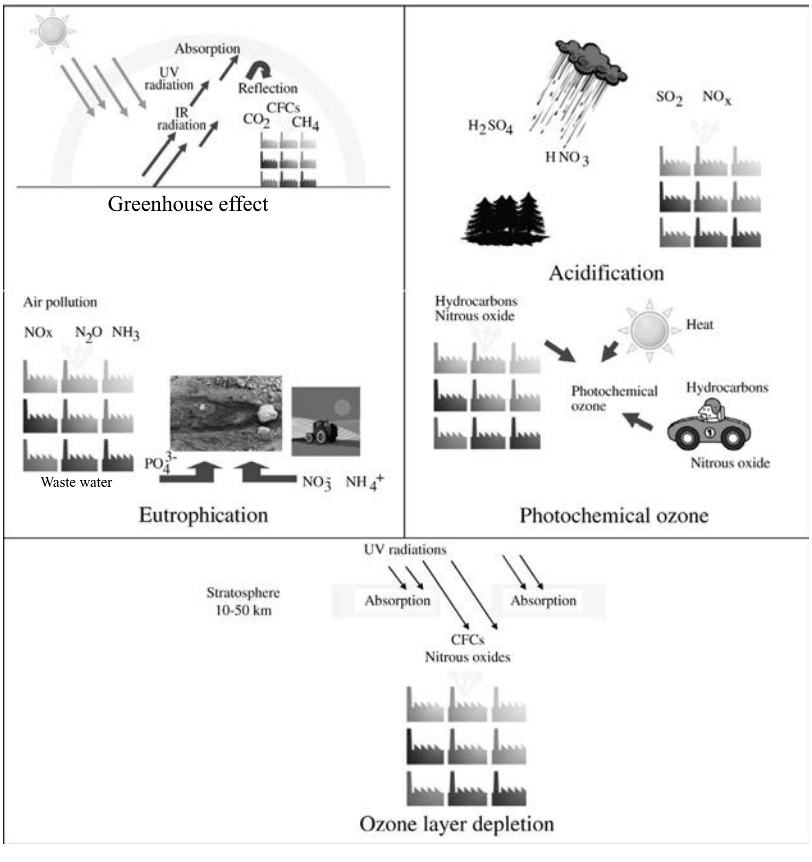

Figure 8.5. *Schematization of the principal environmental impacts*

These four indicators (GWP, AP, ODP, and PCOP) depend on the global or regional atmospheric domain.

The Human Toxicity Potential by Ingestion (HTPI), Human Toxicity Potential by either inhalation or dermal Exposure (HTPE), Aquatic Toxicity Potential (ATP), and Terrestrial Toxicity Potential (TTP) are related to the local toxicological domain. As a first approximation, the lethal dose 50 (LD50) or LC50 (lethal concentration 50) is used to estimate HTPI. This indicator measures the dose of substance causing the death of 50% of a given animal population (often mice or rats) under specific experimental conditions. ATP is estimated from the study of the effects on the "fathead minnow" (*Pimephales promelas*). Data are expressed in the form of a concentration causing death (LC50) for 50% of the organisms exposed to a substance for a given limited duration.

8.3.3. *Application of the WAR algorithm*

The WAR algorithm has been used on many processes and the application process is well illustrated in process test cases (we can refer to the works of [HIL 96] and [DIW 02] on penicillin or benzene by toluene hydrodealkylation production processes).

8.4. SPI (Sustainable Process Index)

Another approach to analyze the sustainability of a process is based on the calculation of an aggregate indicator proposed by Krotscheck and Narodoslawsky [KRO 95], the SPI (Sustainable Process Index), an expression of the ecological footprint concept for a process that measures the total environmental impact of various human activities. The SPI calculation is based on the mass and energy balances of the process. It is independent of the legal standards that can vary over time, making it particularly attractive. The aim of the SPI is to compare the mass and energy flows generated by human activities to natural material flows, on a global and local scale. In this approach, the planet is seen as a thermodynamically "open" system, i.e. open to the flow of solar radiations toward its surface and which emits energy in the universe. Solar radiations are the only natural driving forces for all the environmental processes and those resulting from human activities. They constitute a limited flow, although available indefinitely, which is received by the planet's surface. This means that all natural processes or those induced by human activities require some part of this limited flow and a certain surface: in other words, technological processes compete with each other and with the natural processes for this surface, which is a limited resource. Human activities impact the environment in several ways: any process considered in a "cradle-to-grave" analysis requires raw materials, energy, facilities, staff, and rejects waste or emissions into the environment. The total area to integrate a specific process in the ecosphere in a sustainable manner is then given by:

$$A_{tot} = A_{MP} + A_E + A_I + A_S + A_D \ [m^2] \quad [8.13]$$

where A_{MP} represents the area for the extraction of raw materials, A_E denotes the area relative to the energy resource, A_I denotes the area relative to facilities, A_S denotes the area relative to staff, and A_D denotes the area to discharge all waste and emissions.

Processes produce services or goods. The impact per unit of good or service is represented by a specific area a_{tot}:

$$a_{tot} = \frac{A_{tot}}{N_P} \quad [8.14]$$

where N_P represents the number of goods or services produced by the process, such as the amount of kilowatt per hour produced by a specific energy system. The reference period is generally one year. Finally, we can link this specific area, for the production of a certain good or service, to the statistically available area per person to provide goods or services in a sustainable manner. The following ratio defines SPI as:

$$SPI = \frac{a_{tot}}{a_{in}} \quad [8.15]$$

where a_{in} is the available surface relative to the annual supply of goods and energy per person. It is usually estimated by dividing the total area of a region by the annual number of its inhabitants. Actually, the SPI indicates how much of the area, which is theoretically available per person to ensure their livelihood under sustainable conditions, is used for the production or the service in question: as the SPI (or a_{tot}) gets lower, the impact on the ecosphere to provide the good's or service also becomes lower. A key point of the SPI assessment is the ability to specify and compare the different impacts of a technology. The detailed description of the SPI calculation and application would go beyond the scope of this chapter. Readers may refer to the articles by [NAR 95] and [KRO 96], which illustrate this approach. The authors propose correlations to determine the different areas [NAR 06]. An interesting case study of this indicator is proposed by [STE 99a,b] for the case of a bioprocess (penicillin production).

In order to provide a more comprehensive analysis of the interaction of environmental burdens and financial costs, a environmental performance strategic map has been proposed, based on the combination of different footprints [DEB 09]: carbon footprint [HUI 08, WIE 07], water footprint [HOE 02], energy footprint (renewable, non-renewable) [STO 03], and footprint due to emissions (air, water, and soil) [SAN 07].

8.5. Exergy as a thermodynamic base for a sustainable development metrics

Another way to define a sustainable development indicator is to use exergy. A presentation of all the concepts is proposed in two parts in [GON 01a, GON 01b]. The use of exergy [DEW 08] makes it possible to quantify, on the whole, the resources consumed and the emissions into the environment, to the extent that it is a physical magnitude that can integrate mass and energy transfers.

Exergy analysis is based on the combination of the first (energy conservation) and second principle (development of entropy, consideration of irreversibilities, and energy degradation) of thermodynamics [AHE 80, BEJ 96]. Due to the generation of entropy, the energy available in the outgoing products (exergy of outgoing products) is lower than the one available in the resources. This deterioration in quality is quantifiable by exergy destruction and is involved in physico-chemical processes, either in the natural ecosystem (biomass production, for example) or in the industrial ecosystem (production, consumption, etc.).

The first applications of exergy analysis in the 1980s mostly focused on the analysis of industrial systems. The research in this area includes both methodological developments and applications to specific industrial processes and to their supply chain. Let us note that many studies have been conducted on the combination of exergy analysis and "pinch" methods (e.g. [SOR 99, FEN 97]).

Cumulative exergy consumption (CExC) extends the exergy analysis beyond the simple process to consider all the processes from natural resource extraction up to the final product. Here again, the major interest of this overall analysis is to provide guidelines for the improvement of one of the involved processes and to compare several approaches [MOR 91].

