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Because of the central position of the chemical industries along the value chain, process design has a pivotal role, involving many decision makers and multiple levels of deci sions. To tackle the environmental concern at source, this article presents a methodological framework for process eco design, coupling flowsheeting simulators both for production and energy processes with a Life Cycle Assessment module that generalizes and automates the evaluation of environ mental impacts. The life cycle inventory is carried out through the combined use of mass and energy balances resulting both from the global simulation of the process and its associated energy production requirement and from the use of inventory database (i.e., Ecoinvent v3) embedded in the Life Cycle Assessment software tool used (SimaPro). Dif ferent process alternatives can thus be evaluated in a system atic way and the energy related emissions for any given process that match exactly the real situation can be com puted without introducing a bias in the estimation. Through comparisons between a case base and process alternatives, a systematic decision can be made in terms of whether a solu tion is moving the process towards a more sustainable opera tion. The effectiveness of the proposed framework is first illustrated through the case study of benzene production and second, by a biodiesel production process from waste vegeta ble oils which is one of the foremost alternative fuels to those refined from petroleum products.

Keywords: ecodesign, life cycle assessment, process energy plant simulation, flowsheeting, sustainability

INTRODUCTION

Environmental concerns act as a driving force for chemi cal process designers to change their practices in process design and decision making. In that context, classical process design methods and tools that have been developed over the past decades as emphasized for instance in [1,2] are cur rently adapted or revisited to achieve environmental impact minimization at a desired economic performance. Among the different design approaches, chemical process simulators play a pivotal role both in academics and industry to model, design, and optimize operational conditions and evaluate different process configurations [3 5]. In most cases, the quality of the design is based on techno economic consider ations and the environmental issue is addressed considering either additional constraints to the design problem or valida tion steps of end of pipe treatments. Integrating ecological considerations with environmental impact criteria in the pre liminary stage of the process systematic design has been identified as a better alternative with a larger impact on the design and is often referred as "ecodesign." To improve the overall environmental performance of chemical products and processes, an environmental assessment with a life cycle per spective (Life Cycle Assessment, LCA) following ISO 14040 guidelines is particularly relevant [6]. Despite its interest, the use of LCA tools in the chemical engineering community and even more in the industrial sector is not implemented rou tinely. As reported in [7], the industrial sector is still in search of practical tools to carry out systematic sustainability assess ments of both existing and new processing technologies [8]. It must also be emphasized that "typical" LCAs are generally carried out for given and thus fixed operating conditions of a typical process at environmental evaluation stage. Process design can be viewed as a multi objective problem in the context of cleaner production and can be tackled by several approaches and among others, multiobjective optimization methodologies and multiple criteria decision making techni ques (MCDM) [9]. A framework for optimal design of chemi cal processes with incorporation of environmental concerns based on LCA leading to a multiobjective optimization for mulation is proposed in [10]. Moreover, an MCDM based methodology can be used to evaluate different chemical pro cess routes under sustainability criteria in order to select one process [11].

The analysis of the dedicated literature shows that there is a need to incorporate Life Cycle thinking to produce chemi cals and utilities to find solutions for more efficient process ing and energy systems for the process industries. For this purpose, process modelling, simulation and optimization are particularly useful for design and systems engineering meth odologies as key elements to optimize existing and prospec tive processes. Using process modelling based on eco efficiency and economics can be viewed as a prerequisite for knowledge based decision making to enhance process sus tainability. This work is intended to reach some of these strategic objectives and will be targeted at the development of an integrated approach to take these elements into account.

In this perspective, a systematic, generic approach for sus tainability assessment and design selection is proposed through integrating economic and environmental indicators. It is based on a methodological framework for process eco design, coupling flowsheeting simulators both for production and energy processes with a life cycle assessment module that generalizes and automates the evaluation of the environ mental criteria. The system involves a “cradle to gate” bound ary and a compliant software framework to implement efficient Life Cycle Impact Assessment (LCIA) method and automate environmental impact analysis.

The interest of the methodology is twofold: first, several process variants can be evaluated in a systematic way by use of a process simulator for flowsheet generation. If the com putational time required for simulation is quite acceptable (from several seconds to several minutes for large size prob lems), the situation may be quite different when performing optimization where the various objectives must be evaluated many times by successive use of the process simulator. It must be emphasized that multiobjective optimization does not lead to a single ideal solution but to a set of compromise solutions. This reinforces the need of a good knowledge of the studied system by successive simulations of process options of interest to identify the key optimization variables that must be later encountered in a systematic multiobjective optimization task.

Second, the energy related emissions for any given pro cess that match exactly the real situation can be computed without introducing a bias in the estimation that may occur when using average values of emissions from environmental database.

The article is divided into several sections: a literature review following this introduction section delimits the scope of this work. Modelling/simulation techniques and life cycle assessment (LCA) tools are then to select in the Materials and Methods section the methodological framework that has been developed. The case study of Benzene production presents the sensitivity analysis that has been carried out to assess the behaviour of benzene production by hydrodealky lation (HDA) of toluene from an environmental and eco nomic viewpoint. The methodology is also applied to the biodiesel production process from waste vegetable oils (WVO).

LITERATURE REVIEW AND SCOPE OF THIS WORK

The chemical and petrochemical sector is by far the larg est industrial energy user, accounting for roughly 10% of total worldwide final energy demand and 7% of global greenhouse gases (GHG) emissions [12]. With a reduction of 96 million tons of carbon dioxide equivalents since 1990, the chemical industry alone has achieved nearly one third of the EU commitment under the Kyoto Protocol. Even if environ mental gains are substantial, the chemical industry is commit ted to contributing to the agreed EU target of reducing GHG by 20% by 2020, by further reducing its GHG intensity. So, further GHG abatement opportunities in its sites must be explored.

Only the earlier design stage of a chemical process will be investigated in this work under the following assump tions: (i) the system boundaries include all activities from extraction of raw materials and primary resources, the manufacturing process to the product leaving the factory gate (cradle to gate analysis); this assumption is sound since many products from the chemical industry are intermediates and serve multiple applications: cradle to gate boundaries are thus well fitted for subsequent value chain partners (for instance to supply environmental information on a business to business level, providing environmental data to customers for use in environmental product declarations); cradle to gate studies are also relevant for the comparison of functionally equivalent products. (ii) Only the case of normal operating conditions will be explored. The case of degraded conditions will not be considered. (iii) The case of fugitive emissions will not be considered even if they are among the major concerns of industrial process releases, since they cause problems to various aspects including the environment, health, and economic. We are aware that the early evaluation of process hazards is yet beneficial because process can be made inherently benign at lower cost.

Since the last decades, many tools and indicators for assessing and benchmarking environmental impacts of differ ent chemical production systems have been developed [13]. More generally, sustainability assessment of processes can be found in [14] based on a proposed metrics (the so called Sus tainability Evaluator) or in [15]. Nowadays, Life Cycle Assess ment (LCA) following [16] is an accepted environmental management tool to holistically and systematically quantify environmental burdens and their potential impacts over the whole life cycle of a product, process or activity [17]. So far, LCA has been applied mainly to products. LCA applied to processes has been introduced more recently. The main dif ference between process oriented and product oriented LCA is that rather than evaluating various products that can fulfil a defined function, various process configurations that can produce a defined product are evaluated. When LCA is applied to processes, functional units can be defined as the product from the system. Inventory analysis and impact assessment are then to be carried out for the system evalu ated. The objective consists to evaluate the environmental impact of a process configuration and its associated operat ing conditions. A consistent analysis would consider trans portation and materials involved in the manufacturing of the equipment items of the complete process. At preliminary design stage, these elements are not fully established and will not be considered in what follows. Table 1 presents some examples of eco efficient process design using the LCA methodology exploring the concept of sustainable chemical processes [27].

Several authors [6,28,29] updated regularly literature reviews about eco efficient process design combining simula tors with LCA. In recent years, it must be emphasized that sustainable process design using state of the art process sim ulators has emerged [30 32]. The analysis of the literature reveals that LCA and process simulation can be addressed in two ways, either embedding process description in an LCA tool or embedding LCA in process simulation. The former approach suffers yet from a lack of process models imple mented in current LCA tools while the latter needs to broaden the scope of the studied system. Following these guidelines, a methodology which is intended to design eco efficient processes has been developed in [33] and applied in [34,35], taking into account economic and environmental considerations to obtain an eco friendly and economically viable design. The methodology performed an environmental impact analysis considering not only the process but also its energy requirements by using process models implemented in the Ariane software tool developed by ProSim SA. Gener ally, average values can be found in environmental database concerning energy production, in particular vapour produc tion. The use of a dedicated simulator for utility production in a chemical facility is particularly interesting in the sense that the emissions can be computed from the effective condi tions used and the variation in vapour process conditions can thus be studied by simulation. There is also a specific interest to use such simulators since database and impact assessment are generally affected by incomplete or missing information, or approximate information that does not match

Table 1. Representative works on the application of LCA to process design.

Authors	Case study
(Kikuchi *et al.*, 2010) [18]	Biomass derived Polypropylene
(Othman *et al.*, 2010) [7]	Bio diesel production using alkali based catalyst
(Halim and Srinivasan, 2011) [19]	Benzene production by Hydrodealkylation of Toluene
(Brunet *et al.*, 2012) [20]	Biodiesel production
(Nucci *et al.*, 2014) [21]	Vegetable oil production
(van Boxtel *et al.*, 2015) [22]	Algae cultivation
(Yilmaz *et al.*, 2015) [23]	Iron casting production
(Bisinella de Faria *et al.*, 2015) [24]	Wastewater treatment
(Raman and Gnansounou, 2015) [25]	Bioethanol production
(Christoforou and Fokaides, 2016) [26]	Torrefaction process

exactly the real situation of the studied process so that a bias may be introduced in the environmental impact estimation. A process simulation tool dedicated to utility production, such as Ariane, ProSim SA turns out to be useful to fill envi ronmental database gap, by the design of specific energy sub modules, so that the energy related emissions for any given process can be computed. Despite the assets of the above mentioned work, some drawbacks can be yet highlighted: the methodology proposed in [33] is based on a gate to gate analysis and the used tools have been developed for a spe cific process, thus strongly affecting genericity.

A very interesting contribution is the work presented in [36,37] that deals with the development, implementation and application of the so called "process sustainability prediction (PSP)" framework with CAPE OPEN modules ready to be used in any process simulator which provides CO interfaces, that is intended to be used in the design stage of a chemical process, for selecting the best solution in terms of environ mental impact, among different design variants. It also encompasses a toxicological data estimation methodology, using molecular modelling techniques, and the implementa tion of a toxicological database. This current work aims at extending these concepts by proposing a generic "cradle to gate" approach and a compliant software framework to implement efficient Life Cycle Impact Assessment (LCIA) method and automate environmental impact analysis.

MATERIALS AND METHODS

Design of the Methodological Ecodesign Framework

Basically, the proposed approach for eco efficient process design consists of three main stages: tiers 1 and 2 correspond respectively to process inventory analysis and impact assess ment phases of LCA methodology for identification purpose of the involved chemical components. LCA is used here for partial inventory determination (the inventory phase will also be consolidated by the global simulation of the process) and for impact evaluation at production stage. LCA does not yet embody the whole lifecycle thinking (for instance the dis mantling of the process is not considered). Tier 3 is based on the interaction of the previous steps with process simula tion for environmental impact assessment and cost estimation through a computational framework. Figure 1 shows the interaction between the three stages.

