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Biorefinery supply chain design optimization under sustainability dimensions

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Optimisation de la conception de la chaîne d'approvisionnement pour une bioraffinerie durable

Biorefinery supply chain design optimization under sustainability dimensions

Doctoral Dissertation

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(Spec: Industrial System Engineering)

By

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Optimisation de la conception de la chaîne d'approvisionnement pour une bioraffinerie durable

1. Introduction

Si on considère les défis qualifiés de cruciaux à l'échelle mondiale, la sécurité énergétique et notamment les enjeux liés aux carburants fossiles apparaissent comme prioritaires. Ceci se traduit par une demande croissante du marché en terme de nouveaux carburants et de produits biosourcés, qui ne doit pas être déconnectée d'une préoccupation sociétale telle que la préservation de notre planète pour les générations futures. Ainsi, dès les premières étapes de conception d'un projet de bioraffinerie, il est impératif de considérer des facteurs aussi divers que les émissions de gaz à effet de serre, la sécurité alimentaire, la préservation de la biodiversité, la gestion raisonnée de l'eau, la promotion du secteur rural ou la génération de valeur économique (Department of Energy, 2015).

De fait, un objectif stratégique réside dans une utilisation efficiente des ressources naturelles dans un contexte de développement durable (NNFC, 2007 ; Department of Energy, 2015). Compte tenu de l'abondante disponibilité de biomasse à l'échelle mondiale, il existe un potentiel significatif de produits et de carburants de remplacement de ceux dérivés du pétrole (Kamm and Kamm 2004; Gnansounou, 2011; Department of Energy, 2015). Pour effectuer cette transformation, les bioraffineries se présentent comme une solution alternative aux raffineries traditionnelles (IEA Bioenergy, 2009 ; NREL, 2015). Cependant, cette voie nécessite des recherches plus approfondies avant d'être implémentée (Nguyen et al., 2017).

Une revue de la littérature nous a permis de voir qu'il existait, selon le type et le nombre de matières premières et de produits finaux en jeu, trois typologies de bioraffinerie (Dyne et al. 1999; Kamm and Kamm 2004; Espinoza Pérez et al. 2017):

- ✚ Les bioraffineries de Phase I, qui considèrent un seul type de matières premières et un seul produit final. Elles disposent de technologies de production fixes et sont donc peu flexibles.
- ✚ Les bioraffineries de Phase II, qui visent à l'obtention de plusieurs produits finaux. Elles peuvent donc s'adapter plus facilement aux changements du marché.
- ✚ Les bioraffineries de Phase III, qui intègrent des technologies plus flexibles pouvant utiliser différents types de matières premières pour produire différents types de produits finaux. Ces dernières sont les plus flexibles mais en même temps les plus complexes car pouvant s'adapter à des changements de marchés pour les produits finaux, à des variations de prix ou disponibilité des matières premières ou encore à des changements de fournisseurs.

Nous avons aussi découvert l'existence d'une classification concernant les matières premières qui peuvent être utilisées dans les bioraffineries (Kamm and Kamm 2004; Moncada et al., 2014). Ainsi, les bioraffineries de *première génération* utilisent une biomasse issue des cultures dédiées à

l'alimentation; celles de *seconde génération* utilisent des cultures non-comestibles, des résidus, ou du bois, entre autres. Enfin, les bioraffineries de *troisième génération* utilisent principalement des algues.

Le Tableau 1, fait un état des bioraffineries en fonctionnement en 2016 selon la classification des matières premières .

Tableau 1. Bioraffineries en fonctionnement en 2016 selon la classification des matières premières (Dovetail Partners, 2017)

	Première génération	Seconde génération	Troisième génération
Echelle Commerciale	330	43	1
Usine Pilote	9	25	15

Ces chiffres montrent clairement que les bioraffineries de première génération ont été fortement développées à l'échelle mondiale. C'est pourquoi, elles ont, sans aucun doute, été à l'origine des effets indésirables et inattendus en termes d'impacts environnementaux. De plus, comme nous l'avons expliqué, leur production étant basée sur une matière première comestible, elles obligent les décideurs politiques à faire des choix sur l'usage des terres disponibles, générant de fait des conflits entre un usage pour l'alimentaire ou pour la production de carburants. (Nguyen et al., 2017; Bautista 2015)

Les bioraffineries qui produisent plusieurs produits finaux ne se sont quant à elles pas assez développées (Dovetail Partners, 2017). Deux facteurs sont principalement mis en avant (Valdivia et al., 2016 ; Nguyen et al., 2017):

- ✚ La perception du risque associé à des nouvelles technologies de production par les investisseurs potentiels,
- ✚ La faible rentabilité résultant de la combinaison entre la nécessité d'investissement en procédés coûteux (intensité de capital), les prix bas à l'heure actuelle des produits biosourcés et l'absence de chaînes d'approvisionnement matures et stabilisées.

Enfin, les bioraffineries de Phase III étant en émergence, les perspectives de développement de ces dernières semblent prometteuses.

2. Objectives

Ainsi, dans l'objectif de développer d'avantage des bioraffineries de Phase II, et ce d'une façon durable, quelques aspects doivent être considérés simultanément (Nguyen et al., 2017; Espinoza Pérez et al., 2017; Valdivia et al., 2016; Lamers et al., 2015; Kim et al., 2011; Dunnett et al., 2008) :

- ✚ L'optimisation de la chaîne d'approvisionnement
- ✚ L'intégration des étapes de prétraitement dans la chaîne d'approvisionnement
- ✚ La diversification des matières premières et des produits finis
- ✚ L'intégration de l'analyse de durabilité avant l'implémentation de la bioraffinerie, considérant le contexte de territoire où le projet veut être développé

- ✚ L'investissement privé pour amener la bioraffinerie à un niveau de maturité suffisant et pérenne dans le temps.

Ces derniers n'étant pas de même nature, nous pensons qu'en développant les quatre premiers aspects, le cinquième pourrait être une conséquence ou résultat. C'est le point de vue que nous avons pris pour nos travaux de thèse dont l'objectif général est, in fine : « La création d'un outil d'aide à la décision pour des projets de conception de la chaîne d'approvisionnement d'une bioraffinerie phase III durable, incorporant des critères de diversification des matières premières et des produits finis, de prétraitements nécessaires à l'homogénéisation de la biomasse, et d'application de différentes technologies de production ».

Plus spécifiquement, nos travaux nous ont conduit à :

- ✚ La définition précise des défis et des exigences relatifs à la mise en place d'une chaîne d'approvisionnement pour une bioraffinerie phase III durable,
- ✚ La proposition d'un modèle d'optimisation basé sur des approches méta-heuristiques et,
- ✚ L'application et la validation du modèle proposé sur un cas concret : le territoire colombien.

3. Méthodologie

Pour atteindre ces objectifs, la recherche opérationnelle s'avère être une discipline qui fournit une base scientifique pertinente pour résoudre des problèmes de prise de décision multicritères et multiéchelles. Elle a d'ailleurs été largement appliquée dans l'évaluation des projets *ex-ante* et *ex-post*, selon une approche en six étapes : la formulation du problème, la formulation du modèle, la résolution du modèle, la validation du modèle, la sélection de la solution et, enfin l'implémentation de la solution (Winston 2003; Taha 2010).

3.1. Formulation du problème

Dans la formulation du problème, il est important de décrire de façon détaillée la chaîne d'approvisionnement attendue. Cette dernière doit notamment intégrer des fournisseurs, des usines de prétraitement, des usines de production, des clients pour les produits intermédiaires et finis, et des flux de réutilisation des sous-produits dans les usines de production (Espinoza Pérez et al., 2017).

Il faut également considérer les différents niveaux de prise de décision qui peuvent exister dans une chaîne d'approvisionnement : stratégique, tactique et opérationnel (Iakovou, E., et al., 2010). Ce point est d'autant plus important que selon l'avancée du projet, certaines décisions ne peuvent plus être changées et que l'incertitude dans les données peut varier plus ou moins fortement. Enfin, le concept de durabilité doit être pris en compte. Pour ce faire, nous nous intéressons aux cinq dimensions qui le constituent : Economique, sociale, environnementale, technologique et politique (Bautista et al., 2016a ; Bautista et al , 2016b). La dimension économique intègre l'utilisation de la capacité installée des usines, la maximisation des profits, la valeur des produits, entre autres. La dimension sociale considère par exemple l'emploi généré sur le territoire suite à l'installation des sites de production. La dimension environnementale considère notamment la quantité de gaz à effet serre générée, les eaux résiduelles et les autres émissions potentielles. La dimension technologique considère quant à elle le

degré de maturité de la technologie qui sera utilisée, selon le « technology readiness level (TRL)», ainsi que la réduction des coûts associés à l'apprentissage technologique. Finalement, la dimension politique s'avère être très importante pour ce type d'industrie, car ce sont les gouvernements qui sont les principaux prescripteurs en permettant le développement ou non des bioraffineries. En effet, ils peuvent jouer plusieurs rôles, allant de l'allocation de ressources ou de subventions, à la réduction du taux d'imposition voire à la régulation des prix des biocarburants comme cela est le cas dans certains pays (par exemple, la Colombie).

Sur une base des articles scientifiques publiés sur une période de dix années (2006 à 2016) concernant les recherches spécifiques sur la conception de la chaîne d'approvisionnement des bioraffineries, un total de 84 articles ont été sélectionnés et étudiés en profondeur (Espinoza Pérez et al., 2017). Nous avons ainsi remarqué, que la plupart des recherches se sont focalisées sur la dimension économique et que la grande majorité intègre les trois niveaux de prise de décision de la chaîne d'approvisionnement. Par ailleurs, nous avons trouvé que seulement deux études considèrent quelques-uns des aspects des cinq dimensions de la durabilité. Cela montre que notre recherche développe l'aspect pas assez abordé de l'évaluation intégrale de la durabilité des projets des bioraffineries.

3.2. Formulation du modèle

Concernant l'étape de formulation du modèle, nous pouvons distinguer trois modèles, qui sont différents mais interdépendants, relatifs au niveau de prise de décision pour la chaîne d'approvisionnement :

- ✚ Le modèle pour le design conceptuel (représentant le niveau stratégique),
- ✚ Le modèle de gestion (qui représente le niveau tactique)
- ✚ Et le modèle de planification (qui représente le niveau opérationnelle)

Chacun de ces modèles doit être construit sur la base de une analyse des aspects de la durabilité à son niveau de décision et des caractéristiques de la chaîne d'approvisionnement. Finalement, ces modèles doivent être intégrés dans un modèle général.

Le modèle du design conceptuel est le point de départ du modèle général. Puis, afin de construire ce modèle qui doit représenter au mieux la complexité du phénomène que nous cherchons à formaliser, une stratégie de modélisation est nécessaire. Ainsi, une seconde contribution de nos travaux réside dans la proposition d'une stratégie systématique pas à pas pour développer le modèle. D'abord, intégrant les variables, contraintes et paramètres associés à la chaîne d'approvisionnement. Par la suite, chaque dimension de durabilité doit être analysée et formalisée pour définir les contraintes, les fonction objective et les paramètres qui seront intégrés dans le modèle de manière séquentielle. De cette manière, l'approche proposée permet au développeur de vérifier à chaque étape la cohérence et pertinence du modèle.

Dans notre cas spécifique nous avons commencé par un modèle simple, qui considère seulement des usines de production. Ensuite, dans un deuxième temps, nous avons ajouté des usines de prétraitements, suivi par les flux de réutilisation des produits dans les usines de production. Enfin, la vente des produits intermédiaires a été intégrée dans le modèle. De cette démarche systématique il en résulte un modèle contenant un total de 22 fonctions objectif, de nature linéaire mais aussi non-

linéaire. Le modèle ainsi formalisé est multiobjectifs ; composé par l'ensemble de fonctions objectif énumérés préalablement, mais aussi par un ensemble de contraintes linéaires de égalité et inégalité, et par des variables binaires et continues.

3.3. Résolution du modèle

En ce qui concerne l'étape de résolution du modèle, compte tenu des caractéristiques du problème préalablement décrit, une méthode d'optimisation basée sur des approches métaheuristiques et en particulier basée sur des algorithmes évolutionnaires a été choisie. Parmi les avantages de cet algorithme, nous pouvons citer le fait qu'il n'a pas besoin de continuité ou de convexité de l'espace de solutions; qu'il ne se base pas uniquement sur l'information du gradient pour chercher des solutions; et qu'il peut explorer un grand espace de recherche. Avec les caractéristiques énoncées il y a plus de chances d'éviter, ou bien de sortir des optimums locaux (Sharma Ingalls et al. 2013).

Une nouvelle étude bibliographique a été ensuite menée pour définir les différents types d'algorithmes évolutionnaires existants et la quantité d'études dédiés à chacun d'entre eux. Nous avons trouvé les algorithmes suivants comme étant ceux le plus étudiés et utilisés par la communauté scientifique : « Elitist Non-Dominated Sorting Genetic Algorithm », « Non-Dominated Sorting Genetic Algorithm », « Strength Pareto Evolutionary Algorithm », « Multiobjective Genetic Algorithm », « Vector-Evaluated Genetic Algorithm », « Niche-Pareto Genetic Algorithm » et « Penalty Function Approach ». Plus particulièrement, l'algorithme Elitist Non-Dominated Sorting Genetic Algorithm (NSGA-II) est le plus étudié, et son application continue d'être mise en œuvre aujourd'hui. Pour ces raisons il sera utilisé par la suite afin de résoudre le modèle développé.

4. Cas d'étude et résultats

Une fois développé, l'application et validation du modèle ont été réalisées sur une étude de cas sur la filière biocarburants en Colombie. En effet, la Colombie produit du biodiesel en base à huile de palme depuis 2008, et la filière c'est rapidement développée pour arriver à une production de 514,000 tons de biodiesel par an en 2015, ceci essentiellement dans des bioraffineries phase I et II (Fedebiocombustibles, 2017). Cependant, des impacts négatifs ont été observés depuis comme conséquence de cette activité (Bautista, 2015). Nous pouvons citer :

- ✚ L'augmentation de consommation d'énergie du pays à cause de l'installation des usines de production,
- ✚ L'augmentation des émissions des gaz à effet de serre,
- ✚ Une perte de biodiversité, mais aussi une dégradation de la qualité et de la disponibilité de l'eau,
- ✚ L'apparition des problèmes liés à la sécurité alimentaire, parce que l'huile de palme est utilisée comme huile de friture, margarines et comme émulsifiants

Pour éviter ou minimiser ces impacts négatifs, le cas d'étude cherche à explorer des conditions pour développer des bioraffineries de Phase III de deuxième génération d'un point de vue durable. Les caractéristiques du cas d'étude considérant le contexte spécifique de la Colombie sont:

- ✚ La comparaison de différents types de matières premières : le huile de palme et le huile de Jatropha, une culture non comestible
- ✚ L'intégration de la production de différents types des produits finaux: le biodiesel, le glycérol et le biopolyester aliphatique
- ✚ L'évaluation de six types de technologies de production pour les usines de production principales
- ✚ La proposition de dix-sept potentielles locations pour les usines de prétraitement et autres dix-sept locations sont proposées pour les usines de production principales.
- ✚ La proposition de trois capacités de production pour chaque usine de transformation (40,000 ; 80,000 et 120,000 ton/an)
- ✚ La désignation de cinq marchés pour l'huile de palme raffinée issue des usines de prétraitement, et vingt-trois marchés identifiés pour les produits finaux.

Ainsi, le modèle appliqué au cas d'étude de la Colombie dispose de vingt-trois fonctions objectives, 12,978 variables de décision, parmi lesquelles 357 sont binaires. Il existent 85 contraintes d'égalité et 556 contraintes d'inégalité.

Pour la réalisation des comparaisons parmi les 23 fonctions objectives, il a été décidé de faire une comparaison par paires des fonctions. Cette façon de faire génère moins de combinaisons que si nous comparons par trio ou quartet de fonctions, par exemple.

100 comparaisons des fonctions objectives ont été réalisées. Parmi celles, 57 comparaisons ont généré des fronts de Pareto, lesquelles sont présentées et analysés en détail dans le document principal de la thèse. D'une autre côté, 43 comparaisons présentent fonctions objectives que ne sont pas en conflit. Egalement, quelques solutions optimales sont analysées en détail et les cartes géographiques de la Colombie sont présentées dans ce document.

De ces résultats il peut être conclu qu'un compromis entre les fonctions objectives est nécessaire pour un développement durable des bioraffineries.

Finalement, une analyse de sensibilité a été réalisé à fin de valider le modèle appliqué en Colombie, ainsi comme la « soi-disant » validité, la vérification des données et du code utilisent le logiciel Matlab® et la validation croisée permettent de comparer les résultats obtenus avec ceux des recherches amenés préalablement en Colombie.

5. Conclusions et perspectives

Les conclusions et apports de cette travail peuvent être classées selon quatre points de vue différents : d'abord, si elles sont liées à la formulation du problème. Si elles sont relatives à formulation du modèle, si elles sont liées a la solution du modèle, ou bien, si elles concernent a l'application du modèle.

Formulation du problème :

- ✚ Cette recherche a fait une définition précise des défis et des exigences relatifs à la mise en place d'une chaine d'approvisionnement pour une bioraffineries phase III durable,
- ✚ Ainsi, cette thèse a analysé les outils actuellement utilises pour cette conception

Formulation du modèle:

- ✚ La stratégie pour le développement du modèle en deux axes, en intégrant élément par élément, permet une meilleure compréhension du modèle par les chercheurs
- ✚ Un modèle dédié pour l'étape de design des bioraffineries phase III a été développé d'un un point de vue holistique et durable
- ✚ La grande quantité d'indicateurs pour la durabilité a été traduit en 21 fonctions objectives génériques, celle que peut servir à simplifier l'étape de formalisation des préférences des parties prenantes involucrées dans un tel projet
- ✚ Autres fonctions objective pourraient être intégrées dans le modèle, tels que le temps de retour sur investissement
- ✚ Quelques fonctions objective pourraient être regroupes, principalement dans la dimension environnemental

Solution du modèle :

- ✚ Les algorithmes évolutionnaires ont montré leur adéquation pour résoudre le modèle développé
- ✚ L'algorithme NSGA- II est le plus étudié et développé parmi des différents algorithmes évolutionnaires
- ✚ Cet algorithme a été programmé, adapté et vérifié pour résoudre le modèle
- ✚ Autres tests peuvent être amenés pour évaluer la robustes du modèle et sa vitesse pour trouver le fronts de Pareto

Cas d'application en Colombie:

- ✚ Etant donné que les ratios théoriques de transformation pour les technologies de production, encore en stade de développement sont les plus élevés, ces technologies sont les plus sélectionnés parmi les solutions optimaux
- ✚ Par contre, il faut réaliser d'autres études pour mesurer le potentiel risque et incertitude liée à l'implémentation de ces technologies en développement a une échelle commercial

- ✚ Etant donné que les ratios de transformation pour l'huile de Jatropha sont inférieures que celles du huile de palme, les solutions optimaux pour une maximisation de la performance économique utilisent que du huile de palme. En conséquence, il faut considérer des autres technologies de transformation pour des procédés de production, l'huile de Jatropha ou un autre matière première non-comestible
- ✚ La diversification des produits finaux permettre obtenir une meilleure performance économique. De plus, il est possible de réaliser une analyse pour l'exportation du biopolymère aliphatique ou des autres produits dérivés pour avoir un quantité de demande plus élevée et atteindre des économies d'échelle. En parallèle à l'analyse d'autres types de produits biosourcées peuvent être évalués postérieurement.

Cette recherche a développé les bases pour un outil de d'aide à la décision pour le développement d'un projet d'une bioraffinerie durable. Ainsi, parmi les perspectives, les plus importants sont :

- ✚ La réalisation d'un questionnaire pour formaliser les préférences des involucre, basée sur les fronts de Pareto obtenus de l'optimisation multiobjective
- ✚ Le développement des modèles de gestion et planification pour la chaîne de approvisionnement. Et son intégration au modèle de design conceptuel développé dans cette thèse.

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Preface

The growing global population and its effect on world food security, as well as the urgency for climate change mitigation, are issues that foster technological, social, and political innovations to increase the efficiency of the use of natural resources (Höltinger et al., 2014; Sammons et al., 2007; Sukumara et al., 2013). Among the natural resources recently investigated, biomass has interested researchers because of its widespread availability and its potential applicability as sustainable source of energy and materials (Sukumara et al., 2013). In order to integrate bio-based raw materials and new technologies, the biorefinery concept has been developed, as an industrial facility where biomass is transformed into a wide range of marketable products and energy (Department of Energy, 2015; Sammons et al., 2007). Therefore, the main drivers behind a push towards biorefinery production at industrial scale are: (i) energy supply security and reduction in dependency on oil imports, (ii) support of rural areas development through technology deployment and creation of jobs and (iii) mitigation of the greenhouse gas emission (GHG), and the reduction in emissions of particulate matter that are toxic for the environment, animals and humans —promoting a low carbon and sustainable economy (Bautista et al., 2016; Valdivia et al., 2016).

Unfortunately, the development of the biobased products market has been slower than expected due to the investors' perception of high technological risk, intensive capital costs¹ and the low prices that result in poor economics attractiveness of the biorefineries (Valdivia et al., 2016). As an example of this, for 2015 a total of 67 biorefineries worldwide were producing second-generation ethanol, biodiesel, or aviation biofuel. Only a third of these (24), were operating on commercial scale (Nguyen et al., 2017). Despite government support for the biorefinery technologies and tax credit exemptions has been significant, it is probably still not sufficient (Bautista Rodríguez, 2015; Valdivia et al., 2016). Then, private investors should also play an important role in bringing the biorefinery industry to a mature level, by allocating their resources to green, sustainable and economically viable technology and supporting the development of biorefinery commercial facilities. This will decrease the perceived technological risk for investors, and increase the number of entities, banks and private funds interested in this market (Valdivia et al., 2016).

Concerning the economic results, the availability of enough cost-effective biomass is one of the main challenges for the industry. Because the challenge is not the global amount of feedstock that is available but the logistics for handling and supplying feedstock are not well developed. Another major issue is the cost associated with getting the biobased products to destination (Valdivia et al., 2016). As a consequence of the lack of a well-defined logistical model, biomass supply and biobased products distribution represents the main cost in biorefinery products production (Espinoza Pérez et al., 2017; Kim et al., 2011). Therefore, efforts to optimize the supply chain of biorefineries are needed. Considering that supply is not only a cost problem but it is also a location issue (Valdivia et al., 2016).

¹ The median oil-to-biodiesel plant has a capital expenditure of 465 USD per ton, the median unit capital cost is 757 USD per ton for a dry corn mill ethanol plant, whereas it is 2 899 USD per ton for a lignocellulosic and 3 042 USD per ton for a thermochemical ethanol production biorefinery (Tsagkari, M., Couturier, J., Kokossis, A., & Dubois, 2016);

Another solution to accelerate the market development for biobased products could be to create centralized markets or biomass reference markets that allow homogeneous supply routes. An example could be, as described by (Lamers et al., 2015), to integrate intermediate storage facilities where preprocessing of the biomass will be carried out. This would lead to decreasing logistic costs and provide higher versatility to all facilities (Dunnett et al., 2008; Lamers et al., 2015; Valdivia et al., 2016).

Also, the standardization of biomass coming from different feedstocks, could be seen as a solution, because the industry will reach the flexibility required to provide more freedom for the location of the facilities (Espinoza Pérez et al., 2017), and the number of potential facilities per region will probably increase by making the technology less dependent on local feedstock from a given location (Valdivia et al., 2016).

In order to avoid low prices issues, diversification of final products is one suitable alternative. Because more flexible biorefineries will be able to respond more rapidly to changes in market (Espinoza Pérez et al., 2017; Kamm and Kamm, 2004; Van Dyne et al., 1999).

Then, there is a need for projects to develop the biorefineries and its supply chain, including biomass procurement from different feedstocks, diversification of final products, different production technologies and a preprocessing stage.

However, as biorefineries are an example of large investment projects, it implies a preliminary assessment of the potential project performance, traditionally evaluated through the technical and economic feasibility. These preliminary studies provide information to decisions-makers related to context constraints and opportunities, structural requirements of the project; development time estimated and labor required among other information. Then, depending on decision-maker preferences related to project performances, the project will be deployed or not.

Therefore, regarding the complexity of biorefineries projects, the technical feasibility and economic results evaluation is not enough to estimate accurately the potential project performance. Other aspects should be considered in the preliminary assessment, such as the social and potential environmental impacts of the project. Because nowadays decisions related to launching a project and its success does not depend only in investors' preferences and return of investment, it also depends on factors such as the perceptions of the population and support and environmental policies of the governments involved in the operation area of the project. Thus, to develop a project with a higher probability of being launched and successful, its preliminary assessment should show that the project is sustainable by a compromise between the different sustainability dimensions: Economic, politic, technological, social and environmental.

Nevertheless, complexity also arises when the different dimensions of the project performance are evaluated, and very often there are several performances having conflicting objectives between them. For example, seeking the maximization of economic results as well as minimizing the negative environmental impacts.

The overview carried out to study the supply chain decision-making levels and the sustainability dimensions applied to biorefineries has shown that none of the publications targeted the system complexity as a whole (Espinoza Pérez et al., 2017). From the above evidence, it is clear that the sustainable biorefinery supply chain is still studied in a fragmented and partial manner. Therefore, due to the growing importance of this industry, decision-making approaches and tools are needed to help the development of projects for a sustainable biorefinery supply chain.

Objectives of the research

The overall goal of this research is to lay the foundations for a decision-making tool to support the development of projects for a sustainable biorefinery supply chain conception.

Indeed, as each project is unique it must be evaluated within its own context, taking into account simultaneously: the biomass offer of the territory, the environmental impacts, and a sustainable rural development as mentioned before. So it is a problem that must be treated from a multidisciplinary point of view. This research aims to integrate the point of view of chemical engineering (process design) and industrial engineering (external environment) in a holistic but formal approach to represent the dynamics of the entire industrial ecosystem of a biorefinery project.

Multiobjective optimization by evolutionary algorithms has a proven approach that allows managing simultaneously a set of objective functions with conflicting goals. However, as the reader will further realize, the amount of information and variables to deal with, when modeling such a problem could be significant. So the proposed approach will contribute to formalize the modeling strategy in a systemic way to integrate gradually complexities of the real system and sustainability dimensions, developing an integrated model.

The main contributions of this thesis can be summarized as follows:

- ✚ A detailed bibliographic analysis of the key challenges and requirements for sustainable and industrialized biorefinery supply chain
- ✚ The proposition of a general methodology to assess a sustainable biorefinery supply chain configuration
- ✚ The proposition of a modeling strategy methodology, integrating the sustainability dimensions and the specific requirements for the design of a biorefinery supply chain phase III
- ✚ A bibliographic study for the selection of optimization techniques for the sustainable biorefinery supply chain phase III design model.
- ✚ The development and application of an evolutionary algorithm to handle multi-objectives, binary decision variables and equality and inequality constraints.
- ✚ The development of an integrated model including the specific requirements for the design of a biorefinery supply chain phase III and a set of objective functions related to sustainability dimensions (to find out the decision-maker preferences as perspective).
- ✚ A system behavior comprehension by optimal solutions and sensitivity analyses.

Organization of the thesis

The thesis is organized as follows:

Introduction and context

Chapter I. Why develop a biorefinery? An overview of the biorefinery description and classification is presented, in order to allow the reader to understand the context of this research.

Chapter II. Key challenges and requirements for sustainable and industrialized biorefinery supply chain: A bibliographic analysis. An overview of the supply chain decision-making levels and the sustainability dimensions applied to biorefineries is presented. Furthermore, a comprehensive mapping of the scientific literature is realized to identify the key research challenges and requirements for the biorefinery supply chain design, management and optimization from a sustainable point of view. 182 research articles published from 2006 to 2016 were found and revised. Among them, 84 significant references in terms of sustainable biorefinery supply chain design and management were selected. This chapter distinguishes between existing surveys by the dimensions of sustainability involved and solution methods employed to obtain an optimal configuration for a biorefinery project.

Conceptual Framework

Chapter III. Conceptual framework: Decision-making on sustainable biorefinery supply chain. Operations research discipline fundamentals and its suitability for the conception of a sustainable and industrialized biorefinery project are detailed. Then, the different model classification within the operations research field and the type of model that should describe the biorefinery supply chain is presented. Once, the methodologies to solve the model are detailed and studied is established. To finally propose a general methodology with the process needed to obtain the sustainable biorefinery supply chain configuration.

Model Development

Chapter IV. Methodology proposition: Modeling strategy methodology and bibliographic study for the selection of optimization techniques. This chapter develops an attempt to presenting a methodological proposal for the sustainable Phase III BioRSC design model construction. Then, it presents a first model integrating the biorefinery characteristics and the supply chain strategic decisions. Also, a bibliographic study is carried out to characterize the Multi-Objective Optimization Problem, that will generate the integration of the sustainability dimensions in the model, and to choose the most appropriated optimization technique. Finally, the chosen optimization algorithm is described in detail, as well as its programming and optimization features.

Chapter V. Model construction by sustainability dimensions analysis. The sustainability dimensions description is generalized to implement it in biorefineries projects. In parallel, the model developed in chapter IV is completed thanks to a detailed analysis including each sustainability dimension, principle, criterion and indicator, generating an integrated model that

includes binary and real decision variables; equality and inequality constraints; and several objective functions.

Case study application and results

Chapter VI. Case study parameter description. The parameters to analyze the potential performances of projects to design a sustainable biorefinery supply chain phase III in Colombia are presented in-depth.

Chapter VII. Multiobjective algorithm and optimization results. The algorithm parameters used in the multiobjective optimization by the adapted evolutionary algorithm programming are presented in this chapter, including the strategy for parents' generation. In order to detail the multiobjective optimization results and the obtained Pareto front. A brief sensitivity analysis and the model validation are also presented.

This document finishes then, by presenting the main conclusions and perspectives that synthesize our contributions.

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One scientific paper has been published in the *Renewable and Sustainable Energy Reviews*. And three conferences were presented: *28th European Conference on Operational Research (EURO)* (Poznan, Poland; 2016); *16^{ème} Congrès de la Société Française de Génie des Procédés* (Nancy, France; 2017) and *12th International Conference on Multiple Objective Programming and Goal Programming (MOPGP)* (Metz, France; 2017).

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Contents

Chapter I. Why develop a biorefinery?	1
1.1. Introduction.....	1
1.2. Biorefinery background	1
1.3. Biorefinery integration degree	5
1.4. Special characteristics of biorefineries.....	6
1.5. Summary.....	7
1.6. References	8
Chapter II. Key challenges and requirements for sustainable and industrialized biorefinery supply chain: A bibliographic analysis	11
2.1. Introduction.....	11
2.2. Challenges and requirements for a sustainable biorefinery supply chain conception	11
2.3. Methods	14
2.4. Results	15
2.5. Discussion	20
2.6. Summary.....	21
2.7. References	22
Chapter III. Conceptual framework: Decision-making on sustainable biorefinery supply chain.....	29
3.1. Introduction.....	29
3.2. Operations Research	29
3.3. General methodology proposition for decision-making on sustainable Phase III BioRSC projects.....	42
3.4. Discussion	44
3.5. Summary.....	44
3.6. References	44
Chapter IV. Methodology proposition: Modeling strategy methodology and bibliographic study for the selection of optimization techniques.....	47
4.1. Introduction.....	47
4.2. Model construction proposition for sustainable Phase III BioRSC design.....	47
4.3. Model resolution methodology for a Multi-Objective Optimization Problem.....	59
4.4. NSGA-II programming and optimization features	68
4.5. Summary.....	74
4.6. References	74

Chapter V. Model construction by sustainability dimensions analysis	77
5.1. Introduction.....	77
5.2. Economic dimension analysis.....	78
5.3. Political dimension analysis.....	81
5.4. Technological dimension analysis	87
5.5. Social dimension analysis	90
5.6. Environmental dimension analysis.....	94
5.7. Summary.....	102
5.8. References	104
Chapter VI. Case study parameter description.....	105
6.1. Introduction.....	105
6.2. Parameter definition for strategic decisions in SC and the BioRSC characteristics.....	106
6.3. Parameter definition for the economic dimension equations.....	125
6.4. Political dimension analysis.....	131
6.5. Technological dimension analysis	136
6.6. Social dimension analysis	141
6.7. Environmental dimension analysis.....	148
6.8. Conclusions.....	156
6.9. References	158
Chapter VII. Multiobjective algorithm and optimization results	165
7.1. Introduction.....	165
7.2. NSGA-II parameters and parents production.....	165
7.3. Multiobjective optimization results	166
7.4. An example of optimal solutions with compromises between the sustainability dimensions	181
7.5. Sensitivity analysis.....	182
7.6. Model validation.....	186
7.7. Conclusions.....	188
7.8. References	190
Chapter VIII. Conclusions and perspectives	191
Appendix Chapter V
Appendix Chapter VI

List of Figures

Figure 1. 1 <i>Degree of biorefinery integration based on (Dyne et al. 1999; Kamm and Kamm 2004; Espinoza Pérez et al. 2017b)</i>	5
Figure 2. 1. Triple Bottom Line Extended (TBL+), sustainability dimensions.	12
Figure 2. 2 Main decision variables for each level of decision-making in BioRSC management (Iakovou et al. 2010; Mortazavi et al. 2015).	14
Figure 2. 3 Publication distribution according to the dimensions of sustainability (Ec = Economic, En = Environmental, So = Social, Po = Political, Te= Technological) objective (O = Optimization, S = Simulation) and decision level studied (Espinoza Pérez et al. 2017)	16
Figure 3. 1. Principal steps for solving operational research problems.	30
Figure 3. 2. Optimization model classification resumed.	34
Figure 3. 3. General methodology for design, management and scheduling model construction for a sustainable Phase III BioRSC.....	42
Figure 3. 4. Comparison between stochastic programming multistage and RO application to model construction	43
Figure 4. 1. Phase III BioRSC characteristics, SC strategic decisions and sustainability dimensions model integration.....	49
Figure 4. 2. Model evolution to integrate BioRSC strategic level of decision-making and specific characteristics of a phase III biorefinery (Personal construction).....	50
Figure 4. 3. Adaptation from (Chi-Keong Goh and Kay Chen Tan 2009; Suárez Palacios et al. 2011; Xiong et al. 2015).....	61
Figure 4. 4. Comparison of number of scientific articles related to evolutionary algorithms	64
Figure 4. 5. Research trend of in the use of evolutionary algorithms, Part 1	65
Figure 4. 6. Research trend of in the use of evolutionary algorithms, Part 2	65
Figure 4. 7. Research trend of in the use of evolutionary algorithms, Part 3	65
Figure 4. 8. NSGA-II process structure, based on (Peñuela Meneses and Granada Echeverri 2007; Deb 2008b; Deb 2008a)	66
Figure 5. 1. Sustainability framework.....	77
Figure 5. 2. General model for Phase III BioRSC design	101
Figure 5. 3. Developing model layer-by-layer	102
Figure 6. 1. Geographical distribution of raw material sources.	110
Figure 6. 2. Map with potential pretreatment plants locations and the raw materials sources	113
Figure 6. 3. Map of potential locations of pretreatment plants	114
Figure 6. 4. Principal plant location referred by demand location.....	118
Figure 6. 5. Graphical representation for potential location for main production biorefinery plants	119
Figure 6. 6. Final products demand localization.....	122
Figure 6. 7. Clients for intermediate products at Colombia.....	123

Figure 6. 8. Operational cost for the jatropha oil transformation ($b = 1$) with technology $d = 1$ and production capacity $g = 1$ (40,000 tons/year) at principal plants	138
Figure 6. 9. Indigenous settlements in Colombia in 2012.	143
Figure 6. 10. Density of abandoned properties in Colombia.	145
Figure 7. 1. <i>Steps to population creation and Pareto fronts achievement</i>	165
Figure 7. 2. <i>Pareto front analysis. (a) Net present value (USD 10^8) – Required hectares (10^4). (b) Demand Satisfaction (%) - Required hectares (10^4).</i>	168
Figure 7. 3. <i>BioRSC configuration to obtain a maximal value for the net present value, using the minimum amount of hectares</i>	170
Figure 7. 4 <i>BioRSC configuration to satisfy the 100% of final demand satisfaction, using the minimum amount of hectares.</i>	171
Figure 7. 5. <i>Pareto fronts for net present value comparisons</i>	172
Figure 7. 6. <i>Pareto fronts for demand satisfaction comparisons</i>	175
Figure 7. 7. <i>Pareto fronts for total water use comparisons</i>	178
Figure 7. 8. <i>Pareto fronts for TRL comparisons</i>	179
Figure 7. 9. <i>Pareto fronts for GINI comparisons</i>	180
Figure 7. 10. <i>Net present value sensitivity face price and demand changes</i>	183
Figure 7. 11. <i>Variations over the net present value</i>	184
Figure 7. 12. <i>Net present value optimal solution if final products demand increases 600%</i>	185

List of Tables

Table 1. 1 Bio-refinery definitions	2
Table 1. 2. Raw materials, processing technologies and products in a biorefinery (adapted from Demirbas 2009; Iakovou et al. 2010; Yue et al. 2014b; Clark and Deswarte 2014; Espinoza Pérez et al. 2017b).	2
Table 1. 3 Biorefinery uncertainties (Kim et al. 2011; Sharma et al. 2013; Espinoza Pérez et al. 2017b).	7
Table 2. 1. <i>Search strategy steps (Espinoza Pérez et al. 2017)</i>	15
Table 2. 2 <i>Analysis of the 84 publications selected in this study (Espinoza Pérez et al. 2017)</i>	17
Table 2. 3. <i>Main findings summary (Espinoza Pérez et al. 2017)</i>	21
Table 3. 1. Sustainable Phase III BioRSC model classification	36
Table 3. 2. Principal methodologies for solve OR models description and its suitability for solve MO-BMIP models	39
Table 4. 1. <i>Quantity of Principles, criterion and indicators to analyses for sustainability assessment</i> .	59
Table 4. 2. Different types of MOEAs, based on (Deb 2008a).....	63
Table 4. 3. Keywords used for search on Scopus	64
Table 4. 4. <i>Objective combination for it graphic</i>	68
Table 4. 5. <i>Verification changes in equations to create children and mutants</i>	72
Table 5. 1. <i>Economic analysis by criterion and indicator</i>	78
Table 5. 2 <i>Political analysis by criterion and indicator</i>	82
Table 5. 3 <i>Technology Readiness Level (TRL) description. Based on (Energy 2009; Institute of Medicine and National Research Council 2013; ESA 2015; European Comission 2015; NASA 2015; DTU 2017)</i> .	86
Table 5. 4. <i>Technological analysis by criterion and indicator</i>	88
Table 5. 5. <i>Social analysis by criterion and indicator</i>	91
Table 5. 6. <i>Environmental analysis by criterion and indicator</i>	94
Table 5. 7. <i>Overview of general mathematical expressions in the integrated model</i>	103
Table 6. 1. <i>Model parameters to design a sustainable Phase III BioRSC</i>	105
Table 6. 2. <i>Parameters of the model and equation where they are included</i>	106
Table 6. 3. Raw material availability by raw material type and location	109
Table 6. 4. Hectares availability to jatropha production in Colombia.....	109
Table 6. 5. Jatropha and palm oil production cost (Gaona Currea 2009)	111
Table 6. 6 Estimated oil acquisition cost at Colombia in 2015.....	111
Table 6. 7. Palm and jatropha crude oil physic-chemical characteristics.....	112
Table 6. 8. <i>Material losses in each pretreatment stage for an average oil (Blanco Rodríguez 2007)</i> . 112	112
Table 6. 9. Processing rates for palm oil and jatropha parameters to optimization model ($\alpha n, b, c$) 112	112
Table 6. 10. Potential locations for pretreatment plants in Colombia.....	114
Table 6. 11. Estimated installation cost of pretreatment plants ($Inv_j, c, f, \forall j, c$).....	115
Table 6. 12. Operational cost at pretreatment plants ($ProdCost_{n, j, c} = 1, f, \forall j$)	115
Table 6. 13. Processing rates for intermediate products at principal production plants ($\alpha b, d, a$)....	117
Table 6. 14. Potential location for main production biorefinery plants.....	117

Table 6. 15. Summary of installation cost of main production plants (USD)	119
Table 6. 16. Production cost at principal production plants by intermediate product and technology ($ProdCost_{b,k,d,g,\forall k}$)	120
Table 6. 17. Final products demand by location and product type ($Dem_{l,a}$)	121
Table 6. 18. Refined African palm oil and its fractions sales in Colombia at 2015.....	123
Table 6. 19. Transportation cost at Colombia details (Colombian currency).....	124
Table 6. 20. <i>Economic dimension parameters</i>	125
Table 6. 21. Norms related to pollution in Colombia. Based on UPME (2017a) and Ministerio Medioambiente Colombia (2015).	126
Table 6. 22. TSS rate production at principal plants ($y = TSS, \forall b$)	129
Table 6. 23. BOD rate production principal plants ($y = BOD, \forall b$).....	129
Table 6. 24. Consumer Price Index in Colombia for water supply, sewerage and sanitation based on DANE (2017b) by total revenue (The CPI base is the year 2008, 100)	129
Table 6. 25. Solid waste production rate at pretreatment plants $\forall f$	130
Table 6. 26. Solid waste production rate at principal plants $\forall g$	131
Table 6. 27. <i>Political dimension parameters</i>	131
Table 6. 28. Biodiesel global production in 2015 and percentage of advanced biodiesel produced (REN21 2017; Statista 2017).....	132
Table 6. 29. <i>Biodiesel/diesel</i> rate required globally at 2015	133
Table 6. 30. Parameters for governmental expenditures related to research and development for biorefineries	134
Table 6. 31. <i>Suppliers location RSPO certified in Colombia</i>	136
Table 6. 32. <i>Technological dimension parameters</i>	136
Table 6. 33. Water consumed at principal production plants by technology and capacity (t water/ t intermediate product).....	137
Table 6. 34. Operational cost that integrates technology apprenticeship at pretreatment plants....	138
Table 6. 35. Operational cost that integrates technology apprenticeship at principal plants.....	139
Table 6. 36. TRL at biorefinery principal production plants	140
Table 6. 37. <i>Social dimension parameters</i>	141
Table 6. 38. GINI index related to raw material locations.....	146
Table 6. 39. GINI index related to pretreatment and principal plants locations.	146
Table 6. 40. Employment opportunities at raw material stage	147
Table 6. 41. Employment opportunities at pretreatment plants.....	148
Table 6. 42. Employment opportunities at principal plants.....	148
Table 6. 43. <i>Environmental dimension parameters</i>	149
Table 6. 44. Water degradation rates by raw material type and location ($\vartheta\tau, i, n$).....	151
Table 6. 45. Sewage water rate generation at pretreatment plants (sewage water t/raw material t)	151
Table 6. 46. Sewage water rate generation at principal plants (sewage water t/intermediate product t)	151
Table 6. 47. CO ₂ absorption made in raw material cultivation stage.....	152
Table 6. 48. CO ₂ generation at crude oil extraction stage.....	153
Table 6. 49. CO ₂ generation at pretreatment plants by raw material transformation (CO ₂ equivalent t/t raw material).....	153

Table 6. 50. CO ₂ generation at principal plants by intermediate products transformation (CO ₂ equivalent t/t intermediate products)	153
Table 6. 51. <i>Hectares/t oil production rate</i>	154
Table 6. 52. Energy expenditure to transform products in pretreatment plants	156
Table 6. 53. Energy expenditure to transform products in principal plants	156
Table 6. 54. <i>Total objective functions for the integrated model applied to the Colombian case</i>	157
Table 7. 1. <i>Objective function pairwise comparison</i>	167
Table 7. 2. <i>Optimal solutions detail comparison</i>	169
Table 7. 3. <i>Optimal solution to maximize the demand satisfaction and minimize the CO₂-equivalent emissions</i>	177
Table 7. 4. <i>An optimal solution with compromises between sustainability dimensions.</i>	181
Table 7. 5. <i>Plants selection for demand satisfaction as objective function face to changes in production capacity.</i>	184
Table 7. 6. <i>Plants selection for net present value as objective function face to changes in production capacity.</i>	185
Table 7. 7. <i>Face validity for the integrated model</i>	186
Table 7. 8. <i>Pairwise comparison between all objective functions to sustainable Phase III BioRSC design</i>	189

Chapter I. Why develop a biorefinery?

1.1. Introduction

The growing of global population and its effect on world food security, as well as the urgency for climate change mitigation, are issues that foster technological, social, and political innovations to increase the efficiency of the use of natural resources (Sammons et al. 2007; Sukumara et al. 2013; Höltinger et al. 2014). Among the natural resources recently investigated, biomass has interested researchers because of its widespread availability and its potential applicability as sustainable source of energy and material (Sukumara et al. 2013).

In order to take advantage of the biomass potential, new technologies have been developed to generate alternative energies and new raw materials, which have the potential to reduce greenhouse gas emissions, while increasing energy security and sustainability, reducing petroleum dependency (Kaercher et al. 2013). To integrate these new raw materials and technologies, the biorefinery concept has been developed, as an industrial facility where biomass is transformed into a wide range of marketable products and energy (Sammons et al. 2007; Department of Energy 2015), in the same form oil is transformed in energy, fuels and chemical products in a petroleum refinery. In this chapter, as a starting point, an overview of the biorefinery description and classification is presented, in order to allow the reader to understand the context of this research.

1.2. Biorefinery background

Biorefinery concept involves different industrial sectors, including transport, chemical, energy, agricultural and forest. As a consequence, there is no single definition for that type of industrial facility. However, based on definitions provided by institutions such as the National Renewable Energy Laboratory (NREL 2015), the Energy Research Center of the Netherlands (ECN 2010) and the National Non-Food Crop Centre (NNFCC 2007), presented on Table 1.1, a general definition of the biorefinery concept is proposed (Espinoza Pérez et al. 2017b):

A biorefinery is a facility similar to the traditional oil refinery, where energy, fuels, chemicals and materials are produced through different processes and technologies. Nonetheless, raw materials of biorefineries are any organic material from renewable sources that can be used for industrial purposes. Consequently, there are numerous possibilities for converting it, which multiplies the possible schemes of operation that can be developed.

Main feedstock of a biorefinery is biomass, that is organic material obtained from living or recently living organisms, which can be used for industrial purposes (Kamm and Kamm 2004; García 2009). Regarding the diversity of biomass resources that can be processed in a biorefinery, multiple conversion technologies are required to transform them into end-products with a broad range of chemical structures, properties and applications. The diverse biomass types, processing technologies and end-products involved in a biorefinery are detailed in the next subsections and summarized in Table 1. 2. 1.2 (Espinoza Pérez et al. 2017b).

Table 1. 1 *Bio-refinery definitions*

Organization	Bio-refinery definition
IEA Bioenergy Task 42 (IEA Bioenergy 2009).	Bio-refinery is the sustainable processing of biomass into a spectrum of marketable products (food, feed, materials, chemicals) and energy (fuel, energy, heat)
Nacional Renewable Energy Laboratory (NREL 2015)	It is a facility that integrates the processes and biomass conversion equipment to produce fuels, power and chemicals. The bio-refinery concept is similar to oil refineries, which produce multiple fuels and petroleum products
Department of Energy of United States (US-DOE)(Department of Energy 2015).	It is similar to traditional oil refineries concept, where various types of biomass feedstock are converted into negotiable items, like chemicals, fuels and products. Bio-refineries maximize profits by producing high value low volume products, improving profitability; and lower value but higher volumes to satisfy the energy needs of the country. Products obtained can be used for transportation, energy, chemicals and energy
Energy Research Center of the Netherlands (ECN 2010).	Facilities where green raw materials become valuable products, which should be not only fuel but also chemicals with higher value added, so the use of biomass can be profitable. Bio-based products help the chemical industry to reduce its dependence on fossil raw materials and significantly reduce CO ₂ emissions
Nacional Non-Food Crop Centre (NNFCC 2007).	Bio-refining is the sustainable processing of biomass into a spectrum of marketable products (food, feed, fuel, chemicals, heat and electricity). Bio-refineries provide a way by which renewable materials can be integrated and mass-produced, allowing large-scale replacement of fossil fuels and materials

Table 1. 2. *Raw materials, processing technologies and products in a biorefinery (adapted from Demirbas 2009; Iakovou et al. 2010; Yue et al. 2014b; Clark and Deswarte 2014; Espinoza Pérez et al. 2017b).*

Biomass	Transformation technologies	Products
<i>Residual Biomass</i>	<i>Physical transformation</i>	<i>Energy</i>
Forest residues	<i>Direct extraction</i>	Thermal energy
Agricultural residues	<i>Biochemical transformation</i>	Electrical energy
Municipal waste	<i>Thermochemical transformation</i>	Mechanical energy
<i>Energy Crops</i>		<i>Biofuels</i>
Crops for ethanol production		Bioethanol
Oilseeds		Biodiesel
Lignocellulosic crops		Biogas
Aquatic crops		Synthetic biofuels
		<i>Chemicals and materials</i>
		Carbohydrate-based bio-products
		Lipid-based bio-products
		Protein-based bio-products
		Lignin-based bio-products
		Secondary metabolites

1.1.1. Biomass

Potential raw materials can be divided into residual biomass and energy crops (García 2009). Residual biomass includes forest residues (either residues from wood processing, paper mills and pulp), agricultural residues (either pruning woody crops such as vineyards, arable crops such as cereal straw, cattle residues as manure and slurry, food industry residues) and municipal waste (such as waste oil and wastewater). Energy crops comprise but are not limited to sugar cane, corn, starch sources,

oilseeds, producing terpenes and rubber plants, lignocellulosic crops, herbs and grasses, and aquatic crops (Biomass Research and Development 2013; García 2009).

1.1.2. Biomass transformation technologies

As previously mentioned, because of the diversity in biomass resources used as feedstock, multiple conversion technologies are needed to transform their physical and chemical characteristics into the required products (Biomass Research and Development 2013). Factors that influence the choice of a conversion process include the type and quantity of biomass feedstock, the desired product and internal or external restrictions, i.e. chemical composition of biomass, end-use specifications of the product, economic conditions and other project-specific factors as environmental standards, legal framework, etc. (Hulteberg and Karlsson 2009; Iakovou et al. 2010).

Biomass transformation processes can be classified into physical transformation, direct extraction, thermochemical transformation, chemical transformation and biochemical transformation.

Physical transformation: Also called mechanical transformation, it can occur by changes in temperature or pressure or application of external forces or fields (National Research Council (US) 2013).

Direct extraction: Otherwise known as physicochemical conversion. It is the transformation of biomass, after drying and milling to reduce particle size by extraction process using solvents. This conversion produces products such as fragrances, flavoring substances, colorings, condiments, pharmacological substances, nutraceuticals, oils, hydrocarbons and polyphenols (García 2009; Iakovou et al. 2010).

Thermochemical transformation: It involves changing physical properties and chemical structures of biomass through the use of high temperature processes and catalysis (Yue et al. 2014). Biomass is converted into solid, liquid or gas fuels (e.g.: gasification, pyrolysis and coal) (Balat et al. 2009; Iakovou et al. 2010). These processes can be divided into four categories: direct combustion, gasification pyrolysis and liquefaction (García 2009; Iakovou et al. 2010).

- *Combustion* is used over a wide range of outputs to convert the chemical energy stored in biomass into heat, mechanical power or electricity (De Kam et al. 2009; Iakovou et al. 2010). In this process oxygen is in excess respect to the stoichiometric ratio. Combustion of biomass produces hot gases at temperatures around 800–1,000 °C. In practice, combustion is feasible for biomass with inherent moisture content less than 50%. However, biomass with high moisture content is better suited for biological conversion processes (Velis et al. 2009; Iakovou et al. 2010).
- *Gasification* is the conversion of biomass into a combustible gas mixture by the partial oxidation at high temperatures, typically in the range 800–900 °C (Cao et al. 2006; García 2009). In this kind of process, biomass is heated with limiting amounts of an oxidizer as air, oxygen, steam or hydrogen. Low calorific value gas produced can be burnt directly or it can be used as a fuel for gas engines and gas turbines, as well as feedstock in the production of chemicals (Iakovou et al. 2010).

- *Pyrolysis* is the conversion of biomass into solid, liquid, and gaseous fractions by heating in air absence. In fast pyrolysis (residence time of less than one second and temperatures around 1,000°C) a liquid known as pyrolysis oil fuel can be obtained (García 2009; Yue et al. 2014).
- *Liquefaction* is the conversion of biomass into a stable liquid hydrocarbon by applying high pressure and temperature (Xu and Etcheverry 2008).

Chemical transformation: Involves the change of physical properties and chemical structures of biomass resources by reaction with different transformation agents, usually in presence of catalysts. Probably, production of biodiesel from vegetable oils by transesterification with methanol in presence of alkaline catalyst is the most important application of this kind of biomass transformation.

Biochemical transformation: In this kind of processes, chemical structure of biomass is modified by the action of microorganisms as bacteria, yeasts and fungi (Clark and Deswarte 2014). Microorganisms can be present in biomass or externally added during processing (Yue et al. 2014). Transformation processes include anaerobic digestion, for obtaining biogas and ethanol; transesterification mediated by organisms for producing micro-diesel, and biological hydrogen production (Demirbas 2009), among many other transformations.

1.1.3. Products

Products obtained in a biorefinery can be energy, fuels, chemicals and materials (NNFCC 2007; IEA Bioenergy 2009; ECN 2010; NREL 2015; Department of Energy 2015).

Energy: It includes all forms of energy derived from fuels of biological origin. These include thermal energy, which can be obtained by direct combustion in boilers, electrical energy, from the steam generated by combustion, and mechanical energy ,obtained by engine combustion (García 2009).

Biofuels: It comprises bioethanol, biodiesel, biogas, synthetic biofuels, among others (Kamm and Kamm 2004; Department of Energy 2015).

Chemicals and materials: These can be divided into five categories: bio-products based on carbohydrates (e.g.: lactic acid, succinic acid, butanol, 3-hydroxypropionic acid, 1,3-propanediol, poly-hydroxy-alkanoates (PHAs)), lignin-based bio-products (vanilla, dimetilsulfoxidos, lignosulfonates, phenol formaldehyde resins, epoxy resins), lipid-based bio-products (esters, acids, alcohols, ethoxylated alcohols, amines, amides, polymers, etc.), protein-based bio-products and secondary metabolites (latex, terpenes and PHA) (Kamm et al. 2010; Demirbas 2009; Clark and Deswarte 2014).

1.3. Biorefinery integration degree

Regarding the wide range of raw materials entering the production system and the diversity of processing technologies, three degrees of biorefinery integration can be distinguished, as presented in Figure 1. 1 (Van Dyne et al. 1999; Kamm and Kamm 2004).

A Phase I biorefinery uses a single raw material in a simple and fixed transformation process, yielding one main product, so there is no flexibility in the process (Espinoza Pérez et al. 2017b). A Phase II biorefinery also processes a single raw material, but is able to produce various end-products in response to the market (Espinoza Pérez et al. 2017b). Finally, a Phase III biorefinery uses several types of raw materials and production technologies that enable the production of many industrial products (Espinoza Pérez et al. 2017b).

Biorefineries Phase II and Phase III are able to respond more rapidly to changes in the market environment than a Phase I biorefinery. However, Phase II and Phase III biorefineries design is more complex (Espinoza Pérez et al. 2017b), because there is a set of choices to make that increases the decision-making process. Once the final product features and requirements are defined, these decisions must include biomass selection, transformation technologies and materials management for turning raw materials into end-products, in addition to other constraints and requirements for developing a sustainable biorefinery (Espinoza Pérez et al. 2017b), which will be discussed on Chapter II.

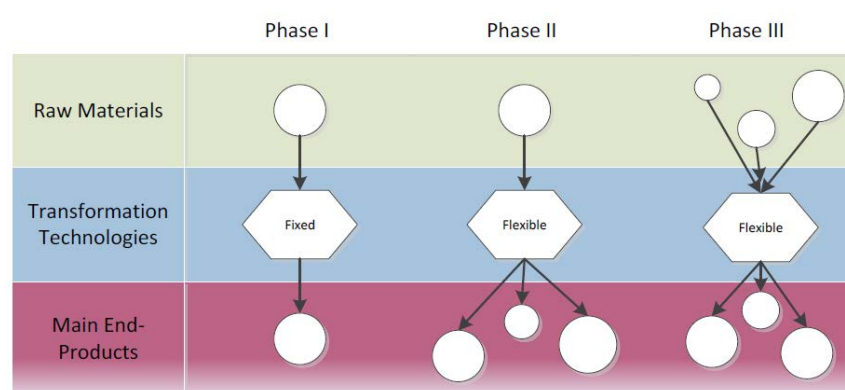


Figure 1. 1 Degree of biorefinery integration based on (Dyne et al. 1999; Kamm and Kamm 2004; Espinoza Pérez et al. 2017b)

Based on this categorization, most of the worldwide current biofuels production plants are part of the biorefineries Phase II, because they valorize by-products. For example, biodiesel production plants produce biodiesel, crude and/or pure glycerin, margarines, food for livestock and organic fertilizers by processing only palm oil as raw material (Grupo Oleoflores 2017; Manuelita 2017).

However, considering problems raised from raw materials price increment in biofuels industry which has impacted negatively its profitability and the negative effect on food security (Espinoza Pérez et al. 2017a), diversification of raw materials is recommended which signifies to develop Phase III biorefineries. Despite this, biorefineries Phase III have not been borne out in practice. Some of the

reasons for this are the high costs of capital investment² and the various uncertainties related to the nature of the biorefinery, which will be discussed on section 1.4.

1.4. Special characteristics of biorefineries

First of all, biomass is usually characterized by seasonal availability (Rentizelas et al. 2009). At the same time, there are high transportation costs because biomass is bulky and difficult to transport. Moreover, harvesting and collection costs are high because their supply is widely dispersed geographically (Ekşioğlu et al. 2009). Furthermore, biomass is a heterogeneous matter, so it requires pre-treatments to homogenize it (Santibañez-Aguilar et al. 2014). Therefore, the form in which biomass will be procured determines a high percentage of the investment and operational costs.

Another characteristic of a biorefinery is their actors are independent and also geographically distributed (Hanafizadeh and Sherkat 2009). This implies that each stakeholder regards its own interests and needs, and focuses on achieving its own targets (Long and Zhang 2014). Therefore, a previous geographical analysis is required, in addition to an analysis for the interest of stakeholders, which is clearly associated with multi-objective management. These actors, interact strongly, thus the system exhibits a wide range of dynamic behaviors, which can interfere with scheduling and control at the enterprise level (Lin et al. 2008). This dynamic behavior is due principally to the competitive environment (White et al. 2005).

The set of characteristics detailed above adds strong uncertainties that affect the efficiency of the biorefinery system, which eventually can lead either to infeasible supply chain network designs or to suboptimal performance (Gebreslassie et al. 2012). These constraints create a complex landscape for biorefinery investors and decision-makers, and consequently tools are needed to help assess these uncertainties (Kim et al. 2011). A detailed list of these uncertainties and their origin is presented in Table 1. 31.3.

The tools to assess these challenges should consider that the biorefinery requires information sharing by rapidly transferring information about customer demand to all supply chain levels (Hanafizadeh and Sherkat 2009), as this enables rapid response to market changes (Newman and Krehbiel 2007). Similarly, a flexible structure is desirable, for example a supply chain that adapts itself to environmental changes (Hanafizadeh and Sherkat 2009).

² The median oil-to-biodiesel plant has a capital expenditure of 465 USD per ton, the median unit capital cost is 757 USD per ton for a dry corn mill ethanol plant, whereas it is 2 899 USD per ton for a lignocellulosic and 3 042 USD per ton for a thermochemical ethanol production biorefinery (Tsagkari, M., Couturier, J., Kokossis, A., & Dubois 2016);

Table 1. 3 *Biorefinery uncertainties (Kim et al. 2011; Sharma et al. 2013; Espinoza Pérez et al. 2017b).*

Classification	Uncertainties
Cost	Cost of transporting biomass
	Operation cost for conversion processing
	Cost of transporting intermediate products
	Cost of transporting final products
	Acquisition cost for each biomass type
	Annualized capital cost of conversion processing
	Expansion plans
Profits (Value)	Value of each intermediate product at conversion processing site
	Sale price of each final product
Production Process	Yield of final product from intermediate product at conversion processing
	Yield of intermediate product from biomass at conversion processing
Extern	Demand fluctuations
	Natural or human disasters
	Weather
	Technology availability
Nature of biomass	Change in regulations and policies
	Biomass availability for each biomass type
	Biomass properties such as moisture content

1.5. Summary

As presented in this chapter, biorefineries Phase III are in theory an opportunity to use natural resources in a sustainable way and to replace pollution elements as oil and petrochemicals. However, currently there exists only biorefineries Phase II. Due to biorefineries Phase III high costs of capital investment, related uncertainties and more complex decision-making process.

Then, it is important to note that before making any investment it is recommendable to understand and try to measure the potential benefits and untoward effects of the business. For avoid the problems presented by biorefineries Phase II currently running worldwide, as negative effect on food security.

In this sense, for the conception of the phase III biorefinery integrating potential benefits and untoward effects, different elements and decisions involved must to be distinguished. Firstly, it should be taken into consideration the biorefinery nature constraint presented on this chapter. In addition to the analysis of the decisions related to the supply chain conception and the inclusion of the sustainability concept that will be detailed in the next chapter.

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Chapter II. Key challenges and requirements for sustainable and industrialized biorefinery supply chain: A bibliographic analysis

2.1. Introduction

Even though, biorefineries Phase III can be designed to transform various types of biomass into a range of marketable products and energy (Sammons et al. 2007; Department of Energy 2015), currently only biorefineries Phase I and Phase II have been implemented. Therefore, potential benefits and untoward effects of biorefineries Phase III have not been borne out in practice. Then, to avoid potential undesirable effects of biorefineries implementation at an industrial scale, as diminishing food security or negative economic performance, a phase III biorefinery have to be design from a holistic point of view (American Society for Cybernetics 2014), considering the relevant and full range of "dimensions" of impact (Bautista et al. 2016). That is, to adopt a sustainability assessment for their conception.

Among the different challenges to be overcome when a phase III biorefinery at an industrial scale and in a sustainable manner is going to be implemented, a well-designed and well managed supply chain (SC) is a key condition (Ekşioğlu et al. 2009). Indeed, the design and management of such a project involves many hierarchical decisions which should be optimized (Kim et al. 2011a).

The SC design, management and optimization is a highly complex problem that cannot be solved using simple heuristics from the viewpoint of a single discipline (Sammons et al. 2007). Recently, many researchers have focused their work on the process of design and optimization of a Biorefinery Supply Chain (BioRSC) from an economic point of view (Sharma et al. 2013b; Yue et al. 2014b). However, other dimensions of sustainability have not been included, which represents a serious drawback for this kind of projects. In this chapter, through a comprehensive mapping of the scientific literature, the key research challenges and requirements for BioRSC design, management and optimization from a sustainable point of view are identified.

182 research articles published from 2006 to 2016 were found and revised. Among them, 84 significant references in terms of sustainable BioRSC design and management were selected. This chapter distinguishes between existing surveys by adopting a sustainability perspective, emphasizing the BioRSC challenges, dimensions of sustainability involved and solution methods employed to obtain an optimal configuration for a phase III biorefinery, considering the relevant and full range of impact dimensions of its implementation.

2.2. Challenges and requirements for a sustainable biorefinery supply chain conception

As stated by Ekşioğlu et al. (2009) and Galvez et al. (2015), a well-designed and well managed SC is needed to conceive an optimal phase III biorefinery at an industrial scale in a sustainable way. Hence, designing and optimizing the entire BioRSC system must be developed in a cost-effective, robust and sustainable form (Yue et al. 2014b; Bautista et al. 2016). In order to accomplish this task, constraints and

requirements related to evaluation of the sustainability dimensions and to the decision-making stages should be considered. Following they are going to be described.

2.2.1. Evaluation of the sustainability dimensions

BioRSC design requires sufficient covering of all the aspects of a sustainable SC and the development of an adequate and realistic representation. This means providing a holistic point of view (American Society for Cybernetics 2014), considering, among several factors, that production of most of the bio-based products is not currently economically attractive in comparison to the petroleum derivatives (Wilda Asmarini 2016), despite the benefits in other fields, such as environmental, that have to be simultaneously considered.

The adoption of sustainability assessment for the BioRSC design from a holistic point of view should consider the relevant dimensions, because decision-makers and other stakeholders should be informed of the full spectrum of impact (Bautista et al. 2016). In terms of the impact, environmental, social and economic dimensions are sometimes referred to as the “three pillars” of sustainability or the “triple bottom-line – TBL” (Seuring and Müller 2008; Brandenburg et al. 2014). Recently, the Triple Bottom Line Extended (TBL+) was proposed, including political and technological dimensions, as represented on Figure 2.1. Although TBL+ approach was applied to biodiesel sustainability assessment, it could also be applied to any type of biorefinery.

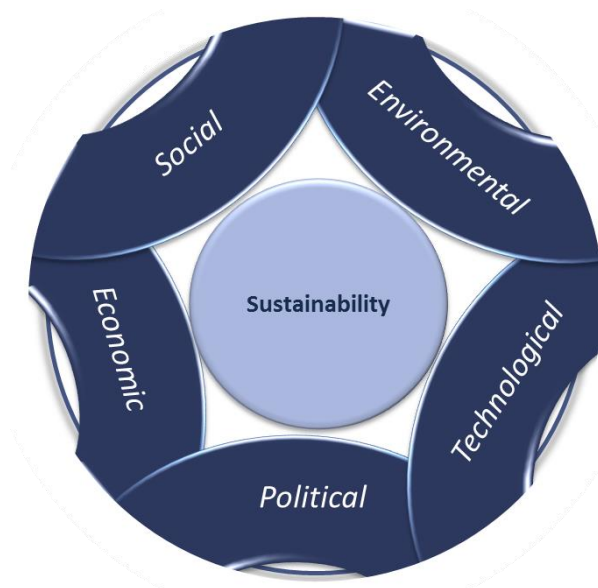


Figure 2. 1. Triple Bottom Line Extended (TBL+), sustainability dimensions.

In particular, political dimension is highly relevant for biorefineries because the governmental policies are essential for promoting its implementation, creating economic conditions and favorable markets through subsidies, tax exemptions, and mandatory consumption as in the case of the diesel-biodiesel mixture (Bautista et al. 2016). Moreover, technological dimension is also relevant, regarding in the field of bio-based products emerging technologies are coming out, and there are concerns about technological learning, royalties or technology substitution among other aspects related to new products and processes (Bautista et al. 2016).

This new concept of five sustainability dimensions, it although was developed for biodiesel systems, can be extended to biorefineries, because current biodiesel production plants constitutes part of a Phase II biorefinery. Therefore, to determine sustainable design criteria and optimization objectives, five dimensions analysis should be considered, as discussed following:

Economic. The main economic objective is to design a self-sustaining biorefinery. It will not need government assistance or reinvestments, because it will have the necessary profitability to be self-sustaining (Cambridge Dictionaries Online 2015). Several metrics can be used to measure this objective. However, in this case, it is necessary to evaluate indicators such as “Maximizing Profit” or “Net Present Value” because minimized cost metrics are not really useful, as a consequence of the high production cost of biodiesel, mainly associated to the high price of vegetable oil (Rincón et al. 2015). Also, regarding prices and market volatility, it is important to include product diversification and the sale of by-products (You et al. 2012).

Social. Regarding the social dimension, studies conducted on BioRSC have measured two edges: the first is related to employment generation and the second to social welfare in terms of food security (Bai et al. 2012; Singh et al. 2014). However, the topics considered in the social dimension must also include respect for property land rights, social acceptability, and promotion of responsible working conditions (Bautista et al. 2016).

Environmental. Among various approaches, life cycle assessment (LCA) is the one most used in studies that consider environmental impact (Yue et al. 2014b). Environmental principles considered in this dimension can be analyzed in regard to issues such as air, soil and water quality, waste and wastewater management, balance of greenhouse gases, conservation and protection of biodiversity and wildlife, and energy efficiency (Ruiz-Mercado et al. 2012).

Technological. This dimension refers to the production technologies available on the industrialized and developing level, as well as its evolution through technological learning based on production (de Wit et al. 2010). It also takes into account technological trends in the use and production of bio-based products.

Political. It refers to promotion or restriction policies that may be promulgated by governments or multi-lateral organizations, as well as possible subsidies and tax reductions to stimulate the market (Bautista et al. 2016). This dimension is one of the most important for a biorefinery because several countries, through governmental incentives, have developed suitable conditions for the emergence of biofuels and bio-based products industries. Some examples are Colombia, Brazil, Argentina, Peru (Falck-Zepeda et al. 2010; Viana Leite 2013), USA (United States Congress 2014) and the European Union (European Parliament 2009), among others.

This enlarged vision of the TBL enabling an improved analysis of the implication of a biorefinery within a particular context. However, the main challenge associated to increasing the dimensions of the sustainability analysis is the availability of reliable information to accomplish it. In addition, in terms of BioRSC modeling, it involves integrating a greater number of variables, parameters, objectives and constraints that may require longer calculation times for simulation and optimization.

2.2.2. Requirements for the decisions involved in the design and management of the biorefinery supply chain

In addition to the previous challenges and requirements, the design and operation of SC networks are also important for the industrialization of biorefineries (Kim et al. 2011a). SC refers to an ideal complete management system as a single entity and not as a disparate group of functions (Keith and Tim 2003; Blanchard 2010). Consequently, the principal challenge in managing SC is the development of decision-making models that can accommodate multiple stakeholders and activities integrated across the SC network (Venugopalan et al. 2014).

The decision-making process through the various activities of the SC is hierarchized under three decision perspectives: strategic, tactical and operational (Mortazavi et al. 2015). Strategic are the basis for tactical and operational decisions, as shown in Figure 2.2. The strategic level covers long-term decisions in the SC design (Chopra and Meindl 2012; De Meyer et al. 2014; Majid Eskandarpour 2015), while the tactical level includes the management of medium-term decisions, which typically range from six months to one year (Guillén et al. 2006; Awudu and Zhang 2012). The operational level corresponds to short-term decisions, weekly and daily, which concern to inventory planning (daily inventory control, lack of inventory at distribution points) and to programming vehicles (Tsolakis et al. 2014).

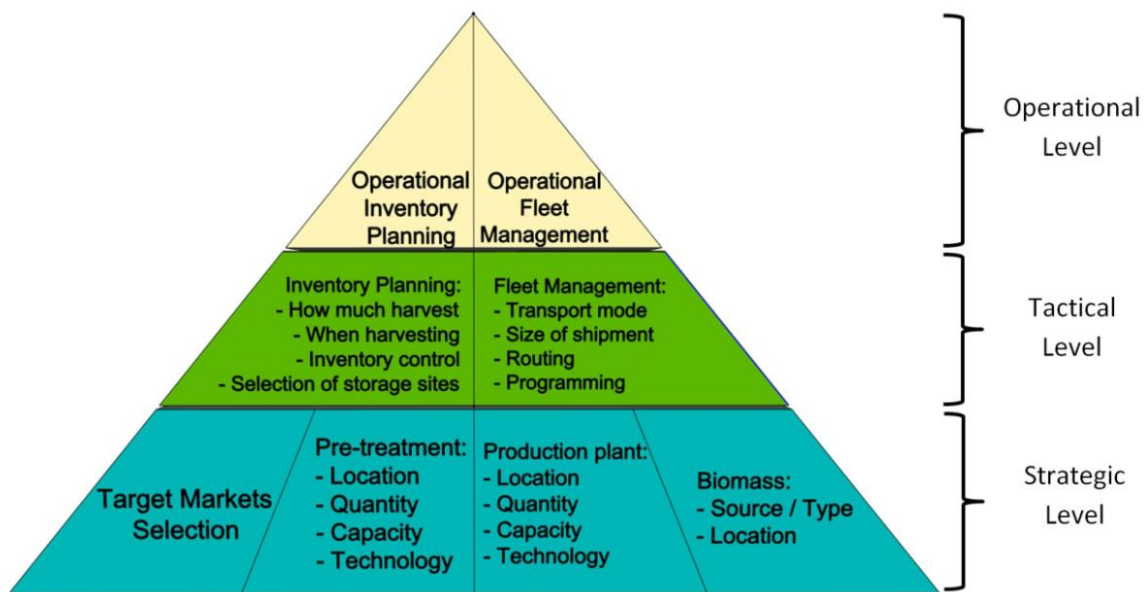


Figure 2. 2 Main decision variables for each level of decision-making in BioRSC management (Iakovou et al. 2010; Mortazavi et al. 2015).

2.3. Methods

Regarding the need to use biomass in a sustainable and industrialized way, the objective of this chapter is to determine how the key challenges and requirements for sustainable BioRSC design and optimization have been addressed by the scientific community. Thus, a systematic literature review method composed by a search strategy and the analysis of the collected documents has been implemented.

2.3.1. Search strategy

In order to determine how the key challenges and requirements for sustainable BioRSC design and optimization have been addressed by other researchers, a search strategy was designed including the following steps: (1) defining keywords to perform the search in databases, (2) establishing sources of information to be employed (databases), (3) delimiting the period to be explored, and (4) making an initial selection of documents. The main characteristics for each step are described in Table 2.1

Table 2. 1. Search strategy steps (Espinoza Pérez et al. 2017)

Steps	Description
Keywords	“Supply Chain” AND “Biorefinery”
Sources of information	Journal articles and conference proceedings searched in databases in English. Specifically in Scopus and Web of Science.
Period of information	Between 2006 and 2016, because the first documents found referring to biorefineries date back to 2006.
Initial selection (First filter)	Document selection related to the whole BioRSC modeling

2.3.2. Descriptive document analysis

After the application of the first component of the method, the selected documents were analyzed in terms of the identification of challenges and requirements, as well as what types of tools have been used for SC design and management. As the challenges generated by the nature of BioRSC are part of the uncertainties that affect BioRSC system efficiency, to the following strategy was implemented:

- ✚ To analyze the inclusion of uncertainty in the model used for SC design and management as the first descriptive analysis.
- ✚ To analyze the presence of any of the five dimensions of sustainability.
- ✚ To identify the decision-making levels and major decision variables included in the research

2.4. Results

According to the search strategy described above, 183 scientific publications were found. Then, after a first selection, 84 scientific publications were chosen to be reviewed in detail. Figure 2.3 presents the distribution of the reviewed publications according to their scope (Economic, Environmental, Social, Technological or Political), the applied approach (simulation and/or optimization) and decision levels studied (strategic, tactical or operational). From the figure, it appears that studies focused exclusively on economic objectives are the most common (30) and they mostly deal with optimization. On the opposite side, the political dimension of sustainability is the least studied, with only five publications that included government incentives. Furthermore, 51% of the publications include the three decision-making levels.

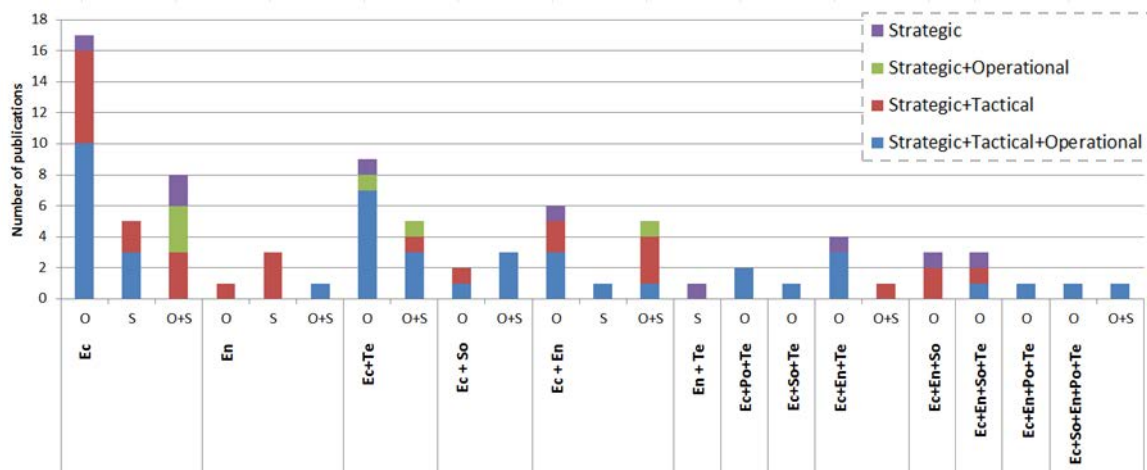


Figure 2. 3 Publication distribution according to the dimensions of sustainability (Ec = Economic, En = Environmental, So = Social, Po = Political, Te= Technological) objective (O = Optimization, S = Simulation) and decision level studied (Espinoza Pérez et al. 2017)

It is noteworthy that most of the investigations were applied to cases in the USA. The remaining publications were applied in Spain, Colombia, Greece, and Iran, among others. Thus, there is a real need to increase the internationalization of the application of both bio-based products and models that helps to facilitate the implementation of these industries.

The objectives pursued on the analyzed documents were optimization, simulation or both. Simulation seeks locally optimal solutions, not necessarily global, to reduce execution times and deal with the complexity and stochastic relationships between variables that represent a system (Winston and Goldberg 2004). Optimization determines the values of the decision variables that minimize or maximize an objective function over a set of values that satisfy a set of constraints (Winston and Goldberg 2004).

Table 2.2 presents a detailed analysis about each publication reviewed. First, they were divided by the dimensions included. Then, it was identified if Optimization, Simulation or both approaches were used. In the following column specific tools applied for optimization or simulation are listed. Next, the uncertainty inclusion is evaluated depending on the model: stochastic or deterministic. Finally, the decision-making levels which have been modeled are presented.

According to the information presented in Table 2.2, most of the recent researches published develop the sustainability analysis in a traditional way, using economic, environmental and social dimensions, as reported in other references, without considering the inclusion of variables such as economies of scale or incentives provided by governments or the integration of assessment of developing technologies with different maturity levels (Lautala et al. 2015; Garcia and You 2015; Ba et al. 2016; Ghaderi et al. 2016). 75% of the documents target economic and environmental dimensions are deterministic, while only five have included pretreatment plants. Some of them have considered the environmental area as objective (Zamboni et al. 2009a; Zamboni et al. 2009b; Santibañez-Aguilar et al. 2013; Rincón et al. 2015) and others have considered the environmental aspect as restrictions for optimization.

Table 2. 2 Analysis of the 84 publications selected in this study (Espinoza Pérez et al. 2017)

Publication	Dimensions	Tool	Specific tool	St/D	Decision-making level								
					Strategic			Tactical		Operational			
					(1)	(2)	(3)	(4)	(5)	(6)	(7)	(8)	
(Ekşioğlu et al. 2009)	Ec	O	MIP	D	X	X			X	X	X		
(Huang et al. 2010)	Ec	O	MILP	D	X	X			X	X	X		
(Kim et al. 2010)	Ec	O	MILP	D	X	X	X	X		X	X		
(Bowling et al. 2011)	Ec	O	MILP	D	X			X		X	X		
(Gao 2011)	Ec	O	MIP	D				X	X	X			
(Sharma et al. 2013a)	Ec	O	MILP	St	X	X			X	X			
(Hajibabai and Ouyang 2013)	Ec	O	MINLP	D	X					X			
(Kazemzadeh and Hu 2013)	Ec	O	SMILP	St	X		X			X			
(Lin et al. 2013)	Ec	O	MILP	D	X	X			X	X			
(Mazzetto et al. 2013)	Ec	O	MILP	St	X	X			X	X	X		
(Duarte et al. 2014)	Ec	O	MILP	D	X	X	X		X	X	X		
(Lin et al. 2014)	Ec	O	MILP	D	X	X			X	X	X	X	
(Yeh et al. 2014)	Ec	O	MILP + LP	D	X	X	X		X	X	X		
(Zhang and Wright 2014)	Ec	O	MINLP	D	X	X	X			X	X		
(Yeh et al. 2015)	Ec	O	SMILP	St	X	X			X		X		
(Castillo-villar et al. 2016)	Ec	O	MIQCP	D	X	X							
(Santibañez-Aguilar et al. 2015)	Ec	O	MIDO	D	X	X	X		X	X			
(Sokhansanj et al. 2006)	Ec	S	EXTENDED tm	D	X	X			X	X	X		
(Panichelli and Gnansounou 2008)	Ec	S	SA	D	X	X			X	X	X		
(Rentizelas et al. 2009)	Ec	S	SA	D		X			X	X	X		
(Mansoornejad et al. 2013)	Ec	S	SA	St	X	X	X		X	X	X		
(Melendez and Stuart 2015)	Ec	S	SA	D		X			X	X			
(Kim et al. 2011b)	Ec	O+S	MILP + Monte Carlo	St	X	X	X	X		X			
(Duarte et al. 2012)	Ec	O+S	MILP + ASPEN	D	X	X			X	X	X		
(Kelloway et al. 2013)	Ec	O+S	MILP + HYSYS / Monte Carlo	St	X	X					X		
(Höltinger et al. 2014)	Ec	O+S	MILP + Montecarlo	St	X								
(Yue and You 2015)	Ec	O+S	MINLP + Stackelberg game	St	X	X	X						
(Sukumara et al. 2015)	Ec	O+S	MILP + Aspen+ Discrete event simulation	St	X	X				X			
(Geraili and Romagnoli 2015)	Ec	O+S	MILP, Scenario-based stochastic programming And Aspen Plus	S	X	X	X				X		
(Geraili et al. 2016)	Ec	O+S	MILP + AspenPlus + Monte Carlo	St	X	X					X		
(Eranksi et al. 2013)	En	O	LP + LCA	D	X	X		X	X	X			
(Nguyen et al. 2014)	En	S	LCA + Monte Carlo	St	X			X	X	X			
(Guo et al. 2015)	En	S	LCA	D	X	X		X		X			
(Reeb et al. 2015)	En	S	LCA	D		X				X			
(van Boxtel et al. 2015)	En	O+S	MINLP + LCA	D	X	X			X	X	X		
(Dunnett et al. 2008)	Ec+Te	O	MILP	D	X	X				X	X		
(Parker et al. 2010)	Ec+Te	O	MILP	D	X		X				X		
(Tittmann et al. 2010)	Ec+Te	O	MIP	D	X					X	X		
(Kim et al. 2011a)	Ec+Te	O	MILP	D	X	X	X	X	X	X	X		
(Elia et al. 2013)	Ec+Te	O	MILP	D	X	X			X	X	X		
(Marvin et al. 2013)	Ec+Te	O	MILP	D	X	X	X			X	X		
(Sharma et al. 2013c)	Ec+Te	O	MILP	D	X	X			X	X	X		
(Azadeh et al. 2014)	Ec+Te	O	MILP	St	X	X			X	X	X		
(Ortiz-del-castillo et al. 2016)	Ec+Te	O	MILP	D	X	X							
(Sammons et al. 2008)	Ec+Te	O+S	MILP + ASPEN	D	X		X				X		

Table 2.2. Analysis of the 84 publications selected in this study (Espinoza Pérez et al. 2017) (Continuation)

Publication	Dimensions	Tool	Specific tool	St/D	Decision-making level								
					Strategic				Tactical		Operational		
					(1)	(2)	(3)	(4)	(5)	(6)	(7)	(8)	
(Leduc et al. 2010)	Ec+Te	O+S	MILP + Steady-state simulation model	D	X	X	X			X	X		
(Sukumara et al. 2012)	Ec+Te	O+S	MILP + ASPEN	D	X	X			X		X		
(Sukumara et al. 2013)	Ec+Te	O+S	MILP + ASPEN	St	X	X			X	X	X		
(Lamers et al. 2015b)	Ec+Te	O+S	Biomass Logistics Model + Aspen	D	X	X		X		X			
(Bai et al. 2012)	Ec + So	O	MIQP	D	X	X			X	X	X		
(Kim and Dale 2015a)	Ec + So	O	MILP	D	X	X				X			
(Chen and Onal 2012)	Ec + So	O+S	MINLP, MIP, MILP + Simulate behavior	D	X	X				X	X		
(Wang et al. 2013)	Ec + So	O+S	NLP + Game-theoretic models	D	X	X				X	X		
(Singh et al. 2014)	Ec + So	O+S	MILP GA + AGENT-BASED	St	X	X	X		X	X	X		
(Zamboni et al. 2009a)	Ec + En	O	MO MILP	D	X	X	X			X	X		
(Zamboni et al. 2009b)	Ec + En	O	MO MILP	D	X	X	X			X	X		
(Santibañez-aguilar et al. 2015)	Ec + En	O	MILP	St	X	X	X		X	X			
(Rincón et al. 2015)	Ec + En	O	MO NLP	D	X	X				X	X		
(Murillo-alvarado et al. 2015)	Ec + En	O	MO MILP	D	X	X	X	X		X			
(Duarte et al. 2016)	Ec + En	O	MILP	D	X	X	X	X					
(Wang et al. 2015)	Ec + En	O+S	MILP + LCA + Aspen	D	X	X				X			
(Kim and Dale 2015b)	Ec + En	O+S	MILP + Aspen + Sensitivity analysis	St	X	X	X		X	X			
(Zhang et al. 2014)	Ec + En	O+S	MILP + ASPEN	D	X	X		X	X	X	X		
(Sammons et al. 2007)	Ec + En	O+S	MILP + ASPEN	D	X		X				X		
(Santibañez-Aguilar et al. 2016)	Ec + En	O+S	MO + Monte Carlo	St	X	X	X	X	X	X			
(Zhang et al. 2012)	Ec+En	S	ARENA + IDEF	D		X		X	X	X	X		
(McKechnie et al. 2015)	En + Te	S	LCA	D	X	X		X					
(Gebreslassie et al. 2012a)	Ec+Po+Te	O	SMILP	St	X				X	X	X		
(Gebreslassie et al. 2012b)	Ec+Po+Te	O	SMILP	St	X				X	X	X		
(Andersen et al. 2012)	Ec+So+Te	O	MILP	D	X	X			X	X	X		
(Santibañez-Aguilar et al. 2013)	Ec+En+Te	O	MO MILP	D	X	X	X	X		X	X		
(Liu et al. 2014)	Ec+En+Te	O	MILP	D	X	X	X	X	X	X	X		
(Osmani and Zhang 2014)	Ec+En+Te	O	MILP	St	X		X		X	X	X		
(Cambero et al. 2015)	Ec+En+Te	O	MIP	D	X	X							
(Lamers et al. 2015a)	Ec+En+Te	O+S	MILP+ Sensitivity analysis	St		X		X		X			
(Miret et al. 2015)	Ec+En+So	O	MILP	D	X	X			X	X			
(Martinez-Guido et al. 2015)	Ec+En+So	O	MILP + Scenario analysis	D	X	X				X			
(Zhang et al. 2016)	Ec+En+So	O	GA	St	X	X		X					
(Santibañez-Aguilar et al. 2014)	Ec+En+So+Te	O	MILP	D	X	X	X	X	X	X	X		
(Bairamzadeh et al. 2016)	Ec+En+So+Te	O	MILP, MORPP approach is developed	St	X	X	X	X	X	X			
(Cambero and Sowlati 2016)	Ec+En+So+Te	O	MILP	D	X	X	X						
(You and Wang 2011)	Ec+En+Po+Te	O	MILP	D	X	X				X	X		
(Yue et al. 2014a)	Ec+So+En+Po+Te	O	MO MILF	D	X	X		X	X	X	X		
(You et al. 2012)	Ec+So+En+Po+Te	O+S	MO MILP + ASPEN	D	X	X		X	X	X	X		

Dimension included: Economic (Ec); Social (So); Environmental (En); Political (Po); Technological (Te). **General tools implemented:** Optimization (O); Simulation (S). **Specific tools used:** Linear Programming (LP), Mixed Integer Programming (MIP), Mixed Integer Linear Programming (MILP), Mixed Integer Non Linear Programming (MINLP), Stochastic Mixed Integer Linear Programming (SMILP), Mixed Integer Quadratic Programming (MIQP), Non Linear Programming (NLP) and Mixed Integer Linear Fractional Programming (MILFP), Multi-objective optimization (MO), Mixed-Integer Dynamic Optimization (MIDO), EXTENDED tm, Scenario analysis (SA), Monte Carlo, ASPEN, HYSYS, Stackelberg game, Discrete event simulation, Scenario-based stochastic programming, Life cycle analysis (LCA), Steady-state simulation model, Biomass Logistics Model, Simulate behavior, Game-theoretic models, Genetic algorithm(GA), AGENT-BASED, Sensitivity analysis, ARENA, IDEF, Multi-objective robust probabilistic programming (MORPP). **Model type:** Stochastic, St; Deterministic, D. **Decision-making Level:** Strategic Level [(1) Factory, (2) Biomass, (3) Market, (4) Pre-treatments], Tactical Level [(5) Inventory, (6) Fleet], Operational Level [(7) Inventory, (8) Fleet]

Publications studying economic, environmental and technical dimensions of sustainability are fairly comprehensive regarding comprised decisions. Santibañez-Aguilar et al. (2013) proposed a general superstructure and a mathematical programming model for the sustainable elimination of water hyacinth through a distributed biorefinery network, considering economic and environmental objectives and several technologies available. Osmani and Zhang (2014) presented a two-stage stochastic optimization model to maximize the expected profit and simultaneously minimize carbon emissions. However, they assumed that the demand for co-products is always greater than supply. Liu et al. (2014) used a model with multi-conversion pathways and propose a framework for economic, energy and environmental performance measures. Finally, Lamers et al. (2015a) made an evaluation limited to a subset of potential depot designs, without including the upstream or downstream supply chain.

Only two studies in Table 2.2 considered the five dimensions of sustainability: You et al. (2012) and Yue et al. (2014a). The first used ASPEN to simulate different possible production lines, to choose the production technology and it included government incentives as incomes. Its objective was to minimize the annualized costs, maximize local job creation and minimize greenhouse gas emissions. The second evaluated the cost of producing electricity, the number of local jobs created and environmental impacts associated to the production of a unit of bioelectricity, by LCA methodology. It also considered government subsidies as income for the biorefinery. In both studies only one production technology per plant can be chosen and no consideration is given to economies of scale in the technological dimension of sustainability. None of these last studies evaluated the target market selection.

