1 **AREA: ECONOMICS, SUSTAINABILITY ANALYSIS AND POLICY**

2
3 **EVALUATING THE SUSTAINABILITY OF BIOREFINERIES AT THE**
4 **CONCEPTUAL DESIGN STAGE**

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10
11 **Abstract**

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13 When traditional process-design methodologies are applied to the conceptual design of
14 biorefineries, the main drivers for their development are poorly considered. Biorefinery
15 plants are facilities integrating biomass-conversion processes and equipment to produce
16 fuels, energy, chemical intermediates, and end-use products. Appropriate design tools must
17 consider their sustainability in terms of: a) potential displacement of fossil fuels and
18 materials, b) mitigation of environmental impacts, c) renewability, d) economic feasibility,
19 e) biodiversity preservation, and f) social responsibility. Performance on addressing these
20 drivers should be assessed from appropriate environmental, social and economic
21 perspectives. This paper illustrates the application of a methodology that incorporates these
22 principles in the conceptual design of a switchgrass-based biorefinery. The results show
23 that the proposed design complies with the definition of sustainability in 10 out of 11
24 indicators. The indicator *Baseline-emissions reduction* fell in the unsustainable range
25 mainly due to the high SO₂-eq and PO₄-eq emissions over the life cycle of the proposed
26 system, derived from fertilizers and pesticides application. The techno-economic analysis
27 showed economic feasibility of the biorefinery when the minimum acceptable rate of return
28 is below 12%. The proposed methodology shows great potential as a valuable complement
29 to classic process-design methodologies, by quantifying their sustainability during the
30 conceptual-design stage, and requiring little extra effort beyond performing the techno-
31 economic analysis and a Life Cycle Assessment.

32
33 **Keywords:**

34 Biorefinery, indicator, sustainability framework, life cycle assessment, techno-economic
35 analysis, switchgrass

1. Introduction

The classic approach to chemical process design relies heavily on techno-economic analysis (Peters, Timmerhaus, & West, 2002). More recently, other tools for considering environmental impacts such as Environmental Impact Assessment (EIA) and Life Cycle Assessment (LCA) are also included in the design process (Allen & Shonnard, 2002). Although there have been some proposals to assess the sustainability of chemical processes (Azapagic, Millington, & Collett, 2006; IChemE, 2003; Ruiz-Mercado, Smith, & Gonzalez, 2012a; Ruiz-Mercado, Smith, & Gonzalez, 2012b; Sikdar, 2003), to date there is no generally acknowledged methodology that systematically integrates these tools in a simple and effective way, targeting a preliminary evaluation of the three sustainability dimensions during the conceptual design of chemical processes. The absence of such a methodology is a most important gap since the sustainability of processes is more and more a pressing matter for the process industries, especially for the bio-based industry. Most (if not all) sustainability-evaluation frameworks for on-going chemical processes require trend-over-time monitoring of usually long lists of indicators. At the design stage, the usual strategy is to compare performance of various indicators, define comparison criteria, and choose the “better” scenario (Mata, Caetano, Costa, Sikdar, & Martins, 2013); with this approach it is not possible to have an informed estimation of the sustainability of any given process design.

On the other hand, biorefineries are part of an emerging industry conceived for converting biomass into a spectrum of valuable products, and are defined as “... facilities that integrate biomass conversion processes and equipments to produce fuels, power, and chemicals from biomass” (Kamm, Gruber, & Kamm, 2006). The development of such an industry sprouts from two main drivers: 1) fossils displacement and 2) mitigation of environmental impacts (mainly global warming, but others should also be considered). Due to their bio-based nature, the high expectations on other sustainability criteria that apply to biofuels also extend to biorefineries, such as: 3) (true) renewability, 4) economic feasibility, 5) biodiversity preservation, and 6) responsible social development, the latter being the most controversial as to what indicators better describe the so-called “social sustainability” of systems, since a variety of social issues could potentially be included, such as justice, equity, acceptability, cultural values, among others. These drivers have been translated into sustainability targets, as those proposed by Dale & Ong (2014), who consider 11 design objectives for bioenergy systems, and even suggest a design approach considering diversification of products, landscape design, and local biomass depots to supply larger scale biorefineries.

There are some specific proposal of indicator frameworks for assessing the sustainability of biorefineries. Some of them are multi-criteria decision analyses which consider the objectives and preferences of the stakeholders in the biofuels production to generate the required sustainability criteria (Elghali et al., 2007, Haywood et al., 2009, Myllyviita et al., 2013). Other frameworks include a set of definite sustainability indicators and methodologies (Gnansounou, 2011, Mata et al., 2013). Sadhukhan et al., (2014) present a highly integrated framework for assessing the environmental and economic aspects in a very detailed manner, considering LCA, Economic Value and Environmental Impact analysis, and multicriteria analysis for designing biorefinery plants. A notable effort for including some of these ideas into biorefinery design was published recently by Nguyen et al. (2015). However, all these frameworks do not holistically address the design targets that

should be considered during for biorefinery *systems* (as opposed to biorefinery *plants*). As a result, this article aims to exemplify the application of one of the first prototype sustainability frameworks designed to include the evaluation of these criteria during the conceptual design stage of biorefineries (Sacramento-Rivero, 2012), and consequently provide a preliminary sustainability assessment of the design.

2. Methods

2.1 The sustainability framework

The framework used for the sustainability evaluation of biorefineries (Sacramento-Rivero, 2012) defines 14 indicators, grouped in 5 categories. This methodology was applied with a few modifications that are explained as follows: The original 5 themes (feedstock, process, products, corporate commitment, and environmental load) were replaced by the six design targets (categories) mentioned in the previous section, as the latter were deemed to be more descriptive of what is expected from a sustainable biorefinery (see Figure 1). This re-categorisation of indicators does not modify in any case the calculation of the indicators nor the evaluation of results. With this new distribution it is easier to locate each category in one or more of the three dimensions of sustainability, recognizing that there is a good balance among dimensions in this framework (four indicator categories per dimension).

Insert Figure 1 here

Another modification to the original methodology is that only one (*Social investment*) out of the five indicators in the “Corporate Commitment” category was considered, and the two components of the *Social investment* indicator (Community Development Investment and Employment extent) were assessed as individual indicators, thus avoiding weighing between them. The remaining four metrics in the Corporate Commitment category were devised for the evaluation of a fully operational biorefinery, and thus they are not applicable as a tool for process design. The indicators used in this study and the new categories are listed in Table 1. These indicators require inputs from two analyses: a LCA and a Techno-Economic Analysis (TEA), which is completed only after completing a process flowsheet, the mass and energy balances of the conceptual design.

Insert Table 1 here

An important highlight of this methodology is the normalised scale it uses for all indicators (Figure 2). The values of all indicators are modified using a simple normalisation formula to return values from zero to infinity, being zero and one values that represent an *ideal sustainability state* and a *critical state*, respectively. The former is a strictly theoretical value describing a system with zero negative impacts. The latter describes a system where a tipping point has been reached that will ultimately lead to a collapse of the system, as per the definition of that indicator. This critical value must be defined using a sound scientific basis, and acknowledged by national or international targets, agreements or certification bodies. The choice of the appropriate critical value will depend on the final use of the results of the LCA and the sustainability evaluation, always making sure that the original intentions of the indicator and the criteria match. When two or more sources propose

different critical values, the general recommendation is choosing the most stringent criterion, following the precautionary principle.

