

1 **Analysis of cost-environmental trade-offs in biodiesel production incorporating waste**  
2 **feedstocks: a multi-objective programming approach**

3 Carla Caldeira<sup>\*,a,b,1</sup>, Fausto Freire<sup>a</sup>, Elsa A. Olivetti<sup>c</sup>, Randolph Kirchain<sup>d</sup>, Luís Dias<sup>b,e</sup>

4 <sup>a</sup> ADAI-LAETA Department of Mechanical Engineering, University of Coimbra, Polo II, Rua Luís  
5 Reis Santos, 3030-788 Coimbra, Portugal

6 Email: caldeira.carla@gmail.com; fausto.freire@dem.uc.pt

7

8 <sup>b</sup> INESC-Coimbra University of Coimbra, Polo II, Rua Sílvio Lima 3030-290 Coimbra, Portugal

9

<sup>c</sup> Department of Materials Science & Engineering, Massachusetts Institute of Technology, 77  
Massachusetts, Cambridge, MA 02139, USA

10 Email: elsao@mit.edu

11

<sup>d</sup> Materials Systems Laboratory, Massachusetts Institute of Technology, 77 Massachusetts Avenue,  
Cambridge, MA 02139, USA

12 Email: kirchain@mit.edu

13

14 <sup>e</sup> CeBER and Faculty of Economics, University of Coimbra, Av Dias da Silva 165, 3004-512

15 Coimbra, Portugal

16 Email: lmcdias@fe.uc.pt

17

18

---

<sup>1</sup> Present address: Joint research Centre of the European Commission, Directorate of Sustainable Resources, Bioeconomy Unit, Ispra, Italy

19 **Abstract**

20 Decision-makers in government and industry must develop policy and strategy for highly  
21 complex systems, trading off competing objectives such as environmental and economic  
22 impact. These trade-offs can be difficult to analyze, which may lead to misinformed  
23 choices. There is lack of decision support tools that both include multiple objectives and  
24 facilitate communication to decision-makers in a comprehensive and simple way. To  
25 address this gap, a mathematical model that facilitates the decision process by allowing an  
26 agent to decide based on an explicit overall economic and environmental performance but  
27 simultaneously visualize graphically the trade-offs among the different objectives was  
28 developed. This model was used to assess the trade-offs of using waste-based feedstocks in  
29 blends with conventional feedstocks for biodiesel production, and explore opportunities to  
30 improve biodiesel cost effectiveness whilst managing environmental impacts, particularly  
31 in the feedstock selection process. The compositional uncertainty of the feedstocks is  
32 considered in the model ensuring that the final quality of the biodiesel is not compromised  
33 by the high uncertainty associated with the composition of waste materials. Reductions on  
34 production costs (3%) and on environmental impacts (from 2% to 32%) were obtained  
35 using this model to select the blend composition. The model was shown to be useful to  
36 inform decision-making by allowing comprehensive, simplified visualization of the trade-  
37 offs among cost and environmental impacts. The model can be used to support biodiesel  
38 production planning with lower environmental impacts.

39 **Keywords:** Biodiesel, waste cooking oil, blending optimization, uncertainty, climate  
40 change, water impacts

## 41 **1. Introduction**

42 The combination of Life-Cycle Assessment (LCA), a tool used to assess environmental  
43 impacts, with multi-objective optimization (MOO), a mathematical modeling tool that  
44 supports decision-making considering multiple objectives, has led to the development of  
45 life-cycle multi-objective (LCMO) frameworks to analyze trade-offs between  
46 environmental and economic aspects in several applications (Jacquemin et al., 2012;  
47 Pieragostini et al., 2012; Yue et al., 2016). Case studies can be found in the literature in  
48 several areas such as processing (Capón-García et al., 2011), recycling (Ponce-Ortega et al.  
49 2011), energy systems (Bamufleh et al., 2012; Cristóbal et al., 2012; Gerber and Gassner,  
50 2011; Gutiérrez-Arriaga et al., 2012; López-Maldonado et al., 2011), or buildings (Carreras  
51 et al., 2015; Safaei et al., 2015). Nevertheless, they are often focused on a single economic  
52 and a single environmental objective, typically greenhouse gas (GHG) emissions. A few  
53 studies include a higher number of objectives, like is the case of the recent work presented  
54 by Vadenbo et al. (2017) that developed an environmental multi-objective optimization  
55 model to determine the environmentally optimal use of biomass for energy using the  
56 Danish energy system as case study. In this work, six environmental impact categories are  
57 considered to be minimized. However, a pitfall of these studies is the lack of a simple and  
58 intuitive visual communication of the trade-offs among the different objectives in order to  
59 facilitate the decision process.

60 The challenge of including more environmental impact categories as objective functions in  
61 a LCMO model is related to the complexity of trade-off analysis when considering many  
62 competing objectives. For example, one may be concerned on minimizing GHG emissions  
63 and costs but in fact, the solution that minimizes these two objectives may bring burdens to  
64 other relevant environmental issues such as water scarcity. For this reason, the development

65 of tools that facilitate the trade-off analysis and the decision process is very important  
66 within the LCMO framework (Tsang et al., 2014). This paper presents an alternative  
67 LCMO decision-aiding approach that facilitates the decision process by allowing the  
68 decision-maker to decide based on an explicit overall environmental performance and, at  
69 the same time, visualize the trade-offs among the different objectives to support decisions  
70 in a more comprehensive manner.

71 The model developed is illustrated by assessing the use of Waste Cooking Oils (WCO) in  
72 blends for biodiesel production. WCO have been gaining prominence as an alternative  
73 feedstock for biodiesel production due to their potential to improve the economic and  
74 environmental performance of biodiesel compared with crop-based oils (e.g. soya, rapeseed  
75 or palm, also designated as virgin oils in this paper) (Caldeira et al., 2015; Carla Caldeira et  
76 al., 2016; Dufour and Iribarren, 2012). However, the high uncertainty and variability in  
77 WCO chemical composition due to a high diversity of sources hinder guaranteeing  
78 biodiesel quality (Knothe and Steidley, 2009). A potential strategy to deal with this issue is  
79 to blend WCO with virgin oils, such as soybean, rapeseed, and palm oil as presented by  
80 Caldeira et al. (2017b). The authors showed that, using chance constrained programming  
81 (CCP) to address compositional uncertainty, blends containing WCO can have the same  
82 technical performance as blends composed only of virgin oils while reducing costs.  
83 However, besides costs, it is also important to assess the potential environmental benefits.  
84 Although the main environmental concern of biodiesel is related to GHG emissions,  
85 another relevant aspect to consider when evaluating the environmental impacts of biodiesel  
86 is water use. Water use impacts have been insufficiently addressed in the literature, but if  
87 the location where the crops are cultivated is water scarce, the water consumption impacts  
88 can be significant (Pfister and Bayer, 2014). Moreover, the water quality may be

89 compromised due to the use of fertilizers and pesticides in the crops cultivation  
90 (Emmenegger et al., 2011).

91 Few studies can be found in the literature that combine LCA and MO under uncertainty.  
92 Some of these studies are focused on the uncertainty of the LCA impact either by using  
93 CCP (Guille and Grossmann, 2009; Guillén-Gosálbez and Grossmann, 2010) or by  
94 describing the LCA uncertain parameters through scenarios with given probability of  
95 occurrence (Sabio et al., 2014). Other studies address uncertainty related to prices and  
96 demand uncertainty, using scenarios with given probability of occurrence in the design of  
97 sustainable chemical supply chains (Ruiz-Femenia et al., 2013) and chemical processes  
98 network (Allothman and Grossmann, 2014) or, uncertainty in several parameters expressed  
99 as fuzzy possibility distributions and probability distributions to help design better waste  
100 management strategies (Zhang and Huang, 2013). No study that optimizes blends for  
101 biodiesel production minimizing costs and multiple environmental impacts considering the  
102 feedstocks compositional uncertainty was found in the literature.

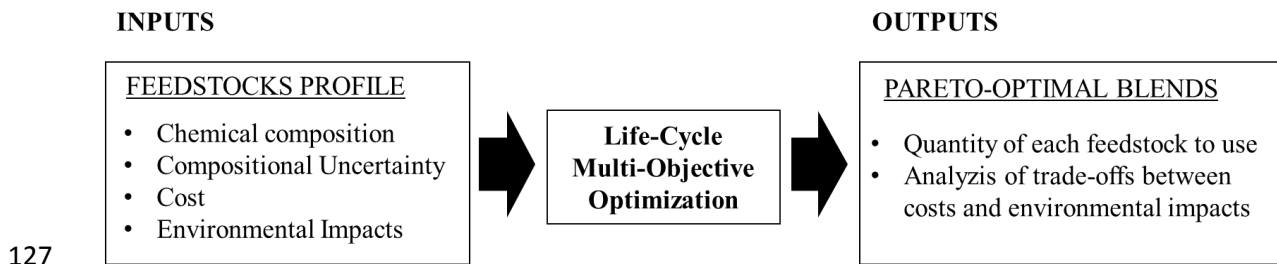
103 This paper presents a model to facilitate trade-off analysis in LCMO problems illustrating  
104 its use in the assessment of the incorporation of secondary material (WCO) in blends for  
105 biodiesel production. The model objectives (to minimize) include feedstock costs, life-cycle  
106 GHG emissions, water scarcity, toxicity, acidification and eutrophication impacts. The oils  
107 compositional uncertainty is incorporated in the model, minimizing the risk of  
108 noncompliance with biodiesel technical requirements. The efficient solutions obtained  
109 allow the production planner to analyze the trade-offs between economic and  
110 environmental performance, and select blends that will lead to a product with lower  
111 environmental impacts.

