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Sustainability Indicators for Chemical Processes: I. Taxonomy

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ABSTRACT: High demand and consumption rates of ecological materials and services to satisfy societal needs and for the dissipation of emissions are quickly exceeding the capacity that nature can provide. To avoid a tipping point situation, where ecological services may no longer be available, society must consider a sustainable path forward. The chemical industry's response is to incorporate a sustainability approach early into process design to reduce the quantity of goods and services needed and to prevent and minimize releases, while increasing their economic and social benefits. This approach leads to design modifications of existing and new chemical processes, which requires a complete sustainability performance assessment that can support a decision-maker to determine whether a process is becoming more or less sustainable. Hence, the development of indicators capable of assessing process sustainability becomes crucial. This work presents a taxonomic classification and definition of sustainability indicators according to the environmental, efficiency, energy, and economic bases proposed by the *GREENSCOPE* methodology for the evaluation and design of sustainable processes. In addition, this work proposes a general scale for measuring sustainability according to the identification and use of best possible target and worst-case scenarios as reference states, as the upper and lower bounds of a sustainability measurement scale. This taxonomy will prove valuable in evaluating chemical process sustainability in the various stages of design and optimization.

■ INTRODUCTION

Releases to the environment and the consumption of raw materials at an elevated rate require ecological goods and services to fulfill human needs, which nature can not satisfy without compromising the ability of future generations to meet their own needs. In the chemical sector, this global challenge can be addressed by the development of sustainable industrial processes. The achievement of this goal involves modifications in the type and magnitude of goods and services used, in preventing and minimizing all type of releases, and in manufacturing the desired product without negatively affecting the economic and societal benefits. These sustainable considerations have to be included into the corporate mission and vision planning at all stages of the industrial supply chain (source, manufacturing plant, product distribution, and disposal).

The integration of sustainability into process design contributes to the prevention and/or minimization of negative circumstances, rather than performing corrective and costly modifications. However, one of the difficulties in quantifying process sustainability is to set the right path to achieve improved sustainability performance. Hence, the development of indicators capable of assessing process sustainability becomes crucial for decision-making and navigates one toward sustainable development goals.[1] These indicators should have the capacity to collect and summarize complex process operations of energy, mass, and momentum transport phenomena into a manageable amount of quantitative information that is easy to analyze and communicate. Various publications propose a list of criteria that sustainability indicators should satisfy.[1−3] Sustainability assessment provides a complete performance evaluation for the designers with the aim to assist them in identifying which procedures are or are not feasible to lead toward a sustainable process.

This sustainability approach is highly recognized as a useful tool at any process scale and category of business, such as unit operation equipment, process, company, country, etc. Therefore, it is necessary to specify that this contribution is focused on sustainability indicators and assessment for chemical industry processes.

Several examples from industry illustrate the benefits of including novel modifications and/or new materials in some processes and unit operations to decrease the demand of material and energy resources,[4,5] needs of separation units[6,7] and solvents,[8−11] and the reduction of byproducts.[12,13] An important motivation for industry to adopt sustainability policies is the intangible cost associated with the business image and perception by society. The public has the buying power to force an industry toward satisfying its sustainable responsibilities. However, the unsystematic implementation of these green chemistry solutions affects the competitiveness of these new process alternatives when compared with conventional manufacturing paths. Therefore, it is necessary to include an economic benefit accompanying the minimization of

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mass and energy resource demand and environmental impacts. The evaluation of these four aspects (economic, energy, environmental, material efficiency) on a manufacturing process provides a sustainable performance status.[14]

Gonzalez and Smith[14] proposed a methodology to evaluate process sustainability called *GREENSCOPE* (Gauging Reaction Effectiveness for the ENvironmental Sustainability of Chemistries with a multi-Objective Process Evaluator), which allows one to quantify process sustainability with metrics in four main areas (bases): Efficiency, Energy, Economics, and Environment (four E's). *GREENSCOPE* can be applied to equipment or process units as well as to the entire process or bench scale, allowing for a direct comparison between several processes manufacturing the same product but employing different raw materials, reaction processes, and separation technologies and producing different byproducts. In addition, the designer or the researcher can implement this methodology to evaluate the sustainability performance after making process modifications. This methodology maintains that the four E bases are interdependent and uses individualized indicators to determine the sustainability of a unit or process.

Other research published to define indicators and metrics for process sustainability includes analyzing environmental, economic, and social areas.[2,3,15−17] These indicator inventories are oriented to the evaluation of existing plants at the business scale. Therefore, their application for making comparisons between process design alternatives and the identification of sustainable solutions is often limited to only process input/output approaches.

The present article aims to describe and discuss sustainability indicators for the design and evaluation of chemical processes, giving an overview of previous publications in the inventory and development of indicators for sustainable production. In addition, this work describes a taxonomic classification and definition of sustainability indicators in accordance with the four main areas proposed by the *GREENSCOPE* methodology to design sustainable processes. This taxonomy of chemical process indicators provides conceptual definition of each indicator, their input variables, and output results. Best-target and worst-case scenarios are proposed as upper and lower sustainability bounds for each indicator, thus normalizing the indicators on a realistic measurement scale. This paper provides a complete discussion of these aspects within the context of a chemical process. The classification, definition, and measurement scale of these indicators provide process designers with a structured methodology, which is easy to reproduce, with the assurance that aspects of process sustainability are integrated in the measurement. This process sustainability assessment provides detailed information to assist decision-makers in assessing whether a process is becoming more or less sustainable.

■ OVERVIEW OF SUSTAINABILITY INDICATOR INVENTORY

In many publications, the authors are agreed that sustainability is satisfying three global requirements or aspects: environment, economy, and society[1−3,18−20] as is shown in Figure 1. Therefore, sustainability indicators often appear classified according to these three areas. Previous works regarding inventory and classification of sustainability indicators are discussed in the text below, describing their contributions and the aspects that have to be addressed in order to propose a new taxonomy of chemical process indicators for use in process design.

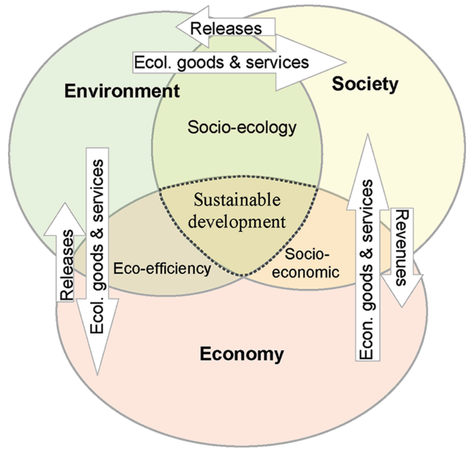

Figure 1. Triple dimensions of sustainable development (adapted from Azapagic and Perdan[3] and Sikdar[19]).

Different international organizations are developing sustainability-reporting frameworks used by diverse types of businesses, corporations, or industries around the world. Usually, they are multinational corporations oriented to realize business sustainability by supporting social activities for the community and applying clean technology at the manufacturing level.[21] The United Nations[22] uses global indicators in environmental, economic, and social areas that could be applicable to an entire country. The Dow Jones corporate sustainability indexes[23] track the performance of companies in terms of corporate sustainability. An interesting work that includes 79 indicators to evaluate sustainability performance in environmental, economic, and social areas is the Global Reporting Initiative.[17] In 2010, there were 450 companies around the world who had shown their sustainability performance using this sustainability-reporting framework. However, all of these indicators are oriented to provide a sustainability assessment at the corporate scale, which does not offer precise enough information to modify a particular process at the design scale. The corporate-scale indicator metrics are defined by the amount of mass and energy consumed per year, by total emissions, and on a revenue basis. These metric reports are useful to track the global performance of a business toward its achievement of environmental corporate goals (e.g., a 10% decrease in CO_2 emissions).