The proposed approach starts with a reference case (i.e., fixed operating conditions) analysis of a given process to identify the chemical components and primary energy sour ces together with process inputs/outputs (dotted line in Fig ure 1). This reference design case serves as an initialization step for the process and energy simulators (stages 1 and 2). These global simulators (COCO, Prosim Plus, Aspen HYSYS, Aspen Plus, CHEMCAD, PRO II ...) have become standard tools to solve mass and energy balances, to calculate flow rates, compositions, temperature, pressure and physical properties for all streams circulating between unit operations [38 40]. The environmental impact evaluation can thus be performed from the calculations of mass flow rates of the process inputs and outputs and as well as from the energy requirements of the process. The framework developed in stage 3 can work with different simulators, since the only requirement is the availability of data through programming scripts for environmental impact assessment. These simula tors are widespread flowsheeting tools with different model ling approaches and interfaces: Aspen HYSYS and COCO have a COM interface whereas ProSim Plus has a program ming interface.

As in our previous work [33], the energy simulator Ariane of ProSim SA was used to compute primary energy require ments (primary resource extraction) and the corresponding environmental emissions and impacts of energy generation. The simulator also allows modelling conventional pollutant emissions such as Nitrogen oxides (NO_x), Sulfur oxides (SO_2), Carbon monoxide (CO), Carbon dioxide (CO_2) and Solid particles.

Concerning tier 1, the data set obtained from the refer ence case is used to perform Life Cycle Inventory (LCI), to identify inventory data of a given chemical process. This refers to the identification of the involved chemical compo nents and energy sources. The inventory data process con siders the components involved in raw material inputs and in waste/purge outputs of a given chemical process as well as the fuels used to produce the energy required for the pro cess and their related emissions.

Environmental Impact Assessment

A key element for the development of the approach is the design of an independent sub database considering the impact factors of all the elements that are reported in the LCI of the process under study. This sub database is extracted from the database considered for the environmental evalua tion of the process. This step only requires that process inventory data and environmental impact assessment results are available to extract the factors for the process under study. Then, in the second stage, the LCIA is implemented to identify the potential environmental impacts in all categories of a chosen impact assessment method. In this work, the SimaPro LCA software tool was selected to perform LCIA [41]. The approach could be reproduced for any other LCA tool i.e. GaBi Software, Umberto, openLCA. It must be yet highlighted that LCA software tools do not exhibit a friendly interface to directly use the embedded LCA models from inventory data. This explains why a preliminary use of LCA tool interface is required. In what follows, the IMPACT 2002+ assessment method is selected for the sake of illustra tion and the LCA process is carried out for the process under

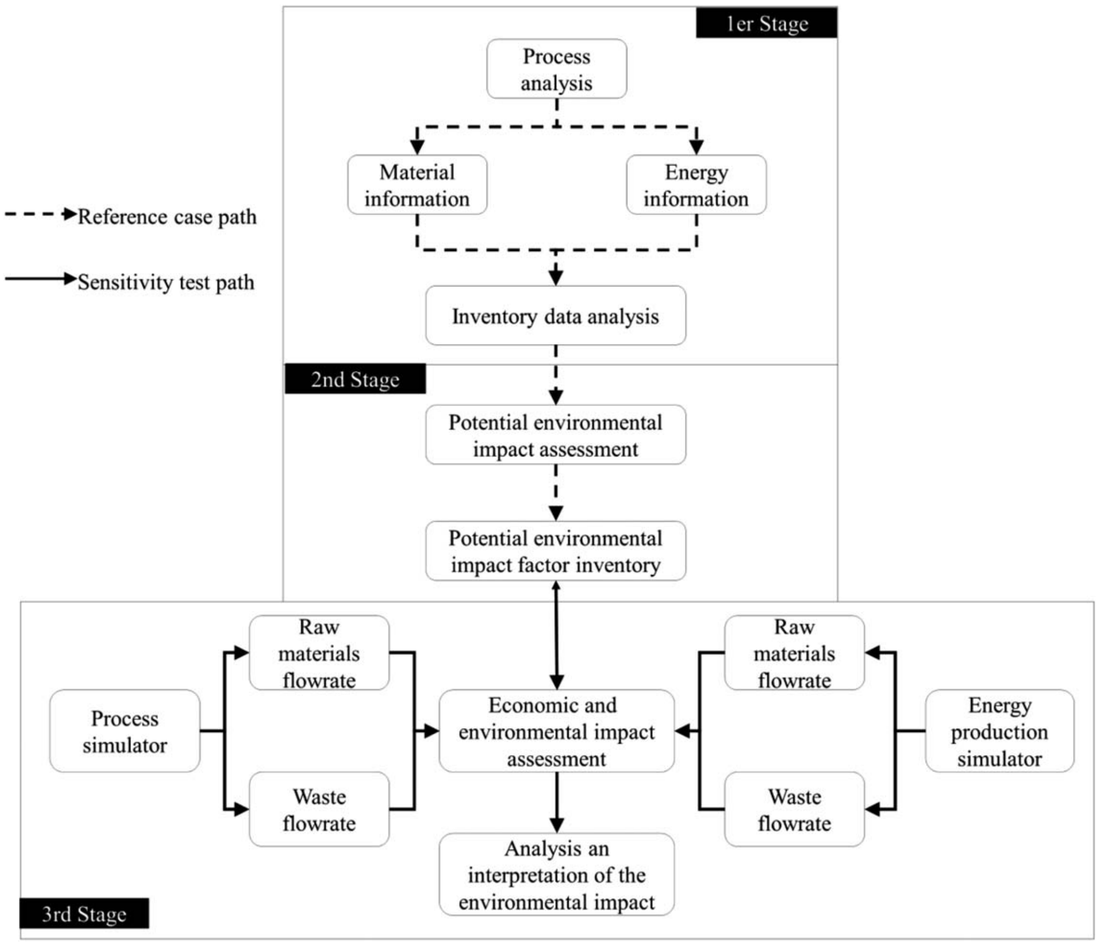

Figure 1. Overview of the proposed approach for eco efficient process design through the integration of the LCA and process simulation.

study. The environmental impacts are calculated using (1) [42]:

$$\text{Impact}_{j,k} \quad \text{Impact Factor}_{j,k} \times \text{Mass}_j \qquad (1)$$

After carrying out LCA, Mass_j and $\text{Impact}_{j,k}$ are known, and the impact factor is computed. The characterization factors of all components in the inventory data can thus be recovered. The damage and normalization factors of the IMPACT2002+ method are presented in [43].

Economic Assessment

Concerning the economic issue, the classical criteria that are reported in the literature involve [44] different types of cost (total cost, operational expenditure or OPEX, investment cost or capital expenditure i.e. CAPEX, etc.); profit or economic potential (a difference between the incomes and the costs); Net Present Value (NPV); other criteria (cumulative cash flow, monetary value added, investment and inventory opportunity costs, etc.); payback time and internal rate of return for instance constitute additional criteria that may be useful to be calculated to have a complete view of the economic assessment of the project without betting on the value of actualization rate and on the lifespan of the process respectively. NPV, profit, payback time, and internal rate of return can been introduced in the economic assessment.

Interconnection between All Components

The ecodesign approach is based on a framework that automates both the environmental impact assessment and the operating cost estimation of a given process. The framework performs the exchange and retrieval of data between the simulation models and the impact factor database. Figure 2 illustrates this data flow between all the components of the framework. Data flow is carried out through the following steps:

1. First, the user enters new values for the process operating variables concerning stream information or/and unit operations in process simulator;
2. A simulation run is performed and the energy requirement and mass flow rates from process inputs/outputs are computed. Concerning steps 1 and 2, sensitivity tests are necessary to detect the significant variables of the process and find their threshold limits. Then, scripting allows configuring the flowsheet with the new values of the variable set.
3. The next step is to transfer energy requirement to energy plant simulator to estimate the emissions from energy production;
4. The characterization, damage and normalized factors are retrieved from the environmental impact database;
5. Finally, environmental impact assessment and cost estimation are carried out and the evaluation criteria are computed.

The main objective of the framework is to link the software tools to analyse the environmental impact and estimate the operating cost of a given process with its associated energy plant. To achieve the objective, it is necessary to use the interoperability feature of process simulators and impact factor database. Figure 3 shows the overall possible architec tures of the framework. The first architecture takes advantage of the programming interface embedded in simulators. Because the approach requires COM interface to link the tools, a programming language interface must support this interface. The second architecture exploits the COM interface that all the software tools involved in the approach have. In this architecture, the framework can be programmed in any language exhibiting a COM feature. Data exchange between the process simulator and the energy simulator is a corner stone of the framework. Figure 4 illustrates data exchange via COM interface.

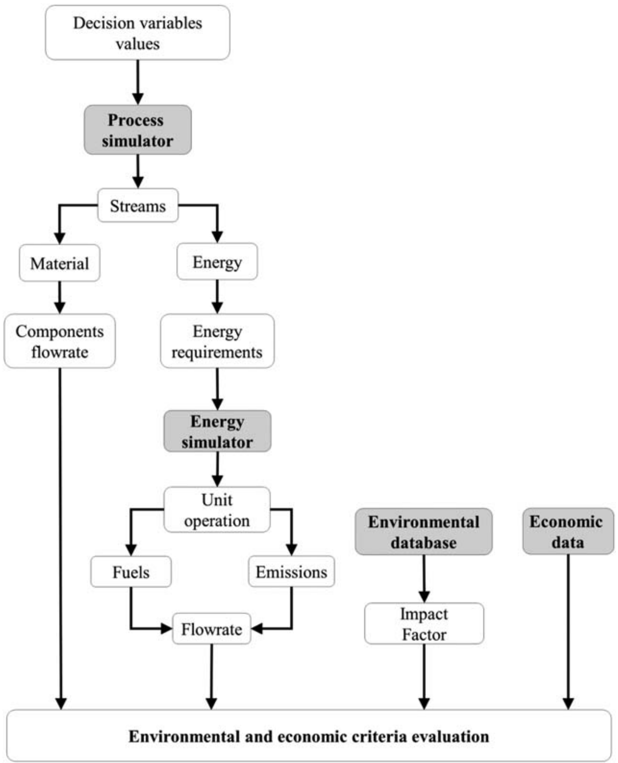

Figure 2. Exchange and retrieval of data between the simu lation models and impact factor database for eco efficient process design.

CASE STUDY: BENZENE PRODUCTION BY HDA PROCESS

HDA process has been studied intensively both in educa tion and research to illustrate fundamental issues in process systems engineering such as process synthesis and energy integration, as well as in integrating design and control [45,46]. This test case was selected since its use is not affected by a lack of process data. Several authors have also used this example to illustrate the potential of their method ology combining Aspen Plus simulator with numerical meth ods to solve multiobjective optimization problem involving environmental impact and profit (see for instance [47]). The PRO/II simulator was also used by [48] to assess different design alternatives of a HDA plant considering the potential environmental impacts and economics. Our objective is not to demonstrate that the case base proposed by Douglas [1] is not satisfactory and could be largely performed from an implementation viewpoint but to show the potential of improvement that can be gained if the hierarchical design strategy initially proposed is extended to take into account environmental assessment. We are also aware that several authors have addressed this case study with environmental issues.

The comparison is not straightforward with other works that address the environmental evaluation of HDA for instance [10] since on the one hand, the structure of the stud ied process is not exactly the same and the impact assess ment method selected is also different on the other hand. The same comment is also valid for the work of [49]. In that case, the indicators used are those of the WAR algorithm and the computation principle is not identical as the process used in Impact 2002+. The hydrodealkylation (HDA) of tolu ene to produce benzene must be viewed here as a bench mark for demonstrating the usefulness of the methodology for ecodesign of chemical processes.

There are different benzene production routes [50] includ ing catalytic reforming, steam cracking and hydrodealkyla tion of toluene. This well known benchmark problem for process design and synthesis studies, was extensively studied [1,51].

