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## Second generation bioethanol production from *Arundo donax* biomass: an optimization method

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### Abstract

In last decades environment has suffered strong and negative consequences resulted by a massive consuming fossil energy. As a result of this process, bioenergy has been intensively increased in recent years. Transportation sector has the largest impact in the use of bioenergy and bioethanol is a type of biofuel which can easily used for transports in place of traditional fossil fuels. Bioethanol production from 1st generation biomass such as corn, sugarcane, has been already commercialized but it is usually not sustainable because it could be seriously damage the food supply. For this reason scientific community has turned his interest to second generation bioethanol from specific energy crops or cultivation of biomass feedstock whose required land for cultivation cannot be used for food cultivations. The case arboreal lingo-cellulose *Arundo donax* is an example of the latter group. The present paper deals with a simulation method to optimize the performances of second generation bioethanol production by using *Arundo donax* as feedstock. The bioethanol production was analyzed by means of a life cycle assessment (LCA). The total energy consumption was calculated thanks to Monte Carlo method. The simulation of this second-generation biomass technology was optimized by considering the reuse of light components and of the energy recovery for the agriculture and industrial process. Thanks to these optimizations it was obtained an Energy Return On Investment (EROI) = 1,52 revealing that this technology may certainly be convenient from the energetic point of view.

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## Nomenclature

$EC_{out}$	Total Energy output
$EC_{in}$	Total Energy input
$EC_{AGRI}$	Total Energy demand in Agricultural processes
$EC_{TRANSPORT}$	Total Energy demand in transports from Agriculture phase to the biorefinery
$EC_{PRETREAT}$	Total Energy demand in the pretreatment phase
$EC_{PROCESS}$	Total Energy demand in the biorefinery processes
$EC_{eth}$	Total Energy in the Bioethanol production
$EC_{lightgas}$	Total Energy from the light gases produced
$EC_{SEED}$	Total Energy demand in the seeds for the crops
$EC_{MAN}$	Total Energy demand in the used manure
$EC_{FUEL}$	Total Energy demand in the agricultural machines
$EC_{MACH}$	Total Energy demand in the machines manufacturing
$EC_{ELEC}$	Total Energy demand in the electricity use in Agriculture
$EC_{FERT}$	Total Energy demand associated with the use of commercial fertilisers
$EC_{CA}$	Total Energy demand associated with the application of calcium
$EC_{PEST}$	Total Energy demand for the production of pesticides

## 1. Introduction

In last decades the use of renewable energy sources has significantly increased in many countries in the world, especially in the EU countries, and this trend is expected to increase more and more [1]. One of the reasons of this increase is due to the application of many directives to incentive renewable energy sources. For example, with the Directive 2009/28/CE about renewable energies promotion, each State has to reach some goals within 2020, in particular about transports, the quote of consumptions from renewable sources has to get at least 10% of the total consumption [2]. Therefore the development of technologies about biofuels becomes crucial. Moreover, the energy produced with biomasses and in particular by the combustion of biodiesel is considered a clean energy thanks to their low emission pollutants, and above all, the zero balance of carbon dioxide [3]. Nowadays there are two main ways to produce biofuels, and especially bioethanol, from biomasses. The so-called first generation bioethanol is produced usually by the alcoholic fermentation. In this process the biomasses are usually simple sugars, starch or generally food crops. Despite the fact the first generation processes are already industrialized with good results [4, 5], they suffer the competition with food production. With the aim at avoiding discrepancies on productions, European community with the Directive 2015/1513 has established a maximum of 7% for the contribution of biofuels produced by food crops. The second generation ethanol production process is usually conducted by fermentation of the sugar originated by the enzymatic hydrolysis of cellulose and hemicellulose, which are the main constituents of plants. This process is still not competitive at an industrial scale [6], but it is not expected any threat of food supplies with respect to crops for human or animal consumption. As result of these considerations the scientific community has turned its interest to the latter technology and a strong enhancement in second generation bioethanol production is expected in the future [7]. Moreover, most of the “energy” crops used for the second generation processes could be planted in marginal lands not suitable for cultivation for food and fodder, including areas even contaminated by human activities. The use of cultivations for energy production implies a verification of the accumulated and used energy in the production processes, because obviously only the crops whose energy balance is positive are adapted for this purpose [8]. Among these possible dedicated cultivations *Arundo donax* deserves a great attention [9]. This crop is

characterized by high resistance to parasites, low nutrients demand and high thermal stress resistance. These and other properties make *Arundo donax* a culture that fits many types of environment and also marginal lands.

