

# Key Performance Indicators for Implementing Sustainability and Environmental Protection in Early Process Design Activities

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The adoption of a sustainability perspective in chemical industry shall start from the early phases of process design (e.g. conceptual design, technology selection, process development) where the key drivers in the environmental, economical, and hazard fingerprint of a process are defined. These phases also allow the opportunities for the lower cost of design change. A sound support of design activities requires quantitative tools, allowing for the assessment of the sustainability profile of a process, the identification of possible improvements and supporting informed tradeoffs.

Though several tools for process development were proposed in last decades, application is still limited in the current practice because of issues on data requirement, indicator definition and customization to specific application needs (e.g. PFD definition in design of polypropylene production plants).

This study focuses on the application to the early process design of environmental and exergy Key Performance Indicators (KPIs) to support sustainability-oriented design activities. It was tailored on the specific industrial application of polypropylene production plants. The choice of a specific sector allowed customization of the method, promoting ease of application and allowing the assessment of multiple scenarios (e.g. sensitivity on material and energy supply strategies, comparison of different technologies). Results obtained draw up sustainable guidelines to improve design activities within the scope in a lifecycle perspective.

## 1. Introduction

In the last decades, society has been asking to the chemical and process industry a growing commitment toward the development of sustainable and safer production processes. Sustainability and green engineering have become, beside conventional economic and technical aspects, a key driver in the development of new production processes.

Early process design (e.g. conceptual design, technology selection, process development) is a key phase in the adoption of the sustainability perspective, as higher degrees of freedom for change are possible at low marginal costs (Sugiyama et al., 2008). Though conceptual guidelines like Green Chemistry principles or Green Engineering principles provide a direction for the actions, a sound support of design activities requires quantitative tools. These allow for the assessment of the sustainability profile of a process, the identification of possible improvements and the evaluation of the effectiveness of alternative design choices (Dal Pozzo et al., 2017). Moreover, they can support informed tradeoffs in case of conflicting issues.

The development quantitative tools for the sustainability analysis of process schemes received significant attention in the last two decades. Metrics based on material and energy flow analysis (Brinkmann et al., 2010), exergy balances (Ren and Toniolo, 2021), midpoint environmental indicators (Brunet et al., 2012), endpoint environmental indicators (Goedkoop and Spriensma, 2001), ecological indexes (Tugnoli et al., 2008), and combinations of indicators (Huijbregts et al., 2017) were proposed. These metrics were adopted for application in the assessment of several kind of chemical and petrochemical processes and technologies. However, the use of these tools for process development is still limited in the current practice. Critical points concern the large amount of data required in relations to the timeframe and the limited information available in early design phases,

the identification of a specific but yet complete set of indicators for the assessment, and the absence of tools specifically tailored to the required application needs (e.g. specific phase of the design lifecycle and industrial sector).

Considering, for example, the case of polypropylene production (a sector currently producing worldwide 130 Mt/y of polypropylene with a growth forecast of 192 Mt/y for 2030 (Fernández, 2021)), a literature review reveals that no approach specifically designed for environmental impacts of alternative technologies during early design phases is proposed. Applicable current literature on process analysis focuses mainly on technical and efficiency issues (Touloupides et al., 2010) or studied quality control mechanism (Ohshima and Tanigaki, 2000). Life Cycle Assessment (LCA) studies on polypropylene, like the one published periodically by PlasticsEurope (PlasticsEurope, 2016), lack of the detail needed to discriminate the effect of process design choices, and focus mainly on factors as nature of raw materials and polymer waste recycling. Moreover, the metrics used in these LCA studied are not directly suitable for application as design support tools in polymerization process development. In fact, LCA metrics are suited to the analysis of the whole environmental performance of the lifecycle system, which is only one of the aspects of concern in process design: they are not, alone, able to analyse the way energy and material are used within the specific process sections and the margins of improvement still available, given the physical (e.g. thermodynamics) constraints, which would require different metrics (e.g. exergy analysis).