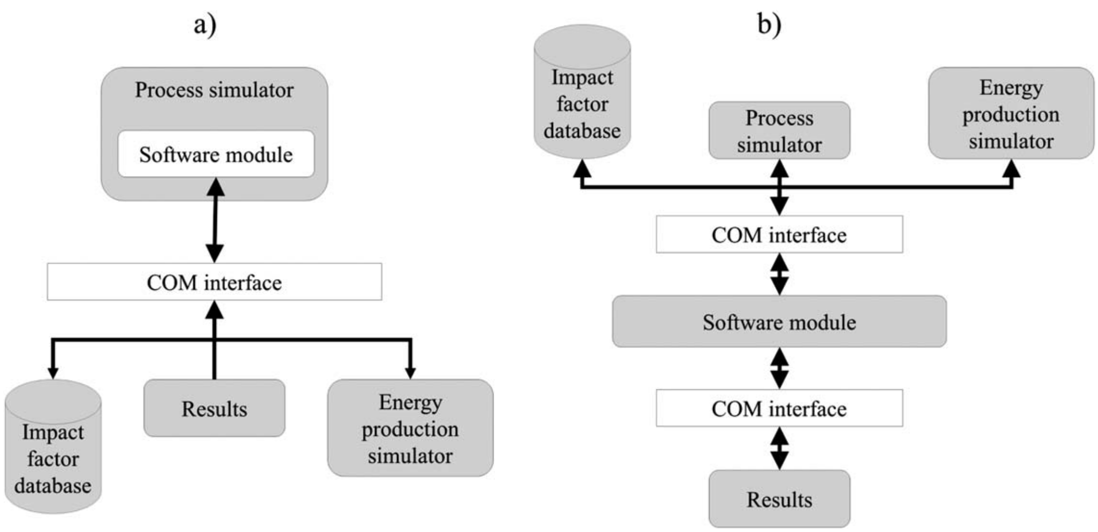

Figure 3. Possible framework architectures: (a) embedded in process simulator with a programming interface and (b) with an independent platform with a COM interface.

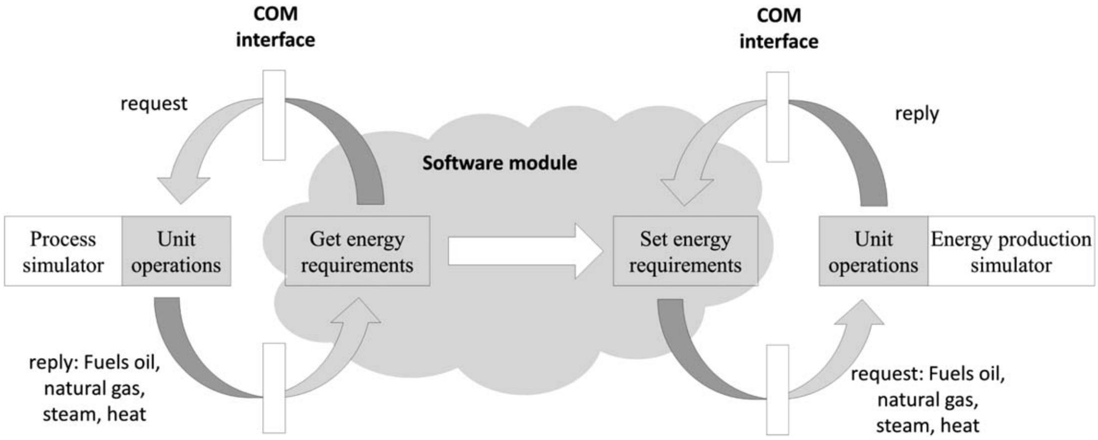

Figure 4. The cornerstone of the proposed framework: data exchange between process and energy simulators via COM interface.

The HDA process involves two reactions, the conversion of toluene to benzene according to:

$$C_7H_8 + H_2 \rightarrow C_6H_6 + CH_4 \quad (2)$$

In addition to this desired reaction, an undesired reaction occurs:

$$2C_6H_6 \leftrightarrow C_{12}H_{10} + H_2 \quad (3)$$

C_7H_8: Toluene, H_2: Hydrogen, C_6H_6: Benzene, CH_4: Methane $C_{12}H_{10}$: Biphenyl

The HDA process is composed of three main steps: (i) reactions between toluene and hydrogen. Two chemical reactions are involved (3) and (4). Reaction kinetics are given as functions of partial pressures of gaseous compo nents. These reactions take place in an adiabatic reactor. (ii) Liquid and steam separation phases. This step involves a two phase separator (flash at a pressure 32 bar) where non condensable gases (methane and hydrogen) are separated from the liquid mixture. Another separation unit (flash at 10 bar) eliminates traces of hydrogen and methane for further separation. A distillation column is used to recover benzene while a second one allows recovery through recycling tolu ene. (iii) Methane purge.

Process energy requirements for the HDA process involve steam for the distillation columns, flashes at high and low pressures and electricity for pumps and compressors. In addition, water is needed to cool effluents leaving the reac tor. As discussed in introduction section, the energy produc tion can be viewed as a separate process, which is generally shared among the various production units. Figure 5 shows the HDA process coupled with an energy production plant and the system boundaries.

The operating conditions of the HDA process are the same as in [1,33,34]. They are specified via the involved streams and the unit operations interface.

HDA Process Simulation

The flowsheets are built within the environment of COCO, ProSim Plus, and Aspen HYSYS process simulators where unit operation blocks, including splitters, separators and reactors are used as building blocks to track the material and energy streams through the complete process. Material and energy balances are computed around each unit and the system state variables are calculated, including component flows and system thermodynamic properties like enthalpy and entropy. The flowsheet design exhibits minor changes with each simulator because of the dedicated interface for unit operations. A good agreement is observed for the results obtained with the three tools for this process under the stud ied operating conditions.

Energy Production Modelling and Emission Computation from Both Process and Energy Production

Ariane simulator can be used to model different routes for energy production. For instance, a gas turbine satisfies the energy requirements of HDA process (steam). Gas turbines equipped with a heat recovery steam generator (HRSG) are widely used in the chemical process industry to satisfy their energy requirements [52]. For the evaluation of the emissions produced by a gas turbine process, the simulation model requires to be calibrated in an iterative process where the following emission factors for both fuels were found. For this purpose, two sets of operating conditions from literature data [53] and experimental outputs were used. Four different configurations were tested with two pressure levels (i.e., 3.4 or 9.3 bar) and fed either with natural gas or fuel oil. It is impossible to strictly reproduce the literature conditions of the steam production process proposed however they have been adapted as much as possible. The model is yet config ured for the two aforementioned pressure values and the parameters shown in Table 2 (pressure, fuel amount, air excess percentage, and fuel).

The major energy related air emissions include CO_2, SO_2, CO, and NO_x. The amount of each kind of emission gener ated is estimated as a linear function of the amount of a given fuel. The simulations results are then compared with the emissions from steam production reported in [53] and also with the emissions from steam production called "Steam, for chemical processes, at plant/RER S" in EcoInvent data base. The identification process shows that a same set of emission factors leads to a good agreement between the pre dicted and experimental results for a given fuel. A larger dis crepancy is observed with the value obtained from EcoInvent data from the average steam production of 11 European chemical sites.

Models have been developed in Ariane to represent first a burner for hydrogen and methane at purge output and second a furnace used to heat the feed at reactor inlet. They are mod elled as furnaces with a dual fuel mixture. Furnace modelling must be calibrated to reproduce emissions of CO_2, CO, NO_x, and SO_2 that can be observed. To accomplish this, a

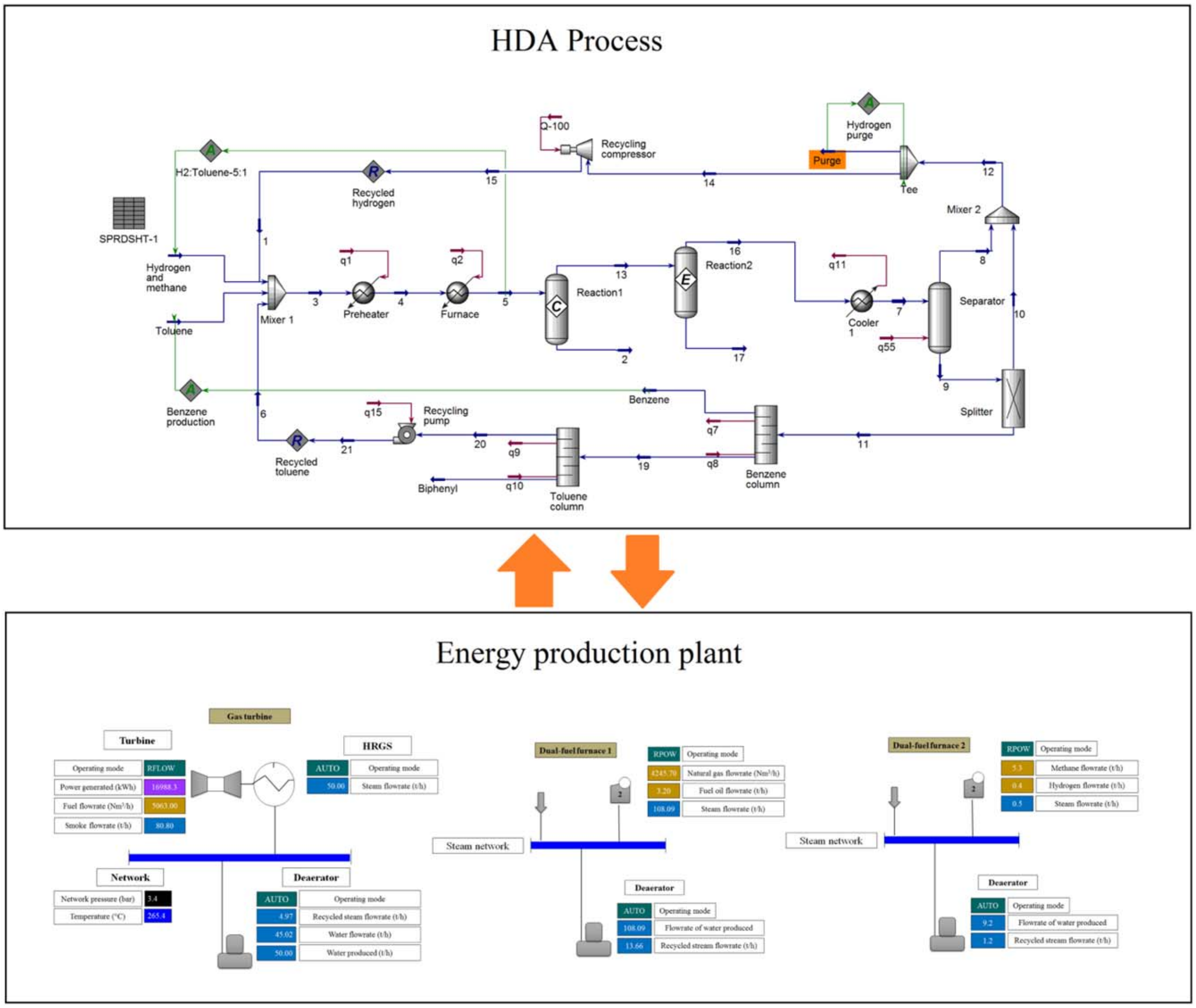

Figure 5. HDA process coupled to an energy production plant and work boundaries.

Table 2. Key parameter specification of the gas turbine in energy simulator.

	Configuration 1	Configuration 2	Configuration 3	Configuration 4
Combustion pressure	3.4 bar	9.3 bar	3.4 bar	9.3 bar
Fuel	Natural gas	Natural gas	Fuel oil	Fuel oil
Air excess	25%	25%	22%	22%
Cogeneration	No	No	No	No
Amount	0.04245 Nm^3	0.03912 Nm^3	0.032 kg	0.03 kg

combination of two sets of operating conditions from literature [53] and their corresponding experimental measurements are taken into account. Each set has a production 1 MJ of steam. The model is configured to operate at a pressure of 9.3 bar and the furnace is fed by natural gas and fuel oil with 25% excess air. The amount of natural gas used is 0.042 Nm^3 and a quantity of 0032 kg fuel oil is used. These are equivalent to those proposed in literature data. Calibration is performed in the same way as with the bi fuel furnace (iterative process). The emission factor of nitrogen oxides is 8714.6 mg Nm ^{3} for natural gas and 2809.3 mg ton ^{1} for fuel oil. Finally, the emission results obtained are shown in Table 3 along with the data found in literature to make a comparison and validate the model of the bi fuel furnace.