The present work focuses on the development of a simulation method to optimize the performances of second generation bioethanol production by using *Arundo donax* as feedstock. The chemical process of bioethanol generation from *Arundo donax* was simulated with PRO/II and thanks to a LCEA analysis it was calculated the Energy Return on Investment (EROI) of such technology.

## 2. The Lyfe Cycle Energy Assessment methodology

In order to analyze from an energetic point of view the efficiency of the second generation bioethanol production process from *Arundo Donax* it was the Life Cycle Assessment (LCA) analysis, one of the most suitable methodology to assess the environment load of different products and processes. This procedure is internationally standardized by ISO 14040 and ISO 14044. In order to perform LCA to this process it was used a “cradle-to-wheel” approach considering the whole process from the agricultural processes to the final production of bioethanol. This analysis was performed considering all the energetic demands of each single process unit and it is called Life Cycle Energy Analysis (LCEA). It was calculated the Energy Return On Investment (EROI), an index used widely in literature [10, 11]. The considered process may be schematized in Figure 1.

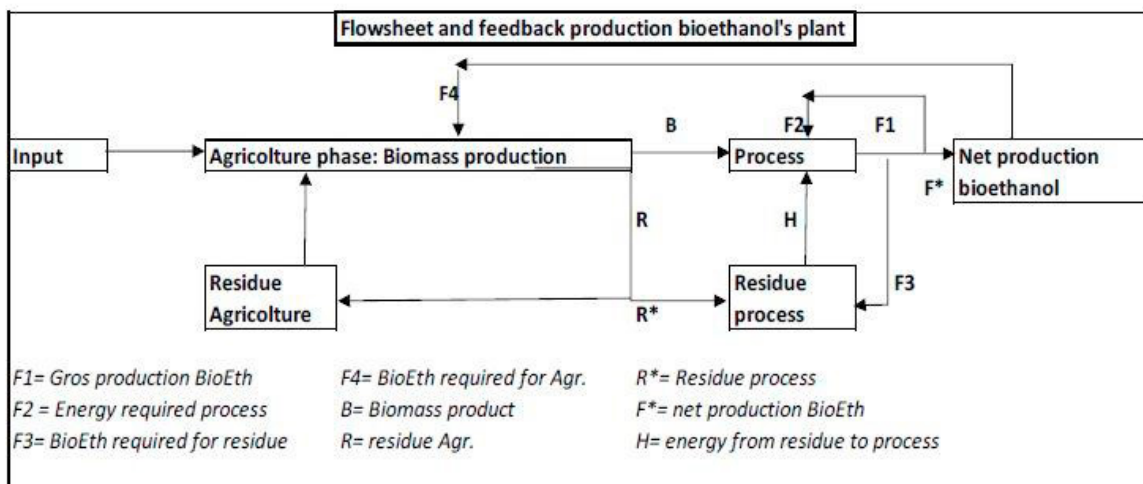


Fig. 1. Flowsheet of the bioethanol production process.

Accordingly Fig. 1 the EROI is mathematically expressed in:

$$EROI = \frac{\text{Energy output}}{\text{Energy input}} = \frac{F^* + H}{F2 + \text{Input} + F4} = \frac{EC_{out}}{EC_{in}} \tag{1}$$

Where:

$$EC_{out} = EC_{eth} + EC_{lightgas} \tag{2}$$

$$EC_{in} = EC_{AGRI} + EC_{TRANSPORT} + EC_{PRETREAT} + EC_{PROCESS} \tag{3}$$

$$EC_{AGRI} = EC_{SEED} + EC_{MAN} + EC_{FUEL} + EC_{MACH} + EC_{ELEC} + EC_{FERT} + EC_{CA} + EC_{PEST} \tag{4}$$

The calculation of EROI presents obviously several complex passages and some variations depends on the complexity of different energy factors. In order to apply this index there were made some assumptions:

- These indexes were converted in [GJ/ha] in order to compare all of them. In the ethanol formation process the inputs were chosen arbitrary.
- The  $EC_{\text{TRANSPORT}}$  is closely related to the available infrastructures presented in the territory of reference. However its contribute to  $EC_{\text{in}}$  is very low (about 2%) so it was reported by literature review.
- $EC_{\text{PRETREAT}}$  was calculated by considering similar cases.
- In order to find an “average” value of  $EC_{\text{AGRI}}$  there was applied a Montecarlo method considering all the variations of the single process units.
- The residues of the process were considered reused in the agricultural phase decreasing its energy demand costs.
- $EC_{\text{PROCESS}}$  and  $EC_{\text{out}}$  were calculated with PROVISION II<sup>TM</sup> with a Montecarlo method.

In table 1 there are reported all singles values and the references with calculation method.

Table 1. Input data for all processes units.

data	Input range	Reference
$EC_{\text{SEED}}$	0,340 - 0,77 [GJ/ha]	[12,13]
$EC_{\text{MAN}}$	0,131 - 2,86 [GJ/ha]	[14]
$EC_{\text{FUEL}}$	4 - 6,75 [GJ/ha]	[14-15]
$EC_{\text{MACH}}$	1,37 - 1,92 [GJ/ha]	[15]
$EC_{\text{ELEC}}$	0,65 - 0,87 [GJ/ha]	[14,16]
$EC_{\text{FERT}}$	2,76 - 7,45 [GJ/ha]	[13]
$EC_{\text{PEST}}$	0,054 - 0,82 [GJ/ha]	[13]
$EC_{\text{CA}}$	0 - 0,03 [GJ/ha]	[13]
$EC_{\text{TRANSPORT}}$	1-2 [GJ/ha]	[17]
$EC_{\text{PRETREAT}}$	6,5 [GJ/ha]	[17]

### 3. Bioethanol generation process simulation

The simulation of the chemical generation process of Bioethanol was performed with the software PRO/II, a modelling software in petrochemical processes. The crop *Arundo Donax* was chosen for many reasons: its high yield (it is estimated that from the third year it is about 30-35 t/ha<sup>-1</sup>yr<sup>-1</sup>), its density (about 40.000 plants ha<sup>-1</sup>), and its poor need of pesticides. The database for biomass components developed by the NREL [18] was used to determinate the lignocellulosic components (cellulose, hemicellulose and lignin) in the PRO II<sup>TM</sup> simulator. The characterization of these three pseudo-components was based on [19]: cellulose 44.1 % wt., hemicellulose 25.7 % wt., lignin 21.3 % wt., ash 1 % wt. and moisture 7,9 % wt. The process simulator estimates energy requirements and equipment parameters for the specified operating scenario. The process simulation is based on the following assumptions:

- The process is isothermal and steady state;
- The processes of drying is managed at the gasifier;
- The considered formed volatiles are H<sub>2</sub>, CO, CO<sub>2</sub>, CH<sub>4</sub>, C<sub>2</sub>H<sub>4</sub>, C<sub>2</sub>H<sub>6</sub>;
- The reactor process is steady state, isothermal and adiabatic;
- The biochemical reactions do not consider the formation of microorganisms;
- The incondensable produced light gases are recycled at the reforming and combustion processes.