Hence, in this *normalised sustainability scale*, values between zero and one represent *sustainable states*, while values equal or greater than one represent *unsustainable operation* of the system. For example, take the indicator “Reduction of Greenhouse Gases (GHGs) emissions”; an ideal system would produce no GHG emissions (that state would be described by a value of zero in the normalised scale), and a critical system would be one that releases exactly the amount of GHGs that the atmosphere is capable of handling without reaching a catastrophic increase in its temperature; since the latter is complicated to define, a critical GHGs reduction would be that required by an appropriate acknowledged target. Thus, if the biorefinery is being designed for a country within the European Union (EU), the reduction targets of the EU Renewable Energy Directive (EU-RED) would define the critical reduction value (in this case, 50% reduction in 2017), and that level of reduction would be described by a value of one in the normalised scale. In the case where two targets apply to the designed biorefinery, the critical value should be set according to the stricter regulation.

Insert Figure 2 here

2.2 The case-study process description

In this paper, the conceptual design of biorefinery transforming switchgrass into lignocellulosic ethanol, methane, heat, electricity, and phenols was used as a case study. According to the classification provided by the International Energy Agency (2014), this is a “4-platform (C5/C6 sugars, biogas, lignin/pyrolysis oil, electricity & heat) biorefinery for the production of ethanol, electricity and heat, and chemicals from lignocellulosic crops”.

The mass and energy balances, as well as the LCA of this system were taken directly from the original publication of Cherubini and Jungmeier (2010). The evaluation methodology requires LCA results using system expansion as opposed to any other allocation method, since it considers as the reference (business as usual) case a fossil-alternative system which produces the same products/services: gasoline (for transportation), natural gas (instead of methane), heat (from heavy oil), electricity (from natural gas), and conventional phenols from oil refinery (as raw material for resin production). However, the reference system is only used in the LCA as a comparison baseline and is not part of the proposed biorefinery design, so it is not included in the TEA. Austria is the reference region as per the original LCA (Cherubini & Jungmeier, 2010), so it is assumed that the biomass production and transformation takes place in that country. Therefore, the critical values were set for Austrian conditions, and where data was not available, values available for other regions were used instead (European Union and Switzerland).

A simplified block diagram showing this process is in Figure 3. All flowrates were calculated based on a plant treating $477 \text{ kton} \cdot \text{a}^{-1}$ of dry switchgrass pellets containing 10% water content. The required cultivation area is 29,810 ha, if a productivity of $16\,000 \text{ kg} \cdot \text{ha}^{-1}$ is assumed. These data and all the assumptions and information regarding the biomass

production stage can be found in the original publication (Cherubini & Jungmeier, 2010), which are not included here due to space limitations. The feedstock is stored under heating to avoid decomposition while waiting for processing. The pellets are treated with an uncatalysed steam explosion pre-treatment, from which a solid fraction (mainly lignin) is set aside for thermochemical conversion. The cellulose/hemicellulose fraction goes to enzymatic cellulose hydrolysis where simultaneous saccharification and co-fermentation of C5/C6 occurs, producing an ethanol/water mixture that is distilled and further purified with a molecular sieve, to produce fuel-grade ethanol. The liquid effluents of the fermentation and distillation operations are sent to anaerobic digesters to produce biogas, which is further upgraded to methane. The anaerobic sludge is disposed off in a wastewater treatment plant. Twenty percent of the lignin recovered from the steam explosion pre-treatment is sent to flash pyrolysis, where it is transformed to pyrolytic oil and char; the phenol fraction in the oil (ca. 32%) is recovered with an efficiency of 50% and the remnant is sent to combustion, along with the pyrolysis char and the remaining lignin fraction. The combustion gases are sent to a Combined Heat and Power (CHP) cycle, producing electricity and excess heat. Ashes are sent to a monitored landfill. More specific details on the considered operational conditions and efficiencies of each process step can be found in the original publication (Cherubini & Jungmeier, 2010).

Insert Figure 3 here

2.3 Techno-economic analysis

The mass and energy balances were completed in a MS Excel® spreadsheet based on the information reported in the original publication. Then, the main equipment pieces were sized using conventional design equations based on the calculated stream flows. For the TEA, purchase costs of common equipment were estimated using the cost correlations in Peters and Timmerhaus (2002), and projected based on a power law with the commonly used scaling factor of 0.6 for chemical processing equipment. The scaled cost was then indexed to a year 2012 dollar value using the Chemical Engineering Plant Cost Index. Once the Total Purchased Equipment Cost (TPEC) is obtained, Fixed Capital Investment (FCI) and Total Project Investment (TPI) were determined from the pre-defined Peters and Timmerhaus factors for a solid-fluid processing plant. Overall, this TEA methodology is expected to be accurate within a 30% error margin, and is regularly used to assess the profitability of chemical processes designs (Brown, Wright, & Brown, 2011; Kazi et al., 2010; Ou, Thilakaratne, Brown, & Wright, 2015; Wright, Satrio, Brown, Daugaard, & Hsu, 2010). The main assumptions of the economic analysis are summarised in Table 2. A factor of 10% of FCI was used as a start-up contingency, given that almost all sections of the plant are based on turn-key commercial technology. The return on investment was evaluated with a 20-year discounted cash-flow rate-of-return spreadsheet. The cost analysis represents an *n*th plant design (that is, assuming that the plant can be built using state-of-the-art, commercially available technology without any delays in start-up and capacity loss). This is a common assumption in publicly available TEAs, thus providing comparable results to similar reports (Kazi et al., 2010; Wright et al., 2010). Annual operating costs include costs for feedstock, natural gas, catalysts and chemicals, waste disposal, utilities, fixed costs (inc. labour and equipment maintenance), and capital depreciation.

1 Insert Table 2 here

2 3 **3. Results and discussion**

4 5 *3.1 Techno-economic analysis results*

6
7 A summary of the mass and energy overall inputs and outputs of this process is presented
8 in Table 3. This particular design favours the production of ethanol, and all other output
9 streams are considered co-products except for the anaerobic digestion sludge which is
10 considered waste. Ideally, the combustion ashes containing nitrogen, phosphorous, and
11 potassium should be returned to the switchgrass plantation reducing the amount of required
12 fertilizers. A careful consideration of this design option might lead to better sustainability
13 performance, but collateral effects such as biomass yield and soil properties should be taken
14 into account. This particular design, however, considered landfilling of ashes and it is
15 evaluated consequently. The energy requirements of the biorefinery plant is fully satisfied
16 by 85% of the produced electricity and virtually all of the generated heat. The remaining
17 electricity is uploaded to the public grid. The main results of the TEA are shown in Table 4.
18 The TPI is 45.1 M\$ (2012 US dollars) and considering a 2% inflation rate, this is recovered
19 during the sixth year of operation. If the minimum acceptable annual rate of return (or
20 annual discount rate) is 10% then the net present worth is 10 M\$ after 20 years. However,
21 the net present worth decreases rapidly and becomes zero when the annual discount rate
22 increases to 12%. All this indicates that the profitability of the plant is feasible, although it
23 may be a major issue to consider when funding from external investors is used, as the
24 investment risk is considered high for this type of processes. Some of the results in Table 4
25 are required data for some sustainability indicators, as is explained in the following
26 sections.

