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Simulation and life cycle assessment of biofuel production via fast pyrolysis and hydroupgrading

Jens F. Peters [a], Diego Iribarren [a,*], Javier Dufour [a,b]

[a] Systems Analysis Unit, Instituto IMDEA Energía, Móstoles 28935, Spain
[b] Department of Chemical and Energy Technology, Rey Juan Carlos University, Móstoles 28933, Spain

HIGHLIGHTS

- Biomass fast pyrolysis and bio-oil hydroupgrading are simulated in Aspen Plus®.
- Bio-oil and synfuels are modeled with high level of detail (83 model compounds).
- Life cycle assessment is carried out based on simulation results.
- Electricity consumption is identified as a key source of environmental impacts.
- Greenhouse gas savings are 54.5% compared to the equivalent fossil fuel.

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ABSTRACT

A biofuel process chain based on fast pyrolysis of hybrid poplar and subsequent hydroupgrading of the obtained bio-oil is simulated using Aspen Plus®. The simulation includes the pyrolysis plant and the biorefinery with its hydrotreating, hydrocracking, distillation and steam reforming sections. All parts of the process are modeled with a high level of detail, using 83 model compounds and a kinetic reaction model for the pyrolysis plant. A cross-check with published experimental data is included in order to validate the model. Based on the simulation results, a Life Cycle Assessment (LCA) is conducted for the biofuel products, identifying the processes with the highest contribution to the environmental impacts. The obtained synthetic biofuels are compared with their fossil fuel equivalents in order to quantify their potential environmental benefits. LCA results show greenhouse gas (GHG) savings of 54.5% for the produced fuel mix compared to conventional gasoline and diesel. Electricity consumption is one of the keys for reducing the overall environmental impact, while GHG savings could be enhanced by improving the thermal efficiency of the combustion processes in the plants. The biofuel pathway assessed is found to be an interesting option to produce second-generation biofuels with optimization potential in all phases of the system.

1. Introduction

As reflected in the EU Renewable Energy Directive 2009/28 (RED) [1], biofuels are considered one of the keys to reduce greenhouse gas (GHG) emissions as well as the high dependency of the European transport sector on imported fossil oil. For 2020, a 10% share of renewable energy is set as a target for the transport sector. This target is not without controversy, as first generation ethanol and biodiesel, which make up virtually all of the current biofuel mix, often show relatively low GHG savings and significant other environmental impacts [2–6]. The proposal for amending the RED in this regard [7] limits the contribution of conventional biofuels to 5% of the final energy consumption in transport, expecting this gap to be filled by second-generation biofuels. These can be produced from non-food crops on unused agricultural land at high yields while requiring little agricultural inputs. Poplar and willow from short-rotation cultivation and perennial grasses like miscanthus or switchgrass are among the most promising energy crops of this type [8].

One of the most efficient options to produce biofuels from this lignocellulosic biomass is its thermochemical conversion by fast pyrolysis [9–14]. The obtained pyrolysis oil (or bio-oil) is a liquid of high density and moderate heating value that can be upgraded in a biorefinery to gasoline and diesel blendstocks [15–17]. Pyrolysis-based biofuels have a high potential for reducing the

* Corresponding author. Tel.: +34 91 737 11 19.
E-mail address: diego.iribarren@imdea.org (D. Iribarren).

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carbon emissions of the transport sector. Potential GHG savings of 60–88% compared to fossil fuels are reported in the literature [18–21]. Nevertheless, in order to provide a comprehensive picture of the environmental performance of biofuel systems, the assessment should not be limited to GHG emissions. Life Cycle Assessment (LCA) is a helpful tool for this purpose, as it comprehensively assesses the impacts of a process or product for a whole set of impact categories [22].

LCA is a standardized methodology [23,24] frequently applied to biofuel systems, mainly to bioethanol and biodiesel processes [25–27]. Nevertheless, only a few works dealing with the LCA of pyrolysis-based biofuels have been published so far [18,20,21,28–31] and there is a lack of detailed inventory data for further studies. This may be partially due to the very limited amount of commercial-scale pyrolysis installations being operative to date [32]. Hence, inventory data are difficult to obtain and assessments have to be based on process simulation. The reference works in this field are the techno-economic studies by Ringer et al. [33], Jones et al. [34] (both based on wood chips as feedstock), and Wright et al. [35] (using corn stover as feedstock), who developed detailed simulations of a complete biofuel process chain [33–36]. Nevertheless, they use black box approaches for modeling the pyrolysis reaction mechanisms and a limited number of model compounds, thus resulting in a considerable simplification of the process. Existing LCA studies on pyrolysis biofuels are usually based on these works, either exclusively [20,21,28,29] or with some modifications according to data retrieved from other literature sources [18,30,31].