112 **2. Material and Methods**

113 **2.1 Life-cycle multi-objective (LCMO) chance constrained model**

114 The model framework is presented in Fig.1. The model determines blends that minimize  
115 costs and environmental impacts by calculating the quantity of each feedstock (palm,  
116 rapeseed, soya and WCO) to use in the blend, addressing the feedstock compositional  
117 uncertainty. The input information is the profile of the different feedstocks: chemical  
118 composition and its associated uncertainty, costs and environmental impacts. The outputs  
119 are optimal blends that are in compliance with the required biodiesel properties with  
120 minimum cost and environmental impact. Typically, there is no feasible solution that  
121 minimizes costs and all the environmental impacts simultaneously thus, the model is a  
122 decision support tool that helps decision-makers find Pareto-optimal solutions, i.e. solutions  
123 such that it is not possible to improve one of the objectives without worsening some other  
124 objective. Decision-makers may thus observe the trade-offs between their objectives and  
125 select their most preferred solution.

126 The model framework is presented in figure 1.



127  
128 **Fig. 1.** Life-cycle multi-objective chance constrained model framework

129

130 Since the biodiesel production cost is mainly attributed to feedstock costs (about 85%)  
131 (Haas et al., 2006), the costs considered in the model concern the purchase of feedstock.

132 Price information from 2011 to May 2014 for palm, canola and soya oils was taken from  
133 IndexMundi (IndexMundi, 2014) and prices for WCO were obtained from a European  
134 broker (Grennea, 2014). The month July 2013 was selected because it is the month when  
135 the price of WCO was closer to the virgin oils price, which represents a conservative  
136 situation to evaluate the benefits of WCO. The prices were 559 €, 767 €, 765 € and 400 €  
137 per ton of palm, rapeseed, soya and WCO. The environmental impacts categories include:  
138 Climate Change (CC), Water Stress Index (WSI), Freshwater Eutrophication (FE), Aquatic  
139 Acidification (AC), Human Toxicity (HT) and Ecotoxicity (ET). The model is illustrated  
140 using the Portuguese context as a case study because the authors had access to primary data  
141 and detailed information about the biodiesel production in Portugal to determine the  
142 environmental impacts of the feedstocks used in the model. Nevertheless, this case is used  
143 to illustrate the model and the assessment herein presented can be replicated for biodiesel  
144 production in other countries.

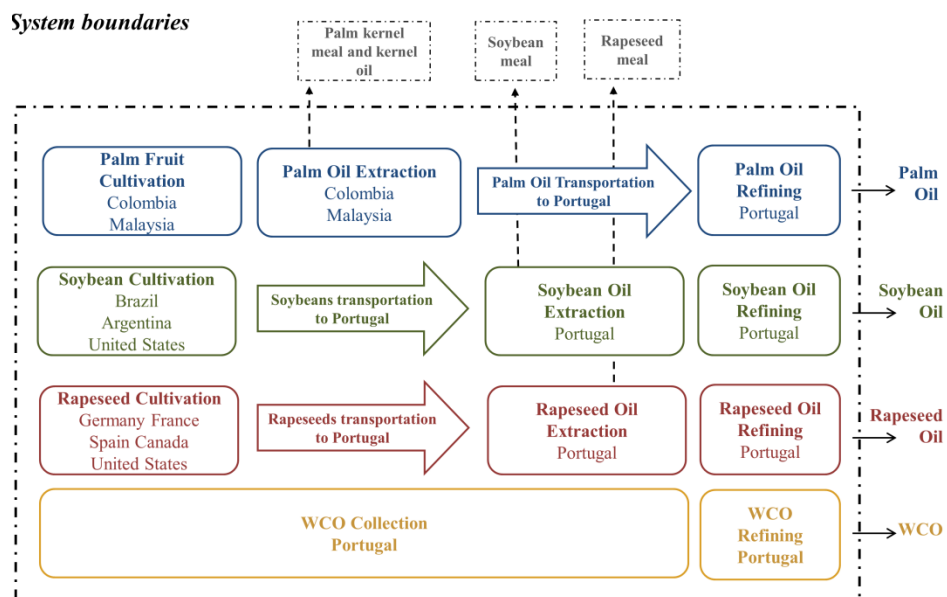
#### 145 **Life-Cycle Assessment model**

146 LCA was used to assess the environmental profile of four feedstocks: three crop-based oils  
147 (palm, soya and rapeseed) and WCO. The data used to build the LCA model was retrieved  
148 from another work done by some of the authors (Caldeira et al., 2018). As the goal of this  
149 paper is to illustrate the LCMO model, the LCA model is briefly described and the impacts  
150 values used in the optimization model are presented in Table 1. The life-cycle (LC) model  
151 was built to assess the GHG emissions impacts (CC), water consumption impacts  
152 (measured by the impact category WSI) and water degradability impacts (measured by the  
153 impact categories FE, AC, HT and ET). The functional unit chosen was 1 kg of vegetable  
154 oil. It is assumed that after the refining step, the virgin oils and the WCO have the required

155 characteristics for the transesterification reaction (biodiesel production). Technically, the  
 156 production of biodiesel from WCO is similar to conventional transesterification processes  
 157 of the virgin oils (Knothe et al., 1997). The variation on the energy content (low heating  
 158 value) of biodiesel produced from palm, soya, rapeseed and WCO is below 1% (Hoekman  
 159 et al., 2012).

160 The system boundaries of the crop-based oils systems, schematically represented in Fig. 2,  
 161 include cultivation, oil extraction, feedstock transportation and oil refining, considering that  
 162 the oils are refined in Portugal. Different cultivation locations were considered: Colombia  
 163 and Malaysia for palm fruit; Argentina, Brazil and US for soybean; and, Germany, France,  
 164 Spain, Canada and US for rapeseed. The palm oil extraction was made in the cultivation  
 165 site while the soya and rapeseed oils were extracted in Portugal. The transportation of the  
 166 palm oil, soybeans and rapeseeds to Portugal was considered in the model.

167



168  
 169  
 170

**Fig. 2.** System boundaries of the oils systems



171 Virgin oil production is a multifunctional system because from the oils extraction phase  
172 other co-products are obtained: from palm oil extraction is also obtained palm kernel meal  
173 and kernel oil; from soybean oil extraction, soybean meal; and, from rapeseed oil, rapeseed  
174 meal. The distribution of the impacts between the oils and the co-products was made using  
175 energy allocation (method suggested in the European Directive 2009/28/EC (European  
176 Comission, 2009) on the promotion of the use of energy from renewable sources).

177 For the WCO, the stages considered within the system boundaries (Fig. 2) are the WCO  
178 collection and refining in Portugal. Depending on the quality of the WCO (mainly related  
179 to the percentage of free fatty acids, FFA) the refining process is different. For low quality  
180 WCO, the refining consists in an acid-catalyzed process to reduce the percentage of FFA  
181 (Jungbluth et al., 2007) while for high quality WCO, the refining consists in filtering to  
182 remove impurities and heating to remove water (above 100° C during approximately 2  
183 hours)(Caldeira et al., 2015). The two alternative WCO refining processes are considered in  
184 the study.

185 The inventory was built with data collected from several references: palm cultivation and  
186 palm oil extraction in Colombia (Castanheira et al., 2014); palm cultivation and palm oil  
187 extraction in Malaysia, Ecoinvent 3.1 database (Jungbluth et al., 2007) soybeans cultivation  
188 in Argentina (considering the reduced tillage cultivation system) (Castanheira and Freire,  
189 2013); soybeans cultivation in Brazil (considering cultivation in Mato Grosso) (Castanheira  
190 et al., 2015); soybeans cultivation in the US, Ecoinvent 3.1 database (Jungbluth et al.,  
191 2007); rapeseed cultivation in Spain, Germany, France, Canada (Malça et al., 2014);  
192 rapeseed cultivation in the US, Ecoinvent 3.1 database; soybean oil extraction in Portugal  
193 (Castanheira et al., 2015); rapeseed oil extraction (Castanheira and Freire, 2016); palm,  
194 soybean and rapeseed oils refining, (Castanheira and Freire, 2016); low quality WCO

195 refining (Jungbluth et al. 2007); high quality WCO refining ( Caldeira et al., 2016) and  
 196 WCO collection (Caldeira et al., 2016; Caldeira et al., 2015).  
 197 Climate Change (CC) and Freshwater Eutrophication (FE) were assessed using the impact  
 198 assessment method ReCiPE (Goedkoop et al. 2009); water consumption impacts (WSI)  
 199 using the method presented by Pfister et al. (2009) and Ridoutt and Pfister (2013); Aquatic  
 200 Acidification (AC) using Impact 2002+ (Jolliet et al., 2003); and Human toxicity (HT) and  
 201 Ecotoxicity (ET) using Usetox recommended version (Rosenbaum et al., 2008).  
 202 **Table 1** Environmental impacts - Climate Change (CC), Water Stress Index (WSI), Freshwater  
 203 Eutrophication (FE), Aquatic Acidification (AC), Human Toxicity (HT) and Ecotoxicity (ET) - for the different  
 204 oils analyzed, palm, soya, rapeseed and WCO (Caldeira et al., 2018).