27
28 Insert Table 3 here

29
30 Insert Table 4 here

31 32 *3.2 Evaluation of the sustainability indicators*

33
34 Table 5 is a summary of the calculated indicator values and the meaning of the
35 sustainability scale for each one of them. This is important information to report with the
36 results of this methodology since the definition of the critical value implicitly defines
37 *sustainability* for every indicator. The calculation procedures are detailed in the next
38 section.

39 40 41 *3.2.1 Calculation of the fossils displacement potential*

42
43 There are three indicators in this category, and together they give an indication of the
44 potential of the designed biorefinery to replace the fossils' derived products and services.
45 While the mass and energy balances give information on the amount of fossil fuel, energy
46 and chemicals that can be substituted by a given amount of feedstock (from the technical
47 point of view), these indicators give further information on how effective the proposed

system is in reducing fossil energy consumption ($NRES$), freshwater consumption (WR), and costs of raw-materials (RCR).

Non-Renewable Energy Share ($NRES$). This is the ratio of the non-renewable energy share of the biorefinery ($NRES_b$) and the targeted share ($NRES_c$). The life-cycle fossil-energy demand of the biorefinery system is $0.93 \text{ PJ}\cdot\text{a}^{-1}$ and the total demand is $9.97 \text{ PJ}\cdot\text{a}^{-1}$ (see Table 3), thus $NRES_b = 0.93/10.9 = 0.085$. The target set by the EU for 2050 aims for a 58% share of bioenergy in utilities and industry. Taking this as the critical value $NRES_c = 1 - 0.58 = 0.42$, so that:

$$NRES = \frac{NRES_b}{NRES_c} = \frac{0.085}{0.42} = 0.203 \quad (1)$$

This low value reflects the fact that almost all the energy demand of the biorefinery comes from self-generated renewable energy. Some countries have lower $NRES$ targets; for example Switzerland aims to achieve a third of its production from renewables ($NRES_c = 0.66$); using those targets would result in even lower (better) values of $NRES$.

Another indicator that is often used for assessing the energetic performance of biofuel systems is the Energy Return Over Investment (EROI). From the original work, the value of the EROI is 3.6, that is, the biorefinery returns 3.6 times the fossil energy consumed. This value is intermediate between the two reported in by Hall et al. (2011), of 0.78 and 17.8 for switchgrass ethanol. However, the EROI is expected to be considerably higher using an integrated biorefinery system like the one presented in this work. The great variations on the EROI might be due to the choice of boundaries of the LCA and/or allocation rules. A standardised protocol for calculating the EROI for fuels has been published by Murphy et al. (2011) and should be followed for allowing comparable results.

While the EROI is not included in this framework as a sustainability metric, it is a key metric for assessing fuel systems and comparing multiple design options, so when the objective of the assessment is comparing various biorefinery systems, the EROI adds important information that this framework does not presently capture.

Freshwater-use reduction (WR). Freshwater is an abundant resource in Austria and it is estimated that only around 4% of the available resources were used in 2013 (OECD, 2015). This means that $W_a/W_d = 1/0.04 = 25$, and thus the critical water-reduction is:

$$WR_c = \frac{0.2W_a}{W_d} = 5 \quad (2)$$

which means that freshwater consumption in Austria can increase 5-fold before reaching the critical point. The total water consumption of the biorefinery system is $0.975 \text{ km}^3\cdot\text{a}^{-1}$ per kg of bioethanol, with a comparable value of $0.707 \text{ km}^3\cdot\text{a}^{-1}$ in the reference system (Cherubini F, 2011, pers. comm.). This gives

$$WR_b = \frac{W_b}{W_f} = \frac{0.975}{0.707} = 1.38 \quad (3)$$

that is, the biorefinery requires 38% more freshwater on its life cycle than the fossil reference system. The final WR indicator is

$$WR = \frac{WR_b}{WR_c} = \frac{1.38}{5} = 0.276 \quad (4)$$

This value is low on the sustainability scale, but only because of the high critical value of Austria. If this same biorefinery design would operate in an average location in Spain, for example, where $WR_c = 0.595$, the sustainability of the freshwater use would be $WR = 2.31$ (well above the critical limit) using the same process design. In this example the calculation of WR was made using the average national consumption of freshwater, which is the simplest calculation that can be done. For more accurate calculations, or for larger countries with large variations on water availability across locations, the available, demand and critical flows should be estimated for the particular locations where water is extracted. Global water models (CESR, 2015) may be used in the absence of available data for specific locations.

Raw-materials cost ratio (RCR). The cost of oil, natural gas, and switchgrass pellets were estimated in $59.75 \$\cdot\text{bbl}^{-1}$ (OCI, 2015), $5.59 \$\cdot\text{GJ}^{-1}$ (Ou et al., 2015), and $0.15 \$\cdot\text{kg}^{-1}$ (eXtension, 2014), respectively. The reference system producing equal amounts of products than the biorefinery consumes $11\,553 \text{ bbl}\cdot\text{a}^{-1}$ of crude oil and $23.9 \text{ Mm}^3\cdot\text{a}^{-1}$ of natural gas (Cherubini, F., Personal Communication). Considering an average of $29.5 \text{ GJ}\cdot\text{m}^{-3}$ in the natural gas, then,

$$RCR = \frac{CF_b}{CF_f} = \frac{477 \times 10^6(0.15)}{(59.75)(11\,553) + (5.59)(23.9 \times 10^6)(29.5 \times 10^6)} = 0.018 \quad (5)$$

The cost of the natural gas required by the reference system is two orders of magnitude larger than the cost of the required switchgrass pellets, thus providing a very low value of the RCR .

Insert Table 5 here

3.2.2 Calculation of the potential mitigation of environmental impacts

This category includes a single metric that reflects the general performance of the biorefinery on reducing emissions of various pollutants and complying with their corresponding reduction targets, as defined by competent authorities, that is, governmental or international agencies, or certification bodies.

Reduction of baseline emissions (RBE). The characterised LCA impacts are summarised in Table 6, which were calculated using the CML-IA method (Impact Assessment method from the Institute of Environmental Sciences (CML) of Leiden University). While acknowledged reduction targets exist for GHG emissions in many countries, reduction targets for other types of emissions that cause other environmental

impacts are rarer (e.g. Acidification Potential, Terrestrial Ecotoxicity Potential, etc.). Due to lack of data for Austrian conditions, the critical reduction values ($\%ER_{c,i}$ values) for all other impact category were taken from the Ecological Scarcity Method (ESM) (R. Frischknecht & Büsser Knöpfel, 2013), which are based on Swiss legislation; the assumption is that the required targets will not depart too much from average Western European conditions, especially when the ESM targets are selected as the more stringent regulations currently applicable to Switzerland.