Decision support systems and techniques based on the combination of exergy and economic analysis concepts have also been developed, thereby leading to an exergy cost.

Exergy analysis was applied to various energy conversion and chemical processes, particularly comparing different energy sectors [DEW 05, DEW 06]. It is particularly interesting for cogeneration systems, ([GOM 09, KAN 09] for example).

8.6. Indicators resulting from a lifecycle assessment

Life Cycle Assessment (LCA) is an environmental management tool that enables us to identify and quantify the environmental impacts of a product, process, or activity from the "cradle to the grave", i.e. from the extraction of raw materials up to its end of life processing (waste discharge, incineration, recycling, etc.).

Its methodology will not be presented here in detail, since it is the subject of a specific chapter of this book (see Chapter 7). An excellent summary of the use of LCA and its prospects is proposed in [GUI 10].

8.6.1. *Main methods of impact categories*

There are different methods to translate the inventory results into environmental impact indicators at different levels. These are generally classified into two broad categories based on their position on the continuum of the cause and effect chain (some examples are shown in Figure 8.6), the "mid-point" methods on the one hand, and the "end-point" methods on the other hand:

– "mid-point" methods, the most recognized and currently used methods, are used to characterize the inventory flows into potential impact indicators (or mid-point indicators), of about a dozen in number. They model the impact relatively closer to the environmental flow and hence consider only part of the environmental mechanism. Their advantage is to reduce uncertainty. Mid-point methods include: the CML 2001 baseline method of the Leiden University in the Netherlands [HEI 92] which has a broad consensus, or the EDIP 97 or 2003 method [HAU 98]. This method, particularly used in Scandinavia, models the impacts corresponding to higher-order effects. It enables a better communication but is more uncertain because of the many hypotheses that it involves. The impact categories commonly considered in mid-point methods generally involve global warming, ozone layer depletion, tropospheric ozone formation, acidification, eutrophication, toxicity, ecotoxicity, resource depletion, and land use;

– "end-point" methods model the impacts relatively far in the environmental mechanism, i.e. which act directly as damages to human health, ecosystems, and resources. These indicators are more relevant in terms of communication and are therefore more simple to use, but their modeling is more uncertain due to the complexity of the mechanism and difficulties to completely model it. Typical methods are the EPS [STE 00] and Eco-Indicator 99 [GOE 01] methods. The damage types concern human health, biotic and abiotic natural environment and resources, and the human environment;

– mid-point and end-point methods: some methods model the impacts both in terms of mid-point and end-point (Impact 2002 + method [JOL 02]).

8.6.2. *Choice of the method of impact categories*

The advantages and disadvantages of the methods of impact categories and indicators have been extensively presented [AZA 06]. Some users prefer mid-point indicators because they describe the impacts in the cause and effect mechanism at the earliest moment and prevent the accumulation of uncertainties when modeling the indicators to the closest end point [PEN 04].

