



Design of integrated biorefineries

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ABSTRACT

The paper outlines a systems approach with capabilities to address common complexities and practicalities in the design of real-life integrated biorefineries. The approach favors a decomposition of the problem into process synthesis, process integration and flowsheeting. The synthesis of paths introduces a graph representation sufficiently generic to model the general problem. Likewise, the development of product portfolios offers a generic cascade representation that combines thermodynamics with mathematical programming. The methodology renders high-throughput capacity and has been exploited to review large combinations of paths through exhaustive screening, subsequently leading to significant savings in capital and operating costs. The paper highlights results from the approach as it has configured the operation and the evolution of existing pilots and demos. The methodology is being extended to address strategic decisions and the better integration of the biorefinery concept. The paper explains limitations and opportunities of existing methods and tools, highlighting the scope for future developments and applications.

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1. Introduction

Strong bio-based economies are expected to create both revenues and jobs, directly and indirectly. They are also expected to increase farmer income and improve economic activity in developing rural regions. To remain competitive, the Chemical Industry will need to perform a progressive shift from petrochemical sources to bio-based resources toward a future bio-economy. McKenzie (Austin, 2009) projects that bio based chemical production (biofuels, polyesters, coatings, glycerol oxidation products, resins, nutraceuticals, prebiotics, and cosmetics) would account for 10 percent of the \$1.5 trillion worldwide annual chemical market (Biomass Magazine, 2012). According to a recent study by the UK Industrial Biotechnology Innovation & Growth Team, the demand for plant-based biochemicals could generate sales of nearly \$600 billion by 2025 (Biomass Magazine, 2012).

Industrial biorefineries have been identified as the most promising route to the creation of the bio based industry (Demirbas, 2009; Kokossis and Yang, 2010). They integrate biomass conversion processes to produce fuels, power, heat, and value-added chemicals. The objective of a biorefinery is to optimize the use of resources and minimize wastes, thereby maximizing benefits and profitability. Whereas state incentives for first generation (1G biorefineries)

biofuels abate quickly, targets to replace fossil transportation fuels become higher counting on second generation (2G biorefineries) production that is taking off in Europe, US, China and South America. 2G plants are expected to decrease oil dependency from high risk countries, stimulate economic growth, and address climate change through emission reductions. The commercial implications of the 'green growth' is explained in a recent study (EuropaBio, 2011). The 'green growth' is estimated to \$300–400 billion whereas the potential for GHG reductions ranges from 60% to 100%. The study explains that significant public investments are available to bring lab-scale developments into commercial scale. With a focus on bioethanol, public support in US has exceeded €1.2 billion over the last 5 years through a wide range of schemes that include grants, tax credits, and loan guarantees. The programs offer lines of assistance to the demand (bio-preferred labeling and procurement, renewable fuel standards, etc.) as well as to the supply end (clean energy loans, crop assistance, and ethanol tax credits); the Biomass Program offers \$2–300 million per year in support for demos. In reference to EU, the EuropaBio explains that, over the same period, government support exceeded €200 million with a mixed focus on fuels and chemicals. Developments include demos for bio-fuels, bio-chemicals, demos for mixed production, pilots, and lighthouse projects (BIOCORE, EuroBioRef, Suprabio) to improve integration and efficiencies. Large-scale investments in biorefineries are similarly reported in China as the country, through the annual production of 1.7 billion gallons of bioethanol, set targets to replace 20% of her crude oil imports by 2020. Meanwhile, several 2G

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bagasse refineries are already in operation in Brazil. Still untapped, the potential of India is huge and larger than that in other regions.

In broad terms, biorefineries process biochemical and thermochemical routes. In the majority of cases, at some point these two would need to integrate with each other. Process systems engineering bears apparent potential to assist with ongoing developments in the field (Kokossis and Yang, 2010; Kokossis et al., 2012). It can be applied to optimize paths, to model, simulate and optimize the unit operations and the plant, or to apply process, energy and water integration when appropriate. Published studies demonstrated the combined use of optimization in techno-economic analysis for bioethanol (Sassner et al., 2008; Martín and Grossmann, 2011; Marvin et al., 2012), biodiesel (Pokoo-Aikins et al., 2010) and mix biofuels (Sen et al., 2012; Luo et al., 2010) with occasional emphasis on the environmental performance and at Life Cycle Analysis (Martinez-Hernandez et al., 2013; Wang et al., 2013; Falano et al., 2014), biorefinery product allocation (Sammons et al., 2008), multiperiod models for optimal planning of resources (Lim et al., 2013) and supply chain network (Kima et al., 2011; Marvin et al., 2011; Yue et al., 2014). Additional work focused on process synthesis. Using all the available methodologies of process synthesis opportunities are available in both microscopic and macroscopic domain (Yuan et al., 2013). Many applications use superstructures to screen paths making decisions about selected flowsheet sections by means of MINLPs (Martín and Grossmann, 2013; Kelloway and Daoutidis, 2013; Zondervan et al., 2011) and/or decomposition methods (Bao et al., 2011; Pham and El-Halwagi, 2012). Other work linked the biorefinery design with product and molecular design (Hechinger et al., 2010; Chemmangattuvalappil and Ng, 2013; Eason and Cremaschi, 2014). Conceptual work further presented methods based on targeting methods, cascade diagrams (Ng, 2010; Tay and Ng, 2012) and the use of C/H/O ternary diagrams (Tay et al., 2011), all particularly useful to preview a seemingly complex problem, to understand trade-offs, and to simplify the complexity before optimization. Robust and shortcut optimization models have been further developed (Zondervan et al., 2011; Bao et al., 2011; Ng et al., 2013) using sequential and branch superstructure development.