Insert Table 6 here

A further complication is that the impact categories in the ESM do not necessarily match those in the methodology developed by the CML-IA method; for this reason, it was necessary to derive equivalent targets ($\%ER_{c,i}$ values) for the CML-IA impacts categories using the critical values defined for the ESM impact categories. The ESM guidelines (Frischknecht & Knöpfel, 2013) report a “current flow” F (the latest record of the annual flow of emission in the country) and a “critical flow” F_c (the minimum acceptable value required for the emission) for each impact category. While some ESM categories match exactly the CML-IA categories (e.g. “CO₂ and further GHG” in the ESM matches “Global-warming potential” in CML-IA), some other ESM categories are very specific and several cause environmental impacts that are considered under a single CML-IA category. Table 7 is a summary of how the impact categories from both methods match. Each ESM impact category has its own current and critical flow, all expressed as an arbitrary unit of measure called Ecopoints (EP), which includes characterisation and normalisation factors, as well as current and critical flows for all associated emissions in that category (Frischknecht & Knöpfel, 2013). Thus, the critical value for the i -th CML-IA impact category that can be matched to n ESM categories, can be calculated by the following formula:

$$\%ER_{c,i} = \frac{\sum_{j=1}^n F_{c,j} \cdot EP_j}{\sum_{j=1}^n F_j \cdot EP_j} \quad (6)$$

where EP_j is the ecofactor for the j -th ESM impact category. For example, the calculation of $\%ER_{c,AP}$ (emission reduction target for the Acidification Potential) integrates two ESM categories (“NH₃” and “SO₂ and further acidifying substances”). The CML-IA characterised value for this category is in ton SO_{2-eq}. The current impact from both ESM categories, in Ecopoints, is $(82 \times 10^6 \text{ EP} \cdot \text{ton}^{-1} \text{ NH}_3) \times (51,463 \text{ ton NH}_3 \cdot \text{a}^{-1}) + (21 \times 10^6 \text{ EP} \cdot \text{ton}^{-1} \text{ SO}_{2\text{-eq}}) \times (12,861 \text{ ton}^{-1} \text{ SO}_{2\text{-eq}}) = 4.49 \times 10^{12} \text{ EP} \cdot \text{a}^{-1}$; if both critical flows are achieved: $(82 \times 10^6) \times (25,000 \text{ ton NH}_3 \cdot \text{a}^{-1}) + (21 \times 10^6) \times (25,000 \text{ ton SO}_{2\text{-eq}}) = 2.58 \times 10^{12} \text{ EP} \cdot \text{a}^{-1}$; thus, the reduction target for the Acidification potential is $\%ER_{c,AP} = 2.58/4.49 = 57.3\%$. With these values, the emission reduction for the i -th category ER_i is calculated by:

$$ER_i = \frac{\%ER_i}{\%ER_{c,i}} \quad (7)$$

where

$$\%ER_i = \frac{EF_{b,i}}{EF_{f,i}} \times 100 \quad (8)$$

The results of these calculations are included in Table 6.

Insert Table 7 here

As explained in the original publication (Sacramento-Rivero, 2012), in order to obtain a single *RBE* value that reflects the various environmental impacts, a squared-weighting factor is applied to aggregate the *ER* values, which follows the same reasoning that the weighting factors in the Ecopoints definition (Frischknecht & Knöpfel, 2013). Thus, the *RBE* is calculated by

$$RBE = \sum_{i=1}^n ER_i \cdot w_i \quad (9)$$

where the weighting factors w_i are

$$w_i = \left(\frac{100}{\%ER_{c,i}} \right)^2 / \sum_{j=1}^n \left(\frac{100}{\%ER_{c,j}} \right)^2 \quad (10)$$

The calculation steps and the final value of the *RBE* are in Table 8. The single value of $RBE = 1.96$ suffers from the disadvantages of any aggregated metric, as it cannot describe in itself the performance of the various indicators composing it. However, it does help to quickly identify that there are some issues with the sustainability of the system related to some of the emissions included in the LCA. Figure 4 helps for understanding where the *hot spots* are. All values of *ER* equal or less than one indicate that the biorefinery achieves the required (critical) reductions or overperforms. Only two categories exceed the critical values: the Eutrophication Potential of the biorefinery is 17 times the critical reduction. This value does not affect as much the final value because the critical reduction required in Western Europe conditions is only about 5.5% ($\%ER_{c,EP} = 94.5$). Since this is a distance to target weighting method, the Eutrophication Potential category has a low weigh. On the other hand, the Acidification Potential is almost two times the critical value and the required reduction is important ($\%ER_{c,AP} = 57.3$). Thus, this category has one of the largest weighting factors and has a prominent contribution to the final *RBE* value.

The effect of the Global-Warming Potential (GWP) *ER* is also interesting for discussion. When compared against the fossil reference, the GHGs emissions of the biorefinery represent only 23% of the fossil system's (see $\%ER$ value in Table 6). This low value is characteristic of second generation biofuel systems (Gnansounou & Dauriat, 2010). The critical target used for the GWP ($\%ER_{c,GWP}$) was taken from the EU-RED (2009), as it is consistent with how the CO_{2-eq} emissions were calculated in the LCA. However, the reduction targets for GWP are subject to rapid

changes and some certification bodies or national policies may demand more strict reductions in the near future.

A sensitivity analysis of the RBE with respect to $\%ER_{c,GWP}$ is in Figure 5. The value of $\%ER_{c,GWP}$ was varied from an overestimated critical target of 15% to the maximum expected value of 50% (which is the current demands of the EU-RED and used in this case study). The value of RBE ranges from 1.6 to 1.96, being the maximum at $\%ER_{c,GWP} = 50$ and the minimum of $RBE = 1.55$ at $\%ER_{c,GWP} = 23$, which is the value that makes the ER_{GWP} equal to unity (i.e. the biorefinery achieving exactly the reduction required by the critical value). As the value of $\%ER_{c,GWP}$ decreases, the weighting factor of the GWP increases at the expense of all the other categories. The largest weighting factor after the GWP is the Acidification Potential (AP). Both are plotted in Figure 5. At the value of $\%ER_{c,GWP}$ decreases the weighting factor of the AP decreases enough to make the relative contribution of this impact category less significant, even though the absolute value of its ER is higher than that of the GWP. This analysis illustrates the relationship among impact categories through the aggregation method proposed for the RBE. In any case, the most importance is given to the impact category farther away from sustainable conditions. In this analysis, even when the main focus switches from the AP to the GWP, the final value of the RBE does not approach sustainable conditions.

Insert Table 8 here

Insert Figure 4 here

Insert Figure 5 here

3.2.3 Calculation of the biorefinery renewability

Normalised biotechnological-valorisation potential (BVP). The scores considered for switchgrass are listed in Table 9; for these scores, the BVP adds up to 23 and normalisation yields:

$$BVP = 1 - \frac{\text{Score} - 21}{36 - 21} = 0.867 \quad (11)$$

Insert Table 9 here

Raw-materials consumption (RMC). Being a perennial crop, switchgrass can be considered to be harvested at the same rate of its replenishment. During the first and second years of production, the productivity is expected to be below the average (33 and 66%, respectively). The considered land for the biorefinery system is the land area required for supplying $477 \times 10^6 \text{ kg} \cdot \text{a}^{-1}$ of pellets since the first year, so that the supply needs a productivity of $RM_b = 16\,000 \text{ kg} \cdot \text{ha}^{-1} \cdot \text{a}^{-1}$ and the regeneration yield on the field is $RM_{re} = 16,850 \text{ kg} \cdot \text{ha}^{-1} \cdot \text{a}^{-1}$, so that

$$RMC = \frac{RM_b}{RM_{re,i}} = \frac{16}{16.85} = 0.95 \quad (12)$$

In other words, the land available is very close to the critical limit so that any decrease on switchgrass productivity may endanger its ability to supply the required feedstock. Planting and maintaining more land surface will decrease the value of this indicator, but changes on the other indicators may be expected by the increase of use of fertilizers and pesticides, as well as energy, transport, etc.