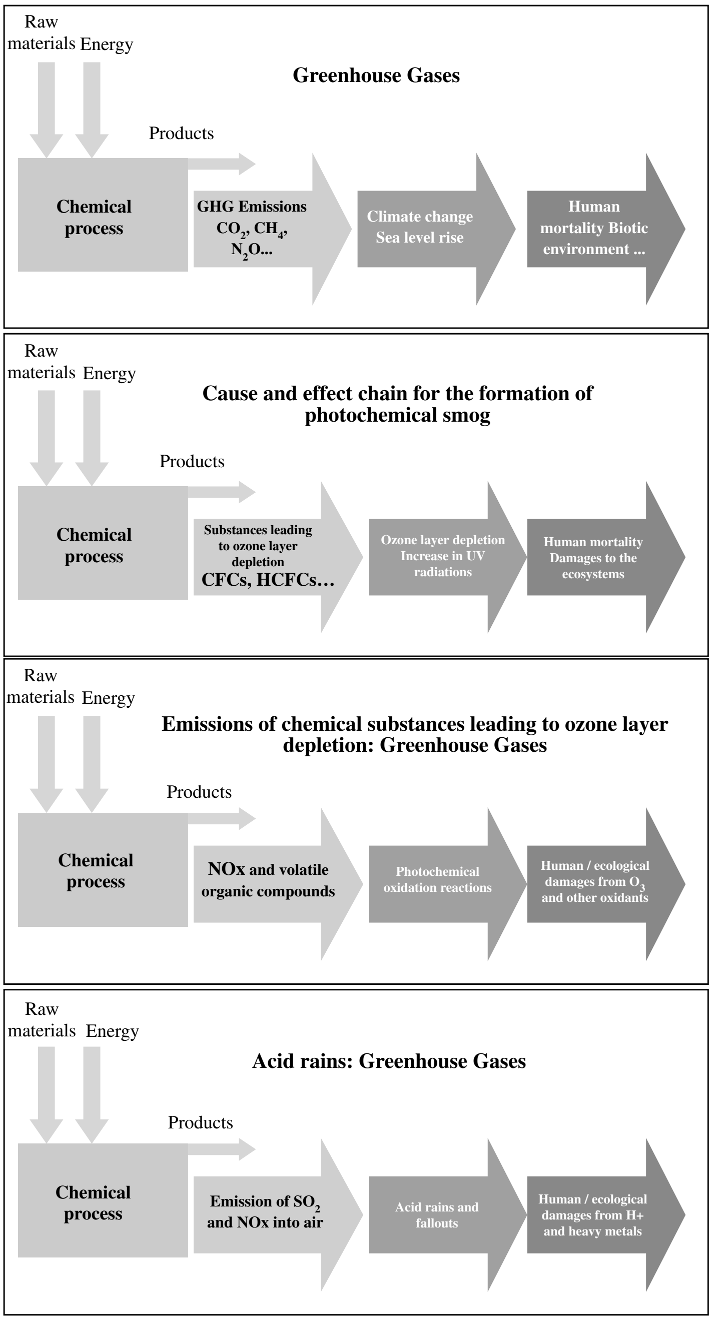

Figure 8.6. *Some examples of cause and effect chains*

These methods are also more transparent to the extent that they do not introduce weighting factors *a priori*. According to [AZA 06], we can also use traditional multicriteria decision support methods (Analytic Hierarchy Process (AHP) and Multi Attribute Utility Theory (MAUT), for example). Other users prefer indicators that are involved later in the cause and effect mechanism, as it makes the weighting of impact categories explicit and structured.

However, the main problem is that it assumes the weighting factors that are universally applicable in all decision-making situations. In addition, the weighted results are often difficult to interpret.

8.6.3. *Toward a sustainable lifecycle assessment*

In a review article on the past, present, and future of LCA [GUI 10], it is mentioned that the development of the LCA has undergone various phases, which eventually included the method as a decisional tool for environmental management, in order to design sustainable products, processes, and systems:

– past of LCA (1970–2000): there were two periods. Initially, the 1970–1990 period with two decades of method *design* with often divergent approaches, terminologies, or even results, thus showing the absence of scientific discussions and exchange platforms about this method. This was followed by a decade of *standardization* with efforts in the scientific activity and coordination of activities (works of the SETAC, definition of standardization activities (especially ISO 14040 Environmental management – lifecycle assessment – principles and framework);

– current LCA (2000–2010): this period is characterized as the decade of *development* of the methodology.

However, the LCA method, as mentioned explicitly, is interested only in the environmental component of the lifecycle assessment. The current challenge is clearly the extension of the methodology to other components of sustainable development (LCSA, Life Cycle Sustainable Analysis).

8.7. Process design methods and sustainable systems

The above analysis shows that the recognition of sustainability criteria in the process design phase is not an easy task. In general, process simulators are used to determine the material and energy flow on a boundary related to the process. Cost models combined with these performance models are used to study the process profitability. Till now, simulation and modeling tools had been used mainly to minimize an economic criterion under environmental constraints.