Economic Assessment

In this case study, only the operating cost has been considered as an economic criterion and will be discussed. The consideration of this kind of cost criterion (instead of net present value for instance) is consistent here since the treated example only involves design variants based on different operating conditions and not on various design configurations. The contribution of the operating cost considered comprises the use of raw materials and the use of required energy by the given process:

$$\textit{Operating Cost} = \sum_{i=1}^{n} (\textit{Unit Cost}_i) x (\textit{amount of raw material})_i + \sum_{i=1}^{m} (\textit{Unit Cost}_i) x (\textit{amount of energy source})_i \quad (4)$$

The operating cost as described in Eq. 2 has been selected for simplicity purpose as it is usually the case at earlier design stage and cannot be considered as a precise estima tion cost as highlighted in [1,50]. Of course, it could be improved at further steps of the process development as the knowledge of the process increases, so that it can be more sensitive to design variants based on different operating con ditions (waste treatment and/or disposal costs, operating labour . . .).

Inventory Data (Tier 1)

The main objective at this first stage of the proposed approach is to identify the inventory data of a given chemical process, e.g. HDA process and its associated energy require ments. Figure 5 indicates that the process has two inputs, on the one hand toluene and a mixture of hydrogen and methane on the other hand. Within the boundaries of the process, the three outputs concern the purge (H_2 and CH_4), the desired product output (benzene) and the by product output (biphe nyl). Because the purge is directed to combustion step, this one was included into the frontier of the studied domain. Ben zene, which is the interest product, was not included in the inventory phase since its impact related to utilization phase will be considered in the further steps of the value chain. The by product, i.e. biphenyl is assumed to be valorised and reused for the formulation of dye carriers for textile dyeing, as an intermediate for polychlorinated biphenyls [54] and as an impregnate paper for citrus fruit where it acts as a fungicide [55]. So, the same assumption as for benzene is adopted.

For energy requirements, the following assumptions are considered: (i) process energy requirement is provided by a gas; (ii) the turbine operates with natural gas; (iii) the fur nace used for heating the mixture of components before entering the reactor operates with a mixture of fuel oil and natural gas; (iv) the burner used for burning hydrogen and methane from the purge stream operates with a mixture of components. This assumption includes the fact that the fuels are recovered in the process to partially satisfy the energy requirements of the process. The inventory data flow obtained from simulations was compared with the flow obtained in [33] under the conditions proposed by [1]. The slight differences can be explained by the fact that [33] uses a simplified model for the simulation of HDA process.

Table 3. Comparison of emissions from two steam produc tions (gate to gate emissions).

	Unit	Ariane model	
Carbon dioxide	Kg	0.182	0.183
Carbon monoxide	Kg	2.01E 3	
Nitrogen oxides	Kg	4.6E 4	4.599E 4
Sulfur dioxide	Kg	1.9E 4	1.99E 4

Identification of Potential Factors (Tier 2)

Table 4 summarizes the inventory data and shows the selected items to represent the inventory data of the HDA process. The characterization factors are obtained by (1) from the characterization results provided by SimaPro. The characterization factors, for mid point evaluation are relative to raw materials, fuels and emissions subcategories. Finally, damage and normalization factors extracted from [43] are used to evaluate the final damage. The identified impact fac tors are stored in a database for further stage of the ecode sign framework.

Integration of All Components (Tier 3)

Figures 6 and 7 show the normalized results of main mid point categories and damage categories (end points) respec tively to compare the environmental impact in all categories. Not surprisingly, it can be observed that the results of the three process simulations are very similar, since the mass and energy balances carried out by the three simulators lead to minor differences. It must be emphasized that the three sim ulators are used to demonstrate that the proposed approach is generic enough to be implemented whatever the simulator used. The results show the contribution of the raw materials and the production of the energy requirements of the pro cess. Energy production contributes to all end point catego ries and to the main mid point categories.

Figure 8 shows a detailed analysis of the mid point cate gories, with the individual contributions of all LCI compo nents. The graphs indicate that the elements of the analysis contribute in different proportions in each category, for example, toluene is the main contributor to the environmen tal impact in the non renewable energy and respiratory organics categories whereas fuel oil is the main contributor in terrestrial and aquatic ecotoxicity, respiratory organics, ionizing radiation, and ozone layer depletion categories. This reveals that a large amount of grey energy *is* involved, the energy hidden in a product, i.e. the amount of energy required to extract that product, i.e., toluene.

Figure 9 shows a more detailed analysis of the terrestrial ecotoxicity and ozone layer depletion categories. In both cat egories, there is a low contribution from the direct emissions of the process and from the raw materials. In contrast, fuels contribute significantly, specifically fuel oil burned in the

Table 4. Inventory data and selected items in the LCA model.

Category	Sub category	Inventory data	Database elements names	Unit
Process	Raw materials	Hydrogen	Hydrogen (reformer)	kg
		Methane	Methane, 96 vol % from synthetic gas, wood, at plant/CH S	m^3
		Toluene	Toluene, liquid, at plant/RER S	kg
Energy	Fuels	Fuel oil	Fuel oil lows 2000 boiler 100 kW U [1]	MJ
		Natural gas	Heat, natural gas, at industrial furnace >100kW/RER S	MJ
	Emissions	Carbon dioxide	Carbon dioxide	kg
		Sulfur dioxide	Sulfur dioxide	kg
		Nitrogen oxides	Nitrogen oxides	kg
		Carbon monoxide	Carbon monoxide	kg

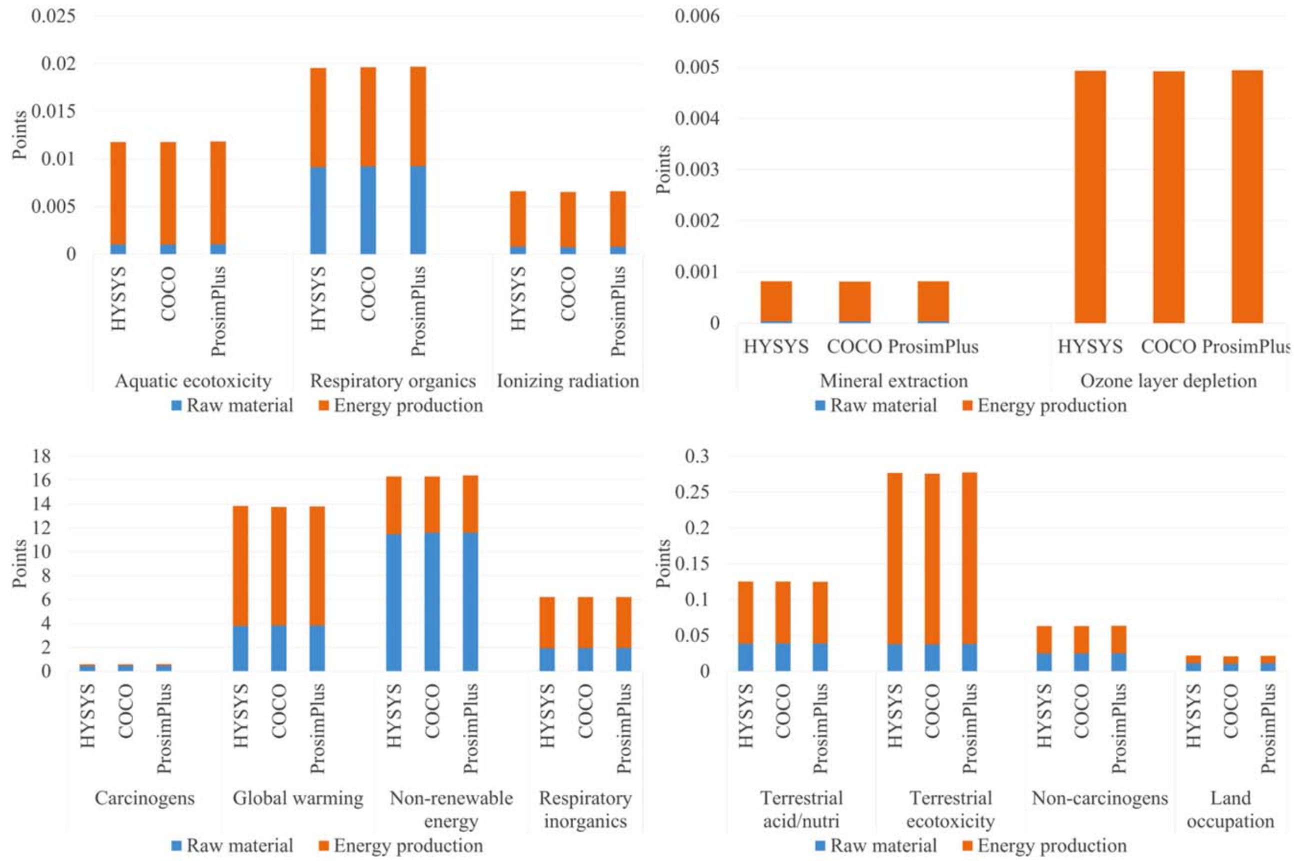

Figure 6. Contribution to mid point categories of the raw materials and the production of the energy requirements of the pro cess (normalization).

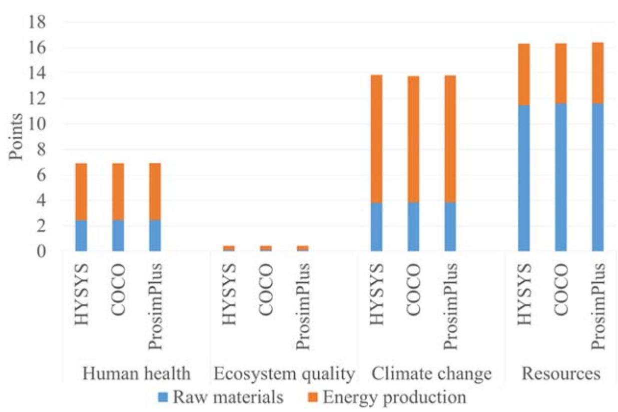

Figure 7. Contribution to end point categories of the raw materials and the production of the energy requirements of the process (normalization).

process furnace, since the impact factor of fuel oil is signifi cantly higher than the impact factor of natural gas. Here, the energetic ratio involved in the calculation of the proportion of fuels used in the furnace process plays a significant role because it allows minimizing the environmental impact by reducing fuel oil utilization.

Figure 10 shows the detailed contribution in end point categories. As for mid point, fuels and raw materials (mainly toluene) are the main contributors to the environmental impact. Carbon dioxide emission, from the furnace with hydrogen and methane as fuels, has a negative scale since the energy produced by the furnace is subtracted from the energy requirements of the process.

Sensitivity Analysis through the Framework

A systematic sensitivity analysis has been performed through the framework and the more significant variables on both economic and environmental viewpoints [1,33 35] have been identified: (i) the conversion rate of toluene in reactor (C_{rate}): lower conversion gives in general better selectivity, but higher costs of recycling. Higher conversion gives more by products and impurities, increasing the cost of separation; (ii) hydrogen flow rate to purge output (F_{H2}): hydrogen is a reactant for the first reaction and a product for the second reaction. In the methane purge, a portion of hydrogen is lost; (iii) Energetic ratio (R_{Fuel}) that represents the ratio fuel flow rate/gas flow rate at the furnace.

Several values of the significant variables are used based in operating conditions of HDA process proposed in [1] as a reference case. It is important to emphasize that the maxi mum and minimum values for the simulation convergence are considered to determine sensitivity analysis values. Table 5 shows the set of values studied for sensitivity analysis. A preliminary study has shown that these variables have a con siderable influence and even an antagonist one on the crite ria that are investigated. According to inventory data flow and environmental impact analysis, the three simulators (HYSYS, COCO, and ProSim) lead to very related results. For the sake of illustration, HYSYS simulator was finally chosen to carry out the sensitivity analysis of HDA process.