While the above is the simplest approach for addressing renewability of feedstocks, a more detailed analysis considering geologic cycles would be a better indicator of its sustainability from the nutrient preservation perspective, in such a way that all the ecosystem limits to replenish the harvested biomass be embedded in a single indicator about the long term renewability. For example, Martinez-Hernandez et al. (2015) determine the rate at which heathland biomass productivity can be maintained in the long term from system dynamics analysis of the biomass and the supporting stocks (such as N and C). However, in the absence of specific data, this approach would require considerable modelling effort, and a rough estimation like the *RMC* may be used.

3.2.4 Calculation of the economic feasibility

Fraction of revenue for feedstock (FRF). Assuming that the cost of switchgrass pellets is 0.15 \$/kg (the estimated market value of switchgrass when corn stover is not available (eXtension, 2014)), the total cost of feedstock is $CF = (0.15)(477 \times 10^6) = 71.6 \times 10^6 \text{ \$} \cdot \text{a}^{-1}$. Assuming conservative sales prices of: ethanol at 0.87 \$·kg⁻¹ (USDA, 2015), 0.20 \$·kg⁻¹ of phenols, 4.47 \$·GJ⁻¹ of methane and 67.15 \$·MWh⁻¹ (80% and 85% the price of natural gas and grid electricity reported by Ou et al. (2015), respectively), the total value of products $VP = (0.87)(103.6 \times 10^6) + (0.20)(2.09 \times 10^6) + (4.47)(179 \times 10^3) + (67.15)(4 \times 10^3) = 91.6 \times 10^6 \text{ \$} \cdot \text{a}^{-1}$. This gives:

$$FRF = \frac{CF}{VP} = \frac{71.6}{91.6} = 0.781 \quad (13)$$

which is a reflection of the results from the TEA reported earlier in this section.

Modified gross margin (GM). This biorefinery is self-sufficient energy-wise: all its energy needs are supplied by the heat and electricity generated. Also, since this is an evaluation at the design stage, it is assumed that the entire production is sold, that is, the Value of Products is equal to the Net Sales, which have an average value of $NS = 116.5 \times 10^6 \text{ \$} \cdot \text{a}^{-1}$, and the total product cost is the average Cost of Sales during the 20 years, which was calculated during the economic evaluation in $COGS = 104.7 \times 10^6 \text{ \$} \cdot \text{a}^{-1}$. Therefore the Modified Gross Margin is $GM = 106.72/165.36 = 0.645$.

$$GM = \frac{COGS}{NS} = \frac{104.7}{116.5} = 0.899 \quad (14)$$

3.2.5 Calculation of the biodiversity preservation potential

This category only measures the potential of losing biodiversity and life-support functions in the switchgrass cropland surface using the Ecosystem Damage Potential (EDP) method, which ‘reflects the anticipated number of (plant) species and the actually encountered number of species for the specific type of land’ (Frischknecht, Steiner, & Jungbluth, 2009). This is only a very crude method for measuring potential biodiversity effects due to land-use change and experimental measurements on biodiversity loss should be preferred. Unfortunately, these data are very scarce and far from becoming available for a generalised use.

Sustainable land-use (SLU). Assuming that the cultivation area is much greater than the land occupied by the biorefinery's facilities, the total area of the biorefinery system is $A = 29,810$ ha. The *SLU* indicator was defined in terms of the characterisation factors presented in the ESM 2006 (R. Frischknecht et al., 2009). It was assumed that the cropland went from “Artificial, non-agricultural areas with vegetation” to “Pastures and meadows”. The characterisation factors for the old and new land uses are: $F_{old} = 1.02$ and $F_{new} = 0.265$, so that the Net Settlement Area is $NSA = (1.02)(0 - 29,810) + (0.265)(29,810 - 0) = -22,506.5$. Thus, according to the *SLU* definition,

$$SLU = 1 + \frac{NSA}{\sum_i A_i} = 1 + \frac{22,506}{29,810} = 0.245 \quad (15)$$

This low value of *SLU* means that the new land use is actually favouring the existence of more species than the reference system (land set-aside unproductive in the “Artificial, non-agricultural areas with vegetation” category). As mentioned before, local measurements of biodiversity in real biofuel production sites may lead to very different results (Gollany et al., 2015). However, at the conceptual design stage of a biorefinery, this indicator is useful for giving an indication of possible impacts to biodiversity.

3.2.6 Calculation of the projected social responsibility

In the previous categories, recurring to benchmarking has been avoided, as per the main intention of the sustainability evaluation methodology. In the case of social indicators, however, it has been unfeasible to choose critical values based on legally binding targets or legislations. Many socioeconomic indicators have been proposed for the evaluation of bioenergy systems (Hilbert & Galligani, 2015) but their interpretation within the normalised sustainability scale has been elusive. Therefore, this is the only category in which the definition of the two proposed socio-economic indicators relies on benchmarking in the chemical processing industry to define the ideal and critical values. Both indicators are taken from the American Institute of Chemical Engineers Sustainability Index (AIChE SI) (Cobb et al., 2009) and the survey therein reported.

Employment extent (EE). This is how the biorefinery performs in terms of job creation, and it is measured according to the number of employees per million dollars of net sales. In the biorefinery design, this number is 74 employees (including only workers in the biorefinery plant), and dividing by the net sales NS the employment extent of the biorefinery plant is $EE_b = 0.635 \text{ M}\$^{-1}$. When normalising within the maximum and minimum (4 and 0.5, respectively (Cobb et al., 2009)) observed in chemical processing plants, the final value for the employment extent is:

$$EE = \frac{EE_{\max} - EE_b}{EE_{\max} - EE_c} = \frac{4.0 - 0.64}{4.0 - 0.50} = 0.961 \quad (16)$$

The number of workers in the biorefinery plant is close to the minimum observed in the chemical processing industry. A more consistent comparison with the other sustainability indicators should take the life-cycle employment within the biorefinery system. It is expected that most of the new jobs will be likely generated in the biomass production stage. If included, the new jobs derived from the biomass production stage would lead to an improvement of the EE indicator. Unfortunately there are no benchmarking values to make comparisons at the life-cycle level. This is why only the biorefinery plant data was used.

Community development investment (CDI). This indicator takes the same idea than the *EE* and provides information on the biorefinery performs in terms of investment in philanthropic and community development projects. In the chemical industry these projects are mostly related to education on science and technology, as well as recreational (Cobb et al., 2009). In the biorefinery design, a 0.05% of the annual net revenue was projected in these types of projects, and averaging the total amount (in inflated dollars) over the 20 years of the projections a total investment of $3.1 \text{ k}\$ \cdot \text{a}^{-1}$ results, corresponding to a $CDI_b = 0.055\%$. When normalising within the maximum and minimum observed in chemical processing plants, the final value for the employment extent is:

$$CDI = \frac{CDI_{\max} - CDI_b}{CDI_{\max} - CDI_c} = \frac{0.13 - 0.055}{0.13 - 0.03} = 0.747 \quad (17)$$

3.3 The sustainability footprint of the proposed design

The 11 indicators can be readily presented graphically in a radar plot like Figure 6. The critical boundary (bold line at the value of one) allows for the quick identification of those indicators that are close or beyond the critical value and therefore deserve most attention to improve the design.

Insert Figure 6 here

All assessed indicators but one fall within the *sustainable* range. The *RBE* is almost twice the critical value. This is due to high values of the Acidification potential, which derive mainly from fertilizer application during the cultivations stage. The Eutrophication Potential is very large (more than 17-fold the critical value) but the critical reduction required for the biorefinery location is low, resulting in a small weighting factor and thus

1 minimizing the negative effects of this large impact. Most analyses comparing
2 environmental burdens of fossil fuels against biofuels conclude that the latter perform better
3 in all impact categories except on the acidification and eutrophication potentials (Cherubini
4 & Jungmeier, 2010; Contreras, Rosa, Pérez, Van Langenhove, & Dewulf, 2009; von
5 Blottnitz & Curran, 2007).

6
7 The *RCR* is very close to the *ideal sustainability* state, given the very large difference
8 between the costs of the raw materials for the reference system, compared to those in the
9 biorefinery. The *SLU* also has a very low value, meaning that there is a significant
10 biodiversity gain due to the projected land-use change; however this value is very
11 preliminary and more specific studies should be done before accepting this result as valid.
12 The *NRES* is also very small due to the little fossil energy requirement of the biorefinery
13 system, which is energetically self-sufficient.

14
15 Indicators very close to the critical state are: *RMC*, due to a projected cultivation area very
16 close to the minimum requirement of switchgrass supply; the *EE* as the number of jobs in
17 the plant are very close to the minimum observed in chemical plants; the *BVP*, since the
18 processing technology for lignocellulosic materials is still not mature, although this is
19 expected to improve substantially in the upcoming years.

20
21 An interesting extension to this work would be to assess how different biorefinery
22 configurations affect the sustainability indicators and the resulting trade-offs. For example,
23 some processes in the biorefinery may lead to the increase of the economic benefit at
24 expense of increasing the environmental load of the biorefinery. As different processes are
25 included in flowsheet designs, some indicators might remain unchanged while others will
26 start to interact with each other. This is a way of identifying which indicators are robust and
27 which are volatile. Pareto analysis may also be applied for this type of analysis. As the
28 objective of the present study is the illustration of the methodology application, this
29 analysis will be the topic of a further paper.

30 31 32 **4. Conclusions**

33
34 The studied methodology is a valuable supplement to classic process design methodologies
35 for biorefineries, since it provides clear definitions of sustainability for various indicators
36 and allows the quantification of key sustainability issues without the need of benchmarking.
37 For its use at the conceptual design stage, performing a techno-economic analysis and a
38 Life Cycle Assessment is required. These three tools together generate enough data to
39 assess the biorefinery design from the economic, social and environmental dimensions in a
40 balanced manner. When applying the methodology to the case study (a switchgrass
41 biorefinery producing ethanol, methane, phenols, and electricity), it was evident that the
42 most urgent areas for improvement are the environmental indicators, more specifically the
43 $\text{PO}_4\text{-eq}$ and $\text{SO}_2\text{-eq}$ emissions, causing that the Acidification and Eutrophication potentials
44 be much larger than critical targets allow. Among the 11 assessed indicators, 10 fell in the
45 sustainable range. Some indicators such as the Employment Extent and Raw Materials
46 Consumption need improvement to fall farther away from the critical limits. Increasing
47 operational jobs within the plant, increasing crop productivity, or increasing the cropland

surface may lead to better results on this indicators, although the effects of these measures on the other indicators should be assessed. Other lessons learned from the application to the case study include:

- a. The choice of critical values for the sustainability scales is of vital importance and must be tied to legally binding, and/or internationally acknowledged targets. If this is not possible, national targets or certification regulations must be used instead, making sure that the original intentions of the indicator and the criteria match. When two or more targets exist, the precautionary principle dictates that the most stringent one should be used.
- b. The methodology is successful in quantifying the dependence of the sustainability of a system to the local conditions. The discussion presented on the *WR* and *RBE* indicators clearly states how local definitions of sustainability (through the critical values of the indicators) can drastically change the perception of the performance of the same biorefinery design.
- c. Indicators tackling the social dimension are difficult to set on a sustainability scale, because commonly there is no possible definition for the ideal sustainability and/or the critical value. For this reason only a couple of social indicators were assessed, and benchmarking was required for these two in order to define the ideal and critical states. This causes that the social aspect is covered only in part by the proposed methodology and a qualitative analysis of social issues is required to complement the information of this methodology.

This methodology should be interpreted as an initial estimation of the overall sustainability of a biorefinery design, useful for making design decisions. It covers the main aspects of a biorefinery, and more importantly, sets quantitative targets for each indicator. A more detailed analysis with other tools is expected to draw similar conclusions, at the cost of extra work and/or on a qualitative/benchmarking basis. Nevertheless, more case studies are needed to validate this conclusion, including evaluations to working biorefineries.

The proposed framework also allows for the inclusion of new indicators, as long as a definition for the normalised sustainability-scale is possible. New indicators can be easily incorporated in the radar plot so that their impact on the overall sustainability assessment can be analysed.

Finally, although the indicators are thought to cover sustainability aspects of biorefineries through the design objectives listed in Table 1, it should be noted that these objectives are shared by all forms of bioenergy processes; therefore, this methodology could also be used to assess the sustainability of simpler bioenergy systems.

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1 Nomenclature

<i>AP</i>	Acidification Potential
<i>BVP</i>	Normalized Biotechnological-Valorisation Potential
<i>CDI</i>	Community Development Investment
<i>CHP</i>	Combined Heat and Power
<i>EDP</i>	Ecosystem Damage Potential
<i>EE</i>	Employment Extent
<i>EIA</i>	Environmental Impact Assessment
<i>EP</i>	Ecofactor, Ecopoints Eutrophication Potential (when used as subindex)
<i>ER</i>	Emissions' Reduction
<i>ESM</i>	Ecological Scarcity Method
<i>EU</i>	European Union
<i>EU-RED</i>	European Union Renewable Energy Directive
<i>FCI</i>	Fixed Capital Investment
<i>FRF</i>	Fraction of Revenue for Feedstock
<i>GHG</i>	Greenhouse Gases
<i>GM</i>	Modified Gross margin
<i>GWP</i>	Global-Warming Potential
<i>LCA</i>	Life Cycle Assessment
<i>NRES</i>	Non-Renewable Energy Share
<i>RBE</i>	Reduction of Baseline Emissions
<i>RCR</i>	Raw-Material cost ratio
<i>RMC</i>	Raw-Materials Consumption
<i>SLU</i>	Sustainable Land-Use
<i>TEA</i>	Techno-Economic Analysis
<i>TPEC</i>	Total Purchased Equipment Cost
<i>TPI</i>	Total Project Investment

WR

Freshwater-use reduction

1
2

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Table 1. Indicator categories of the sustainability framework for biorefineries

Category/Indicators	Category description
Fossils displacement potential (Displacement)	
Non-renewable energy share (<i>NRES</i>)	Determines the potential of a biorefinery system to replace a reference fossil system providing the same products/services.
Freshwater-use reduction (<i>WR</i>)	
Raw-materials cost ratio (<i>RCR</i>)	
Mitigation of environmental impacts (Mitigation)	
Reduction of baseline emissions (<i>RBE</i>)	Estimates the potential mitigation of Global Warming and other environmental impact categories when comparing the emissions of the biorefinery to those of the fossil reference system.
Biorefinery renewability (Renewability)	
Biotechnological-valorisation potential (<i>BVP</i>)	Quantifies the capacity of the designed system for maintaining the required supply within the natural limits of the system's capacity.
Raw-materials consumption (<i>RMC</i>)	
Economic feasibility (Economics)	
Fraction of revenue for feedstock (<i>FRF</i>)	Provides quick estimations of the profitability of the biorefinery system. These indicators are intended to provide essential results from the TEA using the normalised sustainability scale.
Modified gross margin (<i>GM</i>)	
Biodiversity preservation (Biodiversity)	
Sustainable land-use (<i>SLU</i>)	Provides a rough estimation of the loss of biodiversity and loss of life-support functions caused by land-use change associated to the biorefinery.
Community commitment (Community)	
Employment extent (<i>EE</i>)	Measures some benefits of local communities from the biorefinery in terms of jobs creation and monetary investment in community development projects.
Community development investment (<i>CDI</i>)	

Table 2. Major assumptions in the economic analysis

Plant life in years	20
Operating hours per year	7896
Equity	100%
Discount rate	10%
Plant depreciation method	Double Declining Balance
Depreciation period (salvage value = 0) in years	7
Construction period in years	2.5
Fraction of investment in year -3	15%
Fraction of investment in year -2	35%
Fraction of investment in year -1	50%
Start-up time in years	0.5
Income tax rate	39%
Inflation rates	
Construction	2%
Product price	2%
Total Product Cost	2%

Table 3. Main mass and energy inputs and outputs in the biorefinery

Stream	Flow	Stream	Flow
Switchgrass pellets	$477 \times 10^6 \text{ kg} \cdot \text{a}^{-1}$	Ethanol	$103.6 \times 10^6 \text{ kg} \cdot \text{a}^{-1}$
Ashes	$22.8 \times 10^3 \text{ kg} \cdot \text{a}^{-1}$	Methane	$179 \text{ TJ} \cdot \text{a}^{-1}$
Liquid effluent	$718.9 \times 10^6 \text{ kg} \cdot \text{a}^{-1}$	Electricity	$93.0 \text{ TJ} \cdot \text{a}^{-1}$
Phenols	$2.09 \times 10^6 \text{ kg} \cdot \text{a}^{-1}$	Heat	$16.0 \text{ TJ} \cdot \text{a}^{-1}$
Life-Cycle energy demand			
System	Fossil	Renewable	Total
Fossil reference	$4.53 \text{ PJ} \cdot \text{a}^{-1}$	$0.17 \text{ PJ} \cdot \text{a}^{-1}$	$4.7 \text{ PJ} \cdot \text{a}^{-1}$
Biorefinery	$0.93 \text{ PJ} \cdot \text{a}^{-1}$	$9.97 \text{ PJ} \cdot \text{a}^{-1}$	$10.9 \text{ PJ} \cdot \text{a}^{-1}$

Table 4. Main results of the economic analysis

Parameter		M\$
Total purchased equipment cost (TPEC)	100% TPEC	8.3
Direct installed cost	332% TPEC	27.7
Indirect installed cost	139% TPEC	11.5
Fixed Capital Investment (FCI)	471% TPEC	39.2
Working capital	15% FCI	5.9
Land	6% TPEC	0.5
Total project investment (TPI)	541% TPEC	45.1
Annual operating cost		
Feedstock		71.6
Operating labour		1.6
Utilities		5.6
Other variable costs		0.2
Fixed costs		1.2
Total annual operating cost (average, inc. depreciation)		106.5
Average income tax		4.0
Average return on investment	12%	
Average annual net sales		116.5
Payback period (years)	5.4	
Net present worth (at a minimum acceptable annual rate of return of 10%)		10.0

Table 5. Critical value descriptions and results of the sustainability indicators for the case study

Category	Indicator / Equation	Meaning of the critical value (x = 1)	Observations about the critical value	Value
Displacement	Non-Renewable Energy Share (<i>NRES</i>)	The share of non-renewable energy consumption in the biorefinery system is equal to an acknowledged target	The European Union (EU) target of 42% fossil energy share to 2050 was used.	0.20
	Freshwater-use Reduction (<i>WR</i>)	The biorefinery's freshwater consumption represents a reduction on freshwater use (relative to the reference system) equal to an acknowledged target for the plant's location.	The critical water consumption in a region is such that 20% of water reserves are preserved (OECD, 2004). In this case, average national data for Austria were used.	0.28
	Raw-materials Cost Ratio (<i>RCR</i>)	The cost of the biorefinery's raw materials is equal to the cost of the raw materials of the reference system	Raw materials for the reference system: petroleum and natural gas	0.02
Mitigation	Reduction of Baseline Emissions (<i>RBE</i>)	The reduction of baseline emissions in the biorefinery (relative to the reference system) is equal to an acknowledged reduction-target.	Baseline impact categories as per CML-IA methodology. Targets for the EU were taken from the latest Ecological Scarcity Method guidelines (R. Frischknecht & Büsser Knöpfel, 2013)	1.98
Renewability	Biotechnological-Valorisation Potential (<i>BVP</i>)	The economic, technological, geographical and biochemical features of the analysed feedstock are at a predefined minimum acceptable value for bioenergy production	A minimum score of 21 in a 0-36 scale (Duarte, Esteves, Carvalho, & Gírio, 2007)	0.87
	Raw-materials consumption (<i>RCM</i>)	The rates of consumption and regeneration of the renewable raw materials are equal.		0.95
Economics	Fraction of Revenue for Feedstock (<i>FRF</i>)	The market price of the products equals the market price of the feedstock		0.78
	Modified Gross Margin (<i>GM</i>)	The biorefinery's net sales are equal to the cost of goods sold.		0.90

Category	Indicator / Equation	Meaning of the critical value ($x = 1$)	Observations about the critical value	Value
Biodiversity	Sustainable Land-Use (<i>SLU</i>)	The land-use change caused by the biorefinery's operation is at the limit of causing a net biodiversity loss.	Reference land use was “Artificial, non-agricultural area with vegetation”	0.25
	Employment Extent (<i>EE</i>)	The number of employees per million of dollars of net sales is at the minimum value observed in the chemical industry	From the American Institute of Chemical Engineers Sustainability Index (AIChE SI) survey (Cobb, Schuster, Beloff, & Tanzil, 2009), range is 0.5 to 4.0.	0.96
Community	Community Development Investment (<i>CDI</i>)	The annual amount (in % of net revenue) invested in philanthropic and community development projects is at the minimum value observed in the chemical industry	From AIChE SI survey (Cobb et al., 2009), range is 0.03 to 0.13%	0.75

Table 6. Calculation of the Emissions Reduction (ER) values

Impact category	Unit/a	EF_b	EF_f	%ER	%ER _c	ER
Abiotic depletion	kt Sb-eq	0.42	1.94	21.6		
Global Warming Potential (GWP100)	kt CO ₂ -eq	64.6	281.0	23.0	50.0	0.46
Ozone-layer depletion	kg CFC-11-eq	10.5	31.2	33.7	78.5	0.43
Human toxicity	kt 1,4-DB-eq	34.2	187.0	18.3	68.5	0.27
Aquatic ecotoxicity (freshwater)	kt 1,4-DB-eq	4.08	16.8	24.3	172	0.14
Aquatic ecotoxicity (marine)	Mt 1,4-DB-eq	22.8	50.1	45.5	172	0.27
Terrestrial ecotoxicity	kt 1,4-DB-eq	0.35	0.62	56.5	86.5	0.65
Photochemical oxidation	kt C ₂ H ₄ -eq	0.06	0.28	21.4	91.0	0.24
Acidification	kt SO ₂ -eq	1.23	1.17	105.1	57.3	1.83
Eutrophication	kt PO ₄ -eq	2.82	0.17	1658	94.5	17.5

* EF_b and EF_f are the pollutant flows in the biorefinery and the reference systems, respectively. %ER is the percent emission reduction achieved by the biorefinery, and %ER_c is the critical percent reduction.

Table 7. Matching the CML-IA and ESM impact categories for estimating critical reduction targets

Impact category (CML-IA baseline)	Impact category (ESM)	Comments about the ESM targets
Abiotic depletion	NA	The depletion of abiotic resources is not explicitly addressed in the ESM, thus there is no eco-factor derived for an equivalent category of abiotic depletion. In the absence of a critical value, this category is excluded from the <i>RBE</i> calculation.
Global Warming Potential (GWP100)	CO ₂ and further greenhouse gases	The ESM and CML-IA method use the same characterisation factors (time horizon of 100 years). However, the ESM does not consider CO ₂ emissions from land-use change or forest sinks to calculate the eco-factor. The Renewable Energy Directive (RED) and the Roundtable on Sustainability Biomaterials (RSB) have developed commonly accepted regulatory schemes towards the greenhouse gases emissions savings required for the biofuels production which are being implemented (Shonnard et al., 2015). Overall, a 50% emissions saving are required for 2017 and this value is considered in this study.
Ozone-layer depletion	Ozone-depleting substances	The critical value is the ‘tolerated’ level of emissions in 2020 based on a calculated reduction of emissions from chlorofluorocarbon-containing compounds.
Human toxicity	NOx, carcinogenic substances (benzene, dioxin and furans, and PAHs), lead, cadmium, and mercury emissions to air Arsenic, lead, cadmium, chromium, copper, nickel, mercury, and absorbable organic halogenated compounds (as Cl ⁻) emissions to surface water Nitrate emissions to groundwater Lead, cadmium, copper, and zinc emissions to soil	This impact category refers to the toxic effect on humans of substances or interventions released to the air, water, and/or soil. CML-IA method uses fate, exposure/intake, effect, and transfer factors to model the ways the emissions migrate from a compartment to another. On the other hand, the ESM method classifies emissions according to the release compartment. The critical targets are defined then according to emission levels to air, water and soil, and not to the actual toxic loads affecting said compartments.
Aquatic ecotoxicity (freshwater)	Lead, cadmium, chromium, copper, nickel, and mercury emissions to surface water	This impact category refers to the toxic effect on freshwater of substances or interventions released to the air, water, and/or soil. CML-IA considers fate, exposure, transfer, and effect factors, while ESM

Aquatic ecotoxicity (marine)	Lead, cadmium, chromium, copper, nickel, and mercury emissions to surface water	target values are for discharge flows. This impact category refers to the toxic effect on freshwater of substances or interventions released to the air, water, and/or soil. CML-IA considers fate, exposure, transfer, and effect factors, while ESM target values are for discharge flows.
Terrestrial ecotoxicity	Carcinogenic substances, lead, cadmium, and mercury emissions to air Lead, cadmium, chromium, copper, nickel, and mercury emissions to surface water Lead, cadmium, copper, zinc, and plant protection products (as glyphosate equivalent) to soil	This impact category refers to the toxic effect on freshwater of substances or interventions released to the air, water, and/or soil. CML-IA considers fate, exposure, transfer, and effect factors, while ESM target values are for discharge flows.
Photochemical oxidation	NMVOCs emissions.	The critical flow of NMVOCs of the ESM method is based on the targets stated by the Swiss Federal Council.
Acidification	Ammonia (NH ₃), SO ₂ and further acidifying substances emissions to air	The critical flow of ammonia of the ESM method is based on the reduction targets stated by the Swiss Federal Office for the Environment (FOEN) and Federal Office for Agriculture (FOAG), while that of the SO ₂ on the reductions targets defined by the Swiss Air Pollution Control Ordinance and the United Nations (Economics Commission for Europe).
Eutrophication	Nitrogen, phosphorous, and organic Matter (COD) emissions to surface water	The current and critical flows for nitrogen, phosphorous, and organic matter (COD) of the ESM method were calculated from measured and estimated concentration in the Rhine river and normalised to total flows in Switzerland. Although these values are uncertain and may not apply to Austria, they were used in this work due to the lack of a better estimation for critical flows.
No CML-IA baseline equivalent	Radioactive emissions to seas Carbon in material consigned to bioreactive landfills Hazardous wastes in underground repositories Radioactive wastes in final repositories	Some non-baseline impact categories may apply, (e.g. Ionising Radiation Potential)

Table 8. Calculation of the RBE indicator

Impact category	ER_i	w_i	$w_i ER_i$	Notes
Abiotic depletion	NA	NA	NA	No critical value available. The impact is reduced to ca. 21.6% of the reference level.
Global Warming (GWP100)	0.460	0.264	0.122	The critical value is an overestimation due to a very strict target defined for industrial emissions of CO ₂ , as opposed to total emissions.
Ozone-layer depletion	0.429	0.107	0.046	
Human toxicity	0.267	0.141	0.038	The ESM interventions PM10, Diesel soot, and Endocrine disruptors are not aggregated, because are not considered by the CML-IA method.
Aquatic ecotoxicity (freshwater)	0.141	0.022	0.003	
Aquatic ecotoxicity (marine)	0.265	0.022	0.006	
Terrestrial ecotoxicity	0.653	0.088	0.058	
Photochemical oxidation	0.236	0.080	0.019	
Acidification	1.833	0.201	0.368	
Eutrophication	17.554	0.074	1.299	Critical values have large uncertainties; values derived from average Swiss emissions to the Rhine river.
RBE			1.958	

Table 9. Scores from the BVP of switchgrass

<i>Category</i>	<i>Criterion</i>	<i>Score</i>	<i>Category</i>	<i>Criterion</i>	<i>Score</i>
Biological nature	Herbaceous	3	Political or legal constraints	Supported/ Subsidised	2
Macromolecular composition	Cellulose/ Hemicellulose	1	Seasonality	All year	3
Water content (%)	< 40	2	Economic value	40-120 €/ton	1
Physical characteristics	Soft and low density materials	2	Market dependency	Medium	2
Available quantities (ton/a)	> 80 000	3	Current applied technology/ destination	Industrial feedstock	0
Geographical concentration (ton/a region)	> 80 000	3	Development stage of upgrade technology	Development	1

Graphical Abstract