In the last 15 years, a substantial number of works in the PSE (Process Systems Engineering) domain dedicated to these subjects [CAN 98] is reported in the literature. The available methods can be classified into two categories, either qualitative or quantitative methods. The qualitative methods include summary techniques based on the Douglas' hierarchical procedure model [DOU 88], the onion diagram [SMI 95], or environmental optimization ENVOP [ISA 95], which can be applied to identify the solutions for minimizing the potential discharges of a process. Quantitative methods include the pinch technology [LIN 95], mass exchange networks [ELH 97], superstructure optimization [DAN 96], or simulation. All these methods can be used to better integrate the process and/or its utility network.

The process simulator has become a standard tool for process engineers. Its main advantage is the ability to easily evaluate process changes using commercial software (Aspen Plus, CHEMCAD, gPROMS, HYSYS, PRO/II, ProSim, etc.) in a rather short time period without using difficult and expensive experiments or a pilot test. Such simulators have also been used for environmental studies. The Aspen Plus simulator was coupled with an optimizer to determine the optimal superstructure, thereby reducing waste generation and energy consumption while satisfying a profitability criterion. The methodology was applied for the production of methyl chloride. The CHEMCAD simulator coupled with the WAR algorithm was used by [CAB 99] to compare the environmental impacts induced by changes in the production unit. The objective was to reduce the environmental impact by recycling in a methyl ethyl ketone unit and an ammonia unit. Another study [FUD 00] combined the Aspen Plus simulator with multiobjective methods to reduce the environmental impact and maximize profitability. The methodology was illustrated in the process of benzene production by toluene hydrodealkylation (HDA process). The HYSIS simulator was used with an optimization module to evaluate the design alternatives for a maleic anhydride process [CHE 04]. More recently, several design choices relative to a biodiesel production process have been studied by combining the Aspen Plus simulator and multicriteria decision support tools [OTH 10].

Another approach to sustainable design is adopted by [CAR 08], based on a *SustainPro* indicator to identify, screen, and evaluate the design alternatives. *SustainPro* uses the process information in the form of mass and energy balances from a simulator and applies a set of mass and energy indicators. The methodology is based on a reverse design method, where target values are assigned to the indicators and where the most sensitive variables towards indicators are identified.

A study based on the combination of a simulator coupling the process and the utilities producing unit with a multiobjective optimizer of genetic algorithm type is proposed in [AZZ 09]. A key point concerns the use of the ARIANE™ ProSim software, a simulator dedicated to the production of utilities (steam, electricity, process water), to calculate the needs in primary energy and quantify the emissions of pollutants, which come from the energy producing unit. Among the set of optimal solutions in the Pareto sense, it is important to determine the one(s) that correspond(s) to the best choices, in order to guide decision-makers in these final tasks. A method for decision support has thus been used to establish the best compromise between the criteria (TOPSIS (Technique for Order Preference by Similarity to Ideal Solution) method [HWA 81]): the fundamental idea of this method is to choose a solution as close to the ideal solution (better on all criteria) as possible and as far from the negative-ideal solution (which degrades all the criteria) as possible. The general framework is illustrated in Figure 8.7.

8.8. Conclusion

This chapter has presented a review of the various indicators and metrics recommended in the design or the evaluation phase of processes and sustainable systems. It shows a rich literature in the field and various ways of defining indicators or metrics, with different levels of sustainability assessment, for instance the use of a (AIChE, IChemE) metrics, a potential environmental impact, an SPI which can be viewed as a process sustainable footprint, an energy approach or an approach based on lifecycle assessment, etc. The design of processes and sustainable systems involves extremely varied fields or methods, and affects key products and processes.

So far, the developed works have mostly focused on the simultaneous consideration of environmental and economic aspects. The social factors are indirectly addressed through the impacts on human health, process safety, and the reduction in emissions of toxic discharges. This reflects the difficulty of quantifying social indicators and their interconnection with the operational part of the process.

In this context, it seems clear that the systemic approach of process engineering, which bases its methodology on a holistic view combining modeling, simulation, and optimization, integrating and unifying process engineering concepts, must play an important role. This will necessarily lead us to review design methods and operating procedures to make them more reliable and sustainable, but also to propose innovative methodologies integrating products, processes, and systems, following the principles of sustainable development at the preliminary stages.

