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Review

On process optimization considering LCA methodology

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ABSTRACT

The goal of this work is to research the state-of-the-art in process optimization techniques and tools based on LCA, focused in the process engineering field. A collection of methods, approaches, applications, specific software packages, and insights regarding experiences and progress made in applying the LCA methodology coupled to optimization frameworks is provided, and general trends are identified. The "cradle-to-gate" concept to define the system boundaries is the most used approach in practice, instead of the "cradle-to-grave" approach. Normally, the relationship between inventory data and impact category indicators is linearly expressed by the characterization factors; then, synergic effects of the contaminants are neglected. Among the LCIA methods, the eco-indicator 99, which is based on the endpoint category and the panel method, is the most used in practice. A single environmental impact function, resulting from the aggregation of environmental impacts, is formulated as the environmental objective in most analyzed cases. SimaPro is the most used software for LCA applications in literature analyzed. The multi-objective optimization is the most used approach for dealing with this kind of problems, where the ε -constraint method for generating the Pareto set is the most applied technique. However, a renewed interest in formulating a single economic objective function in optimization frameworks can be observed, favored by the development of life cycle cost software and progress made in assessing costs of environmental externalities. Finally, a trend to deal with multi-period scenarios into integrated LCA-optimization frameworks can be distinguished providing more accurate results upon data availability.

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1. Introduction

The development of industrial technology has caused the transformation of the environment in different ways, changing the nature and extent of the environmental impacts of industrial activities. Some activities may not have an immediate effect on environment and others may have a more global impact on it. In addition, some of the environment impacts lead to accumulative and synergistic effects over space and time (Azapagic, 1999).

Since last three decades, chemical and process industries are pushed by pressure groups demanding more environmental friendly processes, products and practices through ideas such as waste minimization, zero emission, and producer responsibility (Azapagic, 1999).

Nowadays, the Life Cycle Assessment (LCA) is an accepted environmental management tool to holistically, systematically and multidisciplinary quantify environmental burdens and their potential impacts over the whole life cycle of a product, process or activity. Although it has been used in some industrial sectors for about 20 years, only since the beginning of the 1990s, when its relevance as an environmental management aid in both private and public decision making became more evident, LCA has received methodological development. Some examples on that direction are the incorporation of LCA within the ISO 14000 Environmental Management Systems EMS (ISO 14001, 1996), EU Eco-Management and Audit Schemes EMAS (Council Regulation (EEC) No. 1836, 1993), and EC Directive on Integrated Pollution, Prevention and Control IPPC (Council Directive 91/61/EC, 1996; Department of the Environment, Transport and the Regions, U.K., 1998), which require companies to have a full knowledge of the environmental consequences of their actions, both on- and off-site (Azapagic, 1999).

In spite of that the LCA methodology has a subjective component in several aspects, such as the system boundaries, goal definition and scoping, and that the LCA results are often determined by limited data with unknown reliability (Georgakellos, 2005; Goedkoop and Oele, 2008), LCA is widely used as a decision-making tool in process selection, design, and optimization in order to identify clean technologies (Del Borghi et al., 2007). On the other

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hand, simulation and optimization methods, which are valuable tools mainly in process systems engineering, have been successfully applying for several decades (Francesconi et al., 2007; Oliva et al., 2008). The incorporation into an optimization framework of environmental criteria, together with the economic and technical ones, results in a powerful computer-aided decision-making tool.

In this context, integration of mathematical optimization techniques with LCA methodology for conceiving environmentally friendly processes, products and/or activities from "cradle-to-grave", in an efficient and flexible way, with less subjectivity as possible, is an ambitious challenge.

The goal of the present work is to investigate the state-ofthe-art in process optimization techniques and tools, LCA methodologies, and the integration of both of them through process engineering case studies. The method and evaluation framework applied was based in an exhaustive, systematic search in the main scientific databases using specific, topic-sensitive keywords for each particular point addressed or criterion considered. The focus was on the retrieved results of applications and experiences coming mainly from the chemical engineering, process engineering and process systems engineering fields concerned about environmental issues. The purpose is to provide a collection of pioneering papers with distinctive features for gathering the general trends in integrating LCA methodologies with optimization strategies. In doing so, the characteristics or features reviewed regarding modeling and optimization aspects were, among others: (a) the type of the resulting model derived, i.e. linear or non-linear models with continuous or mixed continuous and integer decision variables: (b) the nature of the resulting optimization problem, i.e. single-objective or multi-objective optimization problems; (c) the solution methods and/or strategies used (e.g. Pareto set, solution procedure based on local or global optimization approaches, mathematical programming techniques, neural network-based approaches, genetic algorithm methods); (d) the nature of the considered scenarios (e.g. single-period or multi-period analyses). The characteristics or features reviewed regarding LCA methodologies were among others: (a) impact modeling depth categories in the characterization step (midpoints or endpoints), (b) weighting basis in the valuation step (monetization, distance to target, and panel methods); (c) system boundaries considered (e.g. cradle-tograve approach, cradle-to-gate approach, supply chain analysis, product manufacturing stage only). The screening, selection and inclusion of the referenced papers were performed by analyzing the quality and completeness of the information they provide in order to delineate such general trends.

2. Mathematical optimization techniques suitable for process synthesis and design

Traditionally, system optimization in chemical and process engineering applications has focused on maximizing/minimizing economic objective functions. Grossmann et al. (2000) presented an overview of the major advances in mathematical programming techniques and strategies for modeling and solving design and synthesis problems. These problem types can be formulated as follows:

$$\begin{aligned} \min Z &= f(x,y) \\ s.t. & h_i(x,y) &= 0 \quad i = 1,...,m \\ g_i(x,y) &\leq 0 \quad i = 1,...,l \\ x \in X, y \in \{0,1\} \end{aligned} \tag{1}$$

where f(x, y) is the objective function to be optimized (e.g. cost); $h_i(x, y) = 0$ are the equations that describe the performance of the system such as mass and energy balances and design equations; and

 $g_i(x, y) \leq 0$ are inequalities that define the specifications or constraints for feasible choices, such as material availabilities, energy requirements, and capacities. A mixed-integer programming model corresponds to a mixed-integer linear (MILP) or mixed-integer nonlinear (MINLP) programming model depending on whether the functions are linear or not. The variables x are continuous, and generally correspond to the state or design variables (material and energy flows, pressures, compositions, sizes of process units, etc.), while y are integer or discrete variables, which are generally restricted to 0-1 values to define the selection of an item or an action; for example, alternative materials or processing routes in the system. If there are no integer variables, the mixed-integer programming problem reduces to a linear program (LP) or non-linear program (NLP) depending on whether the functions are linear or not.