One early work proposing indicators of sustainable development for industry is that of Azapagic and Perdan.[3] This work provides 35 indicators categorized over the environmental, economic, and social areas in an attempt to contribute toward a standardization of indicators for sustainable development within industry. Different indicators are used according to the type and purpose of analysis to compare various products delivering an equivalent service, to compare various processes producing the same product, and to compare companies producing the same product. These quantitative indicators are expressed per unit mass of the product or total output per year, depending on the goal of the assessment. Life cycle impact assessments are required to evaluate some of the environmental indicators such as global warming potential (GWP), ozone depletion potential (ODP), etc.[24] However, other indicators like abiotic and biotic depletion values depend on global estimations, which do not provide any quantitative output in the design of chemical processes. Additional indicators in these three areas provide just qualitative and/or semiquantitative information with high dependency of intangible scientific parameters that may have significance at some corporate or business levels but not at the process design level. In addition, this work suggests the implementation of indicators from one area first (i.e., environmental) and gradually introduces the other areas. This partial sustainability assessment could generate unsustainable designs having low environmental impacts but higher costs.[25]

Veleva and coworkers[26,27] proposed a set of 22 indicators categorized in environmental, social, and economic areas and subdivided them through five levels relative to the basic principles of sustainability. The proposed framework provides a methodology to connect a set of indicators with different levels and actions of sustainability into the manufacturing process as is described in Figure 2. Level 1 encloses facility compliance/conformance indicators (i.e., costs associated with Environmental, Health, and Safety (EHS) compliance). Level 2 is about facility material use and performance (i.e., materials use, energy use, rate of customer complaints and returns). Level 3 includes facility effects (i.e., acidification potential, percent of workers who report complete job satisfaction). Level 4 encircles supply chain and product life-cycle (e.g., percent of products designed for disassembly, reuse, or recycling). Finally, level 5 encompasses sustainable system indicators (e.g., ecological cumulative exergy consumption,[28] Eco-LCA[29]).

In 2002, a research group belonging to the BRIDGES to Sustainability organization and sponsored by the American Institute of Chemical Engineers (*AIChE*) proposed a set of sustainability indicators to guide decision-making in chemical processes.[16] Six basic indicators, material intensity, energy intensity, water consumption, toxic emissions, pollutant emissions, and greenhouse gas emissions, were designed to evaluate chemical process sustainability. These indicators were designed to meet several criteria such as simplicity, usefulness, reproducibility, and protection of proprietary information. These indicators are more focused on the use of resources and emissions than on the impacts on society and the environment. Later in 2007, with the goal of adding corporate business indicators, the *AIChE*'s Sustainability Index (SI) [30,31] was developed. The *AIChE* SI includes 24 indicators divided in seven groups: strategic commitment to sustainability, sustainability innovation, environmental performance, safety performance, product stewardship, social responsibility, and value chain management. This index is intended for use by executives and business managers for monitoring and providing guidance into what companies should do to improve their sustainability performance. Each sustainability factor is scored on a scale of 0 to 7, and an overall score is shown for each factor. Some indicators can be extrapolated to a process design scale; most of the corporate level indicators do not represent valuable metrics at the smaller scale. The assessment criteria scores do not have defined maximum or minimum scores, and the calculation methods are not available.

Another significant effort was made in 2002 by the Institution of Chemical Engineers, *IChemE*, in the United Kingdom, who proposed 50 sustainability indicators grouped into environmental, economic, and social areas.[15] These indicators cover resource usage (energy, material, water, and land) and emission impacts (atmospheric, aquatic, and land) for the environmental area; profit, value, and investment for the economic category; and the workplace (employment situation, health and safety at work) and society (external stakeholders) for social indicators. Some of the most interesting issues of these indicators are the assessment of economic and social benefits of the employees and the implementation of quantitative measurements for the computation of social indicators. The proposed indicators can be used at different process and industry levels giving a sustainability performance in the form of ratios independent of the scale of operation (per unit of production) or to consider cost alongside benefits (per revenue or value added).

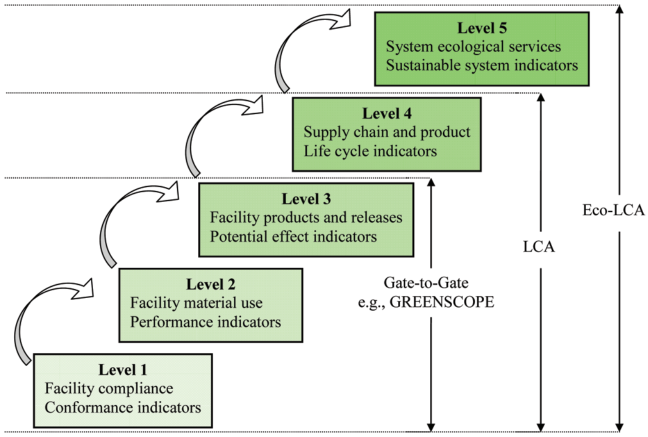

Figure 2. Framework of indicators for sustainable production (adapted from Veleva et al.[27]).

The most extensive recompilation of sustainability indicators in the literature was proposed by Krajnc and Glavic.[2] The inventory consists of 89 indicators classified according to environmental, economic, and social areas. Most of these indicators are found in an official publication by the German Environmental agency and ministry.[32] This guide to corporate environmental indicators allows comparisons with the previous year's data or with other existing companies in a quantifiable way. Krajnc and Glavic categorized the environmental indicators as input (i.e., material, energy, and water use) and output (i.e., product, solid waste, liquid waste, and air emissions) indicators and the economic indicators in financial (e.g., fraction of value added in gross domestic product) and employees (e.g., cost per employee, time of employee education) indicators. Each indicator is described by a semiquantitative expression, symbol, and measurement unit and presented by unit of production or total amount. Some indicators are subjective, based on relative criteria that are not easy to measure, related to the authors' choice of what to measure, and incapable of being used for a comparison between different processes.

Sikdar[19] defines a hierarchical indicator system of three levels or dimensions depending on how many aspects are measured by the indicator. For example, if the indicator measures only one aspect of the process (economic, ecological, and sociological aspects), then it is one-dimensional, 1-D. When two sustainability aspects as described in Figure 1 have been measured using one indicator, then this is a two-dimensional indicator, 2-D (eco-efficiency, socio-economic, and socio-ecological). In addition, three-dimensional, 3-D, indicators are obtained from the intersection of the three aspects, called sustainability indicators. This hierarchical classification is implemented in another publication where four 3-D indicators are proposed.[33] The 3-D indicators are evaluated first, and the 2-D and 1-D indicators are examined for evaluating particular aspects of the process or if the 3-D indicators do not allow clear decision-making. This interesting hierarchical classification could be the base for a sustainability assessment. The procedure could be one of computing 3-D indicators at the first levels of process design, and then when more data are available, 2-D and 1-D indicators are computed giving more detailed sustainability aspects. With this procedure, particular process units with low sustainability can be identified, and the sustainability is always evaluated and improved through all design stages depending on the available data.

As described above, there are several indicators for sustainability assessment of chemical processes, which can be applied at different process or business scales. However, the current indicator reports or methodologies do not establish the activity standards (i.e., they do not define any admissible releases of specific substances contaminating the environment) or a state of reference that can help the designer implement process design modifications and check if the process is moving toward a more sustainable position. This sustainability framework can be approached by the identification and selection of two reference states representing the best target and worst-case for each sustainability indicator. Therefore, this work aims to show the first taxonomy of indicators of chemical process sustainability that contains a suggested sustainability scale for each indicator categorized in four main areas according to the *GREENSCOPE* methodology:[14] Environmental, Efficiency, Economic, and Energy. This process-indicator taxonomy is described in the next section.

■ TAXONOMY OF CHEMICAL PROCESS INDICATORS

Many people classify sustainability indicators according to three main areas: Environmental, Economic, and Social. This general categorization is effective to describe sustainability assessment at the corporate level; however, for design purposes it needs an additional subclassification accounting for the differences between indicators inside one of these three areas. For example, when material and energy process requirements are included as environmental indicators, they are related to each other. But they have to be observed independently for a clear identification of which operating unit, process specification, and/or process operating conditions require adjustments in terms of mass and energy transfer (or both phenomena) for improving process sustainability. Consequently, this work employs the Environment, Efficiency, Economic, and Energy areas to classify the indicators used for sustainability assessment at any stage of the design of chemical processes.

On the other hand, the social area is a fundamental part that has to be considered to measure the impact of chemical products and processes to improve the quality of life of the society (sustainable development). Several social indicators have been proposed in previous publications, most of them representing qualitative or semiquantitative aspects of industry−humanity interactions and the EHS aspects of employees. These social indicator results have a critical relevance at the corporate level to visualize and transmit the intangible costs associated with the EHS effects, business image, and perception by society. However, the image perception indicators are subjective, based on relative criteria that are not easy to measure, related to the business policies of what to measure and report, and are unable to provide a direct relationship through quantitative data to the early stages of process design. Therefore, from a practical point of view, this taxonomy of indicators used for sustainability assessment in the early phases of the design of chemical processes does not include a social category, but quantitative EHS indicators are integrated.