Among the researches focusing on economic and technological dimensions, only two included pretreatment plants (Kim et al. 2011a; Lamers et al. 2015b). This is a very important aspect for biorefinery profitability, because due to the low energy density of biomass and its dispersion, the harvest, logistic and transformation costs are penalized (Kokossis and Yang 2010). Thus, it is essential to consider the localization of pretreatment units to reduce transportation cost and optimize the supply of biomass to biorefineries (Clark and Deswarte 2014). The main economic objective in the reviewed publications is profitability. It was sought by reducing costs, increasing revenues and maximizing the net present value. There are two publications that incorporated uncertainty in the model (Sukumara et al. 2013; Azadeh et al. 2014). In regard to the studies including simultaneously economic and social objectives, most proposed deterministic models and none included pretreatment plants. In other, Bai et al. (2012) considered the objective of maximizing net income for farmers and the biofuel industry, proposing a game theory based model, which included decisions on land use, market selection by manufacturers and the impacts on raw material prices for the food industry. In this section, only Singh et al. (2014) considered the stochastic nature of the problem by applying MILP, a genetic algorithm and simulation based on agents. Market competition was simulated including biorefinery agents, farmers, and food market agents to determine the prices of raw materials that will be used in optimization.

Among the publications that apply optimization, most developed the SC model using MILP, because of the binary nature of decisions. Most of them have applied the ϵ -constraint method to solve optimization, but it has also used a genetic algorithm to solve multi-objective problems.

Only four investigations considered the stochastic nature of the system in the models (Mazzetto et al. 2013; Kazemzadeh and Hu 2013; Sharma et al. 2013a; Yeh et al. 2015). This shows that these models did not consider all the requirements for the design of the bio-based products' SC. There were only three investigations that have integrated optimization and pretreatments, Kim et al. (2010) evaluate both centralized and decentralized SC network configurations and different biomass types. Bowling et al. (2011) also considered distributed and centralized configurations and evaluate the possibility of selling biofuel sub-products. Gao (2011) determined the location of the production plant by the BIOFLAME method prior to modeling and optimization, and then focuses on the quantities of raw materials purchased and stored. The five studies focused on environmental objectives performed a lifecycle analysis to evaluate various impacts. Also, these publications did not consider market selection (Franki et al. 2013; Nguyen et al. 2014; Guo et al. 2015; van Boxstel et al. 2015).

According to the assessment of the information in Table 2.2, it is clear that most of the studies reviewed did not consider daily vehicle scheduling. This occurs because most of the studies that developed daily vehicle scheduling only focus on this decision, and not on the whole BioRSC, which is a criteria for the present mapping study. Finally, as a general rule, analyzed researches focus mainly on one principal final product, mainly a biofuel, but higher added value products and energy integration can further support the sustainability balance of a biorefinery (Belletante et al. 2016).

2.5. Discussion

Although the study of BioRSC started several years ago, almost parallel to sustainability studies based on three dimensions (social, economic and environmental), only six of the studies included in Table 2.2 are based on these. When considering the new sustainability approach based on five dimensions, only two studies considered all the aspects. Few investigations have included the political dimension. These have included the government incentives as a profitability source for the enterprise, leaving behind the political objective of reducing economic incentives when the industry would be self-sustaining. Therefore, it is clear the necessity to consider these two sides of that dimension.

Regarding the inclusion of the technological dimension of sustainability, even though it was considered in 36% of the publications, the vast majority only evaluated the choice of production technologies, without assessing technological learning, economies of scale or the maturity degree of technologies (TRL-Technology Readiness Level). These are issues that could improve the profitability of enterprises, encouraging more private investment.

Some of the investigations took into account the nature of the biomass, but only 29% incorporated uncertainty in their studies. In addition, among the most relevant studies related to sustainability -the last ten publications in Table 2.2- only three considered the target market selection for the different biorefinery final products and sub-products. This means that the integration of high value products has simply been ignored. Incorporating this decision can represent an opportunity to improve economic performance, since profitability is a fundamental pillar for BioRSC industrialization.

These results show that none of the publications targeted system complexity as a whole. From the above evidence, it is clear that the BioRSC is still studied in a fragmented and partial manner. Due to the growing importance of this sector, it is necessary to implement integrated frameworks and operational tools that support the decision-making process. The main findings of this mapping study are included in Table 2.3, as the Current Status of the BioRSC study and the Ideal System Model. The latter presents the characteristics needed for a decision-making support tool that facilitates the sustainable industrialization of BioRSC.

Table 2. 3. *Main findings summary (Espinoza Pérez et al. 2017)*

	<i>Current Status</i>	<i>Ideal System Model</i>
Sustainability: Inclusion of the five dimensions	Early stage for simple systems	Full integration of the five dimensions and scenarios considered
Comprehension	Partial vision approaches	Full integration of stakeholders and the three decision-making levels
Complexity / Completeness	Simple systems, i.e. biodiesel	Integrated biorefinery, with high added value products and pretreatment plants
Modeling and optimization approaches	Use separately: - Sensitivity analysis - Simulate behavior - Multi-Objective optimization - Mixed Integer Linear Programming - Simulation by ASPEN	Integration of tools for robust optimization and behavior comprehension.

2.6. Summary

As shown in this chapter, to conceive an optimal phase III biorefinery at industrial scale and in a sustainable way considering the relevant and full range of impact dimensions of its implementation, BioRSC design and management must integrate the requirements and constraints linked to biorefinery nature, sustainability dimensions and the decision-making levels. Despite decision-making support tools for BioRSC have evolved from first applications, a tool that facilitates sustainable phase III biorefinery implementation has not been developed yet. Therefore, this research lays the basis for the design of a decision-making support tool that facilitates the sustainable industrialization of Phase III BioRSC. This tool would need to incorporate uncertainty, the different decisions for the decision-making levels and the five dimensions of sustainability to cover the requirements that have not been met. Nevertheless, since in the present study only the publications related to the whole BioRSC are considered, another study can be conducted to analyze the research relating specifically to operational and/or tactical aspects. Then, these analyses could be integrated to this research. Furthermore, this bibliographic revision has shown that the discipline Operational Research has been extensively used to develop decision-making support tools linked to biorefinery. Therefore, this is a starter point to determine which one is the suitable methodology to apply, if any, or to develop one, if necessary. Then, the next chapter is dedicated to “Operational Research” description, its methodologies and a general methodology proposition for the tool construction.

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Chapter III. Conceptual framework: Decision-making on sustainable biorefinery supply chain

3.1. Introduction

According to the literature review presented in Chapter II, it can be concluded that the tools for help decision makers (DM) to conceive optimal, industrial and/or sustainable biorefineries have been strongly developed and supported by simulation and optimization techniques. These integrate the Operational Research (OR) discipline.

OR theory had its origin just before the Second World War, in the studies conducted by the British Army about their new radar system installation and their efforts to break the German secret communication code (Bouyssou et al. 2009). It was called OR because the teams of scientist were doing research on how to manage military operations (Hillier and Hillier 2010). However, this discipline has had several names as Operational Analysis, Operations Evaluation, Operations Research, System Analysis, System Evaluation, Systems Research, Quantitative methods and Optimization Techniques and Management Science, but it is most widely known as OR (P. Rama Murthy 2008).

OR was augmented methodologically and computationally by the postwar developments of linear programming, game theory, dynamic programming, discrete-event simulation and digital computer (Saul and Michael 2013). A number of additional ideas and problem types from the pre-war years were incorporated into the field as well (Saul and Michael 2013).

In the next sections, OR fundamentals will be detailed, and then a methodology will be proposed and described for the conception of a sustainable and industrialized Phase III BioRSC project.

3.2. Operations Research

OR is viewed as a body of established mathematical models and methods to solve complex management problems (A. Ravi Ravindran 2008), that provides a scientific method for the quantitative analysis of a problem from which the management can make an objective decision (Saul and Michael 2013). This discipline has drawn upon skills from mathematics, engineering, business, computer science, economics, and statistics to contribute to a wide variety of applications in business, industry, government, and military (A. Ravi Ravindran 2008).

OR can be defined as (Saul and Michael 2013):

- ✚ The application of the scientific methods to complex problems arising in the direction and management of large systems of men, machine, materials, and money in industry, business, government, and defense;
- ✚ The science of deciding how to best design and operate man-machine systems;
- ✚ A scientific method for providing executive departments with a quantitative basis for decision making.

The objective of operations research is (P. Rama Murthy 2008):

“To provide a scientific basis to the decision maker for solving the problems involving the interaction of various components of an organization by employing a team of scientists from various disciplines, all working together for finding a solution which is in the best interest of the organization as a whole. The best solution thus obtained is known as optimal decision”.

Therefore, it is important to define the term “decision making process” which involves all activities and thinking needed to identify the most optimal or preferred choice among the available alternatives (Business Dictionary 2017) through two phases (P. Rama Murthy 2008):

- ✚ Formulation of goals and objectives, enumeration of environmental constraints, identification and evaluation of alternatives.
- ✚ Selection of optimal course of action for a given set of constraints.

In view of the nature and complexity of a Phase III BioRSC, discussed on Chapter I, it can be concluded that it is a large systems of men, machine, materials, and money. This system must to be designed, managed and operated in the best possible way to be sustainable, as discussed on Chapter II. Therefore, it is required to optimize the decisions related to conceive the sustainable Phase III BioRSC. As conclusion, the conception of sustainable Phase III BioRSC can be entirely addressed by OR.

It must not be forgotten the fact that sometimes managers find that qualitative factors are as important as quantitative factors in making decisions (Hillier and Hillier 2010). Thus, this discipline only provides an analysis and recommendations. Then, managers must also take into account various intangible considerations and then use their best judgement to make the decision (Hillier and Hillier 2010).

3.2.1. Phases on solving OR problems

There exist some principal steps for model-building procedure and model solution for the implementation of OR in practice (Winston 2003; Taha 2010). They can be resumed in six steps as shown in Figure 3.1 and explained following.

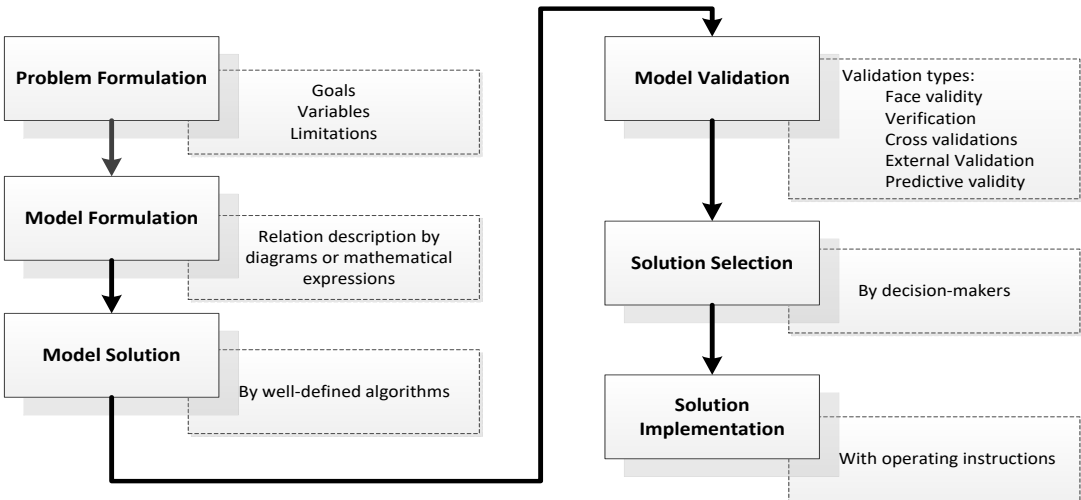


Figure 3. 1. Principal steps for solving operational research problems.

Problem formulation. It involves delimiting the scope of the problem under investigation (Taha 2010). It means to examine the situation and clearly establishes what exactly happens, identifying variables and constraints of the problem to be solved. Similarly, to identify what is the objective and put it, as well as the others aspects, in the form of statement (P. Rama Murthy 2008). The statement must include (P. Rama Murthy 2008; Taha 2010):

- ✚ Description precise of goals or objectives of the study
- ✚ Identification of controllable and uncontrollable variables and
- ✚ Specification of the limitations or restrictions under which the modeled system operates.

Model formulation. In this step a model of the problem is formally developed (Winston 2003). Model construction entails an attempt to translate the problem definition into causal diagrams for its description through mathematical relationships between the variables and constraints (P. Rama Murthy 2008; Taha 2010).

Model solution. It is by far the simplest of all OR phases because it entails the use of well-defined algorithms depending on the model constructed (Taha 2010). An important aspect of the model solution phase is the sensitivity analysis, because it deals with obtaining additional information about the behavior of the optimum solution when the model undergoes some parameter changes (Taha 2010). Sensitivity analysis is particularly needed when parameters of the model cannot be estimated accurately. In these cases, it is important to study the behavior of the optimum solution in the neighborhood of the estimated values.

Model validation. Validation is a set of methods for judging if the model developed is an accurate representation of reality (Winston 2003). That information can be used by DM to determine the applicability of the results (Eddy et al. 2012). Five main types of validation are commonly implemented: face validity, verification (or internal validity), cross validity, external validity, and predictive validity which are below summarized (Eddy et al. 2012);

- *Face validity* is the extent to which a model, its assumptions, and applications correspond to current science and evidence, as judged by people who have expertise in the problem. This process enhances credibility with experts and increases acceptance of results. It can be very difficult for readers to determine whether a model has been properly simplified, oversimplified, or under-simplified for a particular problem. Therefore, it is subjective. Four aspects are particularly important for face validity: *model structure, data sources, problem formulation and results*. For the structure, important questions are whether the model includes all aspects of reality considered important by experts. For problem formulation, whether the setting corresponds to those of interest; for results, whether they match experts' expectations and, if not, whether the model can plausibly explain them. Information about the model and supporting evidence are obtained from documentation provided by the modelers. Information about the problem formulation and results is obtained from the application's report. A description of the process used to evaluate face validity should be made available on request. To the greatest extent possible, evaluation of face validity should be made by people who have

expertise in the problem area, but are impartial, and preferably blinded to the results of the analysis.

- *Verification* is also called internal validity, internal consistency, or technical validity. It examines the extent to which the mathematical calculations are performed correctly, if they are consistent with the specifications of the model and if the model has been implemented correctly. The choice of methods for verification will depend on the complexity of the model. There are two main steps: verifying the individual equations and their accurate implementation in code. Equations and parameters should be validated against their sources, because they might be fitted using good data sources and techniques. Coding accuracy should be checked by using state of the art quality assurance and control methods for software engineering. Examples of techniques include maintaining complete and update documentation of the code; conducting structured “walk through’s” in which the programmer explains the code to other people who search for errors; verification of separate parts of a model one by one; sensitivity analysis; extreme value analysis. Verification helps to ensure there are no unintentional computational errors but it does not evaluate the accuracy of the structure or predictions of the model.
- *Cross-validation* is also called external consistency, comparative modeling, external convergence testing, convergent validity, external consistency, model corroboration. It involves comparing a model with others that address the same problem and determining the extent to which they calculate similar results. The differences among the results and their causes are then examined. Confidence in a result is increased if similar results are calculated by models using different methods. The meaningfulness of this type of validation depends on the degree to which the methods and data sources of the different models are independent. The high degree of dependency among models (e.g., using parameters from other models published earlier) reduces the value of cross-validation.
- *External validation* compares results obtained using the model with actual event data. There are three main steps: identifying the data sources to reproduce, conducting a simulation, and comparing results. Data sources must contain applicable and sufficient described data to enable replication of design and progression (any changes in the design or conduct of the study over the follow up period). External validation tests the ability of the model to calculate actual outcomes. However, this validation can address only the parts covered by data sources. Another limitation is insufficient useful validation data and/or a limited the number of data sources. Even when the information on the source’s design exists, it may not accurately represent what happened because of changes during the study. Another limitation is that the model might not include all elements needed to accurately simulate a source.
- *Predictive validity* involves using a model to forecast events and after some time, comparing the forecasted outcomes with the actual ones. It also ensures a completely independent validation, avoiding opportunities for altering the model to fit observed results. A limitation is that the results are necessarily in the future and rarely in time to be helpful for immediate

decisions. They also require a trial planned or in progress applicable to the decision at hand. Many models are built to synthesize the best available evidence and illuminate a policy decision for which no trial is ongoing, planned, or even feasible. At best, this validation method is applicable only for short term outcomes when research is feasible.

Whether a model is sufficiently valid or accurate for a particular application, who would use its results must determine it. It is recommended that users of a model examine validation results with four criteria:

- ✚ Rigor of the process
- ✚ Quantity and quality of sources used
- ✚ Ability of the model to simulate sources in appropriate detail
- ✚ How closely results match observed outcomes, initially and after making justifiable assumptions about uncertain elements.

Model selection. Given a model and a set of alternatives, the operations researcher should choose the alternative that best meets the research objectives (Winston 2003). In some situations, one might present several alternatives and let the DM to choose the one that best meets its needs (Winston 2003).

Model implementation. Implementation of the solution obtained from a validated model involves the translation of the results into understandable operating instructions to be issued to people who will manage the recommended system (Taha 2010). The system must be constantly monitored (and updated dynamically as the environment changes) to ensure that the recommendations enable the DM to meet its objectives (Winston 2003).

3.2.2. *OR Models*

Reality is at once complex, dynamic and multifaceted. Therefore, it is neither possible nor desirable, to consider each and every element of reality before deciding the courses of action (P. Rama Murthy 2008). In many cases, it will be impossible for a manager to conduct experiments in real environment (Kersten and Amad Saeed 2014). Thus, he can construct a similar model in laboratory and to study the problem to decide (P. Rama Murthy 2008). Hence, for many practical problems a model formulation is necessary because it enables to conduct a number of experiment involving theoretical subjective manipulations to find some optimum solution to the problem on hand (P. Rama Murthy 2008).

i) OR general models classification

An OR model can be defined as some sort of mathematical or theoretical descriptions of the relationship among specified variables and parameters of a system, representing some aspects of a problem on some subject of interest or inquiry (P. Rama Murthy 2008). Models are also categorized depending on their nature of environment, behavior and by method of solution (P. Rama Murthy 2008). The different model classifications are presented in Figure 3.2 and described following.

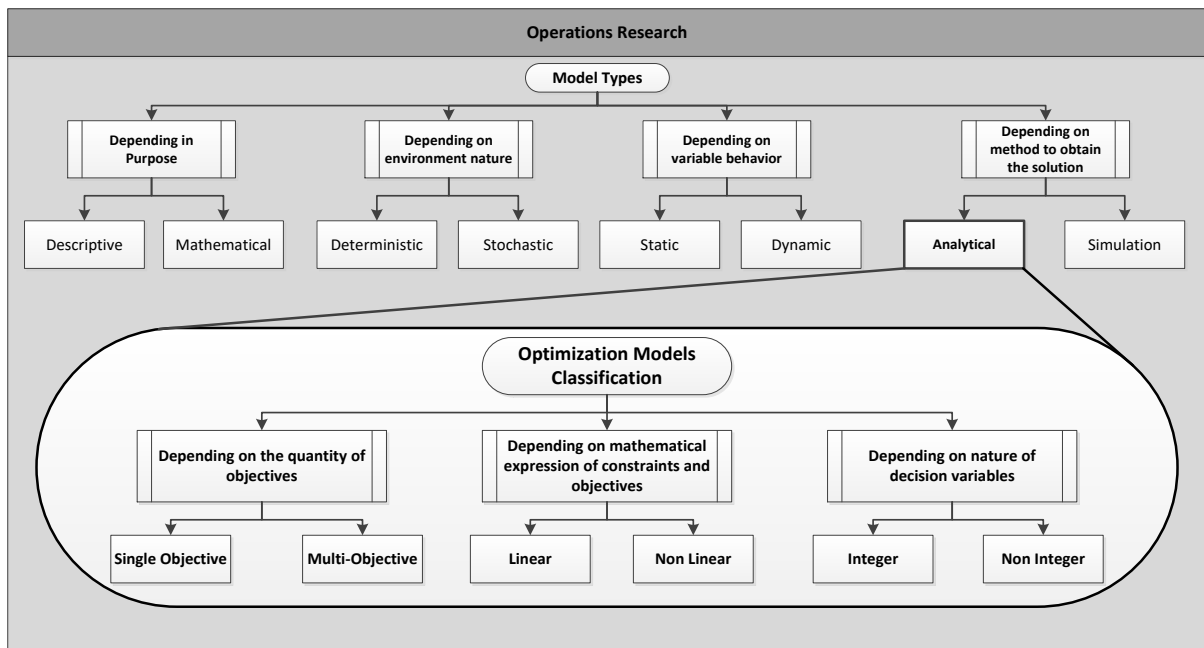


Figure 3. 2. Optimization model classification resumed.

Classification by purpose The models used in OR may be classified depending on their purpose as Descriptive or Mathematical models (A. Ravi Ravindran 2008; P. Rama Murthy 2008).

- *Descriptive models* give a description of certain aspects of the situation or system, giving various variables, constraints and objectives, so that the user can make use for his analysis. These models, though necessary to understand the system.
- *Mathematical models* explain the system or situation in mathematical language and enable the DM to proceed towards solution.

Classification by nature of environment. Depending on the environment in which the problem exists and depending on the variables and conditions, models can be categorized as Deterministic or Probabilistic (P. Rama Murthy 2008).

- *Deterministic models.* There is complete certainty about the values of the available resources and it is assumed that they will not change during the planning horizon (Winston 2003; P. Rama Murthy 2008). The solution of these models often gives the DM an excellent insight for making the best choice (Katta G. Murty 2003). It is also possible to perform sensitivity analysis, studying how the optimum solution varies as the data elements (parameters) in the model vary within a small neighborhood of their current values. DM combine all this information with their judgement to come up with the best decision to implement (Katta G. Murty 2003).
- *Probabilistic or Stochastic models.* When not all the information is available and some parameters should be modeled as random variables (Sen and Hige 1999), models are known as Probabilistic or Stochastic (P. Rama Murthy 2008). As probability distributions are assumed or estimated from past data and, currently, economic conditions and technology change

constantly, probability distributions estimated in a period may no longer be valid in the next (Katta G. Murty 2003).

Classification by the behavior of the problem variables. Depending on the behavior of the variables and constraints of the problem models can be classified as Static or Dynamic (P. Rama Murthy 2008).

- *Static Models.* These models assume that the variables do not depend on other variables and the solution of these models correspond to values (P. Rama Murthy 2008). Consequently, in static models, the decision variables do not involve sequences of decisions over multiple periods (Winston 2003).
- *Dynamic Models.* The dynamic models are expressed in differential equations or in equations of differences, their variables are functions of one or more variables, particularly time is a classic variable of these models (P. Rama Murthy 2008). In this case, the solutions correspond to functions.

The decision variables can involve sequences of decisions over multiple periods (Winston 2003; Zhang et al. 2015). In most multi-period problems, data changes are significant from one period to the next. Therefore, the optimum decisions for the various periods may be different (Katta G. Murty 2003).

Classification by the method of getting the solution. Depending on the methods for getting the solution for a given model and on their purpose, models are classified as follows:

- *Analytical models.* These models will have a well-defined mathematical structure for represent and optimize the studied system. Then, they can be solved by the application of mathematical methods (P. Rama Murthy 2008). Analytic models offer substantial advantages, as they can be integrated in other models to describe large systems and they require far less detailed input than simulation models, which saves both time and money (Ignall et al. 1978).
- *Simulation models.* The meaning of simulation is imitation (P. Rama Murthy 2008). Therefore, the standard use of simulation is direct: to answer a specific question or to obtain a description of the behavior of a system when some of its parameters are changed (Ignall et al. 1978). These models are a mathematical-logical representation, thus the system is not necessarily represented by equations. Then they need certain experimental analysis (P. Rama Murthy 2008). Some distinguished simulation approaches that are used in context of supply chain (SC) management are: spreadsheet simulation, system dynamic, discrete-event simulation, agent-based simulation, business game (Kersten and Amad Saeed 2014).

Therefore, simulation is an excellent tool to reproduce the behavior of complex systems for decision making models (Long and Zhang 2014). Instead, the analytical models are constructed to support DM made better decisions by optimizing the performance of systems in addition to satisfying the requirements on the decision variables (Donald and Chelsea 1990; INFORMS 2017), by identifying

a best possible course of action (Hillier and Lieberman 2001). Furthermore, while a simulation model of a large and complex system can be a very useful, it could be also time-consuming and costly tool to use (Ignall et al. 1978).

ii) Optimization model types

Most of the models solved with analytical methods are prescriptive or optimization models (Winston 2003). These models include: objective function(s), decision variables and constraints (Winston 2003). An optimization model seeks to find values of the decision variables that optimize (maximize or minimize) an objective function among the set of all values for the decision variables that satisfy the given constraints (Winston 2003).

Classification by quantity of objective functions. If there is only one measure of performance, the model will be a single objective model. When there are several measures of performance involved the result is a multi-objective model (Narzisi et al. 2006). The idea of solving a multi-objective problem is understood how helping a human DM in considering the multiple objectives simultaneously and to find a Pareto optimal solution that pleases him/her the most (Branke 2008).

Classification by the mathematical expression of the constraints and objective functions. A linear model is one in which the decision variables, that appear in the objective function and in the constraints, are always multiplied by constants and added together (Poler et al. 2014). Otherwise, while a nonlinear model is similar to a linear model in that is composed of objective function, general constraints and variables bound. The difference is that a nonlinear program includes at least one nonlinear function, which could be the objective function, or some or all of the constraints (Chinneck 2016) . In general, nonlinear models are much harder to solve than linear models (Winston 2003).

Classification by the nature of decision variables. If one or more decision variables must be integer, then this optimization model is an integer model. If all the decision variables are free to assume fractional values, then the optimization model is a non-integer model (Winston 2003).

3.2.3. OR model types and sustainable Phase III BioRSC

In order to define OR models that can represent the sustainable Phase III BioRSC system for its conception, each of the classifications described in section 3.2.2 will be analyzed as shown Table 3.1. First, the general model classification is analyzed according to the sustainable Phase III BioRSC characteristics, to define the model type depending on its purpose, nature of environment, variables behavior and the method to get the solution. The general model to represent the sustainable Phase III BioRSC conception can be developed as mathematical, stochastic, dynamic and analytic. Due the purpose of develop a decision-making tool, the contextual characteristics as uncertainty and the dynamic interrelationship between the decisions of different SC decision-making levels.

Table 3. 1. Sustainable Phase III BioRSC model classification

Model classification	Analysis	Sustainable Phase III BioRSC model
By purpose	As the objective is to develop a decision-making tool for support the conception of a sustainable Phase III BioRSC that could be implemented on different context. There is a need for a general model that can be reutilized on the different application context.	Mathematical model
By nature of environment	As described on Chapter I, the special characteristics and environment of biorefineries adds strong uncertainties that affect the efficiency of the system	Stochastic model
By variables behavior	The whole sustainable Phase III BioRSC system is dynamic. However, two kinds of behaviors can be distinguished regarding the different levels of decision making for the SC. Because strategical decisions must to be taken at the early stage of the project, these variables will be defined as static. Then, decisions associated to the tactical level depend on the strategical decisions made, and, consequently, the operational decisions depend on the tactical ones. This means decisions corresponding to the tactical and operational decisional levels have a dynamic nature.	Mixed, Static and Dynamic model
By the method of getting the solution	Analytical models support DM to take better decisions by optimizing the performance of systems and there is limited information for the description of the system, due to the fact that biorefineries are currently on a development stage, which could impede the development of a simulation model.	Analytical model
By quantity of objective function(s)	As presented on Chapter II, to avoid potential undesirable effects, the phase III biorefinery must to be design from a holistic point of view. It means, to integrate the five sustainability dimensions. Therefore, the definition of several objective functions is expected	Multi-objective model
By the mathematical expression of the constraints and objective function(s)	Many real systems are inherently nonlinear. However, nonlinear programs (NLP) are by nature more difficult to optimize, due to possible discontinuities in space solution, and its execution time is significantly longer than linear programs (LP) (Hamidian et al. 2008; Chinneck 2016). This is the main reason why approximate linear models are frequently used even if the circumstances justify a nonlinear objective (Hochbaum 2007). .	Efforts will focus on developing linear objective functions and constraints as much as possible
By the nature of decision variables	The model must include integer variables to define the installation of the pretreatment plants and the principal production plants. At the same time, it must include fractional variables to raw materials acquired and biobased products produced, among others.	Mixed, integer (binary) and non-integer

Then, as presented in section 3.2.2, due analytical models can support DM to make better decisions by optimizing the performance of systems, the optimization model classification is also analyzed for the sustainable Phase III BioRSC model definition. When an optimization problem involves more than one objective function, as in the case of a sustainable Phase III BioRSC system, the task of finding one (or more) optimum solution(s) is known as the Multi-Objective Optimization Problem (MOOP) (Narzisi et al. 2006). In addition, to facilitate the model solution, efforts will focus on developing a linear model (A. Ravi Ravindran 2008). Finally, analyzing the nature of the variables, this model will include integer and continuous variables. Therefore, the model to develop for these characteristics is a MO-BMIP optimization model (It will be defined as linear or non-linear depending on further sustainability analysis).

3.2.4. OR methodologies

In section 3.2.2, analytical method for getting the solution was chosen to be implemented in the sustainable Phase III BioRSC model to be developed in this project. Then, in section 3.2.3, the sustainable Phase III BioRSC model was described as MO-BMIP optimization model. Therefore, in this section some of the techniques to solve it will be briefly described.

Table 3.2 show the principals methodologies for solve OR models describing briefly their features in the second column (Hillier and Lieberman 2001; A. Ravi Ravindran 2008; P. Rama Murthy 2008; Poler et al. 2014). Linear Programming, Integer Programming, Non-linear Programming, Queueing Theory, Inventory Theory, Simulation and Forecasting, were excluded because these are out of the scope of the model. In the third column, suitability of each methodology for solve MO-BMIP models is analyzed.

In Table 3.2, it can be noted that dynamic programming is not suitable to sustainable Phase III BioRSC conception due to the large amount of decisions related to all the SC decision-making levels. Secondly, game theory and decision analysis have difficulty to be applied due multi-objective nature of sustainability. Then, Markov chains can help to build the probability distribution for the model uncertain parameters. Also, Markov chains and Markov decision process are not suitable for sustainable Phase III BioRSC conception optimization model, as dynamic programming, due to the large amount of decisions related to all the SC decision-making levels and its interrelationship. While, multiple criteria decision making can handle multiple objective functions simultaneously, it does not consider the dynamism and stochasticity of the MO-BMIP for the sustainable Phase III BioRSC conception. Instead, stochastic programming and robust optimization can handle dynamism and stochasticity, and they can be developed as multi-objective models.

Therefore, as conclusion, there are mainly two OR methodologies to conceive the sustainable Phase III BioRSC: stochastic programming and robust optimization. They should ideally be integrated with multiple criteria decision making to include afterwards DM preferences. In section 3.3 two general methodologies are proposed and described.

Table 3. 2. *Principal methodologies for solve OR models description and its suitability for solve MO-BMIP models*

OR Methodology	Characteristics	Suitable for MO-BMIP
Dynamic programming	It transforms a problem with n decision variables into n single-variable sub-problems (A. Ravi Ravindran 2008). It finds the global maxima or minima rather than just the local optima. The key limitation of this methodology is the dimensionality of the state space	No, because the model for the sustainable BioRSC would have a large amount the stages, which could generate difficulties concerning the decision process, the storage of information and time required to perform the computation
Game theory	It features competitive situations, then it allows understanding how the conflicting and cooperation actions between different DM have varied results depending on its pay-off tables (Hillier and Lieberman 2001). It study systems with two or more DM, where the result depend on the actions taken by all the DM and the objectives not always coincide (Poler et al. 2014).	Each player could be associated with several sustainability dimensions and then with different objective function. Further on, the pay-off table must to be constructed for each function combination. Then, it may result in a multi-objective game theory model. That could be translated in a significant time requirement to develop the model, construct the pay-off tables; and to perform the results computation.
Decision analysis	Defined as the process and methodology of identifying, modeling, assessing, and determining an appropriate course of action for a given decision problem (A. Ravi Ravindran 2008). It is integrated by alternatives, states of nature and performances or payoffs (Poler et al. 2014). It can be represented graphically by a combination of lines and nodes called a decision tree (A. Ravi Ravindran 2008)	No, because applicable in case of only one fundamental or end objective.
Markov chains	It is a specific type of stochastic processes based on probabilities instead of certainties (Dictionary 2017). Its ultimate goal is determine what is the probability that the system will find itself in each of the allowed states (Bonamente 2013). Then, Markov chain makes possible to reconstruct the probability distribution of the parameters (Bonamente 2013).	No, because it does not allows the calculation of the optimal decision. However, it allows building the probability distribution for the uncertain parameters for the stochastic model application case.
Markov decision process	It is a tool for optimizing the performance of stochastic processes that can be modeled as a discrete time Markov chain (Hillier and Lieberman 2001). Where a subsequent steps in the chain or sequence are only dependent on the current state of the chain, and not on any of its previous history (Bonamente 2013; Poler et al. 2014).	No, because the different SC decision-making levels depends among them (Tactical on Strategical; Operational on Tactical and Strategical).

Table 3.2. Principal methodologies for solve OR models description and its suitability for solve MO-BMIP models (Continuation)

OR Methodology	Characteristics	Suitable for MO-BMIP
<p>Multiple criteria decision making (MCDM)</p>	<p>It is devoted to problems that involve multiple conflicting objectives that should be considered simultaneously (Branke et al. 2008). MCDM problems are classified depending on the characteristics of the problem or in the timing of the preference information obtained from the DM.</p> <ul style="list-style-type: none"> • <u>By Characteristics</u>: When a discrete and predefined set of alternatives is evaluated to classify or sort them, the process is known as multi-attribute decision analysis or multiple-criteria selection process (A. Ravi Ravindran 2008; Branke et al. 2008). Otherwise, problems that have an infinite number of alternatives, where the alternatives are represented by a set of mathematical constraints; are called multi-criteria mathematical programming (A. Ravi Ravindran 2008; Branke et al. 2008). • <u>By timing of the preference information announcement</u>: No-preference methods are used when there is no DM or his preference is not available. Thus, the problem is solved by finding some compromise solution typically ‘in the middle’ of the optimal solution set (Branke et al. 2008). <p>In a priori methods, the DM specifies his preference. However, the DM does not necessarily know the possibilities and limitations of the problem beforehand and how realistic his expectations are (Branke et al. 2008).</p> <p>In a posteriori methods, a representation of the set of optimal solutions is first generated and then the DM is supposed to select the most preferred one among them (Branke et al. 2008).</p> <p>In interactive approaches, the phases of preference announcement and solution generation alternate (Branke et al. 2008).</p> <p>Therefore, the no-preference methods can be used to produce a starting point for interactive and posteriori methods.</p>	<p>Moderately, because it can be noted that the sustainable Phase III BioRSC can be classified as Multi-criteria mathematical programming, due to the high quantity of decision variables involved and the combination of possible solutions. Also, the use of no-preference methods could be an important starting point for present to DM a holistic but limited solution space to define his preferences avoiding unrealistic expectations.</p> <p>After, depending on the availability of DM it can be decided if the best way is to use interactive or a posteriori methods to obtain the final optimal Phase III BioRSC configuration.</p> <p>However it has found no explicit references to the dynamism and stochastic model characteristics of the Phase III BioRSC model.</p>
<p>Stochastic programming</p>	<p>It studies how to incorporate uncertainty into decision problems with probability distributions (King and Wallace 2012).</p> <p>There are two types of decisions (Wets 2002; Birge and Louveaux 2011):</p> <ul style="list-style-type: none"> • <u>First-stage decisions</u>, also known as <i>here and now decisions</i>, who are taken without full information on some random events. • <u>Second-stage decisions, or control decisions</u>, are taken when full information is received on the realization of some random. 	<p>Yes, because each one of the decision-making levels for SC can be modeled as a stage in a multi-stage model, including the dynamism and the stochasticity of the Phase III BioRSC model.</p> <p>However, it must not be forgotten that each stage model must be developed as mixed integer model and multi-objective to conceive the Phase III BioRSC, if DM preference is not available.</p>

Table 3.2. Principal methodologies for solve OR models description and its suitability for solve MO-BMIP models (Continuation)

OR Methodology	Characteristics	Suitable for MO-BMIP
Stochastic programming	<p>Its main model is the multi-stage stochastic programming model, in which decisions are made subsequently over time, where the next decision takes into account the random effects influencing the system, in addition to available information coming from past history (Prekopa 1995). These models are formulated on the basis of underlying deterministic problems, also called base problems (Prekopa 1995)</p>	<p>Then, the decision related to different SC levels must to be associated to First or Second Stage decisions.</p>
Robust optimization (RO)	<p>It provides a framework to handle the uncertainty of parameters in optimization problems that could immunize the optimal solution for any realization of the uncertainty in a given bounded uncertainty set (Pishvae et al. 2011). The uncertain-but-bounded model of uncertainty needs a priori knowledge; however, it is much easier to point out the support of the relevant distribution than the distribution itself (Pishvae et al. 2011). For a given optimization problem, there can be multiple robust versions depending on the structure of the uncertainty set. When formulating a robust counterpart of an optimization problem, maintaining tractability is an important issue (Neos Guide 2017). Therefore, an optimal solution to this formulation problem is the optimal robust solution of the original uncertainty problem (Pishvae et al. 2011). Such solution satisfies the constraints for all possible realizations of the data, and guarantees an optimal objective function value (Pishvae et al. 2011).</p>	<p>Yes, because the uncertain-but-bounded model includes the stochasticity and dynamism of the Phase III BioRSC model. Then, the model should be developed as mixed integer and multi-objective to conceive the Phase III BioRSC, if DM preference is not available. Therefore, the robust counterpart should be developed.</p>

3.3. General methodology proposition for decision-making on sustainable Phase III BioRSC projects

In this section, two general methodologies considering the integration of MCDM, Stochastic programming multistage and Robust Optimization for the sustainable Phase III BioRSC conception under uncertainty are proposed.

At first step, for any methodology, it should be analyzed the characteristics associated to the Phase III BioRSC, the sustainability dimensions and the SC decision-levels to identify the system elements and develop the correspondent model. Whereby, three different models can be noted, the design, management and scheduling models, related to strategical, tactical and operational SC decision-making level, respectively. Then, each model construction can be described by Figure 3.3. The design model described decisions that must to be taken here and now without information. In the other hand, the management and operational models describe decisions that are made before receive information about the random parameters, known as wait and see decisions.

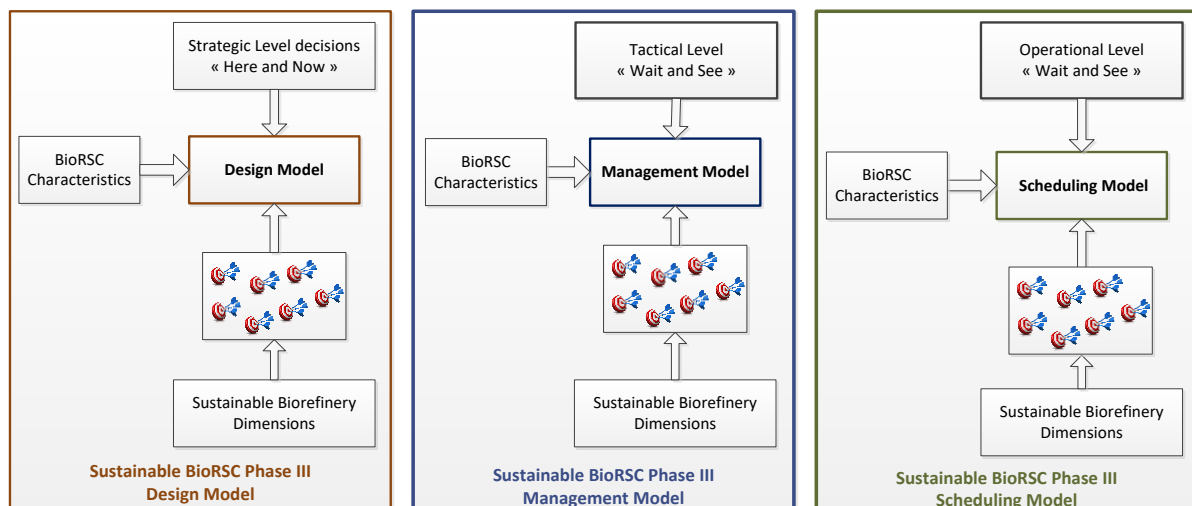


Figure 3. 3. General methodology for design, management and scheduling model construction for a sustainable Phase III BioRSC

The integration of MCDM can be carried out after analyzing the sustainability dimensions, due the objective functions would be identified. However, as seen in section 3.2.4, to avoid unrealistic expectations from DM, a first approach must to be solved with no-preferences. The results must to be presented to the DM to weigh the objective importance. Then the objective functions should be modified according to it. Finally, the modified models are solved to find a realistic solution according the DM preferences.

Returning on the methodology to model and solve the sustainable Phase III BioRSC, it is necessary to keep in mind that tactical decisions depend on strategical decision and parameter uncertainty. Similarly, the scheduling decisions depend on tactical decisions made and the parameter uncertainty. Then, in Figure 3.4 it is described how stochastic programming multistage and RO could be applied to model and optimize the sustainable Phase III BioRSC. In the left side of this figure, stochastic programming multistage is presented. The first step is to build the design model as deterministic. And

then, characterize the probability distribution for the model parameters, along with management model integration. To finish the model construction, the decision variables related to the scheduling model must be defined and added including the probability distribution for the parameters that are added to the model development. Then the model can be solved.

The right side of Figure 3.4 shows RO methodology application. At first, a deterministic model to sustainable Phase III BioRSC design, management and scheduling is developed. Then, a finite set of scenarios to model the uncertain parameters should be constructed. After, the model must be reformulated; to finally solve it.

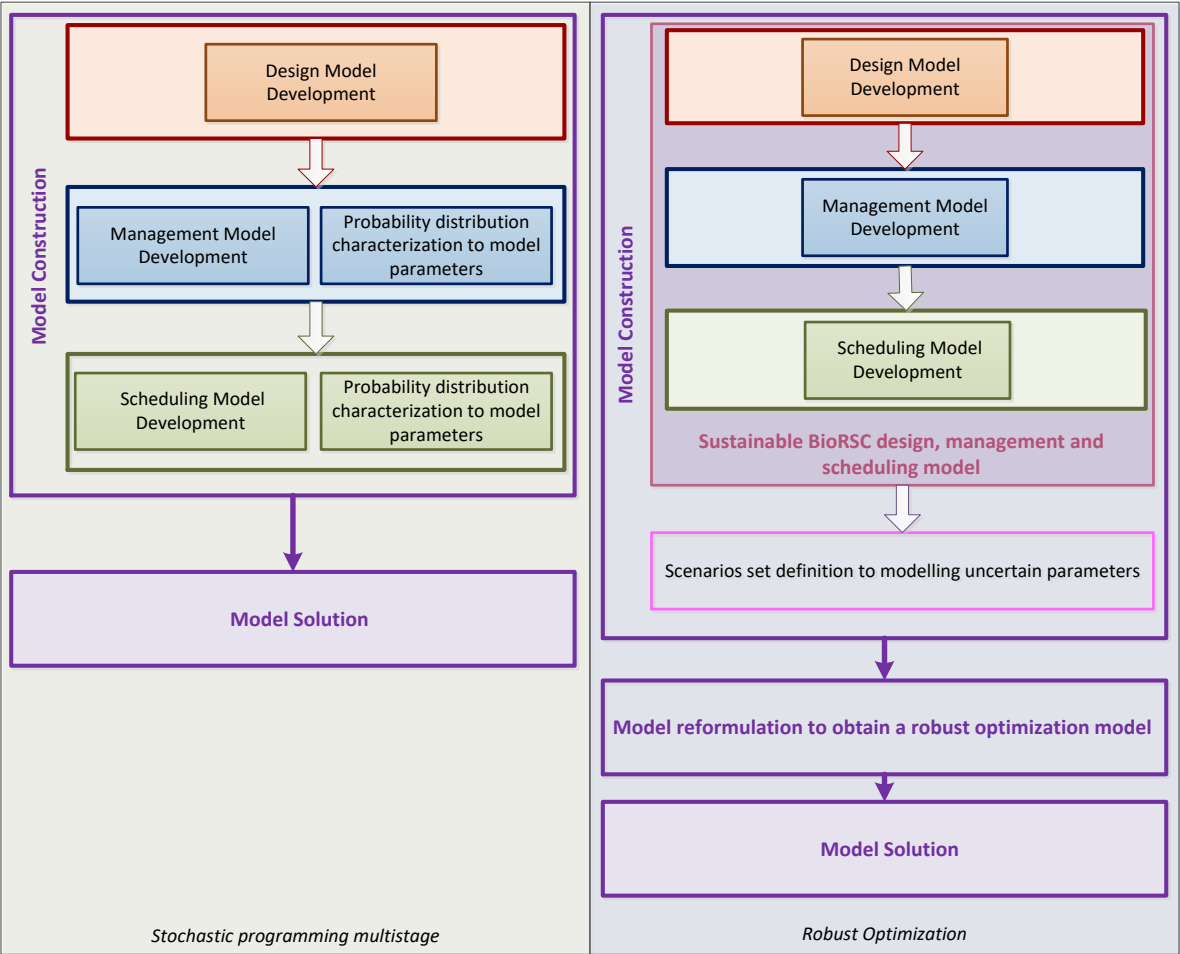


Figure 3. 4. Comparison between stochastic programming multistage and RO application to model construction

It can be noted that the principal difference between both methods is the uncertainty characterization. Then, the methodology to be applied will be selected as a function of available information about uncertain parameters.

Then, the general methodology to obtain the sustainable biorefinery supply chain configuration, integrating MCDM, can be described as:

- ✚ Model construction
- ✚ Model solution
- ✚ DM preferences
- ✚ Model adaptation
- ✚ Model adapted solution.

OR methodologies applied to construct and solve the final complete models will include a large amount of components. Then the optimization model could be classified as *large-scale problem* (Luenberger and Ye 2008). Therefore, to solve this model may be required sophisticated codes and high performing PCs. Also, it is important to highlight that the design model serves as a basis for any of the integrated methodologies to be developed.

3.4. Discussion

In view of the analysis presented below and due to the temporal limitations of the present investigation the aim of this research is to lay the foundations for the model construction and optimization for the sustainable Phase III BioRSC conception; the main contributions related to this goal are:

- ✚ The proposition of a *model construction methodology* for the sustainable Phase III BioRSC design and its application to a case study.
- ✚ A bibliographic study for the selection of optimization techniques to the deterministic sustainable Phase III BioRSC design model.
- ✚ Development and application of an optimization programming to handle multi-objectives, binary decision variables and equality and inequality constraints.
- ✚ Objective functions definition related to sustainability to find out, as perspective, the DM preferences.
- ✚ System behavior comprehension by optimal solutions and sensitivity analyses.

3.5. Summary

In this chapter fundamentals of OR related to the Phase III BioRSC model was discussed. A conceptual framework was presented to select the OR model types and resolution methodologies appropriate for the sustainable BioRSC conception. Subsequently, a general model development is proposed to integrate the decision-making levels on supply chain and the sustainability dimensions.

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Chapter IV. Methodology proposition: Modeling strategy methodology and bibliographic study for the selection of optimization techniques

4.1. Introduction

The bibliographic analysis presented in chapter II allows us to conclude that more comprehensive decision-making tools for conceive sustainable Phase III BioRSC are needed to implement an industrial and sustainable biorefinery. Therefore, in chapter III, the goal was to describe and to select the appropriated methodologies to handle the decision-making tools development. However, while Multiple Criteria Decision Making (MCDM) methods integrated to Multi-stage stochastic programming (MSP) or Robust Optimization (RO) seems the most appropriated, the task to apply them to Phase III BioRSC conception becomes extremely complex due the amount of decision variables, parameters and constraints involved. As the aim of this research is to lay the foundations for the model and optimization for the sustainable BioRSC, therefore, this chapter develops an attempt to presenting a methodological proposal for the sustainable Phase III BioRSC design model construction. Then, it presents a first model integrating the biorefinery characteristics and the supply chain strategic decisions. Also, a bibliographic study is carried out to characterize the Multi-Objective Optimization Problem, that will generate the integration of the sustainability dimensions in the model, and to choose the most appropriated optimization technique. Finally, the chosen optimization algorithm is described in detail, as well as its programming and optimization features.

4.2. Model construction proposition for sustainable Phase III BioRSC design

As presented in Chapter III the model to design a Phase III BioRSC is a BMILP (Binary Mixed Integer Linear Programming) optimization model, regarding the presence of mixed decision variables, for example decision variables for the production plants location, binary in nature. Thus, efforts will focus on continue developing a linear model to avoid possible discontinuities in space solution (Hamidian et al. 2008; Chinneck 2016) to design a sustainable Phase III BioRSC. Moreover, this model will be developed as deterministic to permit the development whether MSP or RO depending on available information about uncertain parameters.

Additionally, sustainability assessment should be multi-objective, because its framework is constituted by principles, criteria and indicators (Bautista et al. 2016), which could translate into more than one objective function. They are defined as:

Principles: The premises, bases or universal principles that define the sustainability of a biorefinery supply chain.

Criteria: Those measurable conditions (qualitative or quantitative) that establish the level of application of the principles of a sustainable biorefinery supply chain.

Indicators: There are observable qualitative or quantitative expressions, which can describe the characteristics, behaviours or phenomena of reality through the development of one or more variables.

The first level in the framework, the principles, represents the interaction between the five dimensions of the sustainability and the biorefinery supply chain stages. The second level is made up of a set of sustainability assessment criteria linked to each principle. These criteria were identified as a measurable condition (qualitative or quantitative) aiming to assess how the sustainability principle was applied to the BioRSC. The first and the second level in the framework were defined in order to make a general sustainability assessment. Therefore, the principles and criteria can be applied regardless of the economic, social, political or biogeographic context, the technological conditions or the raw materials used, among other aspects.

Finally, in the third level, indicators were established to evaluate the characteristics or behaviours of each criterion. Besides principles, and criteria, the indicators must refer to particular conditions of the biorefinery production system, or the assessment scale (national, regional, local).

Therefore the challenge on model construction is the required analysis to determine and integrate the decision variables, constraints and objective functions related to the sustainable Phase III BioRSC characteristics, the SC strategic decisions and the sustainability dimensions (principles, criteria and indicators). This combination results in a highly complex problem due to the amount of components to analyze. Then, for the model construction it is proposed a progressive development, adding elements one at a time. This working-way will permit to start from a simple model to reach a very complex one. Enabling test the model in each element addition.

Considering the mathematical models presented on the literature review, exposed on Chapter II, it can be noted that Phase III BioRSC characteristics and the SC strategic decisions have been quite studied; in contrast to the sustainability dimensions analysis. Therefore, there is ample knowledge about the integration of Phase III BioRSC characteristics and the SC strategic decisions, so these could be analyzed together. Regarding sustainability assessment, dimension analysis and integration is proposed one by one. Therefore, the model construction can be represented by Figure 4.1. In this figure, horizontal axis describes the model statement related to SC strategic level of decision-making and the BioRSC specific characteristics. It considers the integration of n biorefinery characteristics and x SC strategy decisions. The vertical axis corresponds to the inclusion of the sustainability assessment, analyzing each sustainability dimension one by one, indicator by indicator, to define the corresponding decision variables, constraints or objective functions.

The proposal considers starting with the horizontal axis in Figure 4.1 to integrate the Phase III BioRSC strategic level of decision-making and the specific characteristics of biorefineries; as a consequence of the research presented in Chapter II. The economic objective function Maximize net present value (NPV) is defined a priori, in order to test the model and to verify there is at least an optimal solution for the constraints and parameter already defined.

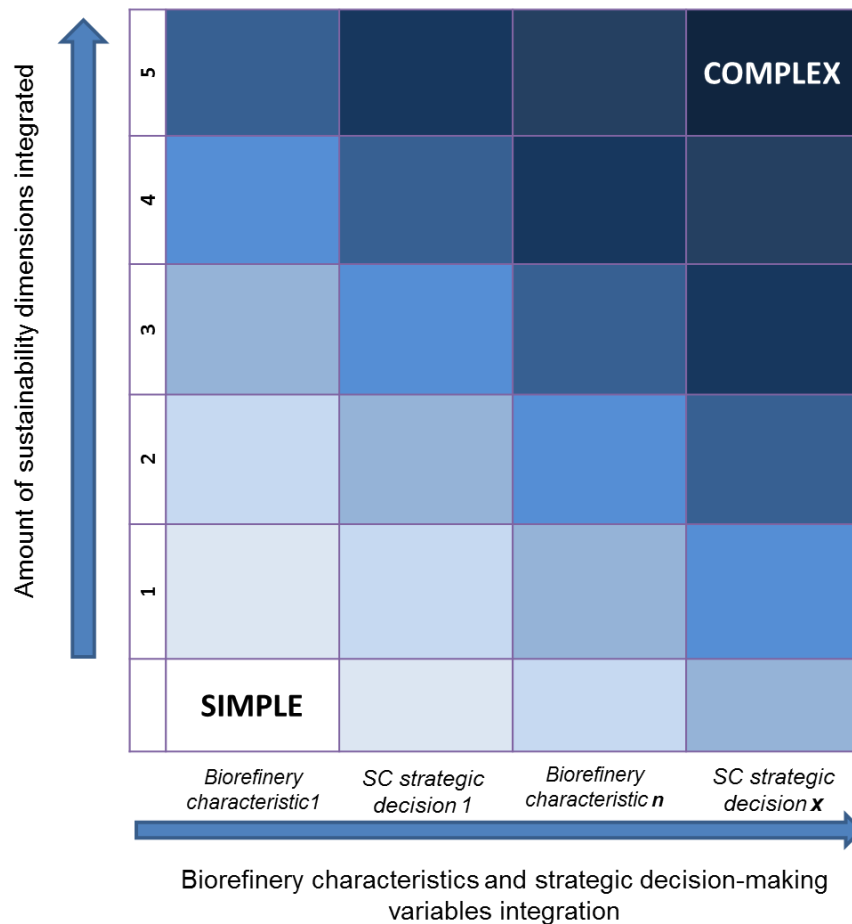


Figure 4. 1. Phase III BioRSC characteristics, SC strategic decisions and sustainability dimensions model integration

4.2.1. Horizontal axis analysis.

Four models have been developed to integrate all Phase III BioRSC strategic level of decision-making and the specific characteristics of biorefineries. These are described below and the procedure is graphically represented in Figure 4.2.

Model 1: The first model allows the decision maker to make only one strategical decision, such as plant localization, and to add the corresponding mass balance restrictions. This model will be more comprehensive by integrating biorefinery characteristics such as the selection between different raw materials and between different final products. Also, the selection of suppliers and final customers, and some strategical decisions, such as the production technology and production capacity at different production plants, could be integrated.

Model 2: The next model integrates another biorefinery characteristic, as the pretreatment implementation, with the corresponding strategic decisions, for example production capacity and production technology selection.

Model 3: Once Model 2 was proposed and tested a third model is developed, integrating the recyclability of some intermediate products and final products in the place where they are produced.

Model 4: In the last step, for the integration of BioRSC strategic level of decision-making and the specific characteristics, the Model 3 is transformed in the Model 4, integrating the possibility of sold the intermediate products, including decisions as customers localization and product quantity requirement.

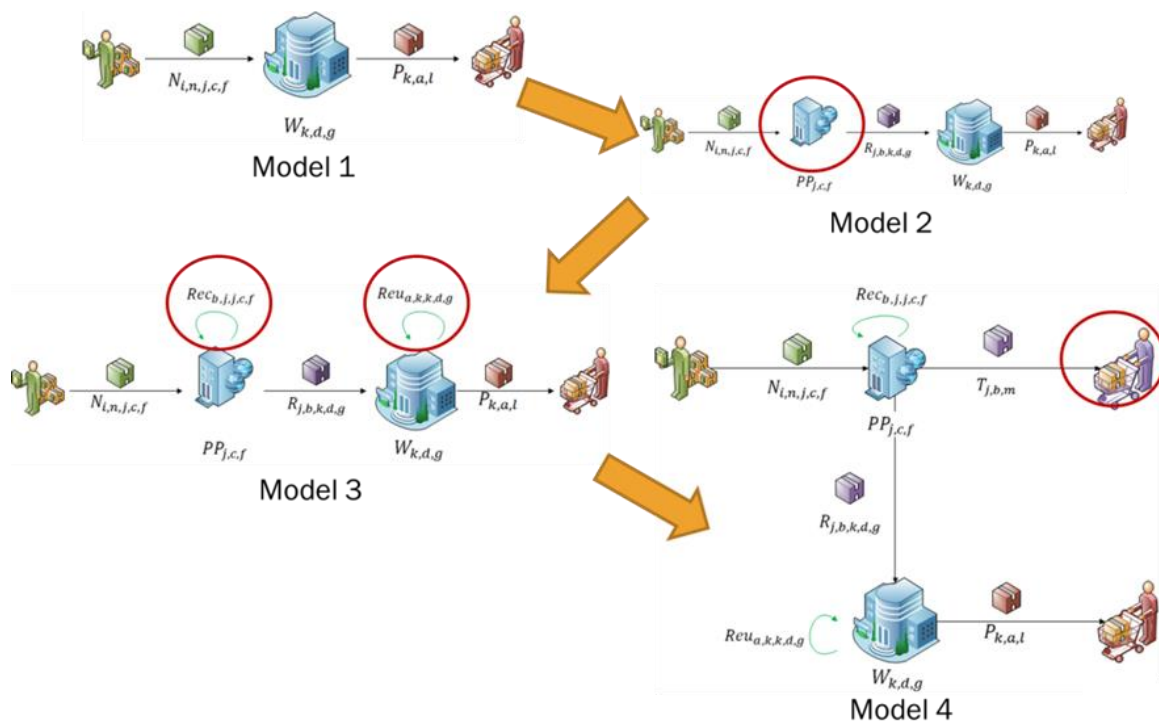


Figure 4. 2. Model evolution to integrate BioRSC strategic level of decision-making and specific characteristics of a phase III biorefinery (Personal construction).

As the Model 4 integrates entirely the Phase III BioRSC strategic level of decision-making and the specific characteristics of biorefineries, it features are described following.

Sub indices

- Raw material type: $n = 1, 2, \dots, N$
- Supplier location: $i = 1, 2, \dots, I$
- Pretreatment plant location: $j = 1, 2, \dots, J$
- Production technology at pretreatment plants: $c = 1, 2, \dots, C$
- Intermediate products type: $b = 1, 2, \dots, B$
- Transformation capacity of income materials at pretreatment plant: $f = 1, 2, \dots, F$
- Intermediate product demand location: $m = 1, 2, \dots, M$
- Main production plants location: $k = 1, 2, \dots, K$
- Production technology at main plants: $d = 1, 2, \dots, D$
- Final products type: $a = 1, 2, \dots, A$
- Transformation capacity of income materials at main plants: $g = 1, 2, \dots, G$
- Final product demand location: $l = 1, 2, \dots, L$

Decision Variables

- *Allocation, technology and capacity:*

$$W_{k,d,g} = \begin{cases} 1 & \text{If the main production plant is built in the location } k \text{ with technology } d \text{ and capacity } g \\ 0 & \text{If not} \end{cases}$$

$$PP_{j,c,f} = \begin{cases} 1 & \text{If the pretreatment plant is built in the location } j \text{ with technology } c \text{ and capacity } f \\ 0 & \text{If not} \end{cases}$$

- *Network:*

$N_{i,n,j,c,f}$ = Flow of tons of raw materials type n from the supplier located at i to the pretreatment plant located at j to be processed by technology c with a processing capacity f

$R_{j,b,k,d,g}$ = Flow of tons of intermediate products type b from the pretreatment plant located at j to the main production plant located at k to be processed by technology d with a processing capacity g

$T_{j,b,m}$ = Flow of tons of intermediate products type b from the pretreatment plant located at j to the client located at m .

$P_{k,a,l}$ = Flow of tons of final products type a from the main production plant located at k to the client located at l .

- *Reuse Flows:*

$Rec_{b,j,c}$ = Reuse flow of intermediate products type b at the pretreatment plant located at j and processed by technology c

$Reu_{a,k,d}$ = Reuse flow of final products type a at the main production plant located at k and processed by technology d

Upper and lower limits

- *Lower limit:* Zero to all variables

- *Upper limit:*

✚ The upper limit for binary variables $PP_{j,c,f}$ and $W_{k,d,g}$ is 1.

✚ For $N_{i,n,j,c,f}$ is the minimum between the availability of raw materials type n located at i and the production capacity f at the pretreatment plant j with technology c .

$$N_{i,n,j,c,f} \leq \text{Min} \{RMAvailability_{i,n} ; CapPP_{j,c,f}\} \quad (1)$$

✚ For $R_{j,b,k,d,g}$ the upper limit is the minimum between the maximum amount of intermediate product type b that could be produced at a pretreatment plant located at j and the production capacity g at the principal production plant located at k with technology d .

The maximum amount of intermediate product type b that could be produced at a pretreatment plant located at j depends on the comparison between the maximal production capacity that could have the pretreatment plant j and the total amount of raw materials that are available to be transformed in that plant. Also, the production of b depends on the transformation rate. Then, it is required to find the maximum transformation rate to obtain b , for all the transformation technologies, because $R_{j,b,k,d,g}$ does not depend on variables as c , and i .

$MaxProduction_{b,j}$

$$= \text{Min} \left\{ \langle \text{Max}_b \{ \alpha_{n,c,b} \} \right. \\ \left. * \text{Max}_j [CapPP_{j,c,f}] ; \sum_n \left(\langle \text{Max}_{b,n} \{ \alpha_{n,c,b} \} \rangle \sum_i RMAvailability_{i,n} \right) \right\} \quad (2)$$

Therefore, the upper limit can be described as:

$$R_{j,b,k,d,g} \leq \text{Min} \{MaxProduction_{b,j} ; CapW_{k,d,g}\} \quad (3)$$

✚ In the same way, the upper limit to $Rec_{b,j,c}$ is the maximum amount of intermediate product type b that could be produced at a pretreatment plant located at j , but with the specific technology c . Therefore, it is required to compare the maximal amount of product b that can be produced at the pretreatment plant depending on its maximal production capacity and the maximal amount that can be produced using all the raw materials available. The mathematical expression is:

$$Rec_{b,j,c} \leq \text{Min} \left\{ \langle \text{Max}_{b,c} \{ \alpha_{n,c,b} \} \rangle * \text{Max}_{j,c} [CapPP_{j,c,f}] ; \sum_n \left(\alpha_{n,c,b} * \sum_i RMAvailability_{i,n} \right) \right\} \quad (4)$$

✚ $Reu_{a,k,d}$ upper limit is the maximum amount of final product type a that could be produced at main production plant located at k . It depends on the comparison between the maximal production capacity that could have the principal plant k with technology d and the total amount of intermediate products that are available to be transformed in that main plant. Also, the production of a depends on the

transformation rate. Then, it is required to find the maximum rate transformation to obtain it, for all intermediate products types. Because $Reu_{a,k,d}$ does not depend on variables as b , g and j .

$$Reu_{a,k,d} \leq \text{Min} \left\{ \left(\text{Max}_{a,d} \alpha_{b,d,a} \right) * \text{Max}_{k,d} [CapW_{k,d,g}] ; \sum_b \left(\alpha_{b,d,a} * \sum_j \text{MaxProduction}_{b,j} \right) \right\} \quad (5)$$

- ✚ $P_{k,a,l}$ upper limit is the minimum value between maximum amount of final product type a that could be produced at main production plant located at k and the final product type a demand by the customer located in l . Therefore, the maximal production capacity of final product a at the main production plant k is defined as:

$$\begin{aligned} & \text{MaxProduction}_{a,k} \\ &= \text{Min} \left\{ \left(\text{Max}_a \alpha_{b,d,a} \right) \right. \\ & \quad \left. * \text{Max}_k [CapW_{k,d,g}] ; \sum_b \left(\text{Max}_{a,b} \{ \alpha_{b,d,a} \} * \sum_j \text{MaxProduction}_{b,j} \right) \right\} \end{aligned} \quad (6)$$

It is used to define the upper limit to $P_{k,a,l}$ as:

$$P_{k,a,l} \leq \text{Min} \{ \text{MaxProduction}_{a,k} ; Dem_{l,a}(\text{Max}) \} \quad (7)$$

- ✚ $T_{j,b,m}$ upper limit is the minimum value between the maximum amount of intermediate product type b that could be produced at a pretreatment plant located at j and the amount of intermediate product type b demanded by a customer located in m , as presented in equation (8)

$$T_{j,b,m} \leq (\text{Min} \{ Dem_{m,b}(\text{Max}); \text{MaxProduction}_{b,j} \}) \quad (8)$$

Parameters

- $RMAvailability_{i,n}$ Is the available amount of raw materials type n at supplier location i .
- $CapPP_{j,c,f}$ Is the transformation capacity in tons of incoming materials at pretreatment plants located at j , equipped with the transformation technology c and the production capacity numbered by f
- $CapW_{k,d,g}$ Is the transformation capacity in tons of incoming materials at main production plants located at k , equipped with the transformation technology d and the production capacity numbered by g
- $\alpha_{n,c,b}$ Transformation rate of raw materials type n to intermediate products type b through technology c .
- $\alpha_{b,d,a}$ Transformation rate of intermediate products type b to final products type a through technology d .
- $Dem_{m,b}(\text{Max})$ Amount of intermediate product type b demanded at client location m
- $Dem_{l,a}(\text{Max})$ Amount of final product type a demanded at client location l

Constraints

- *Mass balances.* These restrictions are an application of the law of conservation of mass to the analysis of physical systems. Therefore, there exists a mass balance for each pretreatment plant and for the main production plants. These balances must be made by differentiating the type of product that is obtained, as a consequence of the different transformation rates, which depend on income materials type and the applied transformation technology.

✚ Intermediate products transformation at Pretreatment Plants

$$\sum_c \sum_n \sum_f \alpha_{n,c,b} \left[\sum_i N_{i,n,j,c,f} \right] = \sum_k \sum_d \sum_g R_{j,b,k,d,g} + \sum_c Rec_{b,j,c} + \sum_m T_{j,b,m} \quad (9)$$

$\forall j, b$

✚ Final products transformation at main production plants

$$\sum_d \sum_b \sum_g \alpha_{b,d,a} * \left[\sum_j R_{j,b,k,d,g} \right] = \sum_l P_{k,a,l} + \sum_d Reu_{a,k,d} \quad (10)$$

$\forall k, a$

- *Raw materials availability.* The raw materials to be consumed in biorefineries are limited by its availability at supplier location.

$$\sum_j \sum_c \sum_f N_{i,n,j,c,f} \leq RMAvailability_{i,n} \quad (11)$$

$\forall i, n$

- *Production Capacity.* The amount of incoming materials is limited by the processing capacity at the pretreatment and at main production plant. They can only receive materials if the plant has been installed with a specific technology and capacity.

✚ Pretreatment plants

$$\sum_n \sum_i N_{i,n,j,c,f} \leq CapPP_{j,c,f} * PP_{j,c,f} \quad (12)$$

$\forall j, c, f$

✚ Main plant

$$\sum_b \sum_j R_{j,b,k,d,g} \leq CapW_{k,d,g} * W_{k,d,g} \quad (13)$$

$\forall k, d, g$

- *Selection of production capacity and technology for each location.* Only one production capacity and one transformation technology can be selected for each plant location

✚ Pretreatment plants

$$\sum_c \sum_f PP_{j,c,f} \leq 1 \quad \forall j \quad (14)$$

✚ Main plants

$$\sum_g \sum_d W_{k,d,g} \leq 1 \quad \forall k \quad (15)$$

- *Minimum number of plants to install.* At least one pretreatment plant and one main production plant must to be installed to have the design of a decentralized system.

✚ Pretreatment plants

$$1 \leq \sum_j \sum_c \sum_f PP_{j,c,f} \quad (16)$$

✚ Main plants

$$1 \leq \sum_k \sum_d \sum_g W_{k,d,g} \quad (17)$$

- *Demand limitations.* Even though raw material seasonality implies its storage, as presented on Chapter II, decisions related to strategical decision-level on SC do not include inventory decision. Therefore, it is not possible to sell more products than the demanded amount in each final selling point, presented on equations (18) and (19). However, in future models including tactical and operational decisions, inventory management is a key decision.

✚ Intermediate Products

$$\sum_j T_{j,b,m} \leq Dem_{m,b}(Max) \quad \forall m, b \quad (18)$$

✚ Final Products

$$\sum_k P_{k,a,l} \leq Dem_{l,a}(Max) \quad \forall l, a \quad (19)$$

Products to be sold only can exist if the plant production is installed. Therefore, two restrictions are required for pretreatment plants, (20) and (21), and another constraint is required to principal plants (22).

✚ Pretreatment plants

$$\sum_b \sum_m T_{j,b,m} \leq M * \sum_c \sum_f PP_{j,c,f} \quad (20)$$

$$\forall j$$

$$\sum_b \sum_k \sum_d \sum_g R_{j,b,k,d,g} \leq M * \sum_c \sum_f PP_{j,c,f} \quad (21)$$

$$\forall j$$

✚ Main plants

$$\sum_a \sum_l P_{k,a,l} \leq M * \sum_d \sum_g W_{k,d,g} \quad (22)$$

$$\forall k$$

These restrictions and the mass balance contribute to limit the values of $Rec_{b,j,c}$ and $Reu_{a,k,d}$, which could only be different from zero if the corresponding production plants are installed.

Objective Function

$$Max NPV = \sum_{i=1}^T \frac{Net\ Cash\ Flow_i}{(1 + Discount\ Rate)^i} - Initial\ Investment \quad (23)$$

Where

$$Net\ Cash\ Flow_i = Incomes_i - Costs_i \quad (24)$$

The assumption for this calculation is that the cash flows will be the same during the time of evaluation of the net present value. Thus, the expression for cash flows becomes:

$$Net\ Cash\ Flow_i = i * (Incomes - Costs) \quad (24)$$

- *Incomes*. It can be described as the products sold in the market by their market value, plus the products that are re-used in the production plants by their value, represented by equation (25).

Incomes =

$$\sum_a Pric_a * \left[\sum_k \sum_l P_{k,a,l} \right] + \sum_b Pric_b * \left[\sum_j \sum_m T_{j,b,m} \right] + \sum_b \sum_j value_{b,j} * \left[\sum_c Rec_{b,j,j,c} \right] + \sum_a \sum_k value_{a,k} * \left[\sum_d Reu_{a,k,k,d} \right] \quad (25)$$

- **Costs.** There are represented by transportation cost, raw material acquisition cost and transformation cost for raw materials and intermediate products, as presented on equation (26).

$$Costs = TransportCost + RawMaterialsCost + ProductionCost \quad (26)$$

The transportation costs consist on the cost of moving the raw materials to pretreatment plants; transport the intermediate products to their respective markets and / or the main production plants, and the transport of the final products to the markets, represented in equation (27)

TransportCost =

$$\sum_i \sum_j TCost_{i,j} * \left[\sum_c \sum_f \sum_n N_{i,n,j,c,f} \right] + \sum_j \sum_k TCost_{j,k} * \left[\sum_d \sum_g \sum_b R_{j,b,k,d,g} \right] + \sum_k \sum_l TCost_{k,l} * \left[\sum_a P_{k,a,l} \right] + \sum_j \sum_m TCost_{j,m} * \left[\sum_b T_{j,b,m} \right] \quad (27)$$

Then, the cost details related to acquisition cost of the raw materials are presented by equation (28).

RawMaterialsCost =

$$\sum_n RMCost_n * \left[\sum_i \sum_j \sum_c \sum_f N_{i,n,j,c,f} \right] \quad (28)$$

The costs of production or operation depend on the incoming materials, the transformation technology used, the production capacity and the plant location.

ProductionCost =

$$\sum_n \sum_j \sum_c \sum_f ProdCost_{n,j,c,f} * \left(\sum_i N_{i,n,j,c,f} \right) + \sum_b \sum_k \sum_d \sum_g ProdCost_{b,k,d,g} * \left(\sum_j R_{j,b,k,d,g} \right) \quad (29)$$

- Initial investment. It is composed by the investment required to install the pretreatment and the principal production plants.

Initial Investment =

$$\sum_j \sum_c \sum_f Inv_{j,c,f} * PP_{j,c,f} + \sum_k \sum_d \sum_g Inv_{k,d,g} * W_{k,d,g} \quad (30)$$

Objective function parameters

- $Prix_a$ and $Prix_b$ are the market value for final products and intermediate products respectively.
- $value_{b,j}$ and $value_{a,k}$ are the value of reuse the intermediate products and the final products in the plants where they were produced, respectively.
- $TCost_{i,j}$, $TCost_{j,k}$, $TCost_{k,l}$, $TCost_{j,m}$ are the transport cost for moving the materials between two points. They are in monetary value divided by material tons to transport. This means that the monetary value must to be previously calculated depending on the distance between the points.
- $RMCost_n$ is the market value of the raw material type n
- $ProdCost_{n,j,c,f}$ is the operation cost at pretreatment plants, depending on the raw materials type n , the transformation technology used c , the production capacity f and the plant location j .
- $ProdCost_{b,k,d,g}$ is the operation cost at main production plants, depending on the intermediate products type b , the transformation technology used d , the production capacity g and the plant location k .
- $Inv_{j,c,f}$ and $Inv_{k,d,g}$ are the inversion monetary value to install the pretreatment and main production plants respectively.

4.2.2. Vertical axis analysis

Regarding the sustainable analysis, vertical axis in Figure 4.1, the economic dimension has been studied deeply, as presented in chapter II. Therefore, it is the most documented and developed, which facilitates its integration to the model.

Then, the economic dimension should be the first sustainability dimension to be incorporated, designing the next Model 5. Nevertheless, the order to incorporate the dimensions should not alter the final optimization model.

For the integration of the subsequent dimensions to the model, the framework proposed by Bautista et al. (2016) within its principles, criteria and indicators, presented at the beginning of section 4.2, should be analyzed generally.

As the challenge on model construction is the required analysis to determine and integrate the decision variables, constraints and objective functions related to the sustainable Phase III BioRSC; and this can be considered as highly complex problem due to the amount of components to analyze; the quantity of indicators or expressions by dimension to analyze is chosen as criteria to select the analysis order of the remaining dimensions. Therefore, Table 4.1 was constructed based on the framework proposed by Bautista et al. (2016) ordering the dimensions according to the number of indicators that each of them has.

It can be seen that the *technological* dimension has the fewest number of principles, criterion and indicators. Therefore, it should be the second dimension to integrate to the model, constructing the Model 6. Following this same logic, the order of incorporation of the remaining dimension analysis is political, social and finally environmental.

The analysis of each sustainability dimension, the resulting models and its application to a study case will be described on chapters V and VI.

Table 4. 1. *Quantity of Principles, criterion and indicators to analyses for sustainability assessment*

Sustainability Dimension	Number of Principles	Number of Criterion	Number of Indicators
Technological	1	4	5
Political	3	9	19
Economic	1	6	40
Social	4	10	42
Environmental	4	11	51

4.3. Model resolution methodology for a Multi-Objective Optimization Problem

The constructed model resulting by the application of the strategy described in the preceding section involves more than one objective function apriori, because there are five dimensions and 157 indicators to analyze. Therefore, several objective functions are expected. As a consequence, the final model should be solved considering multiple objectives simultaneously at first stage, as concluded in Chapter III. This kind of problems with several objective functions is known as Multi-Objective Optimization Problems (MOOP) (Narzisi et al. 2006). Following, the definition of MOOP is described:

Definition 1. A MOOP can be mathematically formulated as shown in equations A to C (Zhou et al. 2011; von Lücken et al. 2014):

$$\begin{aligned}
 & \text{Minimize } F(x) = (f_1(x), \dots, f_m(x))^T \\
 & x = (x_1, \dots, x_n)^T \in \mathcal{X} \subseteq \mathbb{R}^n \\
 & y = (y_1, \dots, y_m)^T \in \mathcal{Y} \subseteq \mathbb{R}^m
 \end{aligned} \tag{A}$$

Subject to

$$g(x) = (g_1(x), \dots, g_k(x))^T \leq 0 \tag{B}$$

$$x_i^{(L)} \leq x_i \leq x_i^{(U)} \quad \forall i \in \{1, \dots, n\} \tag{C}$$

Where

- $F(x)$ corresponds to m objective functions, where \mathbb{R}^m is the objective space.
- x is a vector of n decision variables.
- y represents an m -dimensional objective vector.
- Constraint (C) represents $2n$ variable bounds that help to define the decision variable space or decision space \mathcal{X} .
- y_f is the objective space, it is a multi-dimensional space composed by the objective functions.
- $g(x)$ is a vector composed by k constraint functions which shape the feasible region.

Solutions that do not satisfy constraint functions and/or variable bounds are called infeasible solutions, while solutions that meet all constraints in (B) and (C) are feasible solutions.

The set of all feasible solutions \mathcal{X}_f is known as the feasible region. The domain of each f_i is \mathcal{X}_f . For each solution $x \in \mathcal{X}_f$ a point y exists in the objective space. Thus, \mathcal{X}_f defines the feasible objective space y_f :

$$y_f = F(\mathcal{X}_f) = \bigcup_{x \in \mathcal{X}_f} \{F(x)\}$$

The objectives in MOOP are often in conflict with each other. So, the improvement of one objective may lead to the deterioration of another (Zhou et al. 2011). One solution optimal is one that is non-dominated by any other in the analysis space (Suárez Palacios et al. 2011). Thus, there is no single optimum solution. Instead there is a set of solutions which are all optimal, called the Optimal Pareto Front (Narzisi et al. 2006), showed graphically in figure 4.3. This graph results from the minimization of both objective functions.

Definition 2. A vector $u = (u_1, \dots, u_m)^T$ is said to dominate another vector $v = (v_1, \dots, v_m)^T$, denoted as $u < v$, if $\forall i \in \{1, \dots, m\}, u_i \leq v_i$ and $u \neq v$.

Definition 3. A feasible solution, $x^* \in \mathcal{X}_f$ of problem (A), is called Pareto Optimal Solution, if $\nexists x \in \mathcal{X}_f / F(x) < F(x^*)$. The set of all the Pareto optimal solutions is called the Pareto Set (PS), denoted as

$$PS = \{x \in \mathcal{X}_f | \nexists x' \in \mathcal{X}_f / F(x') < F(x)\}$$

The image of the PS in the objective space is called the *Pareto Front* (PF).

$$PF = \{F(x) | x \in PS\}$$

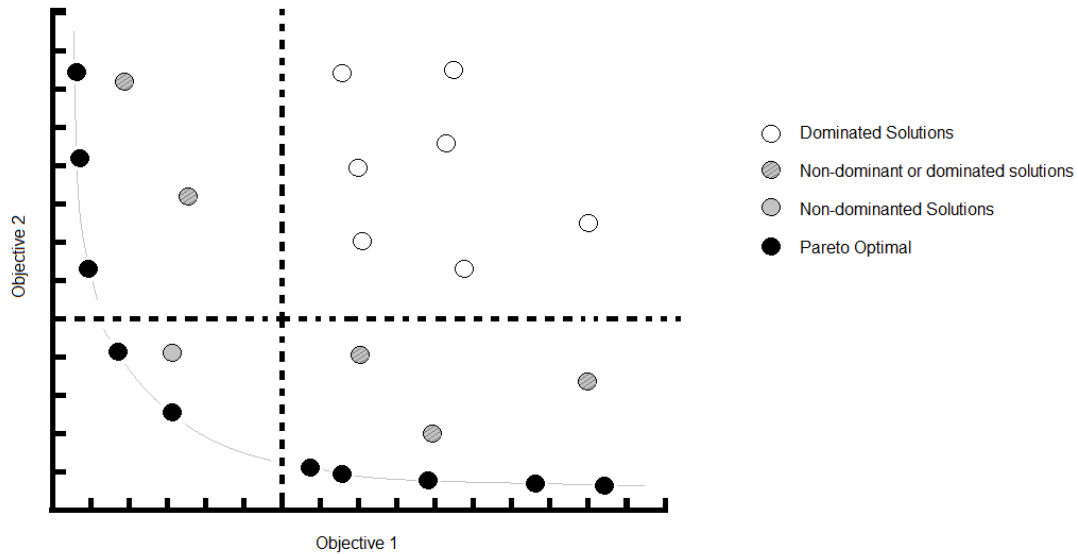


Figure 4. 3. Adaptation from (Chi-Keong Goh and Kay Chen Tan 2009; Suárez Palacios et al. 2011; Xiong et al. 2015).

There are different ways to find the Pareto Front. The first one involves a large amount of optimizations for a unique objective function, minimizing a linear criteria combination. At each optimization the weight of each criterion is modified (Camargo Pardo 2012). However, some problems are so complicated that it may not be possible to solve for obtain the Pareto Front. In such situation it is important to find a good feasible solution that is at least reasonably close to being optimal. Heuristic methods are commonly used to search for such a solution (Frederick S. Hillier 2001).

A heuristic method is a procedure that is likely to discover a very good feasible solution, but not necessarily an optimal solution, for the specific problem being considered (Frederick S. Hillier 2001). The procedure often is a full-fledged iterative algorithm, where each iteration involves conducting a search for a new solution that might be better than the best solution found previously. When the process finished the solution provides by the algorithm is the best one that was found during any iteration (Frederick S. Hillier 2001).

A metaheuristic is a general solution method that provides both a general structure and strategy guidelines for developing a specific heuristic method to fit a particular kind of problem (Frederick S. Hillier 2001). Three prominent types of metaheuristics are Tabu Search, Simulation Annealing and Genetic or Evolutionary Algorithms (Frederick S. Hillier 2001).

Due to their population-based nature, evolutionary algorithms (EAs) are able to approximate the whole PS and PF of an MOOP in a single run (Huband et al. 2006; Zhou et al. 2011). Providing the Decision Maker (DM) with a set of alternatives to choose from (Branke 2008). The ability to handle complex problems, involving features such as discontinuities, multimodality, disjoint feasible spaces and noisy function evaluations, reinforces the potential effectiveness of EAs in multi-objective search and optimization (Fonseca and Fleming 1995).

Some evolutionary algorithms advantages are (Camargo Pardo 2012):

- ✚ Little or no knowledge about the problem to solve is required
- ✚ Insensitivity to the Pareto Front form or continuity
- ✚ Easy to implement and to program

4.3.1. *Multi-Objective Evolutionary Algorithm (MOEA) description*

Multi-Objective Evolutionary Algorithm (MOEA) is a stochastic search methodology to solve multi-objective problems, emulating the Darwinian principle of survival-of-the-fittest in natural selection and adaptation (Chi-Keong Goh and Kay Chen Tan 2009). The evolutionary algorithm is an iterative optimization process. The process starts with the initialization of the population of candidate-solution. Then, the evaluation stage considers the performance of each candidate-solution and the density (diversity) of candidate solutions group. Performance evaluation is calculated on the basis of the criteria optimization problem. After that, the performance of individuals is compared one by one, giving them a rating. Then a classification from highest to lowest is carried out, obtaining an update of candidate-solutions.

The selection of individuals can be performed in different ways. Some MOEAs maintain a fixed amount of the population, while others only keep individuals who are non-dominated, for the next stage of the process. Nonetheless, in most cases, a truncation process will be conducted based on some density assessment to restrict the number of achieved solutions.

The remaining individuals will be eliminated and replaced with new individuals. The objective is generating variation to explore and to exploit the selected individuals to generate a new population of solutions. The variation operators are two mechanisms:

Birth: two surviving individuals are selected randomly and the range of variation of its characteristics is defined. Births are accompanied by a performance test, and the new individual should have better performance to the last survivor of the population to be part of the new population.

Mutation: A predefined percentage of the population chromosomes are mutated at random within a range of calculation. A mutant is taken into account for the new population if their performance is better than the individual who replaced

This process is repeated until fulfill one of two criteria completion:

Number of generations. Security criteria to prevent unnecessary consumption of computer resource.

Loss of biodiversity. When the difference in the performance of the first individual rankings, with respect to the last, is smaller than an error previously established.

4.3.2. Multi-objective evolutionary algorithms bibliometric study

As discussed in the section 4.3.1, there are different types of MOEAs as presented on Table 4.2.

Table 4. 2. Different types of MOEAs, based on (Deb 2008a)

- Non-Elitist Multi-objective Evolutionary Algorithms	
<ul style="list-style-type: none"> ✓ Vector Evaluated Genetic Algorithm ✓ Weight-Based Genetic Algorithm ✓ Random Weighted Genetic Algorithm ✓ Multiple Objective Genetic Algorithm 	<ul style="list-style-type: none"> ✓ Non-Dominated Sorting Genetic Algorithm (NSGA) ✓ Niche-Pareto Genetic Algorithm ✓ Distributed Reinforcement Learning Approach ✓ Nash Genetic Algorithm
- Elitist Multi-objective Evolutionary Algorithms	
<ul style="list-style-type: none"> ✓ Thermodynamical Genetic Algorithm ✓ Pareto-Achieved Evolution Strategy ✓ Pareto Converging Genetic Algorithm ✓ Strength Pareto Evolutionary Algorithm 	<ul style="list-style-type: none"> ✓ Elitist Non-Dominated Sorting Genetic Algorithm (NSGA-II) ✓ Distance-Based Pareto Genetic Algorithm ✓ Multi-objective Micro-Genetic Algorithm
- Constrained Multi-objective Evolutionary Algorithms	
<ul style="list-style-type: none"> ✓ Penalty Function Approach 	<ul style="list-style-type: none"> ✓ Constrained Tournament Method

As it can be seen in Table 4.2, there are at least 17 different types of MOEAs. Consequently, to select one of them, a bibliometric analysis among scientific articles which apply and/or develop optimization evolutionary algorithms should be carried out (Escorcia O. 2008; Bautista et al. 2016). Considering the aim of this research is to solve the MOOP and not to create a new optimization algorithm, the exponential expansion of scientific information is assessed to find the most studied and developed MOEAs, to facilitate their application. To do that, a search was performed in Scopus considering the all period up to September 8th, 2015. The keywords used for the search are presented on Table 4.3.

Then, a first bibliometric analysis of the results is presented on Figure 4.4. It displays each algorithm in circles which differ in size depending on the amount of articles studying each one. It is observed that the NSGA-II, NSGA and Strength Pareto Evolutionary Algorithm are the most studied.

Nevertheless, that fact does not mean currently they are the most studied and developed. Therefore, an historic evolution of the scientific articles number that analyzes each MOEA is presented in Figure 4.5, Figure 4.6 and Figure 4.7. The historical analysis has been separated in three figures due to the great difference in the number of investigations dedicated to the different algorithms, facilitating the observation of the evolution of the scientific interest in each type of algorithm.

