Biodiesel Production from Waste Vegetable Oils: Combining Process Modelling, Multiobjective Optimization and Life Cycle Assessment (LCA)

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Abstract

The objective of this work is to propose an integrated and generic framework for eco-design that generalizes, automates and optimizes the evaluation of the environmental criteria at earlier design stage. The approach consists of three main stages. The first two steps correspond to process inventory analysis based on mass and energy balances and impact assessment phases of LCA methodology. The third stage of the methodology is based on the interaction of the previous steps with process simulation for environmental impact assessment and cost estimation through a computational framework. Then, the use of multi-objective optimization with a multicriteria choice decision making allows to select optimal solutions. The methodology is illustrated through the acid-catalyzed biodiesel production process.

Keywords: multiobjective optimization, biodiesel, process simulation, multiple choice decision making, acid-catalyzed.

1. Introduction

The exhaustion of stocks of fossil fuel supplies in combination with significant environmental and human impacts of petroleum fuel usage make urgent the development of alternative fuels that come from renewable resources. In this context, biofuels are a very promising solution. They include fuels derived from biomass conversion, as well as solid biomass, liquid fuels and various biogases. The scientific community was first interested in the production of biofuel with vegetable oils because it is derived from renewable resources which make biodiesel greener than petroleum diesel (Huynh et al., 2011). However, the main drawback of producing a great quantity of biodiesel from vegetable oil is the lack of feedstock and then, some ethical problems arise because of the utilization of a food product to make biofuel. Recently, lignocellulosic biomass and waste vegetable oils seem to be good candidates to be feedstock for the production of biodiesel (Atapour et al., 2014).

Biodiesel is a renewable fuel for diesel engines and can be produced by vegetable oils or animal fats. Made from agricultural co-products and by-products such as soybean oil, other vegetable oils or animal fats, it is an advanced biofuel. To be called biodiesel, it must meet strict quality specifications and biodiesel can be used in any blend with petroleum diesel fuel. Biodiesel reduces net carbon dioxide emissions by 78 % on a life-cycle basis when compared to conventional diesel fuel. It has also been shown to have dramatic improvements on engine exhaust emissions. Moreover, it is biodegradable and non-toxic and has a more favorable combustion emission profile than diesel, such as lower emissions of carbon monoxide, particulate matter and unburned hydrocarbons. The utilization of waste oils can produce cheap biodiesel and it can also solve the problem of waste oil disposal, so they are very good candidates to the production of biodiesel (Huynh et al., 2011).

In this study, a biodiesel production process design alternative is studied using an approach based on a previous work from Ouattara et al. (2012). This work takes into account economic and environmental considerations to obtain an eco-friendly and economically viable process design. The methodology carried out environmental impact analysis taking into account not only process but also impact of energy requirements. The current work intends to carry on a generic approach cradle-to-gate and a compliant software framework to implement an efficient LCA method and automate environmental impact analysis.

2. Methodology and tools

The originality of this study is to present an approach for eco-efficient process design, coupling process flow-sheeting and an energy plant simulator with a life cycle assessment module that generalizes and automates the evaluation of the environmental criteria. The approach consists of three main stages; the first two correspond to process inventory analysis and impact assessment phases of LCA methodology. The third stage performs environmental impact assessment and cost estimation through a computational framework. Process simulation has been performed with AspenHysys simulation software, and environmental performances are analyzed through Life Cycle Assessment (LCA, Impact 2002+) with Simapro. The energy requirements are evaluated by the use of Ariane software. The criteria are adapted to perform multi-criteria optimization taking into account the economic and environmental aspect by the IMPACT 2002+ method. An attributional LCA is considered: impacts from the production of biodiesel from vegetable oil would be attributed based on the inputs and outputs from the considered system, not taking into account what happened with the other related activities in the economy. In other words, no consequential LCA approach is targeted here. Optimizations have been solved with the genetic algorithm NSGAIIb. This procedure belongs to the genetic algorithm library (MULTIGEN) recently developed in Gomez et al. (2010). The MULTIGEN tools (written in Visual Basic for Applications VBA), use Excel sheets as interface. The general methodology is illustrated on a biodiesel production process from vegetable oils which is one of the foremost alternative fuels to those refined from petroleum products.

3. Biodiesel production simulation with Hysys

3.1. Overview of the biodiesel production process

Among the several routes to transform oil in biodiesel such as pyrolysis or micro-emulsion, the transesterification reaction process is the most common method to obtain biodiesel (Morais et al., 2010). Biodiesel is produced by the transesterification of the oil composing the feedstock (1) in presence of an excess of alcohol and a catalyst:

$$\text{Triglyceride + Alcohol (excess)} \xrightarrow{\textbf{\textit{Catalyst}}} \text{Fatty Acid Ester (BD) + Glycerol} \quad (1)$$

The catalyst can be either a base (alkali-catalyzed process) or an acid (acid-catalyzed process). A particular focus on the latter is made in this study. In this process, methanol (molar ratio methanol: oil of 50:1) and sulphuric acid (used as a catalyzer) feed the transesterification reactor with a stream of pre-heated oil. The excess of methanol is removed from the biodiesel in a distillation column and recycled back to the transesterification reactor. Introduction of calcium oxide is needed to remove sulfuric acid from the transesterification products in the neutralization reactor.