A critical concern after defining sustainability indicators is how to track if progress is made toward sustainable performance. The sustainability indicator scores are not relevant unless reference states are provided or selected. Currently, most sustainability indicator results are expressed in total amounts of material or energy required by the process or per unit of product. For existing processes, this approach can be addressed by comparing the current results with previous trials or by different processes producing the same good. However, this strategy will be more difficult when the analysis is applied at different process design scales and process boundaries or when a new chemistry is proposed. To overcome this issue, this work describes a methodology of identifying and selecting a sustainability scale for each indicator enclosed by two scenarios representing the best target (100% of sustainability) and a worst-case (0% of sustainability). This sustainability scale allows the transformation of any indicator score to a dimensionless form using the worst and best scenarios as is described by eq 1.

$$\text{Percent Score} = \frac{(\text{Actual} - \text{Worst})}{(\text{Best} - \text{Worst})} \times 100\% \qquad (1)$$

This equation helps to visualize and compare the sustainability assessment results of each indicator in the four areas.[34] The indicators' scores are discrete one-dimension values between the selected best target and worst-case scores, where there are not assumptions of relationships or aggregation between different indicators. A linear scale between indicator scores and the percent sustainability is used because it is a simple way to show partial scores of each individual indicator. The next subsections show the indicators for process sustainability, their definitions, and the sustainability values used as reference states.

Environmental Indicators. Preventing negative environmental impacts is one goal in optimizing the design of chemical processes. Reduction or elimination of pollutants through the manufacturing process removes and minimizes the requirements for expensive end-of-pipe remediation treatments. The attainment of these environmental impact minimization goals should start from the process input, such as considering the nature of the raw materials. It is important to mention that indicators and measurements accounting for the use of goods and services (life-cycle raw material inputs) are not considered in *GREENSCOPE*, although these upstream process impacts can be analyzed through life-cycle assessment. This focuses analyses on gate-to-gate processes, where the designer has a strong influence. This is not intended to imply that analyses beyond the process gates are unimportant, just that life cycle effects are not being considered at this time. Therefore, for process inputs only indicators based on hazard categorization are considered. Table 1 shows a list of indicators used for the assessment of process sustainability in the environmental area. Some indicators use the specifications of process input material; other indicators are based on the operating conditions and process operation failures (health and safety hazards), representing the impact of components utilized in the system, and the potential impact of releases.

Different reference states have been chosen according to practical criteria. Usually, zero is the best target (100%) for pollutant releases and hazardous material usage. For the worst-case (0% sustainability), hypothetical scenarios assume that all material and service inputs are classified as hazardous and/or all generated waste for each potential EHS hazard is released out of the process. In addition, other worst-case values are standard measurements and equivalencies given by government agencies and research groups that have developed EHS assessment

Table 1. Environmental Indicators for Sustainability Assessment of Chemical Processes[a]

	indicator	formula	metric	sustainability value: best target (100%)	sustainability value: worst case (0%)
		Process Input (resource use)			
1	Number of hazardous materials input[2]	$N_{\text{haz. mat.}}$ = Number of hazardous substances fed to the process	1	0 No hazardous goods and services inputs	All goods and services inputs are hazardous
2	Mass of hazardous materials input[2]	$m_{\text{haz. mat.}}$ = Total mass of hazardous substances fed to the process	kg	0 No hazardous goods and services inputs	All goods and services inputs are hazardous
3	Specific hazardous raw materials input[15]	$m_{\text{haz. mat. spec.}} = \dfrac{m_{\text{haz. mat.}}}{\text{Mass of product}}$	kg/kg	0	All goods and services inputs are hazardous
		Process			
4	Total mass of persistent, bioaccumulative, and toxic chemicals used[26]	$m_{\text{PBT mat.}}$ = Total mass of PBT substances used by the process	kg	0	All chemicals used are PBT
5	Chemical exposure index[36,37]	CEI = The relative acute health hazard potential from possible chemical release incidents	1	0	1000
6	Health hazard, irritation factor[35,38]	$\text{HH}_{\text{irritation}} = \dfrac{\text{Volume of irritating substances in the workplace}}{\text{Mass of product}}$	m^3/kg	0 m^3/kg	1E6 m^3/kg
7	Health hazard, chronic toxicity factor[35,38]	$\text{HH}_{\text{chronic toxicity}} = \dfrac{\text{Volume of air polluted to a workplace threshold value}}{\text{Mass of product}}$	m^3/kg	0 m^3/kg	1E7 m^3/kg
8	Safety hazard, mobility[35,38]	$\text{SH}_{\text{mobility}} = \dfrac{\text{Mass released into air in case of failure}}{\text{mass of product}}$	kg/kg	0.0001 kg/kg	10 kg/kg
9	Safety hazard, fire/explosion[35,38]	$\text{SH}_{\text{fire/explosion}} = \dfrac{\text{Probable energy potential for reaction with } O_2}{\text{Mass of product}}$	kJ/kg	0	All combustion enthalpy of each process substance is released
10	Safety hazard, reaction/decomposition I[35,38]	$\text{SH}_{\text{reac/dec I}}$ = Probability for undesired reaction or decomposition	1	0	1
11	Safety hazard, reaction/decomposition II[35,38]	$\text{SH}_{\text{reac/dec II}} = \dfrac{\text{Probable energy potential from uncontrolled reactions}}{\text{Mass of product}}$ or $\text{SH}_{\text{reac/dec II}}$ = Probable adiabatic temperature rise	kJ/kg or °C	0 No uncontrolled temperature rise	All reaction enthalpy of each process reaction is released
12	Safety hazard, acute toxicity[35,38]	$\text{SH}_{\text{acute tox.}} = \dfrac{\text{Volume of air polluted to immediate dangerous concentration}}{\text{Mass of product}}$	m^3/kg	0 m^3/kg	1E5 m^3/kg
13	Fault tree assessment[39−41]	FTA = Probability of system failure if the reliability of the individual components is known	1	0	1
		Process Output (releases)			
14	Specific toxic release[1]	$\text{TR}_s = \dfrac{\text{Total mass of toxics (TRI) released}}{\text{Mass of product}}$	kg/kg	0 No releases of TRI toxics	All TRI waste is released

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Table 1. Continued

	indicator	formula	metric	sustainability value: best target (100%)	sustainability value: worst case (0%)
15	Toxic release intensity[1]	$\mathrm{TR} = \frac{\text{Total mass of toxics (TRI) released}}{\text{Sales revenue or value added}}$	kg/\$	0 No releases of TRI toxics	All TRI waste is released
16	Environmental quotient[42,43]	$\mathrm{EQ} = \frac{\text{Total mass of waste}}{\text{Mass of product}} \times \text{Unfriendliness quotient}$	kg/kg	0 no waste production	All waste is released
17	Human health burden, cancer effects[15]	$\mathrm{EB}_{\text{cancer eff.}} = \frac{\text{Total mass of benzene equivalents}}{\text{Sales revenue or value added}}$	kg /\$	0 No carcinogenic releases	All carcinogenic waste is released
18	Environmental hazard, persistency of organic substances[35,38]	$\mathrm{EH}_{\text{degradation}} = \frac{\text{Mass released of organic substances}}{\text{Mass of product}}$	kg/kg	0.01 kg/kg	1 kg/kg
19	Environmental hazard, air hazard[35,38]	$\mathrm{EH}_{\text{air}} = \frac{\text{Volume of limit concentration air emission equivalents}}{\text{Mass of product}}$	m^3/kg	0 m^3/kg	1E7 m^3/kg
20	Environmental hazard, water hazard[35,38]	$\mathrm{EH}_{\text{water}} = \frac{\text{Volume of limit concentration water release equivalents}}{\text{Mass of product}}$	m^3/kg	0 m^3/kg	1E5 m^3/kg
21	Environmental hazard, solid waste (inorganic pollutants)[35,38]	$\mathrm{EH}_{\text{solid}} = \frac{\text{Total mass of inorganic solid waste}}{\text{Mass of product}}$	kg/kg	0 kg/kg	1 kg/kg
22	Environmental hazard, bioaccumulation (the food chain or in soil)[35,38]	$\mathrm{EH}_{\text{bioacc.}} = \frac{\text{Mass of potential releases (incl.product) to accumulate in the food chain}}{\text{Mass of product}}$	kg/kg	1 kg/kg	100 kg/kg
23	Global warming potential[3,15,16,26]	$\mathrm{GWP} = \frac{\text{Total mass of } CO_2 \text{ equivalents}}{\text{Mass of product}}$	kg/kg	0 No GWP gas releases	All GWP waste is released
24	Global warming intensity[2,3,15,16,26]	$\mathrm{GWI} = \frac{\text{Total mass of } CO_2 \text{ equivalents}}{\text{Sales revenue or value added}}$	kg/\$	0 No GWP gas releases	all GWP waste is released
25	Stratospheric ozone-depletion potential[2,3,15,16]	$\mathrm{ODP} = \frac{\text{Total mass of CFC-11 equivalents}}{\text{Mass of product}}$	kg/kg	0 No CFC-11 equivalent releases	All CFC-11 equivalents waste is released
26	Stratospheric ozone-depletion intensity[3,15,16]	$\mathrm{ODI} = \frac{\text{Total mass of CFC-11 equivalents}}{\text{Sales revenue or value added}}$	kg/\$	0 No CFC-11 equivalent releases	All CFC-11 equivalents waste is released
27	Photochemical oxidation (smog) potential[2,15,16]	$\mathrm{PCOP} = \frac{\text{Total mass of ethylene equivalents}}{\text{Mass of product}}$	kg/kg	0 No ethylene equivalent releases	All ethylene equivalents waste is released