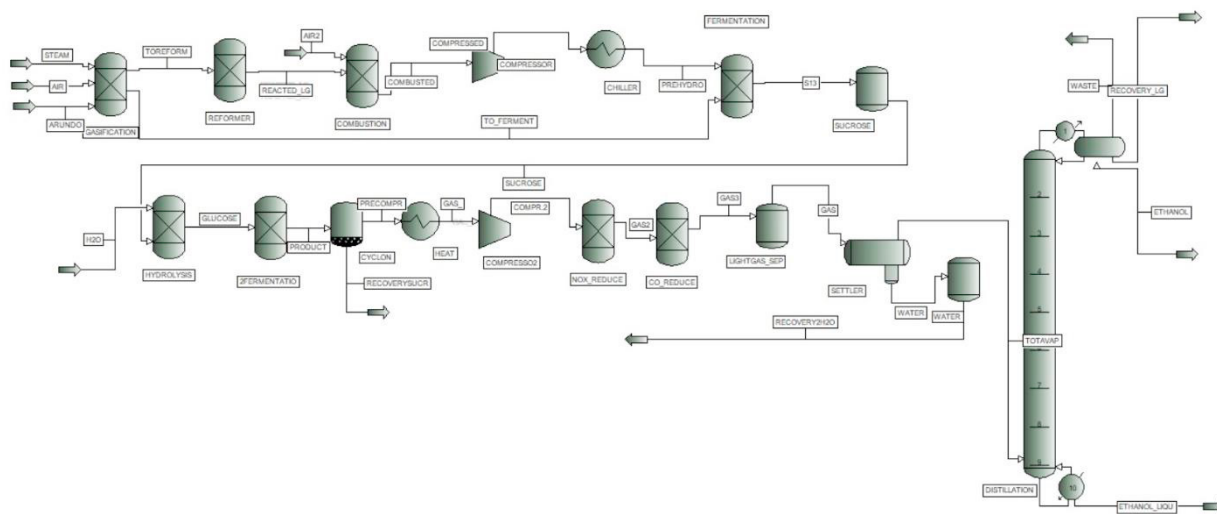


Fig. 2. The flowsheet blocks of the gasification and fermentation of Arundo developed in PRO II.

The different steps that simulate the whole chemical process to convert the biomass to bioethanol are represented in Fig. 2. The main important steps are: biomass drying, biomass pyrolysis, char gasification, gas cleaning and at the end syngas fermentation. The decomposition of the biomass was considered in parallel to its three main components: hemicellulose, cellulose and lignin. In the first pyrolysis the reactions developed in [20] were used for hemicellulose and cellulose. The lignin reaction refers to [21] and the decomposition of sugarcane was developed in [22]. The second pyrolysis was developed according [23]. The complete dehydration was considered at a Temperature of 378 K. The Pre-treat blocks represent the biomass drying. The lignin decomposition begins at a temperature of 563 K with the formation of gases, tar and coal. The block “Gasification” represents the first pyrolysis. In order to lead the process to regime conditions, with the reuse of light gases, it was necessary to consider the minimum data input reported in table 2.

Table 2. Data input in the chemical process.

data	value
Arundo flow rate	4200 [kg/h]
Air flow rate	2900 [kg/h]
Steam flow rate	100 [kg/h]

#### 4. Results

The simulation of the primary energy consumption in Agriculture ( $EC_{AGR}$ ) returns a bell-shaped distribution around a median of 14,56 GJ/ha (with a minimum of 10,275 GJ/ha and a maximum of 18,7 GJ/ha). The simulation of the energy consumption in the chemical process ( $EC_{PROCESS}$ ) returns a bell-shaped distribution around a median of 44,5 GJ/ha (with a minimum of 40,45 GJ/ha and a maximum of 48,67 GJ/ha) as reported in Figure 3.

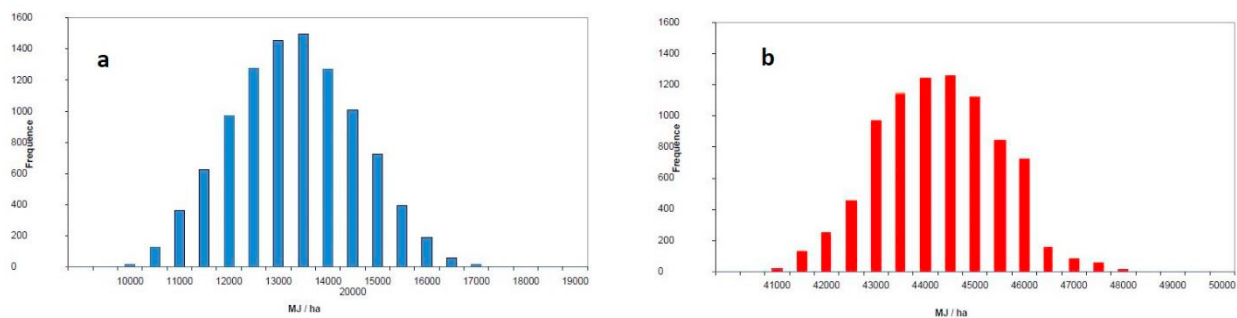


Fig. 3. Simulation of energy consumption in Agriculture (a) and in the chemical process (b) for the production of 1 ha.