Then, an alternative formulation and solution procedure for problems with discrete/continuous variables was described: the generalized disjunctive programming (GDP) approach (Raman and Grossmann, 1994). The basic idea in these models is to use boolean and continuous variables, and a maximization/minimization problem is formulated with an objective function subject to three types of constraints: (a) global inequalities that are independent of discrete decisions; (b) disjunctions that are conditional constraints involving an OR operator; and (c) pure logic constraints that involve only the boolean variables. The GDP optimization problem looks as follows:

$$\min Z = \sum_{k \in K} c_k + f(x)$$
s.t. $g_i(x) \le 0$ $i = 1, ..., l$

$$\begin{bmatrix} y_{jk} \\ h_{jk}(x) = 0 \\ c_k = \gamma_{jk} \end{bmatrix} \quad k \in K$$

$$\Omega(y) = True$$

$$x \in X, \quad y_{jk} \in \{True, False\}$$
(2)

In this form, apart from the term f(x) for the continuous variables, the objective function has the charges c_k that depend on discrete choices. The inequalities $g_i(x) \leq 0$ must hold regardless of the discrete conditions and $h_{ik}(x) = 0$ are conditional equations that must be satisfied when the corresponding boolean variable y_{ik} is True for the jth term of the kth disjunction. The set I_k represents the number of choices for each disjunction defined in the set K. Also, the fixed charge c_k is assigned the value γ_{ik} for that same variable. Finally, the constraints $\Omega(y)$ involve logic propositions in terms of boolean variables. A GDP problem can be reformulated as a mixed-integer programming problem using the convex hull transformation (Turkay and Grossmann, 1996) or with "big-M" constraints for the disjunctions. The propositional logic statements are reformulated as linear inequalities (Raman and Grossmann, 1991, 1994). The GDP technique reduces combinatorial search effort because reduces the number of equations. Grossmann et al. (2000) mention methods for solving those types of problems for both linear and non-linear cases.

Since optimal problem solutions based on an economic objective function usually conflict with those based on an environmental one, multi-objective optimization was proposed to solve this trades-off. In general, a multi-objective (MO) optimization problem can be formulated as follows (Guillén-Gosálbez et al., 2008):

$$\min f(x,y) = [f_1, f_2...f_p]$$
s.t. $h_i(x,y) = 0$ $i = 1,...,m$

$$g_i(x,y) \le 0 \quad i = 1,...,l$$

$$x \in X \subseteq \mathbb{R}^n$$

$$y \in \{0,1\}$$
(3)

where constraints are analogous to those described in (1). Here, the system is optimized simultaneously on a number of objective functions f_1 , f_2 ... f_p to locate the multidimensional noninferior or Pareto frontier. The points that lie in the Pareto curve are the Pareto optimal solutions of the problem and represent the points where no objective can be improved without worsening the value of other objective (Azapagic, 1999; Guillén-Gosálbez et al., 2008; Ngatchou et al., 2005).

One method to solve MO optimization problems is the ε -constraint method, which is based on the optimization of one objective function while treating the other objectives as constraints bounded by some allowable range for ε_i (Azapagic and Clift, 1999a; Guillén-Gosálbez et al., 2008; Ngatchou et al., 2005):

$$\min\{f_k(x,y)\}$$
s.t. $f_i(x) \le \varepsilon_i \quad i = 1,...,n; \quad i \ne k$

$$h_i(x,y) = 0 \quad i = 1,...,m$$

$$g_i(x,y) \le 0 \quad i = 1,...,l$$

$$x \in X \subseteq \mathbb{R}^n$$

$$y \in \{0,1\}$$

$$(4)$$

The problem is repeatedly solved for different values of ε_i to generate the entire Pareto set.

Mussati (2003) and Mussati et al. (2003a, 2003b) proposed an alternative approach for optimal synthesis and design of dualpurpose desalination systems. They determined useful relationships between thermodynamic and economic solutions. Briefly, by applying duality and the Karush-Kuhn-Tucker (KKT) conditions to a thermodynamic problem (maximization of the system efficiency) and to an economic problem (minimization of the total cost), the authors determined the so-called "thermodynamic costs", which relate the main process variables with their corresponding costs. Indeed, for the analyzed system, those thermodynamic costs determine the optimal values range of process variables (lower and upper bounds), which can then be used for initializing the economic optimization problem. Thus, following an analogous approach, it is possible to formulate objective functions for the optimization problem considering environmental indexes (instead of process efficiency), and thus obtaining "environmental costs" (instead of "thermodynamic" ones). The resulting information can be useful not only for having good initial values and bounds, but also for comparing the environmental performance among alternative processes/products/activities.

All mathematical formulations mentioned above are deterministic. However, some system parameter values can be uncertain. A number of inexact programming methods were developed for dealing with uncertainties in planning problems, which were generally based on interval mathematical programming (IMP), fuzzy mathematical programming (FMP) and stochastic mathematical programming (SMP) (Cai et al., 2009). Computationally efficient alternatives to stochastic programming are offered by Fuzzy linear programming (FLP) techniques (Lai and Hwang, 1992; Rommelfanger, 1996; Sadiq and Husain, 2005). Zimmermann (1992) developed a symmetric FLP (SFLP) formulation where constraints are made flexible by introducing the concept of degree of feasibility. In the SFLP model, multiple objective functions can thus be treated as fuzzy constraints, reducing the optimization problem to the maximization of the degree of feasibility of all the fuzzy constraints simultaneously.

The SFLP methodology can be generalized for optimization problems with several objectives, where objective functions are modeled as fuzzy sets and the crisp constraints added to the formulation (Pinto-Varela et al., 2010; Tan, 2005).

Other alternative for solving optimization problems is the approach based on artificial neural networks (ANNs), which mimic

the human brain to learn the relationships between certain inputs and outputs from experience. Particularly, back-propagation-type (BP) neural networks have an input, an output and the interactions between both layers, i.e. hidden layers. Each neuron of a layer is connected to the neurons in the preceding layer, and then, forward-propagating and backward-propagating steps are repeated to perform the learning required. For each input—output pair (i, y), the back-propagation algorithm first calculates the output "y" by propagating "i" forward from input layer to output layer. Then, the network's output is compared with the target vector, and the back propagated from the output layer to the input layer to update the connection weights is started. The training procedure finishes when the network output reaches close enough to the desired output (Yang et al., 2003; Zhou et al., 2009).