Table 1. Continued

	indicator	formula	metric	sustainability value	
				best target (100%)	worst case (0%)
28	Photochemical oxidation (smog) intensity[15,16]	$\mathrm{PCOI} = \frac{\text{Total mass of ethylene equivalents}}{\text{Sales revenue or value added}}$	kg/$	0 No ethylene equivalent releases	All ethylene equivalents waste is released
29	Atmospheric acidification potential[3,15,16,26]	$\mathrm{AP} = \frac{\text{Total mass of } SO_2 \text{ equivalents}}{\text{Mass of product}}$	kg/kg	0 No SO_2 equivalent releases	All SO_2 equivalents waste is released
30	Atmospheric acidification intensity[3,15,16,26]	$\mathrm{API} = \frac{\text{Total mass of } SO_2 \text{ equivalents}}{\text{Sales revenue or value added}}$	kg/$	0 No SO_2 equivalent releases	All SO_2 equivalents waste is released
31	Aquatic acidification potential[15,16]	$\mathrm{WP}_{\text{acid. water}} = \frac{\text{Total mass of released } H^{+} \text{ ions}}{\text{Mass of product}}$	kg/kg	0 No waste with potential to release H^+	All waste with potential to offer H^+ is released
32	Aquatic acidification intensity[15,16]	$\mathrm{WPI}_{\text{acid. water}} = \frac{\text{Total mass of released } H^{+} \text{ ions}}{\text{Sales revenue or value added}}$	kg/$	0 No waste with potential to release H^+	All waste with potential to offer H^+ is released
33	Aquatic basification potential[44]	$\mathrm{WP}_{\text{basi. water}} = \frac{\text{Total mass of released } OH^{-} \text{ ions}}{\text{Mass of product}}$	kg/kg	0 No waste with potential to release OH^-	All waste with potential to offer OH^- is released
34	Aquatic basification intensity[44]	$\mathrm{WPI}_{\text{basi. water}} = \frac{\text{Total mass of released } OH^{-} \text{ ions}}{\text{Sales revenue or value added}}$	kg/$	0 No waste with potential to release OH^-	All waste with potential to offer OH^- is released
35	Aquatic salinization potential[16]	$\mathrm{WP}_{\text{salinity}} = \frac{\text{Total mass of released } Na^{+},\ Cl^{-},\ SO_4^{2-},\ Mg^{2+},\ Ca^{2+},\ K^{+}}{\text{Mass of product}}$	kg/kg	0 No salt releases	All salt waste is released
36	Aquatic salinization intensity[16]	$\mathrm{WPI}_{\text{salinity}} = \frac{\text{Total mass of released } Na^{+},\ Cl^{-},\ SO_4^{2-},\ Mg^{2+},\ Ca^{2+},\ K^{+}}{\text{Sales revenue or value added}}$	kg/$	0 No salt releases	All salt waste is released
37	Aquatic oxygen demand potential[15]	$\mathrm{WP}_{\text{O2 dem.}} = \frac{\text{Total mass of dissolved } O_2 \text{ removed}}{\text{Mass of product}}$	kg/kg	0 No waste with potential to remove dissolved O_2	All waste with potential to remove dissolved O_2 is released
38	Aquatic oxygen demand intensity[15]	$\mathrm{WPI}_{\text{O2 dem.}} = \frac{\text{Total mass of dissolved } O_2 \text{ removed}}{\text{Sales revenue or value added}}$	kg/$	0 No waste with potential to remove dissolved O_2	All waste with potential to remove dissolved O_2 is released
39	Ecotoxicity to aquatic life potential[3,15]	$\mathrm{WP}_{\text{tox. other}} = \frac{\text{Total mass of formaldehyde equivalents}}{\text{Mass of product}}$	kg/kg	0 No formaldehyde equivalent releases	All formaldehyde equivalent waste is released
40	Ecotoxicity to aquatic life intensity[3,15]	$\mathrm{WPI}_{\text{tox. other}} = \frac{\text{Total mass of formaldehyde equivalents}}{\text{Sales revenue or value added}}$	kg/$	0 No formaldehyde equivalent releases	All formaldehyde equivalent waste is released

Table 1. Continued

	indicator	formula	metric	sustainability value	
				best target (100%)	worst case (0%)
41	Ecotoxicity to aquatic life potential by metals[3,15]	$WP_{tox.\ metal} = \frac{\text{Total mass of Cu equivalents}}{\text{Mass of product}}$	kg/kg	0 No dissolved metal releases	All water with dissolved metals is released
42	Ecotoxicity to aquatic life intensity by metals[3,15]	$WPI_{tox.\ metal} = \frac{\text{Total mass of Cu equivalents}}{\text{Sales revenue or value added}}$	kg/$	0 No dissolved metal releases	All water with dissolved metals is released
43	Eutrophication potential[3,15]	$EP = \frac{\text{Total mass of phosphate equivalents}}{\text{Mass of product}}$	kg/kg	0 No phosphate equivalent releases	All phosphate equivalent waste is released
44	Eutrophication potential intensity[3,15]	$EPI = \frac{\text{Total mass of phosphate equivalents}}{\text{Sales revenue or value added}}$	kg/$	0 No phosphate equivalent releases	All phosphate equivalent waste is released
45	Specific emergy intensity[45]	$SMI_M = \frac{\text{Total emergy consumed in the process}}{\text{Mass of product}}$	kSeJ/kg	Minimum theoretical energy, ΔG, as kSeJ	5.846×10^{11} kSeJ/kg[46,47]
46	Emergy intensity[45]	$MI_M = \frac{\text{Total emergy consumed in the process}}{\text{Sales revenue or value added}}$	kSeJ/$	Minimum theoretical energy, ΔG, as kSeJ	2.294×10^{9} kSeJ/$[46,48]
47	Environmental loading ratio[45]	$ELR = \frac{\text{Total emergy supplied from nonrenewable resources}}{\text{Total emergy supplied from renewable resources}}$	kSeJ/kSeJ	0	No emergy supplied from renewable resources
48	Emergy yield ratio[45] or Resource-ECEC efficiency[49]	$EYR = \frac{\text{Total emergy content of the product}}{\text{Total emergy supplied to the process}}$	kSeJ/kSeJ	1	0
49	Emergy sustainability index[49]	$ESI = \frac{\text{Emergy yield ratio}}{\text{Environmental loading ratio}}$	1	1	0
50	Breeding factor[50]	$BF_M = \frac{\text{Total emergy content of the product}}{\text{Total emergy supplied from nonrenewable resources}}$	kSeJ/kSeJ	10	0
51	Renewability index[49]	$RI = \frac{\text{Total emergy supplied from renewable resources}}{\text{Total emergy supplied to the process}}$	kSeJ/kSeJ	1	0
52	Total solid waste mass[32]	$m_{s,\ tot}$ = Total mass of solid waste	kg	No solid waste releases	All solid waste is released
53	Specific solid waste mass[2]	$m_{s,\ spec.} = \frac{\text{Mass of specific type of solid waste}}{\text{Mass of product}}$	kg/kg	0	All types of solid waste are released
54	Solid waste mass for recovery[2]	$m_{s,\ recov.}$ = Mass of recovered solid waste	kg	All solid waste is recovered	All solid waste is released
55	Solid waste mass for disposal[2]	$m_{s,\ disp.}$ = Mass of nonrecovered solid waste	kg	0	All solid waste is released