Recent work (Baliban et al., 2013) highlighted the potential of a layered approach to address complex and large problems in the field. Without compromising on the rigor of the systematic methodology, the layered approach combines advantages of systems engineering with the practicalities of real-life problems.

The design of biorefineries from pilots and installed facilities bears tremendous social and economic benefits. By 2020, “Bloomberg” predicts that, only in Europe, there would be around 1000 of such new units bringing €32.3 trillion revenues and 1 million new jobs (EuropaBio, 2011). Integrated biorefineries are a prerequisite to sustainability. Their sustainability depends on their ability to process alternative feedstocks (multiple wood types, algae; municipal waste), integrate with each other, or colocate with complementary industrial facilities. Even if they stand profitable, stand-alone units tout payback times not particularly attractive; instead, both biochemical and thermochemical routes are possible to demonstrate attractive and sustainable production provided they can scale, integrate and valorize properly the biomass feed. Integration may be applied to combine paths, in the design and development of the plant (e.g. improve efficiencies of raw materials, energy, water), or with the deployment of innovative business models to integrate with upstream and downstream processes. Integration of biochemical and thermochemical plants could be achieved at feedstock-handling and pre-treatment, intermediate stages of biomass conversion, or at downstream stages where products get separated and purified. Examples of co-location (e.g. pulp and paper, heat and power, mills) indicate cost reductions in the range of 20–70% over stand-alone capex; following the claims of the EuropaBio paper, capitalizing on existing demos in

Europe (Bio Base Europe, CPI, BioDemo, BE Basic) estimated benefits close to 50% (Kelloway and Daoutidis, 2013). Due to technological uncertainties and unsettled business models, there is current proliferation of initiatives with different focus to the value chain (e.g. input, conversion technologies, and output) and different emphasis between proprietary technologies and the biorefinery concept installed (e.g. proprietary technologies vs paradigm of integration). Other than supporting individual stages of development (modeling, techno-economic analysis, synthesis and optimization), PSE stands with a strong promise to systematize and build high-throughput capacity assisting structured and methodical manners to evolve small pilots into integrated units. Conventional chemical design technology settled for fixed and known supplies and products. Biorefinery demonstrations depend on product selection; the size required for demonstration depends on what needs be demonstrated; the latter is influenced by technology and subsequently determines the products to select. In biorefineries the feedstocks, the products and the technologies are all degrees of freedom in the design of the plant. The cyclic search for solutions sounds endless with occasional check-points at Life Cycle Analysis (LCA) to review results and validate options for overall impact.

The paper addresses the systems challenge to build a systematic methodology that will assist to scale-up technology in the field. As a matter of good practice, the paper starts with an attempt to describe the problem. Next the systems methodology is outlined in the form of a structured and layered approach. The approach is being applied in two real-life applications, one in a lignocellulosic Biorefinery (BIOCORE: BIOCCommodity Refinery); the other has recently started to upgrade industrial-scale halophytic cultures that process micro-algae (D-Factory: The Micro-Algae Biorefinery). Results are shared for the former work that is now already licensing technology worldwide. Subsequent sections illustrate the application of the approach, highlighting results and achievements, also pointing to a seemingly large number of limitations that need be tackled in future work.

2. Problem description and the outline of a systems methodology

The problem assumes (*given is*) promising work from the lab, possibly already in the form of pilots and demos. Such work typically lead to substrates with a mixture of valuable intermediates and products that one needs to purify and valorize. Typical biochemical substrates include mixtures of C6, C5 and lignin; thermochemical intermediates include syngas; waste and algal substrates relate to mixtures with a potential for energy and chemical products. Also available (*given*) are regional feedstocks and background chemistries (e.g. chemistries not directly related to the pilot but still useful to invoke and build value chains into final products). The problem is then to select (*optimally determine*) the most profitable product portfolio further considering environmental objectives, economic uncertainties in markets, technologies and the security of supplies. In decreasing abstraction, decisions are required to

- (a) Select chemistries and product portfolios to build the biorefinery value chain.
- (b) Set efficiency targets for individual processes and for the total site.
- (c) Develop individual flowsheets for each selected process with respect to the unit operations to integrate.

The paper advocates a structured methodology to address the biorefinery challenge. The methodology is outlined in Fig. 1. It combines three layers of analysis each supported by different

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