Feedstock_origin	CC kg CO <sub>2</sub> eq kg <sup>-1</sup> oil	WSI m <sup>3</sup> eq kg <sup>-1</sup> oil	FE kg P eq kg <sup>-1</sup> oil (*10 <sup>-4</sup> )	AC kg SO <sub>2</sub> eq kg <sup>-1</sup> oil (*10 <sup>-2</sup> )	HT CTUh kg <sup>-1</sup> oil (*10 <sup>-11</sup> )	ET CTUhe kg <sup>-1</sup> oil
Palm_CO	0.90	0.076	3.98	1.24	0.44	0.004
Palm_MY	0.72	0.078	1.83	1.09	0.69	2.47
Soya_AR	0.90	0.264	7.15	0.80	0.74	5.54
Soya_BR	1.29	0.109	7.81	1.08	1.08	8.32
Soya_US	1.23	0.088	1.97	1.02	40.1	0.39
Rapeseed_DE	1.69	0.111	2.62	2.23	1.1	0.45
Rapeseed_FR	1.68	0.182	2.6	2.56	60.2	6.57
Rapeseed_SP	1.85	2.113	2.87	2.88	213.0	23.38
Rapeseed_CN	1.75	0.095	4.42	2.84	79.2	18.06
Rapeseed_US	3.32	0.172	1.88	3.30	52.2	3.09
WCO_PT_Hi*	0.23	0.0020	0.71	0.15	1.37	0.03
WCO_PT_Lo**	0.12	0.0015	0.56	0.01	1.33	0.03

205 CO:Colombia, MY:Malaysia AR:Argentina, BR:Brazil, US:United States, DE:Germany, FR:France, SP:Spain,  
 206 CA:Canada, PT:Portugal  
 207 \*High Quality Waste Cooking Oil  
 208 \*\*Low Quality Waste Cooking Oil

209  
 210  
 211

212 **Addressing feedstock compositional uncertainty using chance constrained**  
213 **optimization**

214 Compositional uncertainty has been addressed by several authors using chance constrained  
215 programming (CCP) optimization (Gaustad et al., 2007; Gülşen et al., 2014; Li et al., 2012;  
216 Sakallı et al., 2011). The application of CCP in blend optimization of conventional  
217 feedstocks (palm, canola, sunflower and soya) used in biodiesel production showed that  
218 feedstock diversification (blending) can: i) help control costs while ensuring fuel quality by  
219 spreading the risk of price volatility across multiple feedstocks (Gülşen et al., 2014); and,  
220 ii) manage GHG emissions uncertainty characteristics of biodiesel (Olivetti et al., 2014).  
221 Using CCP formulation, Caldeira et al. (2017b) analyzed the use of a secondary material  
222 (WCO) in blends with conventional feedstocks. The same set of constraints was used in this  
223 paper to address compliance with technical constraints in face of composition uncertainty.  
224 The constraints were defined based on existing prediction models that relate the  
225 composition, specifically the vegetable oils fatty acids (FA) content of the feedstocks and  
226 biodiesel properties: density (Den), cetane number (CN), cold filter plugging point (CFPP),  
227 iodine value (IV) and oxidative stability (OS) (Caldeira et al., 2017a). The explanation of  
228 these prediction models and derivation of these constraints can be found in previous work  
229 (Caldeira et al., 2017b, 2014).

230

231 **Model formulation**

232 The mathematical formulation of the problem is presented below and the nomenclature  
233 used is described in Table 2. The goal is to determine the Pareto optimal blend that  
234 minimizes production costs and environmental impacts that are calculated according to

235 equation 1, multiplying the quantity of each feedstock used in the blend (the decision  
236 variable in the model,  $QU_i$ ) by the coefficient for each objective  $k$  of each feedstock  $i$  ( $C_{k,i}$ ).  
237 This coefficient indicates the cost or impact on objective  $k$  per unit of feedstock  $i$  used in  
238 the blend. Table 1 presents the coefficients of the environmental impact for each feedstock  
239 and, as explained in the section 2.1 (2<sup>nd</sup> paragraph), the coefficient for the feedstock prices  
240 were 559 €, 767 €, 765 € and 400 € per ton of palm, rapeseed, soya and WCO. The model  
241 is subject to demand and supply constraints (equations 2 and 3). Since the goal is to analyze  
242 the proportion of each feedstock in the blend, the demand was set equal to 1 and no supply  
243 limitations were considered. For each property (Den, CN, CFPP, IV and OS) the final blend  
244 must comply with the technical specifications (equations 4 and 5 for lower and upper  
245 limits).  $\beta$  represents a risk tolerance parameter that determines the maximum accepted non-  
246 compliance rate level chosen by the user. Assuming a normal distribution of the uncertain  
247 parameter ( $q_{i,j}$ ),  $\beta$  is the normal distribution test coefficient (z-value), one-tailed. The  
248 constraints thresholds were defined according to the European Standard EN 14214 (CEN,  
249 2008).

#### Objective functions

$$\min z_k = \sum_{i \in I} (C_{k,i} QU_i) \quad \forall k \quad (1)$$

#### Demand and Supply constraints

$$\sum_{i \in I} QU_i = D \quad (2)$$

$$QU_i \leq S_i \quad \forall i \quad (3)$$

#### Technical Constraints

$$\sum_{j \in J} \left( \text{PropCoef}_{f,j} \sum_{i \in I} QU_i \bar{q}_{ij} \right) + \text{PropConst}_1 - \beta \sqrt{\sum_{j \in J} \text{PropCoef}_{f,j}^2 \sum_{i \in I} QU_i^2 \sigma_{ij}^2} \geq \text{PropGT}_l \quad \forall l \quad (4)$$

$$\sum_{j \in J} \left( \text{PropCoef}_{m,j} \sum_{i \in I} QU_i \bar{q}_{ij} \right) + \text{PropConst}_m + \beta \sqrt{\sum_{j \in J} \text{PropCoef}_{m,j}^2 \sum_{i \in I} QU_i^2 \sigma_{ij}^2} \leq \text{PropLT}_m \quad \forall m \quad (5)$$

$$QU_i \geq 0 \quad \forall i \quad (6)$$

250

251

252 **Table 2** Biodiesel blending optimization problem nomenclature

<b>Indices and sets</b>	$i \in I$	$I = \{\text{soya, canola, palm, WCO}\}$ , feedstock oils
	$k \in K$	$K = \{\text{Cost, CC, WSI, FE, AC, HT, ET}\}$ , objective functions
	$j \in J$	$J = \{1, 2, \dots, 18\}$ , Fatty Acids (FA) 1 to 18 types of FA
	$l \in L$	$L = \{\text{DenLB, CN, OS}\}$ , set of properties with lower limit
	$m \in M$	$M = \{\text{DenUB, IV, CFPP}\}$ , set of properties with upper limit
<b>Parameters</b>	$C_{k,i}$	Coefficient of objective k concerning feedstock i
	D	Demand
	$S_i$	Supply of feedstock i
	$\bar{q}_{i,j}$	Average quantity (%) of FA-j in feedstock i
	$\sigma_{i,j}$	Standard deviation for $\bar{q}_{i,j}$
	$\text{PropCoef}_{l,j}$	Coefficient of FA-j in the prediction model for property l
	$\text{PropCoef}_{m,j}$	Coefficient of FA-j in the prediction model for property m
	$\text{PropConst}_l$	Constant in the prediction model for property l
	$\text{PropConst}_m$	Constant in the prediction model for property m
	$\text{PropGT}_l$	Threshold for property l
	$\text{PropLT}_m$	Threshold for property m
	$\beta$	Test coefficient for normal distribution, one tailed
	<b>Decision Variables</b>	$QU_i$

253

254

## 255 **2.2 An approach to facilitate the trade-off analysis between cost and environmental** 256 **impacts**

257 As typically occurs in multi-objective problems, the competing nature of the objectives  
 258 makes it difficult for decision-makers to identify the “best” solution. Methods exist that use  
 259 “à priori” decision-maker preferences to aggregate the multiple objectives into a single  
 260 objective (by attributing weights to each objective). However, the decision-maker may find  
 261 it hard to define such weights in an explicit way in the absence of a thorough understanding  
 262 of the problem.