Table 1. Continued

				sustainability value	
	indicator	formula	metric	best target (100%)	worst case (0%)
56	Recycling mass fraction[2]	$w_{s,\,recycl.} = \frac{\text{Mass of recycled solid waste}}{\text{Total mass of solid waste}}$	kg/kg	1	0
57	Disposal mass fraction[2]	$w_{s,\,nonrecycl.} = \frac{\text{Mass of nonrecovered solid waste}}{\text{Total mass of solid waste}}$	kg/kg	0	All solid waste is released
58	Hazardous solid waste mass fraction[32]	$w_{s,\,haz.} = \frac{\text{Mass of hazardous solid waste}}{\text{Total mass of solid waste}}$	kg/kg	0	1
59	Total hazardous solid waste disposal[15,32]	$m_{s,\,haz.}$ = Mass of hazardous solid waste released into the environment	kg	0	All hazardous solid waste is released
60	Specific hazardous solid waste[15]	$m_{s,\,haz.\,spec.} = \frac{\text{Mass of hazardous solid waste released}}{\text{Mass of product}}$	kg/kg	0	All hazardous solid waste is released
61	Total nonhazardous solid waste disposal[15,32]	$m_{s,nhaz.}$ = Mass of nonhazardous solid waste released into the environment	kg	All solid waste released is nonhazardous	0
62	Nonhazardous solid waste intensity[15]	$m_{s,\,nhaz.\,spec.} = \frac{\text{Mass of nonhazardous solid waste released}}{\text{Sales revenue or value added}}$	kg/$	All solid waste released is nonhazardous	0
63	Total volume of liquid waste[32]	$V_{l,\,tot.}$ = Total volume of liquid rated as waste	m^3	0	All liquid releases are rated as waste
64	Specific liquid waste volume[32]	$V_{l,\,spec.} = \frac{\text{Total volume of liquid waste}}{\text{Mass of product}}$	m^3/kg	0	All liquid releases are rated as waste
65	Nonpolluted liquid waste volume[32]	$V_{l,\,nonpoll.}$ = Total volume of liquid waste rated as nonpolluted	m^3	All liquid releases are rated as nonpollutant	0
66	Polluted liquid waste volume[32]	$V_{l,\,poll.}$ = Total volume of liquid waste rated as polluted	m^3	0	All liquid releases are rated as pollutant

[a] These indicators describe the environmental impacts of the material inputs to the process, process operation, and process releases. Note that "SeJ" is a solar emjoule used in emergy analysis.

Table 2. Efficiency Indicators for Sustainability Assessment of Chemical Processes[a]

	indicator	formula	metric	sustainability value: best target (100%)	sustainability value: worst case (0%)
1	Reaction yield	$\varepsilon = \dfrac{\text{Mass of product}}{\text{Theoretical mass of product}}$	kg/kg	1	0
2	Atom economy[43,57]	$\text{AE}_i = \dfrac{[(\text{Molecular weight}) \times (\text{stoichiometric coefficient})]_i}{\sum_{\text{reagents}} [(\text{Molecular weight}) \times (\text{stoichiometric coefficient})]_{\text{reagent}}}$	kg/kmol/kg/kmol	1	0
3	Actual atom economy[43]	$\text{AAE} = \text{AE} \times \varepsilon$	kg/kmol/kg/kmol	1	0
4	Stoichiometric factor[53]	$\text{SF} = 1 + \dfrac{\text{Total mass of excess reagents}}{\text{Theoretical total mass of reagents}}$	kg/kg	1	41^{b}
5	Reaction mass efficiency[54,55]	$\text{RME} = \dfrac{\text{Mass of product}}{\text{Total mass of reagents}}$	kg/kg	1	0
6	Total material consumption[26]	$m_{\text{mat., tot.}} = \text{Total mass input}$	kg	Mass of product	40 times mass of product
7	Mass intensity[16,26,58]	$\text{MI} = \dfrac{\text{Total mass input}}{\text{Mass of product}}$	kg/kg	1	40^{b}[52,56]
8	Value mass intensity[3,16,26]	$\text{MI}_{\text{V}} = \dfrac{\text{Total mass input}}{\text{Sales revenue or value added}}$	kg/$	0	52^{b}[53]
9	Mass productivity[56]	$\text{MP} = \dfrac{\text{Mass of product}}{\text{Total mass input to process or process step}}$	kg/kg	1	0
10	Environmental factor[10,52]	$E = \dfrac{\text{Total nonproduct or non-}H_2O\text{ mass out of process}}{\text{Mass of product}}$	kg/kg	0	39^{b}[52]
11	Mass loss index[38,42]	$\text{MLI} = \dfrac{\text{Total nonproduct mass out of process or process step}}{\text{Mass of product}}$	kg/kg	0	100
12	Environmental factor based on molecular weight[54]	$E_{\text{mw}} = \dfrac{[(\text{Molecular weight}) \times (\text{stoichiometric coefficient})]_{\text{waste}}}{[(\text{Molecular weight}) \times (\text{stoichiometric coefficient})]_{\text{product}}}$	kg/kmol/kg/kmol	0	100
13	Effective mass yield[59]	$\text{EMY} = \dfrac{\text{Mass of product}}{\text{Total mass of hazardous reagents}}$	kg/kg	$\text{EMY}^{-1} = 0$	$\text{EMY}^{-1} = 40^{b}$
14	Carbon efficiency[56]	$\text{CE} = \dfrac{\text{Moles of carbon in product}}{\text{Moles of carbon in reagents}}$	kmol/kmol	1	0
15	Material recovery parameter[43,55]	$\text{MRP} = \dfrac{\text{Total mass of reaction and postreaction solvents} + \text{mass of catalysts recovered}}{\text{Total mass of reaction and postreaction solvents} + \text{mass of catalysts used}}$	kg/kg	1	0
16	Solvent and catalyst environmental impact parameter[54,55]	$f = \dfrac{\text{Total mass of reaction and postreaction solvents} + \text{mass of catalysts used}}{\text{Mass of product}}$	kg/kg	0	62[54,55]

Table 2. Continued

	indicator	formula	metric	sustainability value	
				best target (100%)	worst case (0%)
17	Physical return on investment[49]	$\mathrm{pROI_M} = \dfrac{\text{Mass of product}}{\text{Mass input needed in excess}}$	kg/kg	$\mathrm{pROI_M}^{-1} = 0$	$\mathrm{pROI_M}^{-1} = 40^{b}$
18	Renewability material index[49]	$\mathrm{RI_M} = \dfrac{\text{Renewable mass input}}{\text{Total mass input}}$	kg/kg	1	0
19	Breeding material factor[49,50]	$\mathrm{BF_M} = \dfrac{\text{Mass of product}}{\text{Nonrenewable mass input}}$	kg/kg	10	0
20	Recycled material fraction[3,15]	$w_{\text{recycl. mat.}} = \dfrac{\text{Recycled mass input}}{\text{Total mass input}}$	kg/kg	1	0
21	Mass fraction of product from recyclable materials[2,32]	$w_{\text{recycl. prod.}} = \dfrac{\text{Mass of product from recyclable materials}}{\text{Mass of product}}$	kg/kg	1	0
22	Mass fraction of product designed for disassembly, reuse, or recycling[3,26]	$w_{\text{recov. prod.}} = \dfrac{\text{Potential mass of product designed for recovery}}{\text{Total mass of products}}$	kg/kg	1	0
23	Total water consumption[2]	$V_{\text{water, tot.}}$ = Volume of water consumed in the process or process unit	m^3/h	0	All water requirement is supplied by fresh water
24	Fractional water consumption[15,16,26]	$\mathrm{FWC} = \dfrac{\text{Volume of fresh water consumed}}{\text{Mass of product}}$	m^3/kg	0	2.95 m^3/kg[60]
25	Water intensity[15,16,26]	$\mathrm{WI} = \dfrac{\text{Volume of fresh water consumed}}{\text{Sales revenue or value added}}$	$m^3/\$$	0	1.55 $m^3/\$$[60]
26	Volume fraction of water type[2,32]	$\phi_{\text{water type}} = \dfrac{\text{Consumption volume per type of water}}{\text{Total consumption volume}}$; Type of H_2O: drinking water and raw water (surface, well, lake, river, or rainwater)[32]	m^3/m^3	$\phi^{-1}_{\text{water type}} = 0$	$\phi^{-1}_{\text{drinking water}} = 1$

[a] These indicators describe the material demand in a process or unit operation to make the desired product or perform the required function (reaction, separation, purification, etc.). Please note the reference states for some indicators are given as the reciprocal value to avoid indetermination (e.g., EMY, $\mathrm{pROI_M}$). [b] For MI (and the related $\mathrm{MI_V}$, SF, E, EMY, and $\mathrm{pROI_M}$), other values more closely identified with a process sector can be used as shown by Sheldon.[52]