Genetic algorithms (GA) search the optimal solutions by using the biological evolution principles, including natural selection and survival of the fittest. GA can be adopted to select the input variable of the BP neural network, which greatly affects the output variable and can simplify the BP network structure reducing the learning time. Certain numbers of binary digits are assigned to the parameters to be optimized. The binary string creates a chromosome and the algorithm tries to find the best 0 and 1 combination of the string. Penalty functions drastically change the value of the objective function if the parameters get out of the selected range. By combining the BP neural network and GA, a multi-objective optimization model can be built considering the following steps: (1) sample data capturing and processing; (2) applying GA to select and simplify the input variable of the model: (3) building a network model to forecast different objectives, training the BP network. and ensuring that it has forecasting ability; (4) optimizing and analyzing each objective (Yang et al., 2003; Zhou et al., 2009).

3. Life cycle assessment (LCA)

The life cycle assessment has two main objectives. The first one is to quantify and evaluate the environmental performance of a product or a process from "cradle-to-grave", i.e. considering the entire life cycle of the product: extracting and processing raw materials; manufacturing, transportation and distribution; use, reuse, maintenance; recycling and final disposal (Guinée et al., 1993), and thus help decision-makers to choose among alternative products and processes. In addition, LCA provides a basis for assessing potential improvements in the environmental performance of a product system (Azapagic and Clift, 1999a).

Regarding to the LCA framework, in 1990, the Society for Environmental Toxicology and Chemistry (SETAC) initiated activities to define LCA and developed a general methodology for conducting the LCA studies (Udo de Haes et al., 1999). Soon afterward, the International Organization for Standardization (ISO) started similar work on developing principles and guidelines on the LCA methodology (ISO 14040, 1997). Although SETAC and ISO worked independently of each other, a general consensus on the methodological framework has started to emerge, differing in details only (Azapagic, 1999).

The methodological framework for conducting LCA, as defined by both SETAC (Udo de Haes et al., 1999) and ISO (ISO 14040, 1997), comprises four main phases: (1) Goal definition and Scoping, (2) Inventory Analysis, (3) Impact Assessment, and (4) Improvement Assessment in the SETAC or Interpretation in the ISO methodologies, respectively. In the first phase, the system boundaries must be expanded to include the upstream and downstream activities related to the main process itself (Guillén-Gosálbez et al., 2008). The functional unit is also specified within this phase; it enables alternative goods, or services, to be compared and analyzed, and it is not usually just a quantity of material (Rebitzer et al., 2004). In practice,

a functional unit is an equivalent amount of a product, service or process function; its definition should take account the market context of a product and some technological options to perform the same or similar product function (Krozer and Vis, 1991).

The Inventory Analysis involves data collection and calculation procedures to quantify relevant inputs and outputs of a product system (Goedkoop and Oele, 2008; Guinée et al., 1993). In this phase, mass and energy balances are performed to quantify all the material and energy inputs, wastes, and emissions caused by a functional unit of the product studied (Azapagic, 1999; Guinée and Heijungs, 1993; Udo de Haes et al., 1999). Since the data documentation is crucial, there are public standard databases, such as SPINE, from Sweden, developed by the Center for Environmental Assessment of Product and Material Systems CPM (Carlson et al., 1995), and ECOINVENT of the Swiss Center for Life Cycle Inventories (Frischknecht, 2001) that were included in several LCA software in order to increase acceptance and data format compatibility. The format consists of a long list of data fields, which accommodate information about the valid geography, time span, and a description of the technology, among others (Rebitzer et al., 2004).

The Impact Assessment aggregates the inputs and outputs quantified in the Inventory Analysis to approach their potential environmental impacts, which can be done by three classes of indicators: (a) first generation indicators that weight inventory data using policy-based measures or intrinsic properties, i.e. in terms of "policy-based hazard equivalents" (Pennington et al., 2004); (b) marginal approaches that provide estimates of marginal changes (small changes) to the existing risks and (potential) impacts that would be attributable to a change in, or the provision of, different goods and services (Udo de Haes et al., 1999); and (c) average approaches that yield estimates of the contributions of a product to the overall *status quo* of risks and (potential) impacts (Udo de Haes et al., 1999).

A number of different Life Cycle Impact Assessment (LCIA) methods are available, several of which are implemented in commercial software (Dreyer et al., 2003). Most methods are based on impact categories and characterization factors, which consists of the following steps: classification, characterization, normalization (optional) and valuation (Guinée et al., 1993; Huijbregts et al., 2000; Miettinen and Hämäläinen, 1997) In the first step, the environmental burdens, quantified previously in the Inventory Analysis, are aggregated into a limited set of recognized environmental impact categories taking into account the available scientific knowledge about the processes. The selection of the appropriate impact categories is guided by the goal of the study, and its number has to be limited by practicality. In the ISO methodology, they are aggregated into three areas of protection: human health, natural resources and natural environment; while in the SETAC methodology, one more area is considered: man-made environment (Udo de Haes et al., 1999). Pennington et al. (2004) lists the available methods for common impact categories in LCAs. The relative contribution of each environmental impact is assessed in the Characterization step of the LCIA methods (Azapagic and Clift, 1999a). The characterization is performed multiplying the amount of each substance by its characterization factor and all the figures are summed together. Characterization factors, also called "potentials", are substancespecific, quantitative representations of potential impacts per unit emission of a substance. They are calculated for each impact category to which a substance may potentially contribute (Huijbregts et al., 2000). These factors can be generic (eq. (5)) and nongeneric (eq. (6)); the former are typically the outputs of the characterization models, and are available in the literature in the form of databases:

$$S_j = \sum_i Q_{j,i} m_i \tag{5}$$

where S_j is the indicator for impact category j; m_i is the size of the intervention of type i (for instance, the mass of a substance emitted to air), and $Q_{j,i}$ is the characterization factor that links intervention i to impact category j (Pennington et al., 2004). Equation (6) illustrates some of the potential variables of *nongeneric* characterization factors in the context of impacts on human health and the natural environment (analogous equations are available for natural resources) (Pennington et al., 2004):

$$\begin{aligned} Q_{i,s,t} &= \sum_{l} \frac{\text{Effect}(i,l,t)}{\text{Emission}(i,s)} \\ &= \sum_{l} \left(\frac{\text{Fate}(i,l,t)}{\text{Emission}(i,s)} \right) \cdot \left(\frac{\text{Exposure}(i,l,t)}{\text{Fate}(i,l,t)} \right) \cdot \left(\frac{\text{Effect}(i,l,t)}{\text{Exposure}(i,l,t)} \right) \end{aligned}$$

$$(6)$$

Subscript i denotes the substance, s is the location of the emission, l is the related location of exposure of the receptor, and t is the time period during which the potential contribution to the impact is taken into account (Pennington et al., 2004).