Table 4. 3. Keywords used for search on Scopus

Evolutionary Algorithm	Keywords
Vector Evaluated Genetic Algorithm	"VEGA" AND "Genetic Algorithm" "VEGA" AND "Evolutionary Algorithms"
Weight-Based Genetic Algorithm	"Weight-Based Genetic Algorithm"
Random Weighted Genetic Algorithm	"Random Weighted Genetic Algorithm"
Multiple Objective Genetic Algorithm	"Multiple Objective Genetic Algorithm"
Non-Dominated Sorting Genetic Algorithm (NSGA)	"Non-Dominated Sorting Genetic Algorithm" AND NOT "Elitist" AND NOT "NSGA II"
Niched-Pareto Genetic Algorithm	"Niched-Pareto Genetic Algorithm"
Distributed Reinforcement Learning Approach	"Distributed Reinforcement Learning Approach"
Nash Genetic Algorithm	"Nash Genetic Algorithm"
Elitist Non-Dominated Sorting Genetic Algorithm (NSGA-II)	"Elitist Non-Dominated Sorting Genetic Algorithm" "Elitist Non-Dominated Sorting Genetic Algorithm" AND "NSGA II" "NSGA II" AND "Evolutionary Algorithm"
Distance-Based Pareto Genetic Algorithm	"Distance-Based Pareto Genetic Algorithm"
Strength Pareto Evolutionary Algorithm	"Strength Pareto Evolutionary Algorithm"
Thermodynamical Genetic Algorithm	"Thermodynamical Genetic Algorithm"
Pareto-Achieved Evolution Strategy	"Pareto Converging Genetic Algorithm"
Pareto Converging Genetic Algorithm	"Pareto Converging Genetic Algorithm"
Multi-objective Micro-Genetic Algorithm	"Multi objective Micro Genetic Algorithm"
Penalty Function Approach	"Penalty Function Approach" AND "Evolutionary Algorithm"
Constrained Tournament Method	"Constrained Tournament" AND "Evolutionary Algorithm"

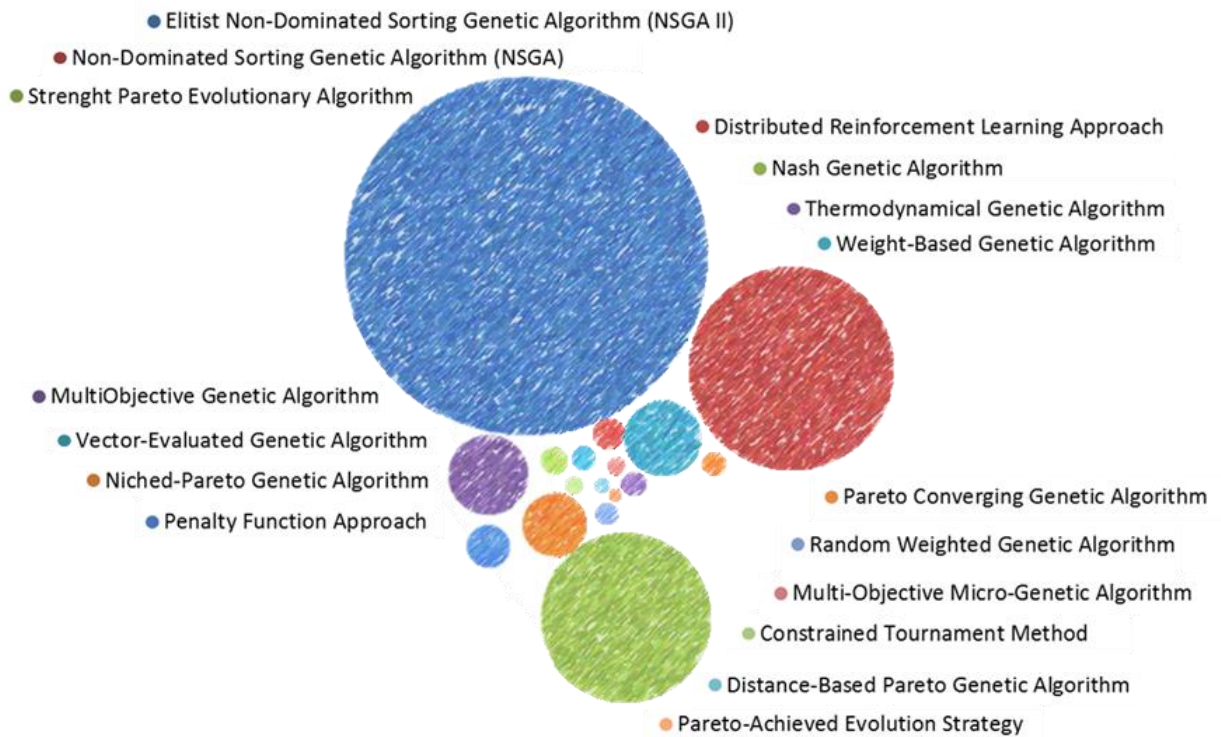


Figure 4. 4. Comparison of number of scientific articles related to evolutionary algorithms

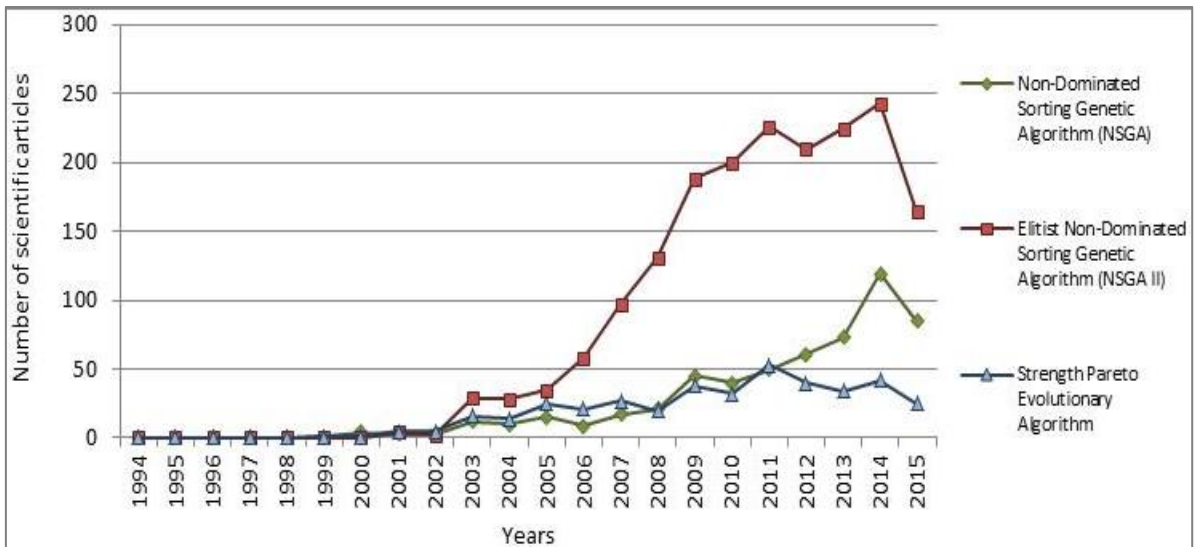


Figure 4.5. Research trend of in the use of evolutionary algorithms, Part 1

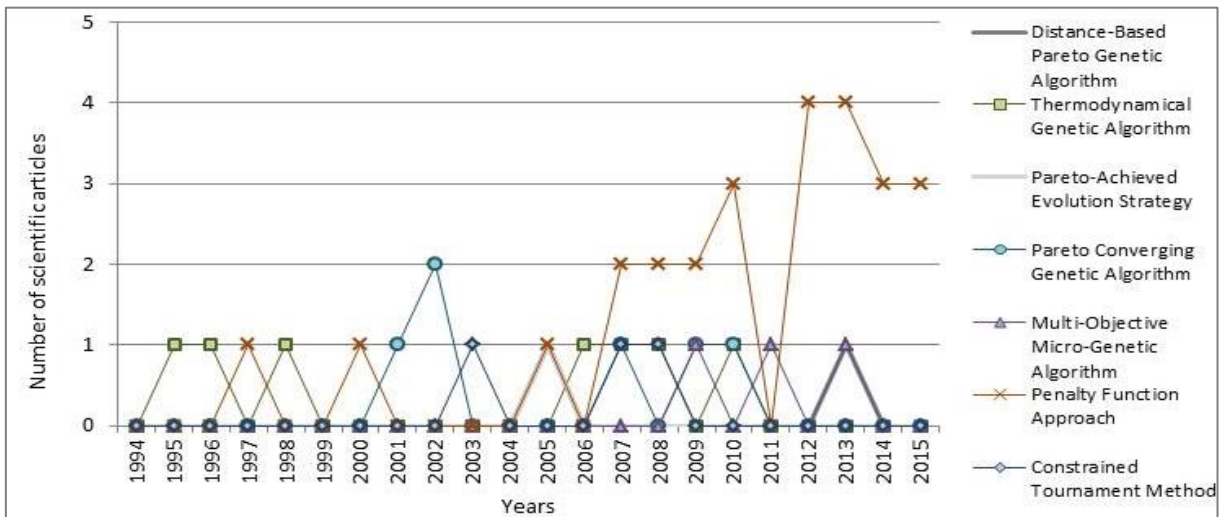


Figure 4.6. Research trend of in the use of evolutionary algorithms, Part 2

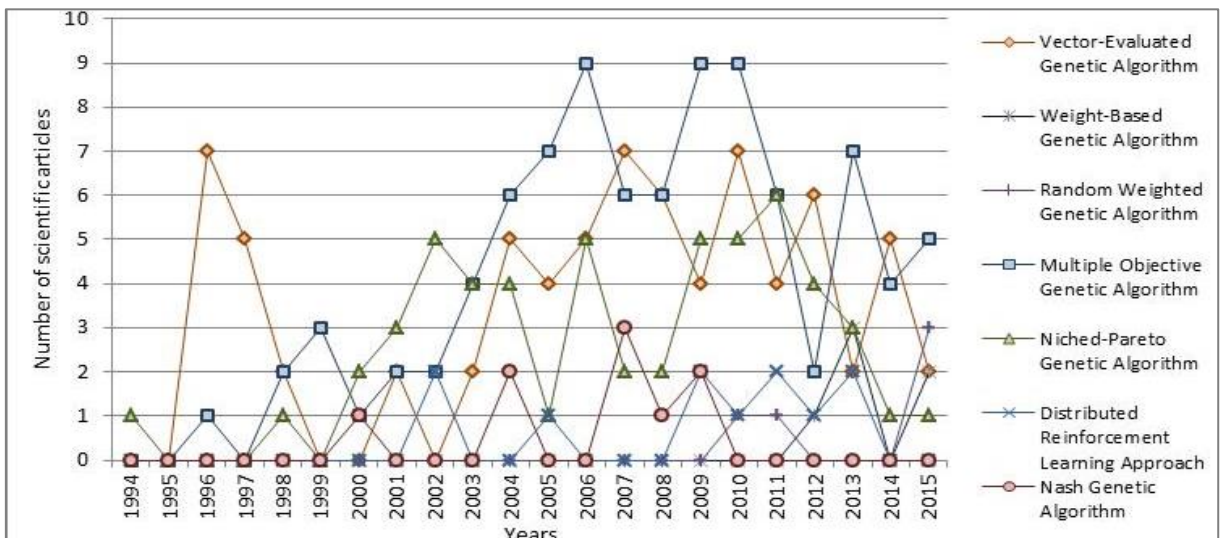


Figure 4.7. Research trend of in the use of evolutionary algorithms, Part 3

Figures 4.5, 4.6 and 4.7, show that NSGA-II, NSGA and Strength Pareto Evolutionary Algorithm had a relatively constant scientific interest between 1994 and 2015. Figure 4.5 shows that the number of scientific articles analyzing NSGA-II increased exponentially from 2005 to 2009. Then, an average of about 200 related investigations were published each year between 2010 and 2015. Therefore, NSGA-II is the MOEA to be used to resolve the MOOP.

4.3.3. Elitist Non-Dominated Sorting Genetic Algorithm (NSGA-II)

The NSGA-II procedure (Deb 2008a) attempts to find multiple Pareto-optimal solutions in a multi-objective optimization problem. It has the following three features:

- ✚ Uses an elitist principle, i.e. it incorporates a mechanism for preserving the dominant solutions through several generations of a genetic algorithm
- ✚ Uses an explicit diversity preserving mechanism
- ✚ Emphasizes non-dominated solutions.

The optimization process that follows this algorithm is detailed below and represented schematically in Figure 4.8 and detailed following.

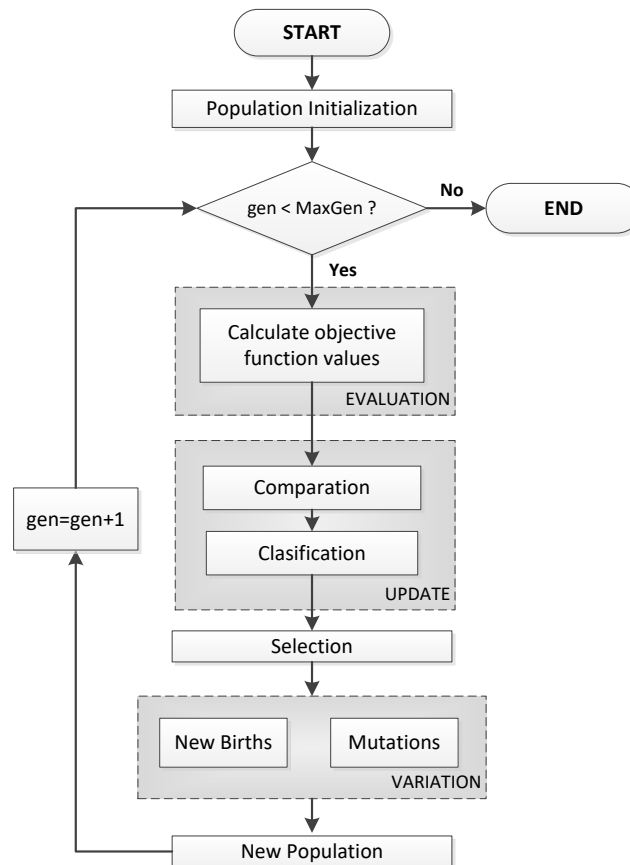


Figure 4. 8. NSGA-II process structure, based on (Peñuela Meneses and Granada Echeverri 2007; Deb 2008b; Deb 2008a)

Population initialization. Creation of a set of potential solutions (Parents) size N for the decision variables, either randomly or through a smooth constructs.

Evaluation. Calculation of objective function values, evaluation of the initial population and calculation of the objective function value and restriction values. In general, the objective function is an expected value.

Update.

- *Comparison:* On the current population (Parents) N pairs of solutions are selected, chosen at random
- *Classification:*
 - ✚ Evaluation of Pareto dominance among individuals of each pair to determine those non-dominated.
 - ✚ Evaluation of the stacking operator, which allows quantifying the space around an alternative that is not occupied by any solution. For this, it must be calculated the perimeter of the cuboid formed by neighboring solutions having the same dominance range as the alternative i , this is:

$$d_i = \sum_{m=1}^M \left| \frac{f_m^{i_{+1}} - f_m^{i_{-1}}}{f_m^{max} - f_m^{min}} \right|$$

Where:

I^m is a vector which indicates the alternative solution neighbor to the alternative i .

f_m^{max} and f_m^{min} are the maximum and minimum values over the solution space of the objective function m .

M is the number of objective functions optimized.

Therefore, the alternative with the highest level of diversity is the one with the largest stacking distance.

Selection: Among the individuals ordered according to dominance, pairs are selected to compete in a tournament, where the alternative that belongs to the best quality range wins. The winners of each tournament are the only empowered to obtain offspring. This procedure replaces the selection used in the traditional genetic algorithm. It consists in comparing two attributes of each pair of individuals:

- ✚ Rank of non-domination r_i according to the Pareto front
- ✚ Stacking distance d_i

The selection returns the winning solution i based on two fundamental criteria:

- ✚ If it has a better non-domination rank: $r_i < r_j$
- ✚ If both alternatives, i and j , has the same non-domination Rank, then the alternative with a higher diversity level is selected: $d_i > d_j$

Variation. The objective of generating variation is to explore and exploit the selected individuals to generate a new population of solutions. The variation operators are two mechanisms: Crossing and mutation, which are handled in the same way as shown by the genetic algorithm.

New Population. Determination of the final descendants set. This is a process of elite solutions preselection and preservation. It is to bring together all, Parent solution and the descendants obtained by operators selection, crossover and mutation. Thus, the current population is increasing at twice the individual's amount of the initial population. Then, it is necessary to classify the complete set on their respective dominance fronts (To evaluate the dominance of all the solutions and to order them in a decreasing way) and to preserve the N individuals belonging to the better quality fronts. This way, the genetic information of the dominant alternatives is presented in the next generations attracting the remaining of the population to their neighborhoods.

gen=gen+1. After defining the individuals that compose the new population, the generation number (gen) must be updated.

The criterion of completion of the process can be set as the maximum number of generations (*MaxGen*), so this process is repeated while $gen < MaxGen$. Or if all the individuals are part of the first Pareto front.

4.4. NSGA-II programming and optimization features

Related to the sustainability analysis and the different objective functions in the integrated model, particular attention should be paid to the amount of objective functions to compare by optimization. Because, in multiobjective problems graphical representation of the optimization results has a great importance in the analysis and decision making process (Blasco et al. 2017). In fact, depending on the number of objective functions to be optimized and the type of graphic to be performed there will be a number of possible combinations. For explain it, on table 4.4 it is presented the quantity of graphics that will be generated depending on the total amount of objective functions and on the graphic type.

Table 4. 4. *Objective combination for it graphic*

Total objective function amount	Graphic type	
	2D: Two functions	3D: Three functions
3	3	1
4	6	4
5	10	10
6	15	20
10	45	120
15	105	455
20	190	1140

Thus, it might be concluded that if the total amount of objective functions to optimize are more than five, it is recommendable to use 2D graphics to represent the solutions. Therefore, due to the integrated model will include at least five objective functions it is much practical to analyses 2D graphics.

Finally, an evolutionary algorithm NSGA-II already programmed for Matlab® was adapted to optimize the model with integer decision variables, equality and inequality constraints. The algorithm was developed by Selvaraj (2015) and it is useful for models with two objectives functions, variable decisions with domain in \mathbb{R} and inequality constraints. Then, the algorithm found is useful to manage the objective function combination and it is structured in modules as follows:

Main_NSGA2. This module controls the optimization algorithm. Here it should be defined the population size, the number of decisional variables, the number of runs, the parameters for crossover and mutation, the maximum number of generations and the number of objectives. Also, it must be entered upper and lower limits for decision variables.

Initial population is created random between boundary limits for variables. Then, population is evaluated in the fitness functions and inequality constraints for it comparison. Therefore, parents are selected to create a population of children with the same size that initial population. This will be compared with parent population to select the best performed individuals.

Test_case. This module include the objective functions and the inequality constraints for evaluate the individuals.

Normalization. As there may be different amounts of constraints, which can be translated to a different range of constraint violation of every candidate, this module normalize it and create only one value for constraint violation.

NDS_CD_cons. This module perform a fast elitist non-domination sorting and crowding distance assignment (Deb et al. 2002).

Tour_selection. In this section parents are selected from the population pool for reproduction by using binary tournament selection based on the rank and crowding distance. An individual is selected if its rank is lesser than the other or if its crowding distance is greater than the other.

Genetic_operator. In this module, the crossover is performed followed by mutation, which is conducted on "Poly_mutation" (Deb et al. 2002).

Replacement. This section take a population sorted by front, and creates the new generation by adding individuals until the population size exceeds the initial population size. If when adding all the individuals of any front, the population exceeds the initial population size, then the required number of remaining individuals alone is selected from that particular front based on crowding distance.

Furthermore, it is necessary to modify the algorithm to use it on the integrated model. Specifically to manage binary variables, equality and inequality constraints. To make it, the original algorithm was analyzed to identify the sections to modify. As result, the modules to modify are Main_NSGA2, Test_case and Genetic_operator.

Starting, Test_case was integrated in Main_NSGA2. Due all optimizations to compare objective functions have the same decision variables, constraints and boundary limits. Therefore, matrix with constraints and boundary limits are linked only once between Microsoft Excel and Matlab® to create a workspace in Matlab®. This will be use in all comparison among objective functions.

The objective functions will be linked in each optimization between Microsoft Excel and Matlab®. The calculation of the function value for each individual is made in this module.

To include the equality constraints in the optimization, a similar procedure to the current one which deals with inequality constraints in Test_case was integrated in Main_NSGA2. Currently, for inequality constraints, if the individual respect each inequality constraint a value of zero is generated by using a logical test from Matlab®. Similarly it was integrated the equality constraints. Where, if the individual respect each equality constraint a value of zero is generated. After, all absolute errors are added and normalized in Normalization.

Regarding the inclusion of binary variables, “Main_NSGA2” must to be modified at first to generate an initial population with binary variables. Therefore, it was decided that the amount of binary variables should be defined as an algorithm parameter and the binary variables will be the first ones. Highlighting that maintain the variable order is important.

Then, as initial population is created random, the Matlab® function *randi*[0 1] was used to create the initial binary variables. However, in children and mutants creation it can be generated decimal values between 0 and 1. Therefore, the follow rules are followed:

$$\begin{aligned} \text{If binary value} < 0,5 &\Rightarrow \text{binary value} = 0 \\ \text{If binary value} > 0,5 &\Rightarrow \text{binary value} = 0 \\ \text{If binary value} = 0,5 &\Rightarrow \text{binary value} = \text{randi}[0 \ 1] \end{aligned}$$

Finally, due several NSGA II algorithms were found (Nieminen et al. 2003; Srivinasan et al. 2003; Butter et al. 2006; Correa Flórez et al. 2008; Seshadri 2009), also different equations were found to create children and mutants. Therefore, they were tested to select the equations that generate the greater number of first Pareto front for the combination of a linear and nonlinear objective function from the integrated model (Net present value and Total water use). Then the equations to create children are:

$$\begin{aligned} u &= \text{rand}(1, nvar); \\ \alpha &= -0.2 + 1.2 \cdot u; \\ bq &= (u \leq 0.5) \cdot ((2 \cdot u)^{\alpha}) + (u > 0.5) \cdot ((1 / (2 \cdot (1 - u)))^{\alpha}); \\ tc &= \text{rand}(1, nvar); \\ \text{Children1} &= (tc \geq \text{probCross}) \cdot \text{Parent1} + \dots \\ &\quad (tc < \text{probCross}) \cdot (0.5 \cdot ((\text{ones}(1, nvar) + bq) \cdot \text{Parent1} + ((\text{ones}(1, nvar) - \\ &\quad bq) \cdot \text{Parent2}))); \\ \text{Children2} &= (tc \geq \text{probCross}) \cdot \text{Parent2} + \dots \\ &\quad (tc < \text{probCross}) \cdot (0.5 \cdot ((\text{ones}(1, nvar) - bq) \cdot \text{Parent1} + ((\text{ones}(1, nvar) + \\ &\quad bq) \cdot \text{Parent2}))); \end{aligned}$$

And the equations to create mutants are:

$$\begin{aligned} mum &= 1; \\ t &= \text{rand}(1, nvar); \\ t2 &= \text{rand}(1, nvar); \\ \text{delta} &= (t < 0.5) \cdot ((2 \cdot t)^{\alpha}) - 1 + (t \geq 0.5) \cdot (1 - (2 \cdot (1 - t))^{\alpha}); \end{aligned}$$


```

loc_mut=(t2<=pm);
Mutant1 =(1 + loc_mut.*delta).*Parent3;
Mutant2=ui+((vi-ui).*rand(1,nvar));

```

Where ui is the upper bound for decision variables and li is the lower bound. *Parent1*, *Parent2* and *Parent3* are individuals of the current generation. *Children1*, *Children2*, *Mutant1* and *Mutant2* are individuals for future generation. *probCross* is defined as the probability to realize the crossover between parents and *pm* is the probability of made a mutation in the individual.

It was decided to create two mutants, due the huge amount of decision variables in the Colombian case study and to preserve diversity among the individuals by creating *Mutant2* at random with boundary values.

The original programming realized by Selvaraj (2015) includes fourteen different cases to test the algorithm. However, only the test cases 10, 11, 12, 13 and 14 include objective function pairwise comparison with a constrained model. Therefore, to validate changes in children and mutant creation in comparison with the original programming, the different optimizations with constraints where tested under the same parameters par default that in the original programming. The results are presented graphically in table 4.5.

In table 4.5 it can be noted that the adapted algorithm results in test cases 11 and 12 reproduces the results of the original program. However, in test cases 10, 13 and 14, the adapted algorithm results cover a broad spectrum of the objective functions. Therefore, the modification in programming allows an extensive research in the solution space.

Even though the adapted algorithm was only tested on inequality constraint models; as the inequality treatment was replicated for equality constraints, it can be expected that the adapted algorithm allows finding optimal solutions for a constrained multiobjective model including equality and inequality constraints.

Finally, modifications to generate binary variables should be verified in the integer constrained model multiobjective optimization. Observing if optimal solutions are generated and constraints error decrease in each new generation.

Table 4. 5. Verification changes in equations to create children and mutants

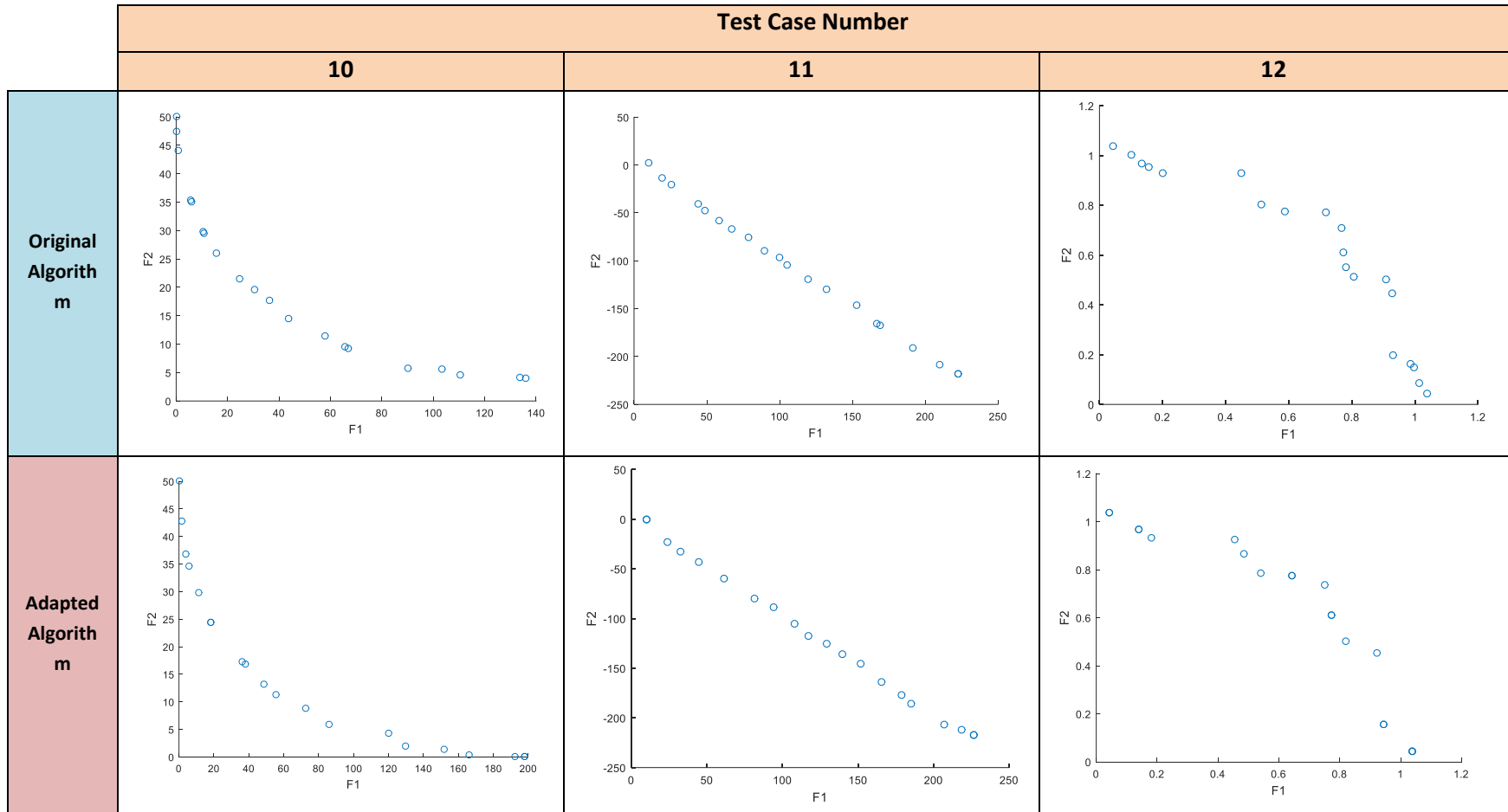
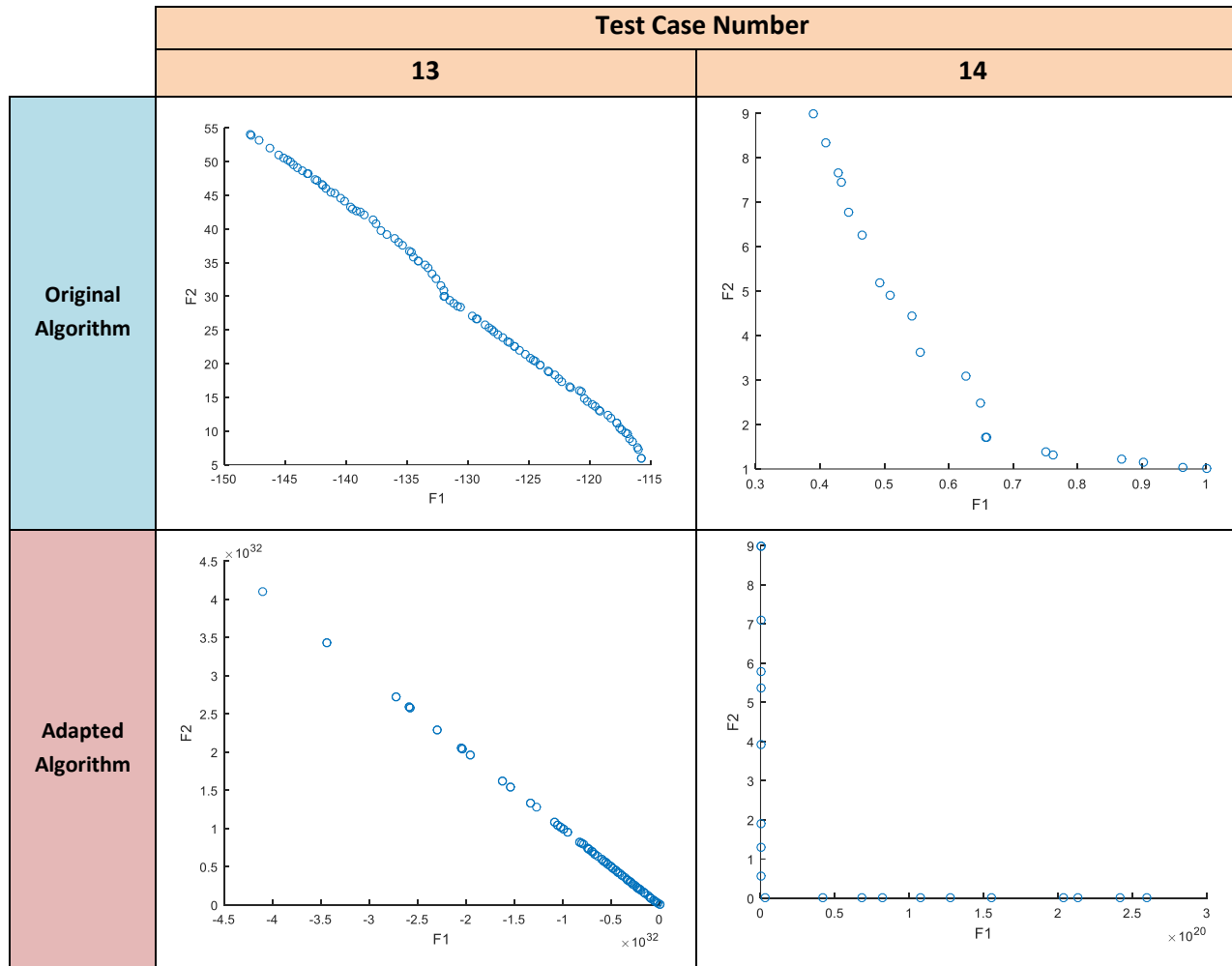


Table 4.5. Verification changes in equations to create children and mutants (Continuation)



4.5. Summary

This chapter presents a methodological approach for the construction of the integrated integer constrained multiobjective model (equality and inequality constraints) required for the sustainable Phase III BioRSC design. Integrating the pretreatment process; the potential diversification at raw material, intermediate products and final products type; the production technology and capacity selection at pretreatment and principal plants; and the sustainability dimensions.

In addition, the selection of an optimization method and an algorithm adaptation to solve the model was realized.

Regarding the methodological approach, to simplify the complexity of the construction model, is necessary carrying out a step-by-step process. Using this methodology is possible to carry out a verification and optimization of the model in the different stages of construction. Also, two axes for model development are proposed to include the characteristics of the Phase III BioRSC, strategic decisions and dimensions of sustainability in stages.

Then, a logical sequence for the model construction that includes the Phase III BioRSC characteristics and strategic decisions was detailed, following the horizontal axis of the designed methodology. Finally, the mathematical formulation of the initial model is presented with the following components:

- ✚ 8 general decision variables,
- ✚ 14 constraints,
- ✚ 20 parameters
- ✚ One objective function

The vertical axis, detailed in the methodology, will be addressed in Chapter V to finish the integrated model. Due the necessary detailed analysis to include each sustainability dimension, principle, criteria and indicator.

Moreover, a bibliographic review was carried out to determine the suitable optimization algorithm for the multiobjective model resolution. The NSGA-II was selected as result of this analysis. Then, its optimization mechanism was detailed. And subsequently the corresponding algorithm programming was described and adapted to optimize an integer constrained multiobjective model.

The adapted algorithm was verified for constrained models; however, the verification for its application on integer constrained multiobjective models remains pending until chapter VII.

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Chapter V. Model construction by sustainability dimensions analysis

5.1. Introduction

As discussed in Chapter IV, the model for the sustainable Phase III BioRSC design is going to be built using a *model construction process*. It means, the first stage is to integrate the strategic decisions for the SC, then the BioRSC characteristics and finally, to integrate the sustainability dimensions. The model implies analyzing the sustainability framework constituted by principles, criteria and indicators (Bautista et al. 2016a), as presented in figure 5.1.

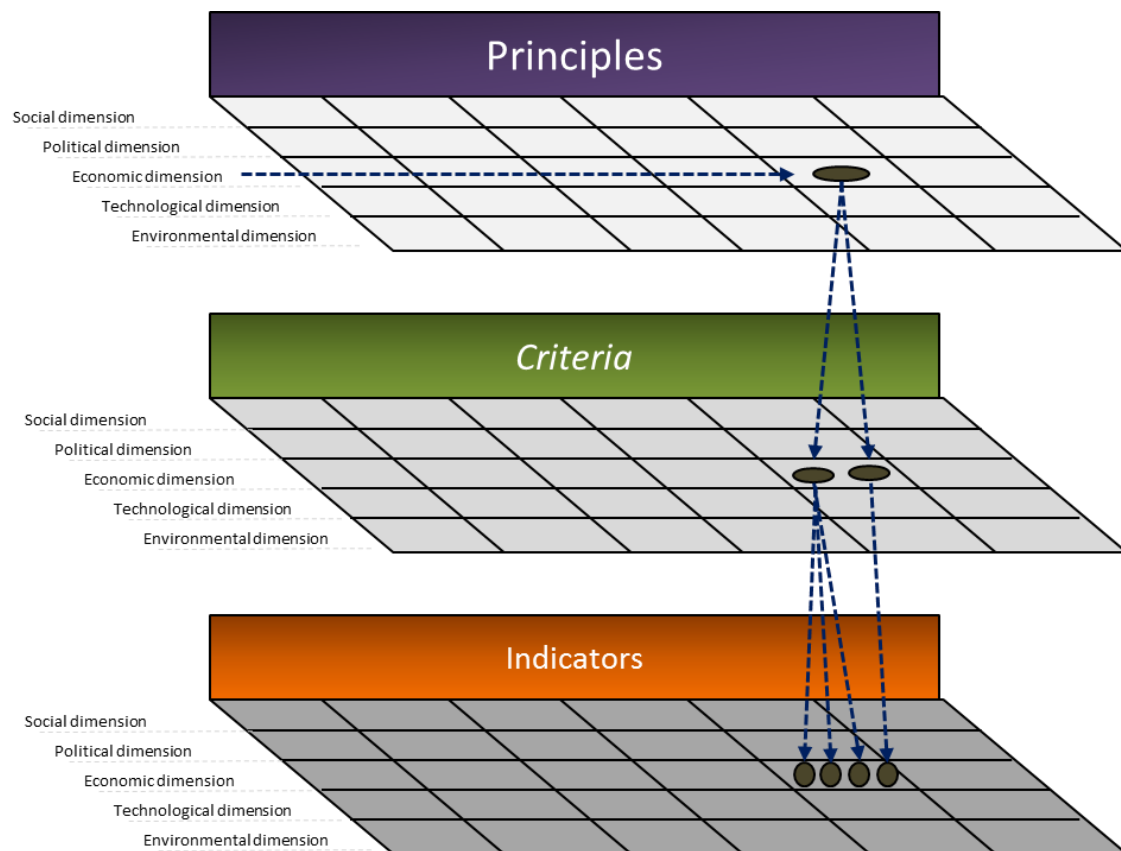


Figure 5. 1. Sustainability framework

However, sustainability dimensions presented on the research developed by Bautista et al. (2016) are dedicated to biodiesel. Therefore, a generalization to biorefineries has to be carried out. Subsequently, the analysis of each sustainability dimension has to be done with the aim of define the associated equality and inequality constraints, objective functions, decision variables and parameters. Then, in this chapter each sustainability dimension is presented in a different section, 77constraint at first the dimension analysis and then the corresponding mathematical expressions to be integrated in the model for the sustainable Phase III BioRSC.

5.2. Economic dimension analysis

For the sustainable Phase III BioRSC analysis, the economic dimension is the first to be studied to complete the mathematical model. It is characterized by one principle: “Biorefinery production must be sustainable at both macroeconomic and microeconomic level” (Bautista et al. 2016b). This principle includes six criteria that are detailed through forty economic indicators, presented in Appendix 5.1.

A comprehensive analysis of economic criteria and indicators is presented in section 5.2.1 to define decision variables, constraints, objectives and/or parameters to be included on the economic dimension in the BioRSC design model. Then, in section 5.2.2, the corresponding model equations are defined.

5.2.1. Economic criteria and indicators analysis

The economic criteria assess the influence level of macroeconomic variables as market variability, on microeconomic variables as raw material, final and intermediate products prices (Bautista et al. 2016b). Therefore, Appendix 5.2 presents a detailed analysis by economic criterion and indicator in order to define which ones should be represented by mathematical expressions to be included in the model for conception of sustainable Phase III BioRSC. Based on that analysis, it can be noted the most of the indicators have been already included in Model 4 presented in Section 4.2.1. However, indicators 83 and 86, presented in table 5.1, can be described as objective functions not mentioned before. Therefore, they should be mathematically expressed. Table 5.1 presents a summary of selected economic criterion and indicators analysis.

Table 5. 1. *Economic analysis by criterion and indicator*

Criterion	Indicator(s)
22	(83)
Production of biobased products (Local capacity production).	
It can be translated as the use of the installed capacity. This can be calculated as a function of the materials entering into the pretreatment plants and principal production plants, divided by the production capacity of the corresponding plant if the plant is installed. The ideal operation of a production plant maximizes the utilization of the installed production capacity, to reduce idle time of machines and workers. Therefore, this indicator can be translated as an objective function for the model in development.	
22	(86)
Production of biobased products (Operational and pollution cost)	
The operating costs associated to each production plant, either main or pre-treatment, have already been considered in Chapter IV. Then, pollution cost associated to the biobased products production must to be determined. In general, there are at least three principal pollution costs that could be associated to the biobased products production in biorefineries (UPME 2017). The existence of such costs will depend on the laws and norms of each country, such as atmospheric resources normativity regulating the concentration of air pollutants that are harmful to health; water resources normativity related to environmental taxes due water use or wastewater stream; and solid waste regulation such as collect solid wastes cost and disposal cost. For the model formulation, these pollution cost must be multiplied by the corresponding rate of pollution production and the amount of transformed products at pretreatment and principal plants. Also, it may be different type of specific pollution, as for example there are different kinds of atmospheric emissions, as CO ₂ , SO ₂ , particulate matter or NO _x , with different impacts.	

5.2.2. Economic dimension related mathematical expressions

As concluded in section 5.2.1; indicators 83 and 86 have to be represented by mathematical equations to complete the whole economic dimension in the developing model. There are described following.

Indicator 83. It is described as the use of the installed capacity. Then, it depends on processed materials at production plants and its production capacities. Therefore, it can be represented as:

$$\frac{\sum_i \sum_n N_{i,n,j,c,f}}{CapPP_{j,c,f} * PP_{j,c,f}} \forall j, c, f \text{ and } \frac{\sum_j \sum_b R_{j,b,k,d,g}}{CapW_{k,d,g} * W_{k,d,g}} \forall k, d, g$$

It is employed to represent the fraction of the installed capacity used in pretreatment plants and principal plants respectively by equations (31) and (32).

$$PretUse = \frac{\sum_j \sum_c \sum_f (\sum_i \sum_n N_{i,n,j,c,f})}{\sum_j \sum_c \sum_f CapPP_{j,c,f} * PP_{j,c,f}} \quad (31)$$

$$PrincUse = \frac{\sum_k \sum_d \sum_g (\sum_j \sum_b R_{j,b,k,d,g})}{\sum_k \sum_d \sum_g CapW_{k,d,g} * W_{k,d,g}} \quad (32)$$

Then, the total capacity use in the biorefinery production system will be:

$$PretUse + PrincUse$$

Considering this value in the range between 0% and 200%, it is needed to normalize in order to know the real percentage of capacity used in the biorefinery production system. Thus, the expression for this objective is formulated as equation (33).

$$Max \left(\frac{PretUse + PrincUse}{2} \right) \quad (33)$$

Indicator 86. Due to different types of pollution costs related to this indicator, there are at least three general equations to represent it. Equations (34), (35) and (36) represent the pollution cost related to pollutant emissions, residual water generation and solid waste production. Also different pollutant components can be detailed for each pollution type.

$TPolCostAtm =$

$$\sum_x \langle PolCostAtm_x * \left[\sum_n \sum_c \sum_f \left\{ \phi_{x,n,c,f} * \left(\sum_j \sum_i N_{i,n,j,c,f} \right) \right\} + \sum_b \sum_d \sum_g \left\{ \phi_{x,b,d,g} * \left(\sum_k \sum_j R_{j,b,k,d,g} \right) \right\} \right] \rangle \quad (34)$$

$$TPolCostWat = \sum_y \left\langle PolCostWat_y * \left[\sum_n \sum_c \sum_f \left\{ \psi_{y,n,c,f} * \left(\sum_j \sum_i N_{i,n,j,c,f} \right) \right\} + \sum_b \sum_d \sum_g \left\{ \psi_{y,b,d,g} * \left(\sum_k \sum_j R_{j,b,k,d,g} \right) \right\} \right] \right\rangle \quad (35)$$

$$TPolCostSolid = \sum_z \left\langle PolCostSolid_z * \left[\sum_n \sum_c \sum_f \left\{ \omega_{z,n,c,f} * \left(\sum_j \sum_i N_{i,n,j,c,f} \right) \right\} + \sum_b \sum_d \sum_g \left\{ \omega_{z,b,d,g} * \left(\sum_k \sum_j R_{j,b,k,d,g} \right) \right\} \right] \right\rangle \quad (36)$$

In Equations 34, 35 and 36 the parameters are:

- $TPolCostAtm$ is the total cost related atmospheric pollution
- $TPolCostWat$ is the total cost related water pollution
- $TPolCostSolid$ is the total cost related solid waste pollution
- $\phi_{x,n,c,f}$ and $\phi_{x,b,d,g}$ are rates of atmospheric pollution type x produced when transforming the raw material type n with technology c and production capacity f at pretreatment plants (t pollution/t raw material) and when transforming intermediate products type b with technology d and production capacity g at principal plants (Ton pollution/Ton intermediate products).
- $PolCostAtm_x$ is the cost related to atmospheric pollution type x production (USD/t pollution)
- $\psi_{y,n,c,f}$ and $\psi_{y,b,d,g}$ are rates of residual water type y production when transforming the raw material type n with technology c and production capacity f at pretreatment plants (t pollution/t raw material) and when transforming intermediate products type b with technology d and production capacity g at principal plants (Ton pollution/Ton intermediate products).
- $PolCostWat_y$ is the cost related to residual water type y production (USD/t pollution)
- $\omega_{z,n,c,f}$ and $\omega_{z,b,d,g}$ are rates of solid waste type z generated when transforming the raw material type n with technology c and production capacity f at pretreatment plants (Ton pollution/Ton raw material) and when transforming intermediate products type b with technology d and production capacity g at principal plants (Ton pollution/Ton intermediate products).
- $PolCostSolid_z$ is the cost related to solid waste type z production (USD/t pollution)

Therefore, the total pollution cost could be used as an objective function itself, minimizing the expenses related to pollution. Another possibility is to integrate it to the calculation of NPV, at the total cost of the entire project (equation 26). Simultaneously, from an environmental point of view, the objective functions can search for minimizing the generation of each type of pollution.

$$Costs = TransportCost + RawMaterialsCost + ProductionCost + TPolCostAtm + TPolCostWat + TPolCostSolid \quad (26)$$

5.3. Political dimension analysis

The inclusion of the political dimension in sustainability assessment enables to perform an analysis of the impact on the social, economic and environmental dimensions of local or international regulatory frameworks implementation, mandatory or voluntary certification systems(Bautista et al. 2016b).

The principles in political dimension are referred to the influence of national and international policies about promotion, market, and sustainable production. There are three principles: “National promotion policies for the production and consumption of first generation biobased products must be in accordance with international policies”, “National policies to the promotion of biobased products production should be consistent with international environmental policies on acceptable forms of allowed thresholds of greenhouse gas emissions in the life cycle of biobased products” and “The actors involved in biorefinery production system should promote commitment to ethics, transparency and compliance with local laws”.

These three principles, which are integrated by four criteria, are composed by the six indicators presented in Appendix 5.3. Its detailed analysis to define decision variables, constraints, objectives and/or parameters required to be including in the political dimension to complete the Phase III BioRSC design model is presented in section 5.3.1. Then, in section 5.3.2, the corresponding model equations are defined.

5.3.1. Political criteria and indicators analysis

The political criteria seek assess the agreement between national and international subsidies schemes, advanced biobased products production and consumption, national capability in biorefinery research and development. Also, it includes the raw material production consistency with international environmental policies, and local perception on ethical and transparency commitment of the actors in the BioRSC (Bautista et al. 2016b). The detailed analysis related to these political criteria and indicators to define model components is presented in the Appendix 5.4. Based on this analysis, indicators 43, 45, 46 and 50 should be represented by mathematical expressions to integrate the political dimension in the model. Table 5.2 presents the summary of selected political criterion and indicators analysis.

Table 5. 2 *Political analysis by criterion and indicator*

<i>Criterion</i>	<i>Indicator(s)</i>
11	(43)
Agreement between local and internationally biobased production (Incentives or tax reduction)	
<p>This indicator measures the variation of government incentives and tax reduction; therefore, it is applicable only if there are incentives or tax reduction related to biobased products. Then, it implies a previous review of each case study on the incentives provided by the government.</p> <p>As the present developed model is static, this indicator could be represented as the amount of government expenditures to encourage the biobased products production. These expenditures are expected to decrease over time when industries are self-sustaining. So it can be deduced that the government's objective, other than incentivize the biobased products industry, is to reduce its government spending associated with it, in order to be able to devote these resources to other projects.</p> <p>Some researches applied this indicator as incentives for installation of production plants, which are given only once when the plant is already installed, either central or pre-treatment (You and Wang 2011; You et al. 2012; Yue et al. 2014). About tax reduction, searches have found no explicit references.</p>	
12	(45)
Agreement between local and internationally first generation biobased production (Production rates)	
<p>It is expected that the objective will be to reach international values on advanced biobased products production. Then, it could be interpreted as maximizing the amount of advanced biobased products produced by the biorefinery.</p>	
13	(46)
Agreement between local and internationally biobased production legal consumption requirements	
<p>At first, it is needed to analyze if there is a percentage of "Biobased product/Total consumed product" required by government. If so, it will be a parameter to determine the biobased product demand. In the other hand, in general it could be concluded that the objective of this indicator is to reach the international values for the percentages of "Biobased product consumption/Total consumed product". However, as there are no consumption regulations for all final biobased products, this objective can be reformulated as the maximization of the demand satisfaction with biobased products.</p>	
16	(50)
Local land used for raw materials cultivation (Land certification)	
<p>To evaluate this indicator is required to study if potential suppliers have a voluntary certification for its land resources. Then, the objective will be to maximize the rate between the biobased products produced by raw materials from certified lands and the total biobased products produced. However, it could be also described in a simplest and linear form as the maximization of the use of raw materials belonging to certified land for biobased products.</p>	

5.3.2. Political dimension related mathematical expressions

As analyzed in section 5.3.1, there are five political indicators that have to be represented by general mathematical equations. They are presented following.

Indicator 43. This indicator can be described in two parts: the government incentives for installation of production plants and tax reduction.

- *Government incentives for production plants installation*

In most cases, the total incentives received for a project ($IncP_j$ and $IncW_k$) cannot exceed the allowable incentive cap ($incCap_j$ and $incCap_k$) and cannot be higher than certain percentage of the total construction cost ($incPerP_j$ and $incPerW_k$); if the plants are not installed, no incentives would be received. This description is translated mathematically in equations (37) and (38).

$$IncP_j \leq Min \left\{ incCap_j \left[\sum_c \sum_f PP_{j,c,f} \right]; incPerP_j \left[\sum_c \sum_f Inv_{j,c,f} \right] \right\} \quad (37)$$

$$IncW_k \leq Min \left\{ incCap_k \left[\sum_d \sum_g W_{k,d,g} \right]; incPerW_k \left[\sum_d \sum_g Inv_{k,d,g} \right] \right\} \quad (38)$$

Where $Inv_{k,d,g}$ and $Inv_{j,c,f}$ are the investment cost for implementing the production technology d in location k with the capacity g for principal plants, and for implementing the production technology c in location j with the capacity f for pretreatment plants.

There is also a restriction related to the maximum budget available for these projects, which can be represented mathematically by equation (39).

$$\sum_j IncP_j + \sum_k IncW_k \leq LimBudget \quad (39)$$

Then, the co-financing (subsidies for construction) amount $\sum_j IncP_j + \sum_k IncW_k$ should be added to NPV because enterprises can consider these incentives as revenues, modifying equation (23) as follows:

$$Max NPV = \sum_{i=1}^T \frac{Net\ Cash\ Flow_i}{(1 + Discount\ Rate)^i} - Initial\ Investment + \left(\sum_j IncP_j + \sum_k IncW_k \right) \quad (23)$$

Also it can be seeing as a governmental objective, due to the government would minimize its expenditures; then the first political objective function will be represented by equation (40).

$$Min \left[\sum_j \{IncP_j\} + \sum_k \{IncW_k\} \right] \quad (40)$$

- *Government revenues not received by tax reduction on biobased products*

A prior tax-related search is required in the country where the study is conducted to determine the type of tax reduction associated with biorefineries.

In general, tax incentives are made by tax reduction or exemption on determined value added biobased products (Colombian Government 2004). Therefore, considering the Government incentives for production plants detailed on the above analysis, and the tax exemption, the objective function to minimize the tax exemption and incentives provided by the government can be described as presented in equation 40.

$$\text{Min} \left\{ \text{Inc}P_j + \text{Inc}W_k + \text{TaxRed}_a * \left(\sum_k \sum_l P_{k,a,l} \right) \right\} \quad (40)$$

Where TaxRed_a is the tax exemption in USD per tonne of bioproduct type a sold. Then, for the new decision variable $\text{Inc}P_j$ and $\text{Inc}W_k$ the lower and upper limits can be described as equations (41) and (42).

$$0 \leq \text{Inc}P_j \leq \text{Min} \left\{ \text{LimBudget} ; \text{incCap}_j \left[\sum_c \sum_f PP_{j,c,f} \right] ; \text{incPer}P_j \left[\sum_c \sum_f \text{Inv}_{j,c,f} \right] \right\} \quad (41)$$

$$0 \leq \text{Inc}W_k \leq \text{Min} \left\{ \text{LimBudget} ; \text{incCap}_k \left[\sum_d \sum_g W_{k,d,g} \right] ; \text{incPer}W_k \left[\sum_d \sum_g \text{Inv}_{k,d,g} \right] \right\} \quad (42)$$

Indicator 45. As presented in section 5.3.1, it can be understood as maximize the biobased products produced from non-edible crops ($n_{NFC} \in \text{non food uses raw material}$) which can be represented in mathematical form as equation (43).

$$\text{Max} \left\langle \sum_{n_{NFC}} \left(\sum_i \sum_j \sum_c \sum_f N_{i,n,j,c,f} \right) \right\rangle \quad (43)$$

Indicator 46. The maximization of the demand satisfaction using biobased products can be mathematically described by equation (44).

$$\text{Max} \left\{ \frac{\sum_k \sum_a \sum_l P_{k,a,l}}{\sum_l \sum_a \text{Dem}T_{l,a}} \right\} \quad (44)$$

Where $\text{Dem}T_{l,a}$ is the total demand for products that are replaced by biobased products type a at location l

Indicator 48. Considering call for projects to develop production technologies, governmental expenditures related to research and development for biorefineries can be modeled as equation (45).

$$\left(\sum_c InvTechP_c + \sum_d InvTechW_d \right) \leq BudgetaryLimProjectValueTech \quad (45)$$

Where

- $InvTech_c$ = Amount invested by the government in technology c
- $InvTech_d$ = Amount invested by the government in technology d
- $BudgetaryLimProjectValueTech$ is the parameter maxime budget intended for technology development

And the limits for $InvTechP_c$ and $InvTech_d$ are represented by equations (46) and (47).

$$0 \leq InvTechP_c \leq \text{Min}\{LimProjectValueTech_c, PerProjTech_c * [ProjectValueTech_c]\} \quad (46)$$

$$0 \leq InvTechP_d \leq \text{Min}\{LimProjectValueTech_d, PerProjTech_d * [ProjectValueTech_d]\} \quad (47)$$

Where $LimProjectValueTech_c$ and $LimProjectValueTech_d$ is the limit amount invested by the government in technology c and d by project. $PerProjTech_c$ and $PerProjTech_d$ are the percentage of total projects value ($ProjectValueTech_c$ or $ProjectValueTech_d$) that will cover the government.

These investments must be added to the other government expenditures updating equation (40).

$$\text{Min} \left\{ IncP_j + IncW_k + \sum_a \left[TaxRed_a * \left(\sum_k \sum_l P_{k,a,l} \right) \right] + \sum_c InvTech_c + \sum_d InvTechW_d \right\} \quad (40)$$

This financial support can be understood as financing to bring technology and products to the final market (COLCIENCIAS 2016), as long as they have been commercially validated. Then, it is needed to understand the technology development levels.

There are different production technologies to obtain the same final products. They can differ in process type and raw materials used, between others. This implies different production cost and transformation yields. The technology development requires several stages to transform scientific research into applied research and development and technologies operating successfully with acceptable performance and reliability in an industrial context (Commercial application) (NASA 2015). These stages are described in the Technology Readiness Level (TRL) (NASA 2015) detailed on table 5.3. It can be deduced that the passage from one stage to another upper level requires an investment in time, money and manpower. Therefore, it can be expected that investors have preferences for those technologies with a higher level on TRL to minimize risk.

Table 5. 3 *Technology Readiness Level (TRL) description. Based on (Energy 2009; Institute of Medicine and National Research Council 2013; ESA 2015; European Commission 2015; NASA 2015; DTU 2017)*

TRL	Description	Supporting information
1	Scientific research begins to be translated into applied research and development. There exist unproven idea/proposal concepts. No analysis or test has been performed	Paper studies of a technology's basic properties. References to who, where and when.
2	Invention begins. Practical applications can be "invented", identified or formulated. But the applications are still speculative: There is not experimental proof or detailed analysis to support the assumptions/conjecture	Examples are limited to analytic studies, analysis to support the concept
3	Active research and development is initiated. This includes both analytical studies to set the technology into an appropriate context and laboratory-based studies to validate the analytical predictions of separate elements of the technology. These studies and experiments should constitute "proof-of-concept"	Results of laboratory test and comparison to analytical prediction for critical sub-systems. Reference to who, where and when these tests and comparisons were performed.
4	Basic technological components are integrated to establish that they will work together. It could be composed of ad hoc discrete components to validate the concept designs or novel features of design through a model or small scale testing in a laboratory. This is relatively "low fidelity" validation.	Results from testing laboratory-scale breadboards. Providing an estimate of how breadboard hardware and test results differ from the expected goals. References to who did this work and when.
5	The basic technological elements must to be integrated with reasonably realistic supporting elements and have a validation in a relevant environment. This will be test over a limited range of operating conditions to demonstrate its functionality (These test can be done on a scale version if scalable). "High fidelity" laboratory integration of components	Testing laboratory breadboard system. How does the "relevant environment" differ from the expected operational environment? How do the test results compare with expectations? Was the breadboard system refined to more nearly match the expected system goals?
6	A representative Full-scale Model or prototype is built. This technology is tested in a high-fidelity laboratory environment (relevant environment) or in a simulated operational environment.	Results from laboratory testing of a prototype system, near to the desired configuration in terms of performance, weight and volume. How did the test environment differ from the operational environment? How did the test compare with expectations? What are/were the plans, options, or actions to resolve problems before moving to the next level?
7	Technology integration is tested using a Full-scale prototype built and tested on the real operational environment	Results from testing a prototype system in an operational environment. How did the test compare with expectations? What are/were the plans, options, or actions to resolve problems before moving to the next level?
8	Full-scale prototype built and integrated into intended operating system with full interface and functionality test program in intended environment. The technology has shown acceptable performance and reliability over a period of time. In almost all cases, this TRL represents the end of true system development.	Results of testing the system in final configuration under the expected range of environmental conditions in which it will be expected to operate. Assessment of whether it will meet its operational requirements.
9	The technology has successfully operated with acceptable performance and reliability within the predefined criteria. Actual application of technology is in its final form.	OT&E (operational test and evaluation) reports

Regarding technology investment, no information or research has been found to know or calculate in a general way the amount necessary to move from one level of TRL to another. Therefore, for each potential technology a specific study should be carried out to define the required investments to reach a high TRL level. Then, $InvTRLPre_{s_c, s_c+1, c}$ can be defined as the investment required for achieve one TRL level up starting from the TRL level s_c for the pretreatment technology c . And $InvTRLW_{s_d, s_d+1, d}$ can be defined as the investment required for achieve one TRL level up starting from the TRL level s_d for the principal production plants technology d . Then these investments should be related with the governmental investments ($InvTech_c$ and $InvTech_d$). However, before describing this relationship, it should be highlighted that there are two possible scenarios for $InvTRLPre_{s_c, s_c+1, c}$ and $InvTRLW_{s_d, s_d+1, d}$ values depending on whether or not the investment amount is related to the TRL level s . If they are related, it is possible that the investment amount required change depending in starting TRL level s to achieve $s + 1$. If they are not related, the investment amount will be the same to reach up a TRL level no matter the TRL level s . Therefore, further analysis for each potential technology to apply in the case study should be carried out to relate TRL and government investment variables.

Indicator 50. The mathematical expression related to maximize the use of raw materials belonging to certified land for biobased products, can be modeled as equation (48).

$$Max \left\{ \sum_i \sum_n \left[Certificate_{i,n} * \sum_j \sum_c \sum_f (N_{i,n,j,c,f}) \right] \right\} \quad (48)$$

Where the parameter is

$Certificate_{i,n}$

$$= \begin{cases} 1 & \text{If the supplier in the location } i \text{ is certified in the production of the raw material type } n \\ 0 & \text{otherwise} \end{cases}$$

5.4. Technological dimension analysis

The inclusion of the technological dimension permits the analysis of the influence of new technological developments on the sustainability of the BioRSC (Bautista et al. 2016b). This dimension is represented by the principle "Technology used in the BioRSC should promote the reduction of negative impacts on the environment, efficiency and cost reduction in process over time", integrated by four criteria and four indicators, detailed in Appendix 5.5.

5.4.1 Technological criteria and indicators analysis

Criteria related to technological sustainability dimension takes into account the influence of emerging technologies for first and advanced biobased products production on the demand of natural resources, pollution generation, and cost reduction. Also, the criteria consider the technological learning linked to technological improvements and cost reduction (Bautista et al. 2016b). Technological criteria and its corresponding indicators are analyzed in detail in Appendix 5.6 to define which ones should be represented in the developing model. Based on this analysis, indicators 102, 103 and 104 are

represented by equations. Also, indicator 106 should be analyzed for each case study to relate TRL levels with cost reduction and, in future work, with uncertainty and risk. The analysis is summarized in Table 5.4

Table 5. 4. *Technological analysis by criterion and indicator*

<i>Criterion</i>	<i>Indicator(s)</i>
26	(102 and 103)
Soils and water requirements depending on technology	
<p>It can be deduced that for indicator 102 is needed to quantify the required hectares to produce the raw materials. Also, for indicator 103 it must to be calculated the amount of water needed to produce the raw materials and for process it with different technologies at biorefineries. Thus, there are two objective functions to define in this section: the minimization of total required hectares for raw material production and the minimization of the total needed water at BioRSC.</p> <p>It can be noted that the installation of biorefineries could affect land use and water resources. Then, as perspective of this developing model, it could be analyzed the model response to the elimination of raw material availability restriction. It allows observing the potential impact of, par exemple; maximize the demand satisfaction with biobased products.</p>	
27	(104)
Influence of technology learning on efficiency of process and cost reduction	
<p>This indicator seeks to measure variations in cost due to efficiency of processes generated for apply different production technologies and apprenticeship. The cost can be reduced in time by technology apprenticeship, which can be described by learning curves (Herrero et al. 1999). These last are related to the experience accumulated by the company in terms of producing each time in a more efficient way (Herrero et al. 1999). Then, know-how of the production process is translated into a decrease in unit cost as the accumulated production increases (Steinberg 2004). Therefore, the relation between the accumulated production and the cost reduction should be mathematically defined.</p>	
29	(106)
Influence of technology developments on cost reduction	
<p>As seen in indicator 48, analysis of the political dimension in section 5.3.2, the TRL levels describe the technology readiness or maturity. Therefore, it can be deduced that a reduction on operation cost could be generated when a high TRL level is achieved. However, in the same way as investment required achieving higher TRL levels depends specifically on each particular case study, the cost reduction related to different TRL levels should be analyzed for each potential technology in the case study.</p> <p>Also, it must be noted that lower TRL levels are related to uncertainties and risk, due necessary investments in technologies that are not yet industrialized are not fixed or fully known. This generates an incentive to install technologies that have an industrialized level to avoid expenses in technological development. Then, as perspective of this work, due to the fact that the developing model is deterministic, uncertainty should also be analyzed for each potential technology in the case study.</p>	

5.4.2 Technological dimension related mathematical expressions

As analyzed in section 5.4.1, there are three technological indicators that should be represented by the following equations.

Indicator 102. To minimize the total hectares required for raw material production there are two different ways: to change cultivation strategies (or technologies) or to reduce the required raw materials. Then, the required raw materials minimization can be represented mathematically by equation (49).

$$Min \left\{ \sum_n \sum_i \sum_j \sum_c \sum_f N_{i,n,j,c,f} \right\} \quad (49)$$

Indicator 103. To calculate the amount of water consumed to produce raw materials and process them at the biorefinery, it is required to compute the amount of water needed to produce raw materials ($WRawMat_n$), then the water needed to transform raw material n with technology c and production capacity f at pretreatment plants ($WPret_{n,c,f}$). And, the amount of water needed to transform the intermediate product b with technology d and production capacity g at the principal production plants ($WPlant_{b,d,g}$). Therefore, the total amount of required water can be mathematically described by equation (50).

$$Min \left\{ \begin{aligned} & \sum_n WRawMat_n * \sum_i \sum_j \sum_c \sum_f N_{i,n,j,c,f} + \\ & \sum_n \sum_c \sum_f \left(WPret_{n,c,f} * \left[\sum_i \sum_j N_{i,n,j,c,f} \right] \right) + \\ & \sum_b \sum_d \sum_g \left(WPlant_{b,d,g} * \left[\sum_j \sum_k R_{j,b,k,d,g} \right] \right) \end{aligned} \right\} \quad (50)$$

However, the present model does not modelize suppliers, its cultivation technologies or strategies. Then, as different technologies are presented at the transformation plants, it is important to differentiate the impacts of water requirements of these transformation technologies, defining the objective function (51).

$$Min \left\{ \sum_n \sum_c \sum_f \left(WPret_{n,c,f} * \left[\sum_i \sum_j N_{i,n,j,c,f} \right] \right) + \sum_b \sum_d \sum_g \left(WPlant_{b,d,g} * \left[\sum_j \sum_k R_{j,b,k,d,g} \right] \right) \right\} \quad (51)$$

Indicator 104. The mathematical expression to represent learning curves is equation (52) (Alberth 2007). Where C_n represent the cost of the unit n , calculated based on first unit cost (C_0), the number of units (n) and a factor related to learning (b).

$$C_n = C_0 * n^b \quad (52)$$

Related to learning factor, there is the *Progress Ratio (PR)*, represented by equation (53).

$$PR = 2^b \quad (53)$$

Then, to analyze how this cost reduction can be included in the model, parameters as PR must be found for each different production technology. Therefore, if it is desired to apply this indicator based on the formula of the learning curves, the operational cost for each plant can be described as equations (54) for pretreatment plants and equation (55) for principal production plants.

$$CostOpP_{n,j,c,f} = \sum_{x=1}^{\sum_i N_{i,n,j,c,f}} C_{x,n,j,c,f} = \sum_{x=1}^{\sum_i N_{i,n,j,c,f}} C_{0,n,j,c,f} * x^\beta = C_{0,n,j,c,f} * \sum_{x=1}^{\sum_i N_{i,n,j,c,f}} x^\beta \quad (54)$$

And

$$\begin{aligned} CostOpW_{b,k,d,g} &= \sum_{x=1}^{\sum_j R_{b,j,k,d,g}} C_{x,b,k,d,g} = \sum_{x=1}^{\sum_j R_{b,j,k,d,g}} C_{0,b,k,d,g} * x^\beta \\ &= C_{0,b,k,d,g} * \sum_{x=1}^{\sum_j R_{b,j,k,d,g}} x^\beta \end{aligned} \quad (55)$$

Where:

- $CostOpP_{n,j,c,f}$ is the operational cost at pretreatment plant j with process technology c and production capacity f to transform the raw material type n
- $C_{x,n,j,c,f}$ is the cost of produce the unit number x based on raw material type n at pretreatment plant j with process technology c and production capacity f
- $C_{0,n,j,c,f}$ is the initial production cost of transform raw material type n at pretreatment plant j with process technology c and production capacity f ($= ProdCost_{n,j,c,f}$ in equation (29))
- $CostOpW_{b,k,d,g}$ is the operational cost at principal production plant k with process technology d and production capacity g to transform the intermediate product type b
- $C_{x,b,k,d,g}$ is the cost of produce the unit number x based on intermediate product type b at principal production plant k with process technology d and production capacity g
- $C_{0,b,k,d,g}$ is the initial production cost of transform intermediate product type b at principal production plant k with process technology d and production capacity g ($= ProdCost_{b,k,d,g}$ in equation (29))
- x is the indicator to account the production amount.
- β is the factor related to learning.

Then, these operational costs can be included in the economical evaluation replacing equation (29), related to production cost, by equation (56). The inclusion of this indicator is possible if there is available information on the progress ratio for each of the technologies applied in the model.

$$ProductionCost = \sum_n \sum_j \sum_c \sum_f CostOpP_{n,j,c,f} + \sum_b \sum_k \sum_d \sum_g CostOpW_{b,k,d,g} \quad (56)$$

5.5. Social dimension analysis

The topics considered in the social dimension include as principles the respect of the property land rights, the social acceptability, the promotion to responsible work conditions and prevention of food supply alteration. The principles are: "Biomass growers and biorefinery companies must respect property rights, land tenure and customary and traditional rights", "BioRSC must be socially acceptable", "BioRSC must promote responsible work conditions through all their activities" and

“Biomass cultivation and biorefinery companies must prevent alteration in food supply or other local uses of biomass (e.g. energy production, as medicine and as building material)” (Bautista et al. 2016b). This dimension is integrated by four principles divided in ten criteria, resulting on forty two indicators, presented in detail in Appendix 5.7.

5.5.1. Social criteria and indicators analysis

The social criteria are defined to assess the conflict level that can generate the raw materials cultivation and the biorefinery production on local communities. Additionally, the criteria permits to analyze the conflicts change with respect to land access and tenure, the community and workers life conditions, and their influence on social acceptability of the biorefinery production (Bautista et al. 2016b).

The criteria and indicators analysis to determine the inclusion of objective functions, restriction or decision variables for the model development are described in Appendix 5.8. Indicators 1, 2 and 3 are defining the model parameters for geographical potential locations, as well as indicator 25. Furthermore, indicators 7 and 22 are related to land concentration that can be represented by GINI land index (Zheng et al. 2013). Therefore, they can be mathematically represented. Also, indicator 11 can be mathematically represented to describe variations in electricity demand as biorefinery final product. Finally, indicators 18, 35 and 36 are related to employment opportunities generation, and should be integrated in the developing model. These metrics are summarized in Table 5.5.

However, as indicators 1, 2, 3 and 25 are defining model parameters and cannot be described as mathematical expressions they are not presented in section 5.5.2.

Table 5. 5. Social analysis by criterion and indicator

Criterion	Indicator(s)
1	(1, 2 and 3)
Respect the rights of land access and land tenure (Indigenous territories)	
This criterion should be used to determine potential locations (geographical parameter) for potential suppliers of raw materials, the potential location of pretreatment plants and main plants, avoiding protected land.	
2	(7)
Conflict over use, access and land tenure (Equitable land ownership)	
This indicator can be understood as a selection criterion for the potential pretreatment and principal production plants and for raw materials production. To characterize equitable land ownership, there is a GINI index that measures the land ownership concentration (Zheng et al. 2013). Therefore, this indicator can be represented mathematically in the model for localization selection.	
3	(11)
National energy security (Government investments)	
If government increases investment in electricity infrastructure to permit a greater and better access to energy, it could mean an increase in electricity demand. Then this indicator must to be considered and mathematically represented if electricity is evaluated as a biobased product produced at biorefineries.	

Table 5.5. *Social analysis by criterion and indicator (Continuation)*

Criterion	Indicator(s)
6	(18)
Local prosperity, reduction of poverty and promotion of human rights (Opportunities for employment)	
The objective of this indicator is to increase the number of employment related to SC biorefinery. Then, it should be mathematically described.	
6	(22)
Local prosperity, reduction of poverty and promotion of human rights (Participation of small farmers)	
This indicator is linked to equitable land ownership. Then, it can be consider that it is evaluated in Indicator 7 with the GINI land index.	
6	(25)
Local prosperity, reduction of poverty and promotion of human rights (National land usurped)	
This indicator is related with Criterion 1; and it can be considered as avoid land conflicts in the present model development. Therefore, it is analyzed together with Criterion1.	
8	(35 and 36)
Respect the labor laws (Numbers of workers with direct and indirect labor contracts)	
These indicators measure the number of workers by recruitment forms. Differentiating between direct and indirect labor contracts, by intermediary companies or associations. Therefore, the objective of maximize the total amount of employment opportunities generated by the SC biorefinery (Indicator 18) can be mathematically represented and differentiate by labor contract type. It is required to characterize the different labor contracts to define which type should be maximized.	

5.5.2. *Social dimension related mathematical expressions*

As concluded in section 5.5.1, six indicators should be described mathematically to be included in the sustainable Phase III BioRSC design model. They are presented below.

Indicators 7 and 22. To characterize land ownership the GINI index ranges from 0 (when everybody has identical amount of land) to 1 (when all lands belongs to only one person) (OECD 2011). Then, the objective function can be described as the average GINI index minimization. This calculation requires the GINI index for raw materials, pretreatments and principal plants locations. Then, only the GINI value for a selected location must be included; which is presented in equation (57). Where $GINI_x$ is the GINI index for land ownership in location x .

$$Min \{GINI\} = \frac{\left[\sum_i GINI_i * \left(\frac{\sum_n \sum_j \sum_c \sum_f N_{i,n,j,c,f}}{\sum_n \sum_j \sum_c \sum_f N_{i,n,j,c,f} + \varepsilon} \right) + \sum_j GINI_j * \sum_c \sum_f (PP_{j,c,f}) + \sum_k GINI_k * \sum_d \sum_g (W_{k,d,g}) \right]}{Amount\ of\ selected\ locations} \quad (57)$$

However, to calculate the *Amount of selected locations* to obtain the average GINI, it is required an auxiliary variable that identifies if a supplier location i is selected or not. Therefore, the auxiliary variable $SupLoc_i$ is defined as:

$$SupLoc_i = \begin{cases} 1 & \text{If } \sum_n \sum_j \sum_c \sum_f N_{i,n,j,c,f} > 0 \\ 0 & \text{Otherwise} \end{cases}$$

And the *Amount of selected locations* can be calculated as:

$$\text{Amount of selected locations} = \sum_i \text{SupLoc}_i + \sum_j \sum_c \sum_f (PP_{j,c,f}) + \sum_k \sum_d \sum_g (W_{k,d,g})$$

Indicator 11. The mathematical equation (58) relates the product demand (Biobased electricity demand: $Dem_{aE,l}$) with governmental investment in electricity infrastructure ($GovInvE$) via a rate that represent the increase in electricity demand by USD of governmental investment in electricity infrastructure (ξ). Generating a new equality restriction for the model to calculate the total product demand (Total biobased electricity demand: $Dem'_{aE,l}$)

$$Dem'_{aE,l} = Dem_{aE,l} + (\xi * GovInvE) \quad (58)$$

Indicators 18, 35 and 36. Employment opportunities are generated at different sections in the BioRSC. As at raw materials production, raw material transformation at pretreatment plants and intermediate products transformation at principal plants, the required employee amount related to transport and sale points. Also, it should be distinguished the labor contract type.

It is important to note that the present model does not modelize the supplier's strategies or cultivation technologies; therefore, the amount of work places generated at raw material production section can be only differentiated by raw material type. Then, the labor opportunities related to supplier's strategies or cultivation technologies should be included as a perspective of this research. In parallel, employee amount related to transport and sale points are related to tactical and operational decisions; therefore, it should be integrated in future model developments.

Finally, for the sustainable Phase III BioRSC design model, two general parameters are required. $DWork_x$ and $IWork_x$, $DWork_x$ represents the amount of workers with direct contract labor required at the SC section x (Raw material cultivation RM , raw material process $Pret$, or intermediate product process $Princ$). $IWork_x$ represents the amount of workers with indirect contract labor required at the SC section x . Then, the total workers amount, to maximize, can be described by equation (59).

$$\text{Max} \left\{ \begin{array}{l} \sum_i \sum_n [DWork_{RM,i,n} + IWork_{RM,i,n}] * \left[\sum_j \sum_c \sum_f (N_{i,n,j,c,f}) \right] + \\ \sum_c \sum_f [DWork_{Pret,j,c} + IWork_{Pret,c,f}] * \left[\sum_j PP_{j,c,f} \right] + \\ \sum_d \sum_g [DWork_{Princ,d,g} + IWork_{Princ,d,g}] * \left[\sum_k W_{k,d,g} \right] \end{array} \right\} \quad (59)$$

Where $DWork_{RM,i,n}$ and $IWork_{RM,i,n}$ are the direct and indirect workers required to obtain 1 Ton of raw material type n at source location i , respectively. $DWork_{Pret,j,c}$ and $IWork_{Pret,c,f}$ are the direct and indirect workers required to operate the pretreatment plants installed with technology c and capacity f . Finally, $DWork_{Princ,d,g}$ and $IWork_{Princ,d,g}$ are the direct and indirect workers required to operated the principal plants installed with technology d and capacity g .

5.6. Environmental dimension analysis

The environmental principles consider issues as air, soil and water quality, waste and wastewater management, balance of greenhouse gas, conservation and protection of biodiversity and wildlife, and energy efficiency (Bautista et al. 2016b). These principles are four: “The actors involved in the BioRSC must ensure their activities maintain or improve the air, soil and water quality, as well as they do a proper management of solid waste and wastewater”, “BioRSC must have a positive balance of greenhouse gas and maintain or promote carbon sinks”, “BioRSC must promote the conservation and protection of biodiversity and wildlife” and “Energy efficiency and use of renewable energy should be promoted in the processes that are part of the BioRSC”. They are described by eleven criteria that are integrated by fifty one indicators, detailed in Appendix 5.9.

5.6.1. Environmental criteria and indicators analysis

In general, the environmental criteria assess the influence of biodiesel supply chain on the environmental conditions, the transformation of natural ecosystems and the quality of natural resources (Bautista et al. 2016b). The environmental criteria and indicators analysis to determine the inclusion of objective functions, restriction or decision variables for the model development is described in Appendix 5.10. The thirty one selected indicators are summarized in Table 5.6.

Table 5. 6. Environmental analysis by criterion and indicator

Criterion	Indicator(s)
30	(107, 108, 109, 110, 111 and 112)
Ensure air quality (Nitrogen oxide, particulate matter, carbon monoxide and hydrocarbons gas emissions ; atmospheric acidification, and persistent organic pollutants)	
These six indicators are related to gas emissions generated by using biobased products. Then, they can be represented as objective functions to minimize.	
31	(113)
Efficient use of water (Available water)	
As this indicator is related to water availability, it can be seen as a restriction to the developing model.	
31	(117)
Efficient use of water (Recycled water)	
Analyzing this indicator, the recycled water amount will depend on plant design, in other words, it depend in use and recycled water by production technology and in special structures to recycle water. Then, it can be mathematically described as function of materials transformed at biorefinery plants.	
32	(119, 120, 121, 122, 124 and 125)
Contaminated effluents generation (Suspended sediments, phosphorus, nitrogen, herbicide concentration and nitrates in wastewater)	
Indicators 119, 120, 121, 122, 124 and 125 are related to different water pollutants generated at raw material cultivation stage. Therefore, as the developing model does not consider supplier strategies or cultivate technologies, it could be only mathematically represented depending on raw material type. However, the raw material cultivation land requirements depending on culture technique could be represented by mathematical expressions as perspective for future work.	

Table 5.6. Environmental analysis by criterion and indicator (Continuation)

Criterion	Indicator(s)
32	(123)
Contaminated effluents generation (Wastewater production)	
Indicator 123 measure the waste water generated by transformation process at biorefinery plants. This is analyzed economically by criterion 22, indicator 86. Then, it can be mathematically represented as objective function to minimize the wastewater generation.	
33	(126 and 129)
Non-hazardous and hazardous waste generation (Solid waste generation)	
Related to indicator 126, it is assumed that all hazardous waste will take a proper final disposal. Then, indicators 126 and 129 can be represented by the objective function of minimize the total hazardous and non-hazardous waste generation Then, they can be mathematically represented. There indicators are represented in the economic dimension by criterion 22, indicator 86.	
33	(128)
Non-hazardous and hazardous waste generation (Waste recovered or valued)	
The model already integrates the valorization of by-products at pretreatment plants and principal production plants. Therefore, waste recovered or valued at pretreatment and principal production plants can be mathematically represented to be included in the developing model.	
34	(130, 131, 132, 133, 134 and 137)
Soil quality at raw material cultivation (Total organic carbon, nitrogen, phosphorus, agrochemicals)	
These indicators are related to raw material cultivation impacts in soils. Therefore, as the developing model does not consider supplier strategies or cultivate technologies, it could be only mathematically represented depending on raw material type. However, the raw material cultivation land requirements depending on culture technique could be represented by mathematical expressions as perspective for future work.	
35	(140, 141 and 143)
Greenhouse gas emitted and captured (CO ₂ equivalent)	
These indicators are related to measure the equivalent CO ₂ emitted at pretreatment plants, principal plants, logistic activities and biobased products use. Then, they can be integrated in an objective function to minimize the emitted total amount of equivalent CO ₂ . It must to be noted that equivalent CO ₂ emitted by logistic activities must be more detailed when model includes tactical and operational SC decision-making levels.	
36	(146)
Transformation of ecosystems (Land used for raw material cultivation)	
Similarly, indicator 146 is related to raw material cultivation land requirements. Then, it can be expected that the objective will be to minimize the hectares required to grow the raw materials devoted to biorefinery and to evaluate potential raw materials with non-food use (advanced generation). It is important to highlight that land requirements for raw material cultivation may vary depending on raw material type and/or culture technique. Therefore, as the developing model does not consider supplier strategies or cultivation technologies, it could be only mathematically represented depending on raw material type. The, the raw material cultivation land requirements depending on a specific culture technique could be represented by mathematical expressions. But this aspect represents a perspective of this work.	
39	(155 and 156)
Energy used in BioRSC (renewable and non-renewable fuel sources)	
These indicators are related to fuel consumption at the BioRSC including fuel types. Therefore, it can be expected the objective of maximize the percentage of renewable sources used. This can be mathematically described for the present model.	
40	(157)
Energy balance in BioRSC	
This criterion, as analyzed in the economic dimension (Criterion 22, indicator 85), should be mathematically represented to evaluate the energy balance.	

5.6.2. *Environmental dimension related mathematical expressions*

The environmental indicators will be mathematically described to its model integration as follows.

Indicators 107, 108, 109, 110, 111 and 112. The objective function to minimize gas emission by gas type can be represented in a general mathematical form by equation (60). Where $GasEm_{\rho,a}$ and $GasEm_{\rho,b}$ represent the gas emission type ρ generated by the consumption of final products type a and intermediate products type b . The gas types ρ are nitrogen oxide, particulate matter, carbon monoxide, hydrocarbons, Sulphur dioxide equivalent and persistent organic pollutants.

$$Min \left[\sum_a \left(GasEm_{\rho,a} * \sum_k \sum_l P_{k,a,l} \right) + \sum_b \left(GasEm_{\rho,b} * \sum_j \sum_m T_{j,b,m} \right) \right] \quad \forall \rho \quad (60)$$

Indicator 113. The water availability is a constraint for the raw material cultivation, transformation and intermediate products transformation. There are two possible ways to represent this restriction, nationally or locally. At first, nationally can be represented by equation (61). Where $WRawMat_n$ represents the amount of water needed to produce raw materials and the water needed to transform raw material n with technology c and production capacity f at pretreatment plants will be $WPret_{n,c,f}$. The amount of water needed to transform the intermediate product b with technology d and production capacity g at principal production plants is $WPlant_{b,d,g}$, as presented in equation (50) in section 5.4.2.

However, if water constraints need to be analyzed locally; then raw material suppliers, pretreatment plants and principal production plants should be grouped by region or locality, to each particular case study, to restrict each group according to the availability of water correspondingly. Therefore, no general constraint could be made without changes on the structure of decision variables (It will be needed a new sub-indices and new decision variables).

$$\left\{ \begin{array}{l} \sum_n WRawMat_n * \sum_i \sum_j \sum_c \sum_f N_{i,n,j,c,f} \\ + \sum_n \sum_c \sum_f \left(WPret_{n,c,f} * \left[\sum_i \sum_j N_{i,n,j,c,f} \right] \right) \\ + \sum_b \sum_d \sum_g \left(WPlant_{b,d,g} * \left[\sum_j \sum_k R_{j,b,k,d,g} \right] \right) \end{array} \right\} \leq TotalWaterAval \quad (61)$$

Indicator 117. The mathematical expression to maximize the total amount of reused water depending on production technologies can be presented by equation (62). Where $RecWatPret_{n,c,f}$ and $RecWatPlant_{b,d,g}$ are the water reuse ratio by transformation of entering materials (n and b) in products related to technologies (c and d) and capacities (f and g).

$$\begin{aligned}
& \text{Max} \left\{ \sum_n \sum_c \sum_f \left(\text{RecWatPret}_{n,c,f} * \left[\sum_i \sum_j N_{i,n,j,c,f} \right] \right) \right. \\
& \quad \left. + \sum_b \sum_d \sum_g \left(\text{RecWatPlant}_{b,d,g} * \left[\sum_j \sum_k R_{j,b,k,d,g} \right] \right) \right\} \quad (62)
\end{aligned}$$

Indicators 119, 120, 121, 122, 124 and 125. The objective function to minimize water degradation due raw materials cultivation can be presented in general mathematical form by equation (63). Where $\vartheta_{\tau,i,n}$ represent the water pollution type τ generated by the raw material cultivation type n at location i . The water pollution types τ are phosphorus and nitrogen discharges.

$$\text{Min} \sum_n \sum_i \vartheta_{\tau,i,n} * \left(\sum_j \sum_c \sum_f N_{i,n,j,c,f} \right) \quad (63)$$

$\forall \tau$

Indicator 123. The wastewater generation by pollution classification is evaluated as a function of raw material conversion at pretreatment plants and function of intermediate products transformation at principal plants. Therefore, to estimate the total amount of wastewater generation, the rate $SW_{n,c,f}$ and $SW_{b,d,g}$ are required to minimize the wastewater generation, as presents equation (64). These rates represents the wastewater generation when transforming the raw material type n with technology c and production capacity f at pretreatment plants (Ton wastewater/Ton raw material) and when transforming intermediate products type b with technology d and production capacity g at principal plants (Ton wastewater /Ton intermediate products)

$$\text{Min} \left[\sum_n \sum_c \sum_f \left\{ SW_{n,c,f} * \left(\sum_j \sum_i N_{i,n,j,c,f} \right) \right\} + \sum_b \sum_d \sum_g \left\{ SW_{b,d,g} * \left(\sum_k \sum_j R_{j,b,k,d,g} \right) \right\} \right] \quad (64)$$

$\forall \gamma$

Indicators 126 and 129. Hazardous and non-hazardous waste generation at pretreatment and principal plants can be represented by equation (65). Where $\omega_{z,n,c,f}$ and $\omega_{z,b,d,g}$ are rates of solid waste type z generated when transforming the raw material type n with technology c and production capacity f at pretreatment plants (Ton pollution/Ton raw material) and when transforming intermediate products type b with technology d and production capacity g at principal plants (Ton pollution/Ton intermediate products) as presented in economic indicator 86.

$$\text{Min} \left[\sum_n \sum_c \sum_f \left\{ \omega_{z,n,c,f} * \left(\sum_j \sum_i N_{i,n,j,c,f} \right) \right\} + \sum_b \sum_d \sum_g \left\{ \omega_{z,b,d,g} * \left(\sum_k \sum_j R_{j,b,k,d,g} \right) \right\} \right] \quad (65)$$

$\forall z$

Indicator 128. If there is available information about waste recover ratio by waste type, the amount of waste recovered or valorized could be represented by:

$RecWasteTotal =$

$$\sum_z \left[WasteRecP_z * \sum_n \sum_c \sum_f \left\{ \omega_{z,n,c,f} * \left(\sum_j \sum_i N_{i,n,j,c,f} \right) \right\} + WasteRecW_z * \sum_b \sum_d \sum_g \left\{ \omega_{z,b,d,g} * \left(\sum_k \sum_j R_{j,b,k,d,g} \right) \right\} \right]$$

Where $WasteRecP_z$ is waste recover ratio by waste type z at pretreatment plants and $WasteRecW_z$ is waste recover ratio by waste type z at principal plants. Then, the percentage of waste recovered or valorized could be represented by equation (66)

$$Max \left\langle \frac{RecWasteTotal}{\sum_z \left[\sum_n \sum_c \sum_f \left\{ \omega_{z,n,c,f} * \left(\sum_j \sum_i N_{i,n,j,c,f} \right) \right\} + \sum_b \sum_d \sum_g \left\{ \omega_{z,b,d,g} * \left(\sum_k \sum_j R_{j,b,k,d,g} \right) \right\} \right]} \right\rangle \quad (66)$$

Indicators 130, 131, 132, 133, 134 and 137. The objective function to minimize soil deterioration due raw materials cultivation can be presented in general mathematical form by equation (67). Where $\varepsilon_{\zeta,n}$ represent the soil deterioration rate due ζ , which is generated by the raw material cultivation type n . The causes of soil deterioration ζ are total organic carbon, nitrogen, extractable phosphorus and agrochemicals.

$$Min \sum_n \varepsilon_{\zeta,n} * \left(\sum_i \sum_j \sum_c \sum_f N_{i,n,j,c,f} \right) \quad (67)$$

$\forall \zeta$

Indicators 140, 141 and 143. The total amount of equivalent CO_2 generated at BioRSC can be represented by equation (68). Where $CO_{2i,n}$ is the equivalent CO_2 generated at raw material type n production at i . $CO_{2n,c,f}$ and $CO_{2b,d,g}$ are the generation rates of equivalent CO_2 at pretreatment plants and principal plants due entering materials transformation, depending in technology and capacity production. CO_{2a} and CO_{2b} are the generation rates of equivalent CO_2 due biorefinery products consumption. Finally, $CO_{2i,n,j}$, $CO_{2j,b,k}$, $CO_{2k,a,l}$ and $CO_{2j,b,m}$ are the generation rates of equivalent CO_2 due to logistic activities.

$$\text{Min} \left\{ \begin{array}{l} \sum_i \sum_n \left[CO_{2i,n} * \left(\sum_j \sum_c \sum_f N_{i,n,j,c,f} \right) \right] + \\ \sum_n \sum_c \sum_f \left[CO_{2n,c,f} * \left(\sum_j \sum_i N_{i,n,j,c,f} \right) \right] + \sum_b \sum_d \sum_g \left[CO_{2b,d,g} * \left(\sum_k \sum_j R_{j,b,k,d,g} \right) \right] + \\ \sum_a \left[CO_{2a} * \left(\sum_k \sum_l P_{k,a,l} \right) \right] + \sum_b \left[CO_{2b} * \left(\sum_j \sum_m T_{j,b,m} \right) \right] + \\ \sum_i \sum_n \sum_j \left[CO_{2i,n,j} * \left(\sum_c \sum_f N_{i,n,j,c,f} \right) \right] + \sum_j \sum_b \sum_k \left[CO_{2j,b,k} * \left(\sum_d \sum_g R_{j,b,k,d,g} \right) \right] + \\ \sum_k \sum_a \sum_l \left[CO_{2k,a,l} * P_{k,a,l} \right] + \sum_j \sum_b \sum_m \left[CO_{2j,b,m} * T_{j,b,m} \right] \end{array} \right\} \quad (68)$$

Indicator 146. To measure the culture land requirements by raw material type for biorefinery activities, it is needed to know the raw material yield by hectare ($RM\text{Yield}_{i,n}$). Then, the amount of required hectares minimization can be represented mathematically as equation (69).

$$\text{Min} \left\{ \sum_n \sum_i \frac{\sum_j \sum_c \sum_f N_{i,n,j,c,f}}{RM\text{Yield}_{i,n}} \right\} \quad (69)$$

Indicators 155 and 156. Fuel requirements should be established to calculate the annual consumption (from renewable and non-renewable sources). Fuel can be required at raw material location for its production, by raw material type and location ($RFuel_{i,n}$ and $NRFuel_{i,n}$). Also fuel can be used at pretreatment and principal plants for transformation procedures ($RFuelPret_{n,c,f}$, $NRFuelPret_{n,c,f}$, $RFuelPrinc_{b,d,g}$ and $NRFuelPrinc_{b,d,g}$). Finally, fuels are needed to transport the products between locations ($NRFuelLog_{n,i,j}$, $NRFuelLog_{b,j,m}$, $NRFuelLog_{b,j,k}$, $NRFuelLog_{a,k,l}$, $RFuelLog_{n,i,j}$, $RFuelLog_{b,j,m}$, $RFuelLog_{b,j,k}$, $RFuelLog_{a,k,l}$). Therefore, the objective function that relate indicator 155 and 156 is the minimization of non-renewable fuels use percentage of the total fuels consumption, represented by equation (70) including equations (a), (b), (c), (d), ϵ and (f).

$$\text{Min} \frac{(b) + (d) + (f)}{(a) + (c) + (e)} \quad (70)$$

Total fuel for raw material production:

$$RFuel_{i,n} * \sum_j \sum_c \sum_f N_{i,n,j,c,f} + NRFuel_{i,n} * \sum_j \sum_c \sum_f N_{i,n,j,c,f} \quad (a)$$

Non-renewable fuel for raw material production:

$$NRFuel_{i,n} * \sum_j \sum_c \sum_f N_{i,n,j,c,f} \quad (b)$$

Total fuel for entering material transformation:

$$RFuelPret_{n,c,f} * \sum_j \sum_i N_{i,n,j,c,f} + NRFuelPret_{n,c,f} * \sum_j \sum_i N_{i,n,j,c,f} + \\ RFuelPrinc_{b,d,g} * \sum_k \sum_j R_{j,b,k,d,g} + NRFuelPrinc_{b,d,g} * \sum_k \sum_j R_{j,b,k,d,g} \quad \text{€}$$

Non-renewable fuel for entering material transformation:

$$NRFuelPret_{n,c,f} * \sum_j \sum_i N_{i,n,j,c,f} + NRFuelPrinc_{b,d,g} * \sum_k \sum_j R_{j,b,k,d,g} \quad \text{(d)}$$

Total fuel consumption by logistic:

$$(NRFuelLog_{n,i,j} * N_{i,n,j,c,f} + RFuelLog_{n,i,j} * N_{i,n,j,c,f}) + \\ (NRFuelLog_{b,j,k} * R_{j,b,k,d,g} + RFuelLog_{b,j,k} * R_{j,b,k,d,g}) + \\ (NRFuelLog_{a,k,l} * P_{k,a,l} + RFuelLog_{a,k,l} * P_{k,a,l}) + \\ (NRFuelLog_{b,j,m} * T_{j,b,m} + RFuelLog_{b,j,m} * T_{j,b,m}) \quad \text{€}$$

Non-renewable fuel consumption by logistic:

$$NRFuelLog_{n,i,j} * N_{i,n,j,c,f} + NRFuelLog_{b,j,k} * R_{j,b,k,d,g} + \\ NRFuelLog_{a,k,l} * P_{k,a,l} + NRFuelLog_{b,j,m} * T_{j,b,m} \quad \text{(f)}$$

Indicator 157. To conduct the energy balance required by this indicator it is required to analyze the energy consumed and the energy generated (Bautista Rodríguez 2015). Therefore, the energy consumed in the production processes, whether steam, electricity, fuel, between other, and the energy value of the raw material, in addition to the energy value of the products obtained, must be considered.

