

1 **Economic and environmental impact marginal analysis of biorefinery products**  
2 **for policy targets**

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8 ABSTRACT. A simple biofuel production system can be first examined for its policy  
9 compliance in terms of GHG emission reduction target relative to fossil-based  
10 counterparts. More integrated and optimised biorefinery systems with polygeneration  
11 can then be evolved with the aid of graphical analysis of marginal emission savings  
12 vs. additional economic margins. This bottom-up approach helps to achieve greater  
13 GHG emission cut by integrated systems design and thereby setting a more stringent  
14 benchmark to support policies towards achieving climate change mitigation goals.  
15 The combined Economic Value and Environmental Impact analysis is a multi-level  
16 methodology that can be used to represent biorefinery system performances as an  
17 aggregate of differential economic and environmental impact margins of biorefinery  
18 products. The methodology is extended in this paper to support process integration  
19 strategies that allow achieving policy compliance of biorefinery products in terms of  
20 GHG emission savings. An economic and environmental impact profile of the  
21 products is introduced for a graphical visualisation of economic costs and values as  
22 well as deficits and surpluses in environmental impact savings. The effectiveness of  
23 the extended methodology has been demonstrated using a *Jatropha*-based biorefinery  
24 system converting *Jatropha* seed into biodiesel, glycerol and cake, as a case study.

1 The biodiesel produced can achieve 53% emission cut, while glycerol and cake can  
2 achieve an emission cut by 57% by displacing similar functionality respective fossil  
3 based products.

4 Keywords: biorefinery process optimisation, value analysis, environmental impact  
5 assessment, policy support, LCA

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## 8 **1 Introduction**

9 The challenge that emerges while selecting a biorefinery system configuration is  
10 to find the appropriate processing pathways and products from a biomass feedstock  
11 in order to achieve profitability and reduce environmental impact. At the least, a  
12 biorefinery must clearly show economic and environmental added value over a  
13 fossil-based reference system that needs to be displaced. This requires careful  
14 assessment of performances in the early stages of process design (Azapagic, 1999;  
15 Bovea and Pérez-Belis, 2012; Poudelet et al., 2012).

16 As biorefinery configurations become more complex with new process and  
17 product developments, integrating process design and sustainability objectives will  
18 become very challenging. Tools based on process integration methodologies have  
19 been developed for biorefinery design and integration (Ng, 2010; Pham and El-  
20 Halwagi, 2012; Tay and Ng, 2012) and other industrial facilities for cleaner  
21 production (Dunn and Bush, 2001; Klemeš et al., 2010; Munir et al., 2012).  
22 Optimisation frameworks have also been developed for the optimum planning and  
23 design of biorefinery systems (Hosseini and Shah, 2011; Ponce-Ortega et al., 2012;

1 Santibañez-Aguilar et al., 2013). Life cycle assessment (LCA) has also been widely  
2 applied to analyse the energy, greenhouse gas (GHG) emissions and other  
3 environmental impacts of biofuel (Arvidsson et al., 2012; Ekman et al., 2013; Patrizi  
4 et al., 2013) and glucose (Tsiropoulos et al., 2013) production systems. Multicriteria  
5 assessment is also becoming prominent for new systems deployment (Myllyviita et  
6 al., 2012; Ning et al., 2013, Santibañez-Aguilar et al., 2013). However, unlike  
7 relatively stable sectors such as crude oil refining and petrochemical production,  
8 biorefining is a highly dynamic sector. For this sector, feedstock supply systems,  
9 conversion technologies and product portfolios are fast changing together with  
10 environmental policies. Policy targets in the European Union affecting biofuel  
11 production currently require 60% of minimum GHG saving from biofuels with  
12 respect to fossil fuels by 2020 (European Union, 2009). The average reported GHG  
13 emission savings are 30-50% for biofuels from dedicated crops and more than 60%  
14 for biofuels from waste (Smyth et al., 2010).

15 Navigating the wide variation of potential GHG savings requires a  
16 methodological approach that is capable of linking every change at the process level  
17 to overall performance at the system level and that is conceptually explicit,  
18 transparent and consistent with the environmental policy (Jänicke, 2012; Poudelet et  
19 al., 2012; Shin et al., 2008). In this sense, multi-level strategies embracing a life  
20 cycle philosophy are needed to analyse a biorefinery from process streams to whole  
21 systems, such that policies can directly influence process design and vice versa  
22 (D'Alessandro et al., 2010; Hildén, 2011; Jänicke, 2012). Such strategies will allow  
23 the life cycle economic and environmental impact (EI) assessment to be done in a  
24 systematic manner from the smallest element in a biorefinery process network (e.g.  
25 material streams and unit operations) to cradle-to-grave systems. The approach must

1 also allow identification and prioritisation of pathways for process integration and  
2 optimisation that can be linked with the policy targets. Furthermore, a process-based  
3 approach will help process engineers to apply life cycle thinking and adopt it in  
4 decision-support systems (Poudelet, 2012).

5 A conceptual graphical analysis of combined effects for more informed decision  
6 analysis can assist process synthesis, integration and optimisation tasks to generate  
7 process configurations with minimum environmental impacts (Majozi et al., 2006;  
8 Tan et al., 2009; Tjan et al., 2010). A methodology to allow the life cycle economic  
9 value and environmental impact (EVEI) assessments of biorefinery systems has been  
10 presented in Martinez-Hernandez et al. (2013a). The EVEI methodology is extended  
11 in this paper by introducing an economic and environmental impact profile of the  
12 biorefinery products. This profile is a graphical visualisation of economic costs and  
13 values as well as deficits and surpluses in environmental impact savings. The  
14 graphical approach allows a direct comparison with policy targets, and hence allows  
15 setting a more stringent benchmark for policy adaptation. The methodology is  
16 demonstrated by analysing a biorefinery system with *Jatropha curcas* seeds as  
17 feedstock.

## 18 **2 Methodology**

### 19 **2.1 Concepts of EVEI analysis**

20 The value analysis tool has been developed for differential economic  
21 marginal analysis from process streams to networks. It enables evaluation and  
22 graphical presentation of a network margin in terms of the cost of production (COP),  
23 value on processing (VOP) and margins of individual streams (Sadhukhan et al.,  
24 2003, 2008). A stream showing a negative economic margin implies that it would be

1 better (if possible) to purchase that stream from the market rather than produce it  
2 within the process.

3 The evaluation of COP starts from the known market prices of feedstocks and  
4 proceeds stream by stream in the forward direction until end products are reached.  
5 The COP of a stream is the summation of all associated cost components (i.e. the  
6 costs of feedstock, auxiliary raw materials, utilities and annualised capital costs) that  
7 have contributed to the production of that stream. This must mean inclusion of only  
8 those fractional costs involved with the stream's production.

9 The calculation of COP and VOP values is illustrated with reference to Figure 1,  
10 which shows a biorefinery system producing biodiesel, glycerol and cake from  
11 *Jatropha curcas* seeds. In Figure 1, the cost of the feedstock is  $296.3 \text{ \$ t}^{-1}$  and it  
12 enters the process at a rate of  $271200 \text{ t y}^{-1}$ . The first operation it undergoes is  
13 dehushing, which entails total operating and annualised capital costs of  $248\,166 \text{ \$ y}^{-1}$ .  
14 Then, the COP of the outlet stream from the dehushing unit going to the oil  
15 extraction unit is the result of the sum of total cost of feedstock ( $271\,200 \times 296.3 \text{ \$ y}^{-1}$ )  
16 and the total costs of the dehushing unit ( $248\,166 \text{ \$ y}^{-1}$ ) multiplied by an  
17 allocation factor  $\alpha$  (0.9478) and divided by the mass flow rate of the stream:  $(271$   
18  $200 \times 296.3 + 248166) \times 0.9478 / 179800 = 424.9 \text{ \$ t}^{-1}$ . Similar calculations proceed  
19 forward for each stream as it travels through the process.

20 The VOP evaluation proceeds in the backward direction from the end product market  
21 prices until the feedstock in a process network is reached. The VOP of a stream at a  
22 point within the process is obtained from the prices of products that will ultimately  
23 be produced from it, minus the costs of auxiliary raw materials and utilities and the  
24 annualised capital cost of equipment that will contribute to its further processing into

1 these final products. For example, in Figure 1, the glycerol product and the stream  
2 going to the distillation unit are the outlet streams from the decantation unit, which  
3 entails total operating and annualised capital costs of 49 160 \$ y<sup>-1</sup>. Then, the VOP of  
4 the inlet stream to the decantation unit is the result of the value of the glycerol  
5 product (10 700×881.8 \$ y<sup>-1</sup>) plus the value of stream going to the distillation unit  
6 (105 300×637.3 \$ y<sup>-1</sup>) minus the total costs of the decantation unit (49 160 \$ y<sup>-1</sup>) and  
7 divided by the mass flow rate of the stream: (10 700×881.8+105 300×637.3–49 160)  
8 /116 200=658 \$ t<sup>-1</sup>. Note that the COP of a feedstock to a process and the VOP of an  
9 end product correspond to their respective market prices.

10           Equivalent to the COP and VOP, the environmental impact (EI) cost of  
11 production and EI credit from fossil-based product displacement can also be  
12 evaluated stream by stream, in order to understand quantitatively the origins of  
13 environmental impacts and the opportunities for reduction through modification of  
14 process configurations. A stream with a positive environmental impact margin  
15 (difference between EI credit and EI cost) would indicate that there are EI benefits  
16 from its processing, while a stream with a negative EI margin would indicate that its  
17 production generates more EI than the EI credit obtained. This basic concept allows  
18 the analysis of the performance of biomass-based products from a biorefinery with  
19 respect to counterpart fossil-based products. A stream with a negative EI margin  
20 would be better (if possible) bought in from a process that produces it with a positive  
21 EI margin. When this is not possible but it has economic value, its production  
22 pathway must be improved by process integration and using energy and raw  
23 materials with a lower embodied EI.

1 In a cradle-to-grave life cycle approach (including biomass production system,  
2 biorefinery process, transportation and end use of products), the CO<sub>2</sub> captured during  
3 photosynthesis, direct wastes and emissions can be taken into account within the EI  
4 variables of feedstock and products. The EI cost (GHG as CO<sub>2</sub> equivalents) of  
5 feedstock  $I_f$  is made up of the CO<sub>2</sub> binding by photosynthesis ( $B_f$ ), the EI cost from  
6 transportation ( $T_f$ ) and EI cost from production ( $G_f$ ), shown in Eq. 1. This equation  
7 shows that for a biorefinery to be environmentally feasible,  $B_f$  must be greater than  
8 the EI added to the system by  $G_f$  and  $T_f$ .

$$I_f = G_f + T_f - B_f \quad (1)$$

9 In that case,  $I_f$  is negative, indicating feasibility of an overall biorefinery system  
10 and that the GHG emission is reduced due to CO<sub>2</sub> capture during photosynthesis.  
11 When the various crop fractions are utilised in a biorefinery e.g. Jatropha oil for  
12 biodiesel and seed husks for combined heat and power, the CO<sub>2</sub> binding may need to  
13 be allocated to various products. This is carried out by carbon content of the products  
14 shown in Table 3 for cake and husk. The carbon content of biodiesel and glycerol is  
15 calculated from compositions resulting from process simulation in section 3.2.

16 The EI credit value of a biorefinery product is the net avoided emission, shown  
17 in Eq. 2. The EI credit value of a biorefinery product ( $D_p$ ) is made up of the emission  
18 from an equivalent product being replaced ( $I_{peq}$ ), multiplied by a unitless equivalency  
19 factor  $\beta$ , minus end use or end of life emissions ( $I_{end}$ ) and the EI cost from  
20 transportation ( $T_p$ ). Emissions from end use or end of life are, for example, the  
21 emissions from combustion of fuel products when used to operate a car or the  
22 emissions from product decomposition disposed in landfill. An equivalent product is  
23 an existing product that can deliver the same functionality or service as the

1 biorefinery product.  $\beta$ , for example, is the ratio between the heating value of a  
2 biofuel produced from a biorefinery (e.g. biodiesel) and that of an equivalent fossil  
3 based fuel (e.g. diesel).

$$D_p = \beta \times I_{peq} - T_p - I_{end} \quad (2)$$

4 This equation shows that for a biorefinery product having environmental  
5 advantage over a fossil-based counterpart,  $D_p$  must be positive. Analogous to the  
6 economic cost of the feedstock,  $I_f$  represents the EI ‘cost’ of the feedstock. Hence,  $I_f$   
7 is the starting point for forward calculation of EI cost of the intermediate and product  
8 streams in a process network, as further explained in the following section.

9 Analogous to the selling price of a product,  $D_p$  represents the environmental impact  
10 credit of a stream. Hence,  $D_p$  is the starting point for the backward EI credit  
11 calculations of intermediate streams and feedstocks in a process network.

## 12 **2.2 Modelling of streams**

13 Equivalent to streams’ economic performance indicators, VOP and COP, their  
14 EI indicators are their individual impact Credit Value on Processing (CVP) and  
15 Impact Cost of Production (ICP), respectively. As noted above, for a final product,  
16  $CVP = D_p$ . For an initial feedstock,  $ICP = I_f$ .

17 *VOP and CVP of streams.* Since VOP and CVP of a biorefinery end product are  
18 known from reported market prices and embodied EI of an existing product being  
19 replaced, respectively, the calculation proceeds backwards from the end products  
20 towards the feedstock. Consider  $\bar{V}$  as a vector containing VOP and CVP of a feed  
21 stream  $f$  to a process unit  $k$  (excluding auxiliary raw materials to avoid double  
22 accounting in Eq. 3). The vector of values of the feeds (i.e. the inlet streams) can be



1 calculated from the known vector of values of the products (i.e. the outlet streams)  $p$   
 2 minus the total costs  $\bar{O}_k$  of process unit  $k$  through Eq. 3:

$$\bar{V}_f = \left[ \sum_{p=1}^q \bar{V}_p P_p - \bar{O}_k \right] / \sum_{f=1}^g F_f \quad (3)$$

3  $P_p$  and  $F_f$  corresponds to the mass flow rates of product (outlet stream) and feed  
 4 (inlet stream), respectively.

5 *COP and ICP of streams.* The ICP of an outlet or product stream from a process  
 6 unit represents the EI incurred from its production. To evaluate the ICP of a product  
 7 or outlet stream from a process unit, the operating and construction EI costs of the  
 8 process unit are added to the total ICP of the feed and divided by the product mass  
 9 flow rate. The COP of a product stream is evaluated in the same way using the  
 10 corresponding economic variables.  $\bar{C}$  in Eq. 4 is a vector containing the costs (COP  
 11 and ICP) of a product (outlet stream)  $p$  from a process unit  $k$  (excluding emission and  
 12 waste streams to avoid double accounting in Eq. 4).  $\bar{C}$  can be predicted for a product  $p$   
 13 (outlet stream) with allocation factor  $\alpha$  from the known vector of costs of the feeds  
 14 (inlet streams) and total costs of process unit  $k$ :

$$\bar{C}_p = \left[ \sum_{f=1}^g \bar{C}_f F_f + \bar{O}_k \right] \alpha / P_p \quad (4)$$

15 The economic operating costs ( $O_k$ ) of a process unit consist of the costs of  
 16 utilities, auxiliary raw materials and the disposal or treatment cost of any  
 17 emission/waste stream produced. The analogous operating EI cost is indicated by  
 18  $IO_k$ . The capital cost can be estimated from equipment sizing and annualised using a  
 19 capital charge determined from the net present value, internal return rate and

1 discounted cash flow calculations (Sadhukhan et al., 2008). The total impact from  
 2 construction can be also estimated from equipment sizing and the type of materials  
 3 and their EI, and then annualised using the life time of a facility. The annualised  
 4 economic capital cost and EI costs of construction are fixed costs that can be added to  
 5 the operating costs to determine the total costs of a unit as shown in Eq. 5.

$$\bar{O}_k = \begin{bmatrix} O_k \\ IO_k \end{bmatrix} = \begin{bmatrix} \bar{C}_{a,k} \\ \bar{I}_{a,k} \end{bmatrix} \times \bar{A}_k + \begin{bmatrix} \bar{C}_{u,k} \\ \bar{I}_{u,k} \end{bmatrix} \times \bar{U}_k + \begin{bmatrix} \bar{C}_{m,k} \\ \bar{I}_{m,k} \end{bmatrix} \times \bar{M}_k + \begin{bmatrix} CC_k \\ CI_k \end{bmatrix} \quad (5)$$

6  $\bar{O}_k$  denotes total costs of a process unit as function of process variables.

7  $\bar{A}_k$ ,  $\bar{U}_k$  and  $\bar{M}_k$  represent single column vectors of mass flow rates of auxiliary  
 8 raw materials, utilities and emissions/wastes, respectively.

9  $\bar{C}_{a,k}$ ,  $\bar{C}_{u,k}$  and  $\bar{C}_{m,k}$  are single row vectors containing economic costs, while  $\bar{I}_{a,k}$ ,  
 10  $\bar{I}_{u,k}$  and  $\bar{I}_{m,k}$  are a one row vector containing the respective EI costs.

11  $CC_k$  and  $CI_k$  are annualised capital cost and annualised EI from construction,  
 12 respectively.

13 The inclusion of the costs from emissions and auxiliary raw materials in the total  
 14 costs allows their allocations amongst process streams and propagation towards end  
 15 streams in both directions. The allocation factor ( $\alpha$ ) shown in Equation 4 is  
 16 determined in case of multi-output process units. For a stream from single output  
 17 units  $\alpha=1$ . Various approaches or methods can be used for the allocation of costs and  
 18 EI including allocation by mass, energy content, carbon content and economic value  
 19 (Dalgaard et al., 2008; Heijungs and Frischknecht, 1998; Kim and Dale, 2002).  
 20 Amongst these methods, mass or carbon content does not indicate energy outputs  
 21 from various energy products, hence is not effective for the allocation of impacts

1 between energy products. The allocation by economic value using VOP has been  
2 adopted here. The reason for this is that VOP allows capturing the interactions  
3 between the economic and environmental values. If the trends in the two values can  
4 be merged together, such that environmentally sustainable products are also  
5 economically profitable products, then the economic value can be regarded as a good  
6 indicator for impact allocation.

7 The difference between  $\bar{V}$  and  $\bar{C}$  of a stream provides its margins ( $\Delta$ ): economic  
8 margin,  $\Delta e = \text{VOP} - \text{COP}$ , and avoided emission or EI saving,  $\Delta i = \text{CVP} - \text{ICP}$ . When  
9 the aim is to improve the percentage GHG savings, hence addressing policy targets  
10 of biorefinery products with reference to fossil-based equivalent products (European  
11 Union, 2009; US Congress, 2007) the relative percentage of EI savings ( $s_p$ ) of a  
12 product can be calculated using Eq. 6.

$$s_p = \frac{\Delta i}{(I_{peq} \times \beta)} \times 100 \quad (6)$$

13 Built upon the principles of environmentally friendly process design with the  
14 most efficient use of energy, raw materials and capital, process integration tools help  
15 to identify a network's bottleneck and shift loads (e.g. energy / water / materials /  
16 environmental impact) from constrained to unconstrained parts for overall improved  
17 performance (Majozi et al., 2006; Ng, 2010, Tan et al., 2009; Tjan et al., 2010). In  
18 order to facilitate compliance with existing legislation, it is possible to shift the  
19 environmental burden from one product to another following a process integration  
20 approach. Consideration of the network connectivity integrates process operations,  
21 economic and environmental indicators to policy drivers. The concepts and  
22 methodological procedures developed above along with the construction of an EVEI

1 profile, presented in the next section, can be effectively used for the targeting of  
2 avoided emissions for future low carbon adaptation under a strict policy scenario.

### 3 **2.3 EVEI profile of a product**

4 An EVEI profile represents the cumulative economic, environmental impact  
5 costs and values and the resulting margins for a biorefinery product. This graphical  
6 representation allows identification of the “distance to target” and quantification of  
7 any deficit or excess of EI savings with respect to a policy target and also the  
8 resulting economic or environmental compromises from any option for performance  
9 improvement. A generic EVEI profile is presented in Figure 2, featuring the  
10 following:

#### 11 **Figure 2**

- 12 • *Costs composite curve* is a plot of cumulative EI costs versus economic costs  
13 from the feedstock, auxiliary raw materials, utilities, process emissions and fixed  
14 costs (annualised capital costs or EI cost from construction) allocated to a  
15 particular product. These costs are plotted as in the order given in a plot of EI in  
16 the y-axis and economic value (EV) in the x-axis. In Figure 2, a steeper slope of  
17 the contributions from utilities and auxiliary raw material compared with  
18 feedstock indicate higher EI contribution per \$ spent, while a very small slope of  
19 process emissions and fixed costs indicates that there is low EI contribution per  
20 \$ spent.
- 21 • *EI cost limiting line* indicates a benchmark for the EI cost target from the  
22 production of a biorefinery product established from policy. The limiting line  
23 starts at (0,0) and the end point is  $(COP_p \times P_p, ICP_{p, limit} \times P_p)$ .  $ICP_{p, limit}$  is  
24 determined using Eq. 6 for the percentage EI saving set by the policy target

1  $(s_{p,target})$  and the definition of  $\Delta i = CVP - ICP$  as:  $ICP_{limit} = CVP - (s_{p,target} \times I_{peq} \times \beta /$   
2 100).

- 3 • *Value line* is a horizontal line drawn from the EI-axis to the point of total EI  
4 credit value ( $CVP_p \times P_p$ ) against the total economic value on processing  
5 ( $VOP_p \times P_p$ ). This line indicates a reference limit to get positive economic and EI  
6 saving margins.
- 7 • *Product EI saving surplus/deficit* is the distance from the value line to the end of  
8 the limiting line indicating the EI saving margin required to meet the policy  
9 target. The distance from the end point of the costs composite curve and the  
10 limiting line determines the difference between the EI saving margin achieved  
11 and the policy target. If the composite curve is below the limiting line, then there  
12 is a surplus EI saving and then stricter policy target for GHG emission reduction  
13 could be met.

14 The application of the EVEI methodology developed above and the use of  
15 product EVEI profiles to analyse options for accomplishing policy targets is  
16 demonstrated in a case study presented in the next section.

### 17 **3 Case study**

18 The Jatropha-based biorefinery configuration in Figure 1, producing  $100 \text{ kt y}^{-1}$   
19 of biodiesel and the corresponding amounts of glycerol, seed cake and husk, has been  
20 selected as case study. The context is that it is located in Mexico within the radius of  
21 a Jatropha plantation in the state of Michoacan. The current 50% GHG emission  
22 reduction target set in US policies (as of 2012) for biofuel production (US Congress,  
23 2012) is the reference point used in the analysis for policy compliance and applied to  
24 all the products. The seeds are assumed to be produced by non-toxic Jatropha

1 provenances native to Mexico. Therefore, seed cake can be used as animal feed. The  
2 various modelling approaches for each biorefinery subsystems are described as  
3 follows.

### 4 **3.1 Feedstock production model**

5 The EI results for Jatropha seeds production system, deduced from the  
6 inventory data given in Table 1, are shown in Table 2. Jatropha cultivation model  
7 (Martinez-Hernandez et al., 2013b.) shows nitrogen fertilisation as the hot spot of  
8 this stage of the Jatropha-based biorefinery system. Since nitrogen fertilisation is a  
9 hot spot in the system and an important decision variable, two different fertilisation  
10 rates were studied to track the effect of reducing current fertilisation rate. It can be  
11 observed that estimated yield from models correlating yield to average annual  
12 rainfall and nitrogen fertilisation is not significantly affected by the reduction in  
13 fertilisation rate resulting in lower EI cost of production.

14 **Table 1**

15 **Table 2**

### 16 **3.2 Biorefinery process model**

17 Models for seed processing were developed in a spreadsheet, while Jatropha oil  
18 conversion into biodiesel was simulated in the commercial process simulation  
19 software Aspen Plus<sup>®</sup> (Aspen Technology, 2012). The heating values of Jatropha  
20 fruit fractions used for mass and energy balance calculations are shown in **Table 3**.  
21 The overall mass balance of the biorefinery process is presented in Figure 1. The  
22 process consists of seed dehusking producing husk as a substitution fuel for natural  
23 gas. The seed kernels are oil extracted, with seed cake meal co-produced as a protein  
24 source substituting soy meal. The oil undergoes transesterification with methanol

1 using heterogeneous catalyst, which allows flexibility on free fatty acid content in the  
2 feedstock and high conversion into biodiesel and high purity glycerol. Methanol is  
3 recovered by distillation and recycled to the transesterification reactor. Glycerol is  
4 separated by decantation and sold to the market, replacing glycerol from fossil  
5 resources.

### 6 **Table 3**

7 The simulation flowsheet of Jatropha oil conversion into biodiesel is shown in  
8 Figure 3. Oil was modelled as a mixture of tryglycerides (TG) made up of triolein,  
9 tripalmitin, trilinolein and tristearin and free fatty acids (FFA, modelled as oleic  
10 acid). Properties of these components and the corresponding fatty acid methyl esters  
11 (FAME) were not available in the Aspen Plus database. The basic properties (e.g.  
12 molecular weight, density, molecular structure) were introduced and the UNIFAC-  
13 Dortmund physical property model was used for predicting remaining properties.  
14 The oil composition and process specifications for the simulation model are  
15 presented in Martinez-Hernandez et al. (2013b). Table 4 summarises the simulation  
16 results.

### 17 **Figure 3**

### 18 **Table 4**

19 Heat integration was carried out to **reduce** the utility requirements as shown in  
20 Figure 2. Composite curves were used with a minimum temperature difference of  
21 10°C between hot and cold streams in the heat exchangers to carry out heat  
22 integration. The following heat integration opportunities identified were also  
23 simulated in Aspen Plus as shown by the dashed lines in Figure 3. The reaction mix  
24 stream is preheated (from 26°C to 70°C) by the bottom stream of the methanol

1 recovery column (from 167°C to 135°C). The crude biodiesel stream fed to the  
2 distillation column can also be preheated (from 25 to 301°C) by the distillate  
3 biodiesel stream (at 317°C cooled to 35°C), thus reducing reboiler duty. The heat  
4 requirements after heat integration were used for the inventories. The operating  
5 inventories and costs are shown in Table 5.

6 The process models developed by Martinez-Hernandez et al. (2013b) are used to  
7 show how a bottom-to-top level analysis can be carried out to comply with and, at  
8 the same time, inform the policy targeting in the case study that follows. Note that  
9 the previous work uses LCA to assess alternatives for more complex biorefinery  
10 schemes by focusing on environmental impact. In the present work, the combined  
11 economic and EI analysis was carried out for the biodiesel production process only.

### 12 **3.3 Other assumptions**

13 From the predicted seed yield of 4213 kg ha<sup>-1</sup> (Table 2) and the total seed  
14 requirement of 271.2 kt y<sup>-1</sup> (Figure 1), the total land use is 64385 ha y<sup>-1</sup>. Thus, a  
15 transportation distance of 14.3 km is obtained assuming a circular shape of the  
16 cultivation land. The same distance is assumed for seed cake and husk being used  
17 locally. For transportation of other products and materials, the distance is assumed to  
18 be 100 km.

19 The EI from construction materials was estimated assuming that process  
20 equipment is made up of 70% steel and 30% aluminium. The mass of steel was  
21 estimated from the preliminary equipment sizing (Turton et al., 2009). Distillation  
22 columns were sized using the built-in feature in Aspen Plus® for such purpose.  
23 Then, the weight of the vessels was determined using a weight calculator tool  
24 (MatWeb LLC, 2012). The weight of dehusking machines was estimated from



1 vendor data. Cost of vessels, pumps and heat exchangers were estimated using the  
2 CapCost software tool (Turton et al., 2009). Prices were levelised using the Chemical  
3 Engineering Plant Cost Index (CEPCI) reported in the Chemical Engineering  
4 Magazine (2012). The cost of transesterification, decantation and distillation units in  
5 the biodiesel process includes pumps and heat exchangers around main equipment.  
6 The resulting total fixed costs (capital and EI from construction) of the units are  
7 summarised in Table 5. To annualise the economic and EI costs of the process units,  
8 the operation time of  $7920 \text{ h y}^{-1}$ , capital interest rate of 10% and plant life time of 15  
9 years were assumed. The resulting annual capital charge ratio was 0.1315.

## 10 **Table 5**

## 11 **4 Results and discussion**

### 12 **4.1 EVEI results and overall biorefinery performance**

13 The VOP, COP and  $\Delta e$  from the EVEI modelling of the streams are presented in  
14 Figure 1. The biodiesel cost of production (COP) was estimated as  $627.7 \text{ \$ t}^{-1}$  or  $0.55$   
15  $\text{ \$ L}^{-1}$  ( $7.44 \text{ MX\$ L}^{-1}$ ,  $1 \text{ \$}=13.5 \text{ MX\$}$ ), which means it has the potential to be  
16 competitive with petro-diesel prices in Mexico ( $10.81 \text{ MX\$ L}^{-1}$ , August 2012). The  
17 methanol recycle has been considered as a utility stream for units 3 and 4 considering  
18 its market price (i.e.  $27.2 \times 1000 \times 372.1 = 10,121,120 \text{ \$ y}^{-1}$ ). For unit 4 (methanol  
19 recovery), the total costs are recalculated as  $O_4'$  by subtracting the economic value of  
20 the methanol recycle. For unit 3 (transesterification), the methanol recycle presents  
21 an additional cost. Thus  $O_3'$  is calculated by adding the economic value of the  
22 methanol recycle to  $O_3$ . The total treatment cost of the oily waste is included in the  
23 total cost of the biodiesel distillation unit (number 6).

1 The calculations of EI cost of feedstock and EI credit value of the products are  
2 shown in Table 6. These values are required to calculate EI cost of production (ICP)  
3 for intermediate streams and end products and EI credit value (CVP) for intermediate  
4 streams and feedstock. Calculations for intermediate streams are exemplified in  
5 Table 7. CO<sub>2</sub> emissions from the processing and end use (e.g. combustion) were  
6 considered as balanced as they originate from the carbon contained in Jatropha seeds.  
7 Within this system's boundaries (from seed production to product distribution point),  
8 Eq. 1 reduces to  $I_f = G_f + T_f$  while Eq. 2 reduces to  $D_p = \beta \times I_{peq} - T_p$ . These are the  
9 equations used to calculate the values shown in Table 6. However, the CO<sub>2</sub> from the  
10 carbon atoms added from fossil-based methanol to methyl esters in biodiesel is  
11 accounted (0.157 kg CO<sub>2</sub> kg<sup>-1</sup>) as shown in Table 6. For seed husk, the heating value  
12 in Table 3 is used as a factor to convert  $D_p$  from kg MJ<sup>-1</sup> to kg kg<sup>-1</sup>.

### 13 **Table 6**

14 The CVP, ICP and  $\Delta i$  are shown in Figure 4. The oil extracted has an ICP (CO<sub>2</sub>  
15 equivalent) of 1.497 kg CO<sub>2</sub>-eq kg<sup>-1</sup> based on the ICP of the incoming seed kernel of  
16 0.909 kg CO<sub>2</sub>-eq kg<sup>-1</sup>, to which is added the fractional EI cost of the utilities and  
17 equipment construction materials using allocation factor and stream mass flow rates  
18 (i.e.  $(0.909 \times 179800 + 30572) \times 0.8079 / 104700 = 1.497$  kg CO<sub>2</sub>-eq kg<sup>-1</sup>). Similarly,  
19 working backwards from the end, the CVP of the stream entering the biodiesel  
20 distillation is 2.605 kg CO<sub>2</sub>-eq kg<sup>-1</sup>, based on the biodiesel CVP minus the total EI  
21 costs of the unit (including EI from oily waste) and the stream flow rates (i.e.  
22  $(2.779 \times 100000 - 3652) / 105300$ ). Table 7 further exemplifies EVEI calculations.

### 23 **Figure 4**

### 24 **Table 7**

1           The economic and environmental impact profiles for the biorefinery marketable  
2 products are shown in Figure 5a and 5b, respectively. The areas between the values  
3 and costs of each product represents its economic margin and potential EI saving.  
4 The sum of areas represents the total biorefinery margins. The profiles show that the  
5 biorefinery is profitable and that all the products provide EI savings (thus, streams  
6 are sustainable according to this criterion).

## 7 **Figure 5**

### 8 **4.2 Policy compliance and EVEI profiles**

9           Substituting  $\beta$ ,  $I_{peq}$  and  $\Delta i$  into Eq. 6, the following % EI savings of end products  
10 are calculated: Biodiesel with respect to petro-diesel = 32%; Glycerol with respect to  
11 fossil-based glycerol = 36% and seed cake with respect to soy meal =31.5%. These  
12 values are lower than the minimum GHG emission reduction target of 50%. Thus,  
13 improvements in the biorefinery process system are required in order to meet the  
14 targets for these two products. The only product that can meet the policy target is  
15 seed husk (used as fuel), which achieves 90.5% savings with respect to natural gas,  
16 well beyond the required target of 50%. This gives scope to move some of this  
17 excess saving to other products, in order that the savings with which these other  
18 products are credited can meet policy targets. This is equivalent to shifting heating  
19 loads within a heat exchanger network to ease bottlenecks without altering the  
20 overall heat recovery of the network. It thus provides a practical approach to meeting  
21 targets in biorefineries that might on the surface appear to be incapable of delivering  
22 policy targets. It also provides targeted guidance for optimal sources of additional  
23 savings if shifting of existing savings is inadequate.

## 24 **Figure 6**

1           Figure 6 shows the EVEI profile of biorefinery products in the base case system.  
2           A composite factor ( $\alpha'$ ), determined from the product of allocation factors of the  
3           outlet streams ( $\alpha$ ) from each process unit in a product path, is used to calculate the  
4           fractional costs for a particular product as shown in Table 8. These factors are used  
5           to generate the data points in the EVEI profile of a product as shown for the  
6           economic costs allocated to biodiesel in Table 9. The data points for EI costs are  
7           determined following a similar approach. The composite factors ( $\alpha'$ ) will change with  
8           any change in economic value of the streams as they determine the allocation factors  
9            $\alpha$ . The data points for the value and the limiting lines are determined as discussed in  
10          Section 2.3.

11          It can be observed that biodiesel fails to meet the policy target with a deficit in  
12          EI saving of 52.3 kt CO<sub>2</sub>-eq y<sup>-1</sup>. Glycerol incurs a deficit by 5.5 kt CO<sub>2</sub>-eq y<sup>-1</sup> while  
13          the deficit from seed cake is 10.1 kt CO<sub>2</sub>-eq y<sup>-1</sup>. Husk exhibits EI saving surplus of  
14          38.5 kt CO<sub>2</sub>-eq y<sup>-1</sup>. If the surplus savings of seed husk are shifted to make up for the  
15          deficits of biodiesel and glycerol, there is still an overall deficit of about 29 kt CO<sub>2</sub>-  
16          eq y<sup>-1</sup>. As the values are interrelated by the EVEI models, the EI saving across the  
17          products can be more evenly distributed and improved by integration strategies. In  
18          Figure 6, the segment with the highest contribution to EI in the cost composite curve  
19          corresponds to the feedstock (labelled as number 1) for all the products. The  
20          segments corresponding to utilities and auxiliary raw materials are also important  
21          contributors to the EI value for the composite curve of biodiesel and glycerol.  
22          Contribution of utilities is not significant for cake production, while only feedstock  
23          EI is relevant for husk EI. These results provide insights into the utilisation of waste  
24          and by-product streams for low impact utility generation.

1 **Table 8**

2 **Table 9**

### 3 **4.3 Process integration and policy support**

4 Streams with potential as fuels for utility supply were ranked from the lowest to  
5 the highest EI saving ( $\Delta e$ ) in order to sequentially apply process integration  
6 strategies: oily waste < husk < seed cake < glycerol. The EVEI analysis results of  
7 modifications a-d below are summarised in Table 10.

- 8 a. Decrease the nitrogen fertilisation rate from  $162 \text{ kg ha}^{-1}$  to  $100 \text{ kg ha}^{-1}$  (Table  
9 2). This modification increased the % saving of all the products. However, the  
10 50% EI saving target for biodiesel, glycerol and cake was not met and thus  
11 modifications b and c were required.
- 12 b. The heat from oily waste stream can be recovered into steam generation for the  
13 methanol and biodiesel distillation columns' reboilers. The total heat in the oily  
14 stream (with a heating value of  $39.63 \text{ MJ kg}^{-1}$ ) is  $209\,266 \text{ GJ y}^{-1}$ . Thus, the heat  
15 requirements for the distillation units of  $148\,833 \text{ GJ y}^{-1}$  can be supplied at an  
16 energy efficiency of 71%. The EI saving margins were increased for all the  
17 products and the policy target is only achieved for glycerol (Table 10) but the  
18 modification was not enough to achieve the target for biodiesel and cake.
- 19 c. Further, a portion of seed husk needs to be used for heat generation for the oil  
20 extraction unit. Since any process modifications affect cost of units, the VOP  
21 results and allocation factors are also affected. The calculation of amount of  
22 husk required to meet biodiesel policy target saving of 50% is iterative. The  
23 solver function in Excel was used to estimate the husk requirement. The EI  
24 saving deficit of bioethanol ( $5.7 \text{ kt CO}_2\text{-eq y}^{-1}$ , after modifications a and b) is  
25 divided by total allocation factor of bioethanol (0.6735, after modifications a and

1 b). This gives an estimate of 8.47 kt CO<sub>2</sub>-eq y<sup>-1</sup> that needs to be saved by  
2 replacing steam from natural gas with steam from husk. Then, an estimate for  
3 husk requirement to give the same heat duty as the natural gas is calculated. The  
4 calculation uses the EI of natural gas (0.06117 kg CO<sub>2</sub>-eq MJ<sup>-1</sup>), heat generation  
5 efficiency of natural gas (0.7), heating value of husk (19.86 MJ kg<sup>-1</sup>) and heat  
6 generation efficiency of husk (0.6). The initial value of husk requirement is  
7 obtained as follows:  $8.47 / (0.06117 / 0.7) / (19.86 \times 0.6) = 8.1 \text{ kt y}^{-1}$ . The Excel  
8 Solver gives the final value of husk requirement of 8.2 kt y<sup>-1</sup> that replaces 36.5%  
9 of the heat demand by the oil extraction unit: The boiler annualised capital cost  
10 and revenue losses from the use of husk can be balanced off by the economic  
11 cost saving due to natural gas replacement. As shown in Table 10, all the  
12 products achieved EI saving equal to or greater than 50% in relation to the  
13 corresponding fossil-based product being displaced.

14 The cost of production of biodiesel was decreased from 627.7 \$ t<sup>-1</sup> in the  
15 initial system to 621.6 \$ t<sup>-1</sup> after the modifications a-c. This is due to a net  
16 saving of about 0.8 M\$ y<sup>-1</sup> from the integrated use of oily waste and husk for  
17 heat generation. The net positive EI saving is 65 kt CO<sub>2</sub>-eq y<sup>-1</sup>. Thus the total  
18 biorefinery margin is increased from 7.0 M\$ y<sup>-1</sup> to about 7.8 M\$ y<sup>-1</sup> (11%  
19 increase) and the EI savings from about 213 kt CO<sub>2</sub>-eq y<sup>-1</sup> to 278 kt CO<sub>2</sub>-eq y<sup>-1</sup>  
20 (30% increase) with respect to the initial system.

21 Figure 7 shows the effect of improvements “a” to “c” in the costs composite  
22 curve of all the biorefinery products. The curve for biodiesel (Figure 7a) is  
23 shown displaced downwards to the limiting line indicating that policy target can  
24 be met. Glycerol, cake and husk display significant surpluses. Note that the  
25 value line for husk (Figure 7d) is also displaced downwards and to the left,

1           indicating the revenue loss and reduction of total EI saving due to use of husk  
2           within the system. The EI saving from utility supply from husk has been shifted  
3           and distributed to the other biorefinery products.

4    d.     Further improvement could be realised by generating the entire heat required  
5           by the oil extraction unit using husk. The effect on the performances is analysed  
6           as in the case of improvement c and the final results are shown in Table 10 under  
7           modification “a to d”. It can be observed that EI savings are increased for  
8           biodiesel to 53% and for glycerol and cake to 57%. The total biorefinery  
9           economic margin remains the same after modifications a-c. The total biorefinery  
10          EI savings are 281 kt y<sup>-1</sup>, a 32% increase with respect to the initial system.

11           As shown in Table 10, the saving from husk relative to its fossil counterpart  
12          remains the same after modifications; this is because the total EI saving from husk  
13          replacing natural gas is reduced in the same proportion as the mass flow rate utilised  
14          within the process as fuel. In addition, utilisation of husk does not modify  
15          performance of the dehusking unit itself as most of the energy generated from husk is  
16          used downstream, affecting the performances of the rest of the units and their  
17          products. It is this propagation towards all the product pathways that allows  
18          achieving the targets for all the products. Thus, improvement implemented at a  
19          certain upstream process unit will improve the EI saving of the products derived  
20          from that unit and from its downstream process units.

21          Figure 8 shows the integrated flowsheet after modifications a to c showing the  
22          integration of steam generation from oily waste and husk to achieve the 50% GHG  
23          emissions reduction target by all products.

24          **Figure 7**

25          **Table 10**

## 1 **5 Conclusions**

2 Economic value analysis results can be combined with environmental impact  
3 analysis results for more integrated process design and decision making. The EI  
4 analysis has been illustrated in the current work using the global warming potential  
5 as a criterion. However, in principle, any environmental impact characterisation can  
6 be presented in the same way as the global warming potential, alongside the  
7 economic assessments. The EVEI tool has proved to be useful to evaluate options for  
8 improvement of biorefinery process designs from differential product EV and EI  
9 marginal analysis. By using a multi-level strategy, the tool is capable of capturing the  
10 effects of process and market variables on the marginal values. Both empirical and  
11 fundamental thermodynamic-based models can be integrated, allowing handling of  
12 non-linear models in the EI allocation problems.

13 Integration strategies similar to those used in the case study can be developed for  
14 a scenario where the rebalancing of EI to achieve policy targets entails an economic  
15 cost – the benefit of meeting the target would then need to be balanced against the  
16 economic cost. Simultaneously, holistic process integration can be applied for  
17 integrated biorefinery design, since not only can the EI be reduced, but also the  
18 emission reduction targets can be increased and a higher biorefinery economic  
19 margin can be obtained. For stricter emission reduction policies in the future,  
20 conversion of husk into methanol, heat and power for the biodiesel production  
21 process could be considered. Analysis including carbon credit trading could also be  
22 used to determine the investment incentives for integrated biorefinery systems.

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