In this context, the presented methodology is developed in a lifecycle perspective supporting technology design activities of chemical processes. The methodology is aimed at the quantification of environmental and exergy Key Performance Indicators (KPIs) of a well-defined system. In this perspective, different scopes for emissions along the lifecycle of the reference can be adopted. Reference system includes a primary process (e.g. polymerization plant) and all the required activities for energy and material supply and waste treatment. Appropriate level of detail is allowed in the definition of required input data for each contribution considered. In fact, inputs/outputs more closely related to the primary process design activities were assessed with greater level of detail than environmental pressures originated by lifecycle processes out of the control. Databases of generic average data for these lifecycle processes were developed to support the final user. Exergy analysis is implemented alongside the use of environmental indicators, with the aim to pinpoint the sources of stronger inefficiencies in the use of energy and the opportunities of improvement. The development of a process flow diagram for a polypropylene production plant was used for demonstration of the proposed methodology, proving the applicability and the typical outcomes.

## 2. Methodology

### 2.1 General overview of the method

The developed methodology is specifically aimed at the quantification of environmental impacts and energy efficiency indicators to be used for supporting Front End Engineering Design (FEED) activities of chemical industries, with particular attention to polyolefin polymerization processes. In particular the method supports the evaluation of the sustainability profile of a process scheme, the identification of critical points of improvement, the screening design of alternatives and the prediction of the operative impacts. The approach implements the concept of Life Cycle Thinking at different levels to compute indicators as a function of chemical processes input and output.

The process object of the design is assumed as *Primary process* of the assessment. Auxiliary technologies (*Background processes*) are required for raw material and energy supply: these are generally out of the scope of design, but must be included in the analysis as they affect the overall environmental performance of the system (i.e. Lifecycle perspective).

A certain level of detail (compatible with the information available in the FEED design phase) is required to characterize energy and material consumption of the *Primary process*. *Background processes* are instead out of the control of designer, and generic datasets that measure the average technologies performances can be used. Figure 1 briefly illustrates the method scope and boundaries. Background datasets can characterize specific site-location technology or average performances. In this perspective, a reference unit (e.g. production potentiality) is required to be defined as comparative basis for the characterization of environmental and exergetic performances of the system. Several environmental problematics are analyzed (e.g. emissions of toxic substances, green house gas emissions, depletion of not renewable resources) (Tugnoli et al., 2011). Site specific information about *Background processes* allow to generate specific case-study applications of a single *Primary process*. Decision regarding site-location and technologies involved in the reference scenario allow to monitor the overall lifecycle perspective of the system. Moreover, the application of exergy balance to the reference scheme allows to evaluate the energy management inside the system. Results obtained can highlight strength and weaknesses of process decisions and draw up guidelines to drive design activities. In this direction, comparative assessment can be carried out and generate informed trade-offs in case of conflicting issues. In

this perspective, the analysis is intended to be a support tool for early design activities (e.g. conceptual design of *Primary process*, process comparison).

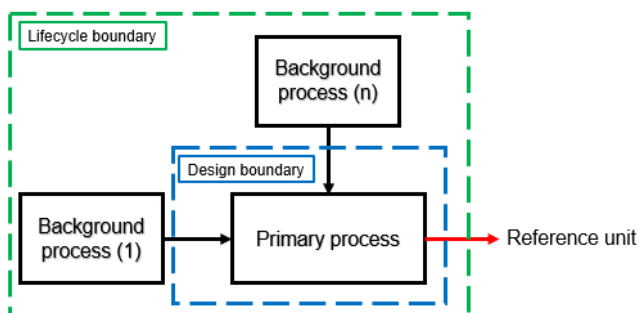


Figure 1: Conceptual definition of scope and boundaries in the application of the proposed method