Analyzing the BioRSC design, presented on figure 5.1, it could be noted that the energy generated is:

- Intermediate products to markets
- Intermediate products in stock at pretreatment plants
- Final product to markets
- Final products in stock at pretreatment plants

And the energy consumed is:

- Energy content of the entering raw material
- Energy expenditure per raw material transport to pretreatment plants
- Energy expenditure to transform raw materials into intermediate products
- Energy expenditure per intermediate product transport to clients
- Energy expenditure per intermediate product transport from pretreatment plants to principal plants
- Energy expenditure to transform intermediate products into final products
- Energy expenditure per final product transport to clients

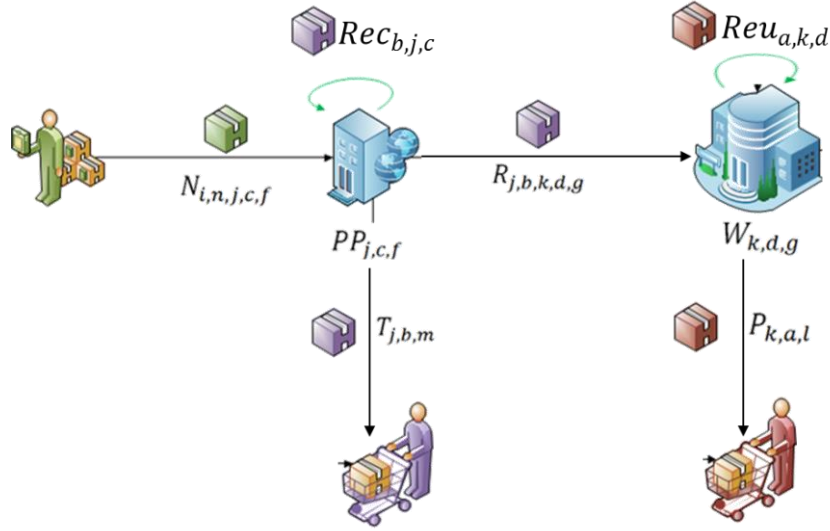


Figure 5. 2. General model for Phase III BioRSC design

The objective is that the energy generated will be greater than the energy consumed. Therefore, this indicator can be translated as an objective function as follows:

$$\text{Generated Energy} > \text{Consumed Energy} \Rightarrow \text{Min} (\text{Consumed Energy} - \text{Generated Energy})$$

Then, it can be expressed by the decision variables as equation (71). Where the parameters are represented by:

- θ_n = Energy content of the raw material type n , in “MJ / Ton of raw material”
- δ = Energy expenditure to transport the products, this factor is in “MJ / (Ton transported * Km traveled)”
- $Dist_{i,j}$ = Distance traveled in Km between supplier i and pretreatment plant j
- $\beta_{n,c,f}$ = Energy consumption to transform incoming raw material type n with technology c and production capacity f (If this value is independent of production capacity, it means that economies of scale are not considered in the production pretreatment plant)
- $Dist_{j,k}$ = Distance traveled in Km between the pretreatment plant j and the main production plant k
- $\beta_{b,d,g}$ = Energy consumption to transform the incoming intermediate products type b with the technology d and the production capacity g (If this value is independent of the production capacity, it means that they are not considered economies of scale in the main production plants)
- $Dist_{k,l}$ = Distance traveled in Km between the main production plant k and the customer located in l
- $Dist_{j,m}$ = Distance traveled in Km between the pretreatment plant j and the intermediate product customer located in m
- θ_b = Energy content of intermediate product type b , in “MJ / Ton of intermediate product”
- θ_a = Energy content of final product type a , in “MJ / Ton of final product”

$$\text{Min} \left\{ \begin{aligned} & \sum_n \left[\left(\sum_i \sum_j \sum_c \sum_f N_{i,n,j,c,f} \right) * \theta_n \right] + \sum_i \sum_j \left[\left(\sum_n \sum_c \sum_f N_{i,n,j,c,f} \right) * \delta * Dist_{i,j} \right] + \\ & \sum_n \sum_c \sum_f \left[\left(\sum_i \sum_j N_{i,n,j,c,f} \right) * \beta_{n,c,f} \right] + \sum_j \sum_k \left[\left(\sum_b \sum_d \sum_g R_{j,b,k,d,g} \right) * \delta * Dist_{j,k} \right] + \\ & \sum_b \sum_d \sum_g \left[\left(\sum_j \sum_k R_{j,b,k,d,g} \right) * \beta_{b,d,g} \right] + \sum_k \sum_l \left[\left(\sum_a P_{k,a,l} \right) * \delta * Dist_{k,l} \right] + \\ & \sum_j \sum_m \left[\left(\sum_b T_{j,b,m} \right) * \delta * Dist_{j,m} \right] - \sum_b \left[\left(\sum_j \sum_m T_{j,b,m} \right) * \theta_b \right] - \\ & \sum_b \left[\left(\sum_j \sum_c Rec_{b,j,c} \right) * \theta_b \right] - \sum_a \left[\left(\sum_k \sum_l P_{k,a,l} \right) * \theta_a \right] - \\ & \sum_a \left[\left(\sum_k \sum_d Reu_{a,k,d} \right) * \theta_a \right] \end{aligned} \right\} \quad (71)$$

5.7. Summary

As shown in chapters IV and V, the inclusion of the strategic decisions for the SC, the BioRSC characteristics and the sustainability dimensions is not a trivial task. Because this involves the analysis of a large amount of indicators that should be represented by decisional variables, parameters and objective functions. Therefore, the model construction process detailed in chapter IV is useful due to the fact that it allows developing the model integrating the system complexity layer-by-layer, maintaining the principal model structure, as presented in figure 5.3.

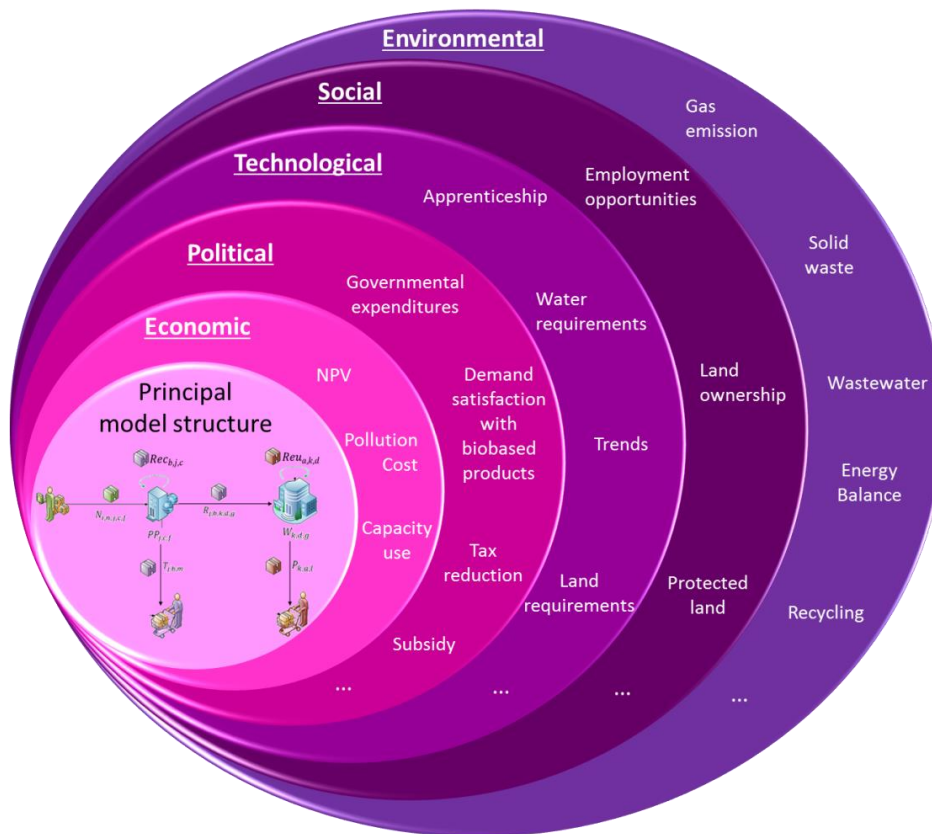


Figure 5. 3. Developing model layer-by-layer

In this chapter, a large amount of objective functions and parameters were described. Resulting in a MO-BMIP (Multi-Objective Binary Mixed Integer Programming) model for the design of a sustainable Phase III BioRSC. An overview of the amount of derived general mathematical expressions by sustainability dimension is presented in table 5.7. Where, it could be observed that 20 objective functions are described in this chapter. If we add the first objective function defined in chapter IV it results in 21 objective functions to sustainable Phase III BioRSC design model. Also, there are 13 decision variables and 19 restrictions general definitions, taking into account model descriptions presented in chapters IV and V. Finally, there are 87 parameters defined to describe the strategical SC decision-making level, biorefinery characteristics and sustainability dimensions. The inclusion of all these equations will depend on case study and available information.

Table 5. 7. *Overview of general mathematical expressions in the integrated model*

Dimension	Mathematical statement	Amount
Initial model	Objective function definition	1
	Decision variable definition	8
	Restriction definition	14
	Parameter definition	20
Economic	Objective function definition	1
	Objective function actualization	1
	Parameter definition	9
Political	Objective function definition	4
	Objective function actualization	3
	Parameter definition	7
	Restriction definition	4
	Decision variable definition	4
Technological	Objective function definition	3
	Objective function actualization	1
	Parameter definition	4
Social	Objective function definition	2
	Parameter definition	11
	Decision variable definition	1
Environmental	Objective function definition	10
	Parameter definition	38
	Restriction definition	1
Total Objective Function		21
Total Parameter Definition		89
Total Restriction Definition		19
Total Decision Variable Definition		13

The next chapter is focused on the presentation of a case study to design a sustainable Phase III BioRSC and the parameter description for the multiobjective optimization.

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Chapter VI. Case study parameter description

6.1. Introduction

The integrated model presented in Chapters IV and V, includes the strategic decisions for the SC, the BioRSC characteristics and the sustainability dimensions analysis. Therefore, in the present chapter the parameters to apply the developed model to a case study will be defined.

It was decided to analyze the case of Colombia to design a sustainable Phase III BioRSC, considering in that country biorefineries Phase II are actually in production and there is a market regulation for biobased products such as biodiesel (Costa et al. 2017). The industry is mainly funded by government subsidies, the principal raw material used is only palm oil and the final product sold is biodiesel (Costa et al. 2017), leaving aside the possibility of selling products with high added value (Bueno et al. 2015).

Thus, the idea is to diversify the raw materials to be used, comparing palm and jatropha oil (Hernández Castiblanco and Amórtegui Gómez 2015). Also, diversifying the final products to be obtained (Bueno et al. 2014), in addition to the evaluation of different production technologies (Basto Aluja 2016).

Therefore, in the present chapter the model parameters are described in six sections, as schematically represented in Table 6.1. In section 6.2 the parameters related to the equations defined in Chapter IV are linked to the economic and political sustainability dimensions. Then, each one of the following sections is dedicated to a specific sustainability dimension and to the model established in Chapter V.

Table 6. 1. Model parameters to design a sustainable Phase III BioRSC

Section	General initial model	Sustainability dimension concerned				
		Economic	Political	Technological	Social	Environmental
6.2.	✓	✓	✓			
6.3.		✓				✓
6.4.			✓			
6.5.				✓		✓
6.6.					✓	
6.7.						✓

6.2. Parameter definition for strategic decisions in SC and the BioRSC characteristics.

In this section, twenty-two parameters are defined, as present table in 6.2. Parameters are part of the equations identified by the numbers in parenthesis. These parameters are required for the general initial model equations and some economic and political related equations.

Table 6. 2. Parameters of the model and equation where they are included.

Parameter	Equation of the General initial model including the parameter	Equations in Chapter V including the parameter				
		Economic	Political	Technological	Social	Environmental
$RMAvailavility_{i,n}$	(1)(2)(4)(11)					
$RMCost_n$	(28)					
$\alpha_{n,c,b}$	(2)(4)(9)					
$CapPP_{j,c,f}$	(1)(2)(4)(12)	(31)				
$Inv_{j,c,f}$	(30)					
$ProdCost_{n,j,c,f}$	(29)		(54)			
$\alpha_{b,d,a}$	(5)(6)(10)					
$CapW_{k,d,g}$	(3)(5)(6)(13)	(32)				
$Inv_{k,d,g}$	(30)					
$ProdCost_{b,k,d,g}$	(29)		(55)			
$Dem_{l,a}(Max)$	(7)(19)					
$Prix_a$	(25)					
$value_{a,k}$	(25)					
$Dem_{m,b}(Max)$	(8)(18)					
$Prix_b$	(25)					
$value_{b,j}$	(25)					
$TCost_{i,j}$	(27)					
$TCost_{j,k}$	(27)					
$TCost_{k,l}$	(27)					
$TCost_{j,m}$	(27)					
Discount Rate	(23)					
i	(23)(24)					

First, the potential raw materials to be used are defined to determine their availability and price in Colombia. Then, the characteristics of pretreatment plants and main production plants, that is, their potential location, production capacity and production technologies, as well as their operation and installation costs, are determined. Afterwards, the potential markets to be covered are defined, that is definition of the potential final products to be sold, the locations of their demands, quantities demanded and market prices. Finally, it is necessary to know the distances and transport costs between the different nodes at the BioRSC.

6.2.1. Raw Materials

As starting point, the raw materials types are chosen for the case study. In Colombia currently, biodiesel is produced from on palm oil (Fedepalma 2015; Fedepalma 2017b). However, it is necessary

to find another raw material for make this industry more flexible, and to change from a biorefinery phase I or II to a complete integrated Phase III biorefinery.

One of the options is to looking for non-edible vegetal oils, in order to produce advanced biodiesel. An example is *Jatropha curcas* oilseed which oil content varies between 30 and 40% (Hernández Castiblanco and Amórtegui Gómez 2015). The plant is used medicinally, in cosmetics, pharmaceutical industry, as a pesticide, lubricant, fertilizer, soil amendment and as a non-conventional source of renewable energy. It is also a plant that by its nature shows high resistance and it is sometimes used for the control of soil erosion (Hernández Castiblanco and Amórtegui Gómez 2015). Also, *Jatropha curcas* has been promoted due to the intention of the Colombian government to promote the crops that would supply the national market of oils demanded as biofuels or biodiesel, through CORPOICA (Hernández Castiblanco and Amórtegui Gómez 2015).

Then, the raw materials to be analyzed and compared in the present case study are the palm oil and *Jatropha curcas* oil.

Raw material availability and location.

- *Palm oil*. The most recent complete information related to hectares in production and oil yield by hectare is for the year 2015 and it is available at the web page of Fedepalma (Fedepalma 2017b).
- *Jatropha curcas oil*. It is a raw material lightly exploited. Colombia has about 135.5 hectares planted, located in the departments of Vichada, Chocó, Santander, Cauca, Antioquia, Cesar and Nariño (Hernández Castiblanco and Amórtegui Gómez 2015). Therefore, the existing analysis developed by Gaona Currea (2009) and Hernández Castiblanco and Amórtegui Gómez (2015) will be used to determine the potential *Jatropha* cultivation locations. Gaona Currea (2009) and Hernández Castiblanco and Amórtegui Gómez (2015) presented a definition for the concept of suitable land for *Jatropha* depending in its agricultural potential and use conflict:

✚ Highly suitable without use conflict (M3A): It corresponds to land without limitations for sustainable *Jatropha* cultivation. The soils are almost flat and the erosion problems are very small. They are deep soils, generally well-drained and easier to work with; they have good water-retention properties, are provided with nutrients and respond to fertilizer additions. They are not subject to flood damage, are productive soils and suitable for intensive cultivation. Climate and height are favorable for optimum growth.

✚ Moderately suitable without use conflict (M3M): It corresponds to land with minor constraints to sustainable *Jatropha* cultivation. Productivity will be lower and inputs will be more expensive than in M3A. These lands have some limitations that reduce the choice of plants or require moderate conservation and management practices, including conservation practices to prevent deterioration or to improve water-air relationships. Limitations may include the following effects: (1) Moderate susceptibility to erosion by water or wind or moderate adverse effects caused by past erosion, (2) Unfavorable structure, (3) Moderate salt or sodium content, easily correctable but likely to reappear,

(4) Occasional flood damage, (5) Humidity correctable by drainage, (6) Climate slight limitations in the use and soil management, and (7) Tolerable height.

It should be noted that there are other areas highly suitable for jatropha production in Colombia. However, they have conflict of use. This could generate potentially negative impacts, as problems of food security due to food price inflation or to use changes in agricultural lands (Gaona Currea 2009; Espinoza Pérez et al. 2017). Therefore, the areas with conflict of use are not considered as potential raw material sources in this research. As well, it was decided to work only with highly suitable lands to jatropha production; because, although they are a smaller amount of hectares, they are easier to work with and they are suitable for intensive cultivation. Therefore, this could ease jatropha exploitation.

According to Gaona Currea (2009) there are different yields of jatropha oil per hectare based on soils type. Moreover, productivity also depends on the oil extraction process implemented.

Based on this information, it was decided to consider the index for the raw materials type (n) as $n = 1,2,3$. Due the fact that integrated model does not include an index for different applied technologies by suppliers. The estimation for palm and jatropha oil availability is presented on Appendix 6.1 and it is summarized on table 6.3. Additionally, it is necessary to include a new restriction associated to the raw materials availability, because, the best extraction method for jatropha oil should be chosen between manual and electric press. Therefore, at each raw material location where jatropha is available, the physical flow to pretreatment plants must to be restricted by the hectares available for jatropha production. Then, the restriction (72) is needed.

$$\frac{\sum_j \sum_c \sum_f N_{i,2,j,c,f}}{RMYield_{i,n=2}} + \frac{\sum_j \sum_c \sum_f N_{i,3,j,c,f}}{RMYield_{i,n=3}} \leq CapHaJat_i \quad (72)$$

$\forall i$ where $CapHaJat_i > 0$

Where:

$RMYield_{i,n}$ = The yield of raw materials type n (tons) obtained per hectare in production at location i

$CapHaJat_i$ = The available hectares amount to obtain jatropha oil at location i .

Table 6. 3. Raw material availability by raw material type and location

<i>i</i>	Location	Biomass Type		
		$RMAvailability_{i,n=1}$	$RMAvailability_{i,n=2}$	$RMAvailability_{i,n=3}$
		Palm oil availability (t/Year)	Jatropha oil availability obtained by manual-extraction (t/Year)	Jatropha oil availability obtained by electric press (t/Year)
(1)	Bosconia / Cesar	281,000.00	0.00	0.00
(2)	María la Baja / Bolívar	55,161.00	36,453.00	43,680.75
(3)	Tumaco / Nariño	23,000.00	0.00	0.00
(4)	Barrancabermeja / Santander	173,400.00	0.00	0.00
(5)	Villanueva / Casanare	111,435.00	0.00	0.00
(6)	San Carlos de Guaroa / Meta	413,300.00	0.00	0.00
(7)	Montería / Córdoba	0.00	332,616.08	398,565.82
(8)	Agustín Codazzi / Cesar	0.00	159,332.96	190,924.84
(9)	Sincelejo / Sucre	0.00	84,512.96	101,269.84
(10)	Santa Marta / Magdalena	198,000.00	55,970.00	67,067.50
(11)	Albania / La Guajira	0.00	53,076.96	63,600.84
(12)	Girardot / Cundinamarca	0.00	35,415.96	42,438.09
(13)	Medellín / Antioquia	0.00	25,439.96	30,484.09
Total		974,296.00	782,817.88	938,031.77

Table 6.4 shows the available hectares to produce jatropha in Colombia by each location *i*, i.e. the parameter $CapHajat_i$. Transformation yields in oil tons per hectare are: $RM Yield_{i,n=2} = 1.16$ and $RM Yield_{i,n=3} = 1.39$. It is assumed that this value does not change with the location, because all the locations are highly suitable for jatropha production without use conflict (Gaona Currea 2009). Finally, the geographical distribution of raw material sources is presented on Figure 6.1.

Table 6. 4. Hectares availability to jatropha production in Colombia

<i>i</i>	Location	$CapHajat_i$
		Jatropha available hectares
(1)	Bosconia / Cesar	0
(2)	María la Baja / Bolívar	31,425
(3)	Tumaco / Nariño	0
(4)	Barrancabermeja / Santander	0
(5)	Villa Nueva / Casanare	0
(6)	San Carlos de Guaroa / Meta	0
(7)	Montería / Córdoba	286,738
(8)	Agustín Codazzi / Cesar	137,356
(9)	Sincelejo / Sucre	72,856
(10)	Santa Marta / Magdalena	48,250
(11)	Albania / La Guajira	45,756
(12)	Girardot / Tolima	30,531
(13)	Medellín / Antioquia	21,931
Total		674,843

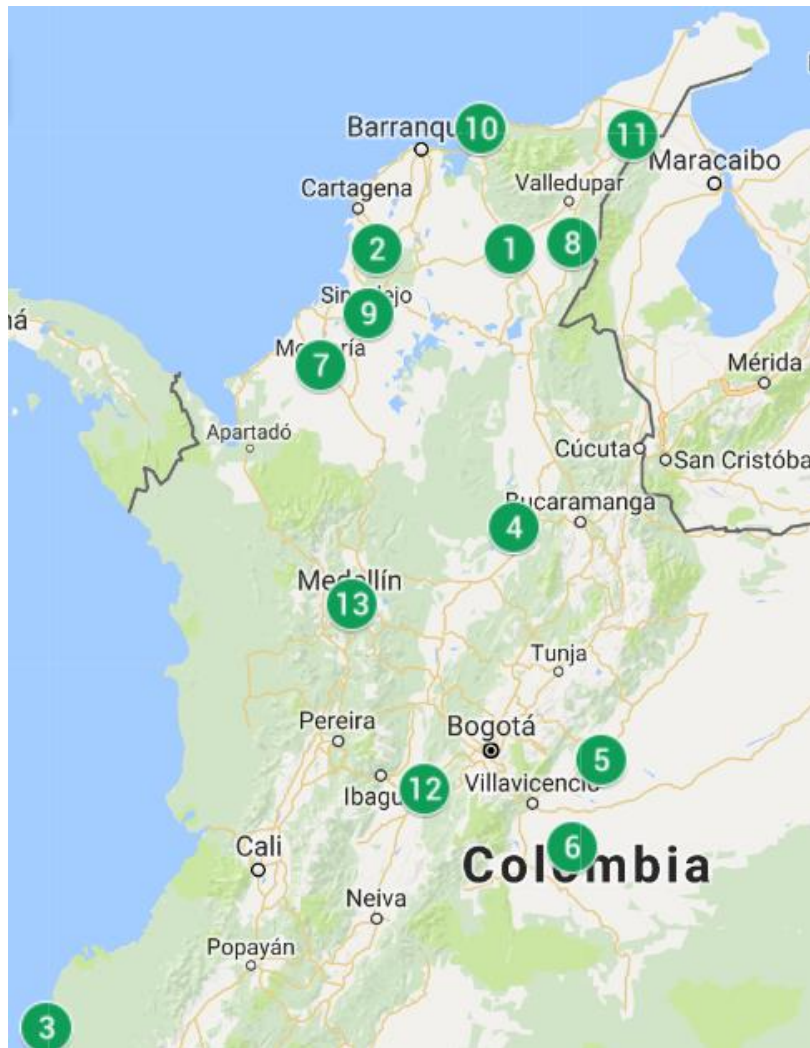


Figure 6. 1. Geographical distribution of raw material sources.

Raw Material cost. Furthermore, it is also necessary to know the market price of the raw materials. To transform the Colombian currency to U.S. dollar, the information corresponding to year 2015 (Banco de la República Colombia 2017) was analyzed to calculate the average: 2,743.39 Colombian currency per U.S. dollar.

Respect to palm oil price, the average value during 2015 was *COP*\$ 2,206,828 per ton (Fedepalma 2015), which can be transformed as:

$$\frac{\$ 2,206,828}{\$ 2,743.39} = 804.42 \text{ USD}/t$$

The market price for jatropha oil acquisition is not available, because it is not currently produced at Colombia. However, the research made by Gaona Currea (2009) assume it is the same price of palm oil, because jatropha oil could be used instead of palm oil for biodiesel production. Nevertheless, in the same research, the production cost for the different raw materials has been estimated for the year 2008, as showed on table 6.5. It can be noted that the production cost is different for each raw material type.

Table 6. 5. Jatropha and palm oil production cost (Gaona Currea 2009)

	Palm	Jatropha	
		Manual-extraction	Electrical Press
Production Cost in 2008 (\$/t)	869,400	841,871	712,675

Therefore, due to lack information and that the most part of biodiesel producers in Colombia are the owners of palm oil plantations (Ecodiesel 2017; Manuelita 2017; Oleoflores 2017), it is assumed that the production cost presented on research can be considered as market price in 2008. Then, as the variation presented by the palm oil market price between 2008 and 2015 can be calculated, this proportional increase will be used to actualize the values for jatropha oil to 2015,

The variation presented by the palm oil market price between 2008 and 2015 is:

$$\frac{\text{Palm oil market price 2008}}{\text{Palm oil market price 2015}} \Rightarrow \frac{869,400}{2,206,828} = 0.393954 (*)$$

Then, the values for jatropha oil market price are divided by value (*) to update the oil production cost in Colombia, as summarized table 6.6; to define the $RMCost_n$.

Table 6. 6 Estimated oil acquisition cost at Colombia in 2015

	Palm oil $n = 1$	Jatropha oil		Year
		By Manual extraction $n = 2$	By Electrical extraction $n = 3$	
Price (\$/t)	869,400.00	841,871.00	712,675.00	2008
Updating (\$/t)	2,206,828.00	2,136,950.80	1,809,008.00	2015
Price updated (USD/t) - $RMCost_n$	804.42	778.95	659.41	2015

6.2.2. Pretreatment plants

In order to characterize the pretreatment plants and to determine the parameters needed for the integrated model, the following variables have to be determined: the production technologies that can be used, the corresponding transformation rates for each type of raw material entering, the potential locations for the pretreatment plants and the installation and operating costs.

Production technologies and transformation yields. Due to the fact that biodiesel is currently produced in Colombia, and there are consumption laws, it is necessary to integrate technologies to prepare the oil for the process of transformation into biodiesel and other products that can be sold in the market. Therefore, the pretreatment process that must be realized is the physical oil refining.

There are two methods of refining oils: chemical refinement and physical refinement (Blanco Rodríguez 2007). The physical refining offers significant advantages over chemical refinement, such as greatest yield in process, recovery of free fat acid of high quality as by-products, reduction of the use of chemical compounds and reduction of water consumption during the process (Blanco Rodríguez 2007). However, the choice of the type of refinement depends on the quality of the oil and its acid

number. In general lines, when the degree of acidity of the oil exceeds approximately 2%, a chemical refining should be made.

The degree of acidity of the oil (%) can be calculated as $(Acid\ number/1,99)$; where the acid number is measured in $mg\ KOH/gr\ sample$ (García Martínez et al. 2014).

According to the literature, the main physicochemical characteristics of crude palm oil and crude jatropha oil are as is presented on table 6.7. Therefore, it can be assumed that both crude oils can be refined physically. Physical refinement includes three steps: degumming; bleaching and deodorization (Blanco Rodríguez 2007).

Table 6. 7. Palm and jatropha crude oil physic-chemical characteristics

Characteristic	Jatropha oil		Palm oil	
	Value	Reference	Value (Max)	Reference
Acid number ($\frac{mg\ KOH}{g\ oil}$)	2.81	(Karaj et al. 2008)	5.00	(UPME et al. 2003)
	6.02	(Yate Segura 2013)		(Fedepalma 2013)
	0.92-6.16	(Castillo Ospina et al. 2011)	2.40	(Rincón M. and Martínez C. 2009)
Moisture or impurities (%)	1.00	(Brossard-González et al. 2010)	1.00	(UPME et al. 2003)
	0.05	(Lafargue-Pérez et al. 2012)		(Fedepalma 2013)
		(S. de Oliveira et al. 2009)		

Table 6.8 presents the usual losses during oil refining in each stage of physical refinement according to the research carried out by Blanco Rodríguez (2007) for an average oil.

Table 6. 8. Material losses in each pretreatment stage for an average oil (Blanco Rodríguez 2007)

Physical refinement stage	Entering mass (Kg)	Outgoing mass (Kg)
Degummed	100.0	94.3
Bleaching	94.3	94.1
Deodorization	94.1	91.4

Due to the lack of information related to jatropha curcas oil, these values will be considered for its pretreatment. However, as there is available information related to crude palm oil (Blanco Rodríguez 2007), the losses in pretreatment process can be estimated, as detailed in Appendix 6.2, to determine the value of $\alpha_{n,b,c}$. Therefore, the processing rates for palm oil and jatropha at pretreatment plants are resumed in table 6.9.

Table 6. 9. Processing rates for palm oil and jatropha parameters to optimization model ($\alpha_{n,b,c}$)

Biomass	Technology	Intermediate Products	
		Refined jatropha oil ($b = 1$)	Refined Palm oil ($b = 2$)
$(n = 1)$ Palm oil	$c = 1$	0.00	97.40%
$(n = 2)$ Jatropha oil by manual extraction	$c = 1$	91.40%	0.00%
$(n = 3)$ Jatropha oil by electrical extraction	$c = 1$	91.40%	0.00%

Potential pretreatment locations. In order to determine the potential locations of pretreatment plants, we searched for cities, where connectivity (transport) and labor force are available (Kalantari 2013). Moreover, these plants need to be located near to the collection points of raw materials, due to the degradation that could suffer these raw materials if they are transported for long distances (Espinoza Pérez et al. 2017). Based on these concepts, most of the potential pretreatment plants were proposed, with exception of plants N° 7 and 12, considered as intermediate points that would centralize the pretreatment process of raw material origination points Nos. 3, 5, 6, 12, 13, 15 and 16, as is shown in figure 6.2.



Figure 6. 2. Map with potential pretreatment plants locations and the raw materials sources

It is necessary to emphasize that these locations could be modified by sustainable analysis requirements. However, they constitute a first approach/proposal to before test new location alternatives. Thus, detailed information about the location of pretreatment plants is presented in the table 6.10. They are shown graphically in Figure 6.3.

Table 6. 10. Potential locations for pretreatment plants in Colombia

<i>j</i>	Location	Department	<i>j</i>	Location	Department
1	San Juan del Cesar	Magdalena	10	Santa Rosa de Cabal	Risaralda
2	Sabanalarga	Atlántico	11	Fundación	Magdalena
3	María La Baja	Bolívar	12	Fusagasugá	Cundinamarca / Bogotá
4	Sahagún	Córdoba	13	Villanueva	Casanare
5	Tumaco	Nariño	14	Aguachica	Cesar
6	Palmira	Valle del Cauca	15	Natagaima	Tolima
7	Garzón	Huila	16	Montería	Córdoba
8	San Carlos de Guaroa	Meta	17	Corozal	Sucre
9	Envigado	Antioquia			

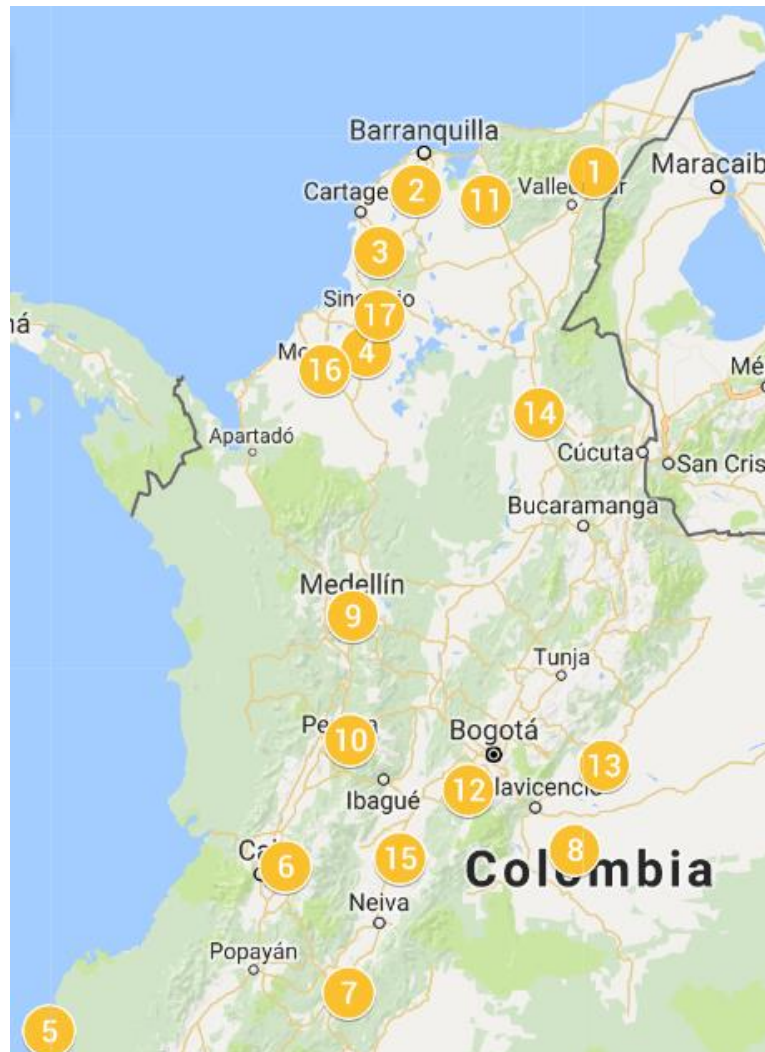


Figure 6. 3. Map of potential locations of pretreatment plants

Installation cost of the pretreatment plants. The research developed by Basto Aluja (2016) has been used to determine the installation costs of pretreatment plants ($Inv_{j,c,f}$) and the plant capacity ($CapPP_{j,c,f}$). Details of the performed analysis for such calculation are found in the Appendix 6.4. Finally, the installation costs are presented in Table 6.11.

Table 6. 11. Estimated installation cost of pretreatment plants ($Inv_{j,c,f}, \forall j, c$)

	Pretreatment Plant Capacity		
	$CapPP_{j,c,f=1} =$ 40 000 Tons/Year	$CapPP_{j,c,f=2} =$ 80 000 Tons/Year	$CapPP_{j,c,f=3} =$ 120 000 Tons/Year
Total Pretreatment Capital Cost $Inv_{j,c,f}$ (USD)	4,500,000	6,240,000	10,850,000

It can be observed that at this stage, there is no differentiation of the investment cost depending on the location of the pretreatment, which is an assumption in the integrated model. However, this factor can be integrated if more information about differences in investment values depending on the location of the production plant in Colombia appears.

Operational cost of pretreatment plants. Regarding the operational cost of pretreatment plants, it is considered a single transformation technology, which is refining. However, there will be different operating costs depending on the type of incoming raw materials (mainly due to their physic-chemical characteristics). Economies of scale are assumed, so the operational cost is lower as production capacity increases. In addition, it is assumed that the operational cost will not be affected by the location of pretreatment plants. The computation of the parameters ($ProdCost_{n,j,c,f}$) is presented in Appendix 6.5 and summarized in table 6.12, based on Basto Aluja (2016) and Bueno et al. (2015).

Table 6. 12. Operational cost at pretreatment plants ($ProdCost_{n,j,c=1,f}, \forall j$)

	Pretreatment Plant Capacity		
	($f = 1$)	($f = 2$)	($f = 3$)
Raw Materials Entering	40,000 t/year	80,000 t/year	120,000 t/year
($n = 1$) Palm oil	42.42	38.96	36.36
($n = 2$) Jatropha oil by manual extraction	39.81	36.56	34.12
($n = 3$) Jatropha oil by electromechanical extraction	39.81	36.56	34.12

6.2.3. Main production plants

In order to characterize the main production plants and to determine the parameters required for the optimization model, the production technologies that can be used have to be described. Additionally, the corresponding transformation rates for each type of intermediate product that can be transformed have to be established, as well as the potential locations of such main production plants should be proposed, and its installation and operating costs.

Production technologies and transformation yields. Considering one of the main objectives of this research is to support the evolution of biorefineries Phase I and II into biorefineries Phase III, the objective in this section is to find and to define the set of transformation technologies that can offer final products with a high added value to the market. In that way, biodiesel, glycerol and polyester were selected as final products to obtain at the main production plants. Biodiesel consumption is mandatory at Colombia (Congreso de la Republica de Colombia 2004) and glycerol is a byproduct of biodiesel obtained by transesterification (University of Strathclyde 2017). Glycerol is widely used in food (11%), pharmaceuticals (18%), cosmetics (16%), tobacco (6%), and other industries depending on its different refining purities (Long and Fang 2012). Aliphatic polyesters can be produced based on

glycerol (Bueno et al. 2015) and used as drug delivery applications (Washington et al. 2016), as hard-tissue engineering synthetic biomaterials (Ozdil and Aydin 2014) and as thermoplastic building-blocks (More et al. 2013). Aliphatic polyesters are low-melting, flexible plastic materials which are used for mulch films and monofilament fibers. They are also used for rather soft and flexible foams and injection-molded parts (Ünkel et al. 2016). The different production technologies to apply in principal production plants are briefly detailed as follows:

- *Base-catalyzed transesterification.* Base-catalyzed transesterification is the most widely used method for biodiesel production obtaining glycerol as the main by-product (TechNotes 2006). The most commonly used base catalyzers are solutions of sodium methoxide (NaOCH₃) or potassium methoxide (KOCH₃) in methanol (TechNotes 2006). Because they are more effective than NaOH and KOH as a catalyst, although they are more expensive (Saifuddin et al. 2015).
- *Base-catalyzed transesterification and polymers production.* This technology is the integration of two different technologies. The first one produces biodiesel and glycerol by base-catalyzed transesterification and the second technology transforms the glycerol into polyester. Because the economy of biofuels is highly dependent on the by-products, recently, the development and design of “green composites” has received great attention representing a new step towards the use of renewable sources (Bueno et al. 2015). Therefore, the production of polyesters from glycerol, for applications such as modifiers for thermosets (epoxy resins) or polyurethanes, plasticizers, and matrices for controlled drug delivery, among others (Bueno et al. 2015), could support the generation of biorefineries phase III.

In addition to above mentioned alkaline transesterification, that is a batch or continuous process in stirred tank reactors, there are another continuous production technology using falling film reactors in two different flow patterns, co-current and counter-current (Basto Aluja 2016).

- *Co-current transesterification.* Its process has a productivity of 1.3 % more than the conventional process, considering the production of biodiesel as a function of the oil consumed.
- *Counter-current transesterification.* Its transformation technology has a productivity of 2.7 % more than the conventional process.

Therefore, there is a combination of six available technologies to transform intermediate products at principal plants, numbered as follows for the integrated model.

- $d = 1$ Base-catalyzed transesterification
- $d = 2$ Base-catalyzed transesterification and polymers production
- $d = 3$ Co-current transesterification
- $d = 4$ Co-current transesterification and polymers production
- $d = 5$ Counter-current transesterification
- $d = 6$ Counter-current transesterification and polymers production

Then, the estimation for the transformation yield for each technology by intermediate product and capacity production ($\alpha_{b,d,a}$) is presented on Appendix 6.3, and is resumed in Table 6.13.

Table 6. 13. Processing rates for intermediate products at principal production plants ($\alpha_{b,d,a}$)

Intermediate Products		Technology at Production Plant	Final Products		
			Biodiesel $a = 1$	Polymer $a = 2$	Glycerol $a = 3$
$b = 1$	Jatropha Oil	$d = 1$	0.97	0.00	0.08
$b = 1$	Jatropha Oil	$d = 2$	0.97	0.19	0.00
$b = 1$	Jatropha Oil	$d = 3$	0.98	0.00	0.08
$b = 1$	Jatropha Oil	$d = 4$	0.98	0.20	0.00
$b = 1$	Jatropha Oil	$d = 5$	1.00	0.00	0.08
$b = 1$	Jatropha Oil	$d = 6$	1.00	0.20	0.00
$b = 2$	Palm Oil	$d = 1$	1.00	0.00	0.08
$b = 2$	Palm Oil	$d = 2$	1.00	0.19	0.00
$b = 2$	Palm Oil	$d = 3$	1.02	0.00	0.08
$b = 2$	Palm Oil	$d = 4$	1.02	0.19	0.00
$b = 2$	Palm Oil	$d = 5$	1.03	0.00	0.08
$b = 2$	Palm Oil	$d = 6$	1.03	0.19	0.00

Potential main production plant locations. In order to determine the potential main production plant locations, first, the current locations of biodiesel production plants in Colombia are considered. Thus, its suitability for location and production capacity can be assessed. In addition, seven new production plant locations are proposed and assessed. These have been located in villages or small towns, to have potential labor workforce and roads that facilitate the transport and connectivity (Kalantari 2013). These locations are close to demand points that are not currently covered by the plants already installed. Figure 6.4 compares the points of demand and production plants. Therefore, the location details are presented on table 6.14 and are represented graphically on figure 6.5.

Table 6. 14. Potential location for main production biorefinery plants

k	Production Plant	Department	Location
1	Biocombustibles sostenibles del Caribe / BioSC S.A	Magdalena	Santa Marta
2	Oleoflores / Agustín Codazzi	Cesar	Agustín Codazzi
3	ROMIL DE COLOMBIA ZONA FRANCA S.A.S.	Atlántico	Barranquilla
4	Biodiesel de la Costa	Atlántico	Galapa
5	Odín Energy	Magdalena	Santa Marta
6	Bio D	Cundinamarca	Facatativá
7	Ecodiesel de Colombia	Santander	Bucaramanga
8	Aceites Manuelita	Meta	San Carlos de Guaroa
9	Biocastilla	Meta	Villavicencio
10	La Paz	Meta	San Carlos de Guaroa
11	Potencial 1 / El Carmen de Bolívar	Bolívar	El Carmen de Bolívar
12	Potencial 2 / Cerete	Córdoba	Cerete
13	Potencial 3 / Fonseca	La guajira	Fonseca
14	Potencial 4 /Ocaña	Norte de Santander	Ocaña
15	Potencial 5 /Cartago	Valle del Cauca	Cartago
16	Potencial 6 / Girardot	Cundinamarca	Girardot
17	Potencial 7 / Pitalito	Huila	Pitalito

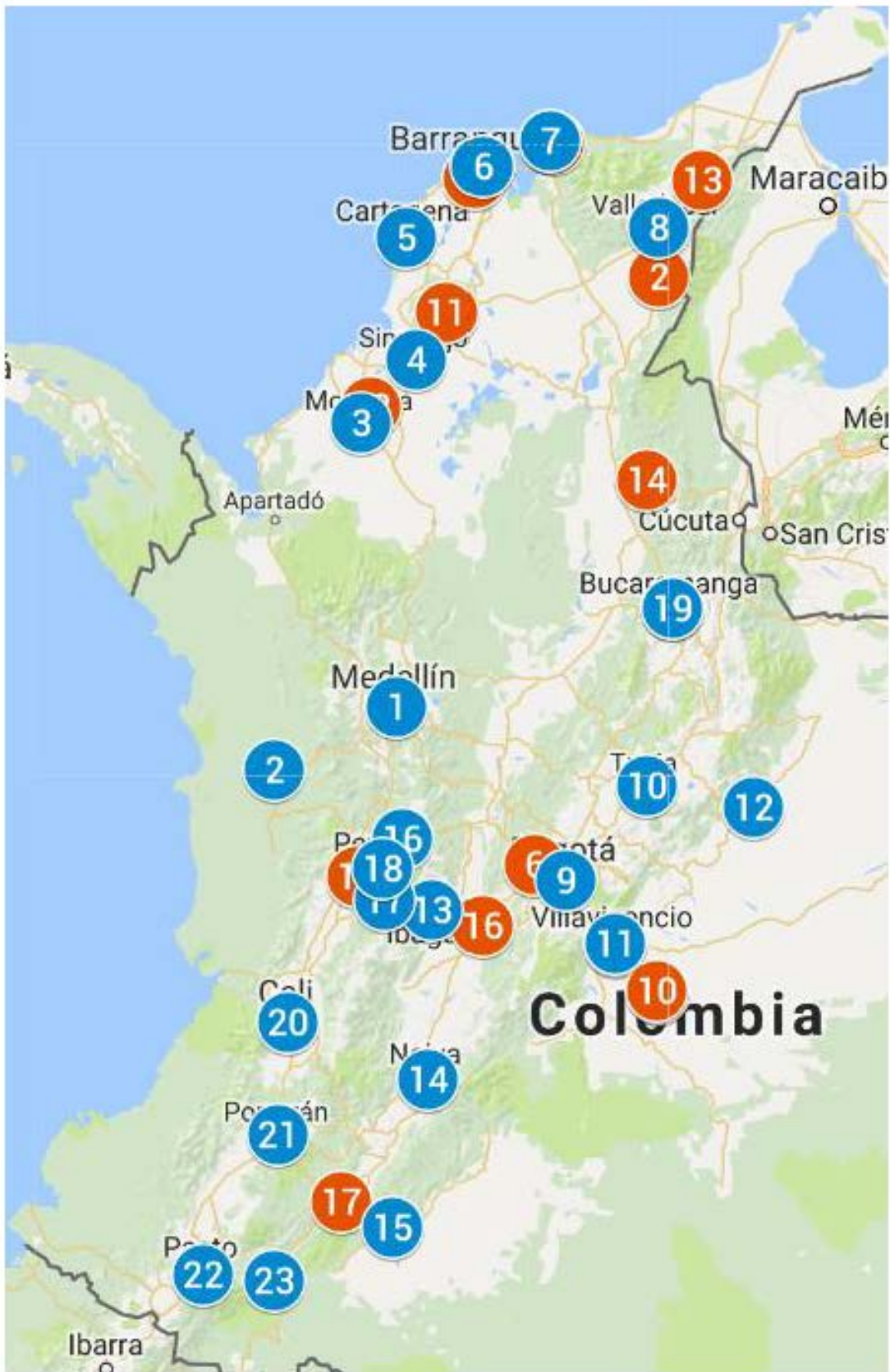


Figure 6. 4. Principal plant location referred by demand location

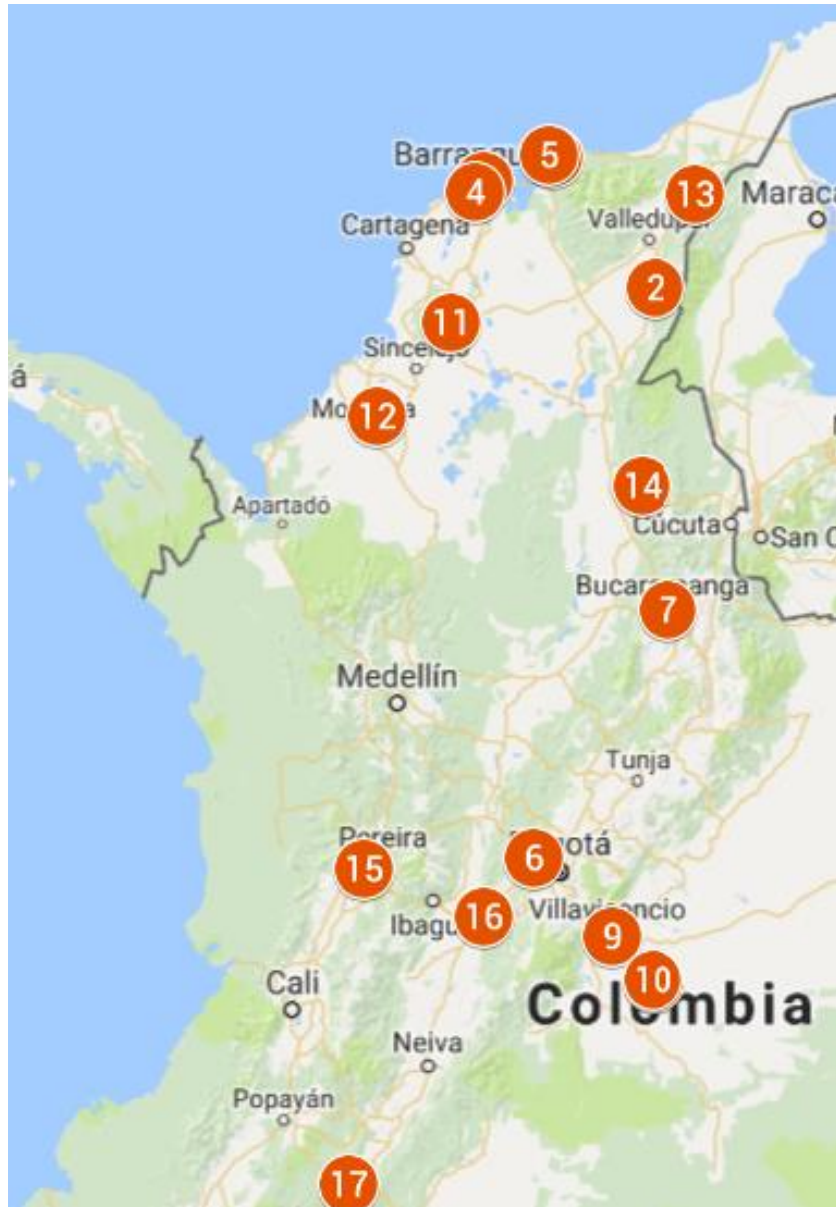


Figure 6. 5. Graphical representation for potential location for main production biorefinery plants

Installation cost of main production plants. Based on Basto Aluja (2016) and Bueno et al. (2015) the installation cost of principal production plant ($Inv_{k,d,g}$) was calculated and the plant capacity ($CapW_{k,d,g}$) was determined, as is detailed on Appendix 6.4 and summarized on Table 6.15.

Table 6. 15. Summary of installation cost of main production plants (USD)

Transformation technology	Production capacity at principal plants		
	$CapW_{k,d,g=1} =$ 40,000 Ton/Year	$CapW_{k,d,g=2} =$ 80,000 Ton/Year	$CapW_{k,d,g=3} =$ 120,000 Ton/Year
$d = 1$	14 200 000	18 800 000	31 500 000
$d = 2$	18 400 000	27 300 000	44 200 000
$d = 3$	9 200 000	11 800 000	20 500 000
$d = 4$	13 500 000	20 400 000	33 400 000
$d = 5$	10 200 000	12 800 000	21 500 000
$d = 6$	14 500 000	30 200 000	34 300 000

As can be noted, it is assumed that there is no difference on installation cost among the different plant localizations. This assumption could be easily adjusted, when the data required will be available. The values calculated are similar to the installation cost found by (Muñoz Baena 2013). Therefore, it is assumed that these values can be used in the integrated model.

Operational cost at the main production plants. Based on Basto Aluja (2016) and Bueno et al. (2015), the operational cost of the principal production plant ($ProdCost_{b,k,d,g}$) was calculated for this particular case. The detailed calculation is presented in Appendix 6.5 and summarized in Table 6.16.

Table 6. 16. Production cost at principal production plants by intermediate product and technology ($ProdCost_{b,k,d,g}, \forall k$)

Intermediate Products		Tech.	Transformation cost (USD/t oil)		
			40,000 t/year $g = 1$	80,000 t/year $g = 2$	120,000 t/year $g = 3$
1	Jatropha Oil	$d = 1$	432	397	371
1	Jatropha Oil	$d = 2$	539	495	462
1	Jatropha Oil	$d = 3$	409	383	366
1	Jatropha Oil	$d = 4$	517	482	458
1	Jatropha Oil	$d = 5$	405	379	362
1	Jatropha Oil	$d = 6$	514	479	455
2	Palm Oil	$d = 1$	448	412	384
2	Palm Oil	$d = 2$	558	513	478
2	Palm Oil	$d = 3$	424	397	379
2	Palm Oil	$d = 4$	535	499	475
2	Palm Oil	$d = 5$	420	393	375
2	Palm Oil	$d = 6$	533	497	472

6.2.4. Final Products

As stated above, one of the main objectives of this research is to design sustainable phase III biorefineries. Therefore, a variety of end-products with high added value must be produced. Accordingly, as presented in section 6.2.3, biodiesel, glycerol and polyester were selected as final products at the main production plants. Therefore, it is necessary to know the corresponding market prices and demands, which are presented below.

Final products demand. To establish biodiesel demand it is necessary to know the diesel consumption (Rincón et al. 2015) and the mandatory percentage of biodiesel consumption per location (Fedebiocombustibles 2017). Based in this information, the biodiesel demand calculation was performed as presented in Appendix 6.6.

Secondly, in order to determine the glycerol demand, the Annual Manufacturing Survey of Colombia (DANE 2017a) is used. The detailed found information of the annual manufacturing survey by location corresponds to 2007. Therefore, the calculation for the glycerol demand by the year 2015 is presented on Appendix 6.7. Finally, to define the polyester demand the unsaturated polyester resin consumption

took into account as aliphatic polyester, as well as its use as additive for polyurethanes production. The data source utilized is the Annual Manufacturing Survey of Colombia (DANE 2017a); and the calculations are presented on Appendix 6.8. The resume to final product demands ($Dem_{l,a}$) is presented on table 6.17 and geographical distributed as shows figure 6.6.

Table 6. 17. Final products demand by location and product type ($Dem_{l,a}$)

<i>l</i>	Final Products (Tons/Year)			Location	Department
	Biodiesel <i>a</i> = 1	Polymer <i>a</i> = 2	Glycerol <i>a</i> = 3		
1	37,382.76	10,922.55	4,282.88	Medellin	Antioquia
2	37,382.76	0.00	0.00	Quibdo	Chocó
3	26,722.28	0.00	0.00	Montería	Cordoba
4	26,722.28	0.00	0.00	Sincelejo	Sucre
5	26,722.28	0.00	1,515.44	Cartagena	Bolivar
6	26,722.28	8.04	605.57	Barranquilla	Atlantico
7	26,722.28	0.01	0.00	Santa Marta	Magdalena
8	26,722.28	0.00	0.00	Valledupar	César
9	59,812.41	13.00	4,036.84	Bogota	Bogotá + Cundinamarca
10	29,906.21	0.00	0.00	Tunja	Boyacá
11	29,906.21	0.00	0.00	Villavicencio	Meta
12	29,906.21	0.00	0.00	Yopal	Casanare
13	12,437.23	0.00	0.00	Ibagué	Tolima
14	12,437.23	0.00	0.00	Neiva	Huila
15	12,437.23	0.00	0.00	Florencia	Caqueta
16	12,437.23	261.78	51.88	Manizales	Caldas
17	12,437.23	0.00	0.00	Armenia	Quindío
18	12,437.23	0.63	0.00	Pereira	Risaralda
19	24,945.53	0.00	4.83	Bucaramanga	Santander
20	28,001.53	175.39	8,938.23	Cali	Valle
21	28,001.53	0.00	628.85	Popayán	Cauca
22	28,001.53	0.00	0.00	Pasto	Nariño
23	28,001.53	0.00	0.00	Mocoa	Putumayo
	596,205.22	11,381.40	20,064.52	Total	



Figure 6. 6. Final products demand localization

Final products prices ($Prix_a$). The Colombian government regulates biodiesel prices, therefore, for 2015 it exists a monthly detail (Fedebiocombustibles 2017), analyzed on Appendix 6.9, which was used to estimate an average price of 1,124.86 USD/t in 2015. The market value for glycerol and polyester were calculated in based on the Annual Manufacturing Survey of Colombia (DANE 2017a). The data considered corresponds to *glycerol* and *unsaturated polyester resin* from the category *raw materials* in the survey, resulting in 3,663,249.4 Colombian peso/t for unsaturated polyester resin and 1,716,175.7 Colombian peso/t for glycerol at year 2015. Afterward, considering the average: 2,743.39 Colombian currency per U.S. (Banco de la República Colombia 2017), the market value for unsaturated polyester resin is 1,335.30 USD/t and for glycerol is 625.57 USD/t.

Product value in reuse at principal plants for final products was not considered ($value_{a,k} = 0 \forall a, k$) because in the present case study, these are not dedicated to any use, such as obtaining energy. Therefore, the reuse variables serve to estimate the annual final product inventory.

6.2.5. Intermediate products

In Colombia, refined palm oil is used as input to food production. Therefore, there exists a well-defined market for it, presented on the Annual Manufacturing Survey of Colombia (DANE 2017a). In contrast, refined jatropha oil is no yet marketable in Colombia and it is non-edible. Finally, the soaps and residues are not valorized in this research. Then, the intermediate product demand ($Dem_{m,b}$) is calculated at Appendix 6.10 and it is summarized in Table 6.18. The geographical localization is showed in figure 6.7. The market value for refined palm oil is calculated from product sales and their value. The data considered correspond to refined palm oil considered as product in Annual Manufacturing Survey of Colombia (DANE 2017a). Then, the price ($Prix_{b=2}$) is 942.19 USD/t.

No product value in reuse at pretreatment plants for intermediate products was considered ($value_{b,j} = 0 \forall b,j$), because in the present study, they were not dedicated to any use, such as obtaining energy. Therefore, the reuse variables serve to know an approximation of the annual intermediate product inventory

Table 6. 18. Refined African palm oil and its fractions sales in Colombia at 2015

m	Department	Location	$Dem_{m,b=2}$ (Ton)
1	Atlántico	Barranquilla	10,071.84
2	Cundinamarca	Bogotá	5,530.46
3	Magdalena	Santa Marta	55,758.15
4	Meta	Villavicencio	32,663.07
5	Valle	Cali	9,831.08
	Total		113,854.59



Figure 6. 7. Clients for intermediate products at Colombia

6.2.6. Distances and transport cost

Once the localization for suppliers, pretreatment plants, principal production plants, markets for intermediate products and final products, were defined, the distance matrix for the transport logistic can be established by using Google Maps. Therefore, four distance matrix were constructed taking into account the kilometers between two points. These matrix are presented on Appendix 6.11.

As the integrated model considers only the strategical supply chain decisions, at this stage only the overland transport cost will be considered, because decision on transport type corresponds to tactical and operational supply chain decisions.

In Colombia exists the “Integral system of efficient costs to transport freight by road” (Sistema integral de costos eficientes al transporte de carga por carretera) (MINTRANSPORTE 2017) presented on table 6.19, to establish transportation costs between two Colombian cities. The data presented is for two axle trucks; and the values are per kilometer and ton.

It is important to note that no restrictions for the truck weight are considered, because the type of transport and its scheduling are part of the tactical and operational supply chain decisions. Therefore, there are parts of the perspectives of this thesis. Also, there is no difference between types of products transported, because the difference will be marked by the quantity of product transferred.

Table 6. 19. Transportation cost at Colombia details (Colombian currency)

Detailed Cost				
Type of cost	Concept	Value per ton	Value per ton KM	Value per loaded trip
	Total Operation Costs	334,632.67	345.83	3,011,693.99
Fixed	Salary	31,281.33	32.33	281,531.93
	Capital	28,579.24	29.54	257,213.17
	Insurance contract	8,269.59	8.55	74,426.30
	Parking	2,177.65	2.25	19,598.85
	Taxes	736.80	0.76	6,631.17
	<i>SUBTOTAL Fixed</i>	<i>71,044.60</i>	<i>73.42</i>	<i>639,401.41</i>
Variable	Fuel	114,490.92	118.32	1,030,418.31
	Maintenance and repair	29,517.49	30.51	265,657.38
	Tolls	26,517.78	27.40	238,660.00
	Tires	17,954.22	18.55	161,587.95
	Lubricants	8,438.86	8.72	75,949.73
	Contingencies	4,483.09	4.63	40,347.84
	Washing and degreasing	2,146.52	2.22	19,318.72
	Filters	1,717.49	1.78	15,457.40
	<i>SUBTOTAL Variable</i>	<i>205,266.37</i>	<i>212.13</i>	<i>1,847,397.34</i>
Other	Fees and commissions	38,550.64	39.84	346,955.75
	Administration factor	15,105.32	15.61	135,947.87
	Retefuente and ICA	4,665.74	4.82	41,991.62
	Additional cost by waiting time	0.00	0.00	0.00
	<i>SUBTOTAL Others</i>	<i>58,321.69</i>	<i>60.27</i>	<i>524,895.24</i>

After searching all available combinations data between cities in Colombia, the transport cost per kilometer and ton, the value must to be exchanged to USD.

The model does not consider detailed transportation cost in the case of two transport points are within the same city. Therefore, it has been decided to define this transportation cost as the average transportation cost of the rest of cities. Furthermore, for the Colombian departments “Choco” and “Arauca” there is no available information. Therefore, the same average value calculated previously is assigned to these departments.

The transportation cost was assigned in the following form: if the document “Integral system of efficient costs to transport freight by road” includes only one city of the department, the value will be assigned to all the cities in that department. Differently, there are some departments with the detail for several cities. If the city searched is between the available cities data, the assigned cost will be the one that corresponds to the determined location. Otherwise, if the city is not among those detailed for department, the value will be taken for the capital. In such cases where the capital of the department does not have data, the average is calculated from cities located after and before in the road, as it is the case of Tunja in Boyacá, where there exists the detail transportation cost for Sogamoso and Duitama. Finally, the transport cost matrices ($TCost_{i,j}$, $TCost_{j,k}$, $TCost_{k,l}$, $TCost_{j,m}$) are presented in Appendix 6.12.

6.2.1. Discount rate for the NPV calculation (Discount Rate)

A five years lifetime for the biorefinery project is proposed for the NPV assessment ($i = 5$ years). This could be modified according to the need of the stake-holders later. A constant cash flow for the assessment period, 5 years, was assumed. However, this assumption could be changed when the model will be integrated with the tactic-operational models, to be developed later. Finally, the *Discount Rate* will be defined in 12%, a typical value for projects developed in Colombia (Departamento Nacional de Planeación Colombia 2013).

6.3. Parameter definition for the economic dimension equations

In this section nine parameters are described to be applied in the equations related to economic dimension in sustainability Phase III BioRSC design model, as present table 6.20. Pollution cost associated to biobased products production has to be determined. Some of the parameters defined in this section are going to be used in the environmental dimension equations too.

Table 6. 20. Economic dimension parameters

Parameter	General initial model	Model Chapter V				
		Economic	Political	Technological	Social	Environmental
$\phi_{x,b,d,g}$		(34)				
$PolCostAtm_x$		(34)				
$\psi_{y,n,c,f}$		(35)				
$\psi_{y,b,d,g}$		(35)				
$PolCostWat_y$		(35)				
$\omega_{z,n,c,f}$		(36)				(65)(66)
$\omega_{z,b,d,g}$		(36)				(65)(66)
$PolCostSolid_z$		(36)				

In Colombia there are several health and environmental regulations (UPME 2017a). Regulations directly related to the environment protection are:

- ✚ Wild flora and forests normativity
- ✚ Atmospheric resources normativity
- ✚ Wildlife and hunting normativity
- ✚ Water resources normativity
- ✚ Solid waste regulation
- ✚ Soil resources normativity

Between the norms associated with these regulations, a specific number of them can be related to the pollution generated by the industries. They are presented in the table 6.21.

Table 6. 21. Norms related to pollution in Colombia. Based on UPME (2017a) and Ministerio Medioambiente Colombia (2015).

Regulation Type	Norms	Description
Atmospheric resources normativity	Decree 2811, 1974	Code of natural resources and the environment Article 33, 192, 193: Noise control in infrastructure works
	Decree 02, 1982	Regulates Title I of Law 09-79 and Decree 2811-74. Sanitary provisions on atmospheric emissions. Article 7 to 9: Definitions and general rules Article 74: Prohibitions and restrictions on the discharge of particulate matter, gases and vapors into the atmosphere Article 75: Prevention of air pollution
	Law 99, 1993	SINA creation and provisions are issued on the environment. Article 5: Functions of the Ministry of Environment to establish standards for prevention and control of environmental deterioration.
	Resolution (0909), June 5, 2008	Establishes the norms and emission standards admissible of pollutants to the atmosphere by fixed sources
Water resources normativity	Decree 1541, 1978	Articles 211 to 219: Control of sewage discharges Articles 220 to 224: Landfills for domestic and municipal use Article 225: Agricultural dumping Articles 226 to 230: Industrial dumping Article 231: Regulation of dumping
	Decree 2858, 1981	Modifies decree 1541 of 1978
	Decree 1594, 1989	Liquid waste disposal regulations: Articles 1 to 21: Definitions Article 22 and 23: Water resource management Article 29: Uses of water; Article 37 to 50: Criteria for water quality Articles 60 to 71: Liquid waste spills Articles 72 to 97: Dumping regulations Article 142: Remuneration fees
	Law 99, 1993	Article 10, 11, 24, 29: Prevention and control of water pollution. Remuneration fees
	Decree 901, 1997	Remuneration fees for specific liquid discharges to bodies of water
	Resolution (631) 2015	Maximum permissible parameters and values in point discharges in surface water bodies
Solid waste regulation	Law 09, 1979	Sanitary measures on solid waste management
	Resolution 2309, 1986	Defines special waste, criteria for identification, treatment and registration. Establishes compliance and security compliance plans.
	CONPES 2750, 1994	Solid waste management policies
	Decree 605, 1996	Regulates Law 142 of 1994, regarding the handling, transportation and final disposal of solid waste.
	Law 430, 1998	Environmental prohibitive regulations are issued on hazardous wastes and other provisions are issued

Therefore, for the Colombian case, as presented in Chapter V, the pollution types are the following.

Atmospheric resources normativity. In Colombia, primary environmental quality standards that regulate the concentration of air pollutants that are harmful to health are related to stationary sources (Ministerio De Ambiente Vivienda Y Desarrollo Territorial et al., 2010). These norms regulate maximum concentrations relative to particulate material (MP10), Sulfur Dioxide (SO₂), Nitrogen Dioxide (NO₂), Lead (Pb) and Cadmium. However, there are no direct taxes or costs associated with the generation of emissions as in countries such as Australia (Nielson, 2010), United Kingdom (UK government, 2017) and Denmark (Bradbury and Van Dender, 2017). Therefore, for this case study the cost related to atmospheric emissions is not considered. However, in environmental dimension the emissions of atmospheric pollutants will be studied (Resolución 0909, 2008).

Water resources normativity. The Law 99 of 1993 provides three types of environmental taxes related to water resources: Retributive fees, compensatory fees and water user charges ("*Tasas Retributivas*", "*Tasas Compensatorias*" and "*Tasas por Utilización de Aguas*", respectively) (Colombian Government 1993).

- *Retributive fees.* The direct or indirect use of the atmosphere, water and soil to introduce or dispose of agricultural, mining or industrial wastes or sewage from any source, smoke, gases and harmful substances that are the result of anthropic or propitious human activities, or economic or service activities, whether or not lucrative, will be subject to the payment of fees for the harmful consequences of the activities expressed (Colombian Government 1993).
- *Compensatory fees.* These fees have been created to offset the costs of maintaining renewable natural resources (Colombian Government 1993).
- *Water uses charges.* The fee for use of water will be charged to all the users of water resource, whether natural or legal persons, public or private (Colombian Government 1993). This fee set by the National Government will be used to pay the costs of protection and renewal of water resources (Colombian Government 1993).

The basis to calculate the retributive and compensatory fees considers the economic evaluation of the social and environmental damages caused by the activity. Social damages, among others, are those caused to human health, landscape, public tranquility, public and private property and other assets with economic value directly affected by the polluting activity. Environmental damage is understood to affect the normal functioning of ecosystems or the renewability of their resources and components (Colombian Government 1993). Retributive and compensatory fees apply even pollution above the permissible limits without prejudice to the imposition of preventive and punitive measures that may be required. The collection of this fees does not imply under any circumstances the legalization of the respective dumping (Colombian Government 1993).

As conclusion, retributive fees are directed to charge for pollution of water, soil and atmosphere, by its harmful effects; while the compensatory fees are set by the use of renewable natural resources to offset the costs of maintaining their renewability (Blanco et al. 2008). In this sense, the water use charge is a compensatory fee for the use of water resources. To date, the Colombian Government has

only regulated the fees for water pollution and water use charges (Blanco et al. 2008). Therefore, as water uses charges are included on price per water consumption, following it only the retributive fees parameters were included in the integrated model.


The Ministry of environment will establish annually the value of the retributive fees (Colombian Government 1993). The minimum retributive fee for 2015 is (Ministerio Medioambiente Colombia 2017a):

$$\begin{aligned} \text{Biochemical Oxygen Demand} - \text{BOD} \text{ (Col \$ / kg)} &= 122.86 \\ \text{Total suspended solids} - \text{TSS} \text{ (Col \$ / kg)} &= 52.54 \end{aligned}$$


As 2,743.39 Cop \$ by USD in Colombia at 2015, then:

$$\begin{aligned} \text{PolCostWat}_{y=\text{BOD}} &= \text{Biochemical Oxygen Demand} - \text{BOD} \text{ (USD / t)} = 44.78 \\ \text{PolCostWat}_{y=\text{TSS}} &= \text{Total suspended solids} - \text{TSS} \text{ (USD / t)} = 19.15 \end{aligned}$$

These values correspond to PolCostWat_y . Therefore, $\psi_{y,n,c}$ and $\psi_{y,b,d}$ will be determined following.

 Pretreatment Plants. In the case of study, pretreatment plants have only one transformation technology. Then, it is necessary to know the sewage water rate generation by ton of raw material type processed. The moisture characteristic of the oil will determine the amount of sewage water generated.

The sewage water production estimation depending in BOD and TSS is presented in Appendix 6.13, and its value is $\psi_{y=\text{BOD},n,c,f} = 5 * 10^{-8} \frac{t \text{ BOD}}{\text{Raw Material } t}$ and $\psi_{y=\text{TSS},n,c,f} = 5 * 10^{-8} \frac{\text{ton TSS}}{\text{Raw Material } t}$, $\forall n, f$, and $c = 1$.

 Principal plants. The wastewater generated at principal production plants depends on the transformed intermediate products. Moreover, it can be analyzed also, depending on the amount of final product to be obtained.

According to Basto Aluja (2016), wastewater is generated from the biodiesel washing operation, required for biodiesel purification. Despite the two different methods of biodiesel washing were used, the amount of water is almost the same, only varying with the production capacity (Effects of production scales) (Basto Aluja 2016). In order to analyze the total wastewater generated in biodiesel production, according to the material balance tables, flows leaving the system with water content of around 90% were considered (Basto Aluja 2016). Thus, it is assumed, according to the simulation Basto Aluja (2016), that the same amount of wastewater is generated, regardless of technology used or type of raw material. Because palm oil and jatropha oil have been pretreated. Then, the sewage water does not depend on the type of incoming raw material, but only on the production capacity.

About polyester production, sewage water is generated due to moisture glycerol elimination in distillation column and as water vapor, which is generated as a by-product in the polycondensation reaction (Bueno et al. 2014). Then, it is required to consider the moisture rate of glycerol generated at biodiesel production, its density and BOD and TSS characteristics Basto Aluja (2016) and Glycerine Producers' Association (1975).

Finally, the wastewater production estimation depending in BOD and TSS at principal plants is presented in Appendix 6.13. It estimation is summarized in table 6.22 and 6.23.

Table 6. 22. TSS rate production at principal plants ($y = TSS, \forall b$)

$\psi_{y=BOD,b,d,g}$		
$\psi_{y=TSS,b,d=1,g=1} = 9,80 * 10^{-8}$	$\psi_{y=TSS,b,d=1,g=2} = 1,33 * 10^{-7}$	$\psi_{y=TSS,b,d=1,g=3} = 1,40 * 10^{-7}$
$\psi_{y=TSS,b,d=2,g=1} = 9,85 * 10^{-8}$	$\psi_{y=TSS,b,d=2,g=2} = 1,34 * 10^{-7}$	$\psi_{y=TSS,b,d=2,g=3} = 1,41 * 10^{-7}$
$\psi_{y=TSS,b,d=3,g=1} = 9,80 * 10^{-8}$	$\psi_{y=TSS,b,d=3,g=2} = 1,33 * 10^{-7}$	$\psi_{y=TSS,b,d=3,g=3} = 1,40 * 10^{-7}$
$\psi_{y=TSS,b,d=4,g=1} = 9,85 * 10^{-8}$	$\psi_{y=TSS,b,d=4,g=2} = 1,34 * 10^{-7}$	$\psi_{y=TSS,b,d=4,g=3} = 1,41 * 10^{-7}$
$\psi_{y=TSS,b,d=5,g=1} = 9,80 * 10^{-8}$	$\psi_{y=TSS,b,d=5,g=2} = 1,33 * 10^{-7}$	$\psi_{y=TSS,b,d=5,g=3} = 1,40 * 10^{-7}$
$\psi_{y=TSS,b,d=6,g=1} = 9,85 * 10^{-8}$	$\psi_{y=TSS,b,d=6,g=2} = 1,34 * 10^{-7}$	$\psi_{y=TSS,b,d=6,g=3} = 1,41 * 10^{-7}$

Table 6. 23. BOD rate production principal plants ($y = BOD, \forall b$)

$\psi_{y=BOD,b,d,g}$		
$\psi_{y=BOD,b,d=1,g=1} = 5,93 * 10^{-7}$	$\psi_{y=BOD,b,d=1,g=2} = 8,05 * 10^{-7}$	$\psi_{y=BOD,b,d=1,g=3} = 8,50 * 10^{-7}$
$\psi_{y=BOD,b,d=2,g=1} = 5,96 * 10^{-7}$	$\psi_{y=BOD,b,d=2,g=2} = 8,08 * 10^{-7}$	$\psi_{y=BOD,b,d=2,g=3} = 8,53 * 10^{-7}$
$\psi_{y=BOD,b,d=3,g=1} = 5,93 * 10^{-7}$	$\psi_{y=BOD,b,d=3,g=2} = 8,05 * 10^{-7}$	$\psi_{y=BOD,b,d=3,g=3} = 8,50 * 10^{-7}$
$\psi_{y=BOD,b,d=4,g=1} = 5,96 * 10^{-7}$	$\psi_{y=BOD,b,d=4,g=2} = 8,08 * 10^{-7}$	$\psi_{y=BOD,b,d=4,g=3} = 8,53 * 10^{-7}$
$\psi_{y=BOD,b,d=5,g=1} = 5,93 * 10^{-7}$	$\psi_{y=BOD,b,d=5,g=2} = 8,05 * 10^{-7}$	$\psi_{y=BOD,b,d=5,g=3} = 8,50 * 10^{-7}$
$\psi_{y=BOD,b,d=6,g=1} = 5,96 * 10^{-7}$	$\psi_{y=BOD,b,d=6,g=2} = 8,08 * 10^{-7}$	$\psi_{y=BOD,b,d=6,g=3} = 8,53 * 10^{-7}$

Solid waste regulation. In Colombia there is a commission for safe drinking water and basic sanitation (CRA 2017) that determines the tariff regime for public sanitation services. Details such as collect solid wastes cost and disposal cost are presented in the research Tello Espinoza et al. (2010) for Latin America and the Caribbean. Specifically to Colombia, the collect solid wastes cost is 34.12 USD/t and the disposal cost were 23.31 USD/t in 2010. These unit costs correspond to ceiling costs adapted to the different municipalities and, in the case of final disposal, also include the cost of treatment. Then, the total solid waste cost in 2010 was about 57.43 USD/t. This value can be updated with the Consumer price index variations between 2010 and 2015, with the detail presented on table 6.24.

Table 6. 24. Consumer Price Index in Colombia for water supply, sewerage and sanitation based on DANE (2017b) by total revenue (The CPI base is the year 2008, 100)

Year	2009	2010	2011	2012	2013	2014	2015
CPI for water supply, sewerage and sanitation	103.87	107.24	110.71	112.64	114.19	116.69	121.72

However, these values are for Colombian currency, reason why the exchange rate between Colombian currency and USD for 2010 is needed. The average exchange rate for 2010 was 1,898.68 Col \$/USD (Banco de la República Colombia 2017).

$$PolCostSolid_{z=1} = 57.43 \frac{USD}{Ton} * 1,898.68 \frac{Col \$}{USD} * \left(\frac{121.72\%}{107.24\%} \right) = 123,764.64 \frac{Col \$}{Ton}$$

And this value must to be actualized with the exchange rate for 2015.

$$PolCostSolid_{z=1} = \frac{123,764.64 \text{ Col \$ /Ton}}{2,743.39 \text{ Col \$ /USD}} = 45.1 \frac{USD}{Ton}$$

Then, the solid waste generation rate at pretreatment and principal production plants is required. Santos Oliveira et al. (2017) reported the most important residue in biodiesel production are the filtration earths impregnated with oil and biodiesel.

Due to the lack information about solid waste generation in Colombia, the research carried out by Santos Oliveira et al. (2017) is considered to calculate the rate of solid waste generation. The biodiesel production process considered in Brazil includes pretreatment units and catalytic reactors (Santos Oliveira et al. 2017). Generating in average 473.2 tons by year per year of filter material, these filters represents the 97% of the total hazardous solid generated at biodiesel plants that produce 100,000 biodiesel tons by year in Brazil (Santos Oliveira et al. 2017).

Then, the total hazardous solid generated will be approximately 473.2 tons by year. Therefore, it means that $473.2/100\,000 = 0.47\%$ is the percentage weight/weight for hazardous solid generation by biodiesel tons produced.

More information cannot be found about the different technologies for principal plants, or any details about the proportion of solid waste generated at pretreatment process and at principal plants for transesterification.

Therefore, it was decided to assume that 0.47% weight of hazardous solid is generated by weight of final products at pretreatment and principal plants for each processing technology.

The solid hazardous rate will be calculated for refined jatropha oil and refined palm oil at pretreatment plants. Also, glycerol is a byproduct in biodiesel production by transesterification; therefore, they should only be considered solid waste generation due to the production of biodiesel and polymers. The estimation detail is presented in Appendix 6.14 and summarized in tables 6.25 and 6.26.

Table 6. 25. Solid waste production rate at pretreatment plants $\forall f$

$\omega_{z=1,n,c,f}$
$\omega_{z=1,n=1,c=1,f} = 0.46\%$
$\omega_{z=1,n=2,c=1,f} = 0.43\%$
$\omega_{z=1,n=3,c=1,f} = 0.43\%$

Table 6. 26. Solid waste production rate at principal plants $\forall g$

$\omega_{z=1,b,d,g}$	
$\omega_{z=1,b=1,d=1,g} = 0.46\%$	$\omega_{z=1,b=1,d=2,g} = 0.55\%$
$\omega_{z=1,b=1,d=3,g} = 0.47\%$	$\omega_{z=1,b=1,d=4,g} = 0.56\%$
$\omega_{z=1,b=1,d=5,g} = 0.47\%$	$\omega_{z=1,b=1,d=6,g} = 0.56\%$
$\omega_{z=1,b=2,d=1,g} = 0.48\%$	$\omega_{z=1,b=2,d=2,g} = 0.57\%$
$\omega_{z=1,b=2,d=3,g} = 0.48\%$	$\omega_{z=1,b=2,d=4,g} = 0.57\%$
$\omega_{z=1,b=2,d=5,g} = 0.49\%$	$\omega_{z=1,b=2,d=6,g} = 0.58\%$

6.4. Political dimension analysis

There are fifteen parameters related to the political dimension in sustainability analysis, as table 6.27 presents. They can be subdivided in parameters related to government incentives for production plants installation, government revenues not received by tax reduction on biobased products, biobased product consumption trends, government technological investments and land certification.

Table 6. 27. Political dimension parameters

Parameter	General initial model	Model Chapter V				
		Economic	Political	Technological	Social	Environmental
$incCap_j$			(37)(41)			
$incPerP_j$			(37)(41)			
$incCap_k$			(38)(42)			
$incPerW_k$			(38)(42)			
$LimBudget$			(39)(41)(42)			
$TaxRed_a$			(40)			
$DemT_{l,a}$			(44)			
$BudgetaryLimProjectValueTech$			(45)			
$LimProjectValueTech_c$			(46)			
$PerProjTech_c$			(46)			
$ProjectValueTech_c$			(46)			
$LimProjectValueTech_d$			(47)			
$PerProjTech_d$			(47)			
$ProjectValueTech_d$			(47)			
$Certificate_{i,n}$			(48)			

6.4.1. Government revenues not received by tax reduction on biobased products

Tax incentives in Colombia are applied under the mechanism of value added tax reduction or exemption on determined products (Congreso de la Republica de Colombia 2004) and the purchase of equipment for certain companies that help promotion, development and use of Non-Conventional Energy Sources (Ministerio de Minas y Energía 2015).

The tax reduction for purchase of this type of equipment is assumed to be included in the estimation of investment costs, since these are based on studies carried out and applied in Colombia. Additionally, among the products obtained in the biorefinery described by the integrated model only biofuels have

tax exemptions (Ministerio de Minas y Energía and UPME 2015). Therefore, tax exemption in USD per ton of bioproduct type $a = 1$ sold must to be determined.

In Colombia, biodiesel is blended with diesel; therefore taxes associated to diesel consumption are the ones that are not collected due the government's incentive to consume biodiesel. According (DIAN 2015):

“The National Tax on gasoline and diesel will be liquidated on February 1, 2015 on taxable bases according to the following general or differential tariffs: For Gasoline Motor Current and ACPM, at a rate of \$ 1,136.62 per gallon.”

To transform this value to $\frac{USD}{Biodiesel\ t}$ it is needed the diesel density: $856\ kg/m^3$ (Universidad Nacional de Colombia 2014) and the equivalence between gallon and m^3 : $264.18\ galones\ U.S. = 1m^3$ (FAO 1983).

Then, the next estimation is made:

$$TaxRed_{a=1} = 1,136.62 \frac{\$Col}{gallon} * \frac{264.18\ gallon}{1\ m^3} * \frac{1\ m^3}{856\ Kg} * \frac{1,000\ kg}{Ton} * \frac{1\ USD}{2,743.39\ \$Col}$$

$$TaxRed_{a=1} = \mathbf{119.15} \frac{USD}{t}$$

6.4.2. Biobased product consumption trends

As global trends, it can be highlighted the fact that currently bioplastics represents about one percent of the about 300 million tons of plastic produced annually (European Bioplastics 2017). However, these bioplastics are mostly made of plants as sugar cane or corn (European Bioplastics 2017), which implies that most of the existing products are first generation biobased products. In the other hand, about the 18% of the international production of biodiesel is advanced, as is detailed on table 6.28.

Table 6. 28. Biodiesel global production in 2015 and percentage of advanced biodiesel produced (REN21 2017; Statista 2017)

Country	Production (in billion liters)	Percentage of advanced biodiesel produced	Reference
U.S.	4.8	28.0%	(EIA 2017)
Brazil	4.1	21.2%	(USDA 2016a)
Germany	2.8	21.9%	(UFOP 2016; USDA 2016b)
France	2.4	-	(USDA 2016b)
Argentina	2.1	-	(USDA 2016c)
Netherlands	1.5	51%	(Grinsven et al. 2015; USDA 2016b)
Indonesia	1.5	-	(USDA 2016d; GreenFacts 2017)
Thailand	1.2	-	(USDA 2016e)
Malaysia	0.7	-	(USDA 2016f)
Belgium	0.6	-	(USDA 2016b; Ecoconso 2017)
Colombia	0.6	-	(USDA 2016g)
Spain	0.6	29.0%	(USDA 2013)
China	0.4	100.0%	(Kang 2014; USDA 2017)
Canada	0.3	44.0%	(USDA 2016h)
India	0.1	-	(USDA 2015)

- : No information about advanced biodiesel produced in these countries.

Therefore, one might expect that the objective will be to reach international parameters on advanced biodiesel production percentage, see Table 6.26, such as China or at least the international value of 18%. Then, it could be interpreted as *maximizing* the amount of advanced biobased products produced by the biorefinery.

Based in this information, one might expect that the Colombian government set as objective to reach international parameters on advanced biodiesel production percentage, such as China or at least the international value of 18%. Then, it could be interpreted as *maximizing* the amount of advanced biobased products produced by the biorefinery. Its means, the biobased products produced based in *jatropha curcas* (raw material type $n = 2,3$).

Considering the same countries detailed in Table 6.28, the $\frac{\text{biodiesel}}{\text{Total diesel}}$ rate established by government mandates are listed on Table 6.29. It can be noted that the blend required in Colombia is above the international average 5.72% and it is very close to developed countries as France, Netherland and U.S. However, little differences between some of these percentages represent a noticeable difference on produced amount of biodiesel, depending on the consumed diesel amount for each country. Specifically, for $\frac{\text{biodiesel}}{\text{Total diesel}}$ rate, there is a 20% blend that cannot be exceeded. Because most of the current diesel engines are only warranted for this blending rate (Australian Government 2012).

Table 6. 29. *Biodiesel/diesel* rate required globally at 2015

Country	%	Reference
U.S.	New York 10% Iowa 11%	(Lane 2016; EIA 2017)
Brazil	7.00	(USDA 2016a)
Germany	4.40	(UFOP 2016; USDA 2016b)
France	7.70	(USDA 2016b)
Argentina	8.40	(USDA 2016c)
Netherlands	6.25	(Grinsven et al. 2015; USDA 2016b)
Indonesia	3.10	(USDA 2016d; GreenFacts 2017)
Thailand	5.80	(USDA 2016e)
Malaysia	7.00	(USDA 2016f)
Belgium	6.00	(USDA 2016b; Ecoconso 2017)
Colombia	7.90	(USDA 2016g)
Spain	4.10	(USDA 2013)
China	0.76	(Kang 2014)
Canada	2.00	(USDA 2016h)
India	0.08	(USDA 2015)

Additionally, for the final products “glycerol” and “polyester” proposed, Colombian or international laws or regulations have not been found. Moreover, as presented before, internationally bioplastics represent only one per cent of the about 3,000 million tons of plastic produced annually (European Bioplastics 2017). Therefore, these are emerging markets.

It could be concluded that the objective is to reach the international values for the percentages of “Biobased product consumption”/“Total consumed product”. However, as no consumption regulation for all final products were found, this objective can be reformulated as the maximization of the demand

satisfaction with biobased products. And the value of $DemT_{l,\alpha=1}$ is the ACPM demand in Colombia, used for the biodiesel demand estimation presented on Appendix 6.6.

6.4.3. Government technological investments

Governmental budgetary support should be an integral part of biobased products policy for suppliers and producers to support livelihood during gestation period (Kumar et al. 2012). It budgetary support include suppression of sales tax on the products, provide minimum support prices for suppliers engaged with raw materials production, subsidies as tax credits, excise duty incentives for products or machines that enhance the use of biobased products (Kumar et al. 2012).

Currently, Colombia has a significant number of incentives for agricultural production, which also apply to crops of raw material for biobased products (García Romero and Calderón Etter 2012). Among them, loans with special interest rates and conditions, and the Incentive to Rural Capitalization (IRC), aimed to improve the competitiveness and sustainability of agricultural production. The latter can be used for the planting and maintenance of crops such as palm, cocoa, and coffee, among others (MinAgricultura 2017), as well as land adequacy, water resources management, acquisition of machinery and equipment for production, infrastructure, development of biotechnology and its incorporation into productive processes (MinAgricultura 2017).

An average subsidy value per hectare of crop or ton of raw material obtained does not exist in Colombia. Therefore, it is not possible to add this type of subsidy to the fiscal cost. However, due to the existence of the ICR, the result of the optimization of the biorefinery supply chain could be analyzed in the presence of variations in the raw materials availability and acquisition price.

An example of projects to develop production technologies for sustainable products is “Portafolio 100” (COLCIENCIAS 2016a), which offers support for eighteen-month projects, with a total budget of 4,000,000,000 Col\$ (1,458,050.08 USD, with 2,743.39 \$Cop/USD) and the value that will be delivered per project is 60% of the investment value or 300,000,000 Col\$ (109,353.76 USD, with 2,743.39 \$Cop/USD) per the project. Only if the project is within the lines of action of the call, among which are "Natural ingredients, bioproducts and bioprocesses for industrial uses and energy production" (COLCIENCIAS 2016b).

Then, considering this call for projects, the parameters for governmental expenditures related to research and development for biorefineries are presented on Table 6.30.