263 Alternatively, an approach to visualize the trade-off among cost and environmental impacts  
 264 without attributing weights to objectives is the  $\varepsilon$ -constraint method, in which one objective  
 265 is minimized while the other are considered as constraints. In particular, if cost is the  
 266 objective being minimized, the following (mono-objective) mathematical program could be  
 267 solved:

Objective function

$$\min z_{\text{Cost}} = \sum_{i \in I} (C_{\text{Cost},i} QU_i) \quad (7)$$

268 Subject to:

$$z_k = \sum_{i \in I} (C_{k,i} QU_i) \leq \varepsilon_k \quad \forall k \neq \text{Cost} \quad (8)$$

269 Demand and Supply constraints, i.e. equations 2 and 3

270 Technical Constraints, i.e. equations 4 to 6.

271 The above mathematical program yields a Pareto-optimal solution for each combination of  
 272 impact limits defined by the  $\varepsilon_k$  right-hand side values, if feasible (some limits might be  
 273 impossible to attain). Hence, different solutions can be obtained by varying these limits.  
 274 However, it might be difficult for a decision-maker to deal with all the  $\varepsilon_k$  parameters  
 275 simultaneously. For this reason, in this work a single parameter  $\Theta$  is used to define Pareto-  
 276 optimal solutions corresponding to cost versus environmental impact trade-offs. This  
 277 approach consists in replacing all the  $\varepsilon_k$ -constraints in equation 8 by the constraints in  
 278 equation 9:

$$\sum_{i \in I} (c_{k,i} \cdot QU_i) \leq \text{Ideal} + \theta (\text{Anti ideal} - \text{Ideal}) \quad \forall k \setminus \{\text{Cost}\}, \theta \in [0,1] \quad (9)$$

279

280 In this equation,  $\Theta$  is a parameter that reflects the constraint level of the environmental  
 281 impacts and ranges from 0 to 1. The so-called “ideal” and “anti-ideal” values are obtained

282 by optimizing each environmental objective at a time. The “ideal” value for each objective  
283 corresponds to minimum impacts on this objective among all the solutions. The “anti-ideal”  
284 value for each objective is the maximum impact found when examining the solutions that  
285 optimize the other objectives. The “ideal” and “anti-ideal” values provide an indication of  
286 the range of impacts obtained by Pareto optimal solutions. When  $\Theta = 1$ , the environmental  
287 impacts are allowed to be as high as the “anti-ideal” value and the solution with the  
288 minimum cost can be obtained. As  $\Theta$  decreases, the upper limit for all environmental  
289 impacts also decreases, departing from the “anti-ideal” values and getting closer to the  
290 “ideal” values (e.g.,  $\Theta = 0.5$  means that the upper limit on each environmental indicator will  
291 be halfway between the ideal and anti-ideal values). Thus, the feasible region decreases  
292 leading to more expensive solutions, up to a minimum value ( $\Theta_{Lim}$ ) such that for  $\Theta < \Theta_{Lim}$   
293 the problem becomes unfeasible. The parameter  $\Theta$  determines if the decision-maker wants  
294 to be closer to the environmental impacts “ideal” value and therefore, having the best  
295 environmental performance (within the constraints of the problem), or to be closer to  
296 minimum costs achievable. The decision-maker can vary  $\Theta$  to learn what the involved  
297 trade-offs are, and results can be conveniently depicted graphically presenting costs as a  
298 function of  $\Theta$ .

299 The model was implemented in GAMS 24.4. (GAMS, 2011). The problem was solved  
300 using the non-linear solver CONOPT (Drud, 2014) which is well suited for models with  
301 nonlinear constraints with a fast method for finding a first feasible solution for very  
302 constrained models. The solver makes use of the Generalized Reduced Gradient (GRG)  
303 method with some extensions added. It has been widely used for solving stochastic and  
304 multi-objective optimization models (Cristóbal et al., 2012; Guillén-Gosálbez &  
305 Grosseman, 2010; López-Maldonado et al., 2011; Sabio et al., 2014). Each run of the

306 model took approximately 40 seconds on an intel (R) Core™ i5-3337U CPU@ 1.8 GHz  
307 machine.

### 308 **3. Results and discussion**

309 It was first analyzed the results of the model minimizing three objectives because this is the  
310 limit of objectives that can be visualized: costs, climate change (CC) and water  
311 consumption impacts (WSI) (section 3.1). Then, the assessment was extended by adding  
312 the other environmental impact categories FE, AC, HT, ET. In this situation, since it is  
313 impossible to visualize the trade-offs the approach described in 2.2 was used. Results are  
314 presented in section 3.2. The analysis was performed for two cases: a) WCO is available to  
315 blend with the virgin oils; and, b) only virgin oils are available (the reference scenario for  
316 biodiesel production in Portugal for the price period considered). The latter is used as  
317 benchmark to evaluate the use of WCO in the blends.

#### 318 **3.1 Cost, Climate Change and water consumption**

319 This section is presented and discussed the results obtained by minimizing costs, CC and  
320 WSI. Table 3 presents the pay-off tables obtained for both scenarios considering three  
321 objectives: Cost, Climate Change (CC) and Water Stress index (WSI). Each row  
322 corresponds to minimizing a different objective. The diagonal of each table (bold values)  
323 presents the “ideal” value of each objective (column) and the shaded area indicates the  
324 “anti-ideal” value of each objective.

325 When WCO is available to blend with the virgin oils, the blends incorporate 34% of WCO  
326 when the cost objective is minimized, 10% when CC is minimized and 32% when WSI is  
327 minimized. The incorporation of WCO allows a reduction of the minimum value obtained  
328 for each objective (“ideal” values) comparatively to the “ideal” values obtained with blends



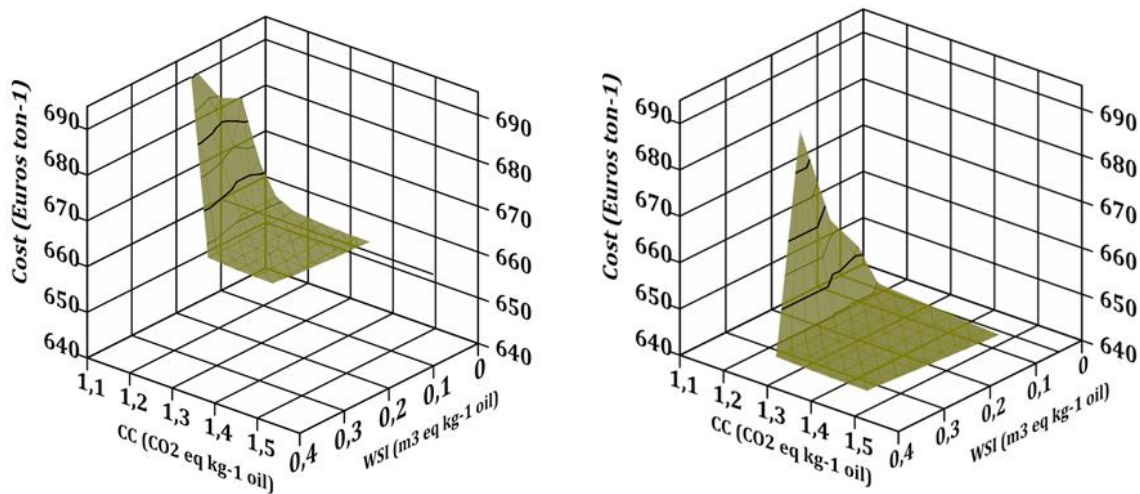
329 composed only of virgin oils (Table 3). The “ideal” value for cost, CC and WSI obtained  
 330 with WCO available are 3%, 2% and 32% lower than the “ideal” values obtained when  
 331 only virgin feedstocks are available. Also the “anti-ideal” value for cost is lower (2%) when  
 332 WCO are included in the blend. Nevertheless, for the “anti-ideal” values for CC and WSI  
 333 there is an increase of 3% and 14%.

334 **Table 3** Pay-off tables obtained by minimizing cost, CC and WSI in two scenarios: a) WCO is available to  
 335 blend with the virgin oils and, b) only virgin feedstocks are available.

Objective minimized	a) With WCO			b) Without WCO		
	Cost (€ ton <sup>-1</sup> )	CC (kg CO <sub>2</sub> eq kg <sup>-1</sup> oil)	WSI (m <sup>3</sup> eq kg <sup>-1</sup> oil)	Cost (€ ton <sup>-1</sup> )	CC (kg CO <sub>2</sub> eq kg <sup>-1</sup> oil)	WSI (m <sup>3</sup> eq kg <sup>-1</sup> oil)
Cost	<b>642.7</b>	1.48	0.354	<b>662.4</b>	1.43	0.304
CC	677.9	<b>1.07</b>	0.149	692.1	<b>1.09</b>	0.159
WSI	650.1	1.31	<b>0.065</b>	689.6	1.26	<b>0.086</b>

336 The diagonal contains “ideal” values of the objective (column)  
 337 The shaded values are “anti-ideal” values of the objective (column)  
 338

339 A set of Pareto optimal solutions were obtained using the  $\epsilon$ -constraint method minimizing  
 340 costs and using CC and WSI as constraints, incorporating them in the constraint part of the  
 341 model. The constraint level ranges, interactively, from the “anti-ideal” to the “ideal” values  
 342 presented in Table 3. The iteration step for each objective is one tenth of the difference  
 343 between the “anti-ideal” and “ideal” value. Fig. 3 shows the Pareto surface obtained  
 344 minimizing cost, CC and WSI for the two scenarios considered: (a) having WCO available  
 345 in the model (right-hand side) and, (b) without WCO available (left-hand side). The Pareto  
 346 surface is displaced to lower costs when WCO is included in the blends. The quantity of  
 347 WCO incorporated in the blends ranges from 10% to 34%. Lower CC and WSI solutions  
 348 can be obtained at a lower cost if WCO is included in the blends.



349 **Fig. 3.** Pareto surface obtained minimizing cost, climate change (CC) and water stress index (WSI) having  
 350 WCO available in the model (right-hand side) and without WCO available (left-hand side).

351

### 352 **3.2 Extended environmental assessment**

353 In this section, the analysis was extended to include the other environmental impacts:  
 354 eutrophication (FE), acidification (AA), human toxicity (HT) and ecotoxicity (ET). The  
 355 pay-off tables obtained for the two scenarios, with and without WCO available, are  
 356 presented in Table 4 and Table 5. Similarly to what was observed for the “ideal” values  
 357 obtained for cost, CC and WSI, the use of WCO also reduces the ideal values in 9% for FE,  
 358 3% for AA and 4% for ET relatively to the situation when only virgin oils are available to  
 359 blend. For HT, the ideal value is the same in both situations. The quantity of WCO  
 360 incorporated in the blend when minimizing FE is 33% and 11% when minimizing AA or  
 361 ET. The blend obtained when minimizing HT has no WCO in its composition.