Table 3. Economic Indicators for Sustainability Assessment of Chemical Processes[a]

	indicator	formula	metric	sustainability value: best target (100%)	sustainability value: worst case (0%)
		Methods for calculating profitability that consider the time value of money			
1	Net present value[38,39,61,62] or Net present worth[61]	NPV = The total of the present value of all cash flows minus the present value of all capital investments	\$	NPV @ discount rate (r_d) = 0%[63]	NPV @ r_d = minimum acceptable rate of return (MARR) = 40% for very high risk projects[40]
2	Present value ratio[40]	$\mathrm{PVR} = \frac{\text{Present value of all positive cash flows}}{\text{Present value of all negative cash flows}}$	\$/\$	Present values @ r_d = 0%[40]	Present values @ r_d = 40%[40]
3	Discounted payback period[40]	DPBP = Time required, after start-up, to recover the fixed capital investment, FCI, required for the project, with all cash flows discounted back to time zero.	yr	DPBP @ r_d = 0%[40]	Plant life cycle
4	Discounted cash flow rate of return[40,61,64]	DCFROR = The highest after-tax interest or discount rate at which the project can just break even (NPV = 0)	%	DCFROR = MARR = 40%[40]	0
5	Capital charge factors[64]	CCF = Revenue − Total production costs	1/yr	CCF @ MARR = 40%[64]	0
6	(Specific) Economic potential[64]	EP = Revenue − Raw material costs − Utility costs	\$/(kg product)	EP that guarantees DCFROR = 40%	0
		Methods for calculating profitability that do *not* consider the time value of money			
7	Rate of return on investment [40,61,64]	$\mathrm{ROI} = \frac{\text{Average annual net profit}}{\text{Fixed capital investment}}$	%/yr	ROI = MARR = 40[61]	0
8	Payback period[40,61,64]	$\mathrm{PBP} = \frac{\text{Fixed capital investment}}{\text{Average annual cash flow}}$	yr	PBP @ MARR = 40[61]	Plant life cycle
9	Turnover ratio[61]	$\mathrm{TR} = \frac{\text{Gross annual sales}}{\text{Fixed capital investment}}$	\$/\$	4[61]	0
10	Cumulative cash position[40]	CCP = The worth of the project at the end of its life	\$	Fixed capital investment	0
11	Cumulative cash ratio[40]	$\mathrm{CCR} = \frac{\text{Sum of all positive cash flows}}{\text{Sum of all negative cash flows}}$	1	CCR that guarantees MARR = 40%[61]	0
12	Net return[61]	R_n = Net profit − Total capital investment	\$	R_n that guarantees MARR = 40%[61]	0
13	Revenues from eco-products[32]	REV = Net revenues from eco-products	\$	Total revenue	0
14	Revenue fraction of eco-products[32]	$\mathrm{REV}_{\text{eco-prod.}} = \frac{\text{Revenues from eco} - \text{products}}{\text{Total revenue}}$	\$/\$	0	1

Table 3. Continued

	indicator	formula	metric	sustainability value: best target (100%)	sustainability value: worst case (0%)
			Processing costs		
15	Equivalent annual cost[63]	C_{eq} = Annual investment cost (AIC) + Annual negative cash flow	\$	AIC @ r_d=MARR	C_{eq} = annual positive cash flow
16	Total product cost[61]	TPC = Manufacturing cost (COM) + General expenses (GE)	\$/kg	TPC that guarantees MARR = 40%[61]	TPC = Product sales price
17	Production cost[38]	E_{PC} = Raw material costs (C_{RM}) + Treatment cost of output flows (C_{WT}) + Labor cost (C_{OL})	\$/kg	C_{WT} = 0, C_{RM} = 10% of Total Product Cost (TPC), C_{OL} = 0.1TPC[61]	All waste is Hazardous, C_{RM} = 0.8TPC, C_{OL} = 0.2TPC[61]
18	Capital cost[61,63]	C_{TM} = Direct costs (C_{direct}) + Indirect costs ($C_{indirect}$) + Working capital (WC)	\$	$C_{direct} = 0.59C_{TM}$, $C_{indirect} = 0.14\ C_{TM}$, WC = 0.1 C_{TM}[61,63]	$C_{direct} = 0.68\ C_{TM}$, $C_{indirect} = 0.28\ C_{TM}$, WC = 0.2 C_{TM}[61]
19	Manufacturing cost[61,63]	COM = Direct manufacturing costs (DMC) + Fixed manufacturing costs (FMC) + Plant overhead costs (POC)	\$/kg	DMC = 0.66TPC, FMC = 0.1TPC, POC = 0.05TPC[61,63]	DMC = 0.66TPC, FMC = 0.2TPC, POC = 0.15TPC[61]
			Process input costs		
20	Specific raw material cost[38]	$C_{SRM} = \dfrac{\text{Raw material costs}}{\text{Mass of product}}$	\$/kg	0.1TPC[61]	0.8TPC[61]
21	Total material cost[2]	$C_{mat,\ tot.}$ = Absolute cost of total material used in the process or process unit	\$	0.1TPC[61]	0.8TPC[61]
22	Total energy cost[2]	$C_{E,\ tot.}$ = Absolute cost of energy used	\$	Only consumed energy from cheapest source, e.g., coal[40] @ 1.72×10^{-6}/kJ	Only consumed energy from expensive source, e.g., electricity[40] @ 1.68×10^{-5}/kJ
23	Specific energy costs[2]	$C_{E,\ spec.} = \dfrac{\text{Total energy cost}}{\text{Total production cost}}$	\$/\$	0	$C_{E,\ spec} \geq 0.2$[61]
24	Average cost of energy source[2]	$C_{E,\ source} = \sum \dfrac{\text{Cost per source of energy}}{\text{Total energy consumption}}$; Energy sources: natural gas, fuel oil (light or heavy), hard coal, brown coal, renewable source, electricity, etc.[32]	\$/kJ	Only consumed energy from cheapest source, e.g., coal[40] @ 1.72×10^{-6}/kJ	Only consumed energy from expensive source, e.g., electricity[40] @ 1.68×10^{-5}/kJ
25	Total water cost[2]	$C_{water\ tot.}$ = Absolute cost of water used in the process or process unit	\$	0	All water required is provided by fresh water at \$0.26/m^3

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Table 3. Continued

	indicator	formula	metric	sustainability value: best target (100%)	sustainability value: worst case (0%)
26	Water cost fraction[2]	$C_{\text{water spec.}} = \dfrac{\text{Total water costs}}{\text{Total production costs}}$	\$/\$	0	$C_{\text{water spec}} \geq 0.2$[61]
27	Average volume water type cost[2]	$C_{\text{water type}} = \sum \dfrac{\text{Cost per type of water}}{\text{Total water consumption}}$ Type of H_2O: drinking water, process use water, boiler feedwater, deionized water, and raw water (surface, well, lake, river, rainwater).[32]	\$/m^3	Only consumed water from cheapest source, e.g., process use water[40] @ \$0.067/m^3	Only consumed water from expensive source, e.g., boiler feedwater[40] @ \$2.45/m^3
		Process output costs			
28	Total solid waste cost[2,32]	$C_{\text{s tot.}}$ = External waste removal fees, internal storage, personnel, waste treatment, and transportation cost	\$	0	\$2/kg[40] All solid waste is Hazardous
29	Solid waste cost fraction[2,32]	$C_{\text{s, spec.}} = \dfrac{\text{Total solid waste costs}}{\text{Total production costs}}$	\$/\$	0	\$0.005/\$[47]
30	Total liquid waste cost[32]	$C_{\text{l tot.}}$ = External waste removal fees, internal storage, personnel, waste treatment, and transportation cost	\$	0	\$2/kg[40] All liquid waste is Hazardous
31	Liquid waste cost fraction[32]	$C_{\text{l, spec.}} = \dfrac{\text{Total liquid waste costs}}{\text{Total production costs}}$	\$/\$	0	\$0.0033/\$[47]
32	Costs of purifying air[32]	$C_{\text{pur. air}}$ = External waste removal fees, internal storage, personnel, waste treatment, and transportation cost	\$	0	All air emissions have to be purified
33	Fractional costs of purifying air[32]	$C_{\text{pur. air fract.}} = \dfrac{\text{Total costs of purifying air}}{\text{Total production costs}}$	\$/\$	0	\$0.0024/\$[47]

[a] These indicators describe the process profitability and costs in a process or unit operation to make the desired product or perform the required function (reaction, separation, purification, etc). Note that all monetary values are given in US dollars.