3.2. Simulation of the process with Aspen Hysys

This section defines the conditions and parameters used to model the bio-diesel process using waste cooking oil with HYSYS software.In this work, tri-olein ($C_{57}H_{104}O_6$). (i.e., triglyceride of oleic acid) is considered as the triglyceride in the waste cooking oil. The reaction set is established before starting flowsheet modelling. Two reactions are involved, one for transesterification and one for neutralization of sulphuric-acid:

Transesterification $$3MeOH + Triolein \rightarrow 3MethylOleate + Glycerol \quad (2)$$

Neutralization $$CaO + H_2SO_4 \rightarrow H_2O + CaSO_4 \quad (3)$$

Raw material inputs are represented as process input streams, Table 1 illustrates the operating conditions.

Table 1. Process inputs for the simulation model in Hysys

	Input 1	**Input 2**	**Input 3**	**Input 4**	**Input 5**
Components	Methanol	Triolein	Sulphuric acid	Water	Calcium oxide
Flow rate	210 kg/h	1,000 kg/h	150kg/h	110 kg/h	80 kg/h
Temperature	25°C	25°C	25°C	25°C	25°C
Pressure	1 bar	1 bar	1 bar	1 bar	1 bar

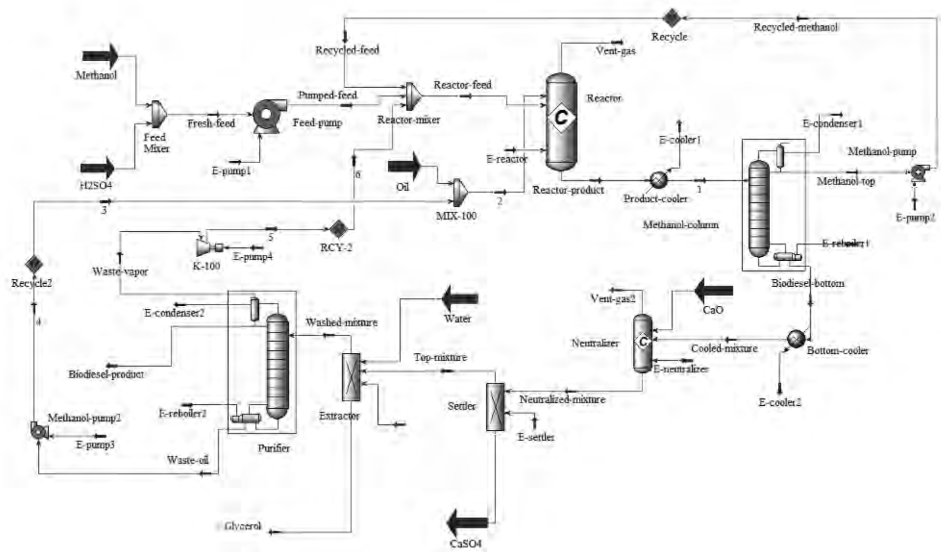

Figure 1. Flowsheet of the acid-catalyzed process obtained with Hysys

The following analysis is based on the environmental impact assessment using the IMPACT 2002+ LCIA (Life cycle impact assessment) method in order to perform a cradle to gate analysis. Methanol in vent gas output of the purifier column and triolein in reboiler liquid output are recycled with a purity of 99.97 % and 99.99 %. Through recycling about 34 kg/h of methanol and 111 kg/h of triolein are recovered and injected into the process

4. Inventory data and identification of potential factors

Inventory data elements are then identified in the EcoInvent database provided in SIMAPRO tool. Table 2 summarizes the inventory data of the biodiesel production process and their related database names.

5. Optimization of biodiesel production

5.1. Formulation of the problem

The formulation optimization problem proposed in this work is to maximize profit and minimize the environmental impact of biodiesel production process. The economic model used is based on the calculation of profit. The calculation is carried out using the basic operation:

$$PROFIT = (Flow_{bd} * \mathrm{Pr}ice_{bd}) - -\sum_{x=1}^{i} QE_x * CostE_x - -\sum_{y=1}^{j} QRM_y * CostRM_y - -\sum_{z=1}^{k} Qw_z * Costw_z \qquad (4)$$

Where:

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

With regard to the environmental aspect, the end-point categories of IMPACT 2002+ LCIA method are used as criteria to minimize.