Table 6. 30. Parameters for governmental expenditures related to research and development for biorefineries

Parameter	Value
<i>BudgetaryLimProjectValueTech</i>	1,458,050.08 USD
<i>LimProjectValueTech_c</i>	109,353.76 USD
<i>PerProjTech_c</i>	60%
<i>ProjectValueTech_c</i>	-
<i>LimProjectValueTech_d</i>	109,353.76 USD
<i>PerProjTech_d</i>	60%
<i>ProjectValueTech_d</i>	-

Considering information on the value of a related project does not exist, it will be assumed that 60% of the value will always be higher than the maximum limit proposed by the government per project (109,353.76 USD); therefore, the limited is defined as follows:

$$0 \leq InvTechP_c \leq 109,353.76 \text{ USD}$$

$$0 \leq InvTechW_d \leq 109,353.76 \text{ USD}$$

This financing can be understood as financing to bring technology and products to the final market (COLCIENCIAS 2016c), as long as they have been commercially validated. Therefore, it is also required to know the technology readiness for the different technologies to apply in the case study ($MatOr_{\mathbb{X}}$: TRL value for technology \mathbb{X}). This will be described in section 6.5.

Returning to the subject of governmental investments in production technologies to move from a prototype stage to a commercial stage of a technology, there is not information or research that permits to know (or calculate) the amount of investment necessary to move from one level of TRL to another, for the technologies applied in the integrated model. It should be noted that some projects can be carried out to allow technology development, but without moving on it to a higher level of TRL; as process improvement to obtain better indicators in the different test environments For this reason, the relations between the amount of funding and the TRL changes are presented as a perspective work.

6.4.4. Land certification

In the case of Colombia, land certification scheme implemented is the “Round Table of Sustainable Palm Oil” (RSPO) (Selfa et al. 2014). This is a non-profit association that brings together various actors in the palm value chain, with the objective of promoting the production and use of palm oil with criteria of environmental, social and economic sustainability. The RSPO is the most recognized initiative in the international sphere in terms of sustainability for the sector (Fedepalma 2017a). Then, the objective will be to maximize the use of certified land for biobased products produced in the biorefinery.

Therefore, the parameter $Certificate_{i,n}$ take the value 1 if the supplier in the location i is RSPO certified in the production of the raw material type n or 0 otherwise. Then, it is needed to know the Colombian suppliers that are RSPO certified. Based on the information available in RSPO (2017), table 6.31 was built based on the suppliers location and the enterprises that are certified RSPO. It is assumed that in the location where a supplier is RSPO certified all other suppliers will also be. Due no production detail has been found for each supplier at each location.

Table 6. 31. Suppliers location RSPO certified in Colombia

<i>i</i>	Departament	RSPO Certification	Reference
1	Bosconia / Cesar	Extractora Palmariguaní S.A; Extractora Sicarare SAS; Industrial Agraria La Palma; Limitada-Indupalma LTDA; Extractora la Gloria SAS; Palmeras de la Costa S.A.; Palmas del Cesar S.A.; Oleoflores S A S	(Fedepalma 2016a)
5	Villa Nueva / Casanare	Extractora del Sur de Casanare S.A.S.	(Mesa Dishington 2013)
6	San Carlos de Guaroa / Meta	Aceites Manuelita S.A.; Fanagra S.A.; Hacienda La Cabaña S.A; Poligrow Colombia Ltda	(Mesa Dishington 2013; Manuelita 2017; Poligrow Colombia 2017)
10	Santa Marta / Magdalena	Palmaceite S.A.; C.I. Biocosta S.A.; Aceites S.A.; Extractora El Roble S.A.S; Extractora Frupalma S.A.	(Fedepalma 2016b; Aceites S.A. 2017; BioCosta S.A. 2017; Extractora El Roble S.A.S. 2017)

6.5. Technological dimension analysis

In this section, the technological dimension parameters can be classified into three groups: water needed in Phase III BioRSC, technological apprenticeship and technology readiness levels, as presented in table 6.32.

Table 6. 32. Technological dimension parameters

Parameter	General initial model	Model Chapter V				
		Economic	Political	Technological	Social	Environmental
$WRawMat_n$				(50)		(61)
$WPret_{n,c,f}$				(50)(51)		(61)
$WPlant_{b,d,g}$				(50)(51)		(61)
β				(54)(55)		
<i>TRL relations</i>				✓		

6.5.1. Amount of water consumed for produce raw materials and process it at biorefinery

To determine $WRawMat_n$, the evapotranspiration or daily water consumption is analyzed. This is equivalent to water lost by direct evaporation from the soil surface plus water lost through transpiration through leaf tissue (Mejía 2000). The complete estimation for palm and jatropha plants is presented on Appendix 6.15, based on (Jongschaap et al. 2007; Abou Kheira and Atta 2009; Alvarez Zarrate 2013; Bautista Rodríguez 2015) it is resumed as:

$$WRawMat_{n=1} = 6,943.62 \frac{t \text{ water}}{t \text{ palm oil}}$$

$$WRawMat_{n=2} = 11,637.93 \frac{t \text{ water}}{t \text{ Jatropha oil}}$$

$$WRawMat_{n=3} = 9,712.23 \frac{t \text{ water}}{t \text{ Jatropha oil}}$$

At pretreatment plants, there are only two stages that use water for the process: Degumming and deodorization, according with the research carried out by (Blanco Rodríguez 2007). Then, the estimation for water required for pretreatment plants is 2.03% of the crude oil utilized as raw material, as presented in Appendix 6.16.

At principal production plants, the main consumption of water is due to washing and equipment cooling. The estimation detail is presented on Appendix 6.16, based on (Bueno et al. 2014; Basto Aluja 2016; VAXA Software 2017). It is resumed in table 6.33, $\forall b$.

Table 6. 33. Water consumed at principal production plants by technology and capacity (t water/ t intermediate product)

Refined oil	Technology (d)	Production capacity at principal plants		
		$CapW_{k,d,g=1} = 40,000 \text{ Ton/Year}$	$CapW_{k,d,g=2} = 80,000 \text{ Ton/Year}$	$CapW_{k,d,g=3} = 120,000 \text{ Ton/Year}$
Jatropha Oil	d=1	6.31	7.27	7.41
Jatropha Oil	d=2	6.34	7.30	7.44
Jatropha Oil	d=3	6.08	7.18	7.34
Jatropha Oil	d=4	6.11	7.21	7.37
Jatropha Oil	d=5	6.06	7.10	7.25
Jatropha Oil	d=6	6.09	7.12	7.28
Palm Oil	d=1	6.36	7.30	7.43
Palm Oil	d=2	6.39	7.32	7.45
Palm Oil	d=3	6.14	7.21	7.36
Palm Oil	d=4	6.17	7.24	7.39
Palm Oil	d=5	6.10	7.11	7.26
Palm Oil	d=6	6.13	7.14	7.29

6.5.2. Technological apprenticeship

Related to the progress ratio, Fatty Acid Methyl Ester Biodiesel (FAME) has a $PR = 98\%$ (Chen et al. 2012). This is the only ratio found; therefore it could be used for all production technologies applied in the integrated model, due to lack of information. Then, the value $\beta = -0.029146346$ and the data about operational cost for pretreatment and principal plants can be used for the cost reduction calculation, as presented on Appendix 6.17.

Based on this information, the figure 6.8 was developed considering the amount of units produced only evaluated up to the maximum production capacity per production plant (120,000 Tons year). In figure 6.8, when producing the first 1,000 t, the cost of produce the 1,000th unit will be 353 USD/t, compared with initial production cost it will signify 78.78 USD/t cost reduction. However, when production reaches 40,000 tons in first year, the cost reduction will be 317 USD/t. Finally, when the accumulated production is 80,000 in the second operation year (because the maximum production capacity by year is 40,000 tons), the cost reduction in comparison with initial production cost will be

only 311 USD/t. It shows that, for the case study with a $PR = 98\%$, the greatest reduction of operational costs occurs in the first year of operation.

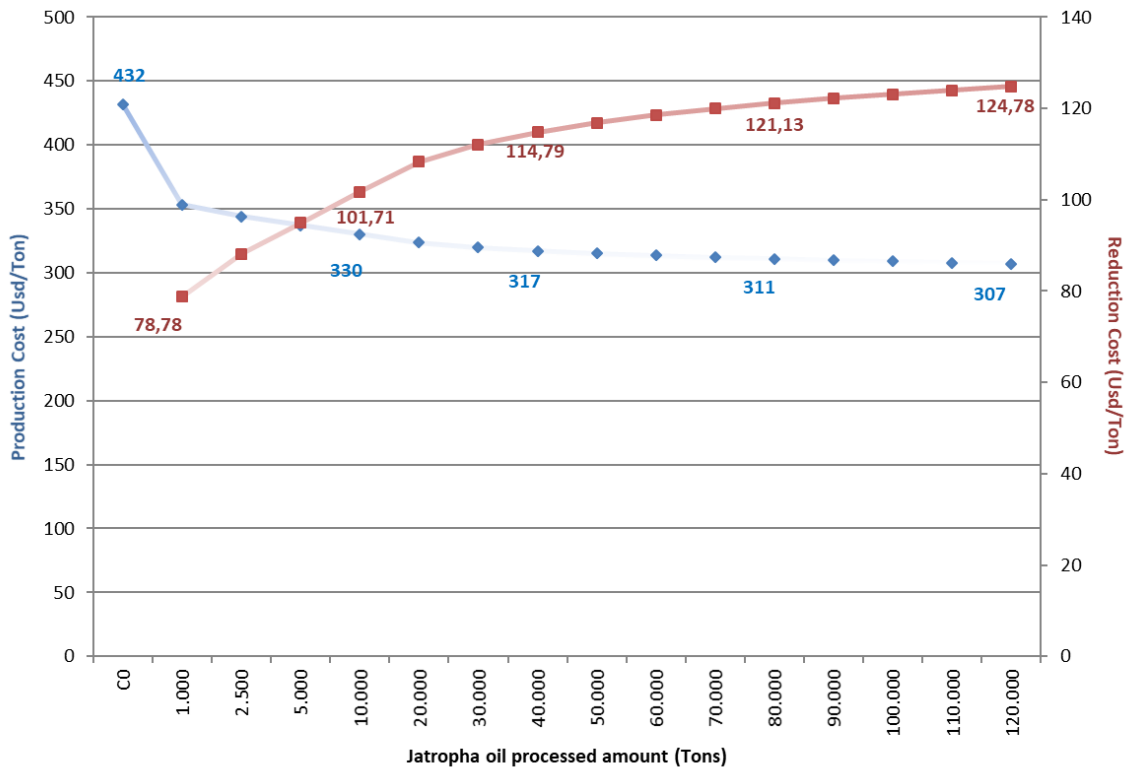


Figure 6. 8. Operational cost for the jatropha oil transformation ($b = 1$) with technology $d = 1$ and production capacity $g = 1$ (40,000 tons/year) at principal plants

Therefore, regarding scarcity of information and trying to simplify the mathematical relationship; it is decided to consider the operational cost including the technology apprenticeship as a model parameter and not as a function. Assuming that the maximum capacity use is searched and as consequence the maximum cost reduction is achieved in the first year of operation.

Then, the operational cost can be calculated as follows: for the capacity of 40,000 tons/year the operational cost considered will be the cost of produce the 40,000-th unit; for the capacity of 80,000 tons/year the operational cost is the cost of produce the 80,000-th unit; and for the capacity 120,000 tons/year the operational cost is the cost of produce the 120,000-th unit. Tables 6.34 and 6.35 presents the operational cost that integrates technology apprenticeship.

Table 6. 34. Operational cost that integrates technology apprenticeship at pretreatment plants

Pretreatment capacity (f)	Raw material type (n)		
	Palm oil	Jatropha oil by manual extraction	Jatropha oil by electrical extraction
40,000	31.15	28.61	26.70
80,000	28.65	26.31	24.55
120,000	28.31	26.00	24.26

Table 6. 35. Operational cost that integrates technology apprenticeship at principal plants

		Initial operational cost		Operational cost integrating technology reductions	
Production technology (d)	Capacity (g)	Entering Materials		Entering Materials (b)	
		Jatropha oil refined (b=1)	Palm oil refined (b=2)	Jatropha oil refined (b=1)	Palm oil refined (b=2)
1	1	432	448	317.21	328.96
1	2	397	412	285.68	296.48
1	3	371	384	263.84	273.08
2	1	539	558	395.78	409.73
2	2	495	513	356.20	369.16
2	3	462	478	328.55	339.93
3	1	409	424	300.32	311.34
3	2	383	397	275.61	285.68
3	3	366	379	260.28	269.53
4	1	517	535	379.63	392.84
4	2	482	499	346.85	359.08
4	3	458	475	325.71	337.80
5	1	405	420	297.39	308.40
5	2	379	393	272.73	282.80
5	3	362	375	257.44	266.68
6	1	514	533	377.42	391.38
6	2	479	497	344.69	357.64
6	3	455	472	323.57	335.66

6.5.3. Technology Readiness Levels

Define the TRL level for each technology proposed for the biorefinery is necessary. Therefore, the analysis for technologies at pretreatment ($MatOr_c$) and principal plants ($MatOr_d$) is detailed following.

Pretreatment plants. The production technology considered is refining. This process is needed because the impurities of the crude oil have an enormous importance in the quality of the biodiesel (BioOILs 2011).

Some of the principal impurities are:

- ✚ Dirt, solids and metal particles from storage and transportation of the oil.
- ✚ Rubbers, naturally occurring in the source material, that hinder the reaction and purification of biodiesel, in addition to affecting its stability and phosphorus content.
- ✚ Metals, also present in naturally occurring oils, that have a huge importance in the stability of the oil against oxidation and for the proper conversion of the oil into biodiesel.
- ✚ Free fatty acids that react with the catalyst used in the production of biodiesel, hindering the complete transformation of the oil to biodiesel.
- ✚ Water, therefore, in the presence of the catalyst, causes oil saponification (formation of soaps).

Each unit that composes the process of pretreatment of crude vegetable oil, is destined to specifically eliminate some of the different impurities mentioned (Degummed, filtration, deacidification). This technology is currently used industrially (Chai et al. 2014), therefore, its TRL is "9" ($MatOr_c = 9$).

Principal plants. There are six different technologies under evaluation, which mix different transesterification process and polyesters production. They are analyzed below.

- *Base – catalyzed transesterification.* The commercial biodiesel is commonly produced by alkali-catalyzed transesterification, because it is the most economical process requiring only low temperatures and pressures and producing a 98% conversion yield (Leung et al. 2010; Lee et al. 2014; University of Strathclyde 2017). Then, as this technology is operating industrially, its TRL is “9”.
- *Polyesters production of from glycerol and adipic acid.* The production technology to obtain polyesters presented on research (“Techno-economic evaluation of the production of polyesters from glycerol and adipic acid”) is at laboratory test level. At this stage, large scale plants are simulated using dedicated software (Bueno et al. 2014). Then, this technology is tested in a high-fidelity laboratory environment and projected to larges scales, which correspond to TRL “6”.
- *Co – current and Counter – current transesterification.* There are registered patents for these two technologies (Veloza Cano 2016). However, they have only been tested at the test-bench scale. It is important to know that the research and development process can be considered divided into five stages, levels or scales: Laboratory, Test bench, Pilot, Semi-industrial and Industrial (González Castellanos 2000). The test-bench scale is the stage that is oriented to the configuration of the experimental units with geometric and operational characteristics similar to the available or recommended pilot or industrial plant equipment, unlike the laboratory stage, where the equipment used differs considerably of the industrial one. Containing a higher level of instrumentation and automation. Test-bench studies are a major step and can contribute to a significant reduction in research costs and in some cases to obviate the need for pilot-scale work. Then, it can be concluded that these technologies where tested on real operational environment using a Full-scale prototype built, which corresponds to TRL “7”.

Then, the lower level of both technologies mixed for each principal plant will be considered for the BioRSC design model, as resumed on table 6.36.

Table 6. 36. TRL at biorefinery principal production plants

Technology (d)	MatOr _d
1. Base-catalyzed transesterification	9
2. Base-catalyzed transesterification and Polyesters production	6
3. Co-current transesterification	7
4. Co-current transesterification and Polyesters production	6
5. Counter-current transesterification	7
6. Counter-current transesterification and Polyesters production	6

Therefore, the maximum TRL value that can be achieved, considering only the installed technologies, needs an auxiliary variable for the calculation of the maximum TRL value that describes if a technology is installed:

$$TechSelection_c = \begin{cases} 1 & \text{if technology } c \text{ is used (If } 0 < \sum_j \sum_f PP_{j,c,f} \text{)} \\ 0 & \text{in other case} \end{cases}$$

$$TechSelection_d = \begin{cases} 1 & \text{if technology } d \text{ is selected (If } 0 < \sum_k \sum_d W_{k,d,g} \text{)} \\ 0 & \text{in other case} \end{cases}$$

So, to calculate the maximum TRL value the objective function can be described as equation (75).

$$Max \left\{ \sum_c MatOr_c * TechSelection_c + \sum_d MatOr_d * TechSelection_d \right\} \quad (75)$$

Where the parameters are:

$MatOr_c$ = Original or current Technology readiness level of technology c

$MatOr_d$ = Original or current Technology readiness level of technology d

6.6. Social dimension analysis

This section includes the potential location restrictions analysis, the GINI values for objective function and the parameters related to employment opportunities generated by the Phase III BioRSC, as presented in table 6.37.

Table 6. 37. Social dimension parameters

Parameter	General initial model	Model Chapter V				
		Economic	Political	Technological	Social	Environmental
$GINI_i$					(57)	
$GINI_j$					(57)	
$GINI_k$					(57)	
$Dem_{aE,l}$					(58)	
$GovInvE$					(58)	
ξ					(58)	
$DWork_{RM,i,n}$					(59)	
$IWork_{RM,i,n}$					(59)	
$DWork_{pret,c,f}$					(59)	
$IWork_{pret,c,f}$					(59)	
$DWork_{princ,d,g}$					(59)	
$IWork_{princ,d,g}$					(59)	

6.6.1. *Potential location social analysis*

This subsection is divided in two analyses. The first one evaluates the proposed locations with indigenous settlements and the second analyzes the density of abandoned properties or stripped, to avoid land title problems.

Indigenous settlements. To define the potential locations for raw material sources, pretreatment plant installations and principal production plants, it is required to analyze the proposed locations in function of protected geographical areas in the case study. In Colombia, there are protected areas due to indigenous settlements, presented in Figure 6.9 (ACNUR 2017; DANE 2017c). This map is compared to proposed locations in Appendix 6.18.

Comparing the proposed locations and the map presented in figure 6.9 it can be observed that among the potential sources of raw materials, position N°9 is next to “San Andres de Sotavento” (40 km), where the indigenous people of Senú are protected. At the same time, the same protected indigenous group is next to the proposed location of the pretreatment N°4 (35 km of distance). However, they are not considered exactly in the same geographical position. Also, none of the potential locations of main plants are proposed in areas belonging to indigenous peoples. Therefore, the proposed locations can be used in the integrated model.

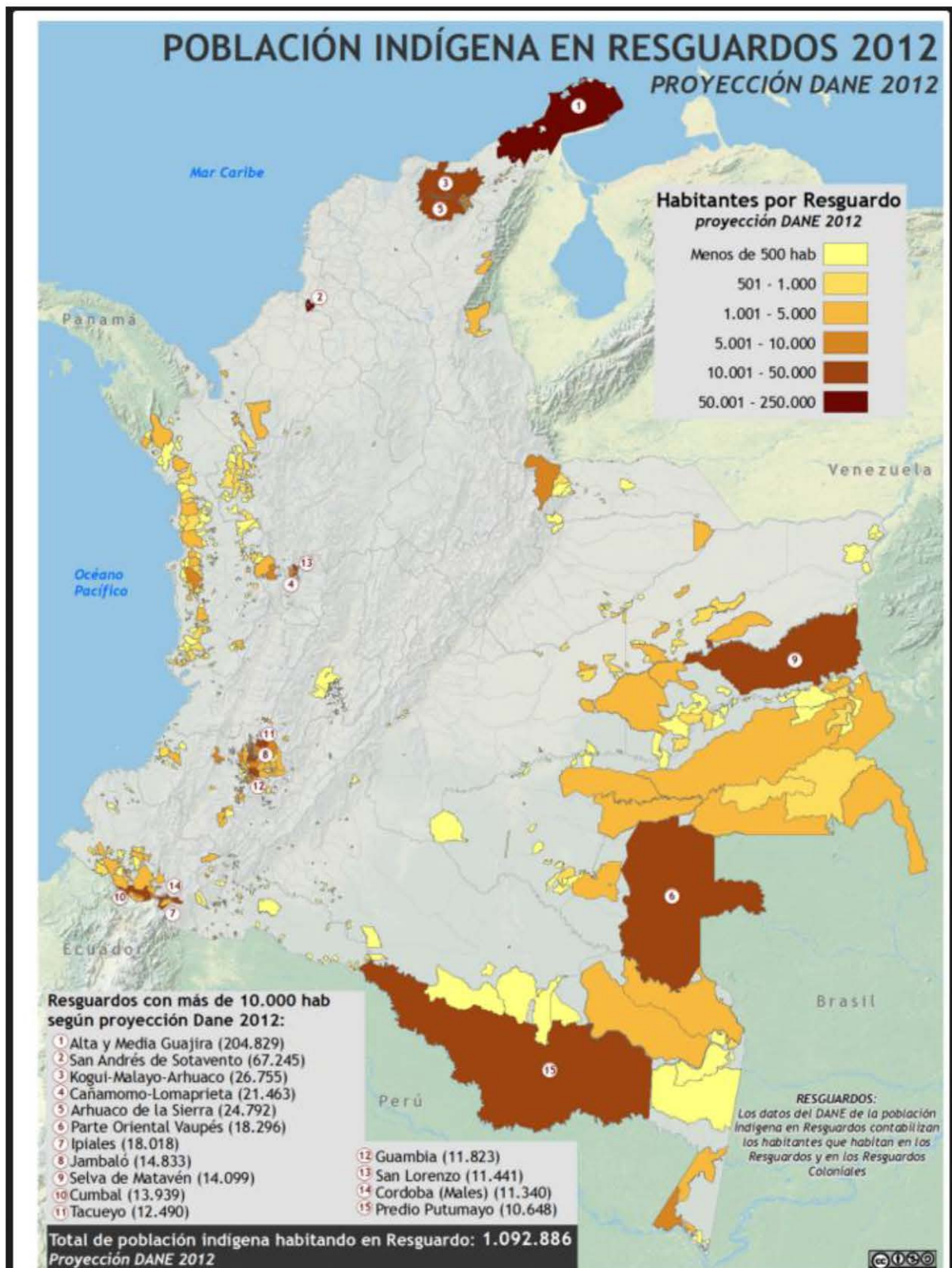


Figure 6. 9. Indigenous settlements in Colombia in 2012.

Density of abandoned of stripped properties. This is analyzed in order to not diminish or threaten land tenure. The distribution of the density of deprived or abandoned properties can be observed in the map presented in Figure 6.10. Thus, the objective would be generate industry directly in these sites after the government has facilitated the recognition of titles and have returned the lands to their owners, trying to not encourage the dispossession or sales of these hectares to large entrepreneurs (Unidad de Restitucion de Tierras 2016). Since it is not known whether the lands belonged previously to indigenous people or whether they were displaced or not, the alternative for this evaluation is the maximization of selection of suppliers of raw materials (locations), pretreatment plant locations and production plants In areas that do not have a high density of abandoned and / or stripped properties. Thinking of minimizing the possibility of affecting and increasing the displacement of existing populations in these areas. Therefore, a new parameter and a new objective function are defined to apply this analysis to the case study specific model.

$$HighDis_x = \begin{cases} 1 & \text{If location } x \text{ is in a high density of abandoned properties or stripped} \\ 0 & \text{In other case} \end{cases}$$

Then, the objective function can be described by equation (76).

$$Min \left\{ \sum_i HighDis_i * \left(\frac{\sum_n \sum_j \sum_c \sum_f N_{i,n,j,c,f}}{\sum_n \sum_j \sum_c \sum_f N_{i,n,j,c,f} + \varepsilon} \right) + \sum_j HighDis_j * \left[\sum_c \sum_f PP_{j,c,f} \right] + \sum_k HighDis_k * \left[\sum_d \sum_g W_{k,d,g} \right] \right\} \quad (76)$$

At potential location for suppliers, the locations that has a high value of density ($HighDis_i = 1$) are $i = 1,2,3,8,10,13$. In the other hand, the pretreatment plants proposed in lands with high density of abandoned properties or stripped are $j = 3,5,9,11$. Finally, for principal production plants, these which a high abandoned land density are $k = 1,2,5,11$.

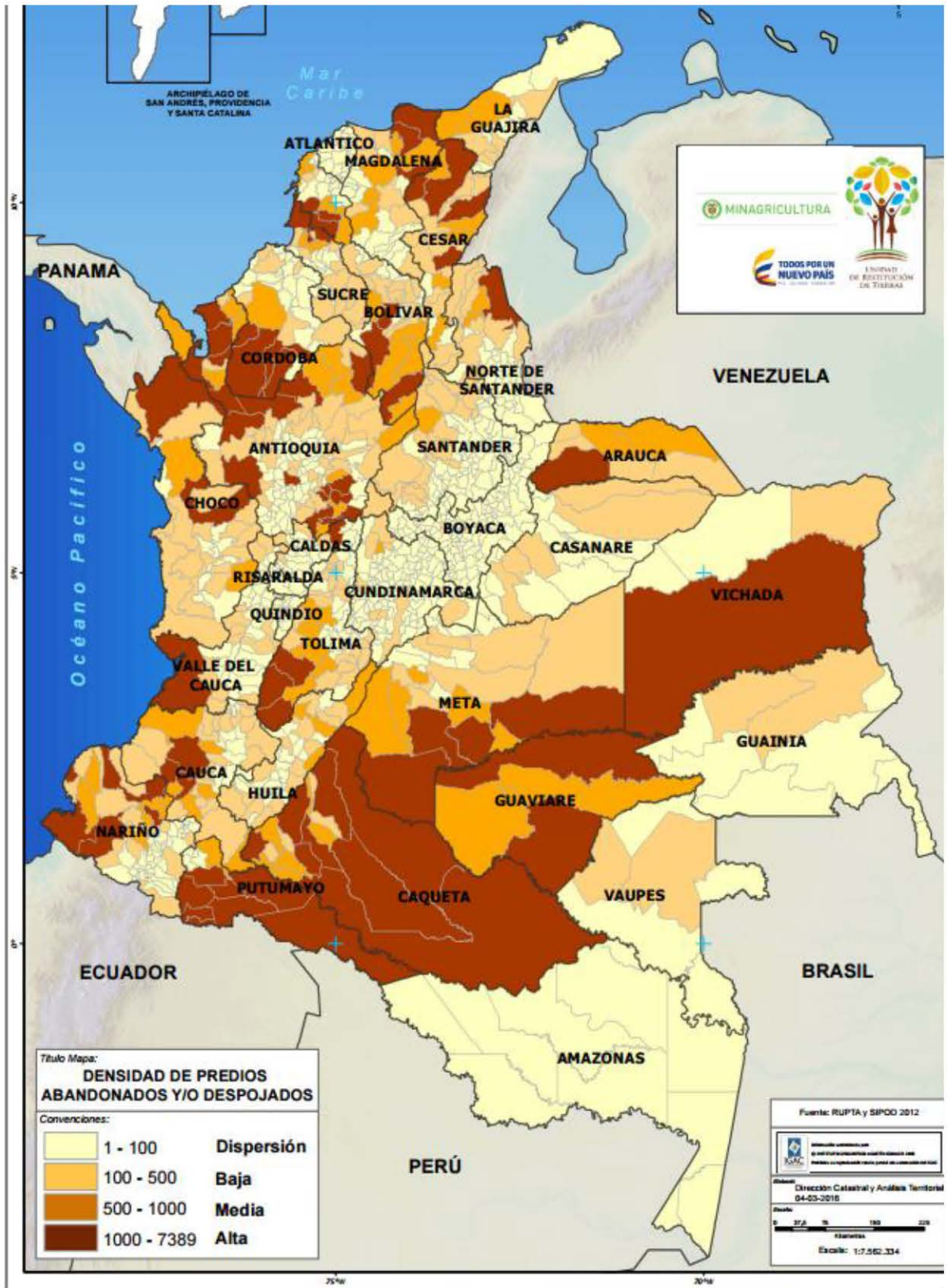


Figure 6. 10. Density of abandoned properties in Colombia.

6.6.2. GINI values

The GINI index for land ownership in Colombia can be found in Gobernación de Cundinamarca (2014) and IGAC (2012). Considering "GINI for owners without repetition" for 2009 (It takes into account for each owner the proportion of area of the property of which it participates), tables 6.38 and 6.39 were constructed. Values for Medellín are not listed; therefore, the national value is considered (GINI=0.885) (CEELAT 2013).

Table 6. 38. GINI index related to raw material locations.

N°	Department	Location	GINI
(1)	Cesar	Bosconia	0.605
(2)	Bolívar	María la Baja	0.753
(3)	Nariño	Tumaco	0.911
(4)	Santander	Barrancabermeja	0.752
(5)	Casanare	Villa Nueva	0.841
(6)	Meta	San Carlos de Guaroa	0.723
(7)	Cordoba	Montería	0.832
(8)	César	Agustín Codazzi	0.712
(9)	Sucre	Sincelejo	0.816
(10)	Magdalena	Santa Marta	0.713
(11)	La Guajira	Albania	0.701
(12)	Cundinamarca	Girardot	0.813
(13)	Antioquia	Medellín	0.885

Table 6. 39. GINI index related to pretreatment and principal plants locations.

Pretreatment Plants				Principal Plants			
	Location	Department	GINI		Location	Department	GINI
1	San Juan del Cesar	Magdalena	0.648	1	Santa Marta	Magdalena	0.713
2	Sabanalarga	Atlántico	0.646	2	Agustín Codazzi	Cesar	0.712
3	María La Baja	Bolívar	0.753	3	Barranquilla	Atlántico	0.289
4	Sahagún	Córdoba	0.744	4	Barranquilla	Atlántico	0.289
5	Tumaco	Nariño	0.911	5	Santa Marta	Magdalena	0.713
6	Palmira	Valle del Cauca	0.897	6	Facatativá	Cundinamarca	0.775
7	Garzón	Huila	0.678	7	Barrancabermeja	Santander	0.752
8	San Carlos de Guaroa	Meta	0.723	8	San Carlos de Guaroa	Meta	0.723
9	Envigado (Next to Medellín)	Antioquia	0.885	9	Castilla la Nueva	Meta	0.769
10	Santa Rosa de Cabal	Risaralda	0.810	10	San Carlos Guaroa	Meta	0.723
11	Fundación	Magdalena	0.767	11	El Carmen de Bolívar	Bolívar	0.659
12	Fusagasuga	Cundinamarca / Bogotá	0.806	12	Cerete	Córdoba	0.800
13	Villanueva	Casanare	0.841	13	Fonseca	La Guajira	0.616
14	Aguachica	Cesar	0.677	14	Ocaña	Norte de Santander	0.650
15	Natagaima	Tolima	0.747	15	Cartago	Valle del Cauca	0.744
16	Montería	Córdoba	0.832	16	Girardot	Cundinamarca	0.813
17	Corozal	Sucre	0.670	17	Pitalito	Huila	0.671

6.6.3. Employment opportunities in the Phase III BioRSC

To calculate the total employment opportunities generated in the Phase III BioRSC implementation the parameters related to raw material production ($DWork_{RM,i,n}$ and $IWork_{RM,i,n}$), pretreatment plants operation ($DWork_{Pret,c,f}$ and $IWork_{Pret,c,f}$) and principal plants operation ($DWork_{Princ,d,g}$ and $IWork_{Princ,d,g}$) are required.

Raw material production. The estimation for direct and indirect workers required by palm hectare are presented in Fedebiocombustibles (2017) (7 Worker/Hectare and 14 Workers/Hectare, correspondingly). Then, these values are multiplied with the palm hectare/pal oil tons rate to obtain the final value for employments opportunities generated by palm oil tons, as presented on Appendix 6.19.

To calculate the direct and indirect employments opportunities at jatropa cultivation, the estimation was made based in the information related to day laborers by harvest for palm and jatropa (Gaona Currea 2009), as presented on Appendix 6.19. Table 6.40 present the final values for the model parameters required.

Table 6. 40. Employment opportunities at raw material stage

i	n	$DWork_{RM,i,n}$ (Worker/Ton)	$IWork_{RM,i,n}$ (Worker/Ton)
1	1	0.04	0.02
2	1	0.07	0.03
2	2	0.22	0.11
2	3	0.17	0.08
3	1	0.10	0.05
4	1	0.05	0.03
5	1	0.04	0.02
6	1	0.04	0.02
7	2	0.22	0.11
7	3	0.17	0.08
8	2	0.22	0.11
8	3	0.17	0.08
9	2	0.22	0.11
9	3	0.17	0.08
10	1	0.03	0.02
10	2	0.22	0.11
10	3	0.17	0.08
11	2	0.22	0.11
11	3	0.17	0.08
12	2	0.22	0.11
12	3	0.17	0.08
13	2	0.22	0.11
13	3	0.17	0.08

Pretreatment plants operation. To determine the direct and indirect amount of workstations at pretreatment plants, the estimation was based on research carried out by Muñoz Baena (2013), who conducted a techno-economic study for a biodiesel plant with 100,000 ton/year production capacity, including the pretreatment stage in the production process.

It is supposed that the number of operators varies according to the capacity of the production plants, but the other types of workers are independent on capacity (Example: manager, administrative workers, security chief and assistant). It is also assumed that the pretreatment plant will have the same personnel requirements as the biodiesel plant presented in such research (Muñoz Baena 2013). Then, as presented in detail on Appendix 6.19, it is calculated that an operator is required for every 20,000 oil t/year processed. Table 6.41 resumes the potential employment opportunities that can be generated at pretreatment plants depending on technology and capacity production.

Table 6. 41. Employment opportunities at pretreatment plants

	Production capacity (<i>f</i>)		
	40,000	80,000	120,000
$DWork_{pret,c,f}$	10	12	14
$IWork_{pret,c,f}$	6	6	6

Principal plants operation. For the estimation of the direct and indirect quantity of workers required in the main plants, it is assumed that for the classical transesterification process ($d = 1$) it will be required the same amount of workers that at the biodiesel plant presented in research Muñoz Baena (2013), with variations according to the capacity of production as in the pretreatment plants. F

For the other technologies, because they are not currently industrialized ($TRL < 9$), it is assumed that at least one specialist must be included (One specialist for the co-current transesterification section, one specialist for the Counter-current transesterification section and one specialist for the production of polyesters). Therefore; the calculation of the number of job positions is summarized in table 6.42.

Table 6. 42. Employment opportunities at principal plants

	$DWork_{Princ,d,g}$			$IWork_{Princ,d,g}$		
	40,000 ($g = 1$)	80,000 ($g = 2$)	120,000 ($g = 3$)	40,000 ($g = 1$)	80,000 ($g = 2$)	120,000 ($g = 3$)
Base-catalyzed transesterification ($d = 1$)	10	12	14	6	6	6
Base-catalyzed transesterification and Polyesters production ($d = 2$)	11	13	15	6	6	6
Co-current transesterification ($d = 3$)	11	13	15	6	6	6
Co-current transesterification and Polyesters production ($d = 4$)	12	14	16	6	6	6
Counter-current transesterification ($d = 5$)	11	13	15	6	6	6
Counter-current transesterification and Polyesters production ($d = 6$)	12	14	16	6	6	6

6.7. Environmental dimension analysis

This section describes the parameters related to the environmental sustainability dimension, as gas emissions, soils and water degradation, wastewater rate production and energy balance for the Colombian case study, as detailed in table 6.43.

Table 6. 43. Environmental dimension parameters

Parameter	General initial model	Model Chapter V				
		Economic	Political	Technological	Social	Environmental
$GasEm_{p,a}$						(60)
$GasEm_{p,b}$						(60)
$TotalWaterAval$						(61)
$RecWatPret_{n,c,f}$						(62)
$RecWatPlant_{b,d,g}$						(62)
$\vartheta_{\tau,i,n}$						(63)
$SW_{n,c,f}$						(64)
$SW_{b,d,g}$						(64)
$WasteRecP_z$						(66)
$WasteRecW_z$						(66)
$\varepsilon_{\zeta,n}$						(67)
$CO_{2i,n}$						(68)
$CO_{2n,c,f}$						(68)
$CO_{2b,d,g}$						(68)
CO_{2a}						(68)
CO_{2b}						(68)
$CO_{2i,n,j}$						(68)
$CO_{2j,b,k}$						(68)
$CO_{2k,a,l}$						(68)
$CO_{2j,b,m}$						(68)
$RM Yield_{i,n}$						(69)
$RFuel_{i,n}$						(70)
$NRFuel_{i,n}$						(70)
$RFuelPret_{n,c,f}$						(70)
$NRFuelPret_{n,c,f}$						(70)
$RFuelPrinc_{b,d,g}$						(70)
$NRFuelPrinc_{b,d,g}$						(70)
$NRFuelLog_{n,i,j}$						(70)
$RFuelLog_{n,i,j}$						(70)
$NRFuelLog_{b,j,k}$						(70)
$RFuelLog_{b,j,k}$						(70)
$NRFuelLog_{a,k,l}$						(70)
$RFuelLog_{a,k,l}$						(70)
$NRFuelLog_{b,j,m}$						(70)
$RFuelLog_{b,j,m}$						(70)
θ_n						(71)
δ						(71)
$Dist_{i,j}$						(71)
$\beta_{n,c,f}$						(71)
$Dist_{j,k}$						(71)
$\beta_{b,d,g}$						(71)
$Dist_{k,l}$						(71)
$Dist_{j,m}$						(71)
θ_b						(71)
θ_a						(71)

6.7.1. Gas emissions generated by product consumption

The unique product that could generate gas emissions is biodiesel when it is burned (Long and Fang 2012; Bueno et al. 2015; Üinkel et al. 2016). Among the different gas emissions that can be generated by product consumption, such as CO, CO₂, CH₄, N₂O or particulate matter, (Antón Vallejo 2004; Bautista Rodríguez 2015), the found values correspond to hydrocarbons (CH₄) and nitrogen oxide (N₂O) emissions to air, which have the same emission rate (Rodríguez et al. 2016). And CO₂ emissions are evaluated in section 6.7.6.

The rate transformation required due measuring units is calculated follows:

$$\begin{aligned}
 GasEm_{\rho=CH_4, \alpha=1} &= \\
 0.034 \frac{\text{gr CH}_4}{\text{gallon biodiesel}} &* \frac{1 \text{Kg CH}_4}{1,000 \text{ gr CH}_4} * \frac{1 \text{ t CH}_4}{1,000 \text{ Kg CH}_4} * \frac{1 \text{ gallon}}{3.78541 \text{ litre}} * \frac{1 \text{ litre}}{0.000875 \text{ t biodiesel}} \\
 &= 1.03 e^{-5} \frac{\text{t CH}_4}{\text{t biodiesel}}
 \end{aligned}$$

$$\text{And then, } GasEm_{\rho=N_2O, \alpha=1} = 1.03 e^{-5} \frac{\text{t N}_2\text{O}}{\text{t biodiesel}}$$

6.7.1. Water availability and recycled water in production process

Insufficient information was available for the integration of water availability restriction and the recycled water objective function in the case study.

6.7.2. Water degradation for raw materials cultivation

Among the different water pollution components (Bautista Rodríguez 2015), nitrates, phosphorus and phosphates information was found in literature. It is important to highlight that these pollutants produce water eutrophication (European Comission - Environment 2006).

The estimation of the rate emission generation is detailed in Appendix 6.20. Based on BID and MMEC (2012) and Quispe et al. (2009). The resume is presented in table 6.44.

Table 6. 44. Water degradation rates by raw material type and location ($\vartheta_{\tau,i,n}$)

Location	Water degradation component								
	$i = 1$			$i = 2$			$i = 3$		
n	Nitrates (NO ₃)	Phosphorus (P)	Phosphates (P)	Nitrates (NO ₃)	Phosphorus (P)	Phosphates (P)	Nitrates (NO ₃)	Phosphorus (P)	Phosphates (P)
1	2.11%	0.33%	0.29%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%
2	4.09%	0.65%	0.55%	8.46%	1.57%	1.02%	7.06%	1.57%	0.85%
3	5.91%	0.94%	0.80%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%
4	3.17%	0.50%	0.43%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%
5	2.58%	0.41%	0.35%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%
6	2.45%	0.39%	0.33%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%
7	0.00%	0.00%	0.00%	8.46%	1.57%	1.02%	7.06%	1.57%	0.85%
8	0.00%	0.00%	0.00%	8.46%	1.57%	1.02%	7.06%	1.57%	0.85%
9	0.00%	0.00%	0.00%	8.46%	1.57%	1.02%	7.06%	1.57%	0.85%
10	2.02%	0.32%	0.27%	8.46%	1.57%	1.02%	7.06%	1.57%	0.85%
11	0.00%	0.00%	0.00%	8.46%	1.57%	1.02%	7.06%	1.57%	0.85%
12	0.00%	0.00%	0.00%	8.46%	1.57%	1.02%	7.06%	1.57%	0.85%
13	0.00%	0.00%	0.00%	8.46%	1.57%	1.02%	7.06%	1.57%	0.85%

6.7.3. Sewage water generation

As presented in Appendix 6.13 based on Basto Aluja (2016), Bueno et al. (2014) and Glycerine Producers' Association (1975) the sewage water generation is resumed in tables 6.45 and 6.46.

Table 6. 45. Sewage water rate generation at pretreatment plants (sewage water t/raw material t)

Raw Material	$SW_{n,c=1,f=1}$	$SW_{n,c=1,f=2}$	$SW_{n,c=1,f=3}$
$n = 1$	1%	0.001	0.001
$n = 2$	1%	0.007	0.007
$n = 3$	1%	0.007	0.007

Table 6. 46. Sewage water rate generation at principal plants (sewage water t/intermediate product t)

$SW_{b,d,g}$	Intermediate product					
	$b = 1$			$b = 2$		
	$g = 1$	$g = 2$	$g = 3$	$g = 1$	$g = 2$	$g = 3$
$d = 1$	5.16%	7.00%	7.39%	5.16%	7.00%	7.39%
$d = 2$	5.19%	7.03%	7.42%	5.19%	7.03%	7.42%
$d = 3$	5.16%	7.00%	7.39%	5.16%	7.00%	7.39%
$d = 4$	5.19%	7.03%	7.42%	5.19%	7.03%	7.42%
$d = 5$	5.16%	7.00%	7.39%	5.16%	7.00%	7.39%
$d = 6$	5.19%	7.03%	7.42%	5.19%	7.03%	7.42%

6.7.4. Solid waste recycled

As presented in Appendix 6.14 based on Santos Oliveira et al. (2017) the solid waste generation is resumed in tables 6.24 and 6.25, section 6.3. However, there was no information found about solid waste recycling. Therefore, the objective function will be evaluated as the minimization of solid waste generation, represented by equation (65), Chapter V.

6.7.5. Soils degradation due raw materials cultivation

Information related to direct discharges of nitrates or phosphorus to land in cultivation process for raw materials is not available. Then, it could be assumed that water discharges with this pollution types will affect land concentrations. Therefore, as perspective of this work it is required to evaluate the eutrophication generated by raw materials cultivation, integrating water and land deterioration.

In the other hand, to evaluate the amount and type of agrochemicals as fertilizers and pesticides, it is required to differentiate in the model the technology of raw materials cultivation. Therefore, it is a perspective of this work.

6.7.6. CO₂ equivalent emissions

To calculate the total CO₂ equivalent emissions generated in the Phase III BioRSC, the parameters related to raw material production ($CO_{2i,n}$), pretreatment plants operation ($CO_{2n,c,f}$), principal plants operation ($CO_{2b,d,g}$), logistics ($CO_{2i,n,j}$, $CO_{2j,b,k}$, $CO_{2k,a,l}$ and $CO_{2j,b,m}$) and product consumption (CO_{2a} and CO_{2b}) are required.

Raw material cultivation and oil extraction. Because raw materials used in this the case of study are cultivated, a CO₂ absorption is made by plants (Bruinsma 2009; Quispe et al. 2009; BID and MMEC 2012; Romero Angulo 2014) although there is a CO₂ generation in the process to transform the plant fruits in crude oil (Bruinsma 2009; Quispe et al. 2009). Therefore, Table 6.47 and 6.48 presents the values for each of these stages, without made assumptions in land use change. The detailed calculation is presented in Appendix 6.23.

Table 6. 47. CO₂ absorption made in raw material cultivation stage

Raw material location (<i>i</i>)	Raw material type (<i>n</i>)		
	1	2	3
1	-3.06	0.00	0.00
2	-5.94	-3.09	-2.58
3	-8.59	0.00	0.00
4	-4.60	0.00	0.00
5	-3.75	0.00	0.00
6	-3.55	0.00	0.00
7	0.00	-3.09	-2.58
8	0.00	-3.09	-2.58
9	0.00	-3.09	-2.58
10	-2.93	-3.09	-2.58
11	0.00	-3.09	-2.58
12	0.00	-3.09	-2.58
13	0.00	-3.09	-2.58

Table 6. 48. CO₂ generation at crude oil extraction stage

Raw material location (<i>i</i>)	Raw material type (<i>n</i>)		
	1	2	3
1	3.23	0.00	0.00
2	6.25	13.40	11.18
3	9.04	0.00	0.00
4	4.84	0.00	0.00
5	3.94	0.00	0.00
6	3.74	0.00	0.00
7	0.00	13.40	11.18
8	0.00	13.40	11.18
9	0.00	13.40	11.18
10	3.08	13.40	11.18
11	0.00	13.40	11.18
12	0.00	13.40	11.18
13	0.00	13.40	11.18

Raw material transformation at pretreatment plants and intermediate product transformation at principal Plants Oil refining is made at pretreatment plants (Basto Aluja 2016). This process is not always performed, transforming directly the crude oil in biodiesel (Wang et al. 2015). However, to obtain a good biodiesel quality it is required to homogenize raw materials (Basto Aluja 2016). Therefore, in order to estimate the CO₂-equivalent emitted in the transformation process at the pretreatment and principal plants the available data from Quantis (2017); Bruinsma (2009) and Renewable Fuels Agency (2010) will be used, as presented in Appendix 6.23 to obtain the values presented in table 6.49. and table 6.50.

Table 6. 49. CO₂ generation at pretreatment plants by raw material transformation (CO₂ equivalent t/t raw material)

Raw Material type	Pretreatment capacity (t/year)		
	40,000	80,000	120,000
<i>n</i> = 1	0.18	0.18	0.18
<i>n</i> = 2	0.17	0.17	0.17
<i>n</i> = 3	0.17	0.17	0.17

Table 6. 50. CO₂ generation at principal plants by intermediate products transformation (CO₂ equivalent t/t intermediate products)

Intermediate product	Technology	Capacity (t/year)		
		40,000	80,000	120,000
<i>b</i> = 1	<i>d</i> = 1	0.47	0.45	0.46
<i>b</i> = 1	<i>d</i> = 2	1.20	1.19	1.19
<i>b</i> = 1	<i>d</i> = 3	0.45	0.44	0.45
<i>b</i> = 1	<i>d</i> = 4	1.19	1.18	1.19
<i>b</i> = 1	<i>d</i> = 5	0.52	0.52	0.53
<i>b</i> = 1	<i>d</i> = 6	1.27	1.27	1.28
<i>b</i> = 2	<i>d</i> = 1	0.47	0.45	0.46
<i>b</i> = 2	<i>d</i> = 2	1.18	1.16	1.17
<i>b</i> = 2	<i>d</i> = 3	0.45	0.44	0.45
<i>b</i> = 2	<i>d</i> = 4	1.17	1.16	1.17
<i>b</i> = 2	<i>d</i> = 5	0.52	0.52	0.53
<i>b</i> = 2	<i>d</i> = 6	1.25	1.25	1.26

Transport. In order to estimate the CO₂ emissions related to raw materials, intermediate products and final products transport, it is assumed that trucks will use only diesel as fuel (without biodiesel blended) for the transport for model simplification due blends disparities between cities in Colombia, as presented in Appendix 6.6. Therefore, as presented in Appendix 6.23, the rate of CO₂ equivalent generated by ton transported and km traveled is 0.0001618, value that should be multiplied by the distance matrix to obtain the final values for $CO_{2i,n,j}$, $CO_{2j,b,k}$, $CO_{2k,a,l}$ and $CO_{2j,b,m}$.

Product consumption. In the Colombian case study presented in this chapter glycerin is used in food, chemicals, pharmaceuticals, and cosmetics industry to produce another products (Glycerine Producers' Association 1975). Also, polymers are principally used in paint and textile industry (Bueno et al. 2015; Üinkel et al. 2016). Therefore, their direct consumption is CO₂ emission-free.

Finally, it is only required to know the CO₂ generated by biodiesel consumption, as calculated in Appendix 6.23, the CO₂ emissions are $0.60 \frac{\text{ton } CO_2}{\text{ton biodiesel}}$ (Fedebiocombustibles 2016).

6.7.7. Hectares required to produce raw materials used at the biorefinery

In this case of study the values for $RM\text{Yield}_{i,n}$ depend on raw material type and location, and the values are presented in table 6.51 (Gaona Currea 2009; Fedepalma 2017c). This estimation is based on the information presented on Appendix 6.1.

Table 6. 51. Hectares/t oil production rate

Raw material location (<i>i</i>)	Raw material type (<i>n</i>)		
	1	2	3
1	24.24%	0.00%	0.00%
2	46.95%	86.21%	71.94%
3	67.92%	0.00%	0.00%
4	36.36%	0.00%	0.00%
5	29.63%	0.00%	0.00%
6	28.11%	0.00%	0.00%
7	0.00%	86.21%	71.94%
8	0.00%	86.21%	71.94%
9	0.00%	86.21%	71.94%
10	23.15%	86.21%	71.94%
11	0.00%	86.21%	71.94%
12	0.00%	86.21%	71.94%
13	0.00%	86.21%	71.94%

6.7.8. Fuels used in the biorefinery SC

For the calculation of the amount of fuels and renewable fuels used in the biorefinery, only information related to transport consumption was found. The transformation process at pretreatment plants and principal plants are detailed in *MJ* consumed but not in fuels or electricity consumption (Bueno et al. 2015; Basto Aluja 2016). Therefore, in order to calculate the amount of fuels consumed by transport it is necessary to know the diesel consumption of trucks. Trucks spends 0.06 USD/(t * km) on average for fuel concept (MINTRANSPORTE 2017) and the average price for diesel in 2015 was 1,204.53 USD/t

(equivalent to 3.87569347 *USD/gal*) (UPME 2017b). Then, the consumption of diesel ACPM per ton transported and kilometer traveled can be calculated as follows:

$$FuelConsumptionLog = 0.06 \frac{USD}{t * km} * \frac{1 t diesel}{1,204.53 USD} = 4.98 * 10^{-5} \frac{t diesel}{t * km}$$

Then, this value must to be multiplied by the amount of *km* between raw material location and pretreatment plants, pretreatment plants and intermediate markets, pretreatment plants and principal plants and between principal plants and final products markets. These tables are presented in Appendix 6.21.

6.7.9. Energy balance

To conduct the energy balance, to analyze the energy consumed and the energy generated is required (Bautista Rodríguez 2015). Then, the values for the Colombian case are defined as follows:

Energy expenditure to transport the products (δ). This value is affected by fuel consumption in transportation and the calorific value, its estimation is presented in Appendix 6.22. The value for the case study is:

$$\delta = 2.1761 \frac{MJ}{t * km}$$

Moreover, it depends on distance transported ($Dist_{i,j}, Dist_{j,k}, Dist_{k,l}, Dist_{j,m}$), which is presented in Appendix 6.22.

Energy content for raw materials and products. Related to the raw materials, the palm oil energy content is $\theta_{n=1} = 36.543 MJ/kg$ (C.A. de Almeida et al. 2002). For jatropha oil two values were found 39.584 *MJ/Kg* (Chauhan et al. 2012) and 38,68 *MJ/kg* (Tiwari et al. 2007), then the average used is $\theta_{n=2} = \theta_{n=3} = 39.132 MJ/kg$. These values will be used for the raw materials and for the intermediate products obtained, because at the pretreatments plants they are only conditionate, but no transformed into different products.

Regarding the final products, Appendix 6.22 presents the obtained data. For all the end products, their characteristics are considered similar regardless the type of raw materials used to obtain them, considering quality standards that regulates the commercialization of these different products. Thus, the average value found in the literature for final products will be taken. For biodiesel, the combustion heat value will be $\theta_{a=1} = 38,943.6 MJ/t$. In the other hand, even though glycerol and aliphatic polymers will not be used for combustion, its value will be used to evaluate the energy generated. Thus, for glycerol it will be $\theta_{a=3} = 22,744.7 MJ/t$ and for polymer it is $\theta_{a=2} = 26,866.7 MJ/t$.

Energy consumption to transform products. The detailed calculation to define the values for $\beta_{n,c,f}$ and $\beta_{b,d,g}$ are presented on Appendix 6.22. Tables 6.52 and 6.53 summarizes the obtained results.

Table 6. 52. Energy expenditure to transform products in pretreatment plants

Raw Material type	Pretreatment capacity (t/year)		
	40,000	80,000	120,000
Palm oil ($n = 1$)	389.67	389.64	389.64
Jatropha oil ($n = 2, 3$)	365.70	365.64	365.64

Table 6. 53. Energy expenditure to transform products in principal plants

Intermediate product	Technology	Capacity (t/year)		
		40,000	80,000	120,000
$b = 1$	$d = 1$	8,294.45	8,068.23	8,190.99
$b = 1$	$d = 2$	21,385.30	21,159.08	21,281.84
$b = 1$	$d = 3$	7,933.33	7,833.97	7,966.68
$b = 1$	$d = 4$	21,194.54	21,095.18	21,227.89
$b = 1$	$d = 5$	9,239.37	9,217.74	9,400.81
$b = 1$	$d = 6$	22,684.58	22,662.95	22,846.02
$b = 3$	$d = 1$	8,294.45	8,068.23	8,190.99
$b = 3$	$d = 2$	20,962.79	20,736.57	20,859.33
$b = 3$	$d = 3$	7,933.33	7,833.97	7,966.68
$b = 3$	$d = 4$	20,765.22	20,665.86	20,798.57
$b = 3$	$d = 5$	9,239.37	9,217.74	9,400.81
$b = 3$	$d = 6$	22,248.44	22,226.81	22,409.88

6.8. Conclusions

As presented at the beginning of this chapter, there is a huge amount of parameters to be determined for each case study. Thus, it is necessary to make a large number of assumptions, estimations and calculations to obtain values close to reality, as well as reliable sources of information.

The idea of the present Colombian case study application is to design a sustainable Phase III BioRSC, due the availability of information, operation plants and many researches and researchers related to BioRSC Phase II in Colombia. For this reason, each source of information used to define the parameters in the Colombian case study proposed is correspondingly referenced and the year 2015 was fixed to use parameters contextualized in the same period of time.

In section 6.2, related to economical dimension parameters, it can be noted that in the Colombian case study presented it is required to integrate a restriction linked to the available hectares for jatropha oil. Even though the integrated model is a generic model that can be applied to any case study, due to the definition of decision variables related to raw material selection. Because, for jatropha oil, there are considered two systems for oil extraction. Then, one of the perspectives of this work is to integrate different cultivation and extraction technologies for biorefineries that use agricultural or cultivable raw materials.

Concerning political dimension analysis presented in section 6.4 and technological section 6.5; it was required to define decision variables, auxiliary variables and constraints in addition to objective functions. Because the TRL analysis must to be done for each technology proposed in the case study. Even though a simple analysis was made in this case study, further researches must to be done to establish the investment and different efforts required to reach each TRL level for each proposed production technology and the impact in uncertainty and risk decrease.

Also, to make more realistic the technological learning impacts in operational cost, to establish or to find the progress ratio for the technologies in development is required. This may be linked to the deeper TRL analysis required, presented as perspective previously.

The social dimension analysis permit the establishment of a new objective function related to the density of abandoned properties. However, it could be used previously, in the potential locations definition. By discarding the potential locations for raw material acquisition, pretreatment and principal production plants situated in high density or deprived or abandoned properties areas. In the same section, the amount of employment opportunities is analyzed. Then, for further research it can be suggested to relate the workstations produced with the production plants installation or operational cost. However, it must to be highlighted that it could result in a nonlinear relation.

Regarding the environmental dimension, it must be noted that some of the emissions can be grouped on Life Cycle Analysis (LCA) categories. As is made in the *CO₂ equivalent* emissions generation analysis, where are included the CO₂, CF₃Br, N₂O and CF₄ emissions. For example, emissions of NH₃, NH₄⁺, NO₂, Phosphates, P, NO₃⁻, NO₂⁻, N₂, N₂O and P₂O₅ can be grouped in LCA categories of eutrophication. This clustering could decrease the quantity of objective functions to evaluate the environmental dimension, facilitating the sustainability analysis. However, it is recommended that this perspective of work will be performed by a specialist in LCA.

Therefore, considering the last objective functions added to integrate the specific conditions of the Colombian case, there are twenty-three objective functions with the corresponding parameters for the multiobjective optimization, summarized in table 6.54.

Table 6. 54. *Total objective functions for the integrated model applied to the Colombian case.*

Eq	Objective functions	Eq	Objective functions
(23)	Net Present Value	(63)	Water deterioration / Nitrates
(33)	Capacity Use	(63)	Water deterioration / Phosphorus
(40)	Governmental expenditures	(63)	Water deterioration / Phosphates
(43)	Use of noon-food crops as raw materials (Advanced)	(64)	Wastewater generation
(44)	Demand satisfaction with biobased products	(65)	Solid waste generation
(48)	Certified land use	(68)	CO ₂ emissions
(49)	Raw material use	(69)	Hectares required
(50)	Total water use	(71)	Energy balance
(51)	Water used in process	(70)	Nonrenewable fuel sources
(57)	GINI	(75)	TRL
(59)	Work generation	(76)	Dispersion
(60)	Gas emissions /CH ₄		

Finally, the multiobjective optimization results for the integrated model applied to the Colombian case study presented in this chapter is presented in the next chapter.

6.9. References

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Chapter VII. Multiobjective algorithm and optimization results

7.1. Introduction

Once the model for a sustainable Phase III BioRSC and the parameters were presented, in this chapter the features of the adapted evolutionary algorithm NSGA-II programming for the multiobjective optimization, including the algorithm parameters used in the optimization and the strategy for the parents' generation are presented. In order to detail the multiobjective optimization results, at the end of this chapter, a brief sensitivity analysis and the model validation are presented.

7.2. NSGA-II parameters and parents production

The parameters utilized for the NSGA-II adapted algorithm programming are a population conformed by 600 individuals and 100 generations. The probability of generate mutation was established in 15% and the probability to generate crossover between parents was 75%. Finally, 75% of the individuals with the best value of Pareto front and crowding distance can be the parents for the next generation.

For the creation of parents for the first generation, it was decided to generate some initial individuals that comply with all the restrictions stated in the integrated model. Therefore, the initial individuals were generated by optimizing the linear objective functions of the integrated model using the *intligprogram* tool in Matlab®. Then, other optimizations were carried out by adding the constraint to satisfy at least the 50% of the final products demand. Then, optimizations were carried out using the integrated model constrains and adding the constraint *Net Present Value* > 0, for fifty-four initial individuals. Therefore, the multiobjective optimization uses these fifty-four initial individuals and generates 546 additional random individuals.

Then, as the integrated model comprises a total of twenty-three objective functions, as described in chapter VI, twenty-two pairwise comparisons were optimized to enlarge the amount of initial solutions. The *Net present value* objective function was selected to integrate the twenty-two possible pairwise comparisons with the remaining functions. 455 different individuals that satisfy with all restrictions stated in the integrated model were obtained. These individuals were used to run the final multiobjective optimizations, as is represented in Figure 7.1. The results related to these finals multiobjective optimizations are presented in section 7.3.

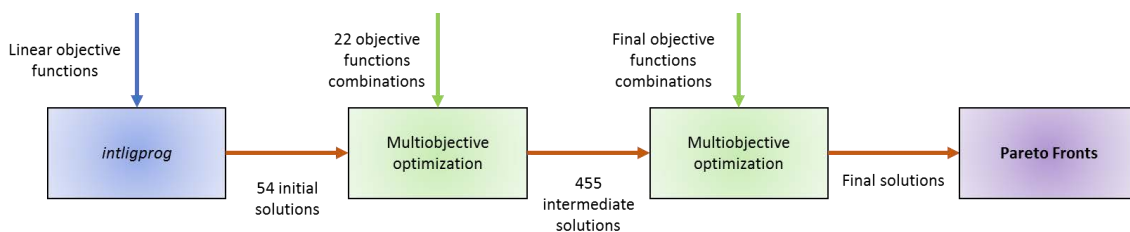


Figure 7. 1. Steps to population creation and Pareto fronts achievement

It must be noted that the NSGA-II adapted algorithm programming reduces the error of population generation after generation and generates new optimal solutions. Then, it verifies that the proposed adapted algorithm programming is suitable for the integrated integer constrained model multiobjective optimization.

7.3. Multiobjective optimization results

As presented in chapter VI, twenty-three objective functions are required for the integrated model applied to the Colombian case. In order to allow the decision maker to have a better representation of the correlation between objective functions, a pairwise comparison must be carried out. Consequently, there are 253 possible combinations for all the defined objective functions. However, to develop a first analysis, one objective function was chosen to represent each sustainability dimension and to compare it with the remaining objective functions. As presented in table 7.1, each cell represents an objective function comparison. Then, the objective functions selected for each dimension were: net present value maximization (economic); the demand satisfaction (political); the minimization of total water use (environmental); the TRL average (technological) and the average GINI index (social). In that way, 100 objective functions pairwise comparisons were made.

To better understand the information contained in table 7.1 the following color convention was used:

Red cells. In upper side of table 7.1, these cells represent comparison between each objective function and itself. Therefore they are not required to be made.

Black cells. They are by symmetry the mirror of the objective functions comparison cells under the red cells.

Then, the multiobjective optimization should be carried out to analyze the pairwise comparison of objective functions under the red cells. However, one of the most important goals when using multiobjective optimization is to find compromises between antagonistic or conflictual objective functions. Therefore, after conducting multiobjective optimization, green, dark blue and light blue cells were defined as:

Green cells. These cells represent pairwise comparison between objective functions in conflict. It means that a Pareto front is generated by the optimization.

Dark blue cells. They represent objective functions that are not in conflict among them.

Light blue cells. They represent multiobjective optimization not realized. Because, after analyze the objective functions comparison already undertaken, it can be expected that comparisons in light blue cells represents objective functions that are not in conflict among them, as dark blue cells.

Pareto fronts generated by each objective function comparison corresponding to the green cells will be analyzed in detail following.

Table 7. 1. *Objective function pairwise comparison*

Eq	Objective functions	Sustainability dimension				
		Economic	Political	Environmental	Technological	Social
		Net Present Value	Demand satisfaction	Total water use	TRL	GINI
(23)	Net Present Value					
(44)	Demand satisfaction with biobased products	✓				
(50)	Total water use	✓	✓			
(75)	TRL	✓	✓	✓		
(57)	GINI	✓	✓	✓	✓	
(33)	Capacity Use	✓	✓	✓	✓	✓
(43)	Use of noon-food crops as raw materials (Advanced)	✓	✓	✓	✓	✓
(48)	Max certified land use	✓	✓	✓	✓	✓
(49)	Min Raw material use	✓	✓	✓	✓	
(69)	Hectares required	✓	✓	✓	✓	
(40)	Governmental expenditures	✓	✓		✓	
(51)	Water in Process	✓	✓	✓	✓	
(76)	Dispersion	✓	✓	✓	✓	
(59)	Work generation	✓	✓	✓	✓	✓
(60)	Gas emissions /CH ₄	✓	✓		✓	
(63)	Water deterioration / Nitrates	✓	✓		✓	
(63)	Water deterioration / Phosphorus	✓	✓		✓	
(63)	Water deterioration / Phosphates	✓	✓		✓	
(64)	Wastewater generation	✓	✓	✓	✓	
(65)	Solid waste generation	✓	✓	✓	✓	
(68)	CO ₂ emissions	✓	✓		✓	
(71)	Energy balance	✓	✓	✓	✓	✓
(70)	Nonrenewable fuel sources	✓	✓		✓	

7.3.1. First Pareto front analysis

Once the whole set of pairwise comparison was established, it is possible to perform it's analysis, which is a very complex process for the decision maker. This complexity is related to the fact that a 2D plot representing a set of solutions could not be analyzed without considering the remaining graphical dimensions (Twenty-three total dimensions determined by the objective functions). Also, it implies a scale adjustment process to enable projection and links between the different pairwise comparisons. In order to illustrate these aspects, a particular example of two pairwise comparisons that integrates different sustainability dimensions is given.

The Pareto fronts analysis for the two pairwise comparisons with yellow border in table 7.1 are presented in Figure 7.2. That comparison was selected because it integrate most of the sustainability dimensions, because the net present value considers pollution cost, governmental subsidy to plant

installation and technology learning cost reductions (economic dimension); the demand satisfaction with biobased products is a governmental objective (political dimension), and the minimization of required hectares for the raw material production is targeted by environmental and technological dimensions.

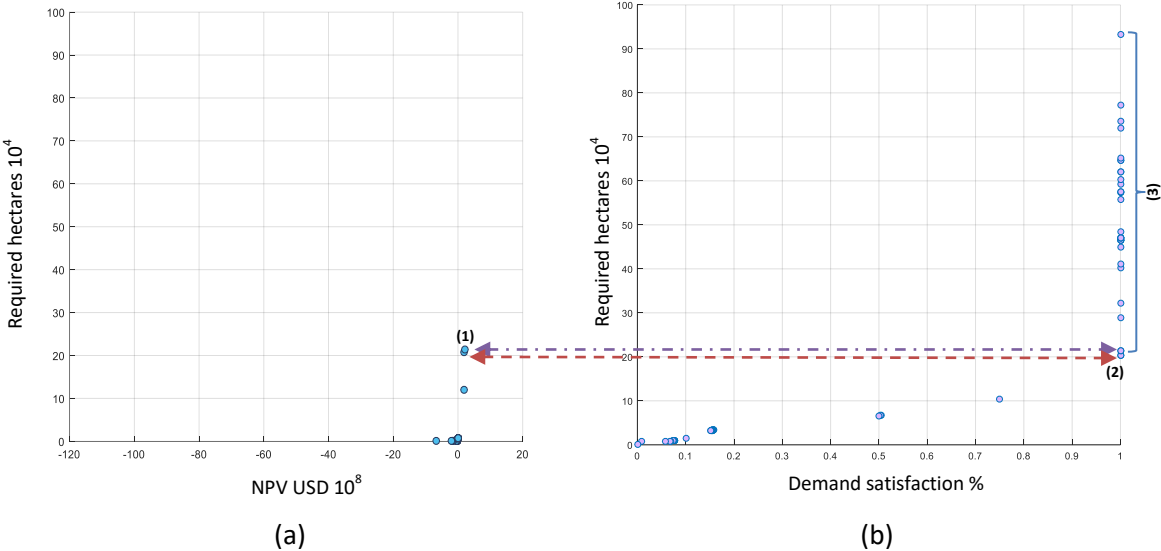


Figure 7.2. Pareto front analysis. (a) Net present value (USD 10⁸) – Required hectares (10⁴). (b) Demand Satisfaction (%) - Required hectares (10⁴).

In figure 7.2 (a), the point (1) represents the maximum value of the net present value, which requires around 214,000 hectares. However, in figure (b) it can be seen that to satisfy the 100% of the final products demand, only 200,000 hectares, approximately, are required (point 2).

A question arises about the previous situation: If the 100% of the demand for final products is satisfied, only with 200,000 hectares, why could the net present value be greater using 214,000 hectares? To solve this question, the solutions obtained by the optimization were analyzed, as presented in table 7.2.

In figure 7.2 (b), the section (3) corresponds to solutions that are normally dismissed by the NSGA-II, because they are all dominated by the condition of the point 2. However, it was decided to represent it to carry out a more complete analysis. Thus, it can be noted that even when the model satisfies completely the final products demand, the production plants can require more raw materials (and consequently, require more hectares) to produce, for example, intermediate products to be sold in intermediate markets or final products that can be stocked or exported.

A question arises about the previous situation: How much more could be surpassed the demand with the potential availability of raw materials? It will be analyzed in the sensitivity analysis.

Table 7. 2. Optimal solutions detail comparison

Max. Net present value Min. Hectares utilized (1)	Max. Demand satisfaction Min. Hectares utilized (2)
Net present value (USD): 224,000,000	Net present value (USD): -434,000,000
Ha: 214,220	Ha: 203,381
Demand satisfaction: 93%	Demand satisfaction: 100%
Raw material used (Tons):	Raw material used (Tons):
<i>Palm oil</i> 670,978	<i>Palm oil</i> 797,214
<i>Jatropha oil</i> 0	<i>Jatropha oil</i> 0
Intermediate product sold (Palm oil Tons):	Intermediate product sold (Palm oil Tons):
113,855	113,191
Amount of pretreatment plants: 10	Amount of pretreatment plants: 8
Total capacity installed (Tons): 680,000	Total capacity installed (Tons): 920,000
Amount of principal plants: 6	Amount of principal plants: 6
Total capacity installed (Tons): 560,000	Total capacity installed (Tons): 720,000
Total investment (USD): 163,000,000	Total investment (USD): 222,000,000
Technologies at principal plants: <i>Counter-current transesterification</i> <i>Counter-current transesterification and polymers production</i>	Technologies at principal plants: <i>Co-current transesterification</i> <i>Counter-current transesterification</i> <i>Counter-current transesterification and polymers production</i>

Regarding table 7.2, it can be concluded that emerging technologies are selected for principal plants, to take advantage of better transformation technologies, characterized by higher yields and high-value product production.

The products flows are geographically represented for optimal solutions in figures 7.3 and 7.4. Figure 7.3 represents the situation in which the maximal value for the net present value is obtained, using the minimum amount of hectares. And figure 7.4 shows the logistics required to satisfy 100% of final products demand with a minimal amount of hectares required.

The left side of figure 7.3 shows the raw material flows and the right side shows the intermediate products and the final product flows. Furthermore, the left side of figure 7.4 shows the raw material and intermediate products flows, while the right side of figures shows the final product flows to facilitate the visualization of the overall products flows.

Comparing figures 7.3 and 7.4, it can be noted that raw material sources (suppliers) are more decentralized when net present value is maximized (Figure 7.3), and distances between pretreatment plants and markets for intermediate product (refined palm oil) are shorter in figure 7.3 than in figure 7.4. However, it can be observed that distances among principal plants and final clients are longer in figure 7.3 than in figure 7.4.

Therefore, it can be concluded that the solution that maximize the net present value using the minimal amount of hectares, results on centralization for biorefinery principal plants production, due, mainly, to high installation cost related to production plants.

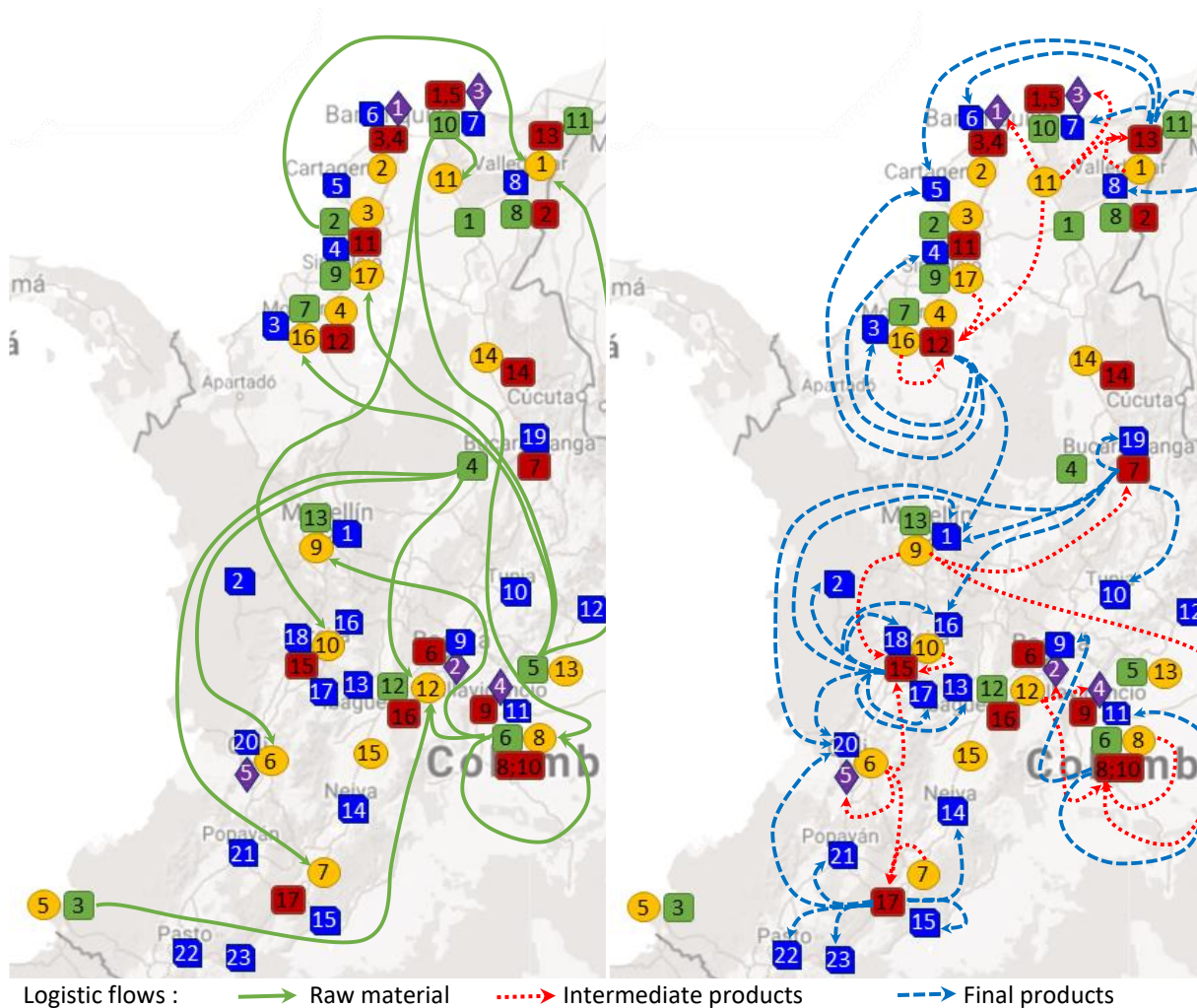


Figure 7. 3. BioRSC configuration to obtain a maximal value for the net present value, using the minimum amount of hectares

Also, a comparison between these optimal solutions with the current situation in Colombia will provide some additional elements. Today, there exist twelve biodiesel plants in operation in Colombia with an installed production capacity of 921,000 t/year (Fedebiocombustibles 2017) in contrast with the ten production plants that were functioning in 2015, with a production capacity of 811,000 t/year (Points 1 to 10 in red in figures 7.3 and 7.4). The total biodiesel demand in 2015 was 596,205 t, as presented in chapter VI. Therefore, a first view, the installed capacity is still higher than the biodiesel demand.

Both optimization solutions, presented geographically in figures 7.3 and 7.4, select a reduced amount of production plants than in current situation at Colombia. Also, the production plants are in a different location to those that are already installed in Colombia. Due the inclusion of pretreatment plants and the option of higher production capacity levels.

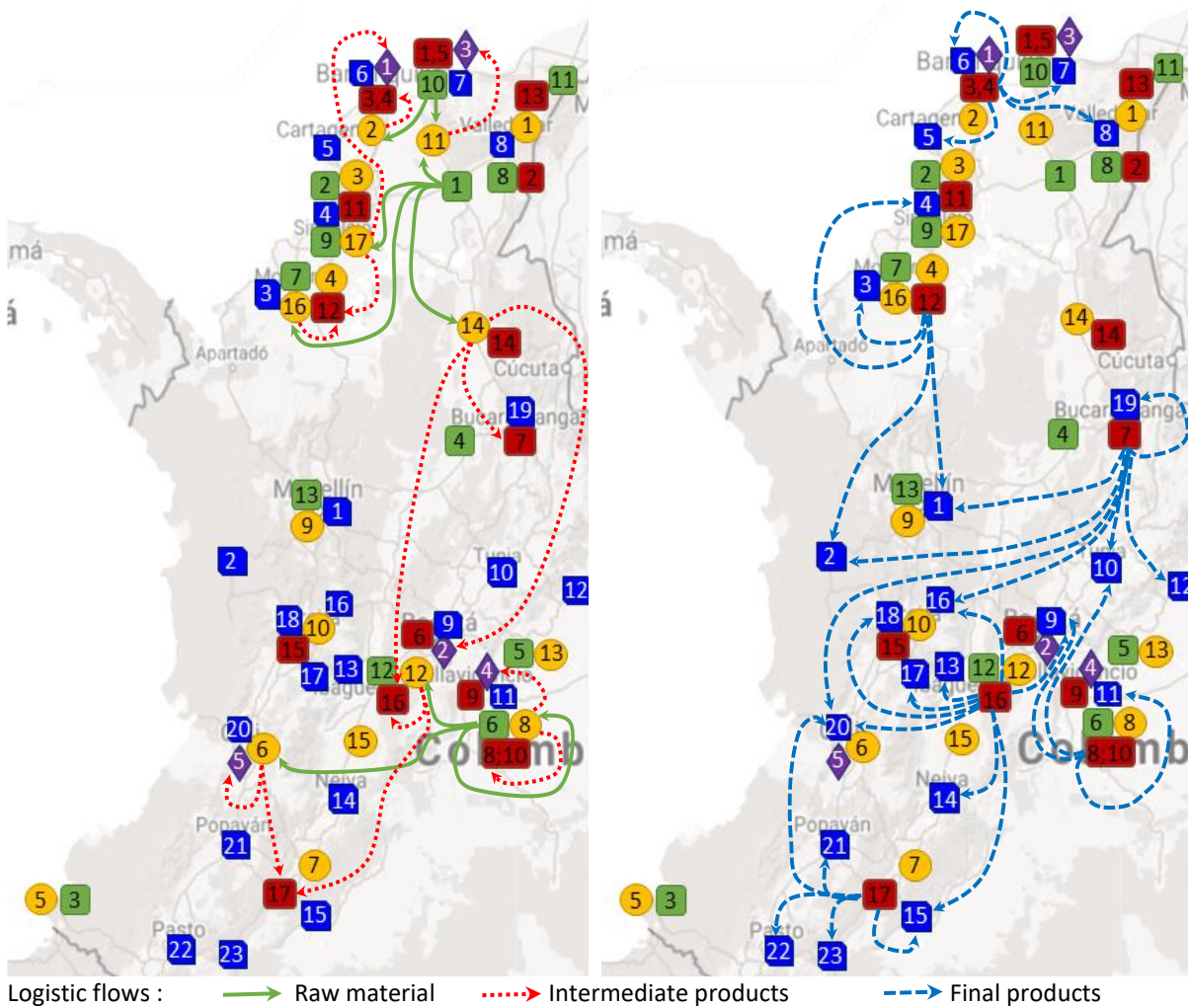


Figure 7. 4 BioRS configuration to satisfy the 100% of final demand satisfaction, using the minimum amount of hectares.

In the next sections the obtained Pareto fronts for the objective functions pairwise comparison are presented and discussed.

7.3.2. Pareto fronts analysis for the pairwise comparison against economic dimension

All the Pareto fronts obtained for the pairwise comparison including the net present value (NPV) are presented in figure 7.5 (a to v). All those figures represent a particular pairwise of antagonist objective functions.

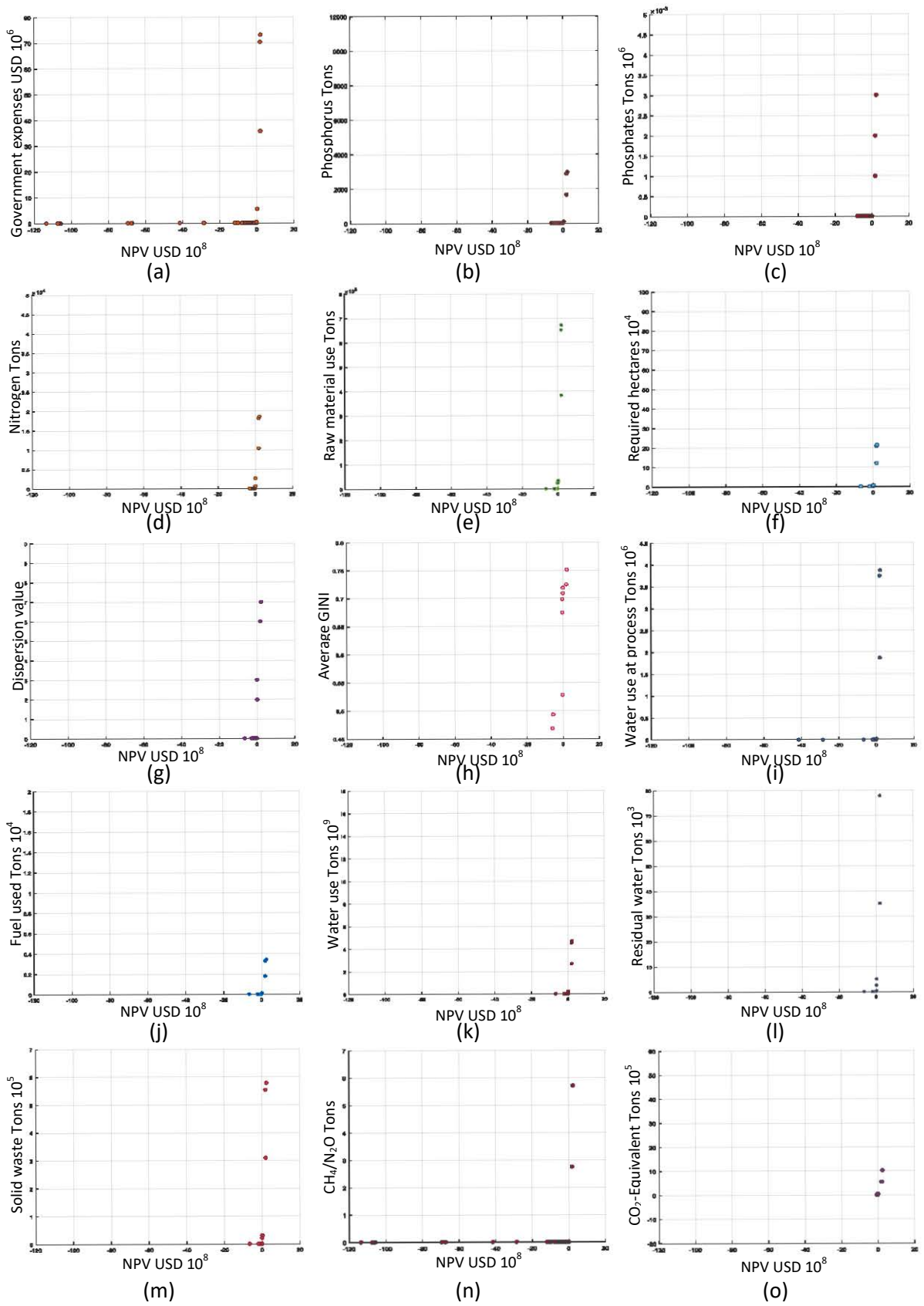


Figure 7. 5. Pareto fronts for net present value comparisons

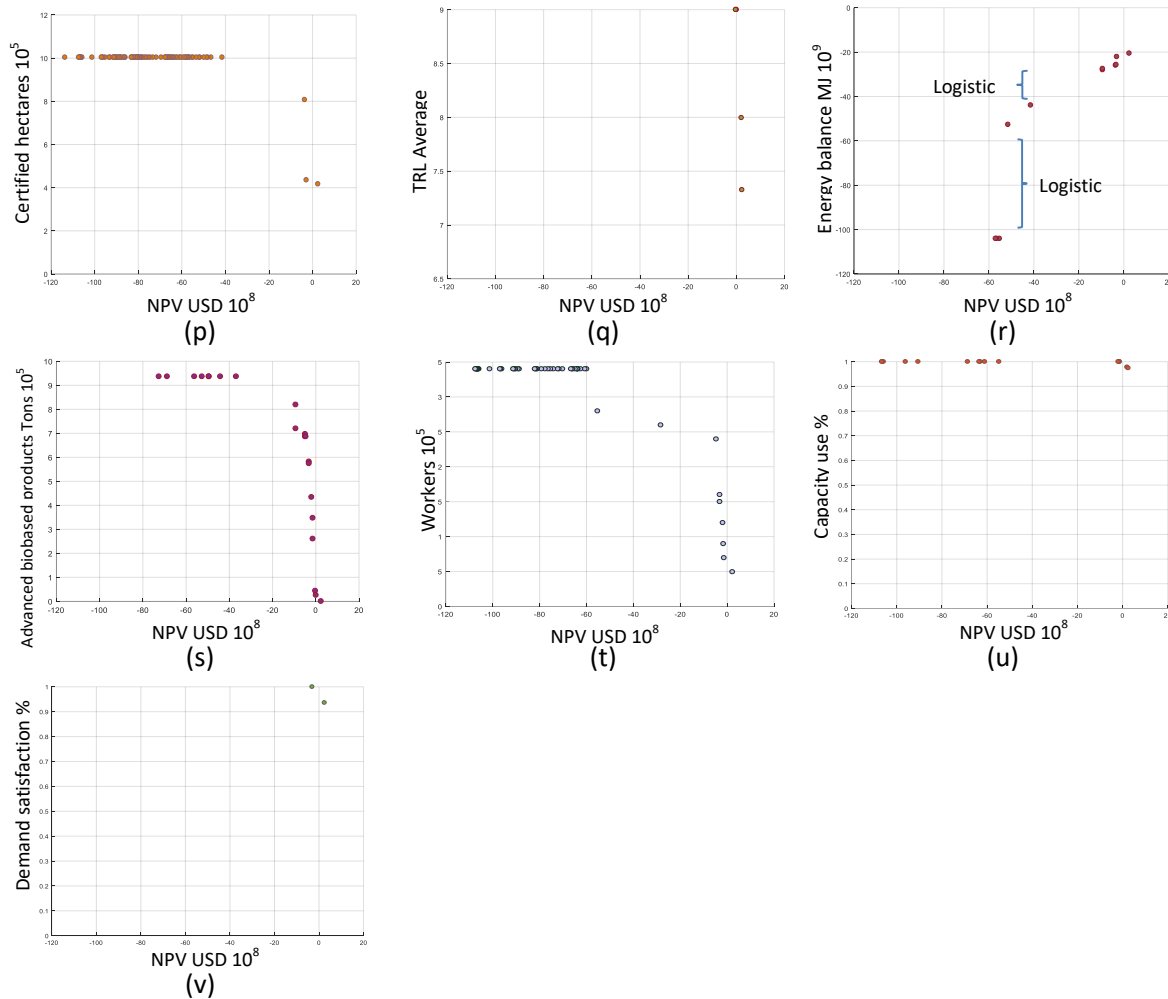


Figure 7.5. Pareto fronts for net present value comparisons (Continuation)

From the results presented in figure 7.5 the following observations are made:

Figure (a). Governmental expenses increase when the net present value rises, due principally to the biodiesel tax reduction, reaching 78,000,000 USD including tax incentives and subsidies for plant installations.

Figures (b), (c) and (d). Water pollution generated by phosphorus, phosphates and nitrates increase due to the higher raw material requirements (e), increasing at the same time the amount of required hectares (f).

Figures (e) and (f). Around 670,000 ton of raw materials are required to maximize the net present value, including intermediate and final products sales. This represents the 31.6% of the total potential availability of jatropha and palm crude oil (around 820,000 t/year and 1,300,000 t/year, respectively).

Figures (g) and (h). When the hectares requirements rise, areas with high dispersion value will be selected. Similarly, if more plants are installed and more suppliers are selected to obtain good economic performance, areas with higher GINI index will be selected as showed by figure (h), reaching an average GINI 0.75. However, despite it is a high value for the index, it must to be considered the special conditions in the Colombian case, where the GINI index is 0.734.

Figures (i), (j), (k), (l) and (m). In the same manner, the use of (i) process water, (j) fuel and (k) total water, also will increase when positive economic results are obtained. At the same time (l) wastewater and (m) solid waste production increases.

Figures (n) and (o). To obtain incomes, intermediate and final products must to be sold. Consequently, gas emissions, as CH₄ and N₂O, increase when net present value rise due to biodiesel sales (n). Likewise, CO₂-equivalent emissions will increase inasmuch as the economical results improve (o). In this figure, negative values for CO₂-equivalent emissions are caused by CO₂ capture at raw material cultivation stage.

Figure (p). The selection of certified hectares decreases when economic results improve, because only some of the palm suppliers are certified in RSPO.

Figure (q). Related to TRL values, it shows that emerging technologies are required to improve economic results.

Figure (r). The comparison between the energy balance and the net present value shows that the net energy consumed (consumption-generation) increases when the economic results improve. This is because energy must to be consumed in logistics to transport products between pretreatment and principal plants when final products will be produced, and energy will be required in transformation process. Also energy must to be consumed in logistics to deliver products to customers.

Figure (s). It shows that diversification of raw materials (maximization of the amount of raw material from non-food crops) is not economically feasible in the case study presented, despite the case study considers lower market value and production cost for jatropha oil and accessibility to jatropha and palm oil in some locations. Then, it can be concluded that raw material diversification is not recommended in the case study, mainly due that transformation rates are lower in the case of jatropha, at pretreatment and principal production plants. It shows the high impact of production technologies in the phase III biorefinery development.

Figure (t). The number of workers decreases when net present value increases, because production plants will be installed only if they allow the stakeholders to obtain better economic performance. Also, the raw material will be the amount required to satisfy the demand that maximizes the economic results. Influencing the amount of workers required at cultivation stage.

Figure (u). It shows that the 93% of the installed capacity is used when the maximum value to net present value is reached.

Figure (v). As presented in section 7.3.1, in order to obtain a better economic performance the final product demand satisfaction should only reach 93%, without satisfying Yopal (12). However, the high-value products demand is completely satisfied. It shows that the scheduling decisions at the tactical an operational level are an important factor to improve economic performance.