## 2.2 Calculation of environmental indicators

The basic set of environmental indicators to be used in the method is proposed in Table 1. These derive from midpoint indicators typically adopted in LCA studies. The basic set of environmental indicators can be adapted in accordance with the specific goal of the considered application. Air, water and solid can be selected as target for environmental analysis. Reference substances are adopted to characterize environmental results in accordance with LCA technique (ISO, 2006). Literature average datasets are used to simulate background processes. Characterization factors ( $CF_i$ ) from the CML-2002 method (Huijbregts, 1999) are introduced to convert specific emissions into their reference substance as shown in Eq(1).

$$I_j = \sum_{i=1}^{n, \text{substances}} \frac{m_i}{P} \cdot CF_i \quad (1)$$

Where  $m_i$  is the mass flow rate of the  $i$ -th substance exchanged with the environment by the studied system,  $P$  is the reference potentiality of the system and  $CF$  is the characterization factor for substance  $i$ .

Table 1: List of environmental indicators.

Indicator ID [ $I_j$ ]	Indicator name	Example of substances (*reference)	Unit of measure
ADI,e	Abiotic Depletion Indicator (elements)	Sb*, Al, Pb, Ti, Na	[kgSb,eq/ref. unit.]
ADI,f	Abiotic Depletion Indicator (fossil fuels)	Fossil fuel*, natural gas, coal, oil crude	[MJ/ref. unit.]
GWI	Global Warming Indicator	CO <sub>2</sub> *, CH <sub>4</sub>	[kg CO <sub>2</sub> ,eq/ref. unit.]
AI	Acidification Indicator	SO <sub>x</sub> , (SO <sub>2</sub> )*, NO <sub>x</sub> , NH <sub>3</sub> , HF	[kg SO <sub>2</sub> ,eq/ref. unit.]
EI	Eutrophication Indicator	PO <sub>4</sub> <sup>3-</sup> *, NO <sub>x</sub> , NH <sub>3</sub>	[kg PO <sub>4</sub> <sup>3-</sup> ,eq/ref. unit.]
POCI	Photochemical Ozone Creation Indicator	C <sub>2</sub> H <sub>4</sub> *, VOCs, NO <sub>x</sub>	[kgEthylene,eq/ref. unit.]
HTI	Human Toxicity Indicator	1,4 – Dichlorobenzene*, Benzene, Acrylonitrile, Arsenic	[kg 1,4 – Dichlorobenzene,eq/ref. unit.]

Star (\*) marks the reference substance used in definition of  $CF$ .

The mass flows in Eq(1) shall be calculated taking into account all the emissions over the “environmental boundary” of Figure 1. Given the additive nature of the indicators, the calculation with reference to the emissions from specific processes within the boundary allows to monitor the entire polymer production chain from environmental standpoint. In this direction, the effect of utilization of different sources for material and energy supply can be quantified. Furthermore, comparative assessment can promote and drive design decisions through the quantification of specific set of indicators. This versatility allows to evaluate the effect of specific background processes (e.g spanning from non-renewable to renewable technologies for electricity and steam generation).

### 2.3 Calculation of exergy indicators

Exergy analysis is based on the simultaneous application of the First and the Second Thermodynamic Laws. It is able to assess the way energy is used in operations, overcoming the limitation of energy balances based only on the First Thermodynamic Law, that do not provide information about the degradation of energy or material sources during a process use. Exergy of a system (e.g. process stream) is assumed equal to zero at environmental equilibrium of pressure and temperature (dead state, e.g. Polymeric outlet stream).

Exergy value of material input and output is calculated by Eq(2). Exergy destruction indicator is derived by the application of exergy balance Eq(3) to the reference system. This approach allows to characterize the exergy lost due to the irreversibility of chemical and physical transformations inside the system.

$$EX_{IN/OUT} = \sum_{i=1}^{N_{comp}} \dot{m}_{i,IN/OUT} [\hat{H}_i - \hat{H}_{i,0} - T_0(\hat{s}_i - \hat{s}_{i,0})] \quad (2)$$

$$Ex, d = \frac{\sum_i^{Streams} (EX_{INi/OUTi} + \dot{W})}{P} \quad (3)$$

Where H is the specific enthalpy of a material stream, T is the temperature of the material stream, s is the specific entropy of the material stream, m is the mass flowrate of the material stream and W is the energy flowrate of an electric stream.