Table 4. Energy Indicators for Sustainability Assessment in Chemical Processes[a]

	indicator	formula	metric	sustainability value: best target (100%)	sustainability value: worst case (0%)
1	Total energy consumption[2,16,26,66]	E_{total} = Total energy consumed by the process or process unit	kJ/h	Minimum theoretical energy ΔG	Max E_{tot}
2	Specific energy intensity[3,16,26,67]	$R_{SEI} = \frac{\text{Net energy used as primary fuel equivalent}}{\text{Mass of product}}$	kJ/kg	0	1.949×10^6 kJ/kg[47]
3	Energy intensity[3,16,26]	$R_{EI} = \frac{\text{Net energy used as primary fuel equivalent}}{\text{Sales revenue or value added}}$	kJ/$	0	3.73×10^4 kJ/$[48]
4	Waste treatment energy[43]	$\text{WTE} = \frac{\text{Waste treatment energy requirements}}{\text{Mass of product}}$	kJ/kg	0	$\frac{\text{Max } E_{\text{waste treat.}}}{\text{kg of product}}$
5	Solvent recovery energy[43]	$\text{SRE} = \frac{\text{Solvent recovery energy requirements}}{\text{Mass of product}}$	kJ/kg	0	$\frac{\text{Max } E_{\text{solvent rec.}}}{\text{kg of product}}$
6	Resource energy efficiency[49]	$\eta_E = \frac{\text{Energy content of the product}}{\text{Total material-input energy}}$	kJ/kJ	0	1
7	Renewability energy index[15,27]	$\text{RI}_E = \frac{\text{Net energy supplied from renewable resources}}{\text{Net energy supplied to the process}}$	kJ/kJ	1	0
8	Breeding energy factor[49,50]	$\text{BF}_E = \frac{\text{Energy content of the product}}{\text{Nonrenewable material-input energy}}$	kJ/kJ	10	0
10	Energy for recycling[2]	$E_{recycl.}$ = Energy used for recycling	kJ	0	Max $E_{recycl.}$
11	Exergy consumption[65,68,69]	Ex_{total} = exergy consumed in all steps of the process or process unit	kJ/h	0	Max $\text{Ex}_{tot.}$
12	Exergy intensity[70]	$R_{Ex} = \frac{\text{Net exergy used}}{\text{Mass of product}}$	kJ/kg	0	$\frac{\text{Max Ex}_{tot.}}{\text{kg of product}}$
13	Resource exergy efficiency[70]	$\eta_{Ex} = \frac{\text{Exergy content of the product}}{\text{Total material-input exergy}}$	kJ/kJ	0	1
14	Renewability exergy index[71]	$\text{RI}_{Ex} = \frac{\text{Net exergy supplied from renewable resources}}{\text{Exergy entering to the process}}$	kJ/kJ	1	0
15	Breeding exergy factor[50]	$\text{BF}_{Ex} = \frac{\text{Exergy content of the product}}{\text{Nonrenewable material-input exergy}}$	kJ/kJ	10	0

[a] These indicators describe the energy demand in a process or unit operation to make the desired product or perform the required operating function (reaction, separation, purification, etc.).

methods to represent the effect of several pollutants.[35] Finally, some potential environmental impacts are quantified by the summation of potency factor contributions of different substances as equivalent amounts of a reference substance with known effect.[15] For example, the global warming burden uses 1 kg of CO_2 as a reference substance and assigns to 1 kg of methane the potency factor of 21 kg of CO_2. This means that methane has a global warming potential 21 times that of CO_2.

Efficiency Indicators. The efficiency of a process or a unit operation can be reflected in terms of the amount of material and services required to generate the desired product (reaction) or complete a specific process task (e.g., separation). Mass transfer operations have an implicit influence on the amount of energy demand, equipment size, costs, raw materials, releases, etc. Therefore, efficiency indicators provide sustainability assessments that are useful for detecting opportunities in process design at the conceptual stages, having predominant influence in all areas of process sustainability. Table 2 describes the proposed indicators to quantify the material requirements for the whole process or a process unit in terms of efficiency. Several indicators are related to unit operation equipment involving chemical reactions, such as classical indicators of chemical reaction efficiency (e.g., reaction yield, atom economy). There are other indicators that employ the total mass or material input to be compared with the product to realize how much mass input is reflected in the product because these values can easily help to quantify the total amount of waste, byproducts, and general releases. However, these pollutants have to be defined to get a realistic estimation of potential effects through specialized environmental indicators. Some indicators describe the renewability and recyclability levels of the material input per mass of product and the amount of solvent and catalyst used in the process. Efficiency indicators focused on water consumption are included. These could be categorized as environmental indicators, but because they only describe the process demand of water and not the pollutant effects in aqueous medium, they are included here.

Most of the efficiency indicators shown here connect material input/output with the product or service generated in the process or operation unit. Therefore, the reference states (best target and worst case) are defined as mass fractions between zero and one (kg of product/kg of reagents). Other indicators (e.g., fractional water consumption, water intensity) have been estimated for the chemical industry, describing their range of values used as a reference for the best and worst cases in the sustainability scale.[10,51] In the case of a total water consumption indicator, the worst case is assumed when all water requirements

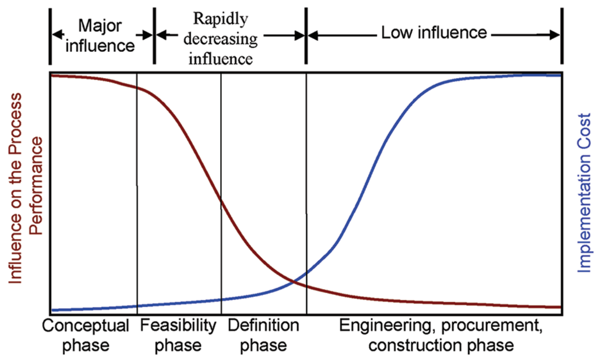

Figure 3. Front-end loading and the implementation of process changes through the process design stages reflected in implementation costs and the potential to influence the process behavior. The cost to implement a process modification at the final design stages is far higher than implementing the same change at the early process design stages, which coincides with the maximum potential to influence the process behavior (adapted from Perry's Chemical Engineers' Handbook[72] Figure 9-23 and Heinzle and Hungerbuhler[73] Figure 2).

are supplied by fresh water, which is when there is no water recycling. An initial assessment can be used as a reference state through comparison with future states when process design modifications are made.

Some worst-case reference values are obtained from previous publications and industry values. For example, the worst case for the environmental factor (E) is the highest score of average E values from chemical industry branches[52] and previous work on reaction analysis.[54,55] Since E and mass intensity (MI) are related[43] by $MI = E + 1$, then a worst case for MI can be obtained from the E value. A worst-case score for the value mass intensity (MI_V) can be suggested using the reference value for MI by selecting a product whose price is affecting the profitability of the process of interest. For the application of this work in the production of biofuels (biodiesel), an October 2010 glycerine price is used as the reference product price[53] in determining a worst-case MI_V score. For the stoichiometric factor (SF) worst case, a value can be proposed by assuming that the total mass of excess reagents is 40 times the mass of product. The worst-case scenario for the solvent and catalyst environmental impact parameter (f) can be assumed from a previous study of 400 organic reactions.[54,55] In the case of renewability indicators such as the breeding material factor indicator (BF_M), a worst-case score can be identified by proposing a hypothetical case where the nonrenewable total mass input is 100 times the mass of the product.

On the other hand, some indicator worst cases are estimated from data describing different chemistries with a small product generation per amount of total material input.[56] Therefore, for some indicators (e.g., mass intensity, mass loss index, physical return of investment) the users can choose their own limits to override the proposed reference states by using values more closely related to their particular process or unit operation.

Economic Indicators. Economic benefit is the main objective of a business. Therefore, a positive economic outcome must be evidenced at the time that a new process technology or modification is proposed to be implemented at commercial scale. Economic objectives for minimizing costs and maximizing profits are used in process system engineering to optimize a process design. Hence, economic indicators describing profitability and costs are fundamental to defining a sustainable process.

Table 3 shows the proposed economic indicators for the assessment of process sustainability in terms of profit and costs. Indicators based on profitability criteria for projects (process, operating unit, equipment) may or may not account for the time value of money (i.e., discounted or nondiscounted values). For evaluating large-scale projects, discounted techniques are recommended; however, for smaller projects (process improvements such as equipment replacement) nondiscounted profitability techniques are still used. Indicators supported in cost criteria can be grouped as processing costs (e.g., capital cost, manufacturing cost), process input costs (raw material cost, utility costs), and process output costs (waste treatment costs).

Three parameters are important for the comparison of different project alternatives, the discount rate (or interest rate) used to move all cash flows back to the beginning of the project, the time required to recover the initial investment, and the minimum rate at which the initial investment is recovered (minimum acceptable rate of return, MARR). Combined aspects of these parameters can be used to propose reference states for economic sustainability indicators. When the interest or discount rate is set equal to zero it gives the best target scenario because this means that future profits keep their value back to time zero, and it generates the shortest time to recover the initial capital investment. The minimum acceptable rate of return is the rate that must be achieved by an investment in order for it to be acceptable to the investor.[61] This parameter has different values according to the level of risk for the investment: for a low risk project (mature technology process) MARR is 4−8%/yr, and for a very high risk investment (unproven technology, high R&D) MARR is 32−48%/yr.[61] In this work a 40% internal rate of return to recover the investment is proposed as the best target. In contrast, a discount rate of 40% to move all cash flows back to the beginning of the project can be used as the worst-case scenario. For other profitability indicators (e.g., discounted cash flow rate of return, turnover ratio), a zero value can represent the lower sustainability limit.