The review of the literature highlights the need to couple process simulators, the tools for quantification of environmental impacts (lifecycle assessment type), and the design optimization methods, in order to achieve an overall acceptable solution. Due to the conflicting nature of the involved criteria, especially related to the presence of many uncertainties in the calculation of impacts, multiobjective optimization, as well as uncertainty analysis methods are an interesting field of investigation.

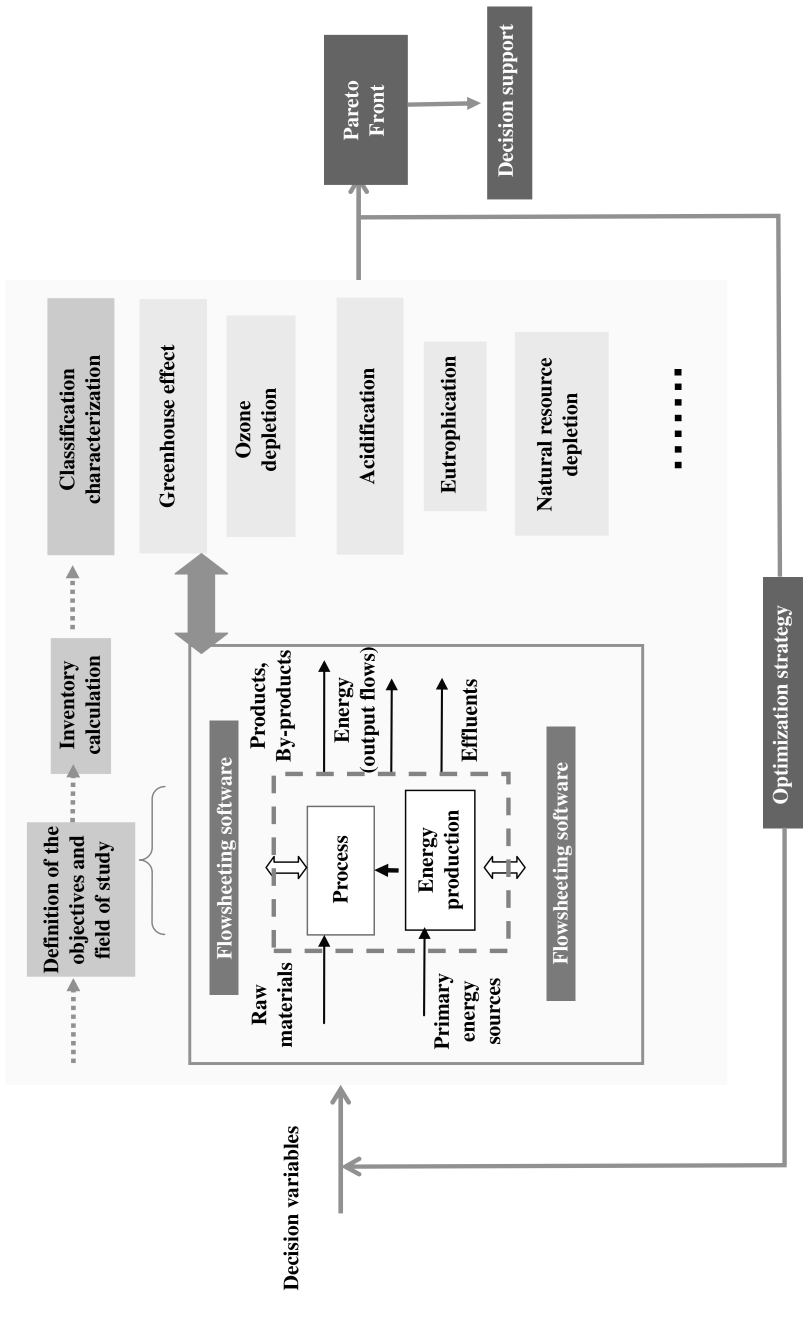

Figure 8.7. *General framework of the study [AZZ 09] coupling process simulator – multiobjective optimization – decision support*

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