Table 2. Inventory data of the biodiesel production process

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

The optimization problem can thus be formulated as follows:

Determine the decision variables (i.e., process operating conditions) in order to satisfy simultaneously the following objectives:

Maximization (Profit)
Minimization (Human Health)
Minimization (Ecosystem Quality)
Minimization (Climate Change)
Minimization (Resources)

Subject to:

Amount of calcium oxide must be exact to remove sulphuric acid
Decision variables ranges

5.2. Optimization results

The eco-design framework was then applied combining the process simulator (HYSYS), the energy plant simulator (Ariane), the environmental sub-module based on life cycle assessment and the genetic algorithm (NSGA IIb in Multigen) and an MCDM tool based on M-TOPSIS (the other decision tools are not applied here). The optimization approach uses the NSGA-IIb genetic algorithm embedded in Multigen environment, with the following parameters: number of individuals in the population: 200; generation number: 50; crossover rate: 0.9; mutation rate: 0.5.

The first step is to carry on a mono-objective optimization by maximizing the profit (Eq.1). The multi-criteria optimization then follows considering simultaneously five criteria i.e.: one economic (Profit) and four environmental ones corresponding to the endpoint of IMPACT 2002+ (Human Health, Ecosystem Quality, Climate Change and Resources). Pareto fronts are represented on figure 2. The results are then analyzed with an M-TOPSIS (Ren et al., 2007) application (Profit and end-point categories) with a same weight allocated for all criteria. The best solution found by M-TOPSIS maintains a balance between all the criteria and, with regard to the mono-criterion solution, (Min Profit) it is not so environmentally unfriendly. The mono-criterion solution is in red in Figure 2 whereas the best solution with TOPSIS is in green in Figure 2.

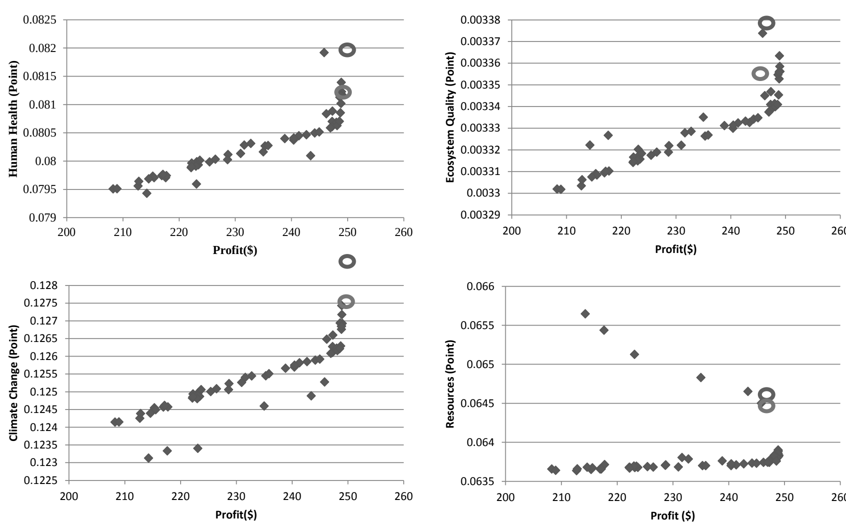

Figure 2. Two dimensionally comparisons of Pareto front (Profit – Environment)

6. Conclusion

The environmental gain obtained by the multi-objective framework is slight which can be attributed to the recycling steps that are introduced in the flowsheet. Figure 3 shows the individual analysis of the environmental impact of M-TOPSIS (Rank 1) solution. The figure confirm the "hot spot" of the system described above, but also indicate other, such as emissions of carbon dioxide and nitrogen oxide in addition to the methanol raw material.

Biodiesel is an alternative to fossil fuel use, which requires further studies to optimize the process in economic and environmental aspects. This work implements an eco-design framework to the production of biodiesel through waste vegetable oils. A cradle-to-gate assessment was then performed and the study was conducted with IMPACT 2002 + LCIA method. The results show that the step of multiple choice decision making with M-TOPSIS leads to an optimal solution not far away from the mono-criterion optimization solution. This kind of analysis can be further developed in order to revisit LCA objectives and carry out consequential analysis that is particularly sound in the case of alternative fuels. Future works will also take into account uncertainties as it was underlined in a recent study of Luna and Martinez (2013).

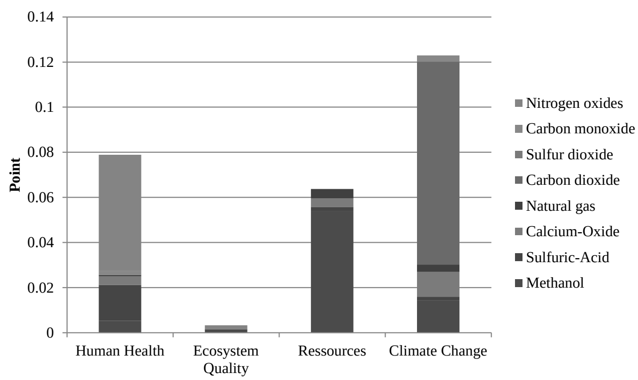

Figure 3. End-point analysis of the M-TOPSIS solution

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