362

363

364

365 **Table 4** Pay-off table for Cost, Climate Change (CC), Water Stress Index (WSI), Freshwater Eutrophication  
 366 (FE), Aquatic Acidification (AC), Human Toxicity (HT) and Ecoxicity (ET) when WCO is available

Objective minimized	Cost € ton <sup>-1</sup>	CC kg CO <sub>2</sub> eq kg <sup>-1</sup> oil	WSI m <sup>3</sup> eq kg <sup>-1</sup> oil	FE kg P eq kg <sup>-1</sup> oil (*10 <sup>-4</sup> )	AC kg SO <sub>2</sub> eq kg <sup>-1</sup> oil (*10 <sup>-2</sup> )	HT CTUh kg <sup>-1</sup> oil (*10 <sup>-11</sup> )	ET CTUhe kg <sup>-1</sup> oil
Cost	<b>642.7</b>	1.48	0.354	4.36	1.87	54.03	6.82
CC	677.9	<b>1.07</b>	0.149	3.62	1.39	13.10	4.09
WSI	650.1	1.31	<b>0.065</b>	3.22	1.98	54.32	12.30
FE	647	1.24	0.101	<b>1.95</b>	1.64	23.62	2.55
AC	676.9	1.11	0.127	3.60	<b>1.34</b>	2.79	2.36
HT	693.7	1.17	0.146	4.49	1.44	<b>0.74</b>	1.86
ET	668	1.32	0.091	3.07	1.74	0.83	<b>0.25</b>

367 The diagonal contains ideal values of the objective (column)  
 368 The shaded values are anti-ideal values of the objective (column)  
 369

370 **Table 5** Pay-off table for Cost, Climate Change (CC), Water Stress Index (WSI), Freshwater Eutrophication  
 371 (FE), Aquatic Acidification (AC), Human Toxicity (HT) and Ecoxicity (ET) when WCO is not available

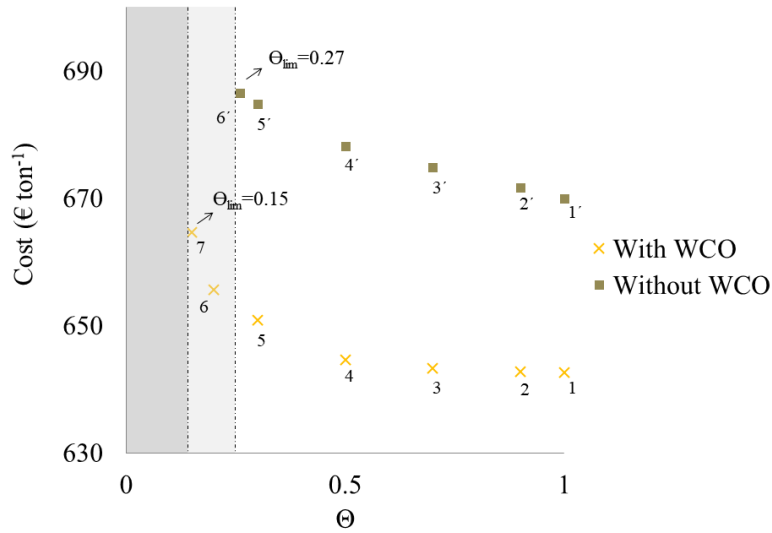
Objective minimized	Cost € ton <sup>-1</sup>	CC kg CO <sub>2</sub> eq kg <sup>-1</sup> oil	WSI m <sup>3</sup> eq kg <sup>-1</sup> oil	FE kg P eq kg <sup>-1</sup> oil (*10 <sup>-4</sup> )	AC kg SO <sub>2</sub> eq kg <sup>-1</sup> oil (*10 <sup>-2</sup> )	HT CTUh kg <sup>-1</sup> oil (*10 <sup>-11</sup> )	ET CTUhe kg <sup>-1</sup> oil
Cost	<b>662.4</b>	1.43	0.304	4.57	1.96	40.60	5.74
CC	692.1	<b>1.09</b>	0.159	3.87	1.43	12.37	4.24
WSI	689.6	1.26	<b>0.086</b>	3.27	1.70	38.73	6.54
FE	693.4	1.20	0.105	<b>2.13</b>	1.50	24.36	2.28
AC	689.7	1.13	0.132	3.85	<b>1.38</b>	3.35	2.57
HT	693.7	1.17	0.146	4.49	1.44	<b>0.74</b>	1.86
ET	676.9	1.35	0.096	3.21	1.80	0.79	<b>0.26</b>

372 The diagonal contains ideal values of the objective (column)  
 373 The shaded values are anti-ideal values of the objective (column)  
 374

375 This analysis shows the potential competing nature of objectives. For example, minimizing  
 376 cost leads to solutions (blends) that correspond to the anti-ideal solution for CC and WSI.  
 377 On the other hand, minimizing WSI leads to the anti-ideal solution for AC, HT and ET  
 378 (Table 4).

379 As the number of objectives increased to seven, it would be impossible to visualize the  
 380 Pareto solutions as it was shown for Cost, CC and WSI in Fig. 3. In this case, the approach

381 described in section 2.2 (equation 9) was applied. Results for the cost obtained for different  
 382  $\Theta$  for the two scenarios, with and without WCO available, are depicted in Fig.4.



383  
 384 **Fig.4.** Blends cost obtained for different  $\Theta$ . For  $\Theta$  lower than 0.15 and 0.27 the problem is unfeasible (shaded  
 385 area) for the situation with and without WCO.  
 386  
 387 Lower cost blends are obtained if WCO is available (yellow crosses). Blend 1 was obtained  
 388 setting  $\Theta=1$  and corresponds to the lowest cost solution (642.7 € ton<sup>-1</sup>). Decreasing the  
 389 value of  $\Theta$  increases the cost and for  $\Theta$  values lower than 0.15 the problem becomes  
 390 unfeasible. For  $\Theta_{Lim}= 0.15$  the solution corresponds to blend 7 which has a cost of 665.1 €  
 391 ton<sup>-1</sup>. In the scenario were WCO is not available (green squares), the cost of blend obtained  
 392 with  $\Theta=1$  (Blend 1') is 670 € ton<sup>-1</sup>, 4% higher than blend 1. The  $\Theta_{Lim}$  for this scenario is  
 393 0.27 and corresponds to blend 6' that has a cost of 686.6 € ton<sup>-1</sup>, 2.3% higher than Blend 7.  
 394 The cost and environmental impacts obtained with  $\Theta=1$  (Blends 1, 1') and  $\Theta= \Theta_{Lim}$  (7, 6')  
 395 in both scenarios (with and without WCO) are presented in Table 6.

396

397 **Table 6** Results for Cost, Climate Change (CC), Water Stress Index (WSI), Eutrophication (FE),  
 398 Acidification (AC), Human Toxicity (HT) and Ecotoxicity (ET) obtained for  $\Theta=1$  and  $\Theta= \Theta_{lim}$  when WCO is  
 399 available (a) and when it is not (b)

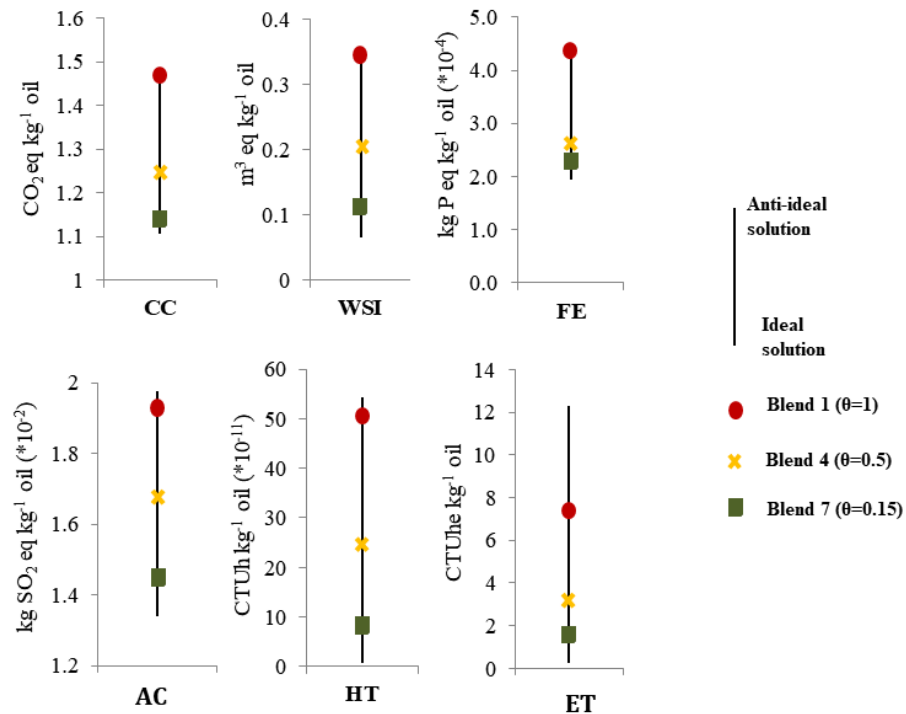
Objective	$\Theta=1$	$\Theta=1$	$\Theta=0.15$	$\Theta=0.27$
	(a)	(b)	(a)	(b)
	(Blend 1)	(Blend 1')	(Blend 7)	(Blend 6')
Cost (€ ton <sup>-1</sup> )	642.7	670.0	665.1	686.6
CC (kg CO <sub>2</sub> eq kg <sup>-1</sup> oil)	1.48	1.22	1.17	1.18
WSI (m <sup>3</sup> eq kg <sup>-1</sup> oil)	0.354	0.304	0.120	0.145
FE (kg P eq kg <sup>-1</sup> oil *10 <sup>-4</sup> )	4.35	3.13	2.41	2.79
AC (kg SO <sub>2</sub> eq kg <sup>-1</sup> oil *10 <sup>-2</sup> )	1.87	1.7	1.44	1.47
HT (CTUh kg <sup>-1</sup> oil *10 <sup>-11</sup> )	54.08	27.83	8.07	11.5
ET (CTUhe kg <sup>-1</sup> oil)	6.82	4.25	1.52	1.94
Quantity of WCO (%)	34	—	18	—

400

401 Using 34% of WCO in Blend 1 needs to be compensated with the use of rapeseed  
 402 feedstocks to comply with the technical constraints, whereas in Blend 1' there is a high  
 403 quantity of palm feedstocks (20% Palm\_CO + 26% Palm\_MY). Since the rapeseed  
 404 feedstocks have higher impacts than the palm ones, the environmental impacts of Blend 1  
 405 are higher than those of Blend 1'. Nevertheless, with decreasing  $\Theta$ , the environmental  
 406 impacts decrease and for  $\Theta=0.15$  (Blend 7) the environmental impacts are lower than the  
 407 ones of Blend 6' (blend with the lowest environmental impacts in the no WCO available  
 408 scenario). This means that lower environmental impacts at a lower cost are obtained when  
 409 WCO is available.

410 Additionally to Fig. 4, that so far was used to analyze the cost savings from using WCO in  
 411 the blends, this approach allows to depict Fig. 5 that shows the value for each  
 412 environmental impact and the position relatively to the “ideal” and “anti-ideal” value for  
 413 the blends. This figure helps the decision-maker to understand in a more comprehensive  
 414 manner the trade-offs associated with different  $\Theta$  values. Fig.4 shows the relative position  
 415 of the solution obtained with  $\Theta =5$  (Blend 4) to the “ideal” and “anti-ideal” values (extreme  
 416 values of the line in the graphs) and also to the solution obtained with  $\Theta =1$  (Blend 1, red

417 dots) and with  $\Theta = 0.15$  (Blend 7, green squares). The combination of Fig.4 and Fig.5  
 418 allows the decision-maker to visualize graphically what happens to cost (Fig. 4) and to each  
 419 impact environmental objective (Fig. 5) for different values of  $\Theta$ . For example, if the  
 420 decision-maker wants to be sure that the blend is closer to the “ideal” value than to the  
 421 “anti-ideal” in all the environmental performance objectives,  $\Theta$  can be set as equal to 0.5  
 422 and the optimal solution is Blend 4 (yellow crosses in Fig. 5). The choice of Blend 4  
 423 represents an increase in the cost of 0.3% relatively to Blend 1 (lower cost blend) but a  
 424 reduction of 11% in AC, 13% in CC, 40% in WSI, 45% in FE, 50% in HT and 72% in ET.

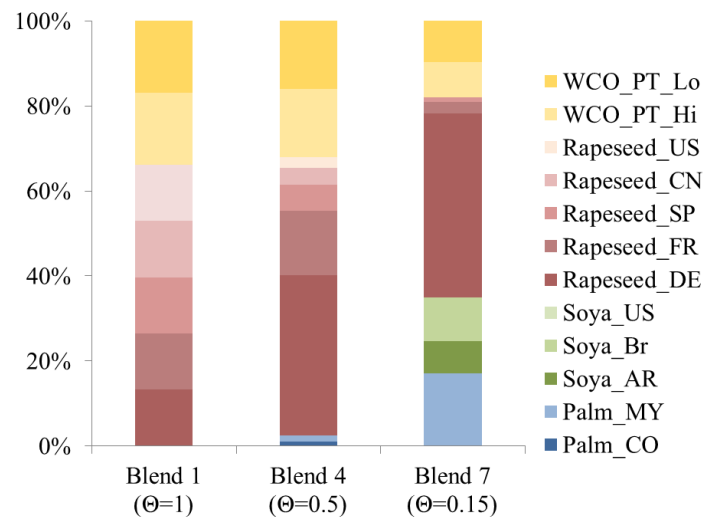


425 **Fig.5.** Relative position to the ideal and anti-ideal values of blend 1 (obtained with  $\Theta = 1$ ), blend 4 (obtained  
 426 with  $\Theta = 0.5$ ) and blend 7 (obtained with  $\Theta = 0.15$ ).

428  
 429 Another interesting aspect of this approach is that, if there is a limit value for a specific  
 430 environmental impact category, this information can be included in the model by limiting  
 431 the specific constraint and performing the analysis having that impact category limited to

432 its threshold. This is the case, for example, for biofuels production in the EU, where the  
 433 Renewable Energy Directive establishes a reduction target of 50% relatively to fossil fuel  
 434 for biofuels produced after 2016 (European Commission, 2009) meaning that the oil blend  
 435 must have at the most a value for CC of 1.395 g CO<sub>2</sub> eq kg<sup>-1</sup> oil blend.

436 The composition of Blends 1, 4 and 7 are presented in Fig.6. Blend 1, the lowest cost blend  
 437 (obtained with  $\Theta=1$ ), is composed of WCO and rapeseed. Since the goal is to minimize cost  
 438 and this blend is obtained for the less stringent constraint level for the environmental  
 439 impacts, the model distributes the quantity of WCO and rapeseed equitably for the different  
 440 “types” of those feedstocks that only differ in the environmental impacts value. Blend 1 is  
 441 the blend that incorporates the highest quantity of WCO, 34% (adding the low and high  
 442 quality WCO).



443

444 **Fig.6.** Blends composition obtained for  $\Theta=1$ ,  $\Theta=0.5$  and  $\Theta=0.15$  ( $\Theta_{Lim}$ )

445

446 When the feasible region contracts by decreasing  $\Theta$ , the quantity of WCO diminishes and  
 447 palm is added to the blend. The quantity of WCO incorporated in Blend 4 is 32%. For  $\Theta_{Lim}$   
 448  $=0.15$ , Blend 7 is the optimal blend obtained and the four types of feedstock compose it:

449 palm, soya, rapeseed and WCO. The quantity of WCO in this blend is 18%. The quantity of  
450 WCO in the blend diminishes with decreasing  $\Theta$  because WCO have higher impacts for HT  
451 and to reduce this category, this feedstock is replaced by others that have lower impacts  
452 such as Palm\_MY, Soya\_US or Rapeseed\_DE.

453 An interesting aspect to analyze is the fact that the blend with lower environmental impacts  
454 (obtained with  $\Theta = 0.15$ ) presents a higher diversity of feedstocks and an uneven  
455 distribution in opposition to what is observed for  $\Theta = 1$ . When the value of  $\Theta$  is decreased  
456 up to the limit of the model feasibility ( $\Theta = 0.15$ ) the constraints for the environmental  
457 impacts are quite demanding (impacts cannot surpass the ideal value plus 15% of the  
458 difference between the anti-ideal and ideal values) and the model selects feedstocks that,  
459 although being more expensive, have lower environmental impacts in some categories  
460 relatively to rapeseed and even WCO. Nevertheless, since each of the feedstocks have  
461 different environmental profiles, the model will blend different proportions of each. For  
462 example, it selects Palm\_MY, Soya\_AR and Soya\_Br because these feedstocks have lower  
463 environmental impacts for HT (table 1). Also the proportion of Rapeseed\_DE is higher in  
464 the blend because among the rapeseeds is the one with lower impacts for HT. Additionally,  
465 the amount of WCO is reduced because these have higher impacts for HT than, for  
466 example, palm. The share of rapeseed has to be kept to comply with the technical  
467 constraints. The proportion of the two WCO feedstocks is the same because both WCO  
468 feedstocks have similar environmental impacts profile (table 1) and the differences between  
469 them is not sufficient to change their proportion in the blend, considering the other  
470 feedstocks environmental impact profile. This is why the lower environmental impacts  
471 solution (obtained with  $\Theta = 0.15$ ) presents more diversity of feedstocks and proportions (the



472 other environmental impact categories are also taken into account but their influence is not  
473 so evident because the values for the alternative feedstocks are not so different).

474 One should have note that the results obtained correspond to a single period price – July  
475 2013. As mentioned in the beginning of this chapter, this period was selected to illustrate  
476 the model because it is the month when the price of WCO is closer to the virgin oils price,  
477 representing a more conservative situation to evaluate the cost benefits of WCO.  
478 Nevertheless, although in the other periods the use of WCO is expected to be beneficial, the  
479 type and quantity of each feedstock used in the blend may change and consequently, the  
480 environmental impacts of the blends may also be different.

481

#### 482 **4. Conclusions**

483 The decision-aiding model herein presented was developed combining environmental LCA  
484 with blending algorithms using multi-objective optimization towards novel engineering  
485 systems methodologies to analyze and better communicate potential trade-offs among  
486 multiple objectives. It was used to assess economic and environmental trade-offs of  
487 decisions at the operational level in biodiesel production, addressing feedstock  
488 compositional uncertainty. Although the model was designed with particularities of the  
489 biodiesel systems, it can be adapted to other industries, particularly recycling industries and  
490 be used to support production planning at the operational level to enhance the technical,  
491 economic and environmental performance of these industries.

492 The application of this tool to assess the use of secondary material (WCO) in blends for  
493 biodiesel production showed that the use of WCO leads to reduction of biodiesel  
494 production costs and environmental impacts relatively to blends composed only with crop-  
495 based oils. Blending WCO with crop-based oils is an attractive approach to reduce costs

496 and environmental impacts of biodiesel while new technologies and alternative feedstocks  
497 for biodiesel production are still evolving and are not yet cost competitive. Moreover, the  
498 collection and use of this residue for biodiesel production avoids its disposal through  
499 sewage systems, reducing economic and environmental burdens by avoiding sewage  
500 treatment at wastewater treatment plants.

501 The technical constraints thresholds used in the model are based on European regulation  
502 but they can be adapted to other standards (for example in the US regulation there is no  
503 threshold for Iodine Value and there is a lower limit for Oxidative Stability (OS)) and the  
504 Cold Filter Plugging Point (CFPP) limit values vary according to the type of climate. Also,  
505 OS and CFPP, that are the binding properties in the model, can be enhanced using additives  
506 and so, the model developed in this work together with these techniques, increases the  
507 spectrum of possible Fatty Acid (FA) based feedstocks to be used in biodiesel production.  
508 Moreover, this model can also be used to assess the use of secondary material like for  
509 example animal fats or the viability of emerging feedstocks such as algae.

510 This study presents some limitations that can be addressed in future research: (i) the  
511 biodiesel production costs considered in the model are the feedstock cost and, although  
512 different cultivation locations were analyzed, the feedstock cost does not take this issue in  
513 consideration; (ii) the technical constraints were defined for properties that are related  
514 directly related to the chemical composition of the oils and other parameters need to be  
515 considered to address other technical difficulties that may be related to the use of WCO;  
516 and (iii) the uncertainty associated with the availability and price of the feedstock (and its  
517 inter-relation based on supply and demand curves), and the uncertainty related to the  
518 environmental impacts are also relevant aspects to be addressed and included in a more  
519 comprehensive uncertainty model.

520

## 521 **Acknowledgements**

522 Carla Caldeira acknowledges financial support from the Portuguese Science and  
523 Technology Foundation (FCT) through grant SFRH/BD/51952/2012. This work has also  
524 been supported by Portuguese Science and Technology Foundation (FCT) projects:  
525 PTDC/AGR-FOR/1510/2014 (POCI-01-0145-FEDER-016764); PTDC/AAG-  
526 MAA/6234/2014 (POCI-01-0145-FEDER-016765). The research presented in this article  
527 was developed under the framework of the Energy for Sustainability Initiative of the  
528 University of Coimbra and the MIT Portugal Program.

529

## 530 **References**

- 531 Alothman, A.M., Grossmann, I.E., 2014. A Bi-Criterion Optimization Planning Model for Process  
532 Networks with Multiple Scenarios and Environmental Impact, 24 European Symposium on  
533 Computer Aided Process Engineering. Elsevier. doi:10.1016/B978-0-444-63456-6.50068-5
- 534 Arne, D., 2014. CONOPT [WWW Document]. ARKI Consult. Dev. A/S, Bagsvaerd, Denmark.  
535 URL [www.conopt.com/](http://www.conopt.com/) (accessed 3.1.14).
- 536 ASTM, 2008. Standard specification for biodiesel fuel blend stock (B100) for middle distillate  
537 fuels. Report no. D6751-08.
- 538 Bamufleh, H.S., Ponce-Ortega, J.M., El-Halwagi, M.M., 2012. Multi-objective optimization of  
539 process cogeneration systems with economic, environmental, and social tradeoffs. *Clean*  
540 *Technol. Environ. Policy* 15, 185–197. doi:10.1007/s10098-012-0497-y
- 541 Caldeira C., Queirós J., Freire, F., 2015. Biodiesel from Waste Cooking Oils in Portugal: alternative  
542 collection systems. *Waste and Biomass Valorization* 6, 771–779. doi:10.1007/s12649-015-  
543 9386-z
- 544 Caldeira, C., Freire, F., Olivetti, E.A., Kirchain, R., 2017a. Fatty acid based prediction models for  
545 biodiesel properties incorporating compositional uncertainty. *Fuel* 196, 13–20.  
546 doi:10.1016/j.fuel.2017.01.074
- 547 Caldeira, C., Gülsen, E., Olivetti, E.A., Kirchain, R., Dias, L., 2014. A Multiobjective Model for  
548 Biodiesel Blends Minimizing Cost and Greenhouse Gas Emissions. In: Murgante B. et al.  
549 (eds) *Computational Science and Its Applications – ICCSA 2014. Lect. Notes Comput. Sci.*  
550 8581, 653–666. doi:10.1007/978-3-319-09150-1\_48
- 551 Caldeira, C., Queirós, J., Noshadravan, A., Freire, F., 2016. Incorporating uncertainty in the Life  
552 Cycle Assessment of biodiesel from Waste Cooking Oil addressing different collection

- 553 systems. *Resour. Conserv. Recycl.* 112, 83-92 doi:10.1016/j.resconrec.2016.05.005
- 554 Caldeira, C., Quinteiro, P., Castanheira, E.G., Boulay, A.-M., Dias, A.C., Arroja, L., Freire, F.,  
555 2018. Water footprint profile of crop-based vegetable oils and waste cooking oil: Comparing  
556 two water scarcity footprint methods *Journal of Cleaner production.* 195, 1190 - 1202
- 557 Caldeira, C., Swei, O., Dias, L., Freire, F., Olivetti, E., Kirchain, R., 2017b. An optimization  
558 approach to increase biodiesel cost effectiveness, addressing compositional and price  
559 uncertainty, in: *Energy for Sustainability 2017 – Designing Cities & Communities for the  
560 Future.* Funchal, Portugal.
- 561 Capón-García, E., Aaron, D.B., Antonio, E., Puigjaner, L., 2011. Multiobjective Optimization of  
562 Multiproduct Batch Plants Scheduling Under Environmental and Economic Concerns. *Alche  
563 J.* 57, 2766-2782 doi:10.1002/aic
- 564 Carreras, J., Boer, D., Guillén-Gosálbez, G., Cabeza, L.F., Medrano, M., Jiménez, L., 2015. Multi-  
565 objective optimization of thermal modelled cubicles considering the total cost and life cycle  
566 environmental impact. *Energy Build.* 88, 335–346. doi:10.1016/j.enbuild.2014.12.007
- 567 Castanheira, É.G., Acevedo, H., Freire, F., 2014. Greenhouse gas intensity of palm oil produced in  
568 Colombia addressing alternative land use change and fertilization scenarios. *Appl. Energy*  
569 114, 958–967. doi:10.1016/j.apenergy.2013.09.010
- 570 Castanheira, É.G., Freire, F., 2016. GHG emissions for the production of biodiesel from rapeseed in  
571 Portugal. Report elaborated for APPB for their ISCC certification. (Cálculo das emissões de  
572 Gases com Efeito de Estufa da Produção de Biodiesel de Rapeseed em Portugal. Relatório  
573 elaborado para a APPB no âmbito do sistema de certificação ISCC - International  
574 Sustainability & Carbon Certification)
- 575 Castanheira, É.G., Freire, F., 2013. Greenhouse gas assessment of soybean production: Implications  
576 of land use change and different cultivation systems. *J. Clean. Prod.* 54, 49–60.  
577 doi:10.1016/j.jclepro.2013.05.026
- 578 Castanheira, É.G., Grisoli, R., Coelho, S., Anderi da Silva, G., Freire, F., 2015. Life-cycle  
579 assessment of soybean-based biodiesel in Europe: comparing grain, oil and biodiesel import  
580 from Brazil. *J. Clean. Prod.* 102, 188–201. doi:10.1016/j.jclepro.2015.04.036
- 581 CEN, 2008. EN 14214: automotive fuels – fatty acid methyl esters (FAME) for diesel engines –  
582 requirements and test methods.
- 583 Cristóbal, J., Guillén-Gosálbez, G., Jiménez, L., Irabien, A., 2012. Multi-objective optimization of  
584 coal-fired electricity production with CO<sub>2</sub> capture. *Appl. Energy* 98, 266–272.  
585 doi:10.1016/j.apenergy.2012.03.036
- 586 Dufour, J., Iribarren, D., 2012. Life cycle assessment of biodiesel production from free fatty acid-  
587 rich wastes. *Renew. Energy* 38, 155–162. doi:10.1016/j.renene.2011.07.016
- 588 Emmenegger, M.F., Pfister, S., Koehler, A., De Giovanetti, L., Arena, A.P., Zah, R., 2011. Taking  
589 into account water use impacts in the LCA of biofuels: An Argentinean case study. *Int. J. Life  
590 Cycle Assess.* 16, 869–877. doi:10.1007/s11367-011-0327-1
- 591 European Commission, 2009. Directive 2009/28/EC of the European Parliament and the Council of 23  
592 April 2009 on the promotion of the use of energy from renewable sources 16–62.

- 593 GAMS, 2011. GAMS Development Corporation: General Algebraic Modeling System (GAMS)  
594 Release 23.7.3 Washington, DC, USA.
- 595 Gaustad, G., Li, P., Kirchain, R., 2007. Modeling methods for managing raw material  
596 compositional uncertainty in alloy production. *Resour. Conserv. Recycl.* 52, 180–207.  
597 doi:10.1016/j.resconrec.2007.03.005
- 598 Gerber, L., Gassner, M., 2011. Systematic integration of LCA in process systems design :  
599 Application to combined fuel and electricity production from lignocellulosic biomass.  
600 *Comput. Chem. Eng.* 35, 1265–1280. doi:10.1016/j.compchemeng.2010.11.012
- 601 Goedkoop M.J., Heijungs R, Huijbregts M., De Schryver A.;Struijs J., V.Z.R., 2009. A life cycle  
602 impact assessment method which comprises harmonised category indicators at the midpoint  
603 and the endpoint level; First edition Report I: Characterisation. ReCiPe 2008.
- 604 Grennea, 2014. Overview of the European double-counting markets and market perspectives.
- 605 Guille, G., Grossmann, I.E., 2009. Optimal Design and Planning of Sustainable Chemical Supply  
606 Chains Under Uncertainty. *Alche J.* 55, 99–121. doi:10.1002/aic
- 607 Guillén-Gosálbez, G., Grossmann, I., 2010. A global optimization strategy for the environmentally  
608 conscious design of chemical supply chains under uncertainty in the damage assessment  
609 model. *Comput. Chem. Eng.* 34, 42–58. doi:10.1016/j.compchemeng.2009.09.003
- 610 Gülşen, E., Olivetti, E., Freire, F., Dias, L., Kirchain, R., 2014. Impact of feedstock diversification  
611 on the cost-effectiveness of biodiesel. *Appl. Energy* 126, 281–296.  
612 doi:10.1016/j.apenergy.2014.03.063
- 613 Gutiérrez-Arriaga, C.G., Serna-González, M., Ponce-Ortega, J.M., El-Halwagi, M.M., 2012. Multi-  
614 objective optimization of steam power plants for sustainable generation of electricity. *Clean  
615 Technol. Environ. Policy.* 15, 551-566 doi:10.1007/s10098-012-0556-4
- 616 Haas, M.J., McAloon, A.J., Yee, W.C., Foglia, T., 2006. A process model to estimate biodiesel  
617 production costs. *Bioresour. Technol.* 97, 671–8. doi:10.1016/j.biortech.2005.03.039
- 618 Hoekman, S.K., Broch, A., Robbins, C., Ceniceros, E., Natarajan, M., 2012. Review of biodiesel  
619 composition, properties and specifications. *Renew. Sustain. Energy Rev.* 16, 143–169.  
620 doi:10.1016/j.rser.2011.07.143
- 621 IndexMundi, 2014. [www.indexmundi.com/](http://www.indexmundi.com/) [WWW Document]. URL [www.indexmundi.com/](http://www.indexmundi.com/)  
622 (accessed 5.19.14).
- 623 Jacquemin, L., Pontalier, P.-Y., Sablayrolles, C., 2012. Life cycle assessment (LCA) applied to the  
624 process industry: a review. *Int. J. Life Cycle Assess.* 17, 1028–1041. doi:10.1007/s11367-012-  
625 0432-9
- 626 Jolliet, O., Margni, M., Charles, R., Humbert, S., Payet, J., Rebitzer, G., 2003. Presenting a new  
627 method IMPACT 2002 + : a new life cycle impact assessment methodology. 8(6):324–330. *Int  
628 J Life Cycle Assess* 8.
- 629 Jungbluth, N., Chudacoff, M., Dauriat, A., Dinkel, F., Doka, G., Faist Emmenegger, M.,  
630 Gnansounou, E., Kljun, N., Spielmann, M., Stettler, C., Sutter, J., 2007. Life Cycle Inventories  
631 of Bioenergy. *Life cycle Invent. bioenergy. Ecoinvent Rep.* .Swiss Cent. LCI, ESU.  
632 Dübendorf, CH. no. 17,.

- 633 Knothe, G., Dunn, R., Bagby, M., 1997. Biodiesel: the use of vegetable oils and their derivatives as  
634 alternative diesel fuels. ACS Symp. Ser. no. 666 fuels Chem. from biomass 172–208.
- 635 Knothe, G., Steidley, K.R., 2009. A comparison of used cooking oils: A very heterogeneous  
636 feedstock for biodiesel. Bioresour. Technol. 100, 5796–5801.  
637 doi:10.1016/j.biortech.2008.11.064
- 638 Li, X., Yu, H., Yuan, M., 2012. Modeling and Optimization of Cement Raw Materials Blending  
639 Process. Math. Probl. Eng. 2012, 1–30. doi:10.1155/2012/392197
- 640 López-Maldonado, L.A., Ponce-Ortega, J.M., Segovia-Hernández, J.G., 2011. Multiobjective  
641 synthesis of heat exchanger networks minimizing the total annual cost and the environmental  
642 impact. Appl. Therm. Eng. 31, 1099–1113. doi:10.1016/j.applthermaleng.2010.12.005
- 643 Malça, J., Coelho, A., Freire, F., 2014. Environmental Life-Cycle Assessment of Rapeseed-Based  
644 Biodiesel: Alternative Cultivation Systems and Locations. Appl. Energy 114, 837–844.  
645 doi:10.1016/j.apenergy.2013.06.048
- 646 Olivetti, E., Gülşen, E., Malça, J., Castanheira, E., Freire, F., Dias, L., Kirchain, R., 2014. Impact of  
647 policy on greenhouse gas emissions and economics of biodiesel production. Environ. Sci.  
648 Technol. 48, 7642–50. doi:10.1021/es405410u
- 649
- 650 Pfister, S., Bayer, P., 2014. Monthly water stress: spatially and temporally explicit consumptive  
651 water footprint of global crop production. J. Clean. Prod. 73, 52–62.  
652 doi:10.1016/j.jclepro.2013.11.031
- 653 Pieragostini, C., Mussati, M.C., Aguirre, P., 2012. On process optimization considering LCA  
654 methodology. J. Environ. Manage. 96, 43–54. doi:10.1016/j.jenvman.2011.10.014
- 655 Ponce-Ortega, J.M., Mosqueda-Jiménez, F.W., Serna-González, M., 2011. A Property-Based  
656 Approach to the Synthesis of Material Conservation Networks with Economic and  
657 Environmental Objectives. AIChE J. 57, 2369–2387. doi:10.1002/aic
- 658 Rosenbaum, R., Bachmann, T., Gold, L., Huijbregts, M., Jolliet, O., Juraske, R., Koehler, A.,  
659 Larsen, H., MacLeod, M., Margni, M., McKone, T., Payet, J., Schuhmacher, M., van de  
660 Meent, D., Hauschild, M., 2008. USEtox— the UNEP-SETAC toxicity model: recommended  
661 characterisation factors for human toxicity and freshwater ecotoxicity in life cycle impact  
662 assessment. Int J Life Cycle Assess 13, 532–546.
- 663 Ruiz-Femenia, R., Guillén-Gosálbez, G., Jiménez, L., Caballero, J.A., 2013. Multi-objective  
664 optimization of environmentally conscious chemical supply chains under demand uncertainty.  
665 Chem. Eng. Sci. 95, 1–11. doi:10.1016/j.ces.2013.02.054
- 666 Sabio, N., Pozo, C., Guillén-Gosálbez, G., Jiménez, L., Karuppiah, R., Vasudevan, V., Sawaya, N.,  
667 Farrell, J.T., 2014. Multiobjective Optimization Under Uncertainty of the Economic and Life-  
668 Cycle Environmental Performance of Industrial Processes. AIChE J. 60, 2098–2121.  
669 doi:10.1002/aic
- 670 Safaei, A., Freire, F., Henggeler Antunes, C., 2015. A life cycle multi-objective economic and  
671 environmental assessment of distributed generation in buildings. Energy Convers. Manag. 97,  
672 420–427. doi:10.1016/j.enconman.2015.03.048

- 673 Sakallı, Ü.S., Baykoç, Ö.F., Birgören, B., 2011. Stochastic optimization for blending problem in  
674 brass casting industry. *Ann. Oper. Res.* 186, 141–157. doi:10.1007/s10479-011-0851-1
- 675 Tsang, M.P., Bates, M.E., Madison, M., Linkov, I., 2014. Benefits and Risks of Emerging  
676 Technologies: Integrating Life Cycle Assessment and Decision Analysis To Assess Lumber  
677 Treatment Alternatives. *Environ. Sci. Technol.* 48, 11543–11550. doi:10.1021/es501996s
- 678 Vadenbo, C., Tonini, D., Astrup, T.F., 2017. Environmental Multiobjective Optimization of the Use  
679 of Biomass Resources for Energy. *Environ. Sci. Technol.* 51, 3575–3583.  
680 doi:10.1021/acs.est.6b06480
- 681 Yue, D.J., Pandya, S., You, F.Q., 2016. Integrating Hybrid Life Cycle Assessment with  
682 Multiobjective Optimization: A Modeling Framework. *Environ. Sci. Technol.* 50, 1501–1509.  
683 doi:10.1021/acs.est.5b04279
- 684 Zhang, X., Huang, G., 2013. Optimization of environmental management strategies through a  
685 dynamic stochastic possibilistic multiobjective program. *J. Hazard. Mater.* 246–247, 257–66.  
686 doi:10.1016/j.jhazmat.2012.12.036
- 687