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## Early-stage decision making approach for the selection of optimally integrated biorefinery processes

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### ABSTRACT

Lignocellulosic biorefineries are the best non-petroleum alternatives for a sustainable development. In the biorefinery process design, it is important to implement an algorithm that allows systematic generation, evaluation of energy conversion chains and making comparison of different pathways, ranking them according to different performance criteria. To achieve these goals, a methodology has been proposed to systematically define an ordered set of solutions using mixed integer linear programming models with integer cut constraints. In this study, we apply a systematic approach which adopts thermo-environmental optimization together with heat integration to assess the economic performance, environmental impact and energy requirement of several process options. Both sugars and syngas platforms are compared considering multiple products (energy services, valuable chemicals, fuels). A superstructure of different processes is developed and heat recovery potentials in the systems are analyzed using pinch analysis. Different pathways are evaluated and ranked according to different objective functions to understand the best combination of products and the synergies between them. Our results provide a set of candidate solutions according to minimum total cost and environmental impact as objective functions, considering benefit of heat integration between different pathways to obtain energy efficient biorefinery systems with improved process economics and reduced environmental impacts.

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### 1. Introduction

The increasing attention towards sustainable development leads researchers to investigate new non-petroleum alternatives. Biomass is one of the most promising renewable resources. The biggest advantage of using biomass derived chemicals and fuels are that the carbon cycle can be closed. In fact biomass resources absorb CO<sub>2</sub> from the atmosphere and the same amount of CO<sub>2</sub> is released into the atmosphere during the decomposition [1]. In an integrated biorefinery, biomass is converted into a variety of products ranging from fuels to higher value chemicals, after many physical and thermal conversion technologies, with minimal waste and CO<sub>2</sub> emissions. Currently the attention on feasible biorefinery concept as well as an inventory of most promising bio-based products is increasing [2]. Future biorefineries would be multi-functional and able to imitate the energy efficiency of modern petroleum refining via extensive energy integration and co-product

development [3]. Biorefinery technologies are still under development and there are challenges for the developers as well as opportunities since a variety of feedstocks, products and processing technologies exist. One of the main challenges is the need of a systematic approach to select and integrate processes in a way that market demand of existing and possible products are satisfied by considering the availability of the biomass feedstocks [4]. A decision needs to be made between bio-based products: bio-energy in terms of heat and power, bio-fuels and bio-chemicals and/or their simultaneous production. The problem to be solved is to identify the competition between these products and to analyze the benefit of co-production in terms of energy efficiency and economics. Integration of the co-production units will maximize the use of biogenic carbon or maximize the impact of biomass as an energy source. Furthermore, closing the energy balance of the whole system by renewable energy sources is essential for actual sustainability of bio-based products. All these features bring the requirement of advanced process synthesis methods which adopts process integration techniques and optimization methods to guarantee the economic viability and minimum environmental

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**Nomenclature**

$C_{tot}$	Annual total cost
$C_{inv}(j)$	Annualized investment cost for unit $j$
$C_{op\&maint}(j)$	Annual operation and maintenance cost for unit $j$
$C_{op}(i)$	Cost for resource $i$
$C_{rev}(k)$	Revenue for selling service $k$
$GWP_{tot}$	Annual global warming potential impact factor
$GWP_{const}(j)$	Annual impact of construction of unit $j$
$GWP_{op}(i)$	Annual impact of consumption of resource $i$
$n(j)$	Lifetime of the plant
$c_{inv}(j)$	Specific investment cost for unit $j$
$c_{op\&maint}(j)$	Annual specific maintenance cost for unit $j$
$c_{op}(i)$	Specific operating cost for resource $i$
$gwp_{const}(j)$	Annual specific impact of construction of unit $j$
$gwp_{op}(i)$	Impact of consumption of resource $i$
$y_{use}$	Binary variable for existence of the technology
$f_{mult}$	Multiplication factor for sizing the technology
$\tau(j)$	Annualization factor

**Abbreviations**

ICC	Integer cut constraint
GWP100a	100-years global warming potential
MILP	Mixed integer linear programming
LCIA	Life cycle impact assessment
LCA	Life cycle assessment
LCI	Life cycle inventory
CFB	Circulating fluidized bed
FICFB	Fast internally circulating fluidized bed
EF	Entrained flow
WGS	Water gas shift
SMR	Steam methane reforming
HMF	Hydroxymethylfurfural
DME	Dimethyl ether
MEA	Monoethanolamine
EtOH	Ethanol
FT	Fischer-Tropsch
MeOH	Methanol
SNG	Synthetic Natural Gas

impact [5].