The simulation process was set to obtain the 99,9 % purity ethanol and it was reached with a distillation Temperature of 372,15 K and a Pressure of around 2,5 – 3,5 atm. At these conditions supposing the plant would working at full capacity there were obtained a mass flow rate of Bioethanol of 1250 kg/h (around the 30 % of the total input Biomass after pretreatment). The light gases that can be recycled ( $H_2$ ,  $CH_4$ ,  $C_2H_6$  and others) presented a total mass flow rate of about 1415 kg/h (around the 45 % of the total input Biomass after pretreatment). In order to calculate the EROI all data input and output were referred to use/production of 1 ha of biomass. In table 3 and Figure 4 all results are reported.

Table 1. Results of all data processes.

<b>INPUT</b>	value	unit	%
$EC_{\text{TRANSPORT}}$	2	[GJ/ha]	2,95
$EC_{\text{PRETREAT}}$	6,5	[GJ/ha]	9,59
$EC_{\text{AGRI}}$	14,56	[GJ/ha]	21,49
$EC_{\text{PROCESS}}$	44,7	[GJ/ha]	65,97
$EC_{\text{in}}$	<b>67,76</b>	[GJ/ha]	-
<b>OUTPUT</b>			
$EC_{\text{eth}}$	29	[GJ/ha]	28,15
$EC_{\text{lightgas}}$	75	[GJ/ha]	72,81
$EC_{\text{out}}$	<b>103</b>	[GJ/ha]	-
<b>EROI</b>	<b>1,52</b>	-	-

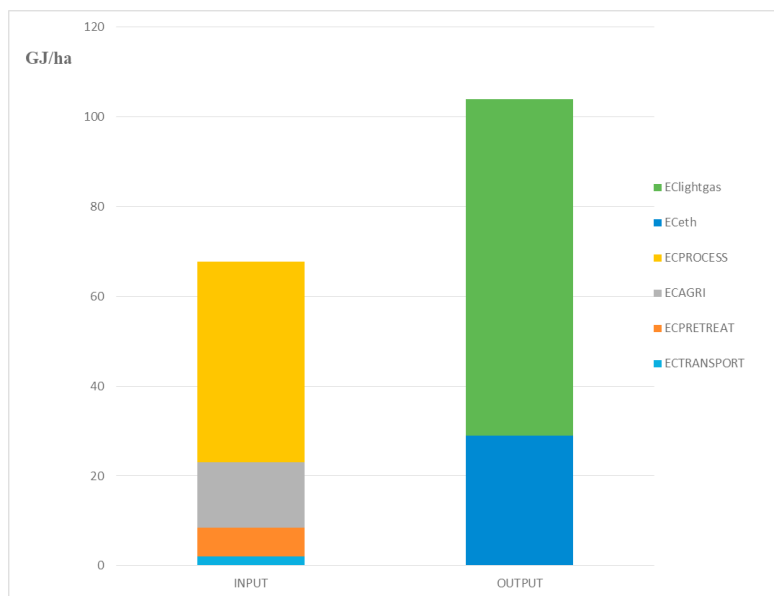


Fig. 4. Contributions from different sources to the total energy of input and output.

## 5. Conclusions

This paper deals with a simulation method to optimize the performances of a second generation bioethanol production process by using *Arundo Donax* as feedstock. The LCEA analysis for this case study reveals that the EROI is about 1,53 making this technology attractive for the energetic market. The agricultural Energy demand is about the 21,5 % of overall demand, the Biorefinery energy demand is the highest request with about the 66 % of the overall demand, a few contribution refers to the pretreatment phase (about the 9,6 %). The Bioethanol energy output is about the 28,1 % of the overall energy output. The process is competitive because of the reuse of lightgases that represents the 73% of the overall energy output. Another great advantage of *Arundo Donax* as “energy” crop is that it could be planted in marginal lands not suitable for cultivation for food and fodder. For future work it is under investigation an optimization GIS model to decrease the energy demand in agricultural pretreatment and transports processes.

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