7.3.3. *Pareto fronts analysis for the pairwise comparison against politic dimension*

Figure 7.6 present the Pareto fronts resulting from the multiobjective optimization carried out between the demand satisfaction for final products and the remaining objective functions, as the fourth column in table 7.1 presents.

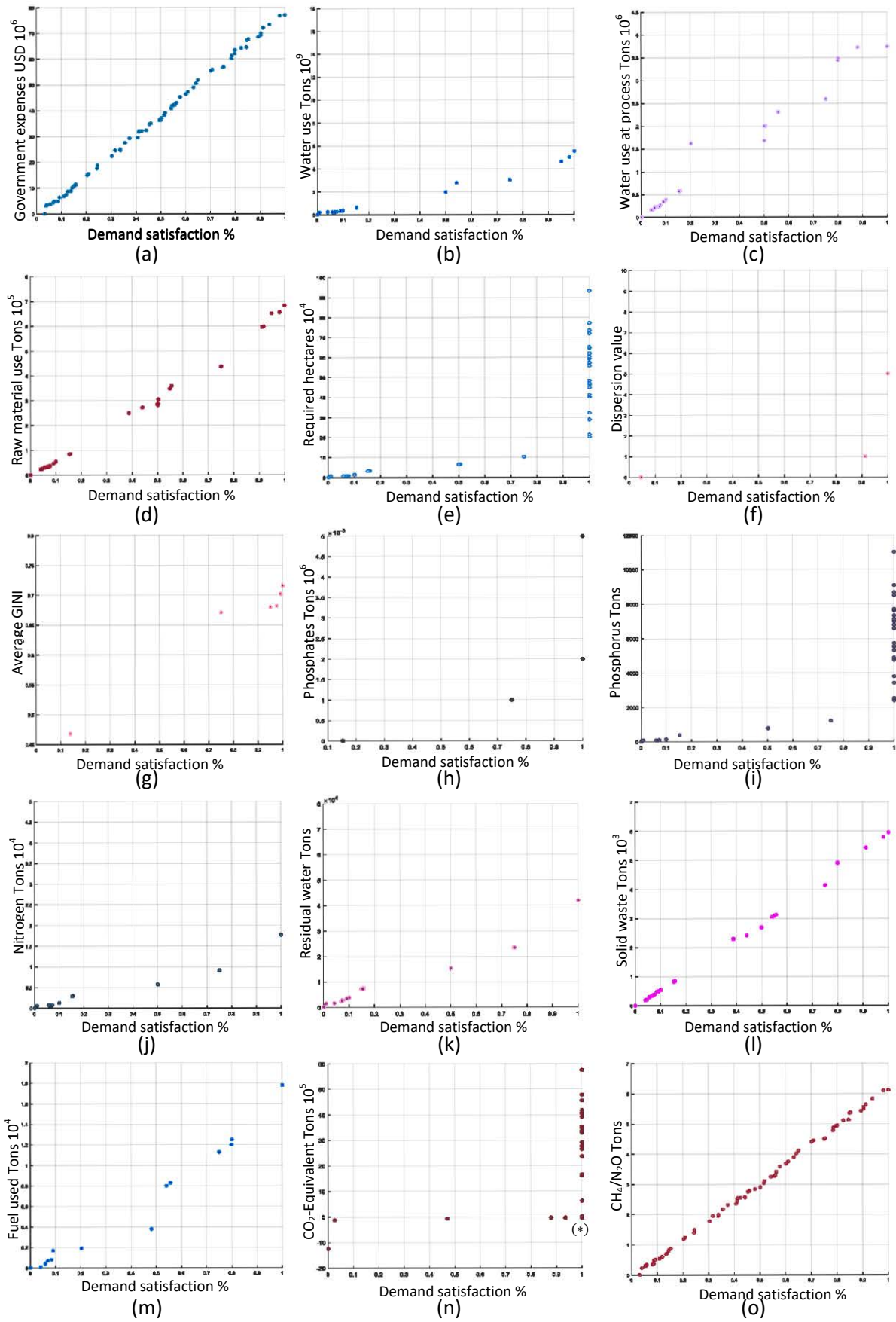


Figure 7. 6. Pareto fronts for demand satisfaction comparisons

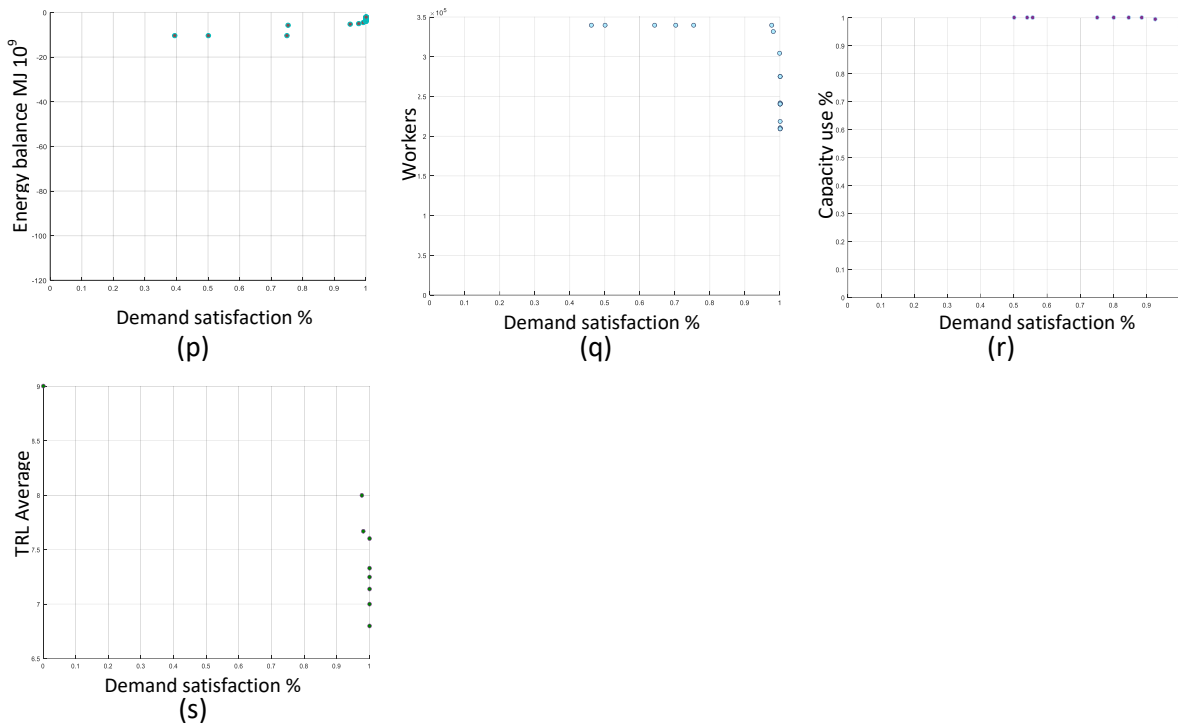


Figure 7.6. Pareto fronts for demand satisfaction comparisons (Continuation)

The analysis of Figure 7.6 is the following:

Figure (a). To increase the demand satisfaction, higher governmental expenses are needed due to investments in plant installation and tax reductions for the biodiesel sales in five years, reaching 80 000 000 USD in expenses. However, as presented in the first analysis on section 7.4.1, the total demand satisfaction for final products does not mean itself a good economic performance. Therefore an intermediate optimal solution should be found to equilibrate among governmental expenses, demand satisfaction rate and net present value results.

Figures (b) and (c). As the demand satisfaction for final products rise, it implies a high amount of final products production without considering the intermediate products sales. It can be expected that the amount of total water required (b) and the water used in process (c) increase in a lesser extent that in section 7.4.2. However, it presents an exponential growth in both cases.

Figures (d) and (e). Similarly to net present value analysis, insofar a greater amount of final products is required, an increase in raw materials is generated and consequently more hectares are required (e). However, only around 700 000 ton of raw materials are required to satisfy the final products demand. It represents 33% of the total potential availability of jatropha and palm crude oil (around 820 000 t/year and 1,300,000 t/year, respectively). This allows selling intermediate products and the increase for local biodiesel consumption blends or the export of final products as polymers.

Figures (f) and (g). Similarly to the analysis presented in section 7.4.2, when the hectares requirements rise, areas with high dispersion value will be selected, as presents figure (f). And therefore, areas with higher GINI index will be selected (g).

Figures (h), (i), (j), (k) and (l). As more raw materials are required, consequently phosphates (h), phosphorus (i) and nitrates (j) are generated as water degradation. A total of 42 000 wastewater

tons (k) and 7 000 tons of solid waste (l) will be generated in production process to satisfy the 100% of final products demand.

Figures (m) and (n). In the same manner, fuel requirements increases due to logistics and plant operations (m). Likewise, CO₂-equivalent emissions will increase in as much as the final products demand satisfaction (n). And it can be observed that the total amount of CO₂-equivalent emissions is negative when the 100% of the demand is satisfied, as a consequence mainly of the CO₂ capture at raw material cultivation stage. It is interesting a deep analysis for the optimal solution (*). As resumed in table 7.3, it can be concluded that the CO₂ capture capacity by raw material type and the technology production yields has a great impact on CO₂-equivalent emissions. Then, more raw materials than required has been cultivated to obtain negative CO₂ emissions in this optimal solution.

Table 7. 3. *Optimal solution to maximize the demand satisfaction and minimize the CO₂-equivalent emissions*

(*) Max. Demand satisfaction and Min. CO ₂ -equivalent emissions	
Net present value (USD):	-367,000,000
Ha:	214,352
Demand satisfaction:	100%
CO₂-equivalent emissions:	-37,100
Raw material used (Tons):	
<i>Palm oil</i>	281,000
<i>Jatropha oil</i>	527,000
Intermediate product sold (Palm oil Tons):	113,854
Amount of pretreatment plants:	7
Total capacity installed (Tons):	840,000
Amount of principal plants:	6
Total capacity installed (Tons):	720,000
Total investment (USD):	214,000,000
Technologies at principal plants:	
<i>Co-current transesterification</i>	
<i>Co-current transesterification and polymers production</i>	
<i>Counter-current transesterification</i>	

Figure (o). As final product demand is integrated to biodiesel demand, when it is consumed, gas emissions as CH₄ and N₂O are produced reaching a maximal value of 7 tons of CH₄ and 7 tons of N₂O by year.

Figure (p). It shows that the energetic balance is not optimal when the demand satisfaction is searched. Because, comparing with results presented in figure 7.4 (r), energy consumption in transformation process and logistic is minimized to reduce related production cost.

Figure (q). While a minimum number of workers is required to satisfy the final product demand (around 200,000 workers), there are no restrictions to generate the maximum potential of employments. This behavior is different to the case presented in figure 7.5 (t), where the maximal number of workers is around 50,000 in order to obtain the maximal value for the net present value.

Figure (r). It shows that the total demand of final products can be satisfied with different rates of capacity use. This is explained because several production plants can be installed, due to the fact that no economical limits are imposed in the integrated model.

Figure (s). It shows that to satisfy final product demand, lower values of TRL are required. Because the technologies proposed to produce polymers are not industrialized ($TRL < 9$).

7.3.4. Pareto fronts analysis for the pairwise comparison against environmental dimension

In figure 7.7 the Pareto fronts obtained in the multiobjective optimizations to compare the minimization of total water use with the advanced biobased products production, the amount of employments generated, the capacity use the energy balance and the maximization of the certified hectares utilized are presented.

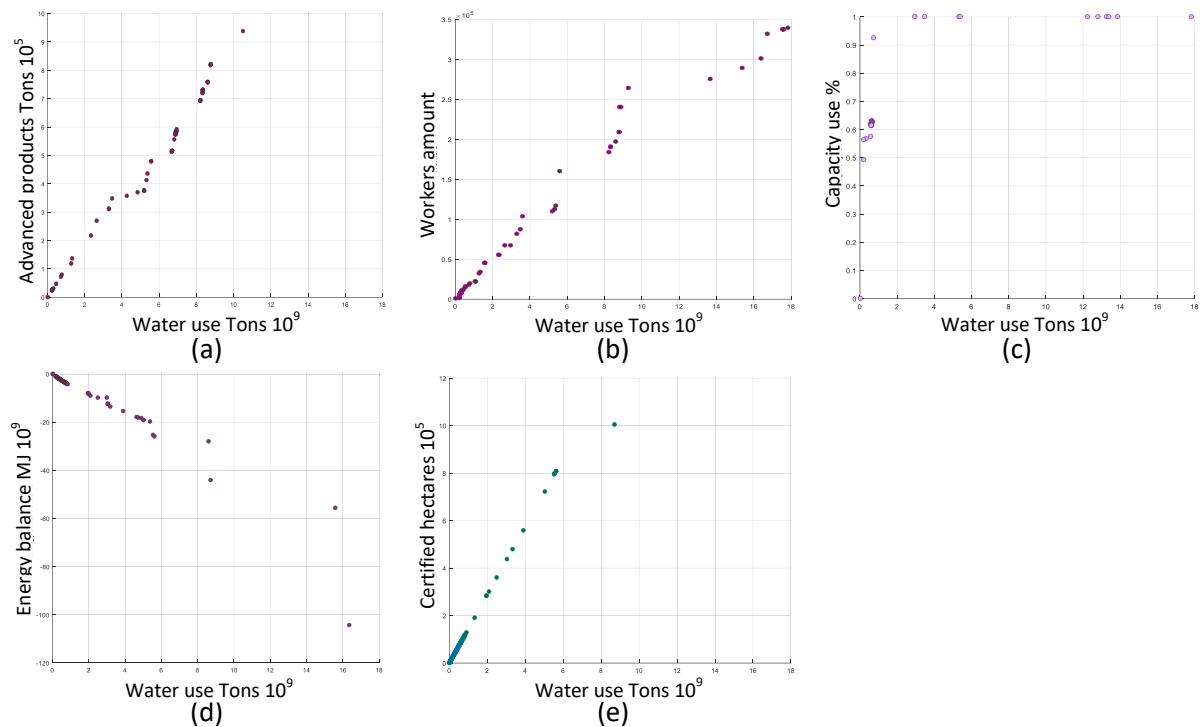


Figure 7. 7. Pareto fronts for total water use comparisons

From the results presented in figure 7.7 the following observations can be made:

Figures (a) and (b). Figure (a) shows that water use increases when non-food crops are used as raw material, due mainly to water required to obtain raw materials. Likewise, in figure (b) the amount of workers is compared to the total amount of water use, showing a direct relation, because both objective functions depend on the amount of raw materials required and the operation of pretreatment and principal plants. However, these objective functions are in conflict because, from a social point of view, the objective is to maximize the amount of employment generated, but it also signifies to increase the total water used due to plants operation. This figure shows that the maximum amount of water use for the case study is around 18×10^9 tons of water when the maximum of employment opportunities are generated (350,000 work places).

Figure (c). It can be noted that the maximal used capacity can be achieved with a minimum of water use of 2.5×10^9 tons. It means to use the maximal capacity at one pretreatment plant and one principal plant installed, as constraints in the integrated model required (Equations 14 and 15 in chapter IV). Because the objective function to maximize the capacity use is an average, it does not

show information related to the amount of production for each plants installed. Therefore, this objective function comparison does not allow a deeper analysis.

Figure (d). It shows that the energy balance will be minimized (energy consumed less energy generated) if large amounts of water are used. Therefore, the production of intermediate and final products is maximized. However, this does not mean that they will be sold.

Figure (e). It shows that the water use will increase if certified hectares are used, due water required to produce raw materials belonging to certified sources.

7.3.5. Pareto fronts analysis for the pairwise comparison against technological dimension

Figure 7.8 was constructed with the Pareto fronts obtained in the multiobjective optimization, to compare the maximization of TRL. In all figures presented in figure 7.8, the maximum value of TRL reached is 9. It can be achieved installing at least one pretreatment plant and at least one principal plant implementing alkaline transesterification ($d = 1$) as biodiesel production technology.

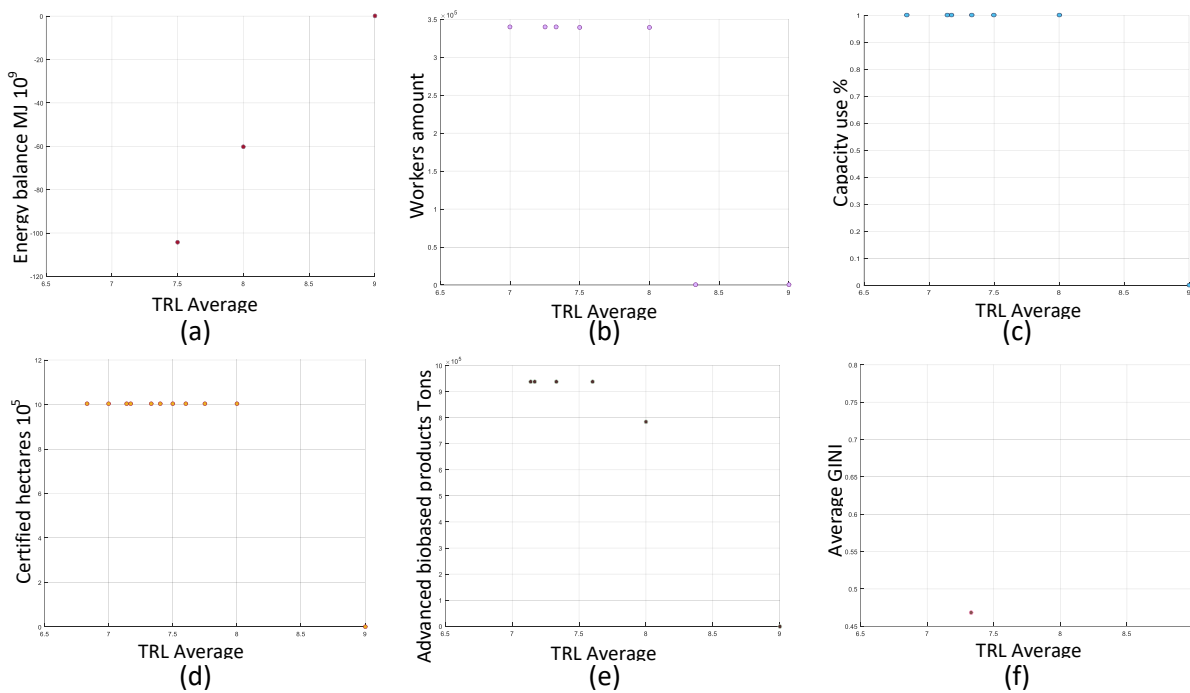


Figure 7. 8. Pareto fronts for TRL comparisons

Based on figure 7.8 that the following analysis is presented:

Figure (a). It shows that to achieve the minimum value to energy balance, the technologies in development should be applied to obtain final products as polymers.

Figure (b). It shows that technologies in development will require greater amounts of workers. It is expected because assumptions made to estimate the amount of workers required at principal plants depending on TRL.

Figures (c), (d), (e) and (f). It is important to identify that the maximum capacity use can be reached regardless of the production technology readiness level. Something similar occurs with the maximization of certified hectares use in figure (d). Installing the principal plant with the transesterification alkaline ($d = 1$) as production technology but it is not necessary that principal

plant start operations. The same analysis can be made for figures (e) and (f), that compares TRL maximization with non-food crops utilization maximization and the minimization of GINI index respectively.

7.3.6. Pareto fronts analysis the pairwise comparison against social dimension

Figure 7.9 presents the Pareto fronts resulting from the multiobjective optimization for the GINI index minimization and the other objective functions.

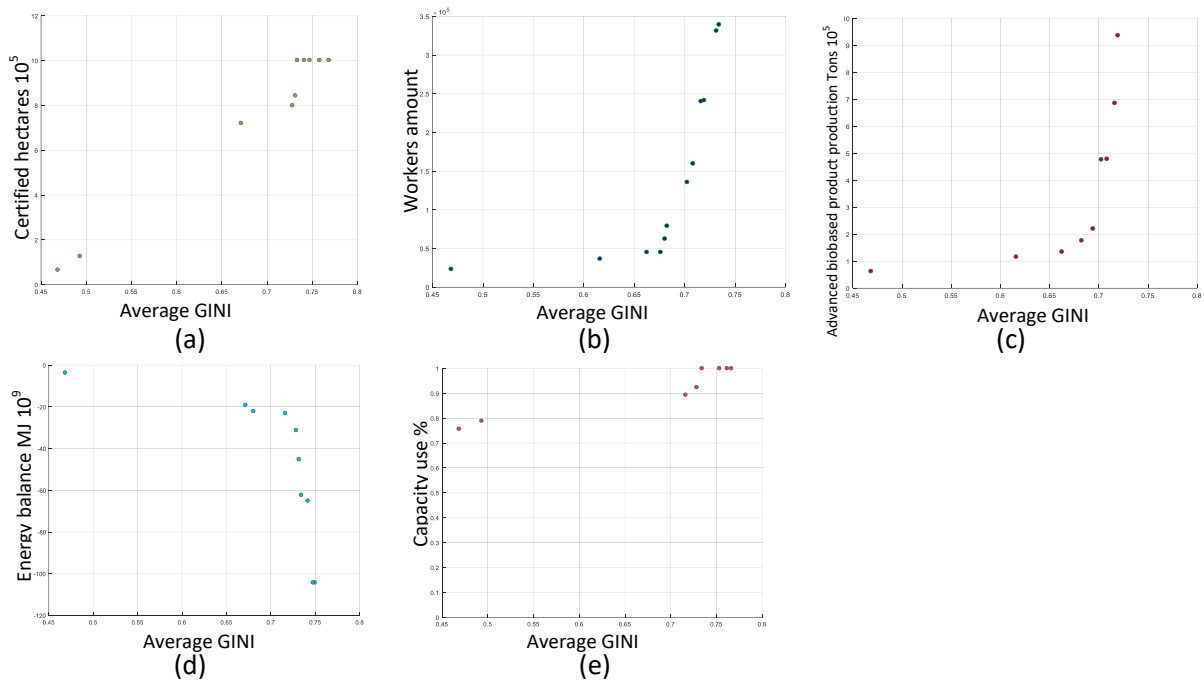


Figure 7. 9. Pareto fronts for GINI comparisons

From figure 7.9 the following analysis can be made:

Figure (a). When few certified hectares are used (150,000) a GINI index around 0.475 is obtained. However, when the amount of required hectares increases (800,000), the average GINI increases considerably (0.73). Due the most of raw material sources has a high GINI index in Colombia. Thus, it reflects the Colombian land ownership issues, where a limited number of people are the owners of large areas.

Figures (b), (c) and (d). A similar trend than in figure (a), is presented in figure (b), where there is an exponential increase in GINI values (0.46 to 0.67 in average GINI, while the amount of works vary between zero and 50,000) to then increase exponentially the amount of workers without high changes in GINI index (the amount of works vary between 50 000 and 350 000, while the average GINI index range from 0.67 to 0.74). This is due to the structural issue of high land ownership concentration in Colombia. Where the average GINI for potential suppliers, pretreatment and principal plants is 0.734 and the mode is 0.723. The same phenomenon can be detected in figures (c) and (d).

Figure (e). It can be noted that for lower values of average GINI the capacity use cannot reach the 100%. Due to process a high amount of raw materials they will belong to suppliers from areas with greater GINI index.

7.4. An example of optimal solutions with compromises between the sustainability dimensions

In table 7.4 the objective functions values for an optimal solution for the pairwise Net present value-GINI that do not represent none of the Pareto front endings, are presented. Also, the bounds found based on Pareto fronts and linear optimizations are presented in the third column, in order to compare these values with the objective function value for the optimal solution.

It can be noted that a compromise between the sustainability dimensions can be found. In this case, for example, the demand of final products will be moderately satisfied and economic benefits will be obtained. However, the payback time will be longer for the optimal solution presented in this section comparing with optimal solution presented in section 7.4.1. Therefore, it will depend on decision maker preferences to define the optimal solution that will represent the best compromise for the sustainable Phase III BioRSC in Colombia.

Table 7. 4. An optimal solution with compromises between sustainability dimensions.

Objective function	Value for optimal solution	Bounds
Net Present Value (USD)	190,000,000	-12,000,000,000 To 225,000,000
Demand satisfaction with biobased products	47%	0 To 100 %
Total water use (t)	2,664,351,000	0 To 17,841,173,500
TRL Average	7.33	6.750 To 9
Average GINI	0.725	0.468 To 0.869
Capacity Use (%)	94%	0 To 100 %
Use of noon-food crops as raw materials (t)	0	0 -938,000
Max certified land use (tons of raw materials)	304,000	0 To 1,004,000
Raw material use (t)	383,000	0 To 2,040,000
Hectares required	119,000	0 To 1,043,000
Governmental expenditures	35,800,000	0 To 78,993,000
Water in Process (t)	1,860,000	0 To 14,500,000
Amounts of locations with high dispersion	5	0 To 27
Work generation	25,698	48 To 339,794
Gas emissions /CH ₄ (t)	3	0 To 6.12
Water deterioration / Nitrates (t)	10,372	0 To 97,500
Water deterioration / Phosphorus (t)	1,650	0 To 12,000
Water deterioration / Phosphates (t)	1,400	0 To 50,000
Wastewater generation (t)	35,000	0 To 304,300
Solid waste generation (t)	3,000	0 To 20,300
CO ₂ emissions (t)	550,000	-2,000,000 To 6,000,000
Energy balance (MJ 10 ⁹)	-12	-105 To 0
Nonrenewable fuel sources (t)	178,000	0 To 236,900

7.5. Sensitivity analysis

The sensitivity analysis, as presented in chapter III, is an important aspect in model solution because it deals with obtaining additional information about the behavior of the optimum solution when the model undergoes some parameter changes (Taha 2010). In order to perform the sensitivity analysis there are two type of parameters that can be modified. First, parameters related to the integrated model constraints; and second, parameters related to the objective functions.

Regarding the present model, the parameters related to the integrated model constraints are the raw material availability, the transformation rates for each production technology, the final and intermediate demand and the production capacity at production plants.




As presented in section 7.4, the potential raw material availability, even considering only the current crude palm oil availability in Colombia, is enough to satisfy the current demand. Therefore it is not a parameter that will affect the optimization results at this stage. However, it could change if tactical and operational decisions are analyzed in future researches, due to raw material seasonality.

The effects of the technology transformation rates on the integrated model solutions can be observed in the current case study. The model considers also emerging (Last generation) technologies. These technologies provide higher transformation rate and allows the project to get better economic performance because the initial investment is not significantly different for the set of potential technologies. Also, technologies with a higher transformation rate are selected to reduce negative impacts in environmental aspects. However, this assumption contrasts with the current Colombian case, where most of the biorefinery production plants use traditional and already industrialized technologies. This can be due to lack of knowledge, uncertainty and risk associated to technologies in development. Thus, a deeper research related to TRL for biorefinery technologies in development should be carried out subsequently.

Moreover, final and intermediate products demand could change the logistic configuration of the optimal solutions. In the same way, the production capacity could have effects on optimal solutions, due it creates changes in constraints and objective function parameters. Consequently, it was decided to carry out the sensitivity analysis considering the last two parameters related to the integrated model constraints.

Concerning the parameters linked to objective functions, and regarding the number of them, as stated in chapter V, only two functions were chosen for the sensitivity analysis: the final product demand satisfaction and the net present value.

Therefore, the sensitivity analysis was designed to vary the parameters related to these objective functions:

-  Refined palm oil demand: Increasing it by 25%, 50%, 75% and 100%
-  Biodiesel demand: Increasing it by 25%, 50%, 75% and 100%
-  Polymer demand: Increasing it by 25%, 50%, 75% and 100%

- ✚ Polymer price: Reduction to 50% and 75% of the current price; raise to 125% and 150% of the current price.
- ✚ Biodiesel price: Reduction to 50% and 75% of the current price; raise to 125% and 150% of the current price.
- ✚ Production capacity at pretreatment plants: Evaluating 20,000, 100,000 and 200,000 tons/year as transformation capacity
- ✚ Production capacity at principal plants: Evaluating 20,000, 100,000 and 200,000 tons/year as transformation capacity
- ✚ Final products total demand: Increasing it by 300% and 600%

As an example to illustrate the sensitivity of objective functions parameters, figure 7.10a presents the results for the net present value sensitivity face to intermediate and final products demand. Figure 7.10b presents the net present value sensitivity face to biodiesel and polymer prices. Comparing both figures; it can be noted that the net present value of the project is more sensible to changes in biodiesel price than to polymer price, refined palm oil demand, biodiesel demand and polymer demand.

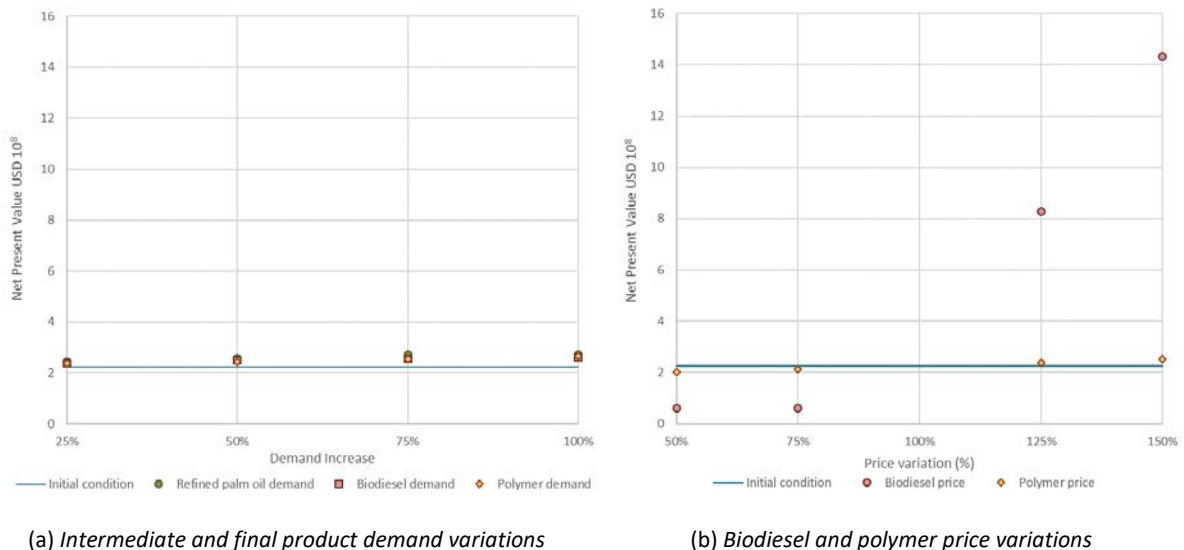


Figure 7. 10. Net present value sensitivity face price and demand changes

The production capacity tests are carried out without changes in investments related to the installation of production plants neither in operational cost to analyze changes in optimal solutions. The final product demand is totally satisfied for the different proposed scenarios and all the proposed pretreatment and principal plants are selected. However, the selection of production capacity is different, as presented in table 7.5. It can be noted that when modifications in production capacity are introduced, there is a higher variability among the production capacities selected than in the initial conditions.

Table 7. 5. Plants selection for demand satisfaction as objective function face to changes in production capacity.

Initial conditions		Pretreatment plant capacity variation		Principal plant capacity variation		Pretreatment and principal plant capacity variation	
Pretreatment plants capacity		Pretreatment plants capacity		Pretreatment plants capacity		Pretreatment plants capacity	
40,000	0	20,000	6	40,000	0	20,000	4
80,000	0	100,000	5	80,000	0	100,000	5
120,000	17	200,000	6	120,000	17	200,000	8
Principal plants capacity		Principal plants capacity		Principal plants capacity		Principal plants capacity	
40,000	1	40,000	0	20,000	1	20,000	2
80,000	2	80,000	3	100,000	2	100,000	4
120,000	14	120,000	14	200,000	14	200,000	11

For the net present value sensitivity analysis, figure 7.11 shows the results face to changes in production capacity at the different stages of the process, as follows: *at pretreatment plants only, at principal plants only, and at pretreatment and principal plants simultaneously*. When the production capacity increases, the net present value also increases. It occurs because, as presented in table 7.6, less production plants are installed, and the production is more centralized. Therefore, it can be concluded that the net present value is highly sensitive to installation cost.

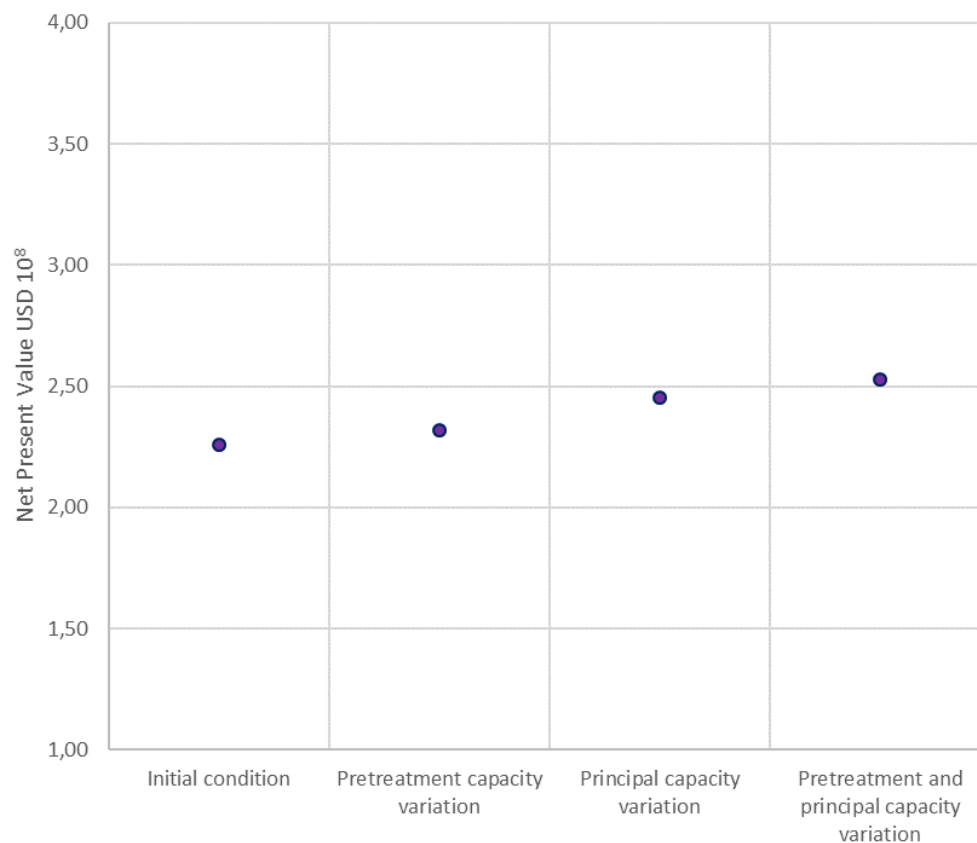


Figure 7. 11. Variations over the net present value

Table 7. 6. Plants selection for net present value as objective function face to changes in production capacity.

Initial conditions	Pretreatment plant capacity variation		Principal plant capacity variation		Pretreatment and principal plant capacity variation	
Pretreatment plants capacity	Pretreatment plants capacity		Pretreatment plants capacity		Pretreatment plants capacity	
40,000	4	20,000	1	40,000	2	20,000
80,000	5	100,000	7	80,000	6	100,000
120,000	1	200,000	0	120,000	1	200,000
Principal plants capacity	Principal plants capacity		Principal plants capacity		Principal plants capacity	
40,000	0	40,000	0	20,000	0	20,000
80,000	4	80,000	1	100,000	2	100,000
120,000	2	120,000	4	200,000	2	200,000

Finally, two scenarios were proposed to determine the maximal demand of final products that will be satisfied with the potential raw material availability. The test carried out increases the final products demand to 300% and 600%, showing that the current demand can be satisfied in 345% using all the current palm oil availability and the potential jatropha oil availability. However, as presented in figure 7.12, only 8,552 tons of refined palm oil will be sold in the intermediate market at Cali ($m = 5$), compared to 113,854 tons sold according to the results in section 7.4.1 (Total intermediate product demand satisfaction). Also, final markets at position 2, 12, 14 and 22 will not be served by the biorefinery system (Departments of Choco, Casanare, Huila and Nariño).

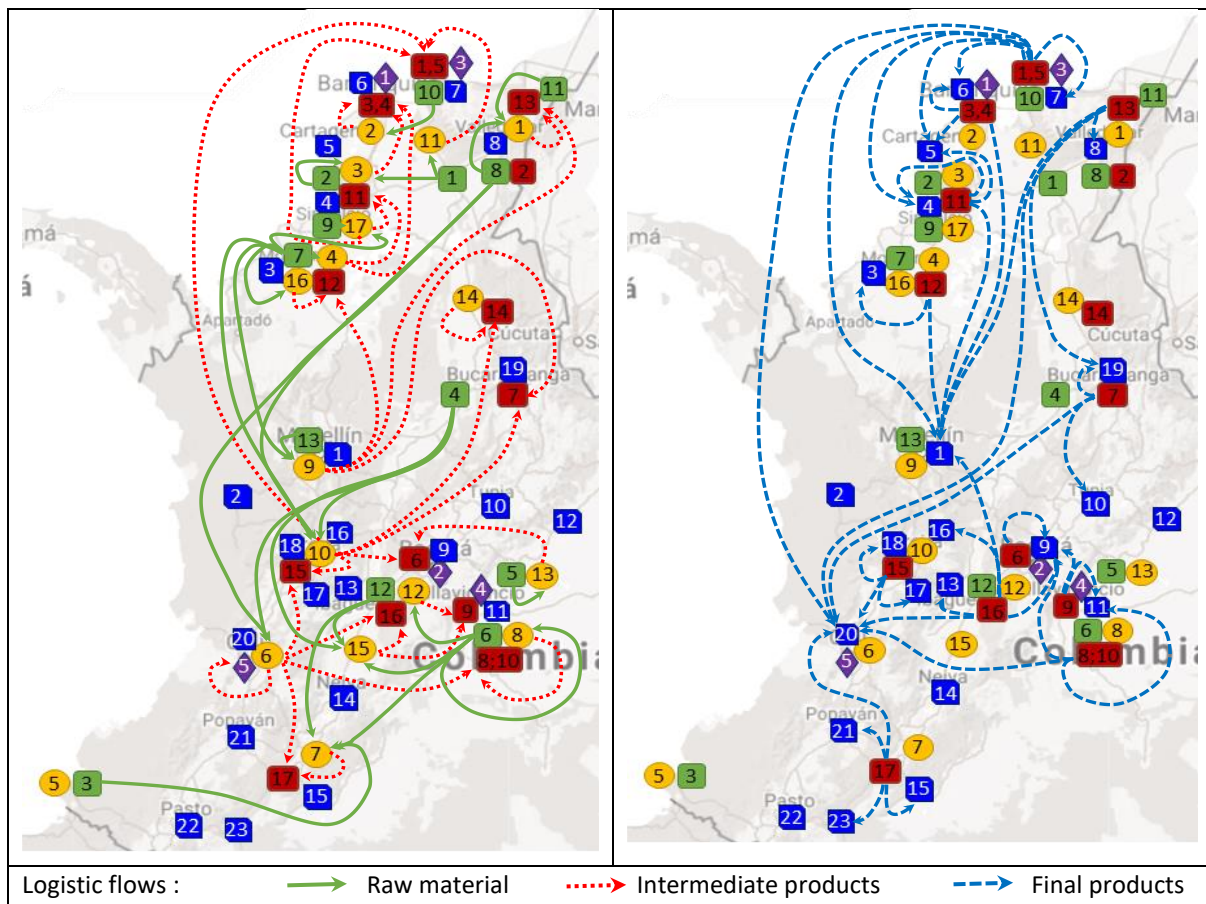


Figure 7. 12. Net present value optimal solution if final products demand increases 600%

7.6. Model validation

As presented in chapter III, model validation corresponds to a set of methods for judging whether the model developed is an accurate representation of reality (Winston 2003). There are five main types of validation commonly implemented: face validity, verification (or internal validity), cross validity, external validity, and predictive validity (Eddy et al. 2012). These validation methodologies are analyzed for the integrated model following.

Face validity. Four aspects are particularly important for face validity: model structure, data sources, problem formulation and results. These aspects are discussed in table 7.7.

Table 7. 7. Face validity for the integrated model

Face validity aspect	Justification
<i>For the structure, important questions are whether the model includes all aspects of reality considered important by experts.</i>	In this case; the model that includes the BioRSC characteristics and SC strategic decision variables was developed based on previous researches carried out about biorefineries supply chains, as presented in chapter IV. Aspects that generate uncertainties for tactical and operational decisions in supply chain are presented as perspectives of the current integrated model. Also, the sustainable aspect of the integrated model was developed based on the principles, criteria, and indicators that were validated with experts about its importance for the sustainability analysis (Bautista et al. 2016). Therefore, it is considered that all the aspects of reality considered important by experts are included in the model or in its perspectives.
<i>For problem formulation; whether the setting correspond to those of interest.</i>	
<i>Information about the model and supporting evidence are obtained from documentation provided by the modelers; information about the problem formulation and results is obtained from the application's report.</i>	The information about the problem formulation is public available and is presented in chapters IV and V, and appendix V. The information related parameters values are presented in chapter VI and appendix VI, with the corresponding information sources.
<i>For results, whether they match experts' expectations and, if not, whether the model can plausibly explain them.</i>	The results presented in this chapter are consistent with current conditions in the case study applied at Colombia and with the research group expectations.

Verification. It examines the extent to which the mathematical calculations are performed correctly, if they are consistent with the specifications of the model and if the model has been implemented correctly. Verification helps to ensure there are no unintentional computational errors.

The integrated model implementation was implemented integrating Microsoft Excel and Matlab®. The optimization results were verified with the values of constraints presented in chapter VI. It corresponds mainly to respect of constraints by the optimal solution verification. However, it can be also used to validate parameters used in the optimization against their sources (Data presented in Microsoft Excel and imported to Matlab® were correct).

The coding accuracy was verified by the fact that optimal solutions are generated in the multiobjective optimization. But also by the explication of code modification to generate the adapted algorithm programming of the NSGA-II algorithm presented in chapter IV, and the sensitivity analysis.

Cross-validation. It involves comparing a model with others that address the same problem and determining the extent to which they calculate similar results.

Results presented in this chapter match with results presented by Duarte et al. (2012), concluding that capacity is an influential factor, because in his research plants with higher capacity were also selected. Also, as concluded by Rincón et al. (2015), other feedstocks, as Jatropha oil, could be combined with palm industry for higher biodiesel blends

External validation. Compares results obtained using the model with actual event data. External validation tests the ability of the model to calculate actual outcomes.

In this chapter, section 7.4.1, a comparison between optimal solutions and the current situation in Colombia is presented. However, it cannot be expected that the model calculate the actual outcomes, because a different scenario is proposed including pretreatment plants and other capacity production levels. Therefore, for future research production capacities of current plants in operation should be considered, as well as they installation investments amounts, operation cost and locations enabling an external validation.

Predictive validity. Involves using a model to forecast events and after some time, comparing the forecasted outcomes with the current ones.

At this stage, models to forecast events are not developed, therefore a predictive validity is not possible.

As conclusion of this section, in order to establish the foundations of a decision-making tool for the sustainable Phase III BioRSC implementation, the developed integrated model is valid or accurate enough. Due to:

- ✚ Rigor of the process to model development
- ✚ Quantity and quality of sources used for the model development and case study application
- ✚ Model behavior and results observed under initially assumptions and after making justifiable assumptions about uncertain elements in sensitivity analysis.

7.7. Conclusions

In order to support a faster convergence of the programming algorithm to optimal solutions, the parameter definition for the NSGA-II adapted algorithm was presented. Also, a strategy to create the first generation of individuals for the multiobjective optimization was detailed.

The strategy to create the first generation of individuals and the adaptation of the NSGA-II programming algorithm showed its suitability for the optimization of the integrated model developed (including binary variables and equality and inequality constraints). Moreover, errors related to the constraints infringements of each individual in the population are reduced generation by generation. Then, the Pareto fronts were generated, when corresponds, in the multiobjective optimizations.

Future research should target the verification of the NSGA-II adapted algorithm with other models that includes: binary variables; equality and inequality constraints; and two objective functions.

Regarding the first results of the multiobjective optimization related to the identification of antagonistic or contradictory objective functions it can be noted that:

The minimization of the total water use is not in conflict with most of the remaining objective functions that includes the environmental dimension (except the energy balance and the net present value). Hence, it can be expected that the same behavior will be reproduced when other objective functions including the environmental dimension be compared with remaining objective functions including the environmental dimension.

It can be graphically explained by Table 7.8; where:

- **Green border.** Highlight the pairwise comparisons realized and analyzed in this chapter.
- **Red cells.** Represent comparison between each objective function and itself. Therefore they are not required to be made.
- **Black cells.** They are, by symmetry, the mirror of the objective functions comparison cells under the red cells.
- **Green cells.** Represent pairwise comparison between objective functions in conflict. It means that a Pareto front is generated by the optimization.
- **Dark blue cells.** Represent objective functions that are not in conflict among them.
- **White cells.** Represent the multiobjective optimizations to realize in future work.

In table 7.8 can be observed there are 72 multiobjective optimizations to be realized in future researches. This will enable to distinguish all the antagonistic objective functions, to subsequently define the preferences of stakeholders based on the Pareto fronts obtained.

The formalization of stakeholder preferences will allow the stakeholders to select an optimal solution with a compromise between sustainability dimensions, as shown by the example presented in section 7.4.

Table 7. 8. Pairwise comparison between all objective functions to sustainable Phase III BioRSC design

Eq	23	44	50	75	57	33	43	48	49	69	40	51	76	59	60	63	64	65	68	71	70	
23	Red																					
44	Green	Red																				
50	Green	Green	Red																			
75	Green	Green	Blue	Red																		
57	Green	Green	Blue	Green	Red																	
33	Green	Green	Green	Green	Green	Red																
43	Green	Blue	Green	Green	Green	White	Red															
48	Green	Blue	Green	Green	Green	White	White	Red														
49	Green	Green	Blue	Blue	Blue	White	White	White	Red													
69	Green	Green	Blue	Blue	Blue	White	White	White	Blue	Red												
40	Green	Green	Blue	Blue	Blue	White	White	White	Blue	Blue	Red											
51	Green	Green	Blue	Blue	Blue	White	White	White	Blue	Blue	White	Red										
76	Green	Green	Blue	Blue	Blue	White	White	White	Blue	Blue	White	White	Red									
59	Green	Green	Blue	Blue	Blue	White	White	White	Blue	Blue	White	White	White	Red								
60	Green	Green	Blue	Blue	Blue	White	White	White	Blue	Blue	Blue	White	White	White	Red							
63	Green	Green	Blue	Blue	Blue	White	White	White	Blue	Blue	Blue	White	White	White	Blue	Red						
64	Green	Green	Blue	Blue	Blue	White	White	White	Blue	Blue	Blue	White	White	White	Blue	Blue	Red					
65	Green	Green	Blue	Blue	Blue	White	White	White	Blue	Blue	Blue	White	White	White	Blue	Blue	Blue	Red				
68	Green	Green	Blue	Blue	Blue	White	White	White	Blue	Blue	Blue	White	White	White	Blue	Blue	Blue	Blue	Red			
71	Green	Green	Blue	Blue	Blue	White	White	White	Blue	Blue	Blue	White	White	White	Blue	Blue	Blue	Blue	Blue	Red		
70	Green	Green	Blue	Blue	Blue	White	White	White	Blue	Blue	Blue	White	White	White	Blue	Blue	Blue	Blue	Blue	Blue	White	Red

Concerning Pareto fronts and sensitivity analysis it can be concluded that:

- High installation investments promote a centralized production in the BioRSC to obtain positive economic performance.
- Emerging technologies are selected in most of the optimal solutions because of their higher transformation yields. However, as presented in chapter VI, the risk and uncertainties related to emerging technologies and its TRL must to be determined in future works for this case study to provide more comprehensive information to decision-makers.
- Jatropa oil was not selected in the optimal solutions that maximize the economic performance, due mainly to lower transformation rates. Thus, future works should take in count emerging technologies for jatropa oil transformation and/or alternative non-edible crops as raw material.
- In the Colombian case studied, the diversification of final products with the production of polymers allows a better economic performance. However, as presented in section 7.5, it does not have high influence on the net present value, compared with biodiesel. Therefore, other types of final high-value products that can be derived from the biodiesel, glycerol or refined oil should be included and evaluated in the case study.

The proposed integrated model has been validated thanks to the Pareto front and sensitivity analysis realized in this chapter, in addition to the detailed description of the model construction and the parameters definition presented in previous chapters. Also, the details related to the programmed algorithm parameters presented and the verification realized for the adaptation of the NSGA-II programmed algorithm supports the integrated model validation and optimization.

Finally, regarding the amount of generic parameters needed for the optimization of the integrated model, it is recommended to develop a case study at a regional scale. To compare results with these presented in this chapter. Also, time should be included in future developments of the integrated model to include the tactical and operational decisions, in addition to uncertainty. It will allow a better approximation of objective functions as the net present value and to evaluate functions as the payback time for the investment.

7.8. References

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Chapter VIII. Conclusions and perspectives

In this document, a methodological approach for strengthening the development of sustainable biorefineries was developed and tested for a specific case related to sustainable Phase III biorefineries. It was done convinced that the development of this kind of industries will open up new possibilities and will generate a positive impact on the society and environment in the near future. From this perspective, this research has been focused around the fundamental question:

To what extent it is feasible to conceive the supply chain for a phase III biorefinery, as well as considering a compromise among the sustainable dimensions?

Beyond answering this question with a Yes/No, what really research is to explore which are the specific characteristics and the decisions that have must be taken at the design stages of a BioRSC. At the same time, this research looked for integrating the aspects of each sustainable dimension that are in conflict with others, seeking a compromise among them. Thus, the overall goal of this thesis was to have a better understanding on the BioRSC design and the concept of sustainability in order to lay the foundations for a decision-making tool to support the development of projects for sustainable BioRSC conception.

The first contribution of this research, based on the literature related to biorefinery characteristic and supply chain design, is a wide range of formalized and detailed key challenges and requirements for sustainable and industrialized BioRSC. Also, it was concluded that Phase III biorefineries are a potential opportunity to use natural resources in a sustainable way and to mitigate negative effects of traditional fossil fuels and related petrochemicals. However, despite its highly documented potential advantages and long term attractiveness, currently, only phase II biorefineries has industrial application. This is mainly because Phase III biorefineries are characterized by high costs of capital investment, related uncertainties and more complex decision-making processes.

A systematic literature review methodology was followed with the aim to map the current researches and methods/tools used for the BioRSC design. It was noted that, although the study of BioRSC started several years ago, almost parallel to sustainability studies including three sustainability dimensions (social, economic and environmental), only six of the registered studies include these dimensions. Likewise, when considering the new sustainability approach based on five dimensions, only two studies integrates all the aspects. In addition, among the most relevant studies related to sustainability only three of them considered the target market selection for the different biorefinery final products and sub-products. It means, the development of Phase III biorefineries has almost been ignored. These results show that none of the publications targeted the sustainable Phase III BioRSC design system complexity as a whole.

In view of the nature and complexity of a Phase III BioRSC, a large system of men, machine, materials, and money; system that must to be designed, managed and operated in the best possible way to be sustainable can be defined. Furthermore, the objective of Operations Research is to provide a scientific basis to the decision maker for solving the problems involving the interaction of various components finding a solution which is in the best interest of the organization as a whole. Therefore, the second contribution is related to the proposition of a general methodology to assess a sustainable Phase III BioRSC conception based on the integration of MCDM, stochastic programming multistage and Robust Optimization (Operations Research methodologies). The general methodology can be described as follows:

Model construction. The general model for the sustainable Phase III BioRSC conception is integrated by three sub models. The first is a deterministic and static model for the SC design decisions. Then, uncertainty and dynamic are included for the management and scheduling models, related to tactical and operational SC decision-making level, respectively.

Model solution. The model should be solved/optimized.

DM preferences. Model results should be presented to decision-maker to evaluate it preferences and to find a compromise among the sustainable dimensions with MCDM.

Model adaptation. Decision-maker preferences are integrated to the general model.

Model adapted solution. The adapted model is solved/optimized to obtain an optimal solution according to the decision-maker preferences.

Once the general methodology was stated, the attention was focused on the development of the first model, devoted to the sustainable Phase III BioRSC design. It was noted that the model construction represent a major challenge due the several decision variables, constraints and objective functions to be defined, related to the sustainable Phase III BioRSC characteristics, the SC strategic decisions and the sustainability dimensions (principles, criteria and indicators) that must be included. Hence, a well-adapted modeling strategy to this particular complex system was required.

Consequently, a progressive development for the model, adding elements one at a time, was proposed. The modelling strategy was conceived in two axes: the first one integrates the Phase III BioRSC characteristics and the SC strategic decisions, thanks to the fact that there is ample knowledge about the integration, and thus they could be analyzed together. The second modeling strategy axis is related to sustainability dimensions, which should be integrated also one by one. This working-way permitted to start from a simply model to reach a very complex one; enabling test the model in each element addition.

The proposed modeling strategy was used to develop the general integrated model that includes thirteen decision variables, nineteen restrictions and twenty-one objective functions (equations presented in Chapters V and VI) including the specific requirements for the design of the Phase III BioRSC and the sustainability dimensions analysis.

Then, in order to validate the applicability of the conceptual integrated model developed, a relevant solving technique enabling to deal multiple objectives have to be used. Thus, a literature review was carried out to study the optimization techniques for multiobjective models. It was observed that multiobjective evolutionary algorithms (MOEA) are suitable to solve the integrated model. Because they are able to handle complex problems, involving features such as discontinuities, multimodality, disjoint feasible spaces and noisy function evaluations. Among the different types of MOEA, the Elitist Non-Dominated Sorting Genetic Algorithm (NSGA-II) is the most studied. It has been developed since 1994 and presents an exponentially increase of related scientific articles from 2005 to 2009. This fact has been highlighted, as the NSGA-II has been enough developed and proven by the scientific community, to facilitate his application on the present research.

Subsequently, in order to solve the integrated model with the NSGA-II, a programed algorithm corresponding to NSGA-II was found and adapted; due to the existence of binary variables, equality and inequality constraints in the integrated model. This adaptation was verified for inequality constrained models and the verification for its application on equality and inequality constrained multiobjective models including binary variables, was performed.

The general integrated model and the adapted NSGA-II programed were applied to the Colombian study case, to design the sustainable Phase III BioRSC. In order to diversify the raw material with non-edible crops, two different types of raw materials were considered in thirteen sources, palm and jatropha crude oil. Also, pretreatment plants were proposed in seventeen locations in Colombia, with three different production capacities and implementing the physical refining to crude oils. The principal production plants are also proposed at seventeen locations with three different production capacities. However, unlike pretreatment plants, six production technologies were proposed to analyze new process to obtain biodiesel, and a set of emerging technologies to obtain high-value products as aliphatic polyesters. Moreover, twenty-three markets were described for the biodiesel, glycerol and aliphatic polyester; and five market locations for refined palm oil.

The results of the multiobjective optimization for the Colombian case study showed that there are several antagonistic or contradictory objective functions among the sustainability dimensions. Then, the corresponding Pareto fronts and the sensitivity analysis allows note that:

- ✚ High installation investments promote a centralized production in the BioRSC to obtain positive economic performance.
- ✚ Emerging technologies with higher transformation yields have a great potential for develop biorefineries. However, its risk and uncertainties must to be determined in future works to provide more comprehensive information to decision-makers.

- ✚ Future works should take in count emerging technologies for jatropha oil transformation and/or alternative non-edible crops as raw material.
- ✚ The diversification of final products with the production of polymers allows a better economic performance. However, it does not have high influence on the net present value, compared with biodiesel. Therefore, other types of final high-value products that can be derived from the biodiesel, glycerol or refined oil should be included and evaluated.

Finally, as consequence of model optimization and the sensitivity analysis, the integrated model for the sustainable Phase III BioRSC design was validated. Nevertheless, further studies should be addressed to construct, validate and integrated the management and scheduling models to the complete conception of the sustainable Phase III BioRSC.

Limits and perspectives of this research

It is well know that in a thesis project, it is difficult to deepen in each field that has been considered. Consequently, some limitations of the contribution are highlighted, in order to put them into a larger perspective.

- ✚ Concerning the contribution of the systematic literature review, in the present study only the publications related to the whole BioRSC were considered. Further studies can be conducted to analyze the research related only to operational and/or tactical aspects.
- ✚ Regarding the proposition of a general methodology to assess a sustainable Phase III BioRSC conception, this thesis sought to obtain an optimal solution respecting the constraints of the model. However, if the target is to analyze the behaviors of the sustainable BioRSC on a time basis, alternative simulation tools such as dynamic system or multiagent simulation could be also considered.
- ✚ Concerning the integrated model developed, it should not be forgotten that it is deterministic and only addresses the SC design decision variables. Therefore, a future work could include SC uncertainties, tactical and operational decision variables, to integrate these models and carry out its validation. Also, other objective functions can be integrated in the model, as the payback time for the investment, in order to evaluate the economic performance of the projects.
- ✚ Although this research contributes to the field of NSGA-II algorithm development in order to compare it robustness and speed to find optimal solutions and the Pareto front, the adapted algorithm programming should be tested on other models including equality and inequality constraints, binary variables and multiobjective functions.
- ✚ In relation with the Colombian case study to design the sustainable Phase III BioRSC, it should be highlighted that jatropha oil is not yet agriculturally developed.

Also, to solve the problem related to lack of information for pretreatment plants, further studies should be undertaken on the field of chemical engineering to analyze the technical and economic feasibility for different levels of capacity production, including environmental analysis.

Related to lack of information for principal production plants, further studies should be undertaken to analyze the technical and economic feasibility for different levels of capacity production to process refined jatropha oil, including environmental analysis.

Moreover, a deeper analysis to the environmental dimension of sustainability should be done with a more formal approach of life cycle analysis to reduce the related objective functions. This can be done by life cycle impacts category indicators (consumption of resources, air pollution, water pollution and waste), in order to facilitate the graphical representation of the optimization results for the decision makers.

Another perspective for the integrated model and the Colombian case is to add a constraint to the optimization model that forces it to consider the principal plants that are currently in operation in Colombia. This could give some guidelines about how to initiate a reconversion process to transform biorefineries phase II in sustainable biorefineries phase III.

Regarding the number of generic parameters needed for the optimization of the integrated model, it is recommended to develop a case study at a regional scale. To compare results with these presented in this research.

- ✚ Concerning the sensitivity analysis, several parameters still can be studied to analyze the behavior of the integrated model applied to the Colombian case. Nevertheless, it will imply time for optimizations and analysis. Then, it is recommended to realize a previous analysis for the parameter uncertainty to realize the sensitivity analysis in a way that contributes to developing tactical and operational models.

Also, other objective functions can be analyzed face to the model constraints parameters variations presented in this thesis.

- ✚ Regarding the multiobjective optimization results, future work can be done with decision makers to give a preference for each objective function and to find compromises among the conflicting objectives to design a sustainable Phase III BioRSC for Colombia.

Appendix Chapter V

Appendix 5.1. Economic dimension in sustainability for biorefineries

Criterion	Indicators
<i>Criterion 20: Level of influence (international and domestic) of availability, production, consumption and prices of the raw materials for products that are intended to be produced from other raw materials over the biobased products production</i>	Indicator 62. Global annual availability of raw materials per years and per global tons of biobased products obtained in biorefineries
	Indicator 63. Global annual production of raw materials per years and per global tons of biobased products obtained in biorefineries
	Indicator 64. Global annual consumption of raw materials per years and per global tons of biobased products obtained in biorefineries
	Indicator 65. Global annual prices of raw materials per years and per global tons of biobased products obtained in biorefineries
	Indicator 66. Local annual availability of raw materials per local tons of biobased products obtained in biorefineries
	Indicator 67. Local annual production of raw materials per local tons of biobased products obtained in biorefineries
	Indicator 68. Local annual consumption of raw materials per local tons of biobased products obtained in biorefineries
	Indicator 69. Local annual prices of raw materials per local tons of biobased products obtained in biorefineries
<i>Criterion 21: Level of influence (international and domestic) of availability, production, consumption and prices of the products that are intended to be produced from other raw materials over the biobased products production</i>	Indicator 70. Global annual production of products that are intended to be produced from other raw materials per global tons of biobased products obtained in biorefineries
	Indicator 71. Global annual consumption of products that are intended to be produced from other raw materials per global tons of biobased products obtained in biorefineries
	Indicator 72. Global annual prices of products that are intended to be produced from other raw materials per global tons of biobased products obtained in biorefineries
	Indicator 73. Local annual production of products that are intended to be produced from other raw materials per local tons of biobased products obtained in biorefineries
	Indicator 74. Local annual consumption of products that are intended to be produced from other raw materials per local tons of biobased products obtained in biorefineries
	Indicator 75. Local annual prices of products that are intended to be produced from other raw materials per local tons of biobased products obtained in biorefineries
	Indicator 76. Local annual quantity of demand sources of products that are intended to be produced from other raw materials per local tons of biobased products obtained in biorefineries
<i>Criterion 22: Annual production (international and domestic) of biobased products obtained in a biorefinery</i>	Indicator 77. Global annual production quantity of biobased products
	Indicator 78. Global annual consumption quantity of biobased products per global tons of biobased products obtained in biorefineries
	Indicator 79. Global annual prices of biobased products per global tons of biobased products obtained in biorefineries
	Indicator 80. Local annual production quantity of biobased products at biorefineries
	Indicator 81. Local annual consumption quantity of biobased products at biorefineries per local tons of biobased products produced
	Indicator 82. Local annual prices of biobased products at biorefineries per local tons of biobased products produced
	Indicator 83. Local production capacity of biobased products at biorefineries per local tons of biobased products produced
	Indicator 84. Local profitability of production of biobased products per local tons of biobased products produced
	Indicator 85. Annual balance energy cost in the biobased products production per local tons of biobased products produced
	Indicator 86. Annual operational and pollution cost in the biobased products production per local tons of biobased products produced
<i>Criterion 23: Level of influence (international and domestic) of availability, production, consumption</i>	Indicator 87. Global annual prices of raw materials for biobased products per global tons of biobased products produced
	Indicator 88. Global total annual production of raw materials for biobased products per global tons of biobased products produced
	Indicator 89. Global annual consumption of raw materials for biobased products per global tons of biobased products produced
	Indicator 90. Global annual consumption of raw materials for different uses to biobased products per global tons of biobased products produced

<i>and prices of raw materials to biobased products over the biobased products production</i>	Indicator 91. Local annual prices of raw materials for biobased products per local tons of biobased products produced.
	Indicator 92. Local total annual production of raw materials for biobased products per local tons of biobased products produced.
	Indicator 93. Local annual consumption of raw materials for biobased products per local tons of biobased products produced.
	Indicator 94. Local annual consumption of raw materials for different uses to biobased products per local tons of biobased products produced.
	Indicator 95. Aboveground net primary productivity (at the state of raw material cultivation) biobased products per annual local tons of biobased products produced. Taking into account the effects of climate change.
<i>Criterion 24: Level of influence (international and domestic) of production, consumption and prices of by-products over the biobased products production.</i>	Indicator 96. Local annual price of by-products per local tons of biobased products produced.
	Indicator 97. Local annual production of by-products per local tons of biobased products produced.
	Indicator 98. Local annual consumption of by-products per local tons of biobased products produced
<i>Criterion 25: Level of influence (international and domestic) of production, consumption and prices of advanced biobased products over the biobased products production.</i>	Indicator 99. Global annual prices of advanced biobased products per global tons of biobased products produced.
	Indicator 100. Global annual production of advanced biobased products per global tons of biobased products produced.
	Indicator 101. Global annual consumption of advanced biobased products per global tons of biobased products produced.

Appendix 5.2. Economic analysis by criterion and indicator

<i>Criterion</i>	<i>Indicator(s)</i>
20	62, 63, 64, 65, 66, 67, 68 and 69
<p>It can be noted at first instance that uncertainty about the availability of raw materials for the production of oil and its derivatives, such as diesel, boost the production and consumption of biobased products such as biodiesel. In general raw materials availability directly affects the production and could affect the product price and offer; also, raw materials limited availability could generate interest in develop new substitute products based on different raw materials. Then, the raw material availability, consumption, production and prices can affect the offer, consumption and prices of the substitute products. Therefore, changes in raw materials availability, production, consumption and prices, of products that are intended to be substituted, could lead to changes on consumption, offer and prices over the biobased products. These last are parameters that serve for the decision of the quantity to produce. Then, these changes in raw materials economic aspects would affect the production of biobased products. In conclusion, a scenario or sensitivity analysis to variations in parameters such as biobased products prices and demand is required.</p> <p>At a later time, a more detailed analysis can be carried out to determine the relations between the availability, production, consumption and prices of the raw materials; for products that are intended to be produced from alternative raw materials and the biobased products consumption and prices. With these relations and forecasting changes on availability, production, consumption and prices of the raw materials the uncertainty of the parameters could be estimated; for the tactical and operational supply chain decision making levels.</p>	
21	70, 71, 72, 73, 74, 75 and 76
<p>The influence that could have the availability, production, consumption and prices of the products that are intended to be produced from other raw materials is observed in the biobased products demand and prices, which are parameters of the model; because they are substitute products. Therefore, a sensitivity analysis to variations in parameters such as biobased products prices and demand is required.</p> <p>As products that are intended to be produced from other raw materials are substitute of biobased products, the local annual consumption of products that are intended to be produced from other raw materials is the biobased products demand utilized in the model. Except if biobased products demand is established by governments, as in Colombia (Colombian Government 2004). Similarly, the local annual prices of products that are intended to be produced from other raw materials are used as biobased products prices. Except if biobased products price is established by the governments, as Colombia (Colombian Government 2014).</p>	
22	77, 78 and 79
<p>The global annual prices, production and consumption of biobased products could affect local prices and demand for biobased products. Because, if global consumption of biobased products increases, local interest can be generated to increase the production of biobased products due to the possibility to penetrate new markets or to cover larger market-share in already established biobased product global markets.</p> <p>On the other hand, variations in international prices of biobased products could generate similar variations in local prices, if there were imports and/or exports of these products. Likewise, the increase in the global production of biobased products could be due to an increase in demand and/or price at worldwide and/or international agreements. That would generate incentives for local biobased products production. Therefore, globally changes related to biobased products generate uncertainty about some parameters of the BioRSC design model, such as prices and demands. Which means that, at supply chain strategic decision level, a sensitivity analysis to variations in parameters such as biobased products prices and demand is required.</p>	
22	80, 81, 82 and 84
<p>Concerning variables at the local level, biobased production is a decision variable in the model. The profitability is represented as objective function to maximize the net present value of the project. The biobased consumption and prices are parameters in the model.</p> <p>It is assumed for the model that there is no import or export of the final products obtained. Therefore, international values for the production, consumption and international prices of the products obtained in biorefining are not included. However, the export of biobased products could be a model perspective.</p>	

Criterion	Indicator(s)
22	83
<p>It can be translated as the use of the installed capacity. This can be calculated as a function of the materials entering into the pretreatment plants and principal production plants, divided by the production capacity of the corresponding plant if the plant is installed.</p> <p>The ideal operation of a production plant maximizes the utilization of the installed production capacity, to reduce idle time of machines and workers. Therefore, this indicator can be translated as an objective function for the model in development.</p>	
22	85
<p>It should be analyzed the cost balance, which would be the analysis and optimization of profits, or the energy balance. Because it is not possible to perform the analysis of the balance energy cost, due to problems in the measurement units. For example, the energy value of the raw material "Palm oil" is 36,543 MJ/Kg. Therefore, it could be multiplied by the quantity of raw materials used to produce biobased products; this will result in the total of MJ consumed by type of raw material "Palm oil". However, if the market value of raw material 392,0459 USD/Ton is used, the result will be in MJ/USD but this parameter can not be multiplied by the quantity of raw materials consumed. Then, it has been decided to calculate the "Energy Balance" in this analysis, which is an environmental indicator. Therefore, it will be analyzed in the corresponding section.</p>	
22	86
<p>The operating costs associated with each production plant, either main or pre-treatment, have already been considered in Chapter IV. Then, the pollution cost associated to the biobased products production must to be determined.</p> <p>In general, it may be at least three principal pollution costs that could be associated to the biobased products production in biorefineries (UPME 2017). The existence of such costs will depend on the laws and norms of the country, such as atmospheric resources normativity regulating the concentration of air pollutants that are harmful to health; water resources normativity related to environmental taxes due water use or water discharges; and solid waste regulation such as collect solid wastes cost and disposal cost.</p> <p>For the model formulation, these pollution cost must be multiplied by the corresponding rate of pollution production and the amount of transformed products at pretreatment and principal plants. Also, it may be different type of specific pollution, as for example there are different kinds of atmospheric emissions, as CO₂, SO₂, particulate matter or NO_x, with different impacts.</p>	
23	87, 88, 89, 90, 91, 92, 93, 94 and 95
<p>The local raw material price is considered as raw material cost acquisition in the model. And the local annual production of raw materials is considered as raw material availability in the model. The local annual consumption of raw materials for biobased products production is a decision variable in the model. And the local annual consumption of raw materials for different uses to biobased products is represented in the model as the intermediate products demand. Then, variations in solution optimizations due to changes in parameters, such as raw material acquisition cost, availability and intermediate product demand should be analyzed to understand their influence on biobased products production.</p> <p>The global values are not considered because the model is projected at local level in the first instance, this means, no imports or exports. Then, its inclusion in the model is a perspective for this research. However, thinking about the influences, in open economies, these values could generate variations in local prices or demands or in production incentives. This indicates the previously described analysis on variations in the parameters related to raw materials and their impacts on the biobased products production.</p>	
24	96, 97 and 98
<p>The local annual price of products that can be replaced by by-products produced at biorefinery plants is the parameter "price" at final markets in the developed model. The local annual consumption is considered as final product demand. And the local annual production of by-products is a decisional variable in the model. The price and demand for products that can be replaced with by-products (biobased) is not supposed to change when the by-product is commercialized. This view is pessimistic, observing the current development of "bio" markets around the world (Ecovia Intelligence 2015; Accurray Research LLP 2017), where "bio" or</p>	

Criterion	Indicator(s)
24	96, 97 and 98 (Continuation)
<p>“organic” products have characteristics similar to those they replace but have similar or higher acquisition costs. Therefore, it is important to evaluate changes in the optimization solution due to variations in by-products parameters. Also it is important to analyze the economic contribution generated by the sale of by-products and/or high value-added products that can be produced at biorefineries.</p> <p>The global values are not considered because the model is projected at local level in the first instance, this means, no imports or exports. Then, its inclusion in the model is a perspective for this research. Some information about biobased products, as bioplastics, can be found in European Bioplastics (2017).</p>	
25	99, 100 and 101
<p>First of all, the <i>advanced</i> concept to biobased products must to be clarified. There are different approaches to classify biobased products because a great diversity of feedstocks and processes are currently being developed to meet sustainability and quality standards (ETIP Bioenergy 2017). A definition of the various generation biofuels can be described based on the carbon source from which the biofuel is derived, as follows (IEA Bioenergy 2008; IEA 2010; ETIP Bioenergy 2017):</p> <p>1st Generation. The crop is actually or potentially considered to be in competition with food (as sugar, lipid or starch as sources).</p> <p>2nd Generation. The biofuel is derived from cellulose, hemicellulose, lignin or pectin; including purpose-grown non-food feedstocks as short rotation coppice and energy grasses.</p> <p>3rd Generation. <i>The biofuel is derived from aquatic autotrophic organism.</i></p> <p>Therefore, making a generalization of this definition towards biobased products, advanced biobased products can be described as those produced from: lignocellulosic feedstocks, non-food crops, or industrial waste and residue streams; having low CO₂ emissions or high GHG reduction; and reaching were or low indirect land use change impact (ETIP Bioenergy 2017).</p> <p>In the current approach of the model are being evaluated different transformation technologies and raw materials, among which can be obtained normal and advanced biobased products.</p> <p>The global values are not considered because the model is projected at local level in the first instance, this means, no imports or exports. Then, its inclusion in the model is a perspective for this research.</p> <p>But, thinking about the influences, in open economies, advanced biobased products production, price and consumption could generate variations in local final product prices or demands or in production incentives, both for normal and advanced biobased products. This means that an analysis on variations in the parameters related to final product demands and prices, and production technologies for pretreatment plants and principal plants is required to study their impacts on the biobased products production</p>	

Appendix 5.3. Political dimension in sustainability for biorefineries

Criterion	Indicators
<i>Criterion 11: Level of agreement between the amount of biobased products produced at local level under a subsidy schema and the amount produced internationally under similar schemes.</i>	Indicator 43. Incentives or tax reduction related to biobased products, variation between years.
	Indicator 44. Local price in USD of biobased products in a price control scheme.
<i>Criterion 12: Level of agreement between first generation bioproducts and advanced bioproducts at international and local level.</i>	Indicator 45. Comparison between first generation bioproducts and advanced bioproducts at international level and first generation bioproducts and advanced bioproducts at local level
<i>Criterion 13. Level of agreement between the national and international percentages of “Biobased product”/“Total consumed product” required by governments</i>	Indicator 46. The national and international percentages of “Biobased product”/“Total consumed product” required by governments
<i>Criterion 14. Level of national research and development capacity in biobased products (first and advanced generation) regarding international capabilities.</i>	Indicator 47. Fiscal cost of the implementation of a biobased product promotion policy
	Indicator 48. Research and development governmental expenditure in biobased products (in terms of percentage of Gross Domestic Product / GDP)
<i>Criterion 15. Amount of biomass produced locally in compliance with international standards (type of biomass or raw materials that does not compete with food crops).</i>	Indicator 49. Annual amount of raw materials for the production in biorefineries, produced compliance with the criteria of renewable biomass.
<i>Criterion 16. National amount of land used for growing biomass for biobased products that meets the international requirements of land suitable for use (i.e. those that do not come from direct exchange of primary forests, exclusion areas with high biodiversity value, land with high carbon stocks and ecologically sensitive areas declared as protected)</i>	Indicator 50. Amount of Biorefinery products produced under voluntary certification criteria (e.g. RSPO, ISCC, NTA 8180) relative to the total amount of Biorefinery products produced globally.
<i>Criterion 17. Amount of domestically produced biobased products that meet international policy on minimum average or threshold of greenhouse gas emissions in their life cycle, including indirect changes in land use.</i>	Indicator 51. Total consumed tons of biobased products that are permitted by international policies at global and local level
<i>Criterion 18. Level of perception of the local community about the degree of ethical commitment by the actor in bio-based products production chain</i>	Indicator 52. Define and communicate the standards of ethical behavior in the organization.
	Indicator 53. Notice the relevant authorities, where appropriate, and complete an Environmental Impact Assessment (EIA).
	Indicator 54. Reports about penalties for non-compliance on labor, taxes or environmental legal issues, between others.
	Indicator 55. Awareness of responsibilities, according to applicable laws (environmental, fiscal, social and labor) can be demonstrated.
<i>Criterion 19. Level of perception of the local community about the commitment to transparency and compliance with local laws by the actors involves in biorefinery's chain.</i>	Indicator 56. Adopt and implement the standards of ethical behavior. Establish mechanism for monitoring and verification.
	Indicator 57. The organization must be transparent in its activities, which makes control over them, how to be making the decisions, and how their functions are defined.
	Indicator 58. The organization must be clear about the source of funds for their activities.

<i>Criterion 19. Level of perception of the local community about the commitment to transparency and compliance with local laws by the actors involved in biorefinery's chain.</i>	Indicator 59. The organization must know the likely effects of their decisions on stakeholders, society, economy and environment.
	Indicator 60. The organization inform to consumers about the environmental effects of products they are consuming and to raise environmental standards in the manufacturing of specific products.
	Indicator 61. Production of any Genetically Modified Organisms must comply with legal requirements

Appendix 5.4. Political analysis by criterion and indicator

<i>Criterion</i>	<i>Indicator(s)</i>
11	43
<p>This indicator measures the variation of government incentives and tax reduction; therefore, it is applicable only if there are incentives or tax reduction related to biobased products. Then, this implies a previous review of each case study on the incentives provided by the government.</p> <p>As the present developed model is static, this indicator could be represented as government expenditures to encourage the biobased products production. These expenditures are expected to decrease over time when industries are self-sustaining. So it can be deduced that the government's objective, other than incentivize the biobased products industry, is to reduce its government spending associated with it, in order to be able to devote these resources to other projects.</p> <p>Some researches applied this indicator as incentives for installation of production plants, which are given only once when the plant is installed, either central or pre-treatment (You and Wang 2011; You et al. 2012; Yue et al. 2014). About tax reduction, searches have found no explicit references.</p>	
11	44
<p>This indicator should be analyzed if government has a price control schema for biobased products. If applicable, it will determine the biobased product price model parameter.</p>	
12	45
<p>One might expect that the objective will be to reach international values on advanced biobased products production. Then, it could be interpreted as maximizing the amount of advanced biobased products produced by the biorefinery.</p>	
13	46
<p>At first, it is needed to analyze if there is a percentage of "Biobased product/Total consumed product" required by government. If so, it will be a parameter to determine the biobased product demand. In the other hand, in general it could be concluded that the objective of this indicator is to reach the international values for the percentages of "Biobased product consumption/Total consumed product". However, as there are no consumption regulations for all final biobased products, this objective can be reformulated as the maximization of the demand satisfaction with biobased products.</p>	
14	47
<p>The governmental budgetary support should be an integral part of biobased products policy for suppliers and producers to support live hood during gestation period (Kumar et al. 2012). It budgetary support include emotion of sales tax on the products, provide minimum support prices for suppliers engaged with raw materials production, subsidies as tax credits, excise duty incentives for products or machines that enhance the use of biobased products (Kumar et al. 2012). And some other measures as presented in the previous indicators, as subsidies for biorefinery construction, pricing of biorefinery products and subsidies to develop production technologies. Most of them have already been analyzed, excepting the subsidies to develop production technologies which will be assessed on Indicator 48, and the raw material subsidies.</p> <p>Raw material subsidies are received by suppliers; then, as in the present model suppliers cash flows have not been represented, these subsidies only can be considered as governmental expenditures (Assuming that the raw material prices are not affected by the existence of this subsidy). Then, the fiscal cost will be the addition of all governmental expenditures. A perspective of the present research is the supplier modelization.</p>	
14	48
<p>The objective of measure this indicator is to compare the local governmental expenditures in research and development for biorefineries to international standards. However, there is not specific data related to research and development governmental expenditures for biorefineries. Instead, there are calls for projects to develop production technologies for sustainable products (COLCIENCIAS 2016).</p>	

Criterion	Indicator(s)
15	49
This could be translated into maximization of the use of advanced biobased products, as they are non-food crops, so this indicator would be represented in the model by indicator 45.	
16	50
To evaluate this indicator is required to study if potential suppliers have a voluntary certification for its land resources. Then, the objective will be to maximize the rate between the biobased products produced by raw materials from certified lands and the total biobased products produced. However, it could be also described in a simplest and linear form as the maximization of the use of raw materials belonging to certified land for biobased products.	
17	51
This could be understood as the produced and/or consumed amount of biobased products that meet international policy related to greenhouse gas emissions in their life cycle. Amount that could be maximized. Therefore, for build this objective it is needed to search the international policy, to classify the products. There exist some information about the carbon foot prints by products (Eurostat 2017) or the greenhouse gas (GHG) emissions by industries and households (Eurostat 2017). However, no specific international regulations have been found on the amount of GHG emissions generated in the entire life cycle of a product in terms of CO ₂ -equivalent, specifically for biobased products from biorefinery. Only it has been found regulations that call for the reduction of GHG generated in the life cycle. Then, this is why this indicator should finally be considered as the search for the minimization of GHG produced in the life cycle of products produced in biorefinery, which is an environmental indicator. Therefore, it will be analyzed in the corresponding section.	
18	52
<p>Ethical behavior in an organization related to current and new biobased products includes human rights, solidarity, sustainability, stewardship and justice (Nuffield Council on Bioethics 2011). The Nuffield Council on Bioethics sets out six ethical principles that policy makers should use to evaluate biofuel technologies and guide policy development (Nuffield Council on Bioethics 2011).</p> <ul style="list-style-type: none"> • Biofuels development should not be at the expense of people's essential rights (including access to sufficient food and water, health rights, work rights and land entitlements) • Biofuels should be environmentally sustainable. • Biofuels should contribute to a net reduction of total greenhouse gas emissions and not exacerbate global climate change. • Biofuels should develop in accordance with trade principles that are fair and recognize the rights of people to just reward (including labor rights and intellectual property rights). • Costs and benefits of biofuels should be distributed in an equitable way. • If the first five principles are respected and if biofuels can play a crucial role in mitigating dangerous climate change then, depending on certain key considerations, there is a duty to develop such biofuels. <p>These principles are considered in the five sustainability dimensions that are being analyzed for the model development. Then, it could be a part of the strategic guidelines of the company to communicate the preferences of its stakeholders to find the balance between the different objectives that are being determined in the present modelization.</p> <p>Therefore, as a future perspective of the present work, the preferences of the investors and/or others involved must be defined. And thus define the ethical behavior of the organization according to preferences for each of the objectives or optimization constraints.</p>	

<i>Criterion</i>	<i>Indicator(s)</i>
18	53
<p>An EIA is a guide to understand the potential environmental impact of a development by an information compilation exercise. Before deciding whether or not it should go ahead. It will serve not only to the investors, but also it allows the local authority and the whole community to properly understand the impact of the proposed development (FOE 2008). This analysis is required for some type of development; if the projects are likely to have a significant impact on the environment as major power plants, chemical works, or waste disposal incineration. It is composed by three stages:</p> <p>Characteristics of development, as size, use of natural resources, waste production, pollution and nuisances, and risk of accidents regarding substances or technologies used. This is already considered in the model development.</p> <p>Location of development, regarding the existing land use, the relative abundance, quality and regenerative capacity of natural resources in the area; and the absorption capacity of the natural environment. This has been considered at the jatropa potential location decision; also, only the hectares of palm currently in production stage have been considered for the model.</p> <p>Characteristics of the potential impact, regarding the extent of the impact (geographical area and size of the affected population); the trans frontier nature of the impact, the magnitude and complexity of the impact, the probability of the impact, its duration, frequency and reversibility. This stage could be analyzed on the environmental dimension analysis, establishing the potential environmental impacts and the associated indicators considering these characteristics.</p> <p>Therefore, an EIA could be realized from the information gathered for the realization of this modelization and the results obtained in the optimization. The investors that carry out the project will be responsible for the completion of the final document and notification to the competent authorities.</p>	
18	54 and 55
<p>The reports about penalties and awareness of responsibilities can be measured and demonstrated once the production plants are installed. Therefore, these indicators are not applicable for the design phase.</p>	
18	56
<p>It is related to <i>Indicator 52</i>, where six ethical principles are represented. These are integrated in the model by the five sustainability dimensions.</p> <p>The verification of these can be done through the measurement of certain indicators (linked to ethical principles), prior to the completion of the project, and compare with the same indicator after the project. Observing if the standards of ethical behavior have been respected. Then, they can trigger action plans to correct certain behaviors that deliver unsatisfactory results.</p> <ul style="list-style-type: none"> • Biobased products development should not be at the expense of people’s essential rights (including access to sufficient food and water, health rights, work rights and land entitlements): <ul style="list-style-type: none"> ✚ Measurement of access to food and water in communities that will be affected ✚ Review of ownership titles of land that will be affected ✚ Measurement of health and health rights levels of the people who will be directly affected by the project. • Biobased products should be environmentally sustainable. <ul style="list-style-type: none"> ✚ Comparison between the indicators of the environmental section that were projected and a study with the already installed project (Including GHG emissions, wastewater generation, among others) • Biobased products should contribute to a net reduction of total greenhouse gas emissions and not exacerbate global climate change. <ul style="list-style-type: none"> ✚ Comparison between the indicators of the environmental section that were projected and a study with the already installed project (Including GHG emissions, wastewater generation, among others) • Biobased products should develop in accordance with trade principles that are fair and recognize the rights of people to just reward (including labor rights and intellectual property rights). <ul style="list-style-type: none"> ✚ Comparison between the indicators of the social section that were projected and a study with the already installed project 	

<i>Criterion</i>	<i>Indicator(s)</i>
18	56 (Continuation)
<ul style="list-style-type: none"> Costs and benefits of Biobased products should be distributed in an equitable way. 	
<ul style="list-style-type: none"> ✚ Measurement of costs and benefits generated by the project 	
19	57 and 58
About Indicator 57 and 58, they are strategic advices to project a good image of the organization.	
19	59
Indicator 59 can be supported by the present model in process and optimization, since it can be observed the results for the five sustainability dimensions and it can be noted how the different objectives are complementary or opposite.	
19	60 and 61
<p>Indicator 60 can be accomplished through the ethical behavior monitoring and the environmental dimension analysis, through which the organization can inform its clients the environmental effects of biorefinery products. This can be taken as an organization marketing strategy.</p> <p>Related Indicator 61, this is a council for organizations. They should review the existing laws in the country where it is desired to carry out the project to know previously the conditions to be achieved related to genetically modified organisms.</p>	

Appendix 5.5. Technological dimension in sustainability for biorefineries

Criterion	Indicators
<p><i>Criterion 26. Level of influence of production of advanced biobased products (international and domestic) on demand of soils and water resources (international and domestic)</i></p>	<p>Indicator 102. Amount of hectares of land required for the production of raw materials for advanced biobased products</p>
	<p>Indicator 103. Amount of water required for the raw material production and biobased products transformation by production technology.</p>
<p><i>Criterion 27. Level of influence of global and domestic production of advanced biobased products by non-conventional technologies on efficiency of processes and cost reduction.</i></p>	<p>Indicator 104. Reduction of production cost dependent on the production technology apprenticeship.</p>
<p><i>Criterion 28. Level of influence of technology trends for systems or elements that can use biorefinery products on the biobased products production (as example, technology trends for engines when biorefinery product is biodiesel)</i></p>	<p>Indicator 105. Demand for biobased products according to the number of systems or elements that does not use the biorefinery specified product.</p>
<p><i>Criterion 29. Level of influence of technological learning (local or international) in the production of biobased products or reducing cost over time.</i></p>	<p>Indicator 106. Reducing cost of production by technological learning independent of accumulate production (associated with technological maturity that can be assessed indirectly by scientific articles and patents related to the technology).</p>

Appendix 5.6. Technological analysis by criterion and indicator

<i>Criterion</i>	<i>Indicator(s)</i>
26	102 and 103
<p>It can be deduced that for indicator 102 is needed to quantify the required hectares to produce the raw materials. Also, for indicator 103 it must to be calculated the amount of water needed to produce the raw materials and for process it with different technologies at biorefineries. Thus, there are two objective functions to define in this section: the minimization of total required hectares for raw material production and the minimization of the total needed water at BioRSC.</p> <p>It can be noted that the installation of biorefineries could affect land use and water resources. Then, as perspective of this developing model, it could be analyzed the model response to the elimination of raw material availability restriction. It allows observing the potential impact of, par example; maximize the demand satisfaction with biobased products.</p>	
27	104
<p>This indicator seeks to measure variations in cost due to efficiency of processes generated for apply different production technologies and apprenticeship. The cost can be reduced in time by technology apprenticeship, which can be described by learning curves (Herrero et al. 1999). These last are related to the experience accumulated by the company in terms of producing each time in a more efficient way (Herrero et al. 1999). Then, know-how of the production process is translated into a decrease in unit cost as the accumulated production increases (Steinberg 2004). Therefore, the relation between the accumulated production and the cost reduction should be mathematically defined.</p>	
28	105
<p>It could be understand as the influence of technology trends on consumption. It will be depending on technology development. Because, if the technology incentives the use of substitute products or if it is more efficient, the biobased product consumption will decrease. At the same time, this could affect product prices. So, technological trends are an uncertainty source. Then, this can be analyzed in a perspective of the actual deterministic model.</p>	
29	106
<p>As seen in indicator 48, analysis of the political dimension in section 5.3.2, the TRL levels describe the technology readiness or maturity. Therefore, it can be deduced that a reduction on operation cost could be generated when a high TRL level is achieved. However, in the same way as investment required achieving higher TRL levels depend specifically in case study, the cost reduction related to different TRL levels should be analyzed for each potential technology in the case study.</p> <p>Also, it must be noted that lower TRL levels are related to uncertainties and risk, due necessary investments in technologies that are not yet industrialized are not fixed or fully known. This generates an incentive to install technologies that have an industrialized level to avoid expenses in technological development. Then, as perspective of this work, due developing model is deterministic, uncertainty should also be analyzed for each potential technology in the case study.</p>	

Appendix 5.7. Social dimension in sustainability for biorefineries

Criterion	Indicators
<i>Criterion 1. Respect the rights of land access and land tenure for peasant and indigenous communities.</i>	Indicator 1. Indigenous peoples shall control biorefinery management on their lands and territories unless they delegate control with free and informed consent to other agencies.
	Indicator 2. Biorefinery management shall not threaten or diminish, directly or indirectly, either the resources or tenure rights of indigenous people
	Indicator 3. Sites of special cultural, ecological, economic or religious significance to indigenous peoples shall be clearly identified in cooperation with such peoples and recognized and protect by Biorefinery managers (all parties involved).
<i>Criterion 2. Promote the minimization of conflict over the use, access and land tenure</i>	Indicator 4. Promotion of the involvement of stakeholders about use of land, management of conflicts and tenure of land
	Indicator 5. Avoidance of land tenure conflicts
	Indicator 6. Projects should not exclude poor people from the land in order to avoid leakage effects
	Indicator 7. Land ownership should be equitable
	Indicator 8. Number of rights granted by constitutions, regulations and official tribunals or other laws: customary, casual, temporary and secondary
	Indicator 9. Number of people in a population with safe titles (for example, registered) in relation to the number of people with insecure titles on the land, in the area of direct influence of the plantations of raw materials and Biorefinery products processing
<i>Criterion 3. Contribute to national energy security and the access of rural communities to energy.</i>	Indicator 10. Index of energy matrix diversification
	Indicator 11. Government investment in electricity infrastructure
<i>Criterion 4. To prevent generation of environmental noise</i>	Indicator 12. Qualitative indicator scale of 1 to 5, 1 being the lower noise impact and 5, a significant impact
<i>Criterion 5. To prevent changes in the landscape generating undesirable visual impact for communities</i>	Indicator 13. Qualitative indicator scale of 1 to 5, 1 being the lower visual impact and 5, a significant visual impact
<i>Criterion 6. To contribute to local prosperity associated with the reduction of poverty and the promotion of human rights.</i>	Indicator 14. Stakeholder involvement in the decisions that concern them
	Indicator 15. Total annual national of households without access to public services of the total number of families, in the direct area influence of raw material plantations/production and mining and transformation Biorefinery plants
	Indicator 16. Access to health care and medication
	Indicator 17. Total annual national of illiteracy people aged 15 or more of the number of persons, in the direct influence of raw materials plantation/production and mining and transformation Biorefinery plants
	Indicator 18. Opportunities for employment: Total annual number of employment in plantation/production of raw materials, and transformation plants
	Indicator 19. Total annual national of head of household's opinion about better living standards of their home, which was about 5 years ago of the total number of families, in the direct area influence of the raw materials plantations /production and mining and processing Biorefinery plants.
	Indicator 20. Unsatisfied basic needs: Weight average of the annual percentages of people in poverty, according to the indicator of unmet basic needs in the municipalities that are part of the zone of influence on the biorefineries production system.
	Indicator 21. Number of organizations of the community partition in Biorefinery production system per year
	Indicator 22. Participation of small farmers (less than 20 ha): Number of small farmers of raw materials for Biorefinery per number of total farmers of raw materials for Biorefinery
	Indicator 23. Land prices of a hectare of land with raw materials for Biorefinery in areas influenced by the production of Biorefinery per year.