Another key issue in the characterization step is the impact modeling depth, i.e. the extent to which environmental mechanisms (cause-effect chains) are modeled (Bare et al., 2002a; Finnveden et al., 1992; Potting and Hauschild, 1997; Udo de Haes et al., 2002). There are two impact modeling depth categories: midpoints and endpoints. The former are considered to be links in the cause-effect chain of an impact category, prior to the endpoints, at which characterization factors or indicators can be derived to reflect the relative importance of emissions or extractions. Common examples of midpoint characterization factors include ozone depletion potentials, global warming potentials, and photochemical ozone (smog) creation potentials. On the other hand, some methodologies have adopted characterization factors at an endpoint level in the cause-effect chain for all categories of impact, i.e. that are of direct societal concern, like incidence of illnesses (e.g. human health impacts in terms of Disability Adjusted Life Years (DALY) due to carcinogenicity, climate change, ozone depletion, photochemical ozone creation; or impacts in terms of changes in biodiversity, etc.) (Bare et al., 2000).

Normalization is a procedure needed to compare across impact categories, or even areas of protection, to prioritize or to resolve trade-offs between product alternatives (Pennington et al., 2004). In addition, this step identifies an impact category that has not a significant contribution to the overall environmental problem, thus reducing the number of issues that need to be evaluated. This is done by dividing the impact category indicators by a "normal" value, adjusting the results to have common dimensions (Goedkoop and Oele, 2008). The most common way to determine the "normal" value is to estimate the impact category indicators for spatial and temporal scale, to clearly define the system (e.g. a region or an economic sector), and to consider a per capita basis (Pennington et al., 2004).

In the Valuation, the final step of the LCIA methods, the impacts can be further aggregated into a single environmental impact function by attaching weights to the impacts to indicate their relative importance (Miettinen and Hämäläinen, 1997). The resulting weighted expressions are often linear relationships, as follows:

$$EI = \sum V_k N_k \quad \text{or} \quad EI = \sum V_k S_k$$
 (7)

where EI is the overall environmental impact indicator, V_k is the weighting factor for impact category k, N is the normalized indicator, and S is the category indicator obtained in the Characterization phase (Pennington et al., 2004). Different authors (Georgakellos, 2005; Goedkoop and Oele, 2008) agree that weighting is a controversial element of LCA because a user might manipulate the

outcome by choosing a method that gives a desired result. However, all weighting methods include scientific aspects, not only from natural sciences, but also from social and behavioral sciences as well as from economics (Pennington et al., 2004). Although ISO does not recommend the application of the Valuation step for public analysis, due its subjectivity, very often it becomes a necessity in LCA to gain manageability (Georgakellos, 2005; Goedkoop and Oele, 2008; Udo de Haes et al., 1999).

Methods for weighting can be classified in three major groups: (a) Monetization, which includes all methods that have a monetary measure involved in the weighting factors. The different types of costs (present cost, willingness to pay and future extraction costs) are added, and all damages are expressed in the same monetary unit; (b) Panel, which involves a group of methods where the relative importance of damages, impact categories or interventions is derived from a group of people through surveys; and (c) Distance to target, where weighting derives from target for each impact category (Finnveden et al., 1992; Goedkoop and Oele, 2008). Table 1 includes some impact assessment methodologies reported in literature and their main characteristics. Specifically, the LCIA methods listed are: CML 92 and 01 developed by the Institute of Environmental Sciences of Leiden University (Guinée, 2001); Ecoindicator 95 and 99 of PRé Consultants (Goedkoop et al., 2000); Environmental Design of Industrial Products (EDIP), EDIP 1997 (Wenzel et al., 1997) and EDIP 2003 (Hauschild and Potting, 2003), of the Danish UMIP; IMPact Assessment of Chemical Toxics (IMPACT 2002+) proposed by the Swiss Federal Institute of Technology (Humbert et al., 2005); the method of the International Panel on Climate Change (IPCC) (Solomon et al., 2007): Tool for the Reduction and Assessment of Chemical and other environmental Impacts (TRACI) developed by the Environmental Protection Agency (EPA) (Bare et al., 2002b); Critical Volume Aggregation and Polygon-based Interpretation developed by the University of Piraeus (Georgakellos, 2005); Custos Ambientais Associados à Geração Elétrica: Hidrelétricas x Termelétricas à Gás Natural of the Instituto Alberto Luiz Coimbra de Pós-graduacao e pesquisa e engenheria (COPPE/UFRJ) (Reis, 2001); Environmental Priority Strategies in product design (EPS 2000) proposed by the Center for Environmental Assessment of Products and Material Systems, Chalmers University of Technology (Steen, 1999); Externalidades na geração hidrelétrica e termelétrica (ELETROBRÁS – Centrais Elétricas S.A., 2000); External costs of Energy (ExternE project) developed by the European Commission (EC – European Commission, 2003); LCA-net scheme of Mie University (Kato and Widiyanto, 2005); and the Waste Reduction Algorithm (WAR) algorithm of National Risk Management Research Laboratory (Cabezas et al., 1999).

The final phase of the LCA methodology, called Interpretation (in the ISO methodology) or Improvement Assessment (in the SETAC methodology), is aimed at identifying the possibilities for improving the performance of the system. In the ISO methodology, in addition to improvements and innovations, this phase covers the identification of major stages in the life cycle contributing to the impacts, a sensitivity analysis, and final recommendations (Azapagic, 1999; Saur, 1997).

3.1. Computation tools and software

There are different computational tools related to the life cycle assessment methodology, such as SimaPro (PRÉ Consultants), Umberto (IFU Hamburg and IFEU Heidelberg), TEAM (Ecobalance), GaBi (Department of Life Cycle Engineering of the Chair of Building Physics at the University of Stuttgart and PE International GmbH), POLCAGE (De La Salle University, Philippines, and University of Portsmouth, UK) and GEMIS (Öko-Institut). These software packages are based on the ISO 14040 methodology and, with the exception of GEMIS and POLCAGE, they are based on general databases. Certainly, ECOINVENT database (Swiss Center for Life Cycle Inventories) is integrated into these software tools providing access to a variety of unit processes as well as to other inventories to cover multiple industrial areas.