Exergy balance is typically applied to a single process boundary aimed at the determination of an index of irreversibility due to chemical and physical operations within the framework. Furthermore, the application of exergy balance to single unit allows to determinate the specific energy efficiency index of the involved operations. In this context, the quantification of single unit exergy destruction terms allows to monitor the efficiency of each single operation inside the boundary pinpointing potential for improvement. In a lifecycle perceptive the minimization of exergy destruction term is an index of the sustainability of the process. The definition of exergy destruction term in a comparative assessment is a key driver for decision making supporting design activities (e.g. technology selection, improvement study).

## 3. Case-study

### 3.1 Set up of the case

The method is demonstrated by the application to the design of a polypropylene production plant. Plant potentiality is assumed to be 400 kt/y of polymeric pellet.

Polypropylene (PP) is a thermoplastic polymer involved in a wide number of applications in packaging, textiles, stationery, containers, and components in the manufactory industry. New plants are continuously built to full fill the ever-increasing plastic demand. Despite the fossil origin of the feedstocks currently used in production of PP, outlooks of the future of the market agree on the expectation that production will increase and new plants will be built in the future.

The *Primary process*, in this case study, is represented by the polymerization technology which convert propylene to polypropylene. Main *Background processes* are:

- Monomer production technologies (Crude oil extraction, Naphtha reforming and Steam Cracker)
- Electricity generation process
- Steam production process

Use and disposal of the polymer are out of the scope of current analysis as they do not depend on the design choices of concern. Reference process scheme to be analyzed is derived by Polypropylene EcoProfile (PlasticsEurope, 2016). Primary process is based on available information on raw material and energy average consumption of Spheripol technology (Axens, 2005) and extruders (Abeykoon et al., 2014).

In this case, 1 kg of polypropylene (PP) with its pellet shape is adopted as reference unit. Indicators are expressed per kg of PP.

The goal of the study is the identification of critical points inside the polymer production chain. In this framework, two nested boundaries are introduced. The first boundary (*Environmental boundary*) includes all the principal process operations (polymerization, monomer production, electricity generation and steam production). This boundary allows to obtain the environmental impact indicators associated to the production of 1 kg of PP. The sensitivity of environmental results regarding raw material and energetic polymerization input can be performed considering different technologies for material and energy supply. In this context, three scenarios are considered in order to measure the effect of different utilization of electricity sources (renewable and non-renewable). A second boundary (*Polymerization boundary*) is introduced tailored to the polymerization process. This boundary

allows to carry out exergy balance and define exergy destruction term associated to polymerization activities. Performances of background processes are obtained by literature datasets (European Commission, 2022). A schematic representation of reference layout is given in Figure 2.