Several researchers have been working in the field of process synthesis and design of large scale biorefinery systems. Most studies in the literature addressed the determination of the single best technology for the production of single product, especially bio-fuels such as ethanol production [6,7], biodiesel production [8] and combined heat and power production [9]. There are also some studies that take into account superstructures with multiple feedstocks, products and conversion pathways for process synthesis and optimization of biorefinery processes. Sammons et al. [10] applied a systematic methodology to evaluate integrated biorefineries in the optimization framework where the candidate configurations are identified based on maximum profitability and ranked according to environmental performance to find the optimal pathway. Ng et al. [11] extended pinch based automated targeting approach of resource conservation networks with maximum fuel production and maximum revenue targets for integrated bio-fuels production from biochemical and thermochemical platforms in biorefineries. Santibañez-Aguilar et al. [12] included epsilon constraint method for multi-objective optimization of ethanol, biodiesel and hydrogen biorefinery but without considering heat integration. Kim et al. [13] proposed a framework for multi-product biorefinery superstructure optimization to evaluate the embedded strategies using alternative criteria and calculated minimum energy consumption for the designs. Few studies comprise a holistic view on the matter while taking into account process integration and thermo-environmental optimization for bio-fuels plants. Gassner and Maréchal [14] developed a methodology based on multi-objective optimization that can be applied to the conceptual design of bio-fuel plants. This approach allows identifying promising flowsheets using process integration methods. Tay et al. [15] developed fuzzy optimization strategy for bio-fuels production pathways where fuzzy optimization needs to be decoupled with incremental values on both economic and environmental objectives to obtain a Pareto optimal front, and energy recovery is considered via steam and electricity production in the syngas platform. Baliban et al. [16] studied biomass to liquids systems under large-scale mixed-integer nonlinear optimization framework to identify best economically and environmentally superior bio-fuels production technologies within heat, power and water integration. Ensinas et al. [17] applied multi-objective optimization using evolutionary algorithms to create a set of candidate solutions

of different configurations for integrated first and second generations sugarcane biorefinery. Albarelli et al. [18] followed the same methodology for the integrated ethanol and methanol production in sugarcane biorefinery.

From process optimization perspective, most of the studies conducted in the literature do not take into account the systematic process integration approach for maximum energy recovery in the integrated multi-platforms (chemical, thermochemical and biochemical conversion platforms) and multi-products biorefineries. The development of cost-effective integrated biorefineries can be only achieved by optimal mass and energy integration. For the bigger scale of production, heat and power demand concerns are quite important. Furthermore, the integration of processes from different platforms and the analysis of the interactions between process units using thermodynamics knowledge are becoming more and more important to improve the efficiency of mass and energy transfer and to reduce the operating cost [19], but it is not widely applied to biorefinery concepts yet. Production of value-added products (e.g., succinic acid, dimethyl ether, etc.), valorization of waste mass and energy streams, and cogeneration are significantly important for the sustainability of the biorefineries.

In this paper, a systematic methodology which adopts energy integration and thermo-environmental optimization techniques is applied to assess the economic performance, environmental impact, and energy requirement for several process options of multiple conversion platforms. A superstructure of different process alternatives based on biochemical and thermochemical conversion pathways is developed. Then, different pathways are systematically compared with each other and ranked according to the objective function with integer cuts constraints (ICC) methodology proposed by Maronese et al. [20] for identification of most promising technologies and optimum configuration and sizes of process units. Optimal integration algorithms between process units of bio-energy, bio-fuels and bio-chemicals production pathways are developed. The method applied in the current study is fast and powerful and it is appropriate for preliminary process design and comparison.

## 2. Methodology

The proposed thermo-environmental optimization methodology

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