The SimaPro software (Goedkoop and Oele, 2008) is nowadays probably the most used software for LCA, in which many published works are based on (Calderón et al., 2010; Chambouleyron et al., 2007; Chen et al., 2010; Fantozzi and Buratti, 2010; Gamberini et al., 2010; Guillén-Gosálbez et al., 2008; Iribarren et al., 2010; Lobendahn Wood et al., 2010; Lunghi et al., 2004; Pizzol et al., 2010; Prudêncio da Silva et al., 2010; Saner et al., 2010; Scacchi et al., 2010; Sebastián et al., 2010; Silva Lora et al., 2010). SimaPro includes several LCIA methods such as Eco-indicator 99, EDIP 1997 and 2003, EPS 2000, among others. It allows viewing parts of the life cycle at different scales, and displaying their contributions to the total score. Currently, SimaPro can be integrated with TCAce (Total Cost Assessment) software developed by Sylvatica and

Table 1Some impact assessment methodologies and their main characteristics.

LCA method	Origin	Indicator basis (impact modeling depth)		Normalization	Weighting basis		
		To midpoint	To endpoint		Monetization	Distance to target	Panel
CML 92 and 01	Netherlands	X		X	_	_	_
CVAPBI ^a	Greece	X		X		X	
CAAGE ^b	Brazil		X	_	X		
Eco-indicator 95, 99	Netherlands		X	X			X
EDIP 1997, 2003	Denmark	X		X		X	
EPS 2000	Sweden		X	X	X		
EGHT ^c	Brazil		X	_	X		
ExternE project	Europe		X	_	X		
IMPACT 2002+d	Switzerland	X	X	X	_	_	_
IPCC	Europe	X		_			
LCA-net scheme	Japan	X		X		X	
TRACI	USA	X		_	_	_	_
WAR algorithm ^e	USA	X		X	_	_	_

^a Critical Volume Aggregation and Polygon-Based Interpretation method.

b "Custos Ambientais Associados à Geração Elétrica: Hidrelétricas x Termelétricas à Gás Natural" method.

^c "Externalidades na Geração Hidrelétrica e Termelétrica" method.

^d It implements a combined midpoint/damage approach for indicator basis. For weighting, self-determined weighting factors or a default weighting factor of 1 are suggested, unless other social weighting values are available.

^e Default weighting factor of 1 is suggested.

member companies of the American Institute of Chemical Engineers (AIChE) Center for Waste Reduction Technologies (CWRT), which provides insights of all potential costs associated with a process or product, by integrating life cycle assessment and scenario-based risk analysis to complement LCA methodology (www.pre.nl/simapro, 2011).

The Umberto software (www.umberto.de/en, 2011) can be used to model, calculate, and visualize material and energy flow systems. It provides a module library that contains several data sets on generic upstream and downstream processes, and it can be used to analyze various scenarios and identify the most ecologically sensible production process. Output results can be assessed using economic and environmental performance indicators addressing companies with cost intensive production that wish to optimize their processes and improve their competitiveness.

The Tools for Environmental Analysis and Management (TEAM) software (Ecobalance-UK, 1998) allows applying similar LCIA methods as SimaPro software. Regards the life cycle cost, it uses POEMS (Product Oriented Environmental Management Systems) for the comparison of different waste management scenarios and their related costs (www.ecobilan.com/uk_team.php, 2011).

The GaBi software (www.gabi-software.com, 2011) provides solutions for the assessment of costs, environmental, social and technical criteria, as well as for the processes optimization. Its available databases include more than 100 agricultural processes.

The Possibilistic LCA using GREET — Greenhouse Gases, Regulated Emissions and Energy use in Transportation - and EDIP -Environmental Design of Industrial Products – method (POLCAGE) software (Tan et al., 2004) focuses on the life cycle of alternative fuels and energy carriers. It uses a simple Multiple-Attribute Decision-Making (MADM) procedure for multiple evaluation criteria and a probabilistic approach based on fuzziness for data uncertainty. The GREET model was developed by the Argonne National Laboratory of U.S. Department of ENERGY, and is used as the inventory sub-model of POLCAGE. It is coded in Microsoft Excel and Visual Basic, and its modular structure allows users to create new fuel pathways or modify existing ones. Possibilistic uncertainty propagation (PUP) is accomplished using a Visual Basic module, which performs iterative calculations through the spreadsheet and subsequently stores output values in a worksheet with its mechanics based on fuzzy arithmetic.

The Global Emission Model for Integrated Systems database (GEMIS) (www.oeko.de/service/gemis/en, 2011) is a computerized life-cycle analysis model, LCA database, and cost-emission analysis system for energy, material, and transport systems. The environmental data cover air emissions, greenhouse gases, liquid effluents, solid wastes, and land-use. The cost data consider investment, fixed annual and variable costs, as well as externality factors for air emissions, and greenhouse gas (GHG).

In addition, there are multimedia fate and exposure models for calculating nongeneric characterization factors such as Uniform System for the Evaluation of Substances (USES) developed by the National Institute of Public Health and the Environment (RIVM et al., 1994), USEtox (Rosenbaum et al., 2008) and CalTOX model (McKone, 1993).

Different commercial specific software packages were used along the stages of the LCA methodology applied in the consulted papers. Indeed, chemical process simulators such as CHEMCAD II and III (Chemstations, 1997); Aspen (Aspen Technology, 1997); the Transient Energy System Simulation Tool — TRNSYS — of the University of Wisconsin, Madison, as well as partial equilibrium models generators such as the MARKet Allocation energy-systems computer model — MARKAL — (Fishbone and Abilock, 1981) and The Integrated MARKAL—EFOM System — TIMES — (Van der Voort et al., 1984) were used in some LCA studies. TIMES is an evolved

version of MARKAL with new functions and flexibilities; its builds on the best features of MARKAL and the Energy Flow Optimization Model EFOM. Both MARKAL and TIMES are linear programming optimization models with multi-period structure. Their source codes are written in General Algebraic Modeling System — GAMS — (Brooke et al., 1998), which process a set of data files and generate a matrix with all the coefficients that specify the economic equilibrium model of the energy system as a mathematical programming problem, and post-process the optimization results. As mentioned, there are general purpose optimization software such as Xpress-MP (Dash Associates, 1993) for LP and MILP problems, Microsoft Excel Solver for LP and NLP, and GAMS and LINGO (LINDO Systems) that allow solving from LP to MINLP optimization problems.

3.2. Applications of LCA methodology

The application type influences the phases' sequence of the LCA methodology and the choices to be made within their different components (Guinée et al., 1993). The application areas of LCA are numerous. The main distinction can be made between applications in the public or private sector. Public sector's LCA studies are used to support the development of environmental legislation and regulation, development of criteria for environmental taxes, standards, or eco-labeling programs, or to provide consumer information. In public studies, the assumptions made, methods and data used, and preferences given, should be clearly presented to make them reproducible as much as possible. In the private sector, companies can use the LCA results to support product development or marketing, to enhance the credibility or the company's environmental policy, or to guide the suppliers to act in an environmentally friendlier way (Miettinen and Hämäläinen, 1997).