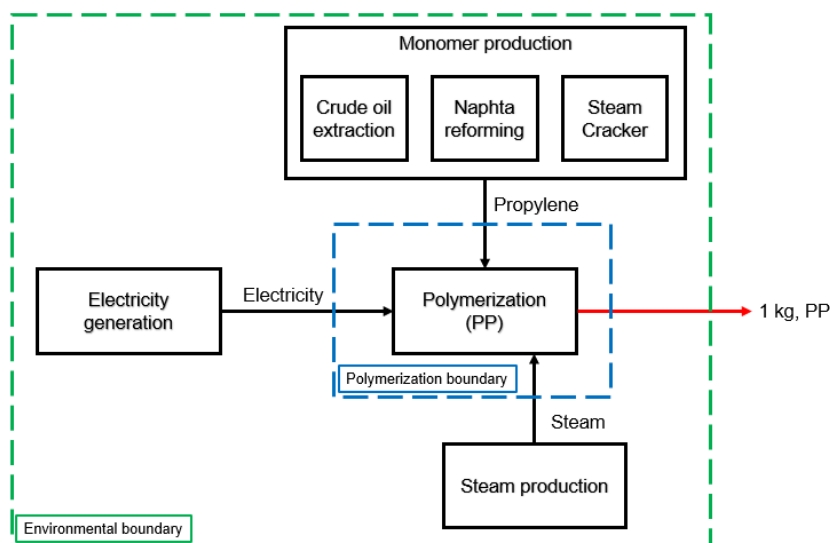


Figure 2: Reference adopted scheme for the application of the presented method

### 3.2 Results and discussion

For sake of brevity only two indicators will be presented in the following: one environmental indicator (GWI) and the Exergy destruction indicator (Ex,d). Global Warming Indicator (GWI) was selected as representative of the environmental performance of the system as strongly related to the energy and material efficiency of the process.

The principal results obtained are reported in Table 2. Eq(1) introduced in section 2.2 allows to estimate the carbon footprint of the *Environmental boundary*. Different scenarios are analyzed for plant location, considering Italy (Scenario 1) and US (Scenario 2); this affects mainly the supply of electricity and steam to the studied system. In addition, the effect of the use of exclusively renewable resource for electricity supply is evaluated (Scenario 3). Eq(3) of section 2.3 applied to the *Polymerization boundary* allows to obtain the exergy destruction indicator.

Table 2: Global Warming Indicator (GWI) and Exergy destruction indicators (Ex,d) of the reference polypropylene production chain

Indicators	Scenario 1	Scenario 2	Scenario 3
GWI [kgCO <sub>2</sub> /kgPP]	1,520	1,556	1,437
Ex,d [kJ/kgPP]	1218,3	1218,3	1218,3

Results are representative of an average situation, therefore specific plant data and information about process configurations can slightly modify the indicators. The effect of site-location dependence on polymer chain is appreciated by the comparison between Scenario 1 and 2. The GWI increases of about 2,6% due to the use of a US electricity grid mix and steam production technology. Regarding Scenario 3, a more sustainable results is achieved for the utilization of renewable resource. The GWI indicator is reduced of about 5,5%. Considering an average polymerization plant with a capability of 400 ktPP/y the reduction of GWI moving from Scenario 1 to Scenario 3 can be quantified in the reduction of approximately 33,4 ktCO<sub>2</sub>/y. Furthermore, considering single processes within the environmental boundary, monomer production activities are responsible of approximately 90% of the indicator. In this direction, other environmental benefits can be achieved for the utilization of renewable resources for monomer supply.

The analysis of the Exergy destruction indicator shows that results are not affected by site-location and technologies for supply of raw material and energy. In addition, Ex,d allows to recognize the principal source of energy consumption inside a reference system. In particular, reference adopted extruder is responsible of

about 52% of the Ex,d. This result shows that more than half of the exergy destructed by polymerization activities is located in the final extrusion section.

#### 4. Conclusions

This work presents a sustainability-oriented design support methodology applied to a polypropylene production. Key Performance Indicators (KPI) are used to measure the environmental impact profile and the energy use efficiency. In the presented case study, Global Warming Indicator (GWI) and Exergy destruction indicator (Ex,d) are calculated to characterize polymerization strategies and auxiliary processes. Results obtained can support design activities pinpointing inefficient operations and potential for improvements. Regarding GWI, the principal source of greenhouse gasses is the monomer production, suggesting that maximisation of process yield is a priority from this point of view. Environmental benefits can be obtained by the utilization of renewable resources (e.g. electricity generation process). Regarding exergy results, extrusion area is the principal source of exergy destruction term due to the high quantity of electricity consumed. In this perspective, it can be reduced by improving the design of this section (e.g. using waste heat or green energy).

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