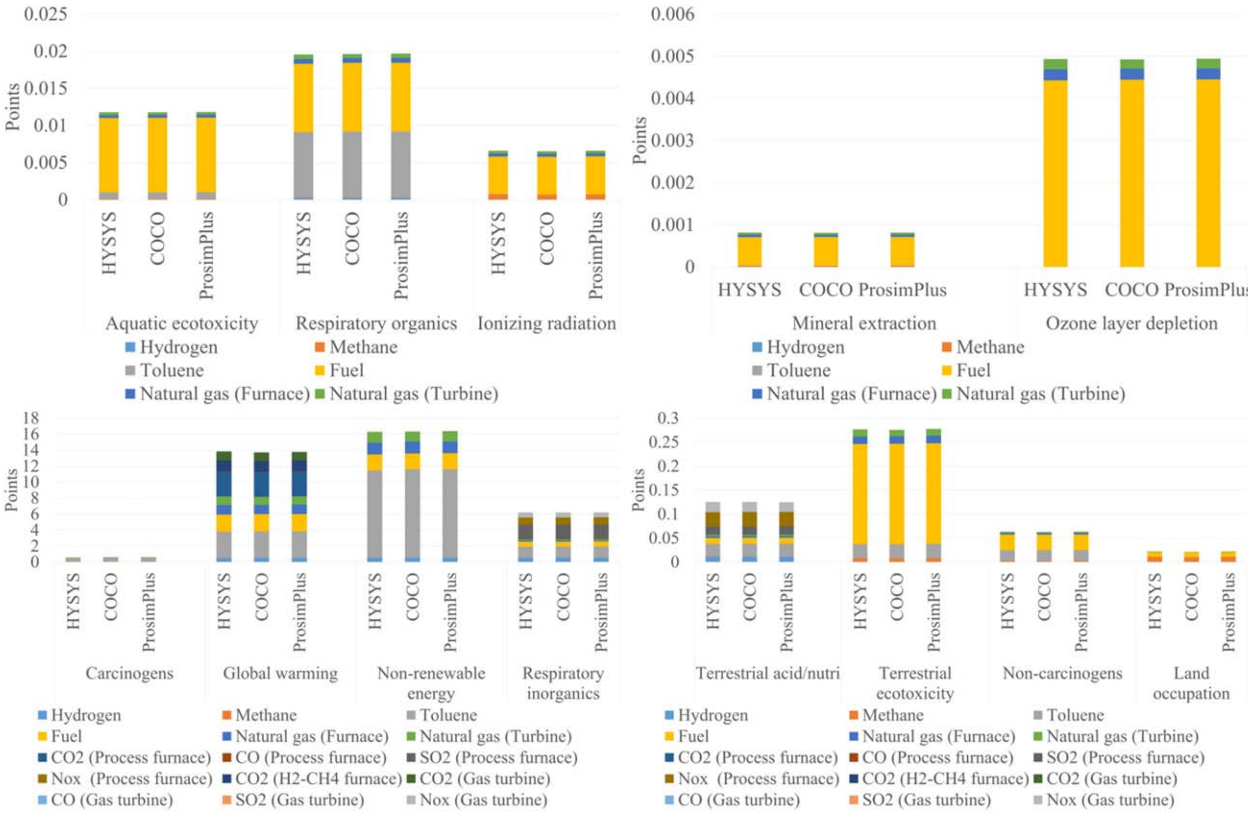

Figure 8. Analysis of the individual impact of the LCI elements in mid point categories.

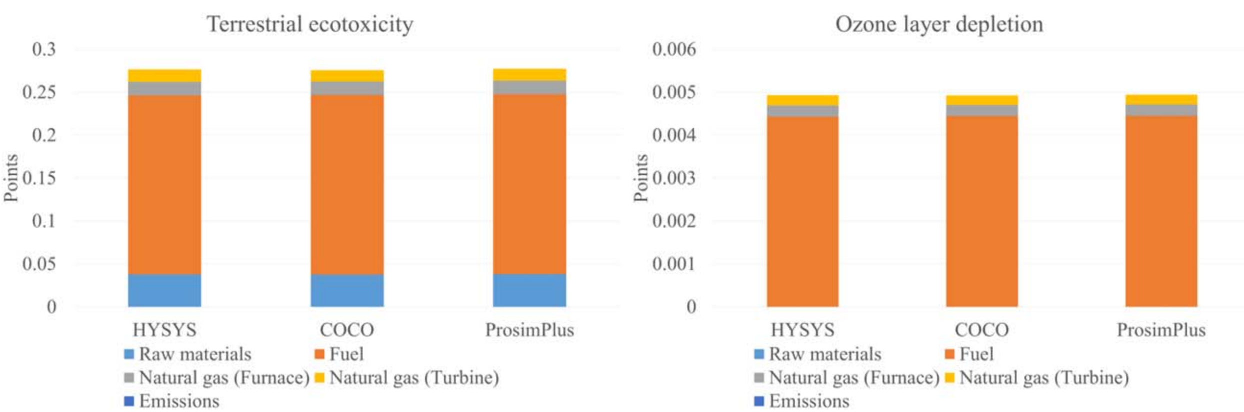

Figure 9. A detailed analysis of the LCI elements contribution in the terrestrial ecotoxicity and ozone layer depletion categories.

Comparison of Process Alternatives in the Midpoint and End Point Categories

Table 6 shows the results obtained for all the tested process options. Not surprisingly, the flowrates of raw materials are very sensitive to F_{H2}, since an increase in the purged hydrogen flowrate leads to an increase in the amount of raw material to satisfy production requirements. The most important variations are observed when varying the energetic ratio at the furnace process, thus leading to a large discrepancy in the associated combustion emissions. All these variations affect the calculation of the cost and environmental impact assessment. Regarding the cost, it fluctuates in all processes based on process and energy variables (C_{rate}, F_{H2}, and R_{Fuel}).

The cost reduction is most significant when the conversion rate in the reactor increases while the other two variables are fixed (Processes proposed by Douglas [1,3,4]).

The results of the environmental impact assessment (mid point and end point categories) and the cost calculation for each configuration are shown in Figures 11 and 12 using radar charts. To facilitate the comparison, a normalization step was performed by assigning the value 1 to the maximum value of each category. The computed relative impacts represent the ratio between the environmental impact and this maximum value.

In both mid point and end point categories (Figures 11 and 12), an antagonism between the environmental and

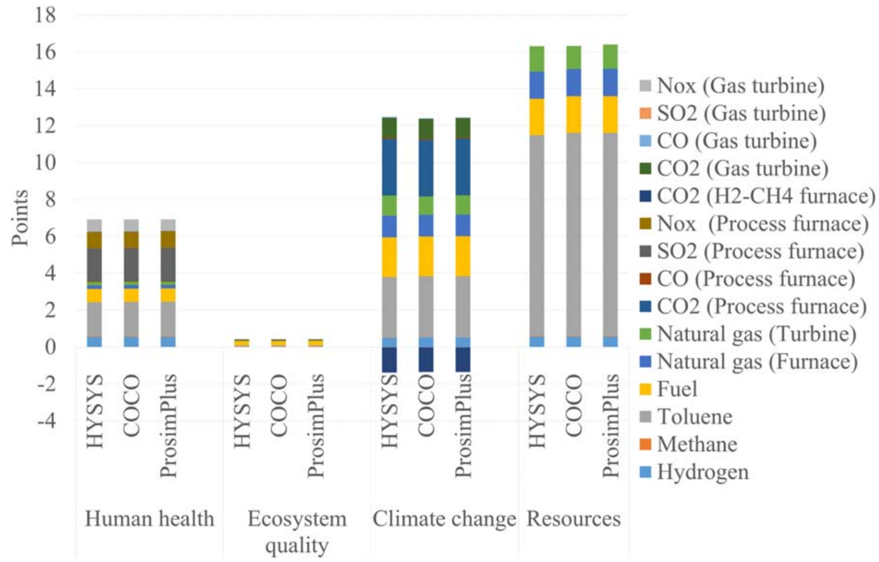

Figure 10. A detailed analysis of the LCI elements contribution in end point categories.

Table 5. Set of values for the sensitivity analysis.

Scenario	R_{Fuel} (%)	C_{rate} (%)	F_{H2} (kmol h ^{1})
Douglas	0.5	0.75	198
1	0.3	0.75	198
2	0.7	0.75	198
3	0.5	0.60	198
4	0.5	0.90	198
5	0.5	0.75	150
6	0.5	0.75	250

economic criteria is observed, which means that the best economic option is not always the best environmentally friendly option and conversely. For example, alternative 2 is the worst from an environmental viewpoint but exhibits a mitigated cost with respect to the other alternatives. As far as alternative 3 is concerned, its highest cost is not associated with the highest environmental impact.

The process proposed by [1] is used as a reference to calculate the gain in the midpoint categories. As reported in Table 7, a positive value represents an improvement in the environmental impact and cost. Conversely, a negative value means that a worse impact. The gain shows the variation in the cost and the mid point categories, some alternatives improve the cost but worsen the environmental impact and vice versa. Only process alternative 4 improves both the cost and environmental impact in relation to the process used by Douglas [1].

Figures 13 and 14 show a classification of the process alternatives according to the variables conversion rate (C_{rate}), hydrogen flowrate (F_{H2}), and energetic ratio (R_{Fuel}) both for mid and end point categories. All the processes are compared with the reference case. It is noteworthy that the increase in the percentage of energetic ratio causes a discrepancy between the environmental impact categories whereas the cost remains apparently unchanged. The process uses the same amount of raw materials and has the same vapour requirements; yet, the ratio of the fuels used in the furnace changes, which leads to different environmental impacts; in addition, natural gas and fuel oil are not so expensive compared to raw materials for the set of economic data considered.

For mid point categories, ozone layer depletion on the one hand and terrestrial and aquatic ecotoxicity on the other hand exhibit the largest variation range among the other criteria.

Environmental Impact Analysis of a Specific Process

Figures 15 17 show the individual analysis of the environmental impact of process alternative 4. Figure 15 shows the contribution to environmental impact according to all subcategories of inventory data as described in previous sections. Ozone layer depletion category is exclusively constituted by fuel requirements. Global warming is equally affected by raw materials, fuels and emissions while raw materials correspond to 80% of carcinogens. Figure 16 shows not surprisingly that the use of fossil fuels contributes to the environmental impact in each of the categories analysed. It must be also pointed out that aquatic ecotoxicity, mineral extraction, ozone layer depletion and terrestrial ecotoxicity categories are exclusively penalized by fuel oil. This confirms the influence of the fuel ratio variable in the HDA process environmental impact.

Figure 17 shows end point categories; here toluene (raw material) is present significantly in resources, human health and climate change categories. Data in Table 6 show that the toluene flow variation is very low between the 7 process alternatives, so that the variation in the categories is mainly attributed to natural gas and fuel through the fuel ratio variable.

CASE STUDY: BIODIESEL PRODUCTION FROM WASTE COOKING OIL

The motivation for development and use of alternative fuels is related to the decreasing stock of readily recoverable oil, the concern about global climate change, the increase in fuel prices and the desire of energy independence. Alternative energy sources and fuels are being developed to make up energy deficit. In this context, producing biodiesel can be a very promising solution to overcome the difficulties linked to the energy crisis. Several processes exist in the literature to produce biodiesel. Among the several routes to transform oil in biodiesel such as pyrolysis or micro emulsion, the transesterification reaction process is the most common method to obtain biodiesel as reported in several works either based on experimental studies [56 58], as on numerical simulation biodiesel production processes [59]. It has been emphasized that lignocellulosic biomass and waste

Table 6. Results of the studied processes.