Briefly, the LCA methodology has been applied for (Azapagic, 1999):

- Strategic planning or environmental strategy development for choosing the Best Practicable Environmental Option BPEO (U.K. Environment Agency); e.g. comparison of the environmental impacts of different products with the same function, and comparison of the environmental impacts of alternative manufacturing processes for the same product;
- Comparison of regional, economical or cultural scenarios for a given product, process and/or activity;
- Identification of environmental improvement opportunities such as identifying "hot spots" i.e. life cycle points critical to the total environmental impact;
- Product and process optimization, design, and innovation;
- Creating a framework for environmental audits, i.e. served as a tool for environmental system management and environmental reporting, e.g. ISO 14001 certificate.

Some different applications of LCA methodology have been described in literature. Kadam (2002) used LCA for quantify and compare two different scenarios for using the excess bagasse (by-product) in the sugarcane production. One option was to burn mass and extra gasoline, and the other one was to produce ethanol and use E10 fuel (10% ethanol and 90% leaded gasoline). In that work, 1 dry ton of bagasse was the functional unit considered; some impact categories of CML and IPCC LCIA methods were selected, and TEAM 3.0 was the software used to carry out the LCA study. Lunghi et al. (2004) used LCA to probe that complete molten carbonate fuel cell (MCFC) power plant fed by LFG (gas generated during wastes digestion in landfills) renders more environmental benefits than an MCFC fed by steam reformed. In this work, they used the SimaPro software, adopted the Eco-Indicator 99 method for impact

assessment, and considered 1 kWhe produced as functional unit. Chambouleyron et al. (2007) used the SimaPro software aiming at identifying the environmental improvement opportunities for producing three different office desks types based on the EDIP LCIA method, assuming 1 desk as the functional unit. Weisser (2007) analyzed a life cycle GHG emission (only one impact category) of electricity generation chains with the IPCC method, based on LCA studies related to fossil, nuclear and renewable technologies published between 2000 and 2006. The key parameters, assessment methodology, conversion efficiency, practices in fuel preparation and transport, technology and fuel choice, the fuel mix assumed for electricity requirement related to plant construction and equipment manufacture, and the system boundaries are compared for each energy technology, taking account the improvements that are likely to occur in the future.

Varun et al. (2009) presented a review of LCAs to compare CO_2 life cycle emissions for generating electricity by different renewable energy sources: wind, solar photovoltaic, solar thermal, biomass, and hydroelectric; and by conventional sources: coal, oil, gas, and nuclear.

4. Frameworks for integration of LCA methodologies and optimization techniques

In this section, a description of proposed frameworks and progress made toward integration of LCA methodologies and optimization techniques is performed. Traditionally, system optimization in chemical and process engineering applications has only focused on maximizing economic objectives. Preliminary works on such integration included various waste minimization approaches, from the concept of mass pinch as a tool to derive cost-optimal Mass Exchange Networks with minimum waste (El-Halwagi and Manousiouthakis, 1990), through minimum waste water generation in process plants (Wang and Smith, 1994) and waste treatment costs (Ciric and Huchette, 1993), to the concept of Zero Avoidable Pollution (Linninger et al., 1994). Although these approaches may have both environmental and economical benefits through reduced wastes and treatment costs, their disadvantage is that they concentrate on emissions from the plant only, without considering other stages in the life cycle (Azapagic, 1999). Most recent works (Bojarski et al., 2009; Gebreslassie et al., 2010; Guillén-Gosálbez et al., 2008; Liu et al., 2010; Pinto-Varela et al., 2010; Zhou et al., 2009) incorporate LCA into the process design and optimization procedures, thus establishing a link between the environmental impacts, operation and economics of the process. In general, the approach for incorporating LCA methodology into system optimization schemes comprises three main steps: (i) carrying out a life cycle assessment study, as discussed in Section 3; (ii) formulating and solving a multi-objective optimization problem in the LCA context, as explained in Section 2; and (iii) selecting the best compromise solution (Azapagic, 1999).

Following, the main approaches for simulation and optimization of chemical and biotechnological processes considering LCA methodology are described.

Hilaly and Sikdar (1994) and Cabezas et al. (1999) presented two preliminary works based on the waste minimization approach. In the former, detergent production is considered as a case study; in the latter, production of methyl ethyl ketone from secondary butyl alcohol and production of ammonia from synthesis gas were chosen as two case studies. In those works, the objective was aimed at minimizing the overall environmental impact of the main process by evaluating and comparing alternative process flow sheets or configurations. To accomplish this, they used a single environmental impact function, a "pollution index", calculated by the waste reduction (WAR) algorithm, which is based on a generic

pollution balance equation of a process flow diagram. Cabezas et al. (1999) presented a generalization of the WAR algorithm considering nine impact categories based on Heijungs et al. (1992), subdivided into four environmental physical potential effects (acidification, greenhouse enhancement, ozone depletion, and photochemical oxidant formation); three human toxicity effects (air, water, and soil); and two ecotoxicity effects (aquatic and terrestrial). Regarding to the weighting factors, although the authors suggested initially setting all factors to one, the users can vary individually each one from 0 to 10 according to local needs and policies. Commercial process simulators CHEMCAD II and III were used for performing all material and energy balances in those works, respectively.

Azapagic and Clift (1999a, 1999b) proposed a MO optimization problem in the LCA methodology context. Specifically, the production of several boron products from two mineral ores, formulated as a LP problem, was the case study considered. In both works, all activities from raw materials extraction to the production of the boron products and materials used are included in the system; however, the use and disposal phases of the products are not considered (i.e. they applied the "cradle-to-gate" approach). Here, the environmental objective function was based on impact categories and characterization factors considering seven impact categories (Heijungs et al., 1992): resource and ozone depletion, global warming potential, acidification, eutrophication, photochemical oxidant creation potential (i.e. photochemical smog), and human ecotoxicity. In this case, the authors did not optimize a single environmental impact function as Cabezas et al. (1999). Prior to the MO optimization, each impact category was optimized as a single-objective optimization problem using LP software Xpress-MP. In some particular cases, the optimization of one or a few critical objectives may lead concomitantly to the optimization of some other associated ones. Azapagic and Clift (1999b) pointed out that the minimization of the global warming potential (GWP) also minimized acidification, nitrification and human toxicity; while the minimization of photochemical oxidant creation potential (POCP) resulted in the optimum value of ozone depletion (OD). In order to include the operating cost and total production, the system was then optimized on three objectives only, i.e. GWP, production (P) and costs (C), as in Azapagic and Clift (1999a). The MO problem was solved by the ε -constraint method to generate a range of noninferior solutions as a three-dimensional Pareto surface. Afterward, the authors also simultaneously optimized the system on OD to generate a four-dimensional Pareto set.