In this study, an innovative Aspen Plus® [37] simulation of a typical pyrolysis and hydrotreating process chain is presented. Within the simulation, a novel kinetic reaction model is used for calculating pyrolysis products based on the atomic and biochemical composition of the lignocellulosic biomass feedstock. In contrast to previous simulation approaches, this leads to a predictive calculation of the pyrolysis products for any lignocellulosic feedstock as well as to a very detailed modeling of the bio-oil, using 33 model compounds. The simulation results are verified against existing experimental data and used as a source of detailed inventory data. According to these results, the life-cycle performance of the produced biofuels is evaluated and compared with that of conventional fossil fuels.

2. Materials and methods

The goal of this study is to evaluate the environmental performance of synthetic biofuels produced via pyrolysis. Bio-oil is obtained through fast pyrolysis of a lignocellulosic feedstock and then upgraded in a biorefinery to synthetic fuels. The pyrolysis plant and the biorefinery are simulated in Aspen Plus® in order to obtain detailed inventory data. The environmental performance of the biofuels is evaluated following an attributional LCA approach. In attributional LCAs, the assessed system is treated like an isolated process that does not interact with global markets. Attributional LCA gives therefore a picture of the impacts directly associated with the life cycle of a product, but it is not suitable for assessing consequences of e.g. policy decisions. In contrast, consequential LCA takes into account the market effects of the production and consumption of a product. This requires explicit modeling of market mechanisms, making the assessment more comprehensive but much more complex and associated with additional uncertainties [38].

2.1. LCA framework

The system boundaries are set according to Fig. 1, including the whole conversion process from feedstock production to the produced biofuels at the refinery gate. Capital goods are not included, assuming that their influence on the final LCA results is negligible [27,39]. Moreover, this assumption facilitates comparison with other studies in this field [18,20,21,28]. Production is assumed to be located in central Spain, one of the countries with the highest agricultural bioenergy potential in Europe [8]. Hence, data specific for Spain are used for all secondary data (electricity mix, average vehicle, etc.) when available.

The functional unit (FU) used in this work is 1 MJ of energy content of the obtained synthetic biofuel mix (gasoline and diesel). This is a common FU for biofuel assessment [20,21,27,40] and allows for comparing the results with the GHG saving targets stated in the RED [1]. According to the lower heating value (LHV) of the fuels and the production rates taken from the simulation results, this corresponds to 0.51 MJ of gasoline and 0.49 MJ of diesel.

The assessed processes are multifunctional, producing more than one product. Allocation is used to deal with this situation. Since all products have energetic uses, allocation is carried out according to their energy content (LHV basis). This is also in accordance with the RED methodology, which defines energy allocation on an LHV basis as the methodology for distributing the GHG emissions in multifunctional systems [1].

In addition to the bio-oil, the pyrolysis reactor yields char as a by-product. Since the char is not further processed to synthetic fuels in the biorefinery and constitutes an independent product, a share of the environmental impacts caused by the pyrolysis process has to be allocated to the char. This allocation is calculated based on the mass flows and the heating values of the bio-oil and char products leaving the plant. The corresponding allocation percentages are presented in Table 1 (‘Pyrolysis’).

In the biorefinery, synthetic gasoline and diesel are produced plus process steam generated by cooling the hydrotreating reactors. Similarly to the char in the pyrolysis plant, this steam is a by-product that does not contribute to the production of the synthetic fuels. It is assumed that this steam constitutes a valuable by-product for use in neighboring industrial facilities. Therefore, allocation is done according to the energy content of the products as obtained from the simulation. The corresponding allocation percentages are given in Table 1 (‘Biorefinery’).

2.2. System description

The system subject to assessment produces biofuels by fast pyrolysis of poplar from hypothetical short-rotation plantations in central Spain. Spain is the country with the third highest agricultural bioenergy potential in the EU-27 and poplar is one of the most suitable energy crops for deployment in this region [8,41]. Biomass is a local resource and small-scale pyrolysis plants are assumed to be located close to the plantation sites for minimizing transport distances [42,43], while the biorefinery is assumed to be part of an existing refinery installation due to economic reasons [34,44]. This decentralized biorefinery configuration has been found to be environmentally more favorable than an integrated pyrolysis/biorefinery configuration in a previous screening assessment comparing different bio-oil use options [45].

For the analysis, the whole system is divided into subsystems. According to Fig. 1, these include agriculture and cropping, biomass transport, the pyrolysis plant, bio-oil transport and the biorefinery plant. The pyrolysis plant and the biorefinery are modeled in Aspen Plus® (shaded grey in Fig. 1), while data for the remaining processes are retrieved from the literature and the ecoinvent database version 2.2 [46–49].

2.2.1. Agriculture and cropping

The agricultural inputs required for poplar short-rotation cultivation (e.g., pesticides and fertilizers) are taken from the literature