	Scenario						
	Douglas	**1**	**2**	**3**	**4**	**5**	**6**
Variables							
C_{rate} (%)	0.75	0.75	0.75	0.6	0.9	0.75	0.75
F_{H2} (kmol/h)	198	198	198	198	198	150	250
R_{Fuel} (%)	0.5	0.3	0.7	0.5	0.5	0.5	0.5
Raw materials							
Hydrogen (kg h ^{1})	949.71	949.71	949.71	947.21	952.34	852.57	1055.27
Methane (kg h ^{1})	397.77	397.77	397.77	396.72	398.87	357.08	441.98
Toluene (kg h ^{1})	25625.24	25625.24	25625.24	25309.01	25881.41	25565.42	25642.15
Purge							
Hydrogen (kg h ^{1})	399.14	399.14	399.14	399.16	398.99	302.38	504
Methane (kg h ^{1})	4997.69	4997.69	4997.69	4615.21	5016.49	4622.32	5002.68
Energy							
Steam (ton h ^{1})	53.78	53.78	53.78	63.2	46.8	56.2	51.5
Fuel Furnace (ton h ^{1})	5.86	4.16	9.70	7.09	4.81	6.58	5.19
Natural gas Furnace (Nm^3 h ^{1})	6236.6	10315.36	4420.87	7544.95	5117.60	6996.76	5523.73
Natural gas Turbine (Nm^3 h ^{1})	5827.14	5827.14	5827.14	7224.23	5187.57	6373.59	5771.76
Electricity (kW)	385.37	385.37	385.37	504.52	296.6	449.71	331.72
Water (Ton)	7918	7918	7918	9596	6649	8795	7191
Emissions							
Process furnace							
CO_2 (ton h ^{1})	30.47	32.83	39.2	36.86	25	34.2	26.98
CO (kg h ^{1})	311.6	445.2	291.2	377	255.7	349.7	276
SO_2 (kg h ^{1})	234.2	166.4	387.7	283.4	192.3	263	207.5
NO_X (kg h ^{1})	70.8	101.6	65.8	85.7	58.1	79.5	62.7
H_2/CH_4 furnace							
CO_2 (ton h ^{1})	13.72	13.72	13.72	12.67	13.77	12.7	13.75
Gas turbine							
CO_2 (ton h ^{1})	11.09	11.09	11.09	13.72	9.87	12.13	10.98
CO (kg h ^{1})	221.8	221.8	221.8	274.3	197.5	242.6	219.7
SO_2 (kg h ^{1})	0.1	0.1	0.1	0.1	0.1	0.1	0.1
NO_X (kg h ^{1})	50.8	50.8	50.8	62.65	45.2	55.5	50.3
Cost ($)	144,636.47	143,066.75	140,591.06	167,390.77	121,799.57	154,818.51	130,320.16

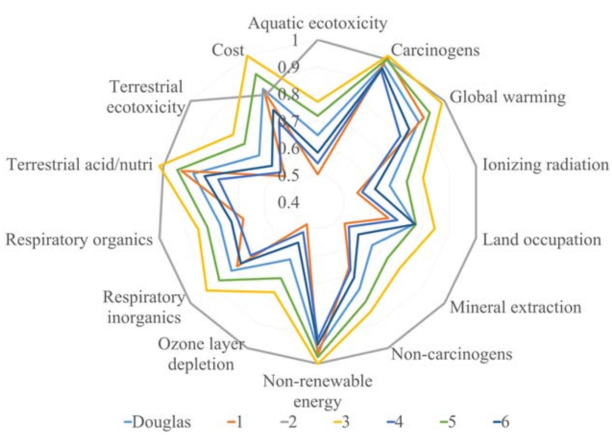

Figure 11. Comparison of the environmental and economic criteria results to show the antagonism between them (mid point categories).

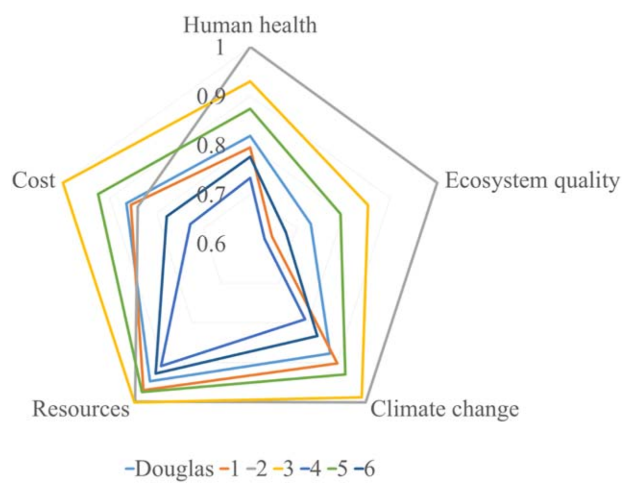

Figure 12. Comparison of the environmental and economic criteria results to show the antagonism between them (end point categories).

vegetable oils seem to be good candidates as feedstock for the production of biodiesel [60 62]. Biodiesel production by acid catalysed process is analysed here as another illustration of the whole methodological framework presented in this work. Contrary to the alkali catalysed process, the main advantage of the acid catalysed over the alkali catalysed pathways is that there is no need to pre treat the oil because the reaction is less sensitive to the free fatty acid's content of the feedstock [63]. In this process, methanol and sulfuric acid (used as a catalyser) feed the transesterification reactor with a stream of pre heated oil. The excess of methanol is then removed from the biodiesel in a distillation column and

Table 7. Increase or decrease cost and environmental impact of IMPACT 2002+ categories.

	Scenario					
	1	2	3	4	5	6
	Gain (%)					
Aquatic acidification	10.61	35.21	15.97	*12.82*	8.53	7.19
Aquatic ecotoxicity	22.38	54.51	19.24	*16.06*	10.99	9.96
Aquatic eutrophication	4.92	19.49	9.40	*7.40*	4.89	4.03
Carcinogens	2.88	2.23	3.63	*2.48*	2.15	1.59
Global warming	2.85	14.06	12.55	*9.83*	6.03	5.02
Ionizing radiation	18.33	48.48	18.76	*15.41*	9.52	8.22
Land occupation	13.06	30.36	10.04	*8.44*	0.64	0.29
Mineral extraction	19.63	52.17	20.29	*16.66*	11.22	9.89
Noncarcinogens	11.68	32.20	12.53	*10.24*	6.87	6.02
Nonrenewable energy	2.34	5.38	5.65	*4.05*	2.86	2.06
Ozone layer depletion	22.70	57.31	21.17	*17.55*	12.10	10.86
Respiratory inorganics	3.32	23.83	14.53	*11.23*	7.11	5.51
Respiratory organics	11.52	29.86	10.77	*8.90*	6.19	5.56
Terrestrial acid/nutri	5.18	13.05	14.78	*10.86*	6.93	4.83
Terrestrial ecotoxicity	18.22	47.74	18.19	*14.98*	10.10	8.95
COST	1.09	2.80	15.73	*15.79*	7.04	9.90

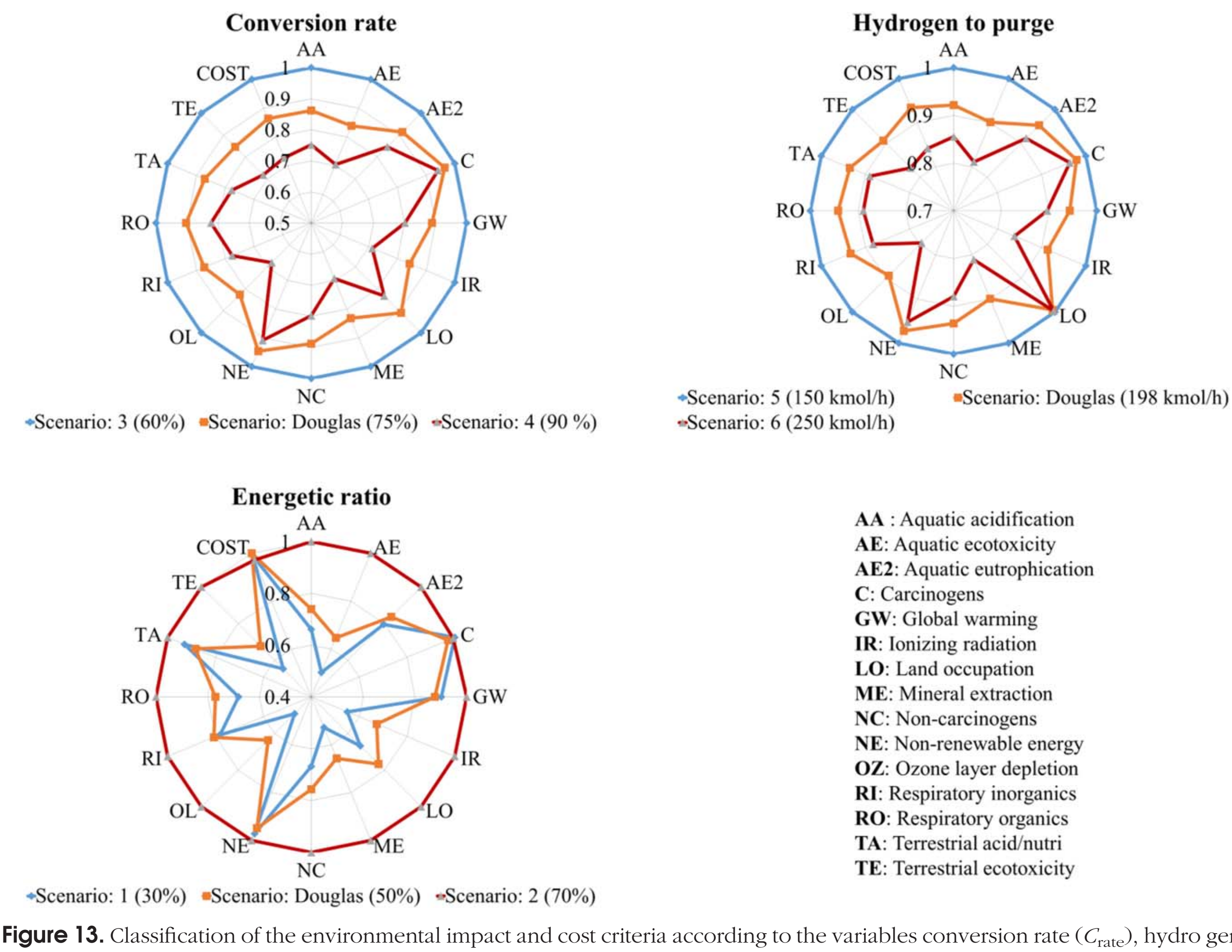

Figure 13. Classification of the environmental impact and cost criteria according to the variables conversion rate (C_{rate}), hydro gen flowrate (F_{H2}), and energetic ratio (R_{Fuel}) (mid points).

recycled back to the transesterification reactor. The introduc tion of calcium oxide [63] in a neutralization reactor leads to remove sulfuric acid from the transesterification products.

The conditions and parameters used to model the biodiesel process using waste cooking oil with HYSYS software are briefly discussed. Vegetable oil is a mixture of triglycerides of

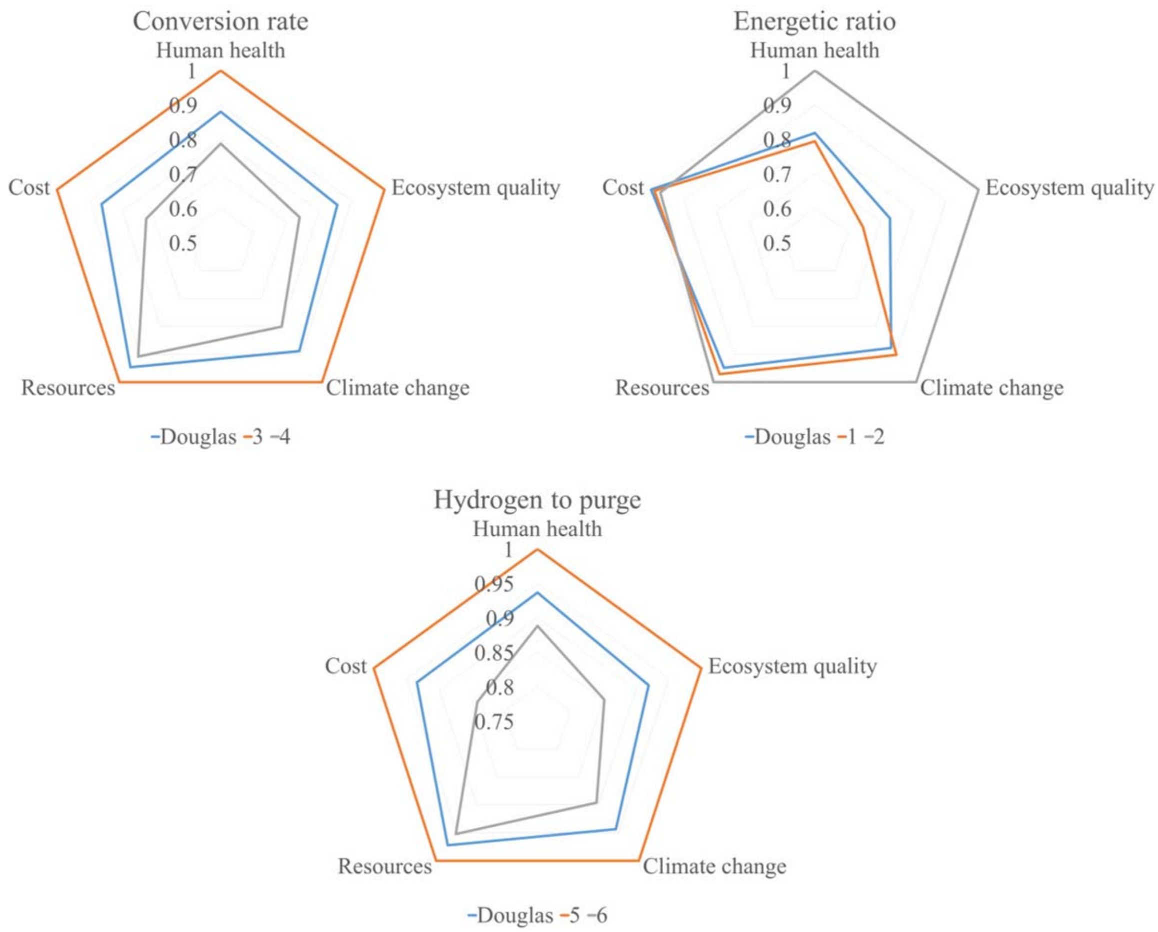

Figure 14. Classification of the environmental impact and cost criteria according to the variables conversion rate (C_{rate}), hydro gen flowrate (F_{H2}), and energetic ratio (R_{Fuel}) (end points).

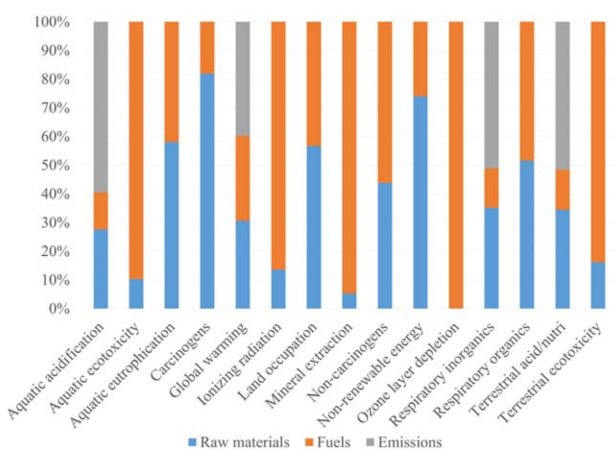

Figure 15. Mid points categories analysis according to inventory data subcategories (characterization).

oleic, linoleic, linolenic, palmitic, stearic, and other acids. The physical properties of different triglycerides present in vegeta ble oil are not much different [64]; hence, one of the triglycer ides can be used to represent the vegetable oil. In this work, triolein ($C_{57}H_{104}O_6$), (i.e., triglyceride of oleic acid) is consid ered as the triglyceride in the waste cooking oil. Because of the high presence of polar components, a combination of thermodynamic/activity models is used (NRTL and UNIQUAC). Different amounts of biodiesel production have been studied.

As previously used for the HDA case study, an attribu tional LCA is considered: the impacts from the production of biodiesel from vegetable oil are attributed to the inputs and outputs of the considered system, without taking account the interactions with the economy. In other words, no conse quential LCA approach is targeted here.

Biodiesel Process Flowsheet

The studied process is a variant of a reported process from the literature [19]. The flowsheet used in the literature was modified to favour stream recycling (Figure 18). Metha nol in vent gas output of the purifier column and triolein in reboiler liquid output are recycled with a purity of 99.97 and 99.99% respectively. Through recycling, about 34 kg h ^{1} of methanol and 111 kg h ^{1} of triolein are recovered and injected into the process. The reaction set is established before starting flowsheet modelling. Two reactions are involved, one for transesterification and one for neutraliza tion of sulfuric acid:

$$\text{Transesterification} \quad 3MeOH + Triolein \rightarrow 3MethylOleate + Glycerol \qquad (5)$$

$$\text{Neutralization} \quad CaO + H_2SO_4 \rightarrow H_2O + CaSO_4 \qquad (6)$$

The transesterification reaction is achieved at 80°C, 4.05 bar. For these conditions, Zheng *et al.* [65] propose a

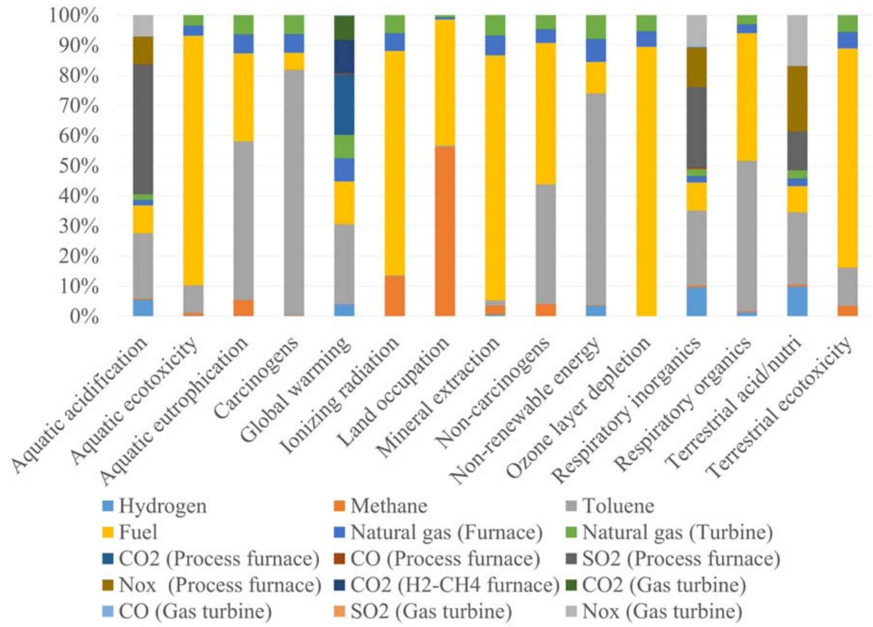

Figure 16. Mid point categories analysis of process alternative 4 (characterization).

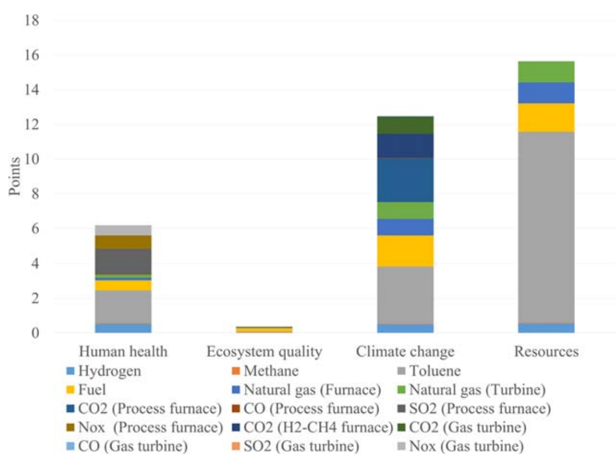

Figure 17. End point categories analysis of process alterna tive 4 (normalization).

conversion of 97% of oil to biodiesel. Also, there are two coolers in the process, the first to cool the effluent from the transesterification reactor outlet and the second to cool the output of the first column responsible for the separation of methanol for recycling. There is another column to sepa rate the biodiesel with a purity of 99.1%. The two columns are composed of 4 and 6 theoretical stages respectively and are set as a "Regular Hysys reboiler." The pressure of the condenser and reboiler is 1 bar. Pumps are positioned one after inputs of raw materials and another in methanol recy cling stream. The pressure is set at 3 and 4 bar, respectively.

Economic and Environmental Assessment

The economic model used in this process is the same as in [19] and the economic criterion is based on the calculation of profit. The calculation is carried out using the basic operation:

$$PROFIT \quad (Flow_{bd} * Price_{bd}) \quad \sum_{y=1}^{i} QE_x * CostE_x \quad \sum_{y=1}^{j} QRM_y * CostRM_y \quad \sum_{z=1}^{k} Qw_z * Costw_z \tag{7}$$

where revenues derived from the sale of biodiesel and costs include raw materials, utilities and a cost for four waste streams: bottom liquid of the acid neutralization column, washwater waste of the extractor column, vent gas of the purifier column, and reboiler liquid.

$CostE_x$;	Energy cost of type × ($/kWh)
$CostRM_y$;	Raw material cost of type y ($/kg)
$Costw_z$;	Waste cost of type z ($/kg)
$Flow_{bd}$;	Biodiesel production in output stream (kg)
$Price_{bd}$;	Price of biodiesel ($/kg)
QE_x;	Energy amount of type x (kWh)
QRM_y;	Raw material amount of type y (kg)
Qw_z;	Waste amount of type z (kg)

The price of biodiesel is 0.6 $/kg and the costs of raw mate rials and utility are shown in Table 8.

Environmental impact assessment uses the IMPACT 2002+ LCIA method to perform a cradle to gate analysis.

Inventory Data and Identification of Potential Factors

Within the cradle to gate boundary, the environmental impact is now considered from the extraction of raw materi als and primary energy needed to satisfy process energy. For the identification of inventory data of the process, some assumptions are made:

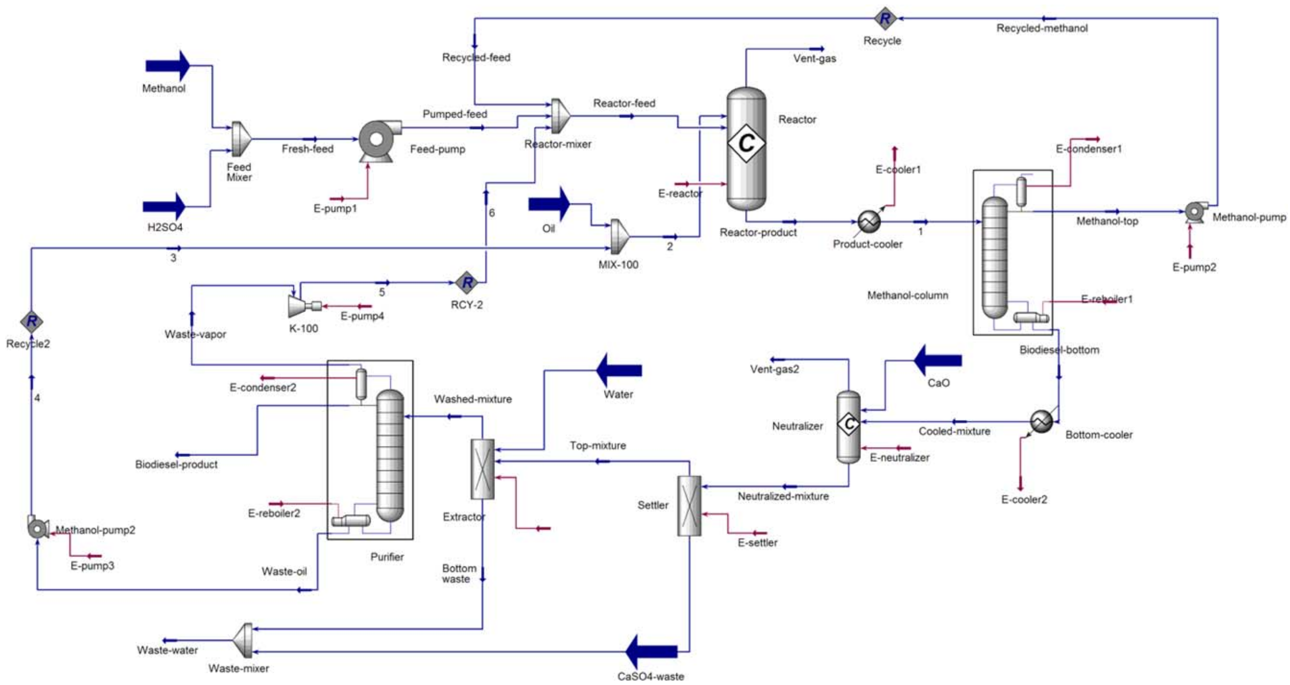

Figure 18. Flowsheet of biodiesel production process.

- The main raw material, triolein, is assumed to have no direct impact, i.e., which means that the production process of vegetable oil is not considered in the analysis.
- In the process, there are two output streams that contain glycerol and calcium sulfate (in a mixture that contains about 45% water for this latter case). These components are not considered in the environmental impact assessment because are considered as by products to be recovered in another process as raw materials. For calcium sulfate commercialization purpose (a purity of 99.9% calcium sulfate is necessary), a separation process is required. This process is not integrated here and the sales of these by products are not considered in the calculation of economic criteria that penalizes profitability.
- The energy requirements are provided by a gas turbine (as in the previous case study) so that the fuel used is analysed from the extraction phase and the generated emissions are considered.

Inventory data elements are then identified in the EcoInvent database provided in SIMAPRO tool. Table 9 summarizes the inventory data of the biodiesel production process and their related database names.

According to the LCIA chosen method, characterization damage and normalization factors belong to Impact 2002+.

Table 8. Summary of raw materials and utility prices of bio diesel production process.

Raw materials	Cost ($/kg)
Methanol	0.18
Sulfuric acid	0.06
Triolein (waste oil)	0.20
Water	0.01
Calcium oxide	0.04
Energy	**Cost ($/kWh)**
Pump	0.062
Cooler	0.003
Reactor	0.003
Condenser	0.003
Reboiler1	0.01
Reboiler2	0.15
Neutralizer	0.03
Waste stream	**Cost ($/kg)**
Waste vapour (vent gas)	0.05
Waste water (bottom liquid, reboiler liquid, washwater waste)	0.12

Sensitivity Analysis

The analysis is carried out by defining four process options (Table 10). The choice of the variables and their values have been defined from a design of experiments that will not presented in detail in this article.

Each variant has a different production capacity and thus an a priori different profit. The profit and environmental impacts of the four alternatives are represented through radar charts representing mid point and end point categories respectively (Figure 19). The radar charts show that all the alternatives exhibit very similar performances for all the environmental indicators. All the values are normalized as previously mentioned. Alternative 4 maintains a balance between environmental and economic criteria while alternative 1 is not so environmentally unfriendly.

The mid point and end point category analysis for variant 4, the most interesting one, is presented in Figures 20 and 21.

As a partial conclusion of the obtained results, this kind of analysis can be further developed to revisit LCA objectives and carry out consequential analysis that is particularly sound in the case of alternative fuels. The eco design framework can be one of the pillars to assess sustainability.

Table 9. Inventory data and selected items in SIMAPRO.

Category	Subcategory	Inventory data	Database elements names	Unit
Process	Raw materials	Methanol		kg
		Sulfuric acid		kg
		Water		kg
		Calcium oxide		kg
Energy	Fuels	Natural gas	Heat, natural gas, at industrial	MJ
			furnace >100kW/RER S	MJ
	Emissions	Carbon dioxide	Carbon dioxide	kg
		Sulfur dioxide	Sulfur dioxide	kg
		Nitrogen oxides	Nitrogen oxides	kg
		Carbon monoxide	Carbon monoxide	kg

Table 10. Process alternatives for biodiesel production.

Variables	Alternative 1	Alternative 2	Alternative 3	Alternative 4
Triolein (kg h ^{1})	1100	1090	975	1047
Methanol (kg h ^{1})	208	208	208	208
Sulfuric acid (kg h ^{1})	139	157	138	139
Calcium oxide (kg h ^{1})	79	90	79	79
Water (kg h ^{1})	111	116	113	111
Energy of cooler 1 (kWh)	18.09	17.86	17.76	17.81
Energy of cooler 2 (kWh)	5	4.89	4.87	4.80

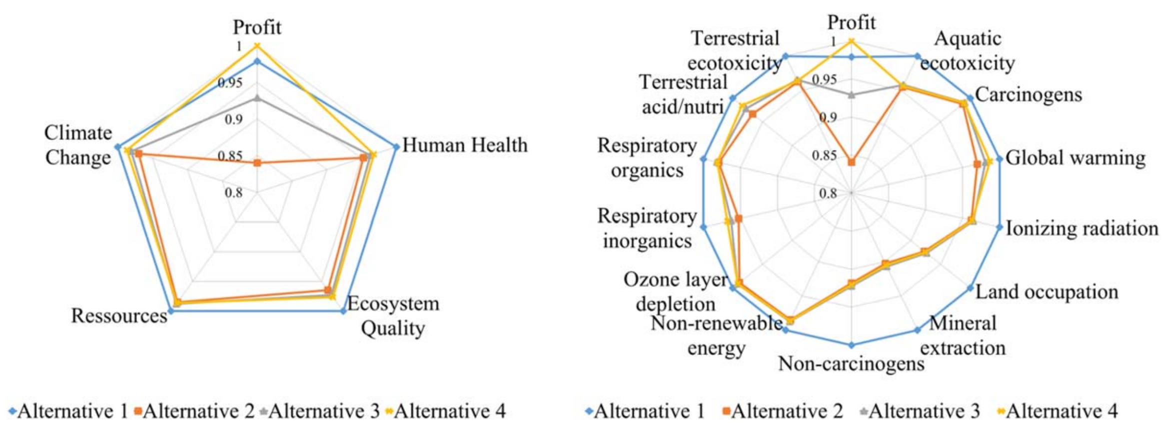

Figure 19. Comparison of profit and environmental criteria of the four process alternatives.

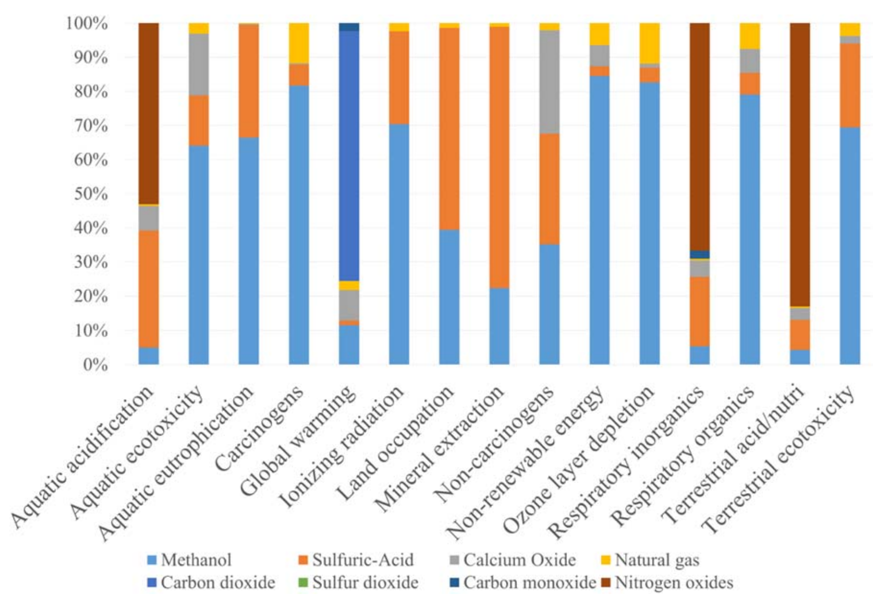

Figure 20. Mid point individual analysis of alternative 4 (characterization score).

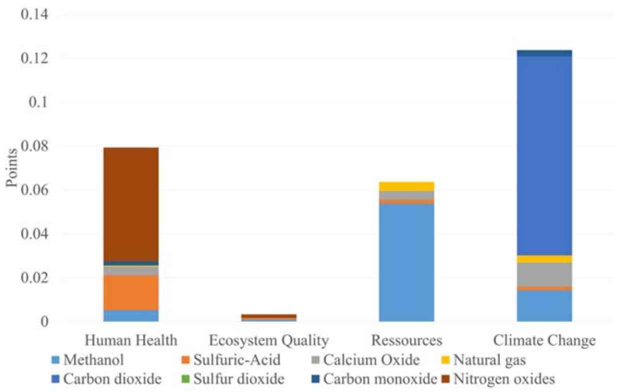

Figure 21. End point individual analysis of alternative 4 (normalization score).

CONCLUSIONS

A major incentive of this work was to apply LCA in com bination with process design. The core of the methodology is based on the link between energy and process simulation tools. The emissions in the system can thus be divided into utility and process waste to increase the knowledge of the origin of the waste and to identify the areas with largest potential for improvement. Even if life cycle assessment is a mature concept and if life cycle inventory databases are now largely implemented, it must be emphasized that data avail ability is one of the most critical issues in LCA. The well known benchmark HDA process first developed by [1] dem onstrates the usefulness of such an approach that must be applied at the very early design stage. Simulation tools for process and energy production can be useful to feed inven tory databases that are embedded in LCA tools. For bridging this gap, this work has proposed the combined use of a pro cess simulation tool dedicated to production utilities, Ariane, ProSim SA, experimental process data, and life cycle assess ment implemented with a commercial software tool SimaPro for the design of specific energy sub modules, so that the life cycle energy related emissions for a given process can be computed. The case study developed has addressed the environmental impact assessment of a bi fuel furnace on the one hand and steam production by a gas turbine on the other hand. The interest of using such an approach is that different operating conditions and technologies can be mod elled and evaluated systematically by the energy simulator. Of course, some experimental data may be necessary to identify the emission profile associated with an energy pro duction unit under specific operating conditions.

Yet, the results that have been presented do not consider confidence limits so that the results may be viewed as ques tionable from the user viewpoint since they may lead to mis judgements. Further improvement of the ecodesign needs to consider the modelling of uncertainty that may occur in the LCA process. The wide spectrum of tools from statistical analysis (for instance Monte Carlo analysis) to fuzzy concepts needs to be studied to be further incorporated in the ecode sign framework. A further extension of the approach is now to embed optimization on top of the ecodesign procedure where LCA and process integration have been used to explore options for a simultaneous improvement of both environmental performance and economic criteria. Because of the ecodesign complexity and of the antagonist behaviour that can be observed among some of the various criteria, multiobjective optimization (MOO) seems particularly attrac tive to automatically find solutions that satisfy both economic and environmental criteria and will play a major role in the « Next generation computer aided process engineering open simulation environment » to design the « Factory of the Future » of the Chemical Process Industries [66].

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