Tan (2005) applied the symmetric fuzzy linear programming SFLP approach to solve a MO-MILP problem taking into account the fuel cycle assessment, i.e. life cycle analysis of the energy carrier used for vehicle propulsion, for a fuel mix as case study. Six impact categories were considered as environmental objective functions: acid rain, smog, global warming, eutrophication, toxicity, and resource depletion. The software POLCAGE and Microsoft Excel Solver were used to solve the multiple environmental objectives. First, weighting factors equal to one were used to give the same importance to the different environmental objectives, and then, different relative relevance was considered by adjusting these factors. The author compared this approach with the ϵ -constraint method described by Azapagic and Clift (1999a). The SFLP approach provided a single solution that embodies a compromise among the multiple conflicting objectives.

Eliceche et al. (2007) formulated a MINLP problem into the LCA methodology context, dealing with an environmentally friendly ethylene process utility plant as case study, where the limits of the plant are extended to include the relevant environmental impacts corresponding to the imported electricity generated in thermoelectric, hydroelectric and nuclear plants. The optimization

objective function was the "pollution index" suggested by Cabezas et al. (1999) using weighting factors equal to one. Seven environmental impact categories (global warming potential, acidification, ozone depletion, human toxicity in air and water, ecotoxicity and eutrophication) were considered (Heijungs et al., 1992). However, the authors observed that evaluating only global warming potential and acidification potential would be sufficient to estimate the overall environmental impact for utility plants as they represented approximately 99.68% of it.

The resulting MINLP problem was implemented in GAMS, and the NLP and MILP sub-problems were solved using CONOPT (Drud, 1994) and OSL (IBM Corp., 1992), respectively. The MINLP model contains 24 binary variables and about 10,500 equations. The solution was found in four major iterations.

Guillén-Gosálbez et al. (2008) applied the MO methodology based on MINLP problem formulations for hydrodealkylation of

toluene, focused on decreasing the environmental impact at the manufacturing stage only. The economic objective function to be optimized was the life cycle operating cost, while the environmental one was the Eco-indicator 99. This LCIA method includes eleven impact categories: (i) carcinogenic effects on humans; respiratory effects on humans caused (ii) by organic substances and (iii) by inorganic substances: (iv) damage to human health caused by climate change: human health effects caused (v) by ionizing radiations and (vi) by ozone layer depletion; damage to the ecosystem quality caused (vii) by toxic emissions, (viii) by the combined effect of acidification and eutrophication, and (ix) by land occupation and land conversion; damage to resources caused (x) by extraction of minerals, and (xi) by extraction of fossil fuels. The integration of the LCA software SimaPro with an optimization approach was performed by using the Eco-indicator 99. Each single-objective optimization problem was implemented

 Table 2

 Integrated LCA-optimization frameworks reported in the consulted literature.

Reference	System boundaries	Objective	Method	Math. form.	Comp. tools
Azapagic and Clift (1999a, 1999b)	Cradle-to-gate approach	i Min. env. impacts ii Min. life cycle op. cost iii Max. annual prod.	Heijungs et al. (1992)	MO LP/Pareto/ε-c M ^a	Xpress-MP
Hugo and Pistikopoulos (2005)	Manufac. stage (SC) ^b	i Max NPV of invest ii Min. env. impacts	Eco-indicator 99	MO MILP multi-period/ param. opt.	n.d.
Tan (2005)	Cradle-to-grave approach	Min.: i acid rain, ii smog, iii global warming, iv eutroph., v tox., vi res. depl.	EDIP	MO LP SFLP	MS Excel Solver POLCAGE
Eliceche et al. (2007)	Cradle-to-gate approach	i Min. overall env. impact	Heijungs et al. (1992) WAR algorithm	MINLP	CONOPT and OSL/GAMS
Guillén-Gosálbez et al. (2008)	Manufac. stage	Min.: i life cycle op. cost ii environ. impacts	Eco-indicator 99	MO MINLP/ Pareto/ε-c M	SimaPro DICOPT, CONOPT, CPLEX/GAMS
Vince et al. (2008)	Cradle-to-grave approach (RO desalination plants)	i Max. TRR ^c Min.: ii electricity consump. iii invest. and op. costs	IMPACT 2002+	MO MINLP Pareto	
Pietrapertosa et al. (2009)	Cradle-to-grave approach	Min. total system cost	ExternE project IPCC method	Multi-period LP	GEMIS MARKAL
Grossmann and Guillén-Gosálbez (2009)	Manufac. stage (Process synthesis and SC manag.)	Min.: i total cost ii env. impacts	Eco-indicator 99	MO MILP and MINLP/ Pareto/ ϵ -c M	SimaPro GAMS
Zhou et al. (2009)	Cradle-to-grave approach (suitable material selection)	Min.: i container weight ii costs iii env. Pollution	Eco-Indicator'99	MO LP BP NNW/GA	SimaPro
Bojarski et al. (2009)	Manufac. stage (SC)	i Min. norm. endpoint damage cat. ii Min. total env. impact iii Max. NPV	IMPACT 2002+	MO MILP/Pareto/ weighted sum method	CPLEX/GAMS SimaPro
Luz Santos and Legey (2010)	Cradle-to-gate approach (const. and op. of hydro/thermal plants)	Min.: i investment ii operation iii env. costs	ExternE project, CAAGE EGHT	Multi-period MILP	Xpress-MP
Pinto-Varela et al. (2010)	Manufac. stage (Elec. and diesel consump. over SC)	i Max. profit ii Min. environ. impacts	Eco-indicator 99 (only damage to human health)	MO MILP SFLP	n.d.
Carvalho et al. (2010)	Cradle-to-gate approach (energy supply)	Min.: i tot. annual CO ₂ emission ii env. impacts iii total annual cost	Eco-indicator 99	MILP	SimaPro LINGO
Gebreslassie et al. (2010)	Cradle-to-gate approach (solar assisted absorption cooling systems)	Min.: i total cost ii env. impacts	Eco-indicator 99	MO MINLP/ Pareto/ε-c M	TRNSYS DICOPT, SNOPT CPLEX/ GAMS
Liu et al. (2010)	Cradle-to-gate approach (energy system)	Min.: i op. and maint. cost ii GHG emissions	Life cycle GHG emission	MO Multi-period MILP/Pareto/ε-c M	CPLEX/GAMS

^a ε-c M: ε-constraint method.