For the economic indicators based on processing, input, and output costs, a zero value could be the best target (100%) for sustainability. Several indicators depend on cost values that have to be accepted or rejected by interdisciplinary business groups; therefore, this work suggests reference states of economic sustainability as percentage values of the total product cost (TPC) applicable to ordinary chemical processing plants.[61] The TPC must guarantee a MARR of 40% for the best target and a TPC equal to the product sales price as reference for the worst-case bound. Most of the worst-case and best target values for processing cost indicators can be proposed from maximum and minimum average values of current chemical company reports (e.g., Tables 6.17 and 6.18 in Peters et al.[61]) as a function of the manufacturing (COM) and capital (C_{TM}) costs. For some utility costs (process input costs) and waste treatment costs (process output costs), the worst-case values are assumed from current industrial values if utility demand is from the most expensive source and the most expensive waste treatments are required (e.g., Table 8.3 in Turton et al.[40]). Finally, as suggested in the previous sustainability area, some indicators (i.e., energy cost, water cost, treatment costs) do not have predefined reference bounds for a sustainability measurement scale because they depend on the particular process or designer to assume which values are acceptable or not. Therefore, an assessment from industry data[51] can be used as a worst-case reference state through comparison with future states when process design modifications are executed.

Energy Indicators. Energy demand is an important issue influencing the sustainability performance of a chemical process or process equipment represented in the total product cost, energy goods and services, and heat emissions. Different thermodynamic properties have been used to obtain an energetic sustainability score including energy, exergy, and emergy.[28,50,65] Calorific energy balances are the most practical methodologies used in industrial processes; however, aggregation rules (efficiency or equivalency factors) are needed to combine energy flows from different sources and work simultaneously with other indicators to account for the value and renewability of the source. Exergy balances offer the advantage to consider the irreversibility of the process (entropy generation), expressing the energy quality by giving the amount of useful work that can be obtained from a source of energy. In addition, the impact of emissions can be represented in terms of exergy loss of the affected system. Emergy explicitly considers substitutability and resource quality and provides results that are more intuitive but plagued by data gaps, controversial aspects, and uncertainties.[65] Similar to all indicators for process sustainability the energy indicators must be scientifically sound, easy to compute, and consistent because the computation of thermodynamic properties depends on several data and reference states that should be available, especially for new chemical processes.

Table 4 describes a set of indicators used to quantify the process performance in the energy base. The indicators are based on calorific energy measurements (such as the energy used per mass of product, waste treatment energy), energy source, renewability, and exergy consumption. Emergy is mentioned here, but it is categorized as an environmental indicator because according to its definition emergy takes into account the energy consumed by ecological goods to produce raw materials and dissipate releases.

For the sustainability values used as reference states, zero energy consumption per unit of product is the best target (more products per unit of consumed energy). A minimum theoretical energy requirement based on Gibbs free energy could be the best target for absolute energy consumption indicators. Most of the worst cases do not have a predefined value because they depend on the particular process or process equipment. The designer has to choose which value is unacceptable. In addition, some worst cases can be assigned by taking the lowest scores found through comparing several sustainability corporate reports,[51] which occurs in the energy intensity indicator. As an alternative, an initial assessment can be used as a reference state for comparison with future states when process design modifications are executed to improve the energy consumption and usage through the chemical process.

DISCUSSION

A combination of performance indicators for chemical processes with a methodology to evaluate sustainability provides the right direction to the designer in the goal of developing more sustainable processes by modifying existing processes as well as by creating new chemistries. According to *GREENSCOPE*, the effects of process changes toward sustainable development must be reflected as performance improvements in the environment, energy, efficiency, and economic areas. It is important to understand that the indicators are related to each other through implicit relationships. For this reason, it can occur that improvements have been achieved in one area and simultaneously other areas are affected negatively. This means that final decisions in process design could be a tradeoff to achieve a net improvement in process sustainability.

When the performance indicators are calculated, the results have to be analyzed and compared with reference states or measurement scales to know what sustainability level has been achieved. Therefore, this work proposes reference states for each indicator based on the identification of a value or scenario corresponding to a highest (best) attained sustainability score and another worst-case value or scenario representing the minimum reached sustainability bound (0%). The best cases are scenarios in which the exceedences of material and energy resources are minimized or eliminated, there are no releases, the potential EHS risks are negligible, a highest industrial profitability is achieved, and the capital, manufacturing, product, production, utility, and treatment costs are minimized or eliminated. In contrast, the worst cases are represented by extreme scenarios where all raw materials are hazardous and nonrenewable; all wastes are released without any treatment, mitigation, or recovery techniques; there are high potential EHS risks; and there is no expected project profitability. These worst states reflect zero efficiency of mass, reaction, and energy transfer operations, and all costs are assumed as the highest standards according to reports from ordinary chemical processing plants.

Since several indicators represent absolute values of mass and energy process consumption, then a worst-case reference state for these assessments can be associated with other indicator results (which have predefined limits) or chosen by interdisciplinary groups of decision-makers (multiobjective decision). These general indicators describe the process sustainability improvements in absolute values (i.e., total energy and material consumption, energy intensity) useful for corporate comparison purposes and global reporting data requirements.

A main issue in developing sustainable processes is to know which stage of the process design is more effective to perform changes having a high potential to influence the sustainability behavior of the process during operation. According to front-end loading[72] management practice, changes performed at early stages of a project life are effective at influencing a project's profitability and less complex to adopt. Figure 3 shows the implementation of process changes at different stages of a project life cycle and the potential to influence a project performance and costs. It is evident that the cost for implementing process modifications at the early design stages is far lower than implementing the same changes at the final process design stages, where there is minimal potential to influence the process behavior. Consequently, specific process changes to improve sustainability at early design stages will have greater potential influence on the sustainability level of the process during operation.

The need for the scalability of the sustainability assessment results has to be addressed in order to make sure that optimized sustainable designs as well as experimental studies at lab scale (giving high sustainability results) will be reflected at the corresponding operative process size or process scale. The chemical process indicators should have the ability to describe the sustainability of the final process scale based on the available data from the experimental results as well as from different process scales (e.g., pilot plant scale to industrial scale).

SUMMARY

Multiple pressures from society, government, trade associations, employees, etc., on the chemical industry regarding the high consumption rates of ecological goods and services as well as negative environmental impacts of releases have been effective in forcing businesses to develop sustainable processes. However, gauging process sustainability and setting the right path to achieve better sustainability performance are challenges in developing sustainable processes. Hence, the development of indicators capable of assessing process sustainability becomes crucial for decision-making and navigates one toward sustainability goals.

This work goes into sustainability assessment by proposing and summarizing chemical process indicators according to the environment, efficiency, energy, and economic bases proposed by the *GREENSCOPE* methodology for the evaluation and design of sustainable processes. The proposed indicators express diverse process performance aspects in a format easy to understand and compare. There are environment indicators showing the hazardous categorization of the material used, operating conditions, and process operation failures and the potential EHS impacts of releases. In addition, several efficiency indicators are proposed to quantify the material requirements for the whole process or a process unit, efficiency of mass transfer processes (e.g., reaction, separation), renewability, material recovery, and water consumption. Economic indicators for the assessment of process sustainability in terms of profit and costs are shown. Furthermore, this work proposed a set of indicators used to quantify the process performance in the energy area based on calorific energy measurements, energy source, renewability, and exergy consumption.

For tracking whether progress is made toward sustainable performance, this work describes a methodology that consists of identifying and selecting a sustainability scale for each indicator enclosed by two scenarios representing the best target (100% of sustainability) and a worst case (0% of sustainability). The best-case scenarios are conditions in which the exceedences of material and energy resources are minimized or eliminated, no pollutant releases, negligible EHS risks, maximum profitability, and all product and processing costs are minimized or eliminated. In contrast, the worst cases are scenarios where all raw materials are hazardous and nonrenewable, all produced wastes are released, higher potential EHS risks, no project profitability, zero efficiency of reaction, mass, and energy transfer operations, and all costs are assumed as the higher averages according to reports from ordinary chemical processing plants.

This work proposes the early process design stages as the most effective time, with the minimum implementation costs, to perform changes having a high potential to influence the sustainability behavior of the process during its operation. It is suggested that indicators must have the ability to describe the sustainability of the final process scale based on the available data from the experimental results, calculations, or simulations, as well as from different process scales. In addition, a synergy between experimental work and the development of conceptual process models to design sustainable processes can be achieved if sustainability assessment is performed in all settings. Namely, sustainability assessment can help to find conditions used in the laboratory that lead to feasible conceptual processes and sustainable processes during operation.

This taxonomy of sustainability indicators for chemical processes provides process designers and decision-makers with a structured methodology easy to reproduce with the assurance that aspects of process sustainability are integrated in the measurement and in determining whether processes are more or less sustainable. Indicator data needs as well as case studies of sustainability assessment in chemical processes will be described in future publications.

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DISCLAIMER

The views expressed in this article are those of the authors and do not necessarily reflect the views or policies of the U.S. Environmental Protection Agency.

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