	Indicator 24. Total national of people displacement from areas affected by the number of persons received by displacement from other areas in the direct influence of raw material plantations and mining and processing Biorefinery plants
	Indicator 25. Total national estimated annual lands usurped hectares in areas of direct influence of the Biorefinery production system
	Indicator 26. Annual amount of conflict associated with guerrilla groups, drug trafficking, or common criminals who present in the direct influence of raw material plantations and mining and processing Biorefinery plants
<i>Criterion 7. Ensure that all their activities are carried out protecting health and promoting safety for employees.</i>	Indicator 27. The process route healthiness index (PRHI)
	Indicator 28. Affiliation of the employees to occupational hazards insurance
	Indicator 29. Hazardous materials protection: Employer provides and employees use adequate protective clothing, appropriate safety equipment, and filtered air respirator systems and/or posited pressure cabs for workers handling highly toxic chemicals.
	Indicator 30. Number of work accidents and occupational sicknesses in the different stages of biobased products production system
	Indicator 31. Sanitation: Employer provides clean drinking water and clean latrines with hand-washing stations to workers
	Indicator 32. Insurance against workplace injury: Employer provides workers compensation and disability insurance for all full time employees.
	Indicator 33. Environmental training of employees, job instructions, on the job training.
	Indicator 34. Fair treatment of worker
<i>Criterion 8. To guarantee the respect of labor laws (associated with forced child labor, discrimination, working hours, salaries, , illness and deaths, forced and compulsory labor).</i>	Indicator 35. Number of workers with direct labor contracts with biorefinery
	Indicator 36. Number of workers employed through other forms of recruitment (associations, intermediary companies).
	Indicator 37. Number of workers who belong to trade unions
	Indicator 38. Number of workers under legal age to work
<i>Criterion 9. To prevent alteration to trade and food supply at the local level</i>	Indicator 39. The consumer price index (CPI) measures changes over time in the general level of prices of consumer goods and services that households acquire, use or pay for consumption
	Indicator 40. Undernourishment: Proportion of undernourished in the population (%). Annual number of undernourished people in the total population of the country.
	Indicator 41. Amount of hectare of agricultural land and livestock research in active production relative to total land available with this vocation, per year.
	Indicator 42. Vulnerability analysis and mapping (VAM) is a network of food security experts who work closely with national governments, United Nations partners and NGOs to inform food insecurity and hunger related programs and policies
<i>Criterion 10. To prevent alteration to biomass production for traditional uses other than biobased products (e.g. as medicine raw material, as building material).</i>	

Appendix 5.8. Social analysis by criterion and indicator

<i>Criterion</i>	<i>Indicator(s)</i>
1	1, 2 and 3
This criterion should be used to determine potential locations (geographical parameter) for potential suppliers of raw materials, the potential location of pretreatment plants and main plants, avoiding protected land.	
2	4, 5 and 6
These indicators are criteria for the selection of potential suppliers, pretreatment and principal production plants. Then, a way to integrate it is to involve the stakeholders in the analysis for the determination of the potential location. Considering where the pretreatment and principal productions plants must not to be installed, and where raw materials cannot be produced, due to land protection or high density of property abandoned or stripped (to avoid tenure land conflicts). Geographical analysis is related to Criterion 1.	
2	7
This indicator can be understood as a selection criterion for the potential pretreatment and principal production plants and for raw materials production. To characterize equitable land ownership, there is a GINI index that measures the land ownership concentration (Zheng et al. 2013). Therefore, this indicator can be represented mathematically in the model for localization selection.	
2	8 and 9
Increasing rights, regulations or laws may lead to changes in potential locations for obtaining raw materials, installation of pretreatment plants and main plants of production; as well as an increase in the amount of safe titles in population possession. Therefore, an uncertainty source is announced by these indicators for the model parameters: raw material location and availability, pretreatment plants location and principal plant location. Therefore, their analysis is needed in the perspective stochastic model of the current deterministic model in development.	
3	10
To contribute to national energy security it is important to generate energy at national level continuously. Related to the energy matrix, it integrates energy sources as oil, coal, nuclear, hydro, biomass and other renewable (Wind, geothermal, solar) (United Nations 2010; IEA 2016). Then, to promote energy matrix diversification it must to be analyzed the energy matrix corresponding to the case study to then choose the source of energy that must to be increased. In general, this indicator can be described as maximize the energy demand satisfaction with biobased products (As indicator 46, which has already been analyzed).	
3	11
If government increases investment in electricity infrastructure to allow a greater and better access to energy, it could mean an increase in electricity demand. Then this indicator must to be considered and mathematically represented if electricity is evaluated as a biobased product produced at biorefineries.	
4	12
This indicator warns about the noise that could be generated by the biorefineries installation. Therefore, the admitted noise limits must to be known to develop mitigation measures if necessary.	
5	13
This indicator is related to potential visual impact that could be generated by the biorefineries installation. It can be measured through communities' opinion by presenting the architecture of production plant projects. To develop mitigation measures with communities and stakeholders.	
6	14
It is an advice to involve stakeholders. Then, stakeholders should be identified to evaluate its interest and ponderation for each objective function established in the current developing model for a future multicriteria analysis as perspective of the present work.	

Criterion	Indicator(s)
6	15, 17, 19, 20, 21, 23, 24 and 26
These indicators aims to evaluate and compare the biorefinery installation effects on public service access, illiteracy, population biorefinery opinion, unsatisfied basic needs, land prices, people displacement and social conflicts. Then, the related data must to be obtained before and after the biorefinery installation. This is no possible to represent it in the current optimization model. So, it should be considered in the perspective work.	
6	16
It is an advice to promote human rights. Then, programs for healthcare and medication should be established at biorefinery plants.	
6	18
The objective of this indicator is to increase the number of employment related to SC biorefinery. Then, it should be mathematically described.	
6	22
This indicator is linked to equitable land ownership. Then, it can be consider that it is evaluated in Indicator 7 with the GINI land index.	
6	25
This indicator is related with Criterion 1; and it can be considered as avoid land conflicts in the present model development. Therefore, it is analyzed together with Criterion1.	
7	27, 28, 29, 30, 31, 32, 33 and 34
The indicators belonging to criterion 7 are basic conditions that must to be accomplished by employers with employees to protect health and promote safety. Therefore, this criterion is an advice to employers and it cannot be mathematically represented for the design phase for the sustainable BioRSC Phase III.	
8	35 and 36
These indicators measure the number of workers by recruitment forms. Differentiating between direct and indirect labor contracts, by intermediary companies or associations. Therefore, the objective of maximize the total amount of employment opportunities generated by the SC biorefinery (Indicator 18) can be mathematically represented and differentiate by labor contract type. It is required to characterize the different labor contracts to define which type should be maximized.	
8	37
This indicator can only be measured if biorefinery is installed. Therefore, it cannot be mathematically represented for the design phase for the sustainable BioRSC Phase III.	
8	38
This indicator is a legal condition that employer must to accomplish in employers recruitment. Therefore, it cannot be mathematically represented for the design phase for the sustainable BioRSC Phase III.	
9	39 and 40
Criterion 9 and its indicators are related to prevent alterations in trade and food supply at local level. Therefore, use of raw materials that are used for food purposes should be avoided in biorefineries. This can be considered as already integrated in the model with the maximization of advanced biobased products production, presented by indicator 45 in political criterion 12.	
10	
Criterion 10, as criterion 9, is linked to prevent alterations in raw materials use. This is directly related with the idea of Biorefinery Phase III, to diversify the types of raw materials used, avoiding excessive use of any of them.	

Appendix 5.9. Environmental dimension in sustainability for biorefineries

Criterion	Indicator
<i>Criterion 30: To ensure that air quality is maintained or improved</i>	Indicator 107. Annual tons of nitrogen oxide gas emissions generated by using biobased products produced at biorefineries.
	Indicator 108. Annual tons of particulate matter gas emissions generated by using biobased products produced at biorefineries.
	Indicator 109. Annual tons of carbon monoxide gas emissions generated by using biobased products produced at biorefineries.
	Indicator 110. Annual tons of total hydrocarbons gas emissions generated by using biobased products produced at biorefineries.
	Indicator 111. Annual tons of total atmospheric acidification burden per unit mass, environmental burden is kg Sulphur dioxide equivalent product
<i>Criterion 13. To promote the efficient use of water to minimize pressure on the local availability of the resource</i>	Indicator 112. Annual tons of total persistent organic pollutants (POP) and substances that deplete the ozone layer
	Indicator 113. Average cubic meters of water available per year in direct area of influence of biobased products production system (taking into account the effects of climate change)
	Indicator 114. Index linking shortage of water available with respect to water consumption in direct area of influence of biobased products production system
	Indicator 115. Water used by hectare in raw material cultivation for biobased products per year
	Indicator 116. Water used annually for biobased products production in the transformation process
<i>Criterion 32. To minimize the generation of pollutant effluents and treat such effluents in order to maintain or improve the local water quality</i>	Indicator 117. Annual quantity or water recycled of the total water utilized in the biobased products production
	Indicator 118. Annual ratio of the amount of water used for growing raw materials and biobased products production of all water used for human consumption and food crops in the area of direct influence (taking into account the effects of climate change)
	Indicator 119. Concentration annual average of suspended sediment in the principal stream (those that are used for human consumption) that are part of the direct influence area (watershed) of raw material plantations.
	Indicator 120. Concentration annual average of phosphorus (P) in the principal stream (those that are used for human consumption) that are part of the direct influence area (watershed) of raw material plantations
	Indicator 121. Concentration annual average of nitrogen in the principal stream (those that are used for human consumption) that are part of the direct influence area (watershed) of raw material plantations
	Indicator 122. Concentration annual average of herbicide concentration in the principal stream (those that are used for human consumption) that are part of the direct influence area (watershed) of raw material plantations
<i>Criterion 33. To ensure that non-hazardous and hazardous wastes are managed responsibly (collection, storage, transportation, treatment and/or disposal) by promoting their minimization, reuse and/or recycling.</i>	Indicator 123. Discharge rate of wastewater generated in the production of one ton of biobased products in transformation industry per year
	Indicator 124. Discharge of nitrate per raw material production for biobased product production per year
	Indicator 125. Discharge of phosphorus per raw material production for biobased product production per year
<i>Criterion 34. The raw material cultivation activities for biobased products must maintain or improve the soil quality (physical, chemical and biological properties) by establishing responsible</i>	Indicator 126. Amount of hazardous waste taken to a proper final disposal of all waste generated in the biorefinery system per year.
	Indicator 127. Amount of waste that are reuse or recycle with relation of total waste generated in stages of raw material cultivation
	Indicator 128. Waste amount that are recovered or valued with relation of total waste generated in stages of raw material transformation to biobased products
	Indicator 129. Total amount of non-hazardous waste generated annually per tons of biobased products produced
<i>Criterion 34. The raw material cultivation activities for biobased products must maintain or improve the soil quality (physical, chemical and biological properties) by establishing responsible</i>	Indicator 130. Amount of total organic carbon (TOC) measured annually in an hectare of raw material cultivation
	Indicator 131. Amount of total nitrogen measured annually in an hectare of raw material cultivation
	Indicator 132. Amount of extractable phosphorus measured annually in an hectare of raw material cultivation
	Indicator 133. Annual measure of bulk density in soils used for growing raw materials

<i>practices of crop management, handling of agrochemicals and pest control.</i>	Indicator 134. Amount of agrochemical (fertilizers minerals or organics and pesticides) used per hectare of cultivation of raw material. In special, the agrochemicals prohibited in the Stockholm and Rotterdam conventions.
	Indicator 135. Quantity annual of land, in region with influence of raw material cultivation for biorefineries, those are degraded due to acidification and salinization
	Indicator 136. Quantity of eroded land in the direct influence of the production of biorefineries.
	Indicator 137. Existence of crop rotation plan/cycle. This plan will identify actual cropping for current year and the intentions for the future (over three years)
<i>Criterion 35. The amount of greenhouse gas captured or stored in carbon sinks (biomass associated) must be greater than the amount of greenhouse gas emitted by the biorefinery supply chain</i>	Indicator 138. Amount of equivalent CO ₂ emitted by direct change of land use in the area of direct influence of biorefinery production system.
	Indicator 139. Generated nitrogen oxide associated with the use of chemical fertilizers and pest control on raw material cultivation land for biorefinery production.
	Indicator 140. Annual amount of equivalent CO ₂ emitted by the raw material adaptation and transformation in biorefinery production system
	Indicator 141. Annual amount of equivalent CO ₂ emitted by the use of biobased products produced in biorefineries.
	Indicator 142. Amount of equivalent CO ₂ emitted by indirect change of land use due to the area of direct influence of biorefinery production system.
	Indicator 143. Amount of equivalent CO ₂ emitted by logistic activities related to biorefinery supply chain.
<i>Criterion 36. Transformation of natural ecosystems and loss of native natural landscape should be avoided during biomass cultivation and biodiesel production.</i>	Indicator 144. Annual amount of equivalent CO ₂ captured or maintained in carbon sinks
	Indicator 145. Land used for food crops different to raw materials used by biorefineries
	Indicator 146. Annual amount of hectare land used for raw material cultivation devoted to biorefinery
	Indicator 147. Conexant index Equivalent Area (ACE) for evaluating the connectivity ecosystem.
	Indicator 148. Annual amount of biodiversity projects and promotion of local traditional knowledge; with participation of communities.
Indicator 149. Annual amount of degraded land (e.g. erosion, salinization, acidification, or other causes) and areas of natural cover change, in areas directly affected by raw material cultivation or biorefinery production plants.	
<i>Criterion 37. Biorefinery supply chain must preserve areas with fragile ecosystems (both terrestrial and aquatic ecosystems) such as nature reserves defined by the national environmental legislation.</i>	Indicator 150. Annual amount of land used for forest and natural ecosystems in direct area of influence of raw materials plantation and biorefinery production plants
	Indicator 151. Annual average temperature of aquatic ecosystems (e.g. estuaries, rivers, lakes, wetlands) located in the area of direct influence of raw material production and biorefinery production system.
	Indicator 152. Aquatic oxygen demand of aquatic ecosystems (e.g. estuaries, rivers, lakes, wetlands) located in the area of direct influence of raw material production and biorefinery production system.
<i>Criterion 38. The number of species of wildlife listed as vulnerable or endangered should not be affected during biomass cultivation and its transformation.</i>	Indicator 153. Number of annual species, flora and fauna, specifically those who are in danger or are considered of special conservation interest, for the International Union for Conservation of Nature (IUCN) and local research organizations.
	Indicator 154. Areas established as wildlife reserves (e.g. national parks, civil society reserves or private reserve areas) located in the area of direct influence of raw material production and biorefinery production system.
<i>Criterion 39. Energy used in the biorefinery supply chain from renewable sources</i>	Indicator 155. Report total annual fuel consumption from renewable fuel sources including fuel types used.
	Indicator 156. Report total annual fuel consumption from non-renewable fuel sources including fuel types used.
<i>Criterion 40: Energy savings in the biorefinery supply chain compared to the previous year.</i>	Indicator 157. Rate among the amount of energy generated by biobased products and the energy consumed for its production.

Appendix 5.10. Environmental analysis by criterion and indicator

<i>Criterion</i>	<i>Indicator(s)</i>
30	107, 108, 109, 110, 111 and 112
These six indicators are related to gas emissions generated by using biobased products. Then, they can be represented as objective functions to minimize.	
31	113
As this indicator is related to water availability, it can be seen as a restriction to the developing model.	
31	114, 115 and 116
Indicators 115 and 116 are related to the amount of water required for raw materials cultivation and its transformation at biorefineries. Then, they can be described as the objective function to minimize the water use. As presented in equation (51) related to technological indicator 103. To measure the effects in water shortage due biorefinery operations, related to indicator 114, it can be compared the total water use (indicator 115 and 116) with water availability (indicator 113). However, it can be represented also as the minimization of total water use (Equation (51)). Therefore, these indicators are already measured and integrated to the model.	
31	117
Analyzing this indicator, the recycled water amount will depend on plant design, in other words, it depend in use and recycled water by production technology and in special structures to recycle water. Then, it can be mathematically described as function of materials transformed at biorefinery plants.	
31	118
This indicator can be analyzed as minimize the objective function that relate the biorefinery water consumption versus the human consumption and requirements for food crops. However, it can be represented also as the minimization of total water use (Equation (51)). Therefore, this indicator is already measured and integrated to the model.	
32	119, 120, 121, 122, 124 and 125
Indicators 119, 120, 121, 122, 124 and 125 are related to different water pollutants generated at raw material cultivation stage. Therefore, as the developing model does not consider supplier strategies or cultivate technologies, it could be only mathematically represented depending on raw material type. However, the raw material cultivation land requirements depending on culture technique could be represented by mathematical expressions as perspective for future work.	
32	123
Indicator 123 measure the waste water generated by transformation process at biorefinery plants. This is analyzed economically by criterion 22, indicator 86. Then, it can be mathematically represented as objective function to minimize the wastewater generation.	
33	126, 129
Related to indicator 126, it is assumed that all hazardous waste will take a proper final disposal. Then, indicators 126 and 129 can be represented by the objective function of minimize the total hazardous and non-hazardous waste generation Then, they can be mathematically represented. There indicators are represented in the economic dimension by criterion 22, indicator 86.	

Criterion	Indicator(s)
33	127
This indicator is related to waste recycled or reuse at raw material cultivation stage. Therefore, as the developing model does not consider supplier strategies or cultivate technologies, waste reuse is out scope for the present model. However, it could be represented by mathematical expressions as perspective of future work.	
33	128
The model already integrates the valorization of by-products at pretreatment plants and principal production plants. Therefore, waste recovered or valued at pretreatment and principal production plants can be mathematically represented to be included in the developing model.	
34	130, 131, 132, 133, 134 and 137
These indicators are related to raw material cultivation impacts in soils. Therefore, as the developing model does not consider supplier strategies or cultivate technologies, it could be only mathematically represented depending on raw material type. However, the raw material cultivation land requirements depending on culture technique could be represented by mathematical expressions as perspective for future work.	
34	135 and 136
Both indicators measure changes in soil characteristics due to biorefinery installation. Then, it should be performed a previous measure in land as reference point for the comparison. Therefore, these indicators are out scope for the present model.	
35	138, 142 and 144
These indicators measure the impact of the biorefinery installation in terms of the equivalent CO ₂ emitted due to direct and indirect change of land use; and the changes in carbon sink. This can be compared only posteriorly. Then, it should be performed a previous measure as reference point for the comparison. Then, these indicators are out scope for the present model.	
35	139
This indicator is related to raw material cultivation impacts due use of chemical fertilizers. Therefore, as the developing model does not consider supplier strategies or cultivate technologies, they are out scope for the present model. However, they could be represented by mathematical expressions as perspective for future work.	
35	140, 141 and 143
These indicators are related to measure the equivalent CO ₂ emitted at pretreatment plants, principal plants, logistic activities and biobased products use. Then, they can be integrated in an objective function to minimize the total amount of equivalent CO ₂ emitted. It must to be noted that equivalent CO ₂ emitted by logistic activities must be more detailed when model includes tactical and operational SC decision-making levels.	
36	145
Indicator 145 can be understood as the impact measure of biorefinery land requirements for raw materials cultivation in land used for another food crops. Then, the objective could be seeing as maximize the use of raw materials that minimize land requirements or to prefer raw materials with no conflict related to land use for food crops. This in general can be described as advanced biobased products. Therefore, this indicator can be represented by equation (44), in political indicator 45.	

Criterion	Indicator(s)
36	146
Similarly, indicator 146 is related to raw material cultivation land requirements. Then, it can be expected that the objective will be to minimize the hectares required to grow the raw materials devoted to biorefinery and to evaluate potential raw materials with non-food use. It is important to highlight that land requirements for raw material cultivation may vary depending on raw material type and/or culture technique. Therefore, as the developing model does not consider supplier strategies or cultivate technologies, it could be only mathematically represented depending on raw material type. The, the raw material cultivation land requirements depending on culture technique could be represented by mathematical expressions as perspective for future work.	
36	147 and 149
These indicators measure the impact of the biorefinery installation on the ecosystem connectivity and land degradation. Then, it should be performed a previous measure as reference point for the comparison. Therefore, these indicators are out scope for the present model.	
36	148
Biodiversity projects could generate governmental expenses, however, there are not related to another model decision variables. Therefore this indicator is out scope for the present model.	
37	150, 151, and 152
These indicators measure the impact of the biorefinery installation on forest and ecosystems. Then, it should be performed a previous measure as reference point for the comparison. Therefore, these indicators are out scope for the present model.	
38	153 and 154
These indicators give a guide to establish the potential location for raw material cultivation, biorefinery pretreatment plants and principal production plants. Then they are considered as geographical constraints.	
39	155 and 156
These indicators are related to fuel consumption at the BioRSC including fuel types. Therefore, it can be expected the objective of maximize the percentage of renewable sources used. This can be mathematically described for the present model.	
40	157
This criterion, as analyzed in the economic dimension (Criterion 22, indicator 85), should be mathematically represented to evaluate the energy balance.	

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Appendix Chapter VI

Appendix 6.1. Raw materials availability estimation.....	1
Appendix 6.2. Processing rates for palm oil and jatropha at pretreatment plants.....	4
Appendix 6.3. Processing rates for palm oil and jatropha at principal plants	6
Annex 6.4. Installation cost at Principal and pretreatment Plants	10
Appendix 6.5. Operational cost estimation for pretreatment and principal production plants	13
Appendix 6.6. Biodiesel demand calculation	17
Appendix 6.7. Glycerin demand calculation.....	20
Appendix 6.8. Polyester demand calculation	21
Appendix 6.9 Biodiesel price estimation.....	24
Appendix 6.10. Palm oil demand calculation	25
Appendix 6.11. Transport distance matrix (km)	26
Appendix 6.12. Transport cost matrix (USD /km t).....	31
Appendix 6.13. Sewage water production parameters estimation	36
Appendix 6.14. Solid waste generation	39
Appendix 6.15. Water consumption for raw materials.....	41
Appendix 6.16. Water required for transformation process at pretreatment and principal plants .	42
Appendix 6.17. Cost reduction due to technology learning	45
Appendix 6.18. Indigenous settlements	48
Appendix 6.19. Workers estimation	51
Appendix 6.20. Water degradation for raw materials cultivation	54
Appendix 6.21. Fuel consumption estimation (t diesel / t product flow).....	56
Appendix 6.22. Energy balance parameters estimation	61
Appendix 6.23. CO2-equivalent emissions.....	67
References	70

Appendix 6.1. Raw materials availability estimation

Related to palm oil production, the information to 2015 is available in Fedepalma (2015) and is resumed in table 1.

Table 1 Palm oil production available as raw material in Colombia (Based on Fedepalma (2015)).

Department	Location	Palm oil trees in production (Ha)	Palm oil trees on development (Ha)	Palm oil production (Tons)	Yield per hectare (Tons/Ha)
Bolívar	Cartagena	25,899	31,563	55,161	2.1299
Casanare	Yopal	33,013	40,092	111,435	3.3755
Meta	Villavicencio	116,161	141,068	413,300	3.5580
Magdalena	Santa Marta	45,834	61,134	198,000	4.3200
Cesar	Valledupar	68,111	85,515	281,000	4.1256
Santander	Bucaramanga	63,044	74,520	173,400	2.7505
Norte de Santander	Cúcuta	12,880	15,224	13,500	1.0481
Nariño	Pasto	15,621	18,346	23,000	1.4724

In the other side, the available land to produce jatropha is estimated on research Gaona Currea (2009) and is presented in table 2. The hectares are classified by suitable degree and use conflict (Gaona Currea 2009; Hernández Castiblanco and Amórtegui Gómez 2015).

Table 2 Available hectares to jatropha production in Colombia by location.

Department	Location	Highly suitable without use conflict M3A (Ha)	Moderately suitable without use conflict M3M (Ha)
Córdoba	Montería	286,738	360,806
Cesar	Valledupar	137,356	262,513
Sucre	Sincelejo	72,856	211,294
Magdalena	Santa Marta	48,250	302,731
La Guajira	Riohacha	45,756	162,888
Bolívar	Cartagena	31,425	398,631
Tolima	Ibagué	30,531	82,194
Antioquia	Medellín	21,931	7,356
Atlántico	Barranquilla	9,056	118,519
Cundinamarca	Bogotá	569	40,513
Huila	Neiva	150	55,231
Nariño	Pasto	0	38,194
Valle del Cauca	Cali	0	18,475
Norte de Santander	Cúcuta	0	10,375
Caldas	Manizales	0	7,969
Choco	Quibdó	0	2,513
Santander	Bucaramanga	0	1,256
Cauca	Popayán	0	200
Total		684,619	2,081,656

It was decided to work only with highly suitable lands to jatropha production; because, though they are a smaller hectares amount, they are easier to work with and they are suitable for intensive cultivation. Therefore, this could ease jatropha exploitation.

According to Gaona Currea (2009) there are different yields of jatropha *oil per hectare cultivated* based on soils type and also the quantity of oil obtained by hectare depends on the system of oil extraction used. These values are presented on table 3.

Table 3. Yields of oil per hectare cultivated based on soils type and the system of oil extraction used. Based on Gaona Currea (2009)

Product	Soil quality	Extraction method	Yield (t/ha)	Oil content (%)	Oil Yield (t/ha)
J. Curcas	Marginal land	Manual-extraction	2.0 – 3.0	35-45	0.8
	Marginal land	Electric press	2.0 – 3.0	35-45	0.9
	Good soils	Manual-extraction	5	37	1.2
	Good soils	Electric press	5	37	1.4

Manual press extraction has an oil extraction efficiency of 62.5% and the electric press has on average 75% (Gaona Currea 2009). Then, the calculation of Oil Yield (Oil t/ha) can be verified, as presents table 4.

Table 4 Oil extraction rate by extraction method

Extraction method	Oil yield by land (t/ha)	Oil content (%)	Oil contained (t/ha)	Extraction efficiency	Oil extracted (t/ha)
Manual-extraction	5	37	=5/37%=1,85	62.5%	1.16
Electric press	5	37	=5/37%=1,85	75.0%	1.39

Then, it is possible to calculate the potential jatropha crude oil by location depending on extraction method, resumed on table 5.

Table 5 Potential available hectares to Jatropha production at Colombia. Based on Gaona Currea (2009)

Department	Location	Highly suitable without use conflict M3A (ha)	Tons of Oil obtained on good soil, Manual extraction	Tons of Oil obtained on good soil, Electric press
Córdoba	Montería	286,738.00	332,616.08	398,565.82
César	Agustín Codazzi	137,356.00	159,332.96	190,924.84
Sucre	Sincelejo	72,856.00	84,512.96	101,269.84
Magdalena	Santa Marta	48,250.00	55,970.00	67,067.50
La Guajira	Albania	45,756.00	53,076.96	63,600.84
Bolívar	Cartagena	31,425.00	36,453.00	43,680.75
Tolima	Girardot	30,531.00	35,415.96	42,438.09
Antioquia	Medellín	21,931.00	25,439.96	30,484.09
Atlántico	Luruaco	9,056.00	10,504.96	12,587.84
Cundinamarca	Bogotá	569.00	660.04	790.91
Huila	Neiva	150.00	174.00	208.50
	Total	684,618.00	794,156.88	951,619.02

Then, joining the availability for the palm and jatropha oils, it may be concluded that the index for the raw materials type is $n = 1,2,3$. And the estimation for palm and jatropha oil availability is presented on table 6.

Table 6 Raw material availability by raw material type and location

N°	Location	Biomass Type		
		1 Palm oil availability (t/Year)	2 Jatropha oil availability obtained by manual- extraction (t/Year)	3 Jatropha oil availability obtained by electric press (t/Year)
(1)	Bosconia / Cesar	281,000.00	0.00	0.00
(2)	María la Baja / Bolívar	55,161.00	36,453.00	43,680.75
(3)	Tumaco / Nariño	23,000.00	0.00	0.00
(4)	Barrancabermeja / Santander	173,400.00	0.00	0.00
(5)	Villanueva / Casanare	111,435.00	0.00	0.00
(6)	San Carlos de Guaroa / Meta	413,300.00	0.00	0.00
(7)	Montería / Córdoba	0.00	332,616.08	398,565.82
(8)	Agustín Codazzi / Cesar	0.00	159,332.96	190,924.84
(9)	Sincelejo / Sucre	0.00	84,512.96	101,269.84
(10)	Santa Marta / Magdalena	198,000.00	55,970.00	67,067.50
(11)	Albania / La Guajira	0.00	53,076.96	63,600.84
(12)	Girardot / Cundinamarca	0.00	35,415.96	42,438.09
(13)	Medellín / Antioquia	0.00	25,439.96	30,484.09
(14)	Luruaco / Atlántico	0.00	10,504.96	12,587.84
(15)	Bogotá / Cundinamarca	0.00	660.04	790.91
(16)	Neiva / Huila	0.00	174.00	208.50
(17)	Cúcuta / Norte de Santander	13,500.00	0.00	0.00

With the information of the table above, it may be concluded that the index for the raw materials location is $i = 1, \dots, 17$

However, there are some suppliers with small amounts of available raw materials, as 14, 15, 16 and 17. Therefore, it is decided to work only with the first thirteen suppliers.

Appendix 6.2. Processing rates for palm oil and jatropa at pretreatment plants

In order to determine the rate of transformation at pretreatment plants, the pre-treatment process is followed stage by stage, determining the quantity of product remaining in each stage. In table 7, the mass balances for the physical refinement stages are presented.

Table 7 Material losses in each pretreatment stage for an average oil (Blanco Rodríguez 2007)

Physical refinement stage	Entering mass (Kg)	Outgoing mass (Kg)
Degummed	100,0	94,3
Bleaching	94,3	94,1
Deodorization	94,1	91,4

Data contained in table 7 corresponds to average oil with the characteristics presented in table 8.

Table 8 Average oil characteristics used in research carried out by Blanco Rodríguez (2007)

Characteristic	%
Phosphatides	0.6
Free fatty acids	10
Waxes	0.06
Humidity / Water	0.27
Pigments	0.2
Volatiles	0.2
Unsaponifiable matter	1.5
Triglycerides	87.17

However, the characteristics for the palm oil are different, as presented in table 9.

Table 9 Palm oil characteristics used in research carried out by Blanco Rodríguez (2007)

Characteristic	%
Phosphatides	0.05 – 0.2 (Average 0.15)
Free fatty acids	2 -5 (Average 3.5)
Unsaponifiable matter	0.4
Triglycerides	90

Then, for the palm oil, the material losses can be calculated as:

Degummed.

Average oil

100 kg to 94.3 kg → Reduction in weight of 5.68% (when the value of phosphatides is 0.6)

If 5.68% matter losses corresponds to 0.6% of phosphatides, then how many loss matter will be loss if oil has 0.15% of phosphatides? We assume a proportional relation.

$$\frac{5.68\% \text{ matter losses}}{0.6\% \text{ of phosphatides}} = \frac{X \text{ matter losses}}{0.15\% \text{ of phosphatides}} \rightarrow X = 1.42\% \text{ matter losses}$$

Bleaching.

Average oil

94.3 kg to 94.1 kg → Reduction in weight of 0.21% (0.2 kg)

There is no information about color in the average oil, and then the same weight reduction value will be assumed for palm oil.

Deodorization.

Average oil

94.1 kg to 91.4 kg → Reduction in weight of 2.87% (when the value of FFA is 10)

If 2.87% matter losses corresponds to 10 FFA, then how many loss matter will be loss if oil has 3.5 FFA? We assume a proportional relation.

$$\frac{2.87\% \text{ matter losses}}{10 \text{ FFA}} = \frac{X \text{ matter losses}}{3.5 \text{ FFA}} \rightarrow X = 1.01\% \text{ matter losses}$$

These estimations are summarized in table 10.

Table 10 Material losses in each pretreatment stage for palm oil

Physical refinement stage	Entering palm oil (Kg)	Outgoing palm oil (Kg)	
Degummed	100.00	100-1.42%*100=	98.58
Bleaching	98.58	98.58-0.2=	98.38
Deodorization	98.38	98.38-1.01%*98.38=	97.39

There was not information found related to jatropha oil characteristics in the same research (Blanco Rodríguez 2007). Thus, values for the average oil will be assumed for jatropha oil physical refinement. Then, the processing rates for palm and jatropha oil at pretreatment plants can be summarized as presented in table 11.

Table 11 Processing rates for palm oil and jatropha parameters to optimization model

Biomass	Technology	Intermediate Products	
		Refined jatropha oil (1)	Refined Palm oil (2)
(1) Palm oil	1	0.00	97.40%
(2) Jatropha oil by manual extraction	1	91.40%	0.00%
(3) Jatropha oil by electrical extraction	1	91.40%	0.00%

Appendix 6.3. Processing rates for palm oil and jatropha at principal plants

i. Base-catalyzed / Conventional transesterification

Base-catalyzed transesterification is made with sodium hydroxide (NaOH). The biodiesel and glycerol production from refined jatropha and palm oil calculation are based on research carried out by Basto Aluja (2016). The material balance presented on it research is summarized in table 22.

Table 12 Material balances in research carried out by Basto Aluja (2016)

	Plant capacity	
	80,000 t/year	120,000 t/year
Incoming Palm oil (Kg/hr.)	10,111.15	15,166.70
Outgoing biodiesel (Kg/hr.)	10,147.00	15,220.04
Outgoing glycerol (Kg/hr.)	806.95	1,225.79

The biodiesel produced based on refined palm oil is:

For 80,000 t/year:

$$\frac{10\,147,00}{10\,111,15} = 1,00355 \frac{\text{biodiesel}}{\text{palm oil}}$$

For 120 000 t/year:

$$\frac{15\,220,04}{15\,166,70} = 1,00352 \frac{\text{biodiesel}}{\text{palm oil}}$$

And the average between these two is:

$$\frac{1,00355 + 1,00352}{2} = 1,003535 \approx \mathbf{1,0035} \frac{\text{biodiesel}}{\text{palm oil}}$$

Then, to obtain the glycerol production amount a similar calculation must to be made.

For 80,000 t/year:

$$\frac{806,95}{10\,111,15} = 0,07976 \frac{\text{glycerol}}{\text{palm oil}}$$

For 120 000 t/year:

$$\frac{1\,225,79}{15\,166,70} = 0,08082 \frac{\text{glycerol}}{\text{palm oil}}$$

And the average between these two is:

$$\frac{0,07976 + 0,08082}{2} = \mathbf{0,08029} \frac{\text{glycerol}}{\text{palm oil}}$$

In order to obtain the amount of biodiesel and glycerol produced based on refined jatropha oil, the research carried out by Bueso et al. (2015) was considered. It research presents the transformation yield of FFA for palm and jatropha oil, presented in table 23.

Table 13 Yield by raw material type (Bueso et al. 2015)

Catalyst	Oil type	Yield %
NaOH	Jatropha	90.0 ± 2.6
	Palm	92.3 ± 1.5

Then, if we suppose that the yield 92.3 % , that correspond to FFA transformation in palm oil, results in $1.0035 \frac{\text{biodiesel } t}{\text{palm oil } t}$ calculated above, the same assumption can be made for jatropha oil:

$$92.3 \% \rightarrow 1.0035 \frac{\text{biodiesel } t}{\text{palm oil } t}$$

$$90.0 \% \rightarrow X \frac{\text{biodiesel } t}{\text{jatropha oil } t}$$

Therefore:

$$\frac{1.0035 * 90.0 \%}{92.3 \%} = \mathbf{0.97113} \frac{\text{biodiesel } t}{\text{jatropha oil } t}$$

Then, for the calculation of glycerol production:

For 80,000 t/year:

$$\frac{806,95}{10\,147,00} = 0,079526 \frac{\text{glycerol } t}{\text{biodiesel } t}$$

For 120 000 t/year:

$$\frac{1\,225,79}{15\,220,04} = 0,080538 \frac{\text{glycerol } t}{\text{biodiesel } t}$$

The average is:

$$\frac{0,080538 + 0,079526}{2} = 0,0800325 \approx 0,08003 \frac{\text{glycerol } t}{\text{biodiesel } t}$$

In order to calculate the glycerol production by jatropha oil, considering that the glycerol is a by-product of biodiesel, and that its production rate related to biodiesel production will be constant, the following estimation can be realized:

$$0.97113 \frac{\text{biodiesel } t}{\text{jatropha oil } t} * 0.08003 \frac{\text{glycerol } t}{\text{biodiesel } t} = 0.077729 \approx \mathbf{0.0777} \frac{\text{glycerol } t}{\text{jatropha oil } t}$$

ii. Base-catalyzed transesterification and polymer production

The research carried out by Bueno et al. (2014) determine that the glycerol available is around 25,600 t/year which would be the quantity fed to the plant. Table 24 presents the products obtained based on this availability, using half of the available glycerol for liquid polymer production, and the other half to solid polymer production.

Table 14 Polymers obtained based on its availability

Product	Quantity (t/year)	Purity degree (%)
Liquid polymer	30,620	72.5
Solid polymer	18,359	100

Then, the required glycerol to produce 30,620 t/year liquid polymers are

$$\frac{25,600}{2} = 12,800 \text{ t/year}$$

The transformation rate between liquid polymer and glycerol can be estimated as:

$$\frac{30,620}{12,800} = 2.3921875 \frac{\text{t liquid polymer}}{\text{t glycerol}}$$

Furthermore, considering the glycerol production depending on entering materials, the calculations presented in table 25 can be made.

Table 15. Polymer production from jatropa and palm refined oil with conventional transesterification

	Refined oil to glycerol	Refined oil to polymer (yield)
Palm oil	$0.08029 \frac{\text{glycerol}}{\text{palm oil}}$	$= 2.3921875 * 0.08029 = 0.1920687$ $\approx \mathbf{0.1921}$
Jatropha oil	$0.0777 \frac{\text{glycerol tons}}{\text{jatropha oil tons}}$	$= 2.3921875 * 0.0777 = 0.1858730$ $\approx \mathbf{0.1859}$

iii. Transformation technology: base-catalyzed transesterification co-current

Based in sections i and ii, and in the research carried out by Basto Aluja (2016), table 26 was constructed. The co-current transesterification has a 1.3% better efficiency that the conventional transesterification in biodiesel production. It means that the biodiesel production at conventional process will be multiplied by 1.013. It is assumed that the same efficiency will be obtained with jatropa refined oil. These estimations are presented in table 26.

Table 16 Polymer production from jatropa and palm refined oil

Raw material	Biodiesel production (Biodiesel tons / Oil tons)	Glycerol production (Glycerol tons / Oil tons)
Jatropha refined oil	$0.9711 * 1.013 = 0.9837$	$0.0777 * 1.013 = 0.0787$
Palm refined oil	$1.0035 * 1.013 = 1.0166$	$0.0803 * 1.013 = 0.0813$

iv. Transformation technology: base-catalyzed transesterification co-current and polymer production

Based in sections I, ii and iii, table 27 was constructed to estimate the production of biodiesel and polymers when the transformation technology at pretreatment plants will be $d = 4$.

Table 17. Polymer production from jatropa and palm refined oil

Raw material	Biodiesel production (Biodiesel tons / Oil tons)	Polymers production (Polymer tons / Oil tons)
Jatropha refined oil	$0.9711 * 1.013 = 0.9837$	$0.1921 * 1.013 = 0.1946$
Palm refined oil	$1.0035 * 1.013 = 1.0166$	$0.1859 * 1.013 = 0.1883$

v. Transformation technology: base-catalyzed transesterification counter-current

Based in sections i and ii, and in the research carried out by Basto Aluja (2016), table 28 was constructed. The counter-current transesterification has a 2.7% better efficiency that the conventional transesterification in biodiesel production. It means that the biodiesel production at conventional process will be multiplied by 1.027. It is assumed that the same efficiency will be obtained with jatropha refined oil. These estimations are presented in table 28.

Table 18 Biodiesel and glycerol production from jatropha and palm refined oil

Raw material	Biodiesel production (Biodiesel tons / Oil tons)	Glycerol production (Glycerol tons / Oil tons)
Jatropha refined oil	$0.9711 * 1.027 = 0.9973197$	$0.0777 * 1.027 = 0.0797979$
Palm refined oil	$1.0035 * 1.027 = 1.0305945$	$0.0803 * 1.027 = 0.0824681$

vi. Transformation technology: base-catalyzed transesterification counter-current and polymer production

Based in sections I, ii and v, table 29 was constructed in order to estimate the production of biodiesel and polymers when the transformation technology at pretreatment plants will be $d = 6$.

Table 19 Polymer production from jatropha and palm refined oil

Raw material	Biodiesel production (Biodiesel tons / Oil tons)	Polymers production (Polymer tons / Oil tons)
Jatropha refined oil	$0.9711 * 1.027 = 0.9973197$	$0.1921 * 1.027 = 0.1972867$
Palm refined oil	$1.0035 * 1.027 = 1.0305945$	$0.1859 * 1.027 = 0.1909193$

Finally, all this information can be resumed in table 30

Table 20 Final products production from jatropha and palm refined oil

Intermediate Products	Technology at Production Plant	Final Products		
		Biodiesel	Polymer	Glycerol
1 Jatropha Oil	1	0.9711	0.0000	0.0777
1 Jatropha Oil	2	0.9711	0.1921	0.0000
1 Jatropha Oil	3	0.9837	0.0000	0.0787
1 Jatropha Oil	4	0.9837	0.1946	0.0000
1 Jatropha Oil	5	0.9973	0.0000	0.0798
1 Jatropha Oil	6	0.9973	0.1973	0.0000
2 Palm Oil	1	1.0035	0.0000	0.0803
2 Palm Oil	2	1.0035	0.1859	0.0000
2 Palm Oil	3	1.0166	0.0000	0.0813
2 Palm Oil	4	1.0166	0.1883	0.0000
2 Palm Oil	5	1.0306	0.0000	0.0825
2 Palm Oil	6	1.0306	0.1909	0.0000

Annex 6.4. Installation cost at Principal and pretreatment Plants

Principal plants investments

In table 12 the installation cost at principal plants by technology and production capacity are presented, according to Basto Aluja (2016).

Table 21 Installation cost at principal production plants

Technology	Production capacity		
	40,000 t/y	80,000 t/y	120,000 t/y
Conventional transesterification	16,000,000	21,000,000	34,000,000
Co-current transesterification	11,000,000	14,000,000	23,000,000
Count-current transesterification	12,000,000	15,000,000	24,000,000

However, these costs include the cost per esterification, which can be considered as pretreatment of the oil. And since this process has been separated and performed in another facility, capital costs must be reduced by the amount associated with esterification equipment (R100, H101; MX-100, P-100 and P-101), summarized in table 13.

Table 22 Installation and purchase cost for esterification equipment

	Production capacity		
	40,000 t/a	80,000 t/a	120,000 t/a
Esterification equipment purchase cost	378,100	453,870	506,733
Esterification equipment installation cost	630,660	757,968	848,905
Total	1,008,760	1,211,838	1,355,638

Then, we will assume that the concept of construction work (pipelines, electrical installation, among others) represents 82% of the equipment cost (Bueno et al. 2015a). Therefore, the total cost related to esterification process is presented in table 14.

Table 23 Total cost related to esterification process by production capacity

	Production capacity		
	40,000 t/y	80,000 t/y	120,000 t/y
Total installation cost related to esterification equipment	1,008,760*(1.82)= 1,835,943	1,211,838*(1.82)= 2,205,545	1,211,838*(1.82)= 2,467,261
Around	1,840,000	2,200,000	2,500,000

Thus, values in table 12 less values in table 14 are the installation cost by technology and production capacity for principal production plants. The resulting around values are presented in table 15.

Table 24 Installation cost at principal production plants without esterification process

	Production capacity		
	40,000 t/y	80,000 t/y	120,000 t/y
Conventional transesterification	14,200,000	18,800,000	31,500,000
Co-current transesterification	9,200,000	11,800,000	20,500,000
Count-current transesterification	10,200,000	12,800,000	21,500,000

In the research carried out by Bueno et al. (2015a), the total investment cost reaches 40M€ for a production plant with capacity to process 25,600 glycerol tons per year. This plant will produce two grades of polyesters, solid and liquid types, using the 50% of glycerol for each final product. Therefore, we will consider only the equipment required for the production of liquid polyesters, and we will assume that the plant will process all the 25,600 glycerol tons per year to produce only liquid polyester. This will require some equipment doubled in capacity. Thus, the required equipment will be:

- Heat exchangers: I01, I02, I03, I04.
- Columns: T01
- Reactors: two R01
- Storage tanks: **two** D02, **two** D04, D06, D07
- Bomb/Pump: **two** B01, **two** B02.

This has a total purchase cost 2,723,000 € and an installation cost of 3,948,350 €. Also, the cost related to piping, instruments, isolation and auxiliaries cost is 5,470,507 € (82%*[purchase cost + installation cost]). Also, there are considered other cost, as fees (540,000 €), laboratory, general and construction cost (11,600,000 €), as in presented by Bueno et al. (2015). These values are added, resulting 24,245,857 €; equivalent to 26,670,443 USD (Considering 1,1€= 1 USD).

Then, the total amount of glycerol that can be processed in the different principal production plants must to be calculated, as presented in table 16 (Glycerol production rates calculation was presented in Appendix 6.3).

Table 25 Glycerol production at principal plants

Entering intermediate products	Technology	Glycerol production rate	Production capacity		
			40,000 t/year	80,000 t/year	120,000 t/year
Jatropha	Conventional	0.0990	0.099*40,000= 3,960	0.099*80,000 =7,920	0.099*120,000= 11,880
	Co-current	0.1003	4,012	8,024	12,036
	Count-current	0.1017	4,068	8,136	12,204
Palm	Conventional	0.1015	4,060	8,120	12,180
	Co-current	0.1028	4,112	8,224	12,336
	Count-current	0.1042	4,168	8,336	12,504

Then, the maximum amount of glycerol that could be produced per technology is presented in table 17.

Table 26 Maximum amount of glycerol that could be produced at principal plants.

	Production capacity		
	40,000 t/year	80,000 t/year	120,000 t/year
Conventional	4,060	8,120	12,180
Co-current	4,112	8,224	12,336
Count-current	4,168	8,336	12,504

In order to estimate the installation cost related to glycerol transformation in polyester, a directly proportional relation is assumed between the amount of glycerol to process and the total investment. As presented in table 27.

Table 27 Investment required for glycerol process.

	Production capacity		
	40,000 t/year	80,000 t/year	120,000 t/year
Conventional	$\frac{26,670,443 \text{ USD}}{25,600 \text{ t glycerol}} * 4,060 \text{ t glycerol} =$	8 459 390,63	12 689 085,94
	4 229 695,31		
Co-current	4 283 868,75	8 567 737,50	12 851 606,25
Count-current	4 342 209,38	8 684 418,75	13 026 628,13

Therefore, the investment presented in table 18 should be added to the investment presented in table 15 in order to calculate the investment required for technologies mixing transesterification and polymerization. The final values for investment are presented in table 18.

Table 28 Investment for principal plants installation by technology and capacity.

Technology	Capacity		
	40,000 t/year	80,000 t/year	120,000 t/year
$d = 1$	14 200 000	18 800 000	31 500 000
$d = 2$	18 400 000	27 300 000	44 200 000
$d = 3$	9 200 000	11 800 000	20 500 000
$d = 4$	13 500 000	20 400 000	33 400 000
$d = 5$	10 200 000	12 800 000	21 500 000
$d = 6$	14 500 000	30 200 000	34 300 000

Pretreatment plants investments

For the pretreatment installation cost, we do not found information related to the investment cost for physical refining installation. Thus, it will be assumed that the pretreatment equipment will represent the same amount that in principal plants (Table 13), and the same proportion than in principal plants, between the equipment investments will be used to estimate the investment values for pretreatment plants.

Table 29 Proportion/Rate of equipment investments versus total investments.

	Capacity		
	40,000 t/year	80,000 t/year	120,000 t/year
Total investment	16,000,000	21,000,000	34,000,000
Total equipment + installation	6,521,267	7,836,620	9,438,165
%	40.76%	37.32%	27.76%

Then, this percentages will be divided by the amount of equipment and installation cost for pretreatment plants, maintaining the same proportion the values can be estimated as presented in table 21.

Table 30 Investments for pretreatment plants

	40,000 t/a	80,000 t/a	120,00 t/a
Equipment and installation cost	1,008,760	1,211,838	1,355,638
% of the total investment	40.76%	37.32%	27.76%
Total investment at pretreatment plants (USD)	4,514,460	6,243,340	10,846,513
Around USD	4,500,000	6,240,000	10,850,000

Appendix 6.5. Operational cost estimation for pretreatment and principal production plants

Principal plants operational cost

In the research carried out by Basto Aluja (2016) the biodiesel production cost by technology and production plants are estimated; then, they are summarized in table 31.

Table 31. Biodiesel production cost by technology and production capacity

	USD/Biodiesel Kg			USD/Biodiesel t		
	40,000 t/year	80,000 t/year	120,000 t/year	40,000 t/year	80,000 t/year	120,000 t/year
Conventional	0.49	0.45	0.42	490	450	420
Co-current	0.46	0.43	0.41	460	430	410
Count-current	0.45	0.42	0.40	450	420	400

However, these costs include the esterification process cost. Therefore, at first it is required to transform the biodiesel production cost to refined oil process cost. This calculation is presented in table 32, using the biodiesel production rates presented in Appendix 6.3.

Table 32. Refined oil processing cost at principal plants including esterification process

Intermediate Products	Technology	Transformation cost for oil (USD/t oil)		
		40,000 t/year	80,000 t/year	120,000 t/year
1 Jatropha Oil	1	476	437	408
1 Jatropha Oil	2	476	437	408
1 Jatropha Oil	3	453	423	403
1 Jatropha Oil	4	453	423	403
1 Jatropha Oil	5	449	419	399
1 Jatropha Oil	6	449	419	399
2 Palm Oil	1	492	452	421
2 Palm Oil	2	492	452	421
2 Palm Oil	3	468	437	417
2 Palm Oil	4	468	437	417
2 Palm Oil	5	464	433	412
2 Palm Oil	6	464	433	412

Then, the esterification process cost should be estimated. But, due to lack information related to the specific process, the values for crude and refined palm oil are analyzed to estimate the production cost at pretreatment plants and utilize the same value as esterification process cost.

Market value for crude palm oil: 804.42 USD/t (Section 6.2.1)

Market value for refined palm oil: 942.19 USD/t (Section 6.2.5)

It is estimated that earnings are the 10% of the market value for the refined palm oil (94.2 USD/t). The difference between the market value for refined and crude palm oil is 137.77 USD/t, less the earnings for the pretreatment enterprise results in 43.55 USD/t. This amount is assumed as refined palm oil production cost at pretreatment plants with a production capacity of 40,000 t/year.

In order to estimate the production cost for the production capacity 80,000 and 120,000 t/year; scale economies presented by the conventional technology at the principal production plants will be assumed in pretreatment plants, as presented in table 33.

Table 33. Pretreatment operational cost estimation with scale economies

Capacity	40,000 t/year	80,000 t/year	120,000 t/year
Conventional technology at principal plants (USD/t)	490	450	420
Refined oil production cost at pretreatment plants (USD/t)	43.55	$=(43,55*450)/490$ =40.00	$=(43,55*420)/490$ =37.33

Then, the production cost at pretreatment plants (assumed as esterification process cost) can be subtracted to the refined oil transformation cost, as presented in table 34.

Table 34 Refined oil processing cost at principal plants excluding esterification process

Intermediate Products	Tech.	Transformation cost for oil (USD/t oil)		
		40,000 t/year	80,000 t/year	120,000 t/year
1 Jatropha Oil	1	$476-43.55=432$	$437-40.00=397$	$408-37.33=371$
1 Jatropha Oil	2	$476-43.55=432$	$437-40.00=397$	$408-37.33=371$
1 Jatropha Oil	3	$453-43.55=409$	$423-40.00=383$	$403-37.33=366$
1 Jatropha Oil	4	$453-43.55=409$	$423-40.00=383$	$403-37.33=366$
1 Jatropha Oil	5	$449-43.55=405$	$419-40.00=379$	$399-37.33=362$
1 Jatropha Oil	6	$449-43.55=405$	$419-40.00=379$	$399-37.33=362$
2 Palm Oil	1	$492-43.55=448$	$452-40.00=412$	$421-37.33=384$
2 Palm Oil	2	$492-43.55=448$	$452-40.00=412$	$421-37.33=384$
2 Palm Oil	3	$468-43.55=424$	$437-40.00=397$	$417-37.33=379$
2 Palm Oil	4	$468-43.55=424$	$437-40.00=397$	$417-37.33=379$
2 Palm Oil	5	$464-43.55=420$	$433-40.00=393$	$412-37.33=375$
2 Palm Oil	6	$464-43.55=420$	$433-40.00=393$	$412-37.33=375$

Finally, in order to estimate the production cost related to aliphatic polymers, as presented by Bueno et al. (2015a), the production cost to obtain aliphatic polyester is 13,695.88 USD/t glycerol processed.

And, as presented in appendix 6.3; the transformation rate between refined oil and glycerol are:

Glycerol t/ Oil t

Technology at principal plants	Jatropha	Palma
Conventional	0.0777	0.08030
Co-current	0.0787	0.0813
Count-current	0.0798	0.0825

Then, the production cost by refined oil ton can be estimated, by multiplying 13,695.88 USD/t glycerol processed with the transformation rate, as presented in table 35.

Table 35 Production cost aliphatic polymers USD/refined oil

Technology at principal plants	Jatropha	Palma
Conventional	$13,695.88 \frac{USD}{t \text{ glycerol}} * 0.0777 = 106.34$	$13,695.88 \frac{USD}{t \text{ glycerol}} * 0.0803 = 109.90$
Co-current	$13,695.88 \frac{USD}{t \text{ glycerol}} * 0.0787 = 107.72$	$13,695.88 \frac{USD}{t \text{ glycerol}} * 0.0813 = 111.32$
Count-current	$13,695.88 \frac{USD}{t \text{ glycerol}} * 0.0798 = 109.21$	$13,695.88 \frac{USD}{t \text{ glycerol}} * 0.0825 = 112.87$

Considering scale economies in the same way that previously, the production cost depending on production capacity can be estimated as presented in tables 36 and 37.

Table 36 Production cost aliphatic polymers USD/refined jatropha oil by technology and production capacity

Jatropha			
Technology at principal plants	40,000 t/year	80,000 t/year	120,000 t/year
Conventional	106.34	$=(106.34*450)/490$ =97.66	$=(106.34*420)/490$ =91.15
Co-current	107.72	$=(107.72*450)/490$ =98.93	$=(107.72*420)/490$ =92.34
Count-current	109.21	$=(109.21*450)/490$ =100.30	$=(109.21*420)/490$ =93.61

Table 37 Production cost aliphatic polymers USD/refined palm oil by technology and production capacity

Palma			
Technology at principal plants	40,000 t/year	80,000 t/year	120,000 t/year
Conventional	109.90	$=(109.90*450)/490$ =100.93	$=(109.90*420)/490$ =94.20
Co-current	111.32	$=(111.32*450)/490$ =102.24	$=(111.32*420)/490$ =95.42
Count-current	112.87	$=(112.87*450)/490$ =103.66	$=(112.87*420)/490$ =96.75

Finally, the total production cost at principal plants can be summarized in table 38.

Table 38 Operational cost at principal production plants by intermediate product, technology and production capacity

Intermediate Products		Tech.	Transformation cost for oil (USD/t refined oil)		
			40,000 t/year	80,000 t/year	120,000 t/year
1	Jatropha Oil	1	432	397	371
1	Jatropha Oil	2	539	495	462
1	Jatropha Oil	3	409	383	366
1	Jatropha Oil	4	517	482	458
1	Jatropha Oil	5	405	379	362
1	Jatropha Oil	6	514	479	455
2	Palm Oil	1	448	412	384
2	Palm Oil	2	558	513	478
2	Palm Oil	3	424	397	379
2	Palm Oil	4	535	499	475
2	Palm Oil	5	420	393	375
2	Palm Oil	6	533	497	472

Pretreatment plants operational cost

The production cost of refined oil was calculated in table 33 is in function of intermediate products generated at pretreatment plants. However, for the optimization model it is required the production cost in function of the raw materials entering in the pretreatment plant. Thus, the transformation rate at pretreatment plants will be used to estimate the production cost (Appendix 6.2). Then the cost production at pretreatment plants depending on raw materials and processing capacity is estimated as presented in table 39.

Table 39 Operational cost at pretreatment plants by raw material and production capacity

Pretreatment production cost refined oil (USD/t)	40,000 t/year	80,000 t/year	120,000 t/year
(1) Palm oil	=43.55*97.40% =42.42	=40.00*97.40% =38.96	=37.33*97.40% =36.36
(2) Jatropha oil by manual extraction	=43.55*91.40% =39.81	=40.00*91.40% =36.56	=37.33*91.40% =34.12
(3) Jatropha oil by electrical extraction	=43.55*91.40% =39.81	=40.00*91.40% =36.56	=37.33*91.40% =34.12

Appendix 6.6. Biodiesel demand calculation

The research carried out by Rincón et al. (2015a) presents the diesel consumption forecast to 2020 by city, as presented in table 40.

Table 40 Biodiesel and diesel consumption forecast to 2020 by city (Rincón et al. 2015)

	Diesel (Million L)	Diesel consumption (%)
Antioquia	1,428.84	5.259%
Chocó	1,428.84	5.259%
Cordoba	1,020.6	3.756%
Sucre	1,020.6	3.756%
Bolivar	1,020.6	3.756%
Atlántico	1,020.6	3.756%
Magdalena	1,020.6	3.756%
Cesar	1,020.6	3.756%
La Guajira	1,020.6	3.756%
Bogotá	1,428.84	5.259%
Cundinamarca	1,428.84	5.259%
Boyacá	1,428.84	5.259%
Meta	1,428.84	5.259%
Casanare	1,428.84	5.259%
Tolima	476.28	1.753%
Huila	476.28	1.753%
Caquetá	476.28	1.753%
Caldas	476.28	1.753%
Quindío	476.28	1.753%
Risaralda	476.28	1.753%
Santander	952.56	3.506%
Norte de Santander	952.56	3.506%
Arauca	952.56	3.506%
Valle	1,071.63	3.944%
Cauca	1,071.63	3.944%
Nariño	1,071.63	3.944%
Putumayo	1,071.63	3.944%
Other departments	23.81	0.088%
Total	27,171.77	Million L
	467,914.07	BDC

Therefore, this data can be considered as the diesel distribution of consumption in Colombia. However, it is required to know the total diesel consumption in 2015.

To determine the amount of ACPM/Diesel consumption in million liters at Colombia in 2015, the information related to 2014 and 2014 were collected.

In 2014, the total ACPM/Diesel consumption, including biodiesel, was 2,047 million gallons equivalent to 133,500 BDC (Ministerio de Minas y Energía and UPME 2015). In 2015, there was a consumption of 139,398.53 BDC (UPME 2016). Regarding the data to 2014, it can be calculated that for 2015 the total ACPM/Diesel consumption, including biodiesel was equivalent to 2,137.44 million gallons.

$$\frac{(2,047 \times 139,398.53)}{133,500} = 2,137.44 \text{ million gallons}$$

Then, these values must to be transformed to liters to relate the information with table 6.8.1. For that, the rate 1 *Gallon* = 3.8 *Liters* was used (U.S. Department of Agriculture 1980).

$$2,137.44 \text{ million gallons} * 3.8 = 8,122.272 \text{ million liters}$$

Therefore, considering the same distribution that presented on Rincón et al. (2015a), the diesel consumption for 2015 is presented in table 41.

Table 41 Diesel consumption in Colombia at 2015 by city.

Departament	%	Diesel Consumption 2015 (Liters)
Antioquia	5.26%	427,231,507
Chocó	5.26%	427,231,507
Cordoba	3.76%	305,397,427
Sucre	3.76%	305,397,427
Bolivar	3.76%	305,397,427
Atlantico	3.76%	305,397,427
Magdalena	3.76%	305,397,427
César	3.76%	305,397,427
La Guajira	3.76%	305,397,427
Bogota	5.26%	427,231,507
Cundinamarca	5.26%	427,231,507
Boyacá	5.26%	427,231,507
Meta	5.26%	427,231,507
Casanare	5.26%	427,231,507
Tolima	1.75%	142,139,760
Huila	1.75%	142,139,760
Caqueta	1.75%	142,139,760
Caldas	1.75%	142,139,760
Quindío	1.75%	142,139,760
Risaralda	1.75%	142,139,760
Santander	3.51%	285,091,747
Norte de Santander	3.51%	285,091,747
Arauca	3.51%	285,091,747
Valle	3.94%	320,017,517
Cauca	3.94%	320,017,517
Nariño	3.94%	320,017,517
Putumayo	3.94%	320,017,517
Otros	0.07%	5,685,590
Total	100%	8,122,272,000

Then, the next step is to calculate the biodiesel consumption for 2015 to stablish it as the biodiesel demand parameters. In Fedebiocombustibles (2014) and Fedebiocombustibles (2017) the legal ACPM-Biodiesel blend is presented for the different cities in Colombia, as presented in the second column in Table 6.8.3.

Since data in Table 6.8.2 integrates ACPM/Diesel and biodiesel consumption, it is required to define the follow relation to calculate the biodiesel demand:

$$\text{Biodiesel demand} = \text{Diesel Consumption}(\text{ACPM} + \text{Biodiesel}) * \text{BiodieselBlend}$$

And also, it is needed to transform the liters to tons of biodiesel with the ration $0.000875 \text{ Ton} = 1 \text{ Liter}$ (Cuellar Sanchez, Monica 2009). With this information table 42 was constructed.

Table 42. Biodiesel demand estimation

Departament	%	Biodiesel Demand (Liters/Year)	Biodiesel Demand (Tons/Year)
Antioquia	10.00%	42,723,150.72	37,382.76
Choco	10.00%	42,723,150.72	37,382.76
Cordoba	10.00%	30,539,742.72	26,722.27
Sucre	10.00%	30,539,742.72	26,722.27
Bolivar	10.00%	30,539,742.72	26,722.27
Atlántico	10.00%	30,539,742.72	26,722.27
Magdalena	10.00%	30,539,742.72	26,722.27
Cesar	10.00%	30,539,742.72	26,722.27
La Guajira	0.00%	0	0.00
Bogota	8.00%	34,178,520.58	29,906.21
Cundinamarca	8.00%	34,178,520.58	29,906.21
Boyacá	8.00%	34,178,520.58	29,906.21
Meta	8.00%	34,178,520.58	29,906.21
Casanare	8.00%	34,178,520.58	29,906.21
Tolima	10.00%	14,213,976.00	12,437.23
Huila	10.00%	14,213,976.00	12,437.23
Caquetá	10.00%	14,213,976.00	12,437.23
Caldas	10.00%	14,213,976.00	12,437.23
Quindío	10.00%	14,213,976.00	12,437.23
Risaralda	10.00%	14,213,976.00	12,437.23
Santander	10.00%	28,509,174.72	24,945.53
Norte de Santander	2.00%	57,018,34.944	4,989.11
Arauca	2.00%	57,018,34.944	4,989.11
Valle	10.00%	32,001,751.68	28,001.53
Cauca	10.00%	32,001,751.68	28,001.53
Nariño	10.00%	32,001,751.68	28,001.53
Putumayo	10.00%	32,001,751.68	28,001.53
Total		692 781 067.97	606 183.43

Appendix 6.7. Glycerin demand calculation

For the glycerol demand estimation the information was searched in DANE (2017) for the crude glycerin consumption; because it is not considered the glycerin refining at biorefinery plants. The information found is presented in Table 43. Due detailed information was found only for 2007, it was required to search the total value of crude glycerin consumption for 2015 and assume that the same % of consumption for 2007 is maintained for 2015.

Table 43. Crude glycerin consumption in Colombia 2007

Department	Total Crude Glycerin Consumption (Kg/Year)	%
Antioquia	1,421,294	21.35%
Atlántico	200,961	3.02%
Bogotá	813,674	12.22%
Bolívar	502,906	7.55%
Caldas	17,217	0.26%
Cauca	208,687	3.13%
Cundinamarca	525,969	7.90%
Santander	1,604	0.02%
Valle	2,966,192	44.55%
Total	6,658,504	100,%

For 2015 the total crude glycerin consumption was 20,064,516 Kg/Year (DANE 2017). Therefore, in base to these assumptions and information, the table 44 was constructed.

Table 44. Crude glycerin demand at Colombia in 2015

Department	Total Crude Glycerin Consumption (Tons/Year)
Antioquia	4,282.8804
Atlántico	605.5692
Bogotá	2,451.8984
Bolívar	1,515.4403
Caldas	51.8811
Cauca	628.8505
Cundinamarca	1,584.9376
Santander	4.8334
Valle	8,938.2250
Total	20,064.5160

Appendix 6.8. Polyester demand calculation

For the polyester demand estimation the information was searched in DANE (2017) for the unsaturated polyester resin consumption. The information found is presented in Table 45. Due detailed information was found only for 2007, it was required to search the total value of unsaturated polyester resin consumption for 2015 and assume that the same % of consumption for 2007 is maintained for 2015.

Table 45. Unsaturated polyester resin consumption in Colombia 2007

Department	Unsaturated polyester resin consumption (Kg/Year)	%
Antioquia	4,721,400	92.17%
Bogota	329,480	6.43%
Cundinamarca	5,432	0.11%
Valle	66,121	1.29%
Total	5,122,433	1

For 2015 the total unsaturated polyester resin consumption was 11,850,302 Kg/Year (DANE 2017). Therefore, in base to these assumptions and information, the table 46 was constructed.

Table 46. Unsaturated polyester demand at Colombia in 2015

Department	Unsaturated polyester resin consumption (Ton/Year)
Antioquia	10,922.55
Bogota	762.22
Cundinamarca	12.57
Valle	152.97
Total	11,850.30

However, polyester can be used as additive with polyurethane in paints production (REPI 2017). Therefore, the polyurethane consumption information was searched in DANE (2017), as presents table 47. Due detailed information was found only for 2007, it was required to search the total value of polyurethane consumption for 2015 and assume that the same % of consumption for 2007 is maintained for 2015.

Table 47. Polyurethane consumption at Colombia in 2007

Department	Polyurethane consumption (Kg/Year)	% of the total
Atlántico	156,099.00	1.7897%
Bogotá	2,694,541.00	30.8935%
Bolívar	15.00	0.0002%
Caldas	5,084,544.00	58.2955%
Cundinamarca	8,458.00	0.0970%
Magdalena	240.00	0.0028%
Norte Santander	330,270.00	3.7866%
Risaralda	12,216.00	0.1401%
Santander	6.00	0.0001%
Valle	435,631.00	4.9946%
Total	8,722,020.00	100.00%

For 2015 the total polyurethane consumption was 17,962,331 Kg/Year (DANE 2017). Therefore, in base to these assumptions and information, the table 48 was constructed.

Table 48. Polyurethane consumption at Colombia in 2015

Department	Polyurethane consumption (t/Year)
Atlántico	321.47
Bogotá	5,549.20
Bolívar	0.03
Caldas	10,471.23
Cundinamarca	17.42
Magdalena	0.49
Norte Santander	680.17
Risaralda	25.16
Santander	0.01
Valle	897.15
Total	17,962.33

Then, to calculate the polyester demand related, it must to be considered that polyester is normally used as additive between 0.1% and 5% (REPI 2017). Therefore, it is assumed that the polyester produced at biorefinery will be consumed as additive in a proportion of 2.5% polyurethane consumption. Therefore, based on this assumption and the information in DANE (2017), table 49 was constructed.

Table 49. Polyester consumption as additive at Colombia in 2015

Department	Polyester demand as additive to Polyurethane consumption (t/Year)
Atlántico	8.03685
Bogotá	138.73001
Bolívar	0.00077
Caldas	261.78071
Cundinamarca	0.43547
Magdalena	0.01236
Norte Santander	17.00414
Risaralda	0.62895
Santander	0.00031
Valle	22.42872
Total	449.05828

Finally, integrating Tables 48 and 49 the polyester total demand for the model is resumes in table 50.

Table 50. Polyester total demand at Colombia in 2015

Department	Polyester demand (t/Year)
Antioquia	10,922.5471
Atlántico	8.0368
Bogotá	900.9533
Bolívar	0.0008
Caldas	261.7807
Cundinamarca	13.0019
Magdalena	0.0124
Norte Santander	17.0041
Risaralda	0.6289
Santander	0.0003
Valle	175.3939
Total	12,299.3603

Therefore the final products demand can be detailed as Table 51

Table 51. Resume for final products demand in Colombian case study.

<i>l</i>	Final Products (t/Year)			Location	Department
	Biodiesel <i>a</i> = 1	Polymer <i>a</i> = 2	Glycerol <i>a</i> = 3		
1	37,382.7569	10,922.5471	4,282.8804	Medellin	Antioquia
2	37,382.7569	0.0000	0.0000	Quibdo	Choco
3	26,722.2749	0.0000	0.0000	Monteria	Cordoba
4	26,722.2749	0.0000	0.0000	Sincelejo	Sucre
5	26,722.2749	0.0008	1,515.4403	Cartagena	Bolivar
6	26,722.2749	8.0368	605.5692	Barranquilla	Atlantico
7	26,722.2749	0.0124	0.0000	Santa Marta	Magdalena
8	26,722.2749	0.0000	0.0000	Valledupar	Cesar
9	59,812.4110	13.0019	4,036.8360	Bogota	Bogotá + Cundinamarca
10	29,906.2055	0.0000	0.0000	Tunja	Boyaca
11	29,906.2055	0.0000	0.0000	Villavicencio	Meta
12	29,906.2055	0.0000	0.0000	Yopal	Casanare
13	12,437.2290	0.0000	0.0000	Igabué	Tolima
14	12,437.2290	0.0000	0.0000	Neiva	Huila
15	12,437.2290	0.0000	0.0000	Florencia	Caqueta
16	12,437.2290	261.7807	51.8811	Manizales	Caldas
17	12,437.2290	0.0000	0.0000	Armenia	Quindío
18	12,437.2290	0.6289	0.0000	Pereira	Risaralda
19	24,945.5279	0.0003	4.8334	Bucaramanga	Santander
20	4,989.1100	17.0041	0.0000	Cúcuta	Norte de Santander
21	4,989.1100	0.0000	0.0000	Arauca	Arauca
22	28,001.5327	175.3939	8,938.2250	Cali	Valle
23	28,001.5327	0.0000	628.8505	Popayán	Cauca
24	28,001.5327	0.0000	0.0000	Pasto	Nariño
25	28,001.5327	0.0000	0.0000	Mocoa	Putumayo

However, the clients in location 20 and 21 have a small demand for the different final biobased products. Therefore, it is decided to no work with these values, resuming it to 23 clients' points.

Appendix 6.9 Biodiesel price estimation

The Colombian government regulates biodiesel prices, therefore, for 2015 exist a monthly detail presented on Table 52 (Fedebiocombustibles 2017). For the conversion of gallons to liters the relation 1 Gallon = 3.785 liters was used. And 2,743.39 Colombian currency per U.S. dollar was utilized to convert Cop to USD (Banco de la República Colombia 2017). Finally, the biodiesel density was used to convert liter to ton (1 liter=0.000875 t). Then, the price average to 2015 is 1,124.8567 USD/t de biodiesel.

Table 52. Biodiesel Price monthly detail for 2015

Biodiesel Price by month in Colombia (Producer Income)				
2015	Cop/gallon	Cop / liter	USD/liter	USD/t
January	9,732.37	2,571.29987	0.9372710	1,071.16685
February	10,248.72	2,707.71995	0.9869978	1,127.99751
March	9,821.42	2,594.82695	0.9458469	1,080.96790
April	10,244.51	2,706.60766	0.9865924	1,127.53414
May	9,708.76	2,565.06209	0.9349972	1,068.56828
June	9,931.74	2,623.97358	0.9564712	1,093.10997
July	10,334.56	2,730.39894	0.9952646	1,137.44525
August	10,352.65	2,735.17834	0.9970067	1,139.43628
September	10,454.71	2,762.14267	1.0068356	1,150.66924
October	10,517.85	2,778.82431	1.0129162	1,157.61857
November	10,734.70	2,836.11625	1.0337999	1,181.48558
December	10,560.21	2,790.01585	1.0169957	1,162.28081
Average				1,124.8567

Appendix 6.10. Palm oil demand calculation

The information related to the refined palm oil sales was found in DANE (2017) and is summarized in table 53.

Table 53 Refined palm oil and its fractions in 2007

Department	Sales (Kg)	Sales (t)	%
Atlántico	7,545,043.00	7,545.04	8.85%
Bogotá	4,142,990.00	4,142.99	4.86%
Magdalena	41,769,695.00	41,769.70	48.97%
Meta	24,468,646.00	24,468.65	28.69%
Valle	7,364,687.00	7,364.69	8.63%
Total	85,291,061.00	85,291.06	100.00%

This detailed data corresponds to 2007. And for 2015 there is only a general value for refined palm oil sales.

Refined Palm oil sales in 2015= 113,854,589 kg/Year

Then, it is assumed that the same percentages by department were sold in 2015, in order to estimate the demand presented in table 54.

Table 54. Refined palm oil estimated demand in Colombia in 2015

Department	Kg
1 Atlántico	10,071,838.24
2 Bogotá	5,530,455.57
3 Magdalena	55,758,146.29
4 Meta	32,663,066.93
5 Valle	9,831,081.96
Total	113,854,589.00

Appendix 6.11. Transport distance matrix (km)

Table 55. Distance matrix between suppliers and pretreatment plants

		Pretreatment Plant Localization																
		1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
Supplier Localization	1	150	248	246	268	1,703	1,026	1,094	955	688	828	69	900	873	213	889	338	210
	2	396	134	1	148	1,647	970	1,340	1,241	580	772	291	1,146	1,119	459	1,135	207	121
	3	1,825	1,747	1,650	1,503	0	687	629	1,297	1,074	883	1,782	1,054	1,327	1,502	891	1,485	1,562
	4	519	655	654	676	1,332	655	722	624	316	456	396	528	502	196	517	602	618
	5	997	1,133	1,132	1,040	1,321	644	627	202	658	538	954	280	0	674	422	1,022	1,096
	6	1,115	1,251	1,251	1,009	1,291	614	597	0	628	508	1,072	249	203	792	392	991	1,214
	7	488	314	207	70	1,482	805	1,087	989	415	607	407	893	1,019	551	882	0	129
	8	104	399	399	421	1,710	1,033	1,100	1,002	694	834	220	906	880	220	895	491	362
	9	373	199	105	46	1,546	869	1,151	1,053	479	670	292	957	1,096	436	946	116	15
	10	231	149	260	370	1,865	1,188	1,256	1,157	850	989	94	1,062	1,035	375	1,051	440	311
	11	76	340	451	493	1,889	1,212	1,280	1,181	874	1,014	292	1,086	1,059	399	1,075	563	434
	12	911	1,047	1,047	805	985	308	291	313	424	202	868	70	343	588	85	788	1,010
	13	797	666	570	423	1,077	400	716	618	10	202	754	522	648	474	511	405	482

Table 56 Distance matrix between pretreatment plants and principal plants

		Principal Plant Localization																
		1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
Pretreatment Plant Localization	1	270	113	363	371	274	876	500	1,116	1,031	1,118	311	476	31	390	986	938	1,288
	2	147	399	51	33	145	1,037	663	1,251	1,212	1,254	128	296	381	517	906	1,048	1,423
	3	258	399	186	164	256	1,036	662	1,251	1,212	1,254	91	189	418	517	809	1,047	1,423
	4	368	421	290	274	366	795	684	1,009	970	1,013	117	53	440	539	662	806	1,182
	5	1,875	1,710	1,908	1,918	1,861	1,136	1,340	1,291	1,252	1,294	1,617	1,499	1,836	1,538	836	985	552
	6	1,193	1,033	1,231	1,241	1,184	458	663	614	575	617	939	822	1,159	861	159	308	305
	7	1,265	1,100	1,299	1,308	1,252	441	730	597	558	600	1,249	1,104	1,227	929	405	290	77
	8	1,165	1,002	1,201	1,210	1,153	237	632	0	58	4	1,151	1,006	1,128	830	518	313	669
	9	857	694	723	707	846	414	324	628	589	632	549	432	821	523	233	425	801
	10	995	834	1,033	1,042	986	302	464	508	469	511	741	624	960	662	42	202	501
	11	93	220	138	147	91	858	484	1,072	1,033	1,075	224	389	239	338	941	869	1,244
	12	1,031	907	1,105	1,114	1,058	94	536	249	210	253	1,055	910	1,033	735	275	70	426
	13	1,047	880	1,078	1,088	1,031	267	510	203	166	206	1,029	1,036	1,006	708	547	343	699
	14	374	220	418	428	371	578	204	792	753	796	369	533	346	59	661	589	965
	15	1,061	895	1,094	1,103	1,047	236	525	392	353	395	1,044	899	1,022	723	264	85	277
	16	438	491	387	344	436	777	610	991	952	995	187	19	510	609	644	788	1,164
	17	309	362	232	216	308	1,000	626	1,214	1,175	1,217	59	112	381	480	721	1,011	1,386

Table 57 Distance matrix between principal plants and final product markets

		Final Product Markets Localization																		
		1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19
Principal Plant Localization	1	838	1,068	438	323	227	102	5	256	955	816	1,071	1,011	950	1,139	1,348	950	1,038	1,003	539
	2	685	915	491	376	425	355	313	63	803	663	919	859	797	986	1,195	797	885	850	386
	3	714	943	360	245	117	3	104	301	1,001	862	1,117	1,057	996	1,185	1,393	995	1,084	1,049	584
	4	698	927	345	229	116	16	113	311	1,010	871	1,126	1,066	1,005	1,194	1,403	1,005	1,093	1,058	594
	5	837	1,066	436	321	226	101	4	254	954	815	1,070	1,010	948	1,137	1,346	948	1,037	1,002	537
	6	405	563	778	841	1,063	993	950	860	48	175	154	391	220	327	536	265	299	318	498
	7	315	544	610	640	689	619	576	486	432	293	548	488	427	616	824	427	515	480	124
	8	619	739	992	1,055	1,277	1,207	1,164	1,074	208	343	89	349	376	483	691	492	455	495	602
	9	580	700	953	1,016	1,238	1,168	1,125	1,035	169	304	53	313	337	444	652	453	416	456	563
	10	623	742	995	1,058	1,280	1,210	1,168	1,078	211	347	92	352	379	486	695	495	458	499	605
	11	540	770	187	72	118	163	252	252	951	812	1,067	1,007	946	1,135	1,343	735	798	757	535
	12	423	652	19	98	245	331	420	416	806	737	922	932	801	990	1,199	618	680	639	699
	13	812	1,041	510	395	444	338	244	79	929	790	1,045	985	923	1,212	1,321	923	1,011	976	512
	14	514	743	609	494	543	474	431	341	631	492	747	687	625	814	1,023	625	713	678	214
	15	240	243	644	707	876	1,077	1,034	944	345	483	434	694	147	354	589	77	51	28	582
	16	416	433	788	851	1,074	1,004	961	871	141	279	230	490	70	176	385	261	149	189	509
	17	792	702	1,164	1,227	1,449	1,379	1,337	1,247	496	634	586	846	398	189	129	537	459	487	884

Table 57 Distance matrix between principal plants and final product markets (Continuation)

		Final Product Markets Localization			
		20	21	22	23
Principal Plant Localization	1	628	1,335	1,582	1,457
	2	475	1,183	1,430	1,304
	3	673	1,381	1,628	1,503
	4	683	1,390	1,637	1,512
	5	626	1,334	1,581	1,456
	6	589	608	855	645
	7	312	812	1,059	934
	8	758	764	1,011	801
	9	719	725	972	762
	10	761	767	1,014	804
	11	623	1,089	1,336	1,453
	12	788	972	1,219	1,308
	13	601	1,309	1,556	1,430
	14	199	1,011	1,258	1,132
	15	770	309	556	575
	16	697	458	705	494
	17	1,072	153	278	132

Table 58 Distance matrix between pretreatment plants and product markets

		Intermediate Product Market Localization				
		1	2	3	4	5
Pretreatment Plant Localization	1	362	918	269	1,033	1,166
	2	51	1,044	148	1,159	1,081
	3	190	1,044	259	1,159	985
	4	282	811	369	926	838
	5	1,908	1,116	1,863	1,206	663
	6	1,239	447	1,194	537	30
	7	1,301	425	1,257	515	252
	8	1,202	207	1,158	88	636
	9	714	429	846	544	409
	10	1,033	330	988	424	221
	11	144	868	99	983	1,116
	12	1,106	76	1,061	166	393
	13	1,053	237	1,008	115	665
	14	423	586	378	701	834
	15	1,097	220	1,052	310	383
	16	352	793	440	908	820
	17	224	1,008	311	1,123	896

Appendix 6.12. Transport cost matrix (USD /km t)

Table 59 Transportation cost matrix between suppliers and pretreatment plants

		Pretreatment Plant Localization																
		1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
Supplier Localization	1	0.13	0.13	0.13	0.13	0.12	0.12	0.13	0.13	0.13	0.13	0.13	0.13	0.13	0.13	0.13	0.13	0.13
	2	0.15	0.15	0.13	0.13	0.13	0.12	0.14	0.11	0.13	0.13	0.15	0.12	0.11	0.13	0.15	0.13	0.13
	3	0.12	0.12	0.13	0.12	0.13	0.14	0.13	0.14	0.14	0.13	0.12	0.13	0.13	0.12	0.14	0.12	0.12
	4	0.12	0.13	0.11	0.13	0.12	0.12	0.12	0.13	0.14	0.13	0.12	0.12	0.14	0.13	0.12	0.13	0.13
	5	0.12	0.12	0.11	0.12	0.13	0.13	0.13	0.94	0.13	0.13	0.12	0.13	0.16	0.13	0.13	0.12	0.12
	6	0.11	0.11	0.11	0.13	0.14	0.14	0.14	0.17	0.15	0.15	0.11	0.18	0.94	0.13	0.15	0.13	0.13
	7	0.14	0.13	0.13	0.13	0.12	0.13	0.13	0.13	0.13	0.13	0.14	0.13	0.12	0.13	0.13	0.13	0.12
	8	0.13	0.13	0.13	0.13	0.12	0.12	0.13	0.13	0.13	0.13	0.13	0.13	0.13	0.13	0.13	0.13	0.13
	9	0.13	0.13	0.13	0.12	0.12	0.13	0.12	0.13	0.13	0.13	0.13	0.13	0.12	0.13	0.13	0.12	0.13
	10	0.13	0.18	0.15	0.14	0.12	0.11	0.13	0.11	0.12	0.11	0.13	0.11	0.12	0.13	0.20	0.14	0.13
	11	0.12	0.13	0.13	0.13	0.13	0.12	0.13	0.12	0.12	0.12	0.12	0.12	0.12	0.12	0.12	0.13	0.13
	12	0.11	0.11	0.12	0.13	0.13	0.13	0.12	0.18	0.14	0.14	0.11	0.13	0.13	0.13	0.14	0.13	0.13
	13	0.12	0.13	0.13	0.13	0.14	0.14	0.11	0.15	0.14	0.16	0.12	0.14	0.13	0.13	0.15	0.13	0.13

Table 60 Transportation cost matrix between pretreatment plants and principal production plants

		Principal Plant Localization																	
		1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	
Pretreatment Plant Localization	1	0.13	0.13	0.18	0.18	0.13	0.11	0.12	0.11	0.11	0.11	0.15	0.14	0.12	0.11	0.19	0.11	0.13	
	2	0.18	0.13	0.13	0.13	0.18	0.11	0.13	0.11	0.11	0.11	0.15	0.13	0.13	0.12	0.13	0.11	0.14	
	3	0.15	0.13	0.15	0.15	0.15	0.12	0.11	0.11	0.11	0.11	0.13	0.13	0.13	0.19	0.14	0.12	0.14	
	4	0.14	0.13	0.13	0.13	0.14	0.13	0.13	0.13	0.13	0.13	0.13	0.13	0.13	0.13	0.13	0.13	0.13	0.13
	5	0.12	0.12	0.12	0.12	0.12	0.13	0.12	0.14	0.14	0.14	0.13	0.12	0.13	0.12	0.13	0.13	0.13	0.13
	6	0.11	0.12	0.12	0.12	0.11	0.13	0.12	0.14	0.14	0.14	0.12	0.13	0.12	0.13	0.13	0.13	0.13	0.12
	7	0.13	0.13	0.14	0.14	0.13	0.12	0.12	0.14	0.14	0.14	0.14	0.13	0.13	0.13	0.13	0.12	0.12	0.13
	8	0.11	0.13	0.11	0.11	0.11	0.18	0.13	0.17	0.17	0.17	0.11	0.13	0.12	0.15	0.15	0.18	0.14	
	9	0.12	0.13	0.13	0.13	0.12	0.14	0.14	0.15	0.15	0.15	0.13	0.13	0.12	0.14	0.16	0.14	0.11	
	10	0.11	0.13	0.13	0.13	0.11	0.14	0.13	0.15	0.15	0.15	0.13	0.13	0.12	0.13	0.18	0.14	0.13	
	11	0.13	0.13	0.18	0.18	0.13	0.11	0.12	0.11	0.11	0.11	0.15	0.14	0.12	0.11	0.19	0.11	0.13	
	12	0.11	0.13	0.11	0.11	0.11	0.13	0.12	0.18	0.18	0.18	0.12	0.13	0.12	0.14	0.13	0.13	0.12	
	13	0.12	0.13	0.12	0.12	0.12	0.13	0.14	0.94	0.94	0.94	0.11	0.12	0.12	0.15	0.13	0.13	0.13	
	14	0.13	0.13	0.13	0.13	0.13	0.13	0.13	0.13	0.13	0.13	0.13	0.13	0.13	0.12	0.12	0.13	0.13	0.13
	15	0.20	0.13	0.15	0.15	0.20	0.14	0.12	0.15	0.15	0.15	0.15	0.13	0.12	0.13	0.15	0.14	0.19	
	16	0.14	0.13	0.13	0.13	0.14	0.13	0.13	0.13	0.13	0.13	0.13	0.13	0.13	0.13	0.13	0.13	0.13	0.13
	17	0.13	0.13	0.13	0.13	0.13	0.13	0.13	0.13	0.13	0.13	0.13	0.12	0.13	0.13	0.13	0.13	0.13	0.12

Table 61 Transportation cost matrix between principal plants and final markets

		Final Product Markets Localization																			
		1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	
Principal Plant Localization	1	0.12	0.13	0.14	0.13	0.15	0.18	0.13	0.13	0.11	0.13	0.11	0.12	0.20	0.13	0.13	0.12	0.19	0.11	0.12	
	2	0.13	0.13	0.13	0.13	0.13	0.13	0.13	0.13	0.13	0.13	0.13	0.13	0.13	0.13	0.13	0.13	0.13	0.13	0.13	0.13
	3	0.13	0.13	0.13	0.13	0.15	0.13	0.18	0.13	0.11	0.13	0.11	0.12	0.15	0.14	0.12	0.12	0.13	0.13	0.13	
	4	0.13	0.13	0.13	0.13	0.15	0.13	0.18	0.13	0.11	0.13	0.11	0.12	0.15	0.14	0.12	0.12	0.13	0.13	0.13	
	5	0.12	0.13	0.14	0.13	0.15	0.18	0.13	0.13	0.11	0.13	0.11	0.12	0.20	0.13	0.13	0.12	0.19	0.11	0.12	
	6	0.14	0.13	0.13	0.13	0.12	0.11	0.11	0.13	0.13	0.14	0.18	0.13	0.14	0.12	0.13	0.15	0.14	0.14	0.12	
	7	0.14	0.13	0.13	0.13	0.11	0.13	0.12	0.13	0.12	0.13	0.13	0.14	0.12	0.12	0.13	0.13	0.12	0.13	0.13	
	8	0.15	0.17	0.13	0.13	0.11	0.11	0.11	0.13	0.18	0.12	0.17	0.94	0.15	0.14	0.13	0.13	0.15	0.15	0.13	
	9	0.15	0.17	0.13	0.13	0.11	0.11	0.11	0.13	0.18	0.12	0.17	0.94	0.15	0.14	0.13	0.13	0.15	0.15	0.13	
	10	0.15	0.17	0.13	0.13	0.11	0.11	0.11	0.13	0.18	0.12	0.17	0.94	0.15	0.14	0.13	0.13	0.15	0.15	0.13	
	11	0.13	0.13	0.13	0.13	0.13	0.15	0.15	0.13	0.12	0.13	0.11	0.11	0.15	0.14	0.12	0.13	0.13	0.13	0.11	
	12	0.13	0.13	0.13	0.12	0.13	0.13	0.14	0.13	0.13	0.12	0.13	0.12	0.13	0.13	0.12	0.13	0.14	0.13	0.13	
	13	0.12	0.12	0.13	0.13	0.13	0.13	0.12	0.12	0.12	0.12	0.12	0.12	0.12	0.13	0.12	0.12	0.13	0.12	0.13	
	14	0.14	0.13	0.13	0.13	0.19	0.12	0.11	0.12	0.14	0.13	0.15	0.15	0.13	0.13	0.12	0.14	0.13	0.13	0.16	
	15	0.16	0.14	0.13	0.13	0.14	0.13	0.19	0.13	0.13	0.13	0.15	0.13	0.15	0.12	0.13	0.15	0.12	0.18	0.13	
	16	0.14	0.13	0.13	0.13	0.12	0.11	0.11	0.13	0.13	0.14	0.18	0.13	0.14	0.12	0.13	0.15	0.14	0.14	0.12	
	17	0.11	0.13	0.13	0.12	0.14	0.14	0.13	0.13	0.12	0.13	0.14	0.13	0.19	0.13	0.12	0.13	0.13	0.13	0.12	

Table 61. Transportation cost matrix between principal plants and final markets (Continuation)

		Final Product Markets Localization			
		20	21	22	23
Principal Plant Localization	1	0.11	0.12	0.12	0.13
	2	0.12	0.12	0.12	0.13
	3	0.12	0.12	0.12	0.12
	4	0.12	0.12	0.12	0.12
	5	0.11	0.12	0.12	0.13
	6	0.14	0.14	0.14	0.13
	7	0.16	0.12	0.13	0.12
	8	0.15	0.15	0.14	0.13
	9	0.15	0.15	0.14	0.13
	10	0.15	0.15	0.14	0.13
	11	0.19	0.12	0.13	0.12
	12	0.13	0.13	0.13	0.12
	13	0.12	0.12	0.12	0.12
	14	0.13	0.12	0.13	0.12
	15	0.13	0.14	0.13	0.13
	16	0.14	0.14	0.14	0.13
	17	0.13	0.12	0.12	0.12

Table 62 Transportation cost matrix between pretreatment plants and product markets

		Intermediate Product Market Localization				
		1	2	3	4	5
Pretreatment Plant Localization	1	0.18	0.11	0.13	0.11	0.11
	2	0.13	0.11	0.18	0.11	0.12
	3	0.15	0.12	0.15	0.11	0.12
	4	0.13	0.13	0.14	0.13	0.13
	5	0.12	0.13	0.12	0.14	0.14
	6	0.12	0.13	0.11	0.14	0.13
	7	0.14	0.12	0.13	0.14	0.12
	8	0.11	0.18	0.11	0.17	0.14
	9	0.13	0.14	0.12	0.15	0.14
	10	0.13	0.14	0.11	0.15	0.13
	11	0.18	0.11	0.13	0.11	0.11
	12	0.11	0.13	0.11	0.18	0.13
	13	0.12	0.13	0.12	0.94	0.13
	14	0.13	0.13	0.13	0.13	0.12
	15	0.15	0.14	0.20	0.15	0.14
	16	0.13	0.13	0.14	0.13	0.13
	17	0.13	0.13	0.13	0.13	0.13

Appendix 6.13. Sewage water production parameters estimation

Pretreatment Plants

As presented in section 6.2.2, crude jatropha an palm oil contains in average 1% of moisture or impurities. Then, $SW_{n,c=1} = 1\%, \forall n$

These percentages must to be multiplied by the characteristic of sewage water generated at pretreatment plants to obtain the values of $\psi_{y,n,c}$ for BOD and TSS. And a density of 1 liter/ton is assumed to sewage water, due to lack information.

The detailed information found for palm oil refinery sewage water is (CHIN and WONG 1981):

$$BOD = 5\,000 \frac{mg}{l} = 0.000005 \frac{t\ BOD}{l}$$

$$TSS = 5\,000 \frac{mg}{l} = 0.000005 \frac{t\ TSS}{l}$$

However, for jatropha oil, there is no data. Therefore, the TSS for palm oil is considered as 1% of impurities, and then $TSS = 15\,000\ mg/l$ will be considered for jatropha oil. Also, it could be noted, at table 5.35, that the acid number is three times of palm oil for jatropha oil, just as impurities. Then it is supposed that the BOD for jatropha oil can be $15\,000 \frac{mg}{l}$ ($= 0,000015 \frac{ton}{l}$).

Finally, the generated amount of **BOD** at pretreatment plants is:

$$\psi_{y=BOD,n,c=1,f} = 1\% * \frac{SW\ t}{Raw\ Material\ t} * 1 \frac{SW\ liter}{SW\ t} * 0,000005 \frac{ton\ BOD}{SW\ liter} = 5 * 10^{-8} \frac{t\ BOD}{Raw\ Material\ t}$$

$$\psi_{y=TSS,n,c=1,f} = 1\% * \frac{SW\ t}{Raw\ Material\ t} * 1 \frac{SW\ liter}{SW\ t} * 0,000005 \frac{ton\ TSS}{SW\ liter} = 5 * 10^{-8} \frac{ton\ TSS}{Raw\ Material\ t}$$

Principal plants

Sewage water generated by biodiesel production

According to research Basto Aluja (2016), wastewater is generated from the biodiesel washes, biodiesel and methanol purification. In this research two different methods of biodiesel washing were used. However, the water needed remained the same for both process, only depending on the production capacities.

In order to analyze the total wastewater generated in biodiesel production, according to the material balance tables, flows leaving the system with water content of around 90% were considered (Basto Aluja 2016), as summarized in table 63.

Table 63. Sewage water generation rate by biodiesel production at pretreatment plants (weight/weight) based on (Basto Aluja 2016)

	Capacity (t/Year)		
	40 000 (g = 1)	80 000 (g = 2)	120 000 (g = 3)
$SW_{b,d,g} = \frac{\text{Sewage water (t)}}{\text{Intermediate products entering (t)}}$	5.16%	7.00%	7.39%

Therefore, it is assumed that the same amount of wastewater is generated, regardless of type of raw material. Because palm oil and jatropa oil have been pre-treated. Thus, the wastewater production rate does not depend on the type of incoming raw material, but only on the production capacity. The amount of wastewater generated by biodiesel production with technologies “Base-catalyzed transesterification” (1), “Co-current transesterification” (3) y “Counter-current transesterification” (5) is calculated on the basis of table 63 and the density of palm and jatropa oil as corresponds.

The sewage water generated by transform jatropa and palm oil in biodiesel by transesterification of intermediate products (*IP*) at principal plants is calculated as:

$$SW_{b=1,2,d,g=1} = 5.16\% \frac{SW \ t}{IP \ t} * 1 \frac{SW \ liter}{SW \ t} = 5.16\% \frac{SW \ liter}{t \ IP}$$

$$SW_{b=1,2,d,g=2} = 7.00\% \frac{SW \ t}{IP \ t} * 1 \frac{SW \ liter}{SW \ t} = 7.00\% \frac{SW \ liter}{t \ IP}$$

$$SW_{b=1,2,d,g=3} = 7.39\% \frac{SW \ t}{IP \ t} * 1 \frac{SW \ liter}{SW \ t} = 7.39\% \frac{SW \ liter}{t \ IP}$$

$$\forall y, d = 1,3,5$$

It is also necessary to know the physicochemical characteristics of this wastewater from biodiesel production in order to evaluate the cost of generating pollution. In the investigation of Rojo Choya (2015) it is detailed that the average value of BOD from biodiesel production is 11.5 *gr/l* and for TSS is 1.9 *gr/l*, which is equivalent to 0.0000115 *t/l* and 0.0000019 *t/l* respectively. If these values are used for sewage water generated from both jatropa and pam oil refined, the quantity of **BOD** produced by transesterification can be calculated as:

$$\psi_{y=BOD,b=1,2,d,g=1} = 5.16\% \frac{SW \ liter}{t \ IP} * 0.0000115 \frac{t \ BOD}{SW \ liter} = 5,93 * 10^{-7} \frac{t \ BOD}{t \ IP}$$

$$\psi_{y=BOD,b=1,2,d,g=2} = 7.00\% \frac{SW \ liter}{t \ IP} * 0.0000115 \frac{t \ BOD}{SW \ liter} = 8,05 * 10^{-7} \frac{t \ BOD}{t \ IP}$$

$$\psi_{y=BOD,b=1,2,d,g=3} = 7.39\% \frac{SW \ liter}{t \ IP} * 0.0000115 \frac{t \ BOD}{SW \ liter} = 8,50 * 10^{-7} \frac{t \ BOD}{t \ IP}$$

$$\psi_{y=TSS,b=1,d,g=1} = 5.16\% \frac{SW \ liter}{t \ IP} * 0.0000019 \frac{t \ TSS}{SW \ liter} = 9,80 * 10^{-8} \frac{t \ TSS}{t \ IP}$$

$$\psi_{y=TSS,b=1,d,g=2} = 7.00\% \frac{SW \ liter}{t \ IP} * 0.0000019 \frac{t \ TSS}{SW \ liter} = 1,33 * 10^{-7} \frac{t \ TSS}{t \ IP}$$

$$\psi_{y=TSS,b=1,d,g=3} = 7.39\% \frac{SW \ liter}{t \ IP} * 0.0000019 \frac{t \ TSS}{SW \ liter} = 1,40 * 10^{-7} \frac{t \ TSS}{t \ IP}$$

$$d = 1,3,5$$

Sewage water generated by polymer production

In the research carried out by Bueno et al. (2014), the sewage water is generated due to moisture glycerol reduction in distillation column and as water vapor, which is generated as a by-product in the polycondensation reaction. Then, it is required to consider the moisture rate of glycerol generated at biodiesel production: 0.342857 % (Basto Aluja 2016).

In this case it is assumed that capacity plant does not generate changes in the amount of sewage water quantity generated, due lack of information. Also, in this case, the sewage water amount will depends on technology, because the glycerol production rate varies with transesterification technology used. Then, the amount of sewage water generated by glycerol (G) volume transformed at principal plants in polymer, related to intermediate product and technology applied is:

$$SW_{b=1,2,d,g=1} = 0.342857\% \frac{SW \text{ liter}}{t G} * 0.0777 \frac{t G}{t IP} + 5.16\% \frac{SW \text{ liter}}{t IP} = 5.19\% \frac{SW \text{ liter}}{t IP}$$

$$SW_{b=1,2,d,g=2} = 0.342857\% \frac{SW \text{ liter}}{t G} * 0.0777 \frac{t G}{t IP} + 7.00\% \frac{SW \text{ liter}}{t IP} = 7.03\% \frac{SW \text{ liter}}{t IP}$$

$$SW_{b=1,2,d,g=3} = 0.342857\% \frac{SW \text{ liter}}{t G} * 0.0777 \frac{t G}{t IP} + 7.39\% \frac{SW \text{ liter}}{t IP} = 7.42\% \frac{SW \text{ liter}}{t IP}$$

$$\forall d = 2,4,6$$

Then, due to information lack about specific characteristics of sewage water by polymer generation, it is assumed that it will have a similar composition to residual water generated by biodiesel production (BOD=0.0000115; TSS=0.0000019). Therefore, the quantity of **BOD** and **TSS** produced can be calculated as:

$$\psi_{y=BOD,b,d,g=1} = 5.19\% \frac{SW \text{ liter}}{t IP} * 0.0000115 \frac{t BOD}{SW \text{ liter}} = 5.96 * 10^{-7} \frac{t BOD}{t IP}$$

$$\psi_{y=BOD,b,d,g=2} = 7.03\% \frac{SW \text{ liter}}{t IP} * 0.0000115 \frac{t BOD}{SW \text{ liter}} = 8.08 * 10^{-7} \frac{t BOD}{t IP}$$

$$\psi_{y=BOD,b,d,g=3} = 7.42\% \frac{SW \text{ liter}}{t IP} * 0.0000115 \frac{t BOD}{SW \text{ liter}} = 8.53 * 10^{-7} \frac{t BOD}{t IP}$$

$$\psi_{y=TSS,b=1,d=2,g=1} = 5.19\% \frac{SW \text{ liter}}{t IP} * 0.0000019 \frac{t TSS}{SW \text{ liter}} = 9.85 * 10^{-8} \frac{t TSS}{t IP}$$

$$\psi_{y=TSS,b=1,d=2,g=2} = 7.03\% \frac{SW \text{ liter}}{t IP} * 0.0000019 \frac{t TSS}{SW \text{ liter}} = 1.34 * 10^{-7} \frac{t TSS}{t IP}$$

$$\psi_{y=TSS,b=1,d=2,g=3} = 7.42\% \frac{SW \text{ liter}}{t IP} * 0.0000019 \frac{t TSS}{SW \text{ liter}} = 1.41 * 10^{-7} \frac{t TSS}{t IP}$$

Appendix 6.14. Solid waste generation

Then, the solid waste generation rate at pretreatment and principal production plants is required. Santos Oliveira et al. (2017) details that the most important residue in biodiesel production is the filter material impregnated with oil and biodiesel. This biodiesel production process includes pretreatment units and catalytic reactors. Between years 2012 and 2014, the maximum amount of spent filter material was 459 tons, representing the 97% of the total hazardous solid generated at biodiesel plants that produce 100 000 biodiesel tons by year in Brazil.

Then, the total hazardous solid generated will be approximately 473,2 tons by year. Therefore, it means that $\frac{473,2}{100\ 000} = 0,4732\%$ is the percentage weight/weight for hazardous solid generation by biodiesel tons produced.

More information cannot be found about the different technologies for principal plants, or any details about the proportion of solid waste generated at pretreatment process and at principal plants for transesterification.

Therefore, it is decided to assume that 0,4732% weight of hazardous solid is generated by weight of final products at pretreatment and principal plants for each processing technology.

At pretreatment plants:

The soaps and residues are intermediate products that are generated as by-products, and then the solid hazardous rate will be calculated only for refined jatropha oil and refined palm oil.

There is assumed that capacity production does not affect the solid waste rate due lack information. As only hazardous solid rate is evaluated as solid waste $z = 1$. Then, the hazardous rate is calculated in table 64.

Table 64 Hazardous generation at pretreatment plants

Biomass type	Refined jatropha oil Rate ($b = 1$)	Hazardous solid rate (by $b = 1$)	Refined Palm oil Rate ($b = 3$)	Hazardous solid rate (by $b = 3$)
Palm oil ($n = 1$)	0.00%	0.00%	97.40%	0.46%
Jatropha oil by manual extraction ($n = 2$)	91.80%	0.43%	0.00%	0.00%
Jatropha oil by electrical extraction ($n = 3$)	91.80%	0.43%	0.00%	0.00%

Then, the parameter is described as:

$$\omega_{z=1,n=1,c=1,f} = 0.0046$$

$$\omega_{z=1,n=2,c=1,f} = 0.0043$$

$$\omega_{z=1,n=3,c=1,f} = 0.0043$$

At principal plants

Glycerol is a byproduct in biodiesel production by transesterification; therefore, they should only be considered solid waste generation due to the production of biodiesel and polymers. The production rates are multiplied by the waste generation percentage defined before (0.4732%) to obtain the hazardous rate by refined oil, summarized in table 65.

Table 65. Hazardous solid waste generated at principal plants depending on production technology and intermediate product transformed

Intermediate Products		Production Technology	Biodiesel ($\frac{t \text{ biodiesel}}{t \text{ refined oil}}$) ($a = 1$)	Hazardous solid rate (by $a = 1$)	Polymer ($\frac{t \text{ polymer}}{t \text{ refined oil}}$) ($a = 2$)	Hazardous solid rate (by $a = 2$)
1	Jatropha Oil	1	0.9711	0.0046	0.0000	0.0000
1	Jatropha Oil	2	0.9711	0.0046	0.1921	0.0009
1	Jatropha Oil	3	0.9837	0.0047	0.0000	0.0000
1	Jatropha Oil	4	0.9837	0.0047	0.1946	0.0009
1	Jatropha Oil	5	0.9973	0.0047	0.0000	0.0000
1	Jatropha Oil	6	0.9973	0.0047	0.1973	0.0009
3	Palm Oil	1	1.0035	0.0048	0.0000	0.0000
3	Palm Oil	2	1.0035	0.0048	0.1859	0.0009
3	Palm Oil	3	1.0166	0.0048	0.0000	0.0000
3	Palm Oil	4	1.0166	0.0048	0.1883	0.0009
3	Palm Oil	5	1.0306	0.0049	0.0000	0.0000
3	Palm Oil	6	1.0306	0.0049	0.1909	0.0009

Then, assuming that there is no difference for solid waste generation by production capacity, due lack information, the mathematical expression to calculate the solid waste amount generated is:

$$\omega_{z=1,b=1,d=1,g} = 0.0046 \frac{t \text{ waste}}{t \text{ refined oil}}$$

$$\omega_{z=1,b=1,d=2,g} = 0.0046 + 0.0009 = 0.0055 \frac{t \text{ waste}}{t \text{ refined oil}}$$

$$\omega_{z=1,b=1,d=3,g} = 0.0047 \frac{t \text{ waste}}{t \text{ refined oil}}$$

$$\omega_{z=1,b=1,d=4,g} = 0.0047 + 0.0009 = 0.0056 \frac{t \text{ waste}}{t \text{ refined oil}}$$

$$\omega_{z=1,b=1,d=5,g} = 0.0047 \frac{t \text{ waste}}{t \text{ refined oil}}$$

$$\omega_{z=1,b=1,d=6,g} = 0.0047 + 0.0009 = 0.0056 \frac{t \text{ waste}}{t \text{ refined oil}}$$

$$\omega_{z=1,b=3,d=1,g} = 0.0048 \frac{t \text{ waste}}{t \text{ refined oil}}$$

$$\omega_{z=1,b=3,d=2,g} = 0.0048 + 0.0009 = 0.0057 \frac{t \text{ waste}}{t \text{ refined oil}}$$

$$\omega_{z=1,b=3,d=3,g} = 0.0048 \frac{t \text{ waste}}{t \text{ refined oil}}$$

$$\omega_{z=1,b=3,d=4,g} = 0.0048 + 0.0009 = 0.0057 \frac{t \text{ waste}}{t \text{ refined oil}}$$

$$\omega_{z=1,b=3,d=5,g} = 0.0049 \frac{t \text{ waste}}{t \text{ refined oil}}$$

$$\omega_{z=1,b=3,d=6,g} = 0.0049 + 0.0009 = 0.0058 \frac{t \text{ waste}}{t \text{ refined oil}}$$

Appendix 6.15. Water consumption for raw materials

Palm oil

In average, it is considered that in Colombia the palm cultivation requires 6.5 mm per day and m² (Extractora Palmariguani S.A. 2011). This value is equivalent to 2,340 mm per year and m² (considering 360 days). Then, considering the water density, this amount is equivalent to 2.34 ton of water per m² or 23,400 water t per hectare.

Considering the average rate of crude palm oil 3.37 t/hectare (Fedepalma 2015), it can be estimated the amount of water required for the palm as:

$$23,400 \frac{t \text{ water}}{ha \text{ palm}} * \frac{1}{3.37} \frac{ha \text{ palm}}{t \text{ palm crude oil}} = 6,943.62 \frac{t \text{ water}}{t \text{ palm crude oil}}$$

Jatropha oil

It is considered that the optimal value for jatropha cultivations related to water requirements is between 1,200 y 1,500 mm per year and m² (Jongschaap et al. 2007; Abou Kheira and Atta 2009; Alvarez Zarrate 2013). Then, the average is 1,350 mm per year and m², value equivalent to 1.35 water tons per year and m² or 13,500 water tons per year and hectare.

Thus, considering the jatropha crude oil production rates with the different extraction methods, it can be estimated the amount of water required for the jatropha as:

Manual extraction

$$13,500 \frac{t \text{ water}}{ha \text{ jatropha}} * \frac{1}{1.16} \frac{ha \text{ jatropha}}{t \text{ jatropha crude oil}} = 11,637.93 \frac{t \text{ water}}{t \text{ jatropha crude oil}}$$

Electric extraction

$$13,500 \frac{t \text{ water}}{ha \text{ jatropha}} * \frac{1}{1.39} \frac{ha \text{ jatropha}}{t \text{ jatropha crude oil}} = 9,712.23 \frac{t \text{ water}}{t \text{ jatropha crude oil}}$$

Appendix 6.16. Water required for transformation process at pretreatment and principal plants

Pretreatment plants

At pretreatment plants there are only two stages that use water for the process: Degumming and deodorization. In the research carried out by Blanco Rodríguez (2007) it can be found the data presented in table 66.

Table 66 Water required for each pretreatment stage for an average oil (entering oil =100 kg/hr) (Blanco Rodríguez 2007)

Physical refinement stage	Water or vapor (kg/hr)
Degummed	2.0200
Bleaching	0.0000
Deodorization	0.0055
Total	2.0255
% related to the initial crude oil	2.03%

Principal plants

It must to be estimated the amount of water required for the biodiesel production with the different production technologies and also the water required for polyester production.

Biodiesel production. As presented in the research carried out by Basto Aluja (2016), there are two water requirements by biodiesel production technologies: to biodiesel washes and to equipment cooling.

a) Washing biodiesel

Water required for washing biodiesel depends only in production capacity (Basto Aluja 2016), the values are summarized in table 67.

Table 67 water required for transesterification process

Production capacity (t/year)	Water t / t entering oil to transesterification
40,000	4.66
80,000	6.47
120,000	6.90

b) Equipment cooling

The amount of water for equipment cooling depends on production capacity and technology. Thus, as stated by Basto Aluja (2016), the amounts are summarized in table 68.

Table 68 Water required for equipment cooling (kg water / kg biodiesel)

	Production capacity		
	40,000	80,000	120,000
Conventional	1.700	0.825	0.525
Co-current	1.450	0.725	0.450
Count-current	1.400	0.625	0.350

These values multiplied by the transformation rate for biodiesel produced with refined oils will give the amounts for water requirements for equipment cooling by refined oil processed, as presented in table 69.

Table 69 Average water required for equipment cooling (t water / t refined oil)

Refined oil	Transesterification process type	Production capacity (t/year)		
		40,000	80,000	120,000
Jatropha Oil	Conventional	1.65	0.80	0.51
Jatropha Oil	Co-current	1.42	0.71	0.44
Jatropha Oil	Count-current	1.40	0.63	0.35
Palm Oil	Conventional	1.70	0.83	0.53
Palm Oil	Co-current	1.48	0.74	0.46
Palm Oil	Count-current	1.44	0.64	0.36

Aliphatic polyester production. The production process does not requires water; however, based in the research carried out by Bueno et al. (2014), the amount of water required for equipment cooling can be estimated with the follow information:

- Cooling water (kJ/kg total polymer)= 621.097
- In order to achieve the cooling of the polymer, freshwater at 283 K that is heated up to 303 K is used.
- To maintain the reaction isothermal, we use jacketed stirred tank reactors with water as cooling agent. Cooling water is introduced at 303.15 K from the condenser (I02) of the distillation column (T01) and exits the jacket at 313.15 K providing heat integration.
- 303,15°K = 30°C
- 283°K = 9.85°C
- Water specific heat average between 30°C and 9.85°C is 4,178 Kj/Kg water (VAXA Software 2017)

Then

$$\frac{621.097 \text{ kJ/kg polyester}}{4,185 \text{ kJ/kg water}} = 0.1484 \frac{\text{kg water}}{\text{kg polyester}} = 0.1484 \frac{\text{t water}}{\text{t polyester}}$$

This value multiplied by the transformation rate for polyester produced with refined oils will give the amounts for water requirements for equipment cooling by refined oil processed. This value is in average $0.03 \frac{\text{t water}}{\text{t polyester}}$

Then, the table 70 summarizes the total amount of water required by technology, raw material and production capacity.

Table 70 Required water at principal production plants (t Water/ t intermediate product)

Refined oil	Technology (<i>d</i>)	Production capacity (t/year)		
		40,000	80,000	120,000
Jatropha Oil	1	6.31	7.27	7.41
Jatropha Oil	2	6.34	7.30	7.44
Jatropha Oil	3	6.08	7.18	7.34
Jatropha Oil	4	6.11	7.21	7.37
Jatropha Oil	5	6.06	7.10	7.25
Jatropha Oil	6	6.09	7.12	7.28
Palm Oil	1	6.36	7.30	7.43
Palm Oil	2	6.39	7.32	7.45
Palm Oil	3	6.14	7.21	7.36
Palm Oil	4	6.17	7.24	7.39
Palm Oil	5	6.10	7.11	7.26
Palm Oil	6	6.13	7.14	7.29

Appendix 6.17. Cost reduction due to technology learning

The production costs at pretreatment plants for the unit produced are summarized in table 71.

Table 71. Production cost at pretreatment plants for crude oil process (USD/Ton)

Raw material	Capacity	Produced units		
		40,000	80,000	120,000
<i>Palm oil</i>	1	31.15	30.53	30.17
<i>Palm oil</i>	2	29.23	28.65	28.31
<i>Palm oil</i>	3	29.23	28.65	28.31
<i>Jatropha oil by manual extraction</i>	1	28.61	28.04	27.71
<i>Jatropha oil by manual extraction</i>	2	26.85	26.31	26.00
<i>Jatropha oil by manual extraction</i>	3	26.85	26.31	26.00
<i>Jatropha oil by electrical extraction</i>	1	26.70	26.16	25.86
<i>Jatropha oil by electrical extraction</i>	2	25.05	24.55	24.26
<i>Jatropha oil by electrical extraction</i>	3	25.05	24.55	24.26

Then, for the maximal capacity per year, the operational cost can be summarized in table 72.

Table 72 Operational cost that integrates technology apprenticeship at pretreatment plants

Pretreatment capacity (<i>f</i>)	Raw material type (<i>n</i>)		
	Palm oil	Jatropha oil by manual extraction	Jatropha oil by electrical extraction
40,000	31.15	28.61	26.70
80,000	28.65	26.31	24.55
120,000	28.31	26.00	24.26

Table 73. Production cost at principal plants for jatropha refined oil process including technological learning (USD/Ton)

<i>d</i>	<i>g</i>	Initial Cost	Produced Unit														
			1,000	2,500	5,000	10,000	20,000	30,000	40,000	50,000	60,000	70,000	80,000	90,000	100,000	110,000	120,000
1	1	432	353	344	337	330	324	320	317	315	313	312	311	310	309	308	307
1	2	397	325	316	310	304	297	294	292	290	288	287	286	285	284	283	282
1	3	371	303	295	289	284	278	275	272	271	269	268	267	266	265	265	264
2	1	539	441	429	421	412	404	399	396	393	391	389	388	387	385	384	383
2	2	495	405	394	386	378	371	367	363	361	359	358	356	355	354	353	352
2	3	462	378	368	360	353	346	342	339	337	335	334	332	331	330	329	329
3	1	409	334	326	319	313	306	303	300	298	297	295	294	293	292	292	291
3	2	383	313	305	299	293	287	284	281	279	278	277	276	275	274	273	272
3	3	366	299	291	286	280	274	271	269	267	266	264	263	262	262	261	260
4	1	517	423	412	403	395	387	383	380	377	375	373	372	371	370	369	368
4	2	482	394	384	376	369	361	357	354	352	350	348	347	346	345	344	343
4	3	458	374	365	357	350	343	339	336	334	332	331	330	328	327	327	326
5	1	405	331	322	316	310	303	300	297	295	294	293	291	290	290	289	288
5	2	379	310	302	296	290	284	281	278	276	275	274	273	272	271	270	270
5	3	362	296	288	282	277	271	268	266	264	263	262	260	260	259	258	257
6	1	514	420	409	401	393	385	381	377	375	373	371	370	369	367	366	366
6	2	479	392	381	374	366	359	355	352	349	348	346	345	344	342	342	341
6	3	455	372	362	355	348	341	337	334	332	330	329	327	326	325	324	324
Reduction cost for: <i>d</i> = 1; <i>g</i> = 1 and jatropha refined oil process			78.78	88.09	94.97	101.71	108.31	112.12	114.79	116.84	118.51	119.92	121.13	122.20	123.15	124.00	124.78

Table 74 Production cost at principal plants for palm refined oil process including technological learning (USD/Ton)

<i>d</i>	<i>g</i>	Initial Cost	Produced Unit														
			1,000	2,500	5,000	10,000	20,000	30,000	40,000	50,000	60,000	70,000	80,000	90,000	100,000	110,000	120,000
1	1	317.21	259	253	247	243	238	235	233	231	230	229	228	227	227	226	226
1	2	285.68	234	227	223	218	214	212	210	208	207	206	206	205	204	204	203
1	3	263.84	216	210	206	202	198	195	194	192	191	191	190	189	189	188	188
2	1	395.78	324	315	309	303	297	293	291	289	287	286	285	284	283	282	281
2	2	356.2	291	284	278	272	267	264	262	260	258	257	256	255	255	254	253
2	3	328.55	269	262	256	251	246	243	241	240	238	237	236	236	235	234	234
3	1	300.32	246	239	234	230	225	222	221	219	218	217	216	215	215	214	214
3	2	275.61	225	219	215	211	207	204	202	201	200	199	198	198	197	196	196
3	3	260.28	213	207	203	199	195	193	191	190	189	188	187	187	186	186	185
4	1	379.63	310	302	296	290	284	281	279	277	275	274	273	272	271	271	270
4	2	346.85	284	276	271	265	260	257	255	253	252	251	250	249	248	247	247
4	3	325.71	266	259	254	249	244	241	239	238	236	235	234	234	233	232	232
5	1	297.39	243	237	232	227	223	220	218	217	216	215	214	213	213	212	211
5	2	272.73	223	217	213	209	204	202	200	199	198	197	196	196	195	194	194
5	3	257.44	210	205	201	197	193	191	189	188	187	186	185	185	184	184	183
6	1	377.42	309	300	294	289	283	279	277	275	274	273	272	271	270	269	268
6	2	344.69	282	274	269	264	258	255	253	251	250	249	248	247	246	246	245
6	3	323.57	265	258	252	247	242	240	238	236	235	234	233	232	231	231	230

Reduction cost for: <i>d</i> = 1; <i>g</i> = 1 and palm refined oil process	57.85	64.68	69.73	74.68	79.53	82.33	84.29	85.80	87.02	88.05	88.94	89.73	90.42	91.05	91.63
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Appendix 6.18. Indigenous settlements

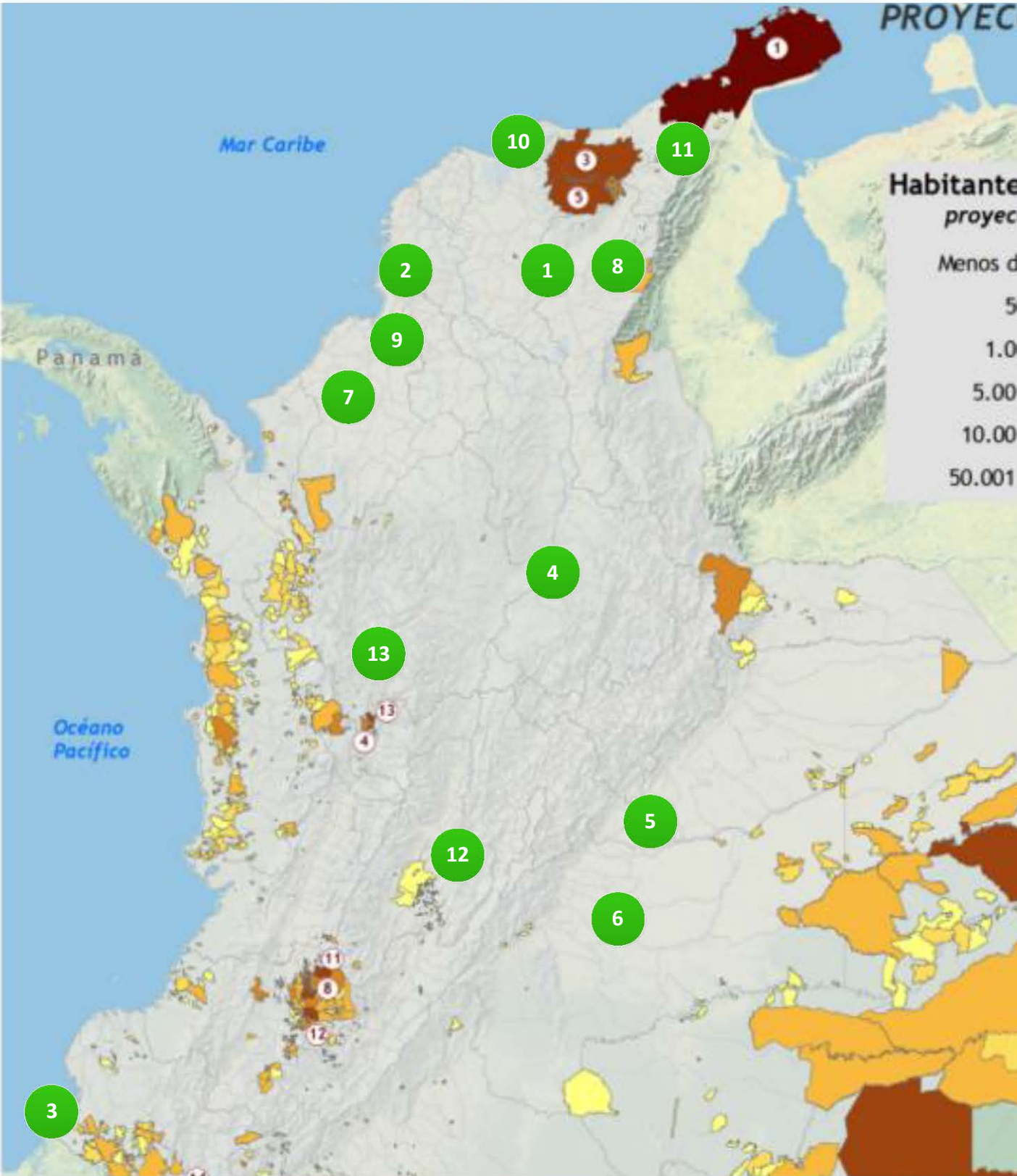


Figure 1 Raw material sources location related to indigenous settlements

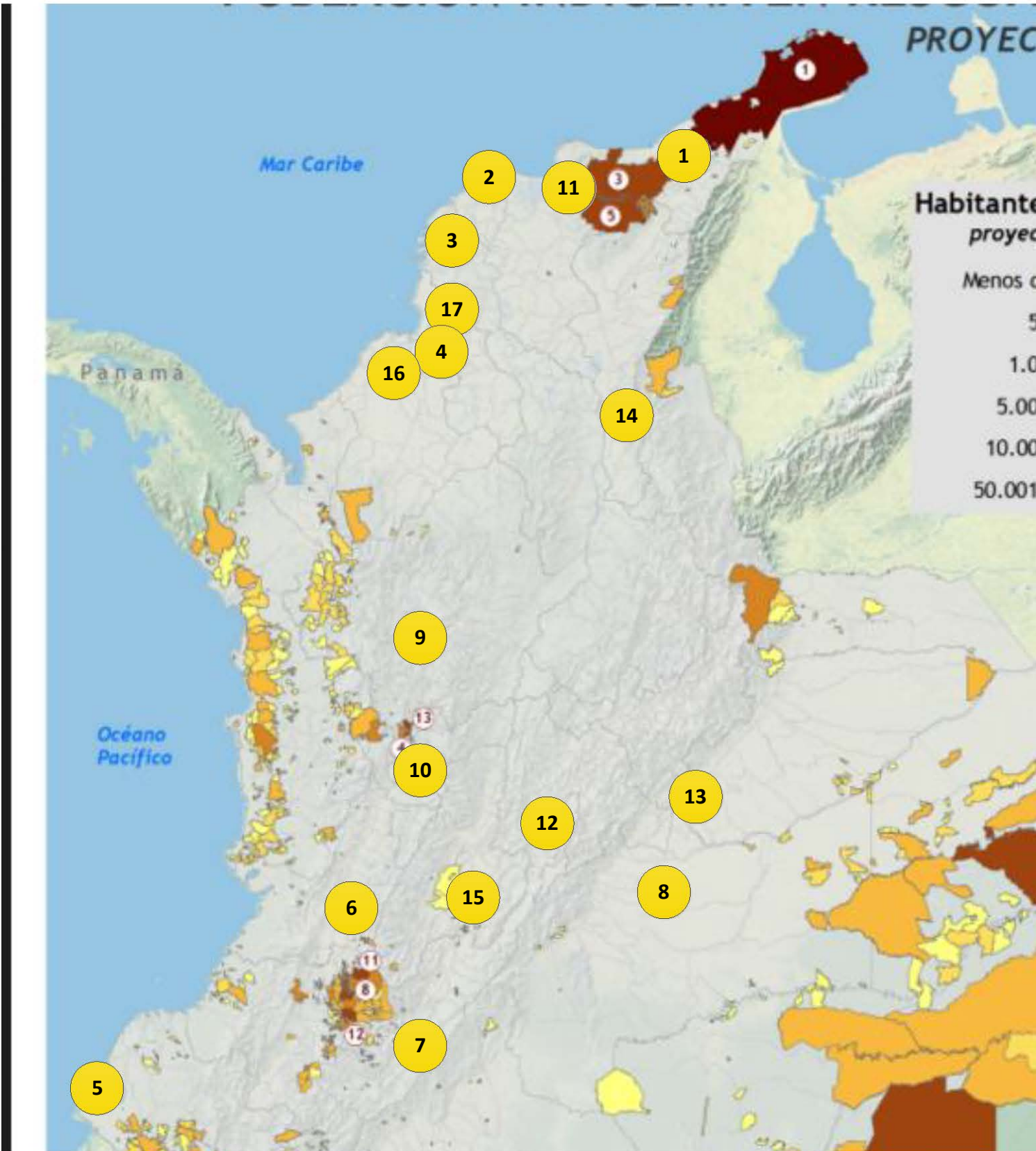


Figure 2 Potential pretreatment plants location related to indigenous settlements

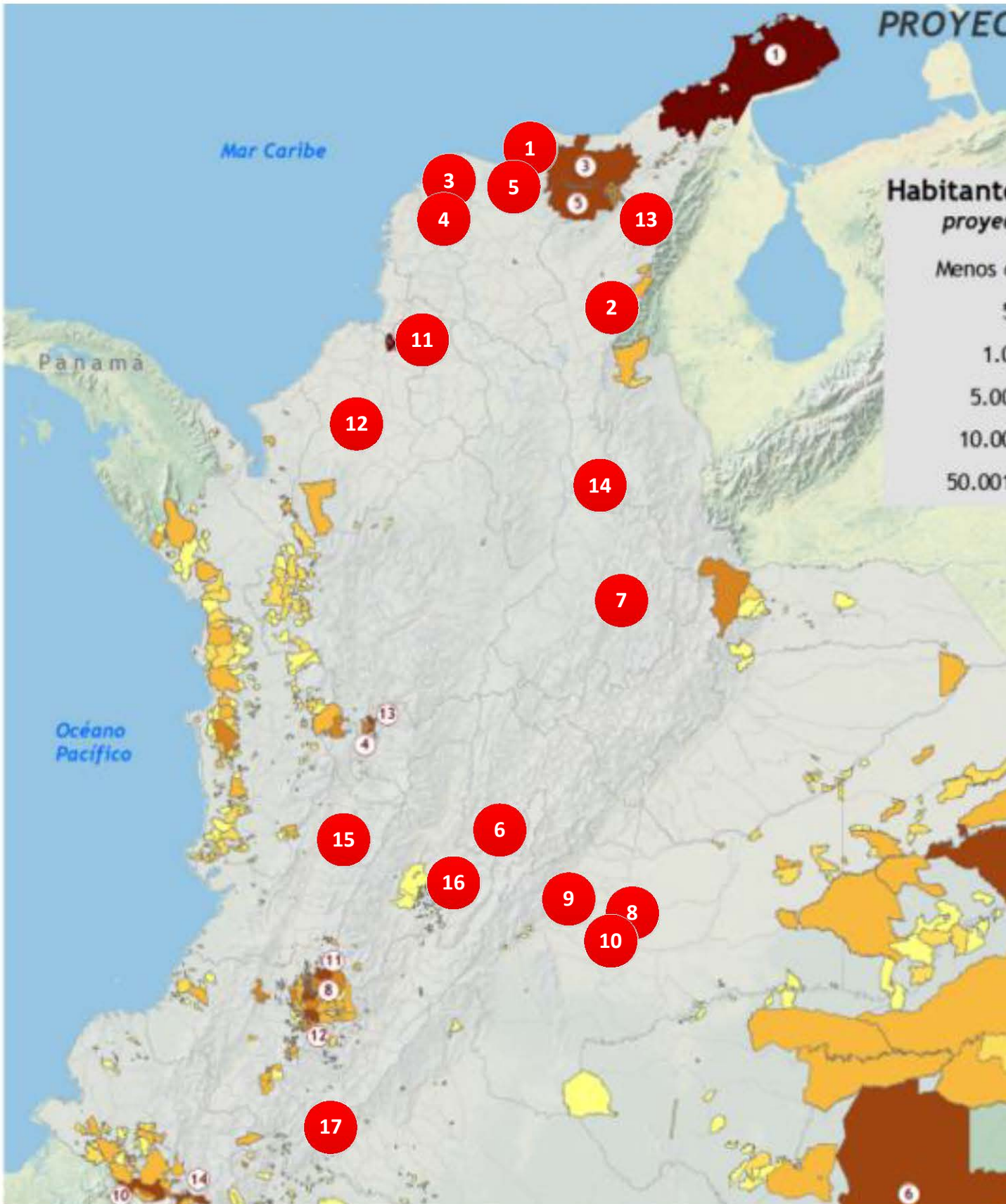


Figure 3 Potential principal production plants location related to indigenous settlements

Appendix 6.19. Workers estimation

Raw material stage

In the case of palm, there are 7 hectares worked by one direct worker and 14 hectare per indirect worker (Fedebiocombustibles 2017).

However, for jatropha the related information considers that depending on extraction method it will be required 18 day-workers per hectare for the manual extraction and 16 day-workers per hectare for the electrical extraction, compared with 10 day-workers per hectare for the palm (Gaona Currea 2009).

Assuming the same proportion between jatropha and palm day-workers, presented in the research carried out by Gaona Currea (2009), the total amount of workers required by raw material type can be estimated as.

Palm

$$\frac{1 \text{ direct worker}}{7 \text{ hectares}} \rightarrow \frac{0.1429 \text{ direct worker}}{1 \text{ hectare}} \text{ and } \frac{10 \text{ day - worker}}{1 \text{ hectare}}$$

Jatropha oil by manual extraction

$$\frac{X \text{ direct worker}}{1 \text{ hectare}} \text{ and } \frac{18 \text{ day - worker}}{1 \text{ hectare}}$$

Then:

$$\frac{X \text{ direct worker}}{1 \text{ hectare}} = \frac{\left(\frac{18 \text{ day - worker}}{1 \text{ hectare}} * \frac{0.1429 \text{ direct worker}}{1 \text{ hectare}} \right)}{\frac{10 \text{ day - worker}}{1 \text{ hectare}}} = 0.2572 \frac{\text{direct worker}}{1 \text{ hectare}}$$

And

$$\frac{0.2572 \text{ direct worker}}{1 \text{ hectare}} = \frac{1 \text{ direct worker}}{3.888 \text{ hectare}}$$

Jatropha oil by electrical extraction

$$\frac{X \text{ direct worker}}{1 \text{ hectare}} \text{ and } \frac{16 \text{ day - worker}}{1 \text{ hectare}}$$

Then:

$$\frac{X \text{ direct worker}}{1 \text{ hectare}} = \frac{\left(\frac{16 \text{ day - worker}}{1 \text{ hectare}} * \frac{0.1429 \text{ direct worker}}{1 \text{ hectare}} \right)}{\frac{10 \text{ day - worker}}{1 \text{ hectare}}} = 0.2286 \frac{\text{direct worker}}{1 \text{ hectare}}$$

And

$$\frac{0.2286 \text{ direct worker}}{1 \text{ hectare}} = \frac{1 \text{ direct worker}}{4.374 \text{ hectare}}$$

Following the same procedure table 75 was constructed.

Table 75 Amount of workers at raw material stage (workers /Ha)

Raw material type	Direct	Indirect	Direct	Indirect
	Ha/Worker	Ha/Worker	Worker/Ha	Worker/Ha
<i>Palm oil</i>	7.0	14.0	0.1429	0.0714
<i>Jatropha oil by manual extraction</i>	3.9	7.8	0.2571	0.1286
<i>Jatropha oil by electrical extraction</i>	4.4	8.8	0.2286	0.1143

Then, these values should be divided by the rate crude oil/ha to obtain the values presented in table 76.

Table 76 Employment opportunities at raw material stage (Workers / crude oil t)

<i>i</i>	<i>n</i>	$DWork_{RM,i,n}$ (Worker/t)	$IWork_{RM,i,n}$ (Worker/t)
1	1	0.04	0.02
2	1	0.07	0.03
2	2	0.22	0.11
2	3	0.17	0.08
3	1	0.10	0.05
4	1	0.05	0.03
5	1	0.04	0.02
6	1	0.04	0.02
7	2	0.22	0.11
7	3	0.17	0.08
8	2	0.22	0.11
8	3	0.17	0.08
9	2	0.22	0.11
9	3	0.17	0.08
10	1	0.03	0.02
10	2	0.22	0.11
10	3	0.17	0.08
11	2	0.22	0.11
11	3	0.17	0.08
12	2	0.22	0.11
12	3	0.17	0.08
13	2	0.22	0.11
13	3	0.17	0.08

Pretreatment plants

To determine the direct and indirect amount of workstations at pretreatment plants, the estimation was based on research carried out by Muñoz Baena (2013), who conducted a techno-economic study for a biodiesel plant with 100,000 t/year production capacity, including the pretreatment stage in the production process.

It is supposed that the number of operators varies according to the capacity of the production plants, but the other types of workers are independent on capacity (Example: manager, administrative workers, security chief and assistant). It is also assumed that the pretreatment plant will have the same personnel requirements as the biodiesel plant presented in such research (Muñoz Baena 2013).

Then, the direct workers required independently of production capacity are (8):

- 1 Director
- 2 Administrative staff
- 1 Store worker
- 1 Electrician
- 1 Worker to installation control
- 1 Security manager
- 1 Assistant security manager

And the direct workers required by production capacity are the production operators.

There are 5 production operators required for a production capacity plant of 100,000 t/year. Then, it is assumed that one production operator will be required each 20,000 t/year.

The indirect workers required are 2 persons for cleaning service and four persons in surveillance service.

Finally, table 77 summarizes these assumptions and estimations to present the amount of workers required by production capacity at pretreatment plants.

Table 77 Employment opportunities at pretreatment plants

	Production capacity (t/year)		
	80,000	80,000	80,000
<i>DWork_{pret,c,f}</i>	10	12	14
<i>IWork_{pret,c,f}</i>	6	6	6

Appendix 6.20. Water degradation for raw materials cultivation

Based on the information presented in table 58, on research carried out by BID and MMEC (2012), the average of nitrates, phosphorus and phosphates has been estimated as follows (Considering 21.38 tons of crude oil by 100 tons of fresh palm fruit):

$$\text{Nitrates} = 0.0871 \text{ t nitrate / ha palm}$$

$$\text{Phosphorus} = 0.0138 \text{ t phosphorus / ha palm}$$

$$\text{Phosphates} = 0.0118 \text{ t phosphates / ha palm}$$

Then, these values are divided by the production rate for palm crude oil by hectare to obtain the values presented in table 78.

Table 78 Water discharges related to palm crude oil (t/ t palm crude oil)

<i>n</i>	Nitrates (NO ₃)	Phosphorus (P)	Phosphates (P)
1	2.11%	0.33%	0.29%
2	4.09%	0.65%	0.55%
3	5.91%	0.94%	0.80%
4	3.17%	0.50%	0.43%
5	2.58%	0.41%	0.35%
6	2.45%	0.39%	0.33%
7	0.00%	0.00%	0.00%
8	0.00%	0.00%	0.00%
9	0.00%	0.00%	0.00%
10	2.02%	0.32%	0.27%
11	0.00%	0.00%	0.00%
12	0.00%	0.00%	0.00%
13	0.00%	0.00%	0.00%

Then, to estimate the values for jatropha crude oil, the estimation is based on researches carried out by BID and MMEC (2012) and Quispe et al. (2009). This last presents the following data:

Table 79 Water discharges in Peru due palm cultivation stages

	Ton/Ha
Nitrates	1.66%
Phosphorus	0.07%
Phosphates	0.04%

Table 80 Water discharges in Peru due jatropha cultivation stages

	Ton/Ha
Nitrates	1.87%
Phosphorus	0.09%
Phosphates	0.04%

The same proportion will be assumed in Colombia; then, the calculations are the follows:

$$\text{Nitrates} = \frac{0.0871 \text{ palm col} * 1.87\% \text{ jatropha peru}}{1.66\% \text{ palm peru}} = 9.81\% \text{ t nitrate / ha jatropha}$$

$$\text{Phosphorus} = \frac{0.0138 \text{ palm col} * 0.09\% \text{ jatropha peru}}{0.07\% \text{ palm peru}} = 1.83\% \text{ t phosphorus / ha jatropha}$$

$$\text{Phosphates} = \frac{0.0118 \text{ palm col} * 0.04\% \text{ jatropha peru}}{0.04\% \text{ palm peru}} = 1.18\% \text{ t phosphates / ha jatropha}$$

Then, these values are divided by the production rate for jatropha crude oil by hectare to obtain the values presented in table 81.

Table 81 Water pollution by type

n	Jatropha oil availability obtained by manual-extraction (t/Year)			Jatropha oil availability obtained by electric press (t/Year)		
	Nitrates (NO ₃)	Phosphorus (P)	Phosphates (P)	Nitrates (NO ₃)	Phosphorus (P)	Phosphates (P)
1	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%
2	8.46%	1.57%	1.02%	7.06%	1.57%	0.85%
3	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%
4	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%
5	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%
6	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%
7	8.46%	1.57%	1.02%	7.06%	1.57%	0.85%
8	8.46%	1.57%	1.02%	7.06%	1.57%	0.85%
9	8.46%	1.57%	1.02%	7.06%	1.57%	0.85%
10	8.46%	1.57%	1.02%	7.06%	1.57%	0.85%
11	8.46%	1.57%	1.02%	7.06%	1.57%	0.85%
12	8.46%	1.57%	1.02%	7.06%	1.57%	0.85%
13	8.46%	1.57%	1.02%	7.06%	1.57%	0.85%

Appendix 6.21. Fuel consumption estimation (t diesel / t product flow)

Table 82 Fuel consumption to transport products between suppliers and pretreatment plants

		Pretreatment Plant Localization																
		1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
Supplier Localization	1	0.0075	0.0124	0.0123	0.0133	0.0848	0.0511	0.0545	0.0476	0.0343	0.0412	0.0034	0.0448	0.0435	0.0106	0.0443	0.0168	0.0105
	2	0.0197	0.0067	0.0000	0.0074	0.0820	0.0483	0.0067	0.0618	0.0289	0.0384	0.0145	0.0571	0.0557	0.0229	0.0565	0.0103	0.0060
	3	0.0909	0.0870	0.0082	0.0748	0.0000	0.0342	0.0313	0.0646	0.0535	0.0440	0.0887	0.0525	0.0661	0.0748	0.0444	0.0740	0.0778
	4	0.0258	0.0326	0.0326	0.0337	0.0663	0.0326	0.0360	0.0311	0.0157	0.0227	0.0197	0.0263	0.0250	0.0098	0.0257	0.0300	0.0308
	5	0.0497	0.0564	0.0564	0.0052	0.0658	0.0321	0.0312	0.0101	0.0328	0.0268	0.0475	0.0139	0.0000	0.0336	0.0210	0.0509	0.0546
	6	0.0555	0.0623	0.0623	0.0502	0.0643	0.0306	0.0297	0.0000	0.0313	0.0253	0.0534	0.0124	0.0101	0.0394	0.0195	0.0494	0.0605
	7	0.0243	0.0156	0.0103	0.0035	0.0738	0.0401	0.0541	0.0493	0.0207	0.0302	0.0203	0.0445	0.0507	0.0274	0.0439	0.0000	0.0064
	8	0.0052	0.0199	0.0199	0.0210	0.0085	0.0514	0.0005	0.0499	0.0346	0.0415	0.0110	0.0451	0.0438	0.0110	0.0446	0.0245	0.0180
	9	0.0186	0.0099	0.0052	0.0023	0.0770	0.0433	0.0573	0.0524	0.0239	0.0334	0.0145	0.0477	0.0546	0.0217	0.0471	0.0058	0.0007
	10	0.0115	0.0074	0.0129	0.0184	0.0929	0.0592	0.0625	0.0576	0.0423	0.0493	0.0047	0.0529	0.0515	0.0187	0.0523	0.0219	0.0155
	11	0.0038	0.0169	0.0225	0.0246	0.0941	0.0604	0.0064	0.0588	0.0435	0.0505	0.0145	0.0541	0.0527	0.0199	0.0535	0.0280	0.0216
	12	0.0454	0.0521	0.0521	0.0401	0.0491	0.0153	0.0145	0.0156	0.0211	0.0101	0.0432	0.0035	0.0171	0.0293	0.0042	0.0392	0.0050
	13	0.0397	0.0332	0.0284	0.0211	0.0536	0.0199	0.0357	0.0308	0.0005	0.0101	0.0375	0.0260	0.0323	0.0236	0.0254	0.0202	0.0240

Table 83 Fuel consumption to transport products between pretreatment plants and principal plants location

		Principal Plant Localization																
		1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
Pretreatment Plant Localization	1	0.0134	0.0056	0.0181	0.0185	0.0136	0.0436	0.0249	0.0556	0.0513	0.0557	0.0155	0.0237	0.0015	0.0194	0.0491	0.0467	0.0641
	2	0.0073	0.0199	0.0025	0.0016	0.0072	0.0516	0.0330	0.0623	0.0604	0.0624	0.0064	0.0147	0.0190	0.0257	0.0451	0.0522	0.0709
	3	0.0128	0.0199	0.0093	0.0082	0.0127	0.0516	0.0330	0.0623	0.0604	0.0624	0.0045	0.0094	0.0208	0.0257	0.0403	0.0521	0.0709
	4	0.0183	0.0210	0.0144	0.0136	0.0182	0.0396	0.0341	0.0502	0.0483	0.0504	0.0058	0.0026	0.0219	0.0268	0.0330	0.0401	0.0589
	5	0.0934	0.0085	0.0950	0.0955	0.0927	0.0566	0.0067	0.0643	0.0623	0.0644	0.0805	0.0747	0.0914	0.0766	0.0416	0.0491	0.0275
	6	0.0594	0.0514	0.0613	0.0618	0.0590	0.0228	0.0330	0.0306	0.0286	0.0307	0.0468	0.0409	0.0577	0.0429	0.0079	0.0153	0.0152
	7	0.0630	0.0005	0.0647	0.0651	0.0623	0.0220	0.0364	0.0297	0.0278	0.0299	0.0622	0.0550	0.0611	0.0463	0.0202	0.0144	0.0038
	8	0.0580	0.0499	0.0598	0.0060	0.0574	0.0118	0.0315	0.0000	0.0029	0.0002	0.0573	0.0501	0.0562	0.0413	0.0258	0.0156	0.0333
	9	0.0427	0.0346	0.0360	0.0352	0.0421	0.0206	0.0161	0.0313	0.0293	0.0315	0.0273	0.0215	0.0409	0.0260	0.0116	0.0212	0.0399
	10	0.0496	0.0415	0.0514	0.0519	0.0491	0.0150	0.0231	0.0253	0.0234	0.0254	0.0369	0.0311	0.0478	0.0330	0.0021	0.0101	0.0249
	11	0.0046	0.0110	0.0069	0.0073	0.0045	0.0427	0.0241	0.0534	0.0514	0.0535	0.0112	0.0194	0.0119	0.0168	0.0469	0.0433	0.0620
	12	0.0513	0.0452	0.0550	0.0555	0.0527	0.0047	0.0267	0.0124	0.0105	0.0126	0.0525	0.0453	0.0514	0.0366	0.0137	0.0035	0.0212
	13	0.0521	0.0438	0.0537	0.0542	0.0513	0.0133	0.0254	0.0101	0.0083	0.0103	0.0512	0.0516	0.0501	0.0353	0.0272	0.0171	0.0348
	14	0.0186	0.0110	0.0208	0.0213	0.0185	0.0288	0.0102	0.0394	0.0375	0.0396	0.0184	0.0265	0.0172	0.0029	0.0329	0.0293	0.0481
	15	0.0528	0.0446	0.0545	0.0549	0.0521	0.0118	0.0261	0.0195	0.0176	0.0197	0.0520	0.0448	0.0509	0.0360	0.0131	0.0042	0.0138
	16	0.0218	0.0245	0.0193	0.0171	0.0217	0.0387	0.0304	0.0494	0.0474	0.0496	0.0093	0.0009	0.0254	0.0303	0.0321	0.0392	0.0580
	17	0.0154	0.0180	0.0116	0.0108	0.0153	0.0000	0.0312	0.0605	0.0585	0.0606	0.0029	0.0056	0.0190	0.0239	0.0359	0.0503	0.0690

Table 84 Fuel consumption to transport products between principal production plants and final product markets

		Final Product Markets Localization																		
		1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19
Principal Plant Localization	1	0.0417	0.0532	0.0218	0.0161	0.0113	0.0051	0.0002	0.0127	0.0476	0.0406	0.0533	0.0503	0.0473	0.0567	0.0671	0.0473	0.0517	0.0499	0.0268
	2	0.0341	0.0456	0.0245	0.0187	0.0212	0.0177	0.0156	0.0031	0.0400	0.0330	0.0458	0.0428	0.0397	0.0491	0.0595	0.0397	0.0441	0.0423	0.0192
	3	0.0356	0.0470	0.0179	0.0122	0.0058	0.0001	0.0052	0.0150	0.0498	0.0429	0.0556	0.0526	0.0496	0.0590	0.0694	0.0496	0.0540	0.0522	0.0291
	4	0.0348	0.0462	0.0172	0.0114	0.0058	0.0008	0.0056	0.0155	0.0050	0.0434	0.0561	0.0531	0.0500	0.0595	0.0699	0.0500	0.0544	0.0527	0.0296
	5	0.0417	0.0531	0.0217	0.0160	0.0113	0.0050	0.0002	0.0126	0.0475	0.0406	0.0053	0.0050	0.0472	0.0566	0.0670	0.0472	0.0516	0.0499	0.0267
	6	0.0202	0.0280	0.0387	0.0419	0.0529	0.0495	0.0473	0.0428	0.0024	0.0087	0.0077	0.0195	0.0110	0.0163	0.0267	0.0132	0.0149	0.0158	0.0248
	7	0.0157	0.0271	0.0304	0.0319	0.0343	0.0308	0.0287	0.0242	0.0215	0.0146	0.0273	0.0243	0.0213	0.0307	0.0410	0.0213	0.0256	0.0239	0.0062
	8	0.0308	0.0368	0.0494	0.0525	0.0636	0.0601	0.0580	0.0535	0.0104	0.0171	0.0044	0.0174	0.0187	0.0241	0.0344	0.0245	0.0227	0.0247	0.0300
	9	0.0289	0.0349	0.0475	0.0506	0.0617	0.0582	0.0560	0.0515	0.0084	0.0151	0.0026	0.0156	0.0168	0.0221	0.0325	0.0226	0.0207	0.0227	0.0280
	10	0.0310	0.0370	0.0496	0.0527	0.0064	0.0060	0.0582	0.0537	0.0105	0.0173	0.0046	0.0175	0.0189	0.0242	0.0346	0.0247	0.0228	0.0249	0.0301
	11	0.0269	0.0383	0.0093	0.0036	0.0059	0.0081	0.0125	0.0125	0.0474	0.0404	0.0531	0.0501	0.0471	0.0565	0.0669	0.0366	0.0397	0.0377	0.0266
	12	0.0211	0.0325	0.0009	0.0049	0.0122	0.0165	0.0209	0.0207	0.0401	0.0367	0.0459	0.0464	0.0399	0.0493	0.0597	0.0308	0.0339	0.0318	0.0348
	13	0.0404	0.0518	0.0254	0.0197	0.0221	0.0168	0.0122	0.0039	0.0463	0.0393	0.0520	0.0491	0.0460	0.0604	0.0658	0.0460	0.0503	0.0486	0.0255
	14	0.0256	0.0370	0.0303	0.0246	0.0270	0.0236	0.0215	0.0170	0.0314	0.0245	0.0372	0.0342	0.0311	0.0405	0.0509	0.0311	0.0355	0.0338	0.0107
	15	0.0120	0.0121	0.0321	0.0352	0.0436	0.0536	0.0515	0.0470	0.0172	0.0241	0.0216	0.0346	0.0073	0.0176	0.0293	0.0038	0.0025	0.0014	0.0290
	16	0.0207	0.0216	0.0392	0.0424	0.0535	0.0500	0.0479	0.0434	0.0070	0.0139	0.0115	0.0244	0.0035	0.0088	0.0192	0.0130	0.0074	0.0094	0.0253
	17	0.0394	0.0350	0.0580	0.0611	0.0722	0.0687	0.0666	0.0621	0.0247	0.0316	0.0292	0.0421	0.0198	0.0094	0.0064	0.0267	0.0229	0.0243	0.0440

Table 84 Fuel consumption to transport products between principal production plants and final product markets (Continuation)

		Final Product Markets Localization			
		20	21	22	23
Principal Plant Localization	1	0.0313	0.0665	0.0788	0.0726
	2	0.0237	0.0589	0.0071	0.0649
	3	0.0335	0.0688	0.0811	0.0748
	4	0.0340	0.0069	0.0815	0.0753
	5	0.0312	0.0664	0.0787	0.0725
	6	0.0293	0.0303	0.0426	0.0321
	7	0.0155	0.0404	0.0527	0.0465
	8	0.0377	0.0380	0.0503	0.0399
	9	0.0358	0.0361	0.0484	0.0379
	10	0.0379	0.0382	0.0505	0.0400
	11	0.0310	0.0542	0.0665	0.0724
	12	0.0392	0.0484	0.0607	0.0651
	13	0.0299	0.0652	0.0775	0.0071
	14	0.0099	0.0503	0.0626	0.0564
	15	0.0383	0.0154	0.0277	0.0286
	16	0.0347	0.0228	0.0351	0.0246
	17	0.0534	0.0076	0.0138	0.0066

Table 85 Fuel consumption to transport products between pretreatment plants and product markets

		Intermediate Product Market Localization				
		1	2	3	4	5
Pretreatment Plant Localization	1	0.0180	0.0457	0.0134	0.0514	0.0581
	2	0.0025	0.0520	0.0074	0.0577	0.0538
	3	0.0095	0.0520	0.0129	0.0577	0.0491
	4	0.0140	0.0404	0.0184	0.0461	0.0417
	5	0.0950	0.0556	0.0928	0.0601	0.0330
	6	0.0617	0.0223	0.0595	0.0267	0.0015
	7	0.0648	0.0212	0.0626	0.0256	0.0125
	8	0.0599	0.0103	0.0577	0.0044	0.0317
	9	0.0356	0.0214	0.0421	0.0271	0.0204
	10	0.0514	0.0164	0.0492	0.0211	0.0110
	11	0.0072	0.0432	0.0049	0.0490	0.0556
	12	0.0551	0.0038	0.0528	0.0083	0.0196
	13	0.0524	0.0118	0.0502	0.0057	0.0331
	14	0.0211	0.0292	0.0188	0.0349	0.0415
	15	0.0546	0.0110	0.0524	0.0154	0.0191
	16	0.0175	0.0395	0.0219	0.0452	0.0408
	17	0.0112	0.0502	0.0155	0.0559	0.0446

Appendix 6.22. Energy balance parameters estimation

Energy expenditure to transport the products

To calculate this value is necessary to know the diesel consumption in trucks transportation. On average spending of $0.06 \text{ USD} / (t * km)$ is observed for fuel concept (MINTRANSPORTE 2017). And the average price for diesel in 2015 is $1,204.53 \text{ USD}/t$, or $3.87569347 \text{ USD}/gal$ (UPME 2017).

Then, the consumption of diesel per ton transported and kilometer travel can be calculated as follows:

$$0.06 \frac{\text{USD}}{t * km} * \frac{1 t \text{ diesel}}{1,204.53 \text{ USD}} = 4.9812 * 10^{-5} \frac{t \text{ diesel}}{t * km}$$
$$0.06 \frac{\text{USD}}{t * km} * \frac{1 gal \text{ diesel}}{3.87569347 \text{ USD}} = \frac{0.0154811 gal \text{ diesel}}{t * km}$$

After, the ACPM calorific value is required to finally calculate the parameter δ . Its calorific value is $133,230.5 \text{ BTU}/gal$ (Ministerio de Minas y Energía and UPME 2009) and $1 \text{ MJ} = 947.817 \text{ BTU}$. Therefore, the conversion is:

$$\frac{133,230.5 \text{ BTU}}{gal} * \frac{1 \text{ MJ}}{947.817 \text{ BTU}} = 140.5656 \frac{\text{MJ}}{gal}$$

Finally, the energy consumption by transport is:

$$\delta = 0.0154811 \frac{gal}{t * km} * 140.5656 \frac{\text{MJ}}{gal} = 2.1761 \frac{\text{MJ}}{t * km}$$

Energy content for final products.

About final products, table 86 present the data found. For all end products, their characteristics are considered to be similar regardless of the type of raw materials used to obtain them. Since there are quality standards to be able to market these different products. Thus, the average value found in the literature for final products will be taken. For biodiesel, the calorific value will be $38,943.625 \text{ MJ}/t$. In the other hand, even though glycerol and aliphatic polymers will not be used for combustion, its value will be used to evaluate the energy generated. Thus, for glycerol it will be $\theta_{\alpha=3} = 22,744.7 \text{ MJ}/t$ and for polymer it is $\theta_{\alpha=2} = 26,866.7 \text{ MJ}/t$.

Table 86 Final products calorific value

Final Product	Value	Reference
Palm biodiesel	37.5 MJ/Kg	www.esru.strath.ac.uk/EandE/Web_sites/06-07/Biodiesel/experiments.html
	36.764 MJ/Kg	www.greencarcongress.com/2006/11/comparing_the_e.html
	39.866 MJ/Kg	“POSIBILIDADES OSIBILIDADES DEL BIODIÉSEL BIODIÉSEL DE PALMA y sus mezclas con diésel en Colombia” (https://publicaciones.fedepalma.org/index.php/palmas/article/download/1291/1291)
	40.025 MJ/Kg	“POSIBILIDADES OSIBILIDADES DEL BIODIÉSEL BIODIÉSEL DE PALMA y sus mezclas con diésel en Colombia” (https://publicaciones.fedepalma.org/index.php/palmas/article/download/1291/1291)
Jatropha Biodiesel	39.340 MJ/Kg	www.greencarcongress.com/2006/11/comparing_the_e.html
	39.230 MJ/Kg	Comparison of palm oil, jatropha curcas and calophyllum inophyllum for biodiesel: a review
	39.594 MJ/Kg	A study on the performance and emission of a diesel engine fueled with jatropha biodiesel oil and its blends
	39.23 MJ/Kg	Biodiesel production from jatropha oil (jatropha curcas) with hijf free fatty acids: An optimized process
Crude Glycerol	25.3 MJ/Kg	www.esru.strath.ac.uk/EandE/Web_sites/06-07/Biodiesel/experiments.html
	22 MJ/Kg	Effectiveness and mechanism of crude glycerol on the biofuel production from swine manure through hydrothermal pyrolysis
	20.934 MJ/Kg	The glycerine glut: Options for the value-added conversion of crude glycerol resulting from biodiesel production
Polyester or Aliphatic polyester	25-30 MJ/Kg	Fire.nist.gov/bfr/pubs/fire86/PDF/f86012.pdf
	(Real) 25.6 MJ/Kg (Theoric) 24 Mj/Kg	www.hanserpublications.com/SampleChapters/9781569904619_9781569904619_Engineering%20Biopolymers_Endres_Siebert-Raths.pdf

Energy expenditure by transformation

Pretreatment plants

Due lack information it is assumed that the consumed energy in physical refining will be similar to energy consumption in esterification process. Then, based on research carried out by Basto Aluja (2016), the pretreatment process includes the equipment detailed in table 87.

Table 87 Equipment power (kJ/h) for esterification

Equipment		Pretreatment capacity (Ton/year)			
		40,000	80,000	120,000	
Reactors	RE-100	3,762.87	7,525.73	11 288,60	
Heat exchangers	H-100	267,480.00	534,960.00	802 440,00	
	H-101	240,732.00	481,464.00	722 196,00	
Mixers	MX-100	297.60	595.20	892,80	
Pumps	P-100	254.92	509.84	764,76	
	P-101	216.68	433.36	650,05	
	P-102	242.17	484.35	726,52	
Towers	TW-100	Condenser,	860,579.63	1 721 159,27	2 581 738,90
		Reboiler	480,656.59	961 313,17	1 441 969,76
Total (kJ/hr)		1 854 222,46	3,708,444.93	5,562,667.39	

The refined oil flows for each production capacity are presented in table 88.

Table 88 Refined oil flows

	Capacity (ton/year)		
	40,000	80,000	120,000
Palm crude oil (t/hr)	5.05	10.10	15.15

Thus, the consumed energy related to equipment power, to realize the pretreatment process for the palm crude oil, can be summarized in table 89.

Table 89 Consumed energy related to equipment power (MJ/ t oil)

	Capacity (ton/year)		
	40,000	80,000	120,000
Energy consumption (MJ) per palm crude oil ton	367.17	367.14	367.14

Also, methanol used in pretreatment process can be considered in the estimation. Table 90, presents the percentage of methanol used by palm crude oil weight.

Table 90 Methanol used by palm crude oil weight

	Capacity (Ton/year)		
	40,000	80,000	120,000
Palm crude oil (Kg/hr)	5,050.50	10,101.10	15,151.51
Methanol flow (Kg/hr)	4.93	9.86	14.79
Methanol/Palm crude oil (% weight/weight)	0.0976%	0.0976%	0.0976%

Considering the specific heat for methanol as 23 MJ/kg (Laby and Kaye 1995); the energy consumed at pretreatment process related to methanol can be estimated as:

$$23 \frac{MJ}{kg \text{ Meth}} * 0.000976 \frac{kg \text{ meth}}{kg \text{ palm}} = 0.0225 \frac{MJ}{kg \text{ palm oil}} * \frac{1,000 \text{ kg palm oil}}{1 \text{ t palm oil}}$$

$$= 22.5 \frac{Mj}{t \text{ palm crude oil}}$$

And the energy consumed in palm crude oil pretreatment can be summarized in table 91.

Table 91 Energy consumed in palm crude oil pretreatment

Raw material	Pretreatment capacity (t/year)		
	40 000	80 000	120 000
Palm crude oil (1)	389,67	389,64	389,64

Then to estimate the energy consumed for jatropha crude oil pretreatment, the production cost estimated in Appendix 6.5 will be utilized. Considering that changes in production cost are linked to equipment energy consumption and materials required for the pretreatment process. Thus, table 92 present the estimation for energy consumption for jatropha pretreatments.

Table 92 estimation for energy consumption for jatropha pretreatments

	40,000 t/year	80,000 t/year	120,000 t/year
(1) Palm oil	42.42 USD/t → 389.67 MJ/t	38.96 → 389.64 MJ/t	36.36 → 389.64 MJ/t
(2) Jatropha oil by manual extraction	$=(39.81 * 389.67) / 42.42$ =365.70	$=(36.56 * 389.64) / 38.96$ =365.64	$=(34.12 * 389.64) / 36.36$ =365.64
(3) Jatropha oil by electrical extraction	$=(39.81 * 389.67) / 42.42$ =365.70	$=(36.56 * 389.64) / 38.96$ =365.64	$=(34.12 * 389.64) / 36.36$ =365.64

Principal Plants:

In order to estimate the energy consumed related to equipment power at principal plants the equipment required for the biodiesel production without esterification is detailed as follows (Basto Aluja 2016):

Conventional process

Reactors: **RT-100 RT-101 RN-100 RN-101**
 Heat exchangers **H-102 H-103 H-104 H-105**
 Mixers **MX-101 MX-102 MX-103 MX-104 MX-105 MX-106**
 Decanters **D-100 D-102**
 Centrifuge **C-100**
 Pumps **P-102 P-103**
 Splitters **SP-100 SP-101**
 Towers **TB-100 TG-100 TW-100 TW-101**
 Extractor/Reactor **W-100**

Co-current process

Reactors **RT-100 RT-101 RN-100 RN-101**
 Heat exchangers **H-102 H-103 H-104 H-105**
 Mixers **MX-101 MX-102 MX-103 MX-104 MX-105 MX-106**
 Decanters **D-100 D-102**
 Centrifuge **C-100**
 Pumps **P-102 P-103**
 Splitters **SP-100 SP-101**
 Towers **TB-100 TG-100 TW-100 TW-101**
 Extractor/Reactor **W-100**

Count-current process

Reactors **RT-100 RN-100 RN-101**
 Heat exchangers **H-102 H-103 H-104 H-105**
 Mixers **MX-101 MX-102 MX-103 MX-104 MX-105 MX-106**
 Centrifuge **C-100**
 Pumps **P-102 P-103**
 Splitters **SP-100 SP-101**
 Towers **TB-100 TG-100 TW-100 TW-101**
 Extractor/Reactor **W-100**

Thus, based on research carried out by Basto Aluja (2016) and the previous equipment detail, table summarized the equipment power requirements by technology and production capacity.

Table 93 Equipment power requirements by technology and production capacity

Technology	Energy consumption	Production capacity (t/year)		
		40,000	80,000	120,000
Conventional	TOTAL (KJ/hr)	10,633,994.5	18,985,689.6	30,337,567.4
	TOTAL (MJ/Ton refined oil entering)	2,105.7	1,879.6	2,002.3
Co-current	TOTAL (KJ/hr)	8,808,027.4	16,619,402.4	26,938,955.4
	TOTAL (MJ/Ton refined oil entering)	1,744.2	1,645.3	1,778.0
Count-current	TOTAL (KJ/hr)	7,491,629.1	14,768,236.0	24,925,058.3
	TOTAL (MJ/Ton refined oil entering)	1,483.5	1,462.1	1,645.1

Then, in order to include the methanol used in the transesterification process, based on research carried out by Basto Aluja (2016), table 94 summarized the methanol flows to determine the percentage of methanol used by palm oil weight.

Table 94 Percentage of methanol used by palm oil weight

	Capacity (Ton/year)		
	40,000	80,000	120,000
Palm oil flow (Kg/hr)	5,050.50	10,101.10	15,151.51
Conventional			
Methanol flow (Kg/hr)	1,358.96	2,717.92	4,076.88
Methanol/ Palm oil (Kg/Kg)	26.91%	26.91%	26.91%
Co-current			
Methanol flow (Kg/hr)	1,359.06	2,717.92	4,076.88
Methanol/ Palm oil (Kg/Kg)	26.91%	26.91%	26.91%
Count-Current			
Methanol flow (Kg/hr)	1,703.09	3,406.13	5,109.19
Methanol/ Palm oil (Kg/Kg)	33.72%	33.72%	33.72%

Therefore, the energy consumed related to methanol utilization at principal plants can be summarized in table 95 ($\frac{MJ}{t \text{ palm oil}}$).

Table 95 Energy consumed related to methanol utilization at principal plants

Technology	Capacity (Ton/year)		
	40,000	80,000	120,000
Conventional	=0.2691*23*1000= 6,188.71	6,188.65	6,188.71
Co-current	6,189.17	6,188.65	6,188.71
Count-current	7,755.88	7,755.69	7,755.75

Table was constructed by adding data in table and table (the energy consumed by the equipment).

Table 96 Energy consumptions by equipment and methanol flows (MJ/t refined oil)

Technology	Capacity (Ton/year)		
	40,000	80,000	120,000
Conventional	8,294.45	8,068.23	8,190.99
Conventional	7,933.33	7,833.97	7,966.68
Co-current	9,239.37	9,217.74	9,400.81

However, in order to estimate the energy consumption by all the production technologies mixes at principal plants, the energy consumed at the polymer production must to be considered. Bueno et al. (2014) estimate that 68,146 KJ are required to produce 1 kg of aliphatic polyester. Then, the production rates are required to estimate the energy to produce aliphatic polyester by refined oils, as presented in table 97.

Table 97 energy to produce aliphatic polyester by refined oils (MJ/ t refined oil)

Technology	Intermediate Products	Production rate polyester/refined oil	MJ/ t refined oil
1	Jatropha	0	0.00
2	Jatropha	0.1921	13,090.85
3	Jatropha	0	0.00
4	Jatropha	0.1946	13,261.21
5	Jatropha	0	0.00
6	Jatropha	0.1973	13,445.21
1	Palm	0	0.00
2	Palm	0.1859	12,668.34
3	Palm	0	0.00
4	Palm	0.1883	12,831.89
5	Palm	0	0.00
6	Palm	0.1909	13,009.07

Finally, table 98 summarizes the consumed energy by entering materials, technology and production capacity at principal plants.

Table 98 Consumed energy by entering materials, technology and production capacity at principal plants

Intermediate Products	Technology	Capacity (ton/year)		
		40,000	80,000	120,000
Jatropha	1	8,294.45	8,068.23	8,190.99
Jatropha	2	21,385.30	21,159.08	21,281.84
Jatropha	3	7,933.33	7,833.97	7,966.68
Jatropha	4	21,194.54	21,095.18	21,227.89
Jatropha	5	9,239.37	9,217.74	9,400.81
Jatropha	6	22,684.58	22,662.95	22,846.02
Palm	1	8,294.45	8,068.23	8,190.99
Palm	2	20,962.79	20,736.57	20,859.33
Palm	3	7,933.33	7,833.97	7,966.68
Palm	4	20,765.22	20,665.86	20,798.57
Palm	5	9,239.37	9,217.74	9,400.81
Palm	6	22,248.44	22,226.81	22,409.88

Appendix 6.23. CO₂-equivalent emissions

At raw materials cultivation stage

According to Romero Angulo (2014), when palm is developed in arable agroforestry areas, the CO₂ capture is 12.64 t CO₂ per palm hectare in Colombia. However, there is no available data in Colombia related to jatropha cultivation. Therefore a direct relation will be assumed with the jatropha cultivation information from Peru. Where, 8.1 t CO₂ are captured per palm hectare and 2.3 t CO₂ are captured per jatropha hectare (Quispe et al. 2009).

Then,

$$\frac{-8.1 \frac{\text{t CO}_2}{\text{ha palm}}}{-2.3 \frac{\text{t CO}_2}{\text{ha jatropha}}} \rightarrow \frac{-12.64 \frac{\text{t CO}_2}{\text{ha palm}}}{X \frac{\text{t CO}_2}{\text{ha jatropha}}} \Rightarrow \frac{-2.3 * -12.64}{-8.1} = -3.6 \frac{\text{CO}_2}{\text{ha jatropha}}$$

Therefore, these values assumed for Colombia should be divided by the yield for crude oil production per hectare, in Appendix 6.1, as presented in table 99.

Table 99 CO₂ capture at raw material cultivation stage (t CO₂ captured / crude oil t)

Raw material location (i)	Raw material type (n)		
	1	2	3
1	$=(-12.64/4.13)=-3.06$	0.00	0.00
2	-5.94	$=(-3.6/1.16)=-3.09$	$=(-3.6/1.39)=-2.58$
3	-8.59	0.00	0.00
4	-4.60	0.00	0.00
5	-3.75	0.00	0.00
6	-3.55	0.00	0.00
7	0.00	-3.09	-2.58
8	0.00	-3.09	-2.58
9	0.00	-3.09	-2.58
10	-2.93	-3.09	-2.58
11	0.00	-3.09	-2.58
12	0.00	-3.09	-2.58
13	0.00	-3.09	-2.58

However, there are CO₂ emissions related to oil extraction that should be also considered. The data presented by Bruinsma (2009) for the Peru study case concludes that 8.53 t CO₂ per hectare are emitted due palm crude oil extraction and 9.96 t CO₂ per hectare are emitted due jatropha crude oil extraction.

Then, due lack information for Colombia, using the same direct relation that in CO₂ captures estimation, it can be estimated that the CO₂ emissions related to oil extraction are the following:

$$\frac{-8.1 \frac{\text{t CO}_2}{\text{ha palm}}}{8.53 \frac{\text{t CO}_2}{\text{ha palm}}} \rightarrow \frac{-12.64 \frac{\text{t CO}_2}{\text{ha palm}}}{X \frac{\text{t CO}_2}{\text{ha palm}}} \Rightarrow \frac{8.53 * -12.64}{-8.1} = 13.31 \frac{\text{t CO}_2}{\text{ha palm}} \text{ in Colombia}$$

$$\frac{-8.1 \frac{\text{t CO}_2}{\text{ha palm}}}{9.96 \frac{\text{t CO}_2}{\text{ha jatropha}}} \rightarrow \frac{-12.64 \frac{\text{t CO}_2}{\text{ha palm}}}{X \frac{\text{t CO}_2}{\text{ha jatropha}}} \Rightarrow \frac{9.96 * -12.64}{-8.1} = 15.54 \frac{\text{t CO}_2}{\text{ha jatropha}} \text{ in Colombia}$$

Therefore, these values assumed for Colombia should be divided by the yield for crude oil production per hectare, in Appendix 6.1, as presented in table 100.

Table 100 CO₂ emission at raw material crude oil extraction stage (t CO₂/crude oil t)

Raw material location (<i>i</i>)	Raw material type (<i>n</i>)		
	1	2	3
1	$\frac{13.31}{4.13}$ =3.23	0.00	0.00
2	$\frac{13.31}{2.13}$ =6.25	$\frac{15.54}{1.16}$ =13.40	$\frac{15.54}{1.39}$ =11.18
3	$\frac{13.31}{1.47}$ =9.04	0.00	0.00
4	$\frac{13.31}{2.75}$ =4.84	0.00	0.00
5	$\frac{13.31}{3.38}$ =3.94	0.00	0.00
6	$\frac{13.31}{3.56}$ =3.74	0.00	0.00
7	0.00	13.40	11.18
8	0.00	13.40	11.18
9	0.00	13.40	11.18
10	$\frac{13.31}{4.32}$ =3.08	13.40	11.18
11	0.00	13.40	11.18
12	0.00	13.40	11.18
13	0.00	13.40	11.18

Pretreatments

Due the information related to physical refining carried out by Blanco Rodríguez (2007) does not includes environmental impact analysis, other research was found.

According to Quantis (2017), pretreatment plants generate 185.94 CO₂-equivalent kg per biodiesel ton (Considering a biodiesel rate production 0.95 per crude oil), which is equivalent to 176.64 CO₂-equivalent kg per palm crude oil ton.

It is assumed that these values are for a pretreatment plants with a production capacity 40,000 tons per year, due lack of information. Then, considering the energy expenditure estimated in Appendix 6.22 at pretreatment plants, a direct relation is assumed between the energy consumption and the CO₂-equivalent emissions generated, as presented in table

Table 101 CO₂-equivalent emissions at pretreatment plants (CO₂-equivalent t/ crude oil t)

	40,000 t/year	80,000 t/year	120,000 t/year
(1) Palm oil	389.67 MJ/t → 0.17664 t CO ₂ /t oil =0.1766	$\frac{(389.64 \cdot 17.66\%)}{389.67}$ =0.1766	$\frac{(389.64 \cdot 17.66\%)}{389.67}$ =0.1766
(2) Jatropha oil by manual extraction	$\frac{(365.70 \cdot 17.66\%)}{389.67}$ =0.1658	$\frac{(365.64 \cdot 17.66\%)}{389.67}$ =0.1657	$\frac{(365.64 \cdot 17.66\%)}{389.67}$ =0.1657
(3) Jatropha oil by electrical extraction	$\frac{(365.70 \cdot 17.66\%)}{389.67}$ =0.1658	$\frac{(365.64 \cdot 17.66\%)}{389.67}$ =0.1657	$\frac{(365.64 \cdot 17.66\%)}{389.67}$ =0.1657

Principal plants

Due the information related to biodiesel production carried out by Basto Aluja (2016) does not includes a detailed environmental impact analysis, other research should be found.

According to Quantis (2017), there are 480 CO₂-equivalent kg generated per biodiesel ton (Considering a biodiesel rate production 0.95 per crude oil). It is assumed that these values are for a plant with production capacity 40,000 tons per year and the conventional technology, due lack of information. Then, the 480 CO₂-equivalent kg generated per biodiesel ton are equivalent to 466 CO₂-equivalent kg per palm refined oil ton processed with conventional technology.

Then, considering the energy expenditure estimated in Appendix 6.22 at principal plants, a direct relation is assumed between the energy consumption and the CO₂-equivalent emissions generated, as presented in table 102.

Table 102 CO₂-equivalent emissions at principal plants (CO₂-equivalent t/refined oil)

Int. Products	Technology	Capacity (ton/year)		
		40,000	80,000	120,000
Jatropha	1	0.47	$=(8,068.23*0.47)/8,294.45=0.45$	0.46
Jatropha	2	$=(21,358.30*0.47)/8,294.45=1.20$	1.19	1.19
Jatropha	3	0.45	0.44	0.45
Jatropha	4	1.19	1.18	1.19
Jatropha	5	0.52	0.52	0.53
Jatropha	6	1.27	1.27	1.28
Palm	1	0.47	0.45	0.46
Palm	2	1.18	1.16	1.17
Palm	3	0.45	0.44	0.45
Palm	4	1.17	1.16	1.17
Palm	5	0.52	0.52	0.53
Palm	6	1.25	1.25	1.26

Transport

The CO₂-equivalent transport emissions factor for the liquid diesel is $10.45 \frac{Kg CO_2 e}{gal ACPM}$ (Carrasco Leal 2014) [and the diesel consumption per km and transported ton is:](#)

$$4.9812 * 10^{-5} \frac{t diesel}{t * km} = \frac{0.0154811 gal diesel}{t * km}$$

Then, the CO₂-equivalent transport emissions [per km and transported ton are:](#)

$$0.0154811 \frac{gal diesel}{t * km} * 10.45 \frac{Kg CO_2 e}{gal diesel} = 0.1618 \frac{Kg CO_2 e}{t * km} = 0.0001618 \frac{t CO_2 e}{t * km}$$

This value should be multiplied for the distance matrix to obtain the matrix with the CO₂-equivalent transport emissions [per transported ton](#).

CO₂ equivalent per biorefinery product consumption

The CO₂ equivalent emissions by biodiesel consumption are $0.002 t CO_2/gal$ (Fedebiocombustibles 2016). [Thus:](#)

$$0.002 \frac{t CO_2 e}{gal biodiesel} * \frac{1 gal}{3.78541 litre} * \frac{1 litre}{0.000875 t biodiesel} = 0,6038 \frac{t CO_2 e}{t biodiesel}$$

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Optimisation de la conception de la chaîne d'approvisionnement pour une bioraffinerie durable

La croissance de la population mondiale et son effet sur la sécurité alimentaire et l'urgence du changement climatique, sont des facteurs qui favorisent des diverses innovations pour accroître l'efficacité de l'utilisation des ressources naturelles. Parmi lesquelles la biomasse est une ressource renouvelable d'une grande disponibilité.

Une bioraffinerie peut transformer la biomasse en énergie durable, matériaux et des produits chimiques. Par contre, au début d'un projet de bioraffinerie, des décisions stratégiques doivent être prises. Et ainsi, le processus de décision doit tenir en compte diverses aspects, comme des conditions spécifiques du territoire où le projet est destiné à être déployé.

Une étude récente montre que, bien que ce problème ait été traité par la communauté scientifique, l'accent est mis sur les facteurs de rentabilité économique. Cependant, considérer toutes les dimensions de la durabilité, «Économique», «Social», «Environnemental», «Technologique» et «Politique» est essentielle dans ce type de projets.

Dans ces conditions, tous les outils d'optimisation disponibles ne conviennent pas. Par conséquent, une étude préliminaire sur les outils d'optimisation multi-objectifs est réalisée. Par la suite, une stratégie d'optimisation intégrant les dimensions de durabilité dans la phase amont du projet a été développée.

En fin, le modèle développé a été appliqué à l'étude du déploiement de bioraffineries en Colombie. Ce modèle et son optimisation permettent une meilleure visibilité pour les décideurs, grâce à sa capacité de proposer des scénarios et d'évaluer les compromis de la durabilité en intégrant les préférences des parties prenantes.

Mots clés : Bioraffinerie, durabilité, optimisation, chaîne d'approvisionnement

Biorefinery supply chain design optimization under sustainability dimensions

The growing global population and its effect on food security and the urgency for climate change mitigation, are issues that foster innovations to increase the efficiency of the use of natural resources. Among them, biomass is a renewable resource highly available.

A biorefinery can transform biomass in source of energy, materials and chemical products. However, at the early stage of a biorefinery project, strategic decisions have to be made, including location, production capacity or technology to be used, determining the project's feasibility. As a consequence, the decision process needs to consider several aspects, as the specific conditions of the territory where the project is supposed to be deployed.

A recent study shows that despite this problem has been treated by the multiple objective programming community, the main focus has been centered on factors of economic profitability. However, consider the whole dimensions of sustainability, "Economical", "Social", "Environmental", "Technological" and "Political" is essential in this kind of project.

Under these conditions, not all available optimization tools are suitable. Hence, a preliminary study about multi-objective optimization tools is realized. Then, a general optimization modeling strategy integrating the sustainability dimensions at the early stage of a biorefinery project is developed.

To finish, the developed model is applied to the case study of biorefinery deployment in Colombia. It will permit a better visibility for decision makers, because its capability to propose scenarios and evaluate sustainability trade-offs by integrating stakeholders preferences.

Keywords: Biorefinery, sustainability, optimization, supply chain