^b SC: supply chain.

^c TRR: Total recovery rate.

in GAMS and solved with DICOPT (Viswanathan and Grossmann, 1990); the NLP sub-problems were solved with the code CONOPT and the MILP master problems with CPLEX (ILOG Inc., 2005).

The problem was first solved by minimizing costs neglecting the environmental concerns. The Eco-indicator 99 value was then reduced by imposing more restrictive limits on the ε -value of the ε -constraint method. The resulting MO-MINLP problem contains 724 constraints, 710 continuous variables, and 13 binary variables. The authors pointed out that the low CPU time required to generate each trade-off solution (about 1–10 s on a 1.4 GHz Pentium III processor) avoided resorting to specific sampling techniques to reduce the number of single-objective problems required for generating the Pareto set.

Pietrapertosa et al. (2009) presented a multi-period LP model for different fossil, nuclear and renewable fuel cycles for power generation. Energy and material flows from extraction to end-use demands/waste management (i.e. "cradle-to-grave" approach), and a 27-year time horizon divided into nine equal-length periods were considered. A linear partial equilibrium model generated by MARKAL was set up to represent the relationships among the system's components and boundaries over the planning time horizon stipulated. MARKAL's main inputs were the demand for energy services together with resources availability and environmental constraints, while the total system cost was the objective function minimized. For examining and comparing the effects on the energy system's configuration, costs of constraints on environmental impacts, and eco-taxes on the main pollutants, three scenarios were defined: (i) the Reference scenario (Business As Usual-BAU case), (ii) the Impacts scenario, and (iii) the Eco-taxes scenario, respectively. The first scenario describes the contribution of renewable energy sources (photovoltaic, wind, biomass and mini-hydroelectric) modeling the evolution of the reference energy system without exogenous environmental constraints, providing the baseline for scenarios analysis. The second scenario includes the software GEMIS as the modeling tool for LCA analysis to evaluate the effects of exogenous constraints on three impact categories: acidification, global warming and smog, and a combination of them, using a single environmental impact function. This analysis included the typical primary pollutants (NO_x, CO, CO₂, SO₂, TSP) and used the IPCC method. Finally, in the Eco-taxes scenario, the damage costs of pollutants (ExternE values) were inserted by a damage function attribute that represents the estimated external cost per unit of emitted pollutant using the ExternE project method. In this scenario, cases for six taxes were presented; five taxes on each air pollutant and one on the sum of them to evaluate their influence on the system configuration and to assess their synergies. Regarding external costs, two kinds of evaluation were considered: ex post, in which the environmental damage is computed without feedback into the optimization process, and ex ante. in which the internalization of external costs is done by introducing eco-taxes to consider the external costs in the optimization of the energy system costs. In the former, the overall external costs are simply added to the cost function with no effect on the determination of the optimal solution, estimating in monetary terms the environmental impacts of atmospheric emissions in different scenario hypotheses. Instead, in the latter, the introduction of environmental taxes emphasizes the role of environmental damage in the definition of resources prices and in the comparison of technologies' performances in terms of both direct and indirect effects.

Zhou et al. (2009) formulated a MO LP problem applying BP neural networks and GA for suitable materials selection for sustainable drink containers considering the "cradle-to-grave" approach. The materials considered were: aluminum, HDPE, PVC,

polypropylene, soda glass, steel, and zinc. Three objective functions were formulated: minimization of (i) the weight of the container; (ii) life cycle costs; and (iii) the environmental pollution, evaluated by the Eco-indicator'99 method using the software SimaPro.

The main characteristics of the consulted literature such as system boundaries, optimization objectives, LCIA methods used, nature of the optimization problems solved, and computational tools used, are summarized and compared in Table 2.

5. Conclusions

Life Cycle Assessment is an accepted environmental management tool to compare goods and services (products), as well as for process selection, design and optimization in order to identify opportunities for reducing the impacts attributable to associated wastes, emissions and resource consumption. On the other hand, optimization strategies and techniques are valuable tools in many engineering and scientific areas. A trend toward developing general theoretical LCA frameworks including optimization approaches could be clearly noted.

Due to the several points addressed, this article is not aiming at being a "formal" paper review, but it is intended to provide a collection of methods, approaches, applications, specific software packages, and general insights regarding experiences and progress in applying the LCA methodology coupled to optimization frameworks or schemes, through some case studies.

So far, most LCA methods have been developed in a few countries or territorial areas (mainly in Western Europe and USA), in which companies, organizations, and research centers are associated to develop their specific, large databases, and eventually software tools based on local/regional considerations and standards. However, efforts and attempts for applying the LCA methodology in practice can be observed in many countries. In this regard, it should be noted that most data cannot be reliably used in regional/economic/environmental scenarios different from those they were estimated for, as the obtained LCA results hardly depend upon them.

The system boundaries, goal and scope definitions provide to the LCA concept with an inevitable subjectivism, which should be reduced as much as possible. In fact, it can be concluded that the "cradle-to-gate" concept to define the system boundaries is the most used approach in practice, instead of the "cradle-to-grave" approach.

Normally, the relationship between inventory data and impact category indicators is linearly expressed by the characterization factors. In this way, synergic effects of the contaminants are neglected, which may underestimate the impact assessment.

For both impact modeling depth and weighting basis no prevalence among their categories or groups, respectively, was observed in the LCIA methods described. However, the eco-indicator 99, which is based on the endpoint category and the panel method, is the most used in practice.

In most analyzed cases, a single environmental impact function, resulting from the aggregation of environmental impacts, was formulated as the environmental objective function. It should be noted that the ISO methodology does not recommend its use for LCA analysis in the public sector because its subjectivity.

Regarding the software packages for LCA applications, SimaPro resulted to be the most used or referenced one in the papers analyzed.

With respect to optimization aspects, the multi-objective optimization is the most used approach for dealing with this kind of problems, where the ε -constraint method for generating the Pareto set was found to be the most applied technique. However, a renewed interest in formulating a single economic objective function in optimization frameworks could be observed. This fact is

favored with the development of life cycle cost software that can be coupled to LCA software, and the progress made in assessing costs of environmental externalities. This seems to be an alternative scheme to the multi-objective optimization approach.

A trend to deal with multi-period scenarios into integrated LCAoptimization frameworks is a welcome one, as it should provide more accurate results upon data availability